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Computer Science Theory for the Information Age*

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1 Introduction

Computer science as an academic discipline began in the 60's. Emphasis was on programming languages, compilers, operating systems and the mathematical theory that supported these areas. Courses in theoretical computer science covered finite automata, regular expressions, context free languages, and computability. In the 70's, algorithms was added as an important component of theory. The emphasis was on making computers useful. Today, a fundamental change is taking place and the focus is more on applications. The reasons for this change are many. Some of the more important are the merging of computing and communications, the availability of data in digital form, and the emergence of social and sensor networks.

Although programming languages and compilers are still important and highly skilled individuals are needed in these area, the vast majority of researchers will be involved with applications and what computers can be used for, not how to make computers useful. With this in mind we have written this book to cover the theory likely to be useful in the next 40 years just as automata theory and related topics gave students an advantage in the last 40 years. One of the major changes is the switch from discrete mathematics to more of an emphasis on probability and statistics. Some topics that have become important are high dimensional data, large random graphs, singular value decomposition along with other topics covered in this book.

The book is intended for either an under graduate or a graduate theory course. Significant back ground material that will be needed for an under graduate course has been put in the appendix. For this reason the appendix has homework problems.

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2 High-Dimensional Space

Consider representing a document by a vector each component of which corresponds to the number of occurrences of a particular word in the document. The English language has on the order of 25,000 words. Thus, such a document is represented by a 25,000-dimensional vector. The representation of a document is called the *word vector model* [SWY75]. A collection of n documents may be represented by a collection of 25,000-dimensional vectors, one vector per document. The vectors may be arranged as columns of a 25,000 × n matrix.

Another example of high-dimensional data arises in customer-product data. If there are 1,000 products for sale and a large number of customers, recording the number of times each customer buys each product results in a collection of 1,000-dimensional vectors.

There are many other examples where each record of a data set is represented by a high-dimensional vector. Consider a collection of n web pages that are linked. A link is a pointer from one web page to another. Each web page can be represented by a 0-1 vector with n components where the j^{th} component of the vector representing the i^{th} web page has value 1, if and only if there is a link from the i^{th} web page to the j^{th} web page.

In the vector space representation of data, properties of vectors such as dot products, distance between vectors, and orthogonality often have natural interpretations. For example, the squared distance between two 0-1 vectors representing links on web pages is the number of web pages to which only one of them is linked. In Figure 2.2, pages 4 and 5 both have links to pages 1, 3, and 6 but only page 5 has a link to page 2. Thus, the squared distance between the two vectors is one.

When a new web page is created a natural question is which are the closest pages to it, that is the pages that contain a similar set of links. This question translates to the geometric question of finding nearest neighbors. The nearest neighbor query needs to be answered quickly. Later in this chapter we will see a geometric theorem, called the Random Projection Theorem, that helps with this. If each web page is a d-dimensional vector, then instead of spending time d to read the vector in its entirety, once the random projection to a k-dimensional space is done, one needs only read k entries per vector.

Dot products also play a useful role. In our first example, two documents containing many of the same words are considered similar. One way to measure co-occurrence of words in two documents is to take the dot product of the vectors representing the two documents. If the most frequent words in the two documents co-occur with similar frequencies, the dot product of the vectors will be close to the maximum, namely the product of the lengths of the vectors. If there is no co-occurrence, then the dot product will be close to zero. Here the objective of the vector representation is information retrieval.



Figure 2.1: A document and its term-document vector along with a collection of documents represented by their term-document vectors.

After preprocessing the document vectors, we are presented with queries and we want to find for each query the most relevant documents. A query is also represented by a vector which has one component per word; the component measures how important the word is to the query. As a simple example, to find documents about cars that are not race cars, a query vector will have a large positive component for the word car and also for the words engine and perhaps door and a negative component for the words race, betting, etc. Here dot products represent relevance.

An important task for search algorithms is to rank a collection of web pages in order of relevance to the collection. An intrinsic notion of relevance is that a document in a collection is relevant if it is similar to the other documents in the collection. To formalize this, one can define an ideal direction for a collection of vectors as the line of best-fit, or the line of least-squares fit, i.e., the line for which the sum of squared perpendicular distances of the vectors to it is minimized. Then, one can rank the vectors according to their dot product similarity with this unit vector. We will see in Chapter 4 that this is a well-studied notion in linear algebra and that there are efficient algorithms to find the line of best fit. Thus, this ranking can be efficiently done. While the definition of rank seems ad-hoc, it yields excellent results in practice and has become a workhorse for modern search, information retrieval, and other applications.

Notice that in these examples, there was no intrinsic geometry or vectors, just a collection of documents, web pages or customers. Geometry was added and is extremely useful. Our aim in this book is to present the reader with the mathematical foundations to deal with high-dimensional data. There are two important parts of this foundation. The first is high-dimensional geometry along with vectors, matrices, and linear algebra. The second more modern aspect is the combination with probability. When there is a stochastic model of the high-dimensional data, we turn to the study of random points. Again, there are domain-specific detailed stochastic models, but keeping with our objective of introducing the foundations, the book presents the reader with the mathematical results needed to tackle the simplest stochastic models, often assuming independence and uniform or Gaussian distributions.

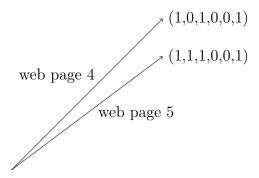


Figure 2.2: Two web pages as vectors. The squared distance between the two vectors is the number of web pages linked to by just one of the two web pages.

2.1 Properties of High-Dimensional Space

Our intuition about space was formed in two and three dimensions and is often misleading in high dimensions. Consider placing 100 points uniformly at random in a unit square. Each coordinate is generated independently and uniformly at random from the interval [0, 1]. Select a point and measure the distance to all other points and observe the distribution of distances. Then increase the dimension and generate the points uniformly at random in a 100-dimensional unit cube. The distribution of distances becomes concentrated about an average distance. The reason is easy to see. Let \mathbf{x} and \mathbf{y} be two such points in d-dimensions. The distance between \mathbf{x} and \mathbf{y} is

$$|\mathbf{x} - \mathbf{y}| = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}.$$

Since $\sum_{i=1}^{d} (x_i - y_i)^2$ is the summation of a number of independent random variables of bounded variance, by the law of large numbers the distribution of $|\mathbf{x} - \mathbf{y}|^2$ is concentrated about its expected value. Contrast this with the situation where the dimension is two or three and the distribution of distances is spread out.

For another example, consider the difference between picking a point uniformly at random from the unit-radius circle and from a unit radius sphere in d-dimensions. In d-dimensions the distance from the point to the center of the sphere is very likely to be between $1 - \frac{c}{d}$ and 1, where c is a constant independent of d. Furthermore, the first coordinate, x_1 , of such a point is likely to be between $-\frac{c}{\sqrt{d}}$ and $+\frac{c}{\sqrt{d}}$, which we express by saying that most of the mass is near the equator. The equator perpendicular to the x_1 axis is the set $\{\mathbf{x}|x_1=0\}$. We will prove these facts in this chapter.

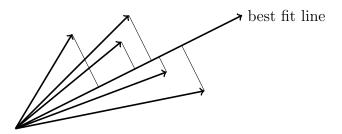


Figure 2.3: The best fit line is that line that minimizes the sum of perpendicular distances squared.

2.2 The High-Dimensional Sphere

One of the interesting facts about a unit-radius sphere in high dimensions is that as the dimension increases, the volume of the sphere goes to zero. This has important implications. Also, the volume of a high-dimensional sphere is essentially all contained in a thin slice at the equator and is simultaneously contained in a narrow annulus at the surface. There is essentially no interior volume. Similarly, the surface area is essentially all at the equator. These facts are contrary to our two or three-dimensional intuition; they will be proved by integration.

2.2.1 The Sphere and the Cube in Higher Dimensions

Consider the difference between the volume of a cube with unit-length sides and the volume of a unit-radius sphere as the dimension d of the space increases. As the dimension of the cube increases, its volume is always one and the maximum possible distance between two points grows as \sqrt{d} . In contrast, as the dimension of a unit-radius sphere increases, its volume goes to zero and the maximum possible distance between two points stays at two.

Note that for d=2, the unit square centered at the origin lies completely inside the unit-radius circle. The distance from the origin to a vertex of the square is

$$\sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2} = \frac{\sqrt{2}}{2} \cong 0.707$$

and thus the square lies inside the circle. At d=4, the distance from the origin to a vertex of a unit cube centered at the origin is

$$\sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2} = 1$$

and thus the vertex lies on the surface of the unit 4-sphere centered at the origin. As the dimension d increases, the distance from the origin to a vertex of the cube increases as $\frac{\sqrt{d}}{2}$, and for large d, the vertices of the cube lie far outside the unit sphere. Figure 2.5 illustrates conceptually a cube and a sphere. The vertices of the cube are at distance $\frac{\sqrt{d}}{2}$

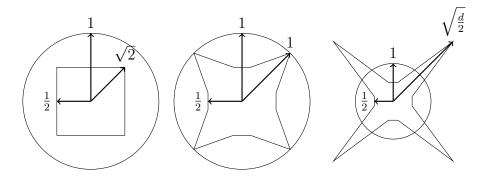


Figure 2.4: Illustration of the relationship between the sphere and the cube in 2, 4, and d-dimensions.

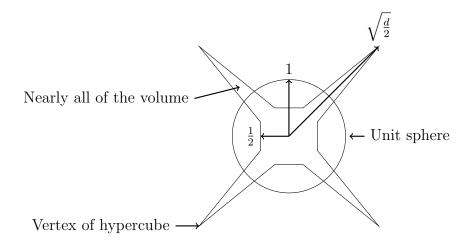


Figure 2.5: Conceptual drawing of a sphere and a cube.

from the origin and for large d lie outside the unit sphere. On the other hand, the mid point of each face of the cube is only distance 1/2 from the origin and thus is inside the sphere. For large d, almost all the volume of the cube is located outside the sphere.

2.2.2 Volume and Surface Area of the Unit Sphere

For fixed dimension d, the volume of a sphere is a function of its radius and grows as r^d . For fixed radius, the volume of a sphere is a function of the dimension of the space. What is interesting is that the volume of a unit sphere goes to zero as the dimension of the sphere increases.

To calculate the volume of a sphere, one can integrate in either Cartesian or polar

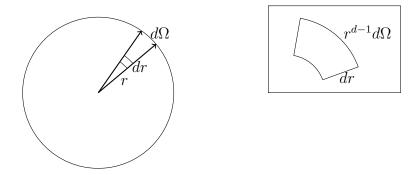


Figure 2.6: Infinitesimal volume in d-dimensional sphere of unit radius.

coordinates. In Cartesian coordinates the volume of a unit sphere is given by

$$V(d) = \int_{x_1=-1}^{x_1=1} \int_{x_2=-\sqrt{1-x_1^2}}^{x_2=\sqrt{1-x_1^2}} \cdots \int_{x_d=-\sqrt{1-x_1^2-\cdots-x_{d-1}^2}}^{x_d=\sqrt{1-x_1^2-\cdots-x_{d-1}^2}} dx_d \cdots dx_2 dx_1.$$

Since the limits of the integrals are complex, it is easier to integrate using polar coordinates. In polar coordinates, V(d) is given by

$$V(d) = \int_{S^d} \int_{r=0}^1 r^{d-1} d\Omega dr.$$

Here, $d\Omega$ is the surface area of the infinitesimal piece of the solid angle S^d of the unit sphere. See Figure 2.6. The convex hull of the $d\Omega$ piece and the origin form a cone. At radius r, the surface area of the top of the cone is $r^{d-1}d\Omega$ since the surface area is d-1 dimensional and each dimension scales by r. The volume of the infinitesimal piece is base times height, and since the surface of the sphere is perpendicular to the radial direction at each point, the height is dr giving the above integral.

Since the variables Ω and r do not interact,

$$V(d) = \int_{S^d} d\Omega \int_{r=0}^{1} r^{d-1} dr = \frac{1}{d} \int_{S^d} d\Omega = \frac{A(d)}{d}.$$

The question remains, how to determine the surface area $A\left(d\right)=\int\limits_{S^{d}}d\Omega$?

Consider a different integral

$$I(d) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\left(x_1^2 + x_2^2 + \cdots x_d^2\right)} dx_d \cdots dx_2 dx_1.$$

Including the exponential allows one to integrate to infinity rather than stopping at the surface of the sphere. Thus, I(d) can be computed by integrating in Cartesian coordinates. Integrating in polar coordinates relates I(d) to the surface area A(d). Equating the two results for I(d) gives A(d).

First, calculate I(d) by integration in Cartesian coordinates.

$$I(d) = \left[\int_{-\infty}^{\infty} e^{-x^2} dx\right]^d = \left(\sqrt{\pi}\right)^d = \pi^{\frac{d}{2}}$$

Next, calculate I(d) by integrating in polar coordinates. The volume of the differential element is $r^{d-1}d\Omega dr$. Thus

$$I\left(d\right) = \int\limits_{\mathbb{S}^{d}} d\Omega \int\limits_{0}^{\infty} e^{-r^{2}} r^{d-1} dr.$$

The integral $\int_{S^d} d\Omega$ is the integral over the entire solid angle and gives the surface area,

A(d), of a unit sphere. Thus, $I(d) = A(d) \int_{0}^{\infty} e^{-r^2} r^{d-1} dr$. Evaluating the remaining integral gives

$$\int_{0}^{\infty} e^{-r^{2}} r^{d-1} dr = \frac{1}{2} \int_{0}^{\infty} e^{-t} t^{\frac{d}{2}} - 1 dt = \frac{1}{2} \Gamma\left(\frac{d}{2}\right)$$

and hence, $I(d) = A(d) \frac{1}{2} \Gamma\left(\frac{d}{2}\right)$ where the gamma function $\Gamma\left(x\right)$ is a generalization of the factorial function for noninteger values of x. $\Gamma\left(x\right) = \left(x-1\right) \Gamma\left(x-1\right)$, $\Gamma\left(1\right) = \Gamma\left(2\right) = 1$, and $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$. For integer x, $\Gamma\left(x\right) = \left(x-1\right)!$.

Combining $I(d) = \pi^{\frac{d}{2}}$ with $I(d) = A(d) \frac{1}{2} \Gamma(\frac{d}{2})$ yields

$$A(d) = \frac{\pi^{\frac{d}{2}}}{\frac{1}{2}\Gamma(\frac{d}{2})}.$$

This establishes the following lemma.

Lemma 2.1 The surface area A(d) and the volume V(d) of a unit-radius sphere in d-dimensions are given by

$$A\left(d\right) = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \quad and \quad V\left(d\right) = \frac{\pi^{\frac{d}{2}}}{\frac{d}{2}\Gamma\left(\frac{d}{2}\right)}.$$

To check the formula for the volume of a unit sphere, note that $V(2)=\pi$ and $V(3)=\frac{2}{3}\frac{\pi^{\frac{3}{2}}}{\Gamma(\frac{3}{2})}=\frac{4}{3}\pi$, which are the correct volumes for the unit spheres in two and three dimensions. To check the formula for the surface area of a unit sphere, note that $A(2)=2\pi$ and $A(3)=\frac{2\pi^{\frac{3}{2}}}{\frac{1}{2}\sqrt{\pi}}=4\pi$, which are the correct surface areas for the unit sphere in two and three dimensions. Note that $\pi^{\frac{d}{2}}$ is an exponential in $\frac{d}{2}$ and $\Gamma\left(\frac{d}{2}\right)$ grows as the factorial of $\frac{d}{2}$. This implies that $\lim_{d\to\infty}V(d)=0$, as claimed.

2.2.3 The Volume is Near the Equator

Consider a high-dimensional unit sphere and fix the North Pole on the x_1 axis at $x_1 = 1$. Divide the sphere in half by intersecting it with the plane $x_1 = 0$. The intersection of the plane with the sphere forms a region of one lower dimension, namely $\{\mathbf{x} | |\mathbf{x}| \leq 1, x_1 = 0\}$ which we call the equator. The intersection is a sphere of dimension d-1 and has volume V(d-1). In three dimensions this region is a circle, in four dimensions the region is a three-dimensional sphere, etc. In general, the intersection is a sphere of dimension d-1.

It turns out that essentially all of the mass of the upper hemisphere lies between the plane $x_1=0$ and a parallel plane, $x_1=\varepsilon$, that is slightly higher. For what value of ε does essentially all the mass lie between $x_1=0$ and $x_1=\varepsilon$? The answer depends on the dimension. For dimension d it is $O(\frac{1}{\sqrt{d-1}})$. To see this, calculate the volume of the portion of the sphere above the slice lying between $x_1=0$ and $x_1=\varepsilon$. Let $T=\{\mathbf{x}|\,|\mathbf{x}|\leq 1, x_1\geq \varepsilon\}$ be the portion of the sphere above the slice. To calculate the volume of T, integrate over x_1 from ε to 1. The incremental volume is a disk of width dx_1 whose face is a sphere of dimension d-1 of radius $\sqrt{1-x_1^2}$ (see Figure 2.7) and, therefore, the surface area of the disk is

$$(1-x_1^2)^{\frac{d-1}{2}}V(d-1).$$

Thus,

Volume
$$(T) = \int_{\epsilon}^{1} (1 - x_1^2)^{\frac{d-1}{2}} V(d-1) dx_1 = V(d-1) \int_{\epsilon}^{1} (1 - x_1^2)^{\frac{d-1}{2}} dx_1.$$

Note that V(d) denotes the volume of the d-dimensional unit sphere. For the volume of other sets such as the set T, we use the notation Volume(T) for the volume. The above integral is difficult to evaluate so we use some approximations. First, we use the inequality $1 + x \le e^x$ for all real x and change the upper bound on the integral to be infinity. Since x_1 is always greater than ε over the region of integration, we can insert x_1/ε in the integral. This gives

Volume
$$(T) \le V(d-1) \int_{\varepsilon}^{\infty} e^{-\frac{d-1}{2}x_1^2} dx_1 \le V(d-1) \int_{\varepsilon}^{\infty} \frac{x_1}{\varepsilon} e^{-\frac{d-1}{2}x_1^2} dx_1.$$

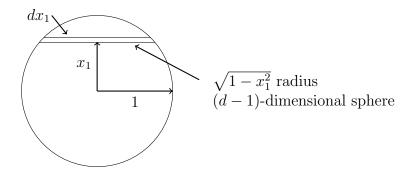


Figure 2.7: The volume of a cross-sectional slab of a d-dimensional sphere.

Now, $\int x_1 e^{-\frac{d-1}{2}x_1^2} dx_1 = -\frac{1}{d-1}e^{-\frac{d-1}{2}x_1^2}$ and, hence,

Volume
$$(T) \le \frac{1}{\varepsilon(d-1)} e^{-\frac{d-1}{2} \varepsilon^2} V(d-1)$$
. (2.1)

Next, we lower bound the volume of the entire upper hemisphere. Clearly the volume of the upper hemisphere is at least the volume between the slabs $x_1 = 0$ and $x_1 = \frac{1}{\sqrt{d-1}}$, which is at least the volume of the cylinder of radius $\sqrt{1 - \frac{1}{d-1}}$ and height $\frac{1}{\sqrt{d-1}}$. The volume of the cylinder is $1/\sqrt{d-1}$ times the d-1-dimensional volume of the disk $R = \{\mathbf{x} | |\mathbf{x}| \leq 1; x_1 = \frac{1}{\sqrt{d-1}}\}$. Now R is a d-1-dimensional sphere of radius $\sqrt{1 - \frac{1}{d-1}}$ and so its volume is

Volume(R) =
$$V(d-1) \left(1 - \frac{1}{d-1}\right)^{(d-1)/2}$$
.

Using $(1-x)^a \ge 1 - ax$

Volume
$$(R) \ge V(d-1)\left(1 - \frac{1}{d-1}\frac{d-1}{2}\right) = \frac{1}{2}V(d-1).$$

Thus, the volume of the upper hemisphere is at least $\frac{1}{2\sqrt{d-1}}V(d-1)$. The fraction of the volume above the plane $x_1 = \varepsilon$ is upper bounded by the ratio of the upper bound on the volume of the hemisphere above the plane $x_1 = \varepsilon$ to the lower bound on the total volume. This ratio is $\frac{2}{\varepsilon\sqrt{(d-1)}}e^{-\frac{d-1}{2}\varepsilon^2}$ which leads to the following lemma.

Lemma 2.2 For any c > 0, the fraction of the volume of the hemisphere above the plane $x_1 = \frac{c}{\sqrt{d-1}}$ is less than $\frac{2}{c}e^{-c^2/2}$.

Proof: Substitute $\frac{c}{\sqrt{d-1}}$ for ε in the above.

For a large constant c, $\frac{2}{c}e^{-c^2/2}$ is small. The important item to remember is that most of the volume of the d-dimensional sphere of radius r lies within distance $O(r/\sqrt{d})$ of the

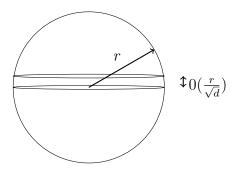


Figure 2.8: Most of the volume of the d-dimensional sphere of radius r is within distance $O(\frac{r}{\sqrt{d}})$ of the equator.

equator as shown in Figure 2.8.

For $c \geq 2$, the fraction of the volume of the hemisphere above $x_1 = \frac{c}{\sqrt{d-1}}$ is less than $e^{-2} \approx 0.14$ and for $c \geq 4$ the fraction is less than $\frac{1}{2}e^{-8} \approx 3 \times 10^{-4}$. Essentially all the mass of the sphere lies in a narrow slice at the equator. Note that we selected a unit vector in the x_1 direction and defined the equator to be the intersection of the sphere with a (d-1)-dimensional plane perpendicular to the unit vector. However, we could have selected an arbitrary point on the surface of the sphere and considered the vector from the center of the sphere to that point and defined the equator using the plane through the center perpendicular to this arbitrary vector. Essentially all the mass of the sphere lies in a narrow slice about this equator also.

2.2.4 The Volume is in a Narrow Annulus

The ratio of the volume of a sphere of radius $1 - \varepsilon$ to the volume of a unit sphere in d-dimensions is

$$\frac{(1-\varepsilon)^d V(d)}{V(d)} = (1-\varepsilon)^d$$

and thus goes to zero as d goes to infinity, when ε is a fixed constant. In high dimensions, all of the volume of the sphere is concentrated in a narrow annulus at the surface.

Indeed, $(1-\varepsilon)^d \leq e^{-\varepsilon d}$, so if $\varepsilon = \frac{c}{d}$, for a large constant c, all but e^{-c} of the volume of the sphere is contained in a thin annulus of width c/d. The important item to remember is that most of the volume of the d-dimensional sphere of radius r < 1 is contained in an annulus of width O(1-r/d) near the boundary.

2.2.5 The Surface Area is Near the Equator

Just as a 2-dimensional circle has an area and a circumference and a 3-dimensional sphere has a volume and a surface area, a d-dimensional sphere has a volume and a surface area. The surface of the sphere is the set $\{\mathbf{x} | |\mathbf{x}| = 1\}$. The surface of the equator is the

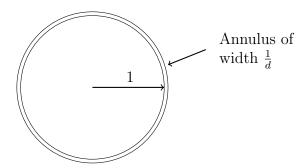


Figure 2.9: Most of the volume of the d-dimensional sphere of radius r is contained in an annulus of width O(r/d) near the boundary.

set $S = \{\mathbf{x} | |\mathbf{x}| = 1, x_1 = 0\}$ and it is the surface of a sphere of one lower dimension, i.e., for a 3-dimensional sphere, the circumference of a circle. Just as with volume, essentially all the surface area of a high-dimensional sphere is near the equator. To see this, calculate the surface area of the slice of the sphere between $x_1 = 0$ and $x_1 = \varepsilon$.

Let $S = \{\mathbf{x} | |\mathbf{x}| = 1, x_1 \ge \varepsilon\}$. To calculate the surface area of S, integrate over x_1 from ε to 1. The incremental surface unit will be a band of width dx_1 whose edge is the surface area of a d-1-dimensional sphere of radius depending on x_1 . The radius of the band is $\sqrt{1-x_1^2}$ and therefore the surface area of the (d-1)-dimensional sphere is

$$A(d-1)(1-x_1^2)^{\frac{d-2}{2}}$$

where A(d-1) is the surface area of a unit sphere of dimension d-1. Thus,

Area
$$(S) = A(d-1) \int_{0}^{1} (1-x_1^2)^{\frac{d-2}{2}} dx_1.$$

Again the above integral is difficult to integrate and the same approximations as in the earlier section on volume leads to the bound

$$\operatorname{Area}(S) \le \frac{1}{\varepsilon(d-2)} e^{-\frac{d-2}{2}\varepsilon^2} A(d-1). \tag{2.2}$$

Next we lower bound the surface area of the entire upper hemisphere. Clearly the surface area of the upper hemisphere is greater than the surface area of the side of a d-dimensional cylinder of height $\frac{1}{\sqrt{d-2}}$ and radius $\sqrt{1-\frac{1}{d-2}}$. The surface area of the cylinder is $\frac{1}{\sqrt{d-2}}$ times the circumference area of the d-dimensional cylinder of radius $\sqrt{1-\frac{1}{d-2}}$ which is $A(d-1)(1-\frac{1}{d-2})^{\frac{d-2}{2}}$. Using $(1-x)^a \geq 1-ax$, the surface area of the hemisphere is at

most

$$\frac{1}{\sqrt{d-2}} (1 - \frac{1}{d-2})^{\frac{d-2}{2}} A(d-1) \ge \frac{1}{\sqrt{d-2}} (1 - \frac{d-2}{2} \frac{1}{d-2}) A(d-1)
\ge \frac{1}{2\sqrt{d-2}} A(d-1)$$
(2.3)

Comparing the upper bound on the surface area of S, in (2.2), with the lower bound on the surface area of the hemisphere in (2.3), we see that the surface area above the band $\{\mathbf{x} | |\mathbf{x}| = 1, 0 \le x_1 \le \varepsilon\}$ is less than $\frac{2}{\varepsilon\sqrt{d-2}}e^{-\frac{d-2}{2}\varepsilon^2}$ of the total surface area.

Lemma 2.3 For any c > 0, the fraction of the surface area above the plane $x_1 = \frac{c}{\sqrt{d-2}}$ is less than or equal to $\frac{2}{c}e^{-\frac{c^2}{2}}$.

Proof: Substitute $\frac{c}{\sqrt{d-2}}$ for ε in the above.

So far we have considered unit-radius spheres of dimension d. Now fix the dimension d and vary the radius r. Let V(d,r) denote the volume and let A(d,r) denote the surface area of a d-dimensional sphere. Then,

$$V(d,r) = \int_{x=0}^{r} A(d,x)dx.$$

Thus, it follows that the surface area is the derivative of the volume with respect to the radius. In two dimensions the volume of a circle is πr^2 and the circumference is $2\pi r$. In three dimensions the volume of a sphere is $\frac{4}{3}\pi r^3$ and the surface area is $4\pi r^2$.

2.3 The High-Dimensional Cube and Chernoff Bounds

We can ask the same questions about the d-dimensional unit cube $C = \{\mathbf{x} | 0 \le x_i \le 1, i = 1, 2, ..., d\}$ as we did for spheres. First, is the volume concentrated in an annulus? The answer to this question is simple. If we shrink the cube from its center $(\frac{1}{2}, \frac{1}{2}, ..., \frac{1}{2})$ by a factor of 1 - (c/d) for some constant c, the volume clearly shrinks by $(1 - (c/d))^d \le e^{-c}$, so much of the volume of the cube is contained in an annulus of width O(1/d). See Figure 2.10. We can also ask if the volume is concentrated about the equator as in the sphere. A natural definition of the equator is the set

$$H = \left\{ \mathbf{x} \left| \sum_{i=1}^{d} x_i = \frac{d}{2} \right. \right\}.$$

We will show that most of the volume of C is within distance O(1) of H. See Figure 2.11. The cube does not have the symmetries of the sphere, so the proof is different. The starting point is the observation that picking a point uniformly at random from C is

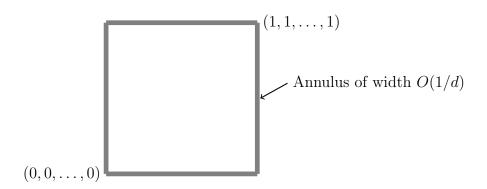


Figure 2.10: Most of the volume of the cube is in an O(1/d) annulus.

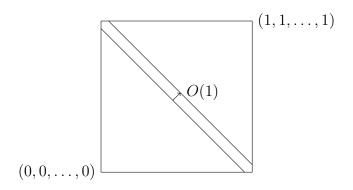


Figure 2.11: Most of the volume of the cube is within O(1) of equator.

equivalent to independently picking x_1, x_2, \ldots, x_d , each uniformly at random from [0, 1]. The perpendicular distance of a point $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ to H is

$$\frac{1}{\sqrt{d}} \left| \left(\sum_{i=1}^{d} x_i \right) - \frac{d}{2} \right|.$$

Note that $\sum_{i=1}^d x_i = c$ defines the set of points on a hyperplane parallel to H. The perpendicular distance of a point \mathbf{x} on the hyperplane $\sum_{i=1}^d x_i = c$ to H is $\frac{1}{\sqrt{d}} \left(c - \frac{d}{2} \right)$ or $\frac{1}{\sqrt{d}} \left| \left(\sum_{i=1}^d x_i \right) - \frac{d}{2} \right|$. The expected squared distance of a point from H is

$$\frac{1}{d}E\left[\left(\left(\sum_{i=1}^{d} x_i\right) - \frac{d}{2}\right)^2\right] = \frac{1}{d}\operatorname{Var}\left(\sum_{i=1}^{d} x_i\right).$$

By independence, the variance of $\sum_{i=1}^{d} x_i$ is the sum of the variances of the x_i , so $\operatorname{Var}(\sum_{i=1}^{d} x_i) = \sum_{i=1}^{d} \operatorname{Var}(x_i) = d/4$. Thus, the expected squared distance of a point

from H is 1/4. By Markov's inequality

$$\operatorname{Prob}\left(\begin{array}{c} \operatorname{distance\ from}\ H\ \operatorname{is\ greater}\\ \operatorname{than\ or\ equal\ to\ } t\end{array}\right) = \operatorname{Prob}\left(\begin{array}{c} \operatorname{distance\ squared\ from}\ H\ \operatorname{is}\\ \operatorname{greater\ than\ or\ equal\ to}\ t^2\end{array}\right) \leq \frac{1}{4t^2}.$$

Lemma 2.4 A point picked at random in a unit cube will be within distance t of the equator defined by $H = \left\{ \mathbf{x} \mid \sum_{i=1}^{d} x_i = \frac{d}{2} \right\}$ with probability at least $1 - \frac{1}{4t^2}$.

The proof of Lemma 2.4 basically relied on the fact that the sum of the coordinates of a random point in the unit cube will, with high probability, be close to its expected value. We will frequently see such phenomena and the fact that the sum of a large number of independent random variables will be close to its expected value is called the *law* of large numbers and depends only on the fact that the random numbers have a finite variance. How close is given by a Chernoff bound and depends on the actual probability distributions involved.

The proof of Lemma 2.4 also covers the case when the x_i are Bernoulli random variables with probability 1/2 of being 0 or 1 since in this case $Var(x_i)$ also equals 1/4. In this case, the argument claims that at most a $1/(4t^2)$ fraction of the corners of the cube are at distance more than t away from H. Thus, the probability that a randomly chosen corner is at a distance t from H goes to zero as t increases, but not nearly as fast as the exponential drop for the sphere. We will prove that the expectation of the t^{th} power of the distance to t^{th} is at most some value t^{th} and t^{th} is at the probability that the distance is greater than t^{th} is at most t^{th} ensuring a faster drop than t^{th} . We will prove this for a more general case than that of uniform density for each t^{th} . The more general case includes independent identically distributed Bernoulli random variables.

We begin by considering the sum of d random variables, x_1, x_2, \ldots, x_d , and bounding the expected value of the r^{th} power of the sum of the x_i . Each variable x_i is bounded by $0 \le x_i \le 1$ with an expected value p_i . To simplify the argument, we create a new set of variables, $y_i = x_i - p_i$, that have zero mean. Bounding the r^{th} power of the sum of the y_i is equivalent to bounding the r^{th} power of the sum of the $x_i - p_i$. The reader my wonder why the $\mu = \sum_{i=1}^d p_i$ appears in the statement of Lemma 2.5 since the y_i have zero mean. The answer is because the y_i are not bounded by the range [0,1], but rather each y_i is bounded by the range $[-p_i, 1-p_i]$.

Lemma 2.5 Let x_1, x_2, \ldots, x_d be independent random variables with $0 \le x_i \le 1$ and $E(x_i) = p_i$. Let $y_i = x_i - p_i$ and $\mu = \sum_{i=1}^d p_i$. For any positive integer r,

$$E\left[\left(\sum_{i=1}^{d} y_i\right)^r\right] \le \operatorname{Max}\left[(2r\mu)^{r/2}, r^r\right]. \tag{2.4}$$

Proof: There are d^r terms in the multinomial expansion of $E((y_1 + y_2 + \cdots y_d)^r)$; each term a product of r not necessarily distinct y_i . Focus on one term. Let r_i be the number

of times y_i occurs in that term and let I be the set of i for which r_i is nonzero. The r_i associated with the term sum to r. By independence

$$E\left(\prod_{i\in I} y_i^{r_i}\right) = \prod_{i\in I} E(y_i^{r_i}).$$

If any of the r_i equals one, then the term is zero since $E(y_i) = 0$. Thus, assume each r_i is at least two implying that |I| is at most r/2. Now,

$$E(|y_i^{r_i}|) \le E(y_i^2) = E(x_i^2) - p_i^2 \le E(x_i^2) \le E(x_i) = p_i.$$

Thus, $\prod_{i \in I} E(y_i^{r_i}) \le \prod_{i \in I} E(|y_i^{r_i}|) \le \prod_{i \in I} p_i$. Let p(I) denote $\prod_{i \in I} p_i$. So,

$$E\left[\left(\sum_{i=1}^{d} y_i\right)^r\right] \le \sum_{\substack{I\\|I| \le r/2}} p(I)n(I),$$

where n(I) is number of terms in the expansion of $\left(\sum_{i=1}^{d} y_i\right)^r$ with I as the set of i with nonzero r_i . Each term corresponds to selecting one of the variables among y_i , $i \in I$ from each of the r brackets in the expansion of $(y_1 + y_2 + \cdots + y_d)^r$. Thus $n(I) \leq |I|^r$. Also,

$$\sum_{\substack{I \\ |I|=t}} p(I) \le \left(\sum_{i=1}^{d} p_i\right)^t \frac{1}{t!} = \frac{\mu^t}{t!}.$$

To see this, do the multinomial expansion of $\left(\sum_{i=1}^d p_i\right)^t$. For each Iwith|I|=t, we get $\prod_{i\in I} p_i$ exactly t! times. We also get other terms with repeated p_i , hence the inequality. Thus, using the Stirling approximation $t! \cong \sqrt{2\pi t} \left(\frac{t}{e}\right)^t$,

$$E\left[\left(\sum_{i=1}^{d} y_i\right)^r\right] \le \sum_{t=1}^{r/2} \frac{\mu^t t^r}{t!} \le \sum_{t=1}^{r/2} \frac{\mu^t}{\sqrt{2\pi} t^t e^{-t}} t^r \le \frac{1}{\sqrt{2\pi}} \left(\operatorname{Max}_{t=1}^{r/2} f(t)\right) \sum_{t=1}^{r/2} t^r,$$

where $f(t) = \frac{(e\mu)^t}{t^t}$. Taking logarithms and differentiating, we get

$$\ln f(t) = t \ln(e\mu) - t \ln t$$

$$\frac{d}{dt} \ln f(t) = \ln(e\mu) - 1 + \ln t$$

$$= \ln(\mu) - \ln(t)$$

Setting $\ln(\mu) - \ln(t)$ to zero, we see that the maximum of f(t) is attained at $t = \mu$. If $\mu < r/2$, then the maximum of f(t) occurs for t = u and $\operatorname{Max}_{t=1}^{r/2} f(t) \le e^{\mu} \le e^{r/2}$. If

 $\mu \ge r/2$, then $\max_{t=1}^{r/2} f(t) \le \frac{(2e\mu)^{r/2}}{r^{r/2}}$. The geometric sum $\sum_{t=1}^{r/2} t^r$ is bounded by twice its last term or $2(r/2)^r$. Thus,

$$E\left[\left(\sum_{i=1}^{d} y_i\right)^r\right] \le \frac{2}{\sqrt{2\pi}} \operatorname{Max}\left[\left(\frac{2e\mu}{r}\right)^{\frac{r}{2}}, e^{\frac{r}{2}}\right] \left(\frac{r}{2}\right)^r$$
$$\le \operatorname{Max}\left[\left(\frac{er\mu}{2}\right)^{\frac{r}{2}}, \left(\frac{e}{4}r^2\right)^{\frac{r}{2}}\right]$$
$$\le \operatorname{Max}\left[\left(2r\mu\right)^{r/2}, r^r\right]$$

proving the lemma.

Theorem 2.6 (Chernoff Bounds): Suppose x_i , y_i , and μ are as in the Lemma 2.5. Then

$$\operatorname{Prob}\left(\left|\sum_{i=1}^{d} y_i\right| \ge t\right) \le 3e^{-t^2/12\mu}, \qquad \text{for } 0 < t \le 3\mu$$

$$\operatorname{Prob}\left(\left|\sum_{i=1}^{d} y_i\right| \ge t\right) \le 4 \times 2^{-t/3}, \qquad \text{for } t > 3\mu.$$

Proof: Let r be a positive even integer. Let $y = \sum_{i=1}^{d} y_i$. Since r is even, y^r is nonnegative. By Markov inequality

$$\operatorname{Prob}(|y| \ge t) = \operatorname{Prob}(y^r \ge t^r) \le \frac{E(y^r)}{t^r}.$$

Applying Lemma 2.5,

$$\operatorname{Prob}\left(|y| \ge t\right) \le \operatorname{Max}\left[\frac{(2r\mu)^{r/2}}{t^r}, \frac{r^r}{t^r}\right]. \tag{2.5}$$

Since this holds for every even positive integer r, choose r to minimize the right hand side. By calculus, the r that minimizes $\frac{(2r\mu)^{r/2}}{t^r}$ is $r=t^2/(2e\mu)$. This is seen by taking logarithms and differentiating with respect to r. Since the r that minimizes the quantity may not be an even integer, choose r to be the largest even integer that is at most $t^2/(2e\mu)$. Then,

$$\left(\frac{2r\mu}{t^2}\right)^{r/2} \le e^{-r/2} \le e^{1-(t^2/4e\mu)} \le 3e^{-t^2/12\mu}$$

for all t. When $t \leq 3\mu$, since r was choosen such that $r \leq \frac{t^2}{2eu}$,

$$\frac{r^r}{t^r} \le \left(\frac{t}{2e\mu}\right)^r \le \left(\frac{3\mu}{2e\mu}\right)^r \le \left(\frac{2e}{3}\right)^{-r} \le \left(\sqrt{e}\right)^{-r} \le e^{-r/2},$$

which completes the proof of the first inequality.

For the second inequality, choose r to be the largest even integer less than or equal to 2t/3. Then, $\operatorname{Max}\left[\frac{(2r\mu)^{r/2}}{t^r}, \frac{r^r}{t^r}\right] \leq 2^{-r/2}$ and the proof is completed similar to the first case.

Concentration for heavier-tailed distributions

The only place $0 \le x_i \le 1$ is used in the proof of (2.4) is in asserting that $E|y_i^k| \le p_i$ for all k = 2, 3, ..., r. Imitating the proof above, one can prove stronger theorems that only assume bounds on moments up to the r^{th} moment and so include cases when x_i may be unbounded as in the Poisson or exponential density on the real line as well as power law distributions for which only moments up to some r^{th} moment are bounded. We state one such theorem. The proof is left to the reader.

Theorem 2.7 Suppose x_1, x_2, \ldots, x_d are independent random variables with $E(x_i) = p_i$, $\sum_{i=1}^d p_i = \mu$ and $E|(x_i - p_i)^k| \le p_i$ for $k = 2, 3, \ldots, \lfloor t^2/6\mu \rfloor$. Then,

$$Prob\left(\left|\sum_{i=1}^{d} x_i - \mu\right| \ge t\right) \le \operatorname{Max}\left(3e^{-t^2/12\mu}, 4 \times 2^{-t/e}\right).$$

2.4 Volumes of Other Solids

There are very few high-dimensional solids for which there are closed-form formulae for the volume. The volume of the rectangular solid

$$R = \{ \mathbf{x} | l_1 \le x_1 \le u_1, l_2 \le x_2 \le u_2, \dots, l_d \le x_d \le u_d \},$$

is the product of the lengths of its sides. Namely, it is $\prod_{i=1}^{d} (u_i - l_i)$.

A parallelepiped is a solid described by

$$P = \{ \mathbf{x} \mid \mathbf{l} \le A\mathbf{x} \le \mathbf{u} \},$$

where A is an invertible $d \times d$ matrix, and \mathbf{l} and \mathbf{u} are lower and upper bound vectors, respectively. The statements $\mathbf{l} \leq A\mathbf{x}$ and $A\mathbf{x} \leq \mathbf{u}$ are to be interpreted row by row asserting 2d inequalities. A parallelepiped is a generalization of a parallelegram. It is easy to see that P is the image under an invertible linear transformation of a rectangular solid. Indeed, let

$$R = \{ \mathbf{y} \mid \mathbf{l} \le \mathbf{y} \le \mathbf{u} \}.$$

Then the map $\mathbf{x} = A^{-1}\mathbf{y}$ maps R to P. This implies that

$$Volume(P) = |Det(A^{-1})| Volume(R).$$

Simplices, which are generalizations of triangles, are another class of solids for which volumes can be easily calculated. Consider the triangle in the plane with vertices $\{(0,0),(1,0),(1,1)\}$ which can be described as $\{(x,y)\,|\,0\leq y\leq x\leq 1\}$. Its area is 1/2 because two such right triangles can be combined to form the unit square. The generalization is the simplex in d-space with d+1 vertices,

$$\{(0,0,\ldots,0),(1,0,0,\ldots,0),(1,1,0,0,\ldots,0),\ldots,(1,1,\ldots,1)\},\$$

which is the set

$$S = \{ \mathbf{x} \mid 1 \ge x_1 \ge x_2 \ge \dots \ge x_d \ge 0 \}.$$

How many copies of this simplex exactly fit into the unit square, $\{\mathbf{x} \mid 0 \leq x_i \leq 1\}$? Every point in the square has some ordering of its coordinates and since there are d! orderings, exactly d! simplices fit into the unit square. Thus, the volume of each simplex is 1/d!. Now consider the right angle simplex R whose vertices are the d unit vectors $(1,0,0,\ldots,0),(0,1,0,\ldots,0),\ldots,(0,0,0,\ldots,0,1)$ and the origin. A vector \mathbf{y} in R is mapped to an \mathbf{x} in S by the mapping: $x_d = y_d; x_{d-1} = y_d + y_{d-1}; \ldots; x_1 = y_1 + y_2 + \cdots + y_d$. This is an invertible transformation with determinant one, so the volume of R is also 1/d!.

A general simplex is obtained by a translation (adding the same vector to every point) followed by an invertible linear transformation on the right simplex. Convince yourself that in the plane every triangle is the image under a translation plus an invertible linear transformation of the right triangle. As in the case of parallelepipeds, applying a linear transformation A multiplies the volume by the determinant of A. Translation does not change the volume. Thus, if the vertices of a simplex T are $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_{d+1}$, then translating the simplex by $-\mathbf{v}_{d+1}$ results in vertices $\mathbf{v}_1 - \mathbf{v}_{d+1}, \mathbf{v}_2 - \mathbf{v}_{d+1}, \ldots, \mathbf{v}_d - \mathbf{v}_{d+1}, \mathbf{0}$. Let A be the $d \times d$ matrix with columns $\mathbf{v}_1 - \mathbf{v}_{d+1}, \mathbf{v}_2 - \mathbf{v}_{d+1}, \ldots, \mathbf{v}_d - \mathbf{v}_{d+1}$. Then, $A^{-1}T = R$ and AR = T. Thus, the volume of T is $\frac{1}{d!}|\mathrm{Det}(A)|$.

2.5 Generating Points Uniformly at Random on the surface of a Sphere

Consider generating points uniformly at random on the surface of a unit-radius sphere. First, consider the 2-dimensional version of generating points on the circumference of a unit-radius circle by the following method. Independently generate each coordinate uniformly at random from the interval [-1,1]. This produces points distributed over a square that is large enough to completely contain the unit circle. Project each point onto the unit circle. The distribution is not uniform since more points fall on a line from the origin to a vertex of the square, than fall on a line from the origin to the midpoint of an edge of the square due to the difference in length. To solve this problem, discard all points outside the unit circle and project the remaining points onto the circle.

One might generalize this technique in the obvious way to higher dimensions. However, the ratio of the volume of a d-dimensional unit sphere to the volume of a d-dimensional

unit cube decreases rapidly making the process impractical for high dimensions since almost no points will lie inside the sphere. The solution is to generate a point each of whose coordinates is a Gaussian variable. The probability distribution for a point (x_1, x_2, \ldots, x_d) is given by

$$p(x_1, x_2, \dots, x_d) = \frac{1}{(2\pi)^{\frac{d}{2}}} e^{-\frac{x_1^2 + x_2^2 + \dots + x_d^2}{2}}$$

and is spherically symmetric. Normalizing the vector $\mathbf{x} = (x_1, x_2, \dots, x_d)$ to a unit vector gives a distribution that is uniform over the sphere. Note that once the vector is normalized, its coordinates are no longer statistically independent.

2.6 Gaussians in High Dimension

A 1-dimensional Gaussian has its mass close to the origin. However, as the dimension is increased something different happens. The d-dimensional spherical Gaussian with zero mean and variance σ has density function

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} \sigma^d} \exp\left(-\frac{|\mathbf{x}|^2}{2\sigma^2}\right).$$

The value of the Gaussian is maximum at the origin, but there is very little volume there. When $\sigma=1$, integrating the probability density over a unit sphere centered at the origin yields nearly zero mass since the volume of such a sphere is negligible. In fact, one needs to increase the radius of the sphere to \sqrt{d} before there is a significant nonzero volume and hence a nonzero probability mass. If one increases the radius beyond \sqrt{d} , the integral ceases to increase even though the volume increases since the probability density is dropping off at a much higher rate. The natural scale for the Gaussian is in units of $\sigma\sqrt{d}$.

Expected squared distance of a point from the center of a Gaussian

Consider a d-dimensional Gaussian centered at the origin with variance σ^2 . For a point $\mathbf{x} = (x_1, x_2, \dots, x_d)$ chosen at random from the Gaussian, the expected squared length of \mathbf{x} is

$$E(x_1^2 + x_2^2 + \dots + x_d^2) = dE(x_1^2) = d\sigma^2.$$

For large d, the value of the squared length of \mathbf{x} is tightly concentrated about its mean. We call the square root of the expected squared distance (namely $\sigma\sqrt{d}$) the radius of the Gaussian. In the rest of this section we consider spherical Gaussians with $\sigma=1$; all results can be scaled up by σ .

The probability mass of a unit variance Gaussian as a function of the distance from its center is given by $r^{d-1}e^{-r^2/2}$ times some constant normalization factor where r is the

distance from the center and d is the dimension of the space. The probability mass function has its maximum at

$$r = \sqrt{d-1}$$

which can be seen from setting the derivative equal to zero

$$\frac{\partial}{\partial r}e^{-\frac{r^2}{2}}r^{d-1} = (d-1)e^{-\frac{r^2}{2}}r^{d-2} - r^de^{-\frac{r^2}{2}} = 0$$

which implies $r^2 = d - 1$.

Calculation of width of the annulus

We now show that most of the mass of the Gaussian is within an annulus of constant width and radius $\sqrt{d-1}$. The probability mass of the Gaussian as a function of r is $g(r) = r^{d-1}e^{-r^2/2}$. To determine the width of the annulus in which g(r) is nonnegligible, consider the logarithm of g(r)

$$f(r) = \ln g(r) = (d-1)\ln r - \frac{r^2}{2}.$$

Differentiating f(r),

$$f'(r) = \frac{d-1}{r} - r$$
 and $f''(r) = -\frac{d-1}{r^2} - 1 \le -1$.

Note that f'(r) = 0 at $r = \sqrt{d-1}$ and f''(r) < 0 for all r. The Taylor series expansion for f(r) about $\sqrt{d-1}$, is

$$f(r) = f(\sqrt{d-1}) + f'(\sqrt{d-1})(r - \sqrt{d-1}) + \frac{1}{2}f''(\sqrt{d-1})(r - \sqrt{d-1})^2 + \cdots$$

Thus,

$$f(r) = f(\sqrt{d-1}) + f'(\sqrt{d-1})(r - \sqrt{d-1}) + \frac{1}{2}f''(\zeta)(r - \sqrt{d-1})^2$$

for some point ζ between $\sqrt{d-1}$ and r.¹ Since $f'(\sqrt{d-1}) = 0$, the second term vanishes and

$$f(r) = f(\sqrt{d-1}) + \frac{1}{2}f''(\zeta)(r - \sqrt{d-1})^{2}.$$

Since the second derivative is always less than -1,

$$f(r) \le f(\sqrt{d-1}) - \frac{1}{2}(r - \sqrt{d-1})^2.$$

Recall that $g(r) = e^{f(r)}$. Thus

$$g(r) \le e^{f(\sqrt{d-1}) - \frac{1}{2}(r - \sqrt{d-1})^2} = g(\sqrt{d-1})e^{-\frac{1}{2}(r - \sqrt{d-1})^2}$$

¹see Whittaker and Watson 1990, pp. 95-96

Let c be a positive real and let I be the interval $[\sqrt{d-1}-c,\sqrt{d-1}+c]$. We calculate the ratio of an upper bound on the probability mass outside the interval to a lower bound on the total probability mass. The probability mass outside the interval I is upper bounded by

$$\int_{r \notin I} g(r) \, dr \leq \int_{r=0}^{\sqrt{d-1}-c} g(\sqrt{d-1}) e^{-(r-\sqrt{d-1})^2/2} \, dr + \int_{r=\sqrt{d-1}+c}^{\infty} g(\sqrt{d-1}) e^{-(r-\sqrt{d-1})^2/2} \, dr
\leq 2g(\sqrt{d-1}) \int_{r=\sqrt{d-1}+c}^{\infty} e^{-(r-\sqrt{d-1})^2/2} \, dr
= 2g(\sqrt{d-1}) \int_{y=c}^{\infty} e^{-y^2/2} \, dy
\leq 2g(\sqrt{d-1}) \int_{y=c}^{\infty} \frac{y}{c} e^{-y^2/2} \, dy
= \frac{2}{c} g(\sqrt{d-1}) e^{-c^2/2}.$$

To get a lower bound on the probability mass in the interval $[\sqrt{d-1}-c,\sqrt{d-1}+c]$, consider the subinterval $[\sqrt{d-1},\sqrt{d-1}+\frac{c}{2}]$. For r in the subinterval $[\sqrt{d-1},\sqrt{d-1}+\frac{c}{2}]$, $f''(r) \geq -2$ and

$$f(r) \ge f(\sqrt{d-1}) - (r - \sqrt{d-1})^2 \ge f(\sqrt{d-1}) - \frac{c^2}{4}.$$

Thus

$$g(r) = e^{f(r)} \ge e^{f\sqrt{d-1}}e^{-\frac{c^2}{4}} = g(\sqrt{d-1})e^{\frac{c^2}{4}}.$$

Hence, $\int_{\sqrt{d-1}}^{\sqrt{d-1}+\frac{c}{2}}g(r)\ dr \ge \frac{c}{2}g(\sqrt{d-1})e^{-c^2/4}$ and the fraction of the mass outside the interval is

$$\frac{\frac{2}{c}g(\sqrt{d-1})e^{-c^2/2}}{\frac{c}{2}g(\sqrt{d-1})e^{-c^2/4} + \frac{2}{c}g(\sqrt{d-1})e^{-c^2/2}} = \frac{\frac{2}{c^2}e^{-\frac{c^2}{4}}}{\frac{c}{2} + \frac{2}{c^2}e^{-\frac{c^2}{4}}} = \frac{e^{-\frac{c^2}{4}}}{\frac{c^2}{4} + e^{-\frac{c^2}{4}}} \le \frac{4}{c^2}e^{-\frac{c^2}{4}}.$$

This establishes the following lemma.

Lemma 2.8 For a d-dimensional spherical Gaussian of variance 1, all but $\frac{4}{c^2}e^{-c^2/4}$ fraction of its mass is within the annulus $\sqrt{d-1} - c \le r \le \sqrt{d-1} + c$ for any c > 0.

Separating Gaussians

Gaussians are often used to model data. A common stochastic model is the mixture model where one hypothesizes that the data is generated from a convex combination of simple probability densities. An example is two Gaussian densities $F_1(\mathbf{x})$ and $F_2(\mathbf{x})$ where data is drawn from the mixture $F(\mathbf{x}) = w_1 F_1(\mathbf{x}) + w_2 F_2(\mathbf{x})$ with positive weights w_1 and w_2 summing to one. Assume that F_1 and F_2 are spherical with unit variance. If their

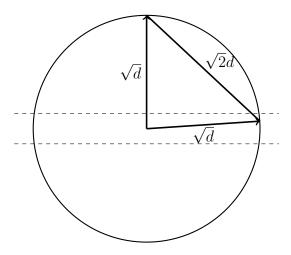


Figure 2.12: Two randomly chosen points in high dimension are almost surely nearly orthogonal.

means are very close, then given data from the mixture, one cannot tell for each data point whether it came from F_1 or F_2 . The question arises as to how much separation is needed between the means to tell which Gaussian generated which data point. We will see that a separation of $\Omega(d^{1/4})$ suffices. Later, we will see that with more sophisticated algorithms, even a separation of $\Omega(1)$ suffices.

Consider two spherical unit variance Gaussians. From Lemma 2.8, most of the probability mass of each Gaussian lies on an annulus of width O(1) at radius $\sqrt{d-1}$. Also $e^{-|\mathbf{x}|^2/2}$ factors into $\prod_i e^{-x_i^2/2}$ and almost all of the mass is within the slab $\{\mathbf{x}|-c \leq x_1 \leq c\}$, for $c \in O(1)$. Pick a point \mathbf{x} from the first Gaussian. After picking \mathbf{x} , rotate the coordinate system to make the first axis point towards \mathbf{x} . Then, independently pick a second point \mathbf{y} also from the first Gaussian. The fact that almost all of the mass of the Gaussian is within the slab $\{\mathbf{x}|-c \leq x_1 \leq c, c \in O(1)\}$ at the equator says that \mathbf{y} 's component along \mathbf{x} 's direction is O(1) with high probability. Thus, \mathbf{y} is nearly perpendicular to \mathbf{x} . So, $|\mathbf{x}-\mathbf{y}| \approx \sqrt{|\mathbf{x}|^2 + |\mathbf{y}|^2}$. See Figure 2.12. More precisely, since the coordinate system has been rotated so that \mathbf{x} is at the North Pole, $\mathbf{x} = (\sqrt{d} \pm O(1), 0, \ldots)$. Since \mathbf{y} is almost on the equator, further rotate the coordinate system so that the component of \mathbf{y} that is perpendicular to the axis of the North Pole is in the second coordinate. Then $\mathbf{y} = (O(1), \sqrt{d} \pm O(1), \ldots)$. Thus,

$$(\mathbf{x}-\mathbf{y})^2=d\pm O(\sqrt{d})+d\pm O(\sqrt{d})=2d\pm O(\sqrt{d})$$
 and $|\mathbf{x}-\mathbf{y}|=\sqrt{(2d)}\pm O(1).$

Given two spherical unit variance Gaussians with centers \mathbf{p} and \mathbf{q} separated by a distance δ , the distance between a randomly chosen point \mathbf{x} from the first Gaussian and a randomly chosen point \mathbf{y} from the second is close to $\sqrt{\delta^2 + 2d}$, since $\mathbf{x} - \mathbf{p}$, $\mathbf{p} - \mathbf{q}$, and $\mathbf{q} - \mathbf{y}$

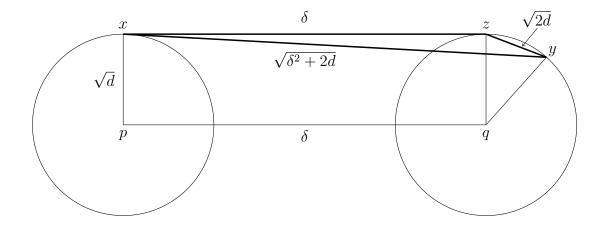


Figure 2.13: Distance between a pair of random points from two different unit spheres approximating the annuli of two Gaussians.

are nearly mutually perpendicular. To see this, pick \mathbf{x} and rotate the coordinate system so that \mathbf{x} is at the North Pole. Let \mathbf{z} be the North Pole of the sphere approximating the second Gaussian. Now pick \mathbf{y} . Most of the mass of the second Gaussian is within O(1) of the equator perpendicular to $\mathbf{q} - \mathbf{z}$. Also, most of the mass of each Gaussian is within distance O(1) of the respective equators perpendicular to the line $\mathbf{q} - \mathbf{p}$. Thus,

$$|\mathbf{x} - \mathbf{y}|^2 \approx \delta^2 + |\mathbf{z} - \mathbf{q}|^2 + |\mathbf{q} - \mathbf{y}|^2$$
$$= \delta^2 + 2d \pm O(\sqrt{d}).$$

To ensure that the distance between two points picked from the same Gaussian are closer to each other than two points picked from different Gaussians requires that the upper limit of the distance between a pair of points from the same Gaussian is at most the lower limit of distance between points from different Gaussians. This requires that $\sqrt{2d} + O(1) \le \sqrt{2d} + \delta^2 - O(1)$ or $2d + O(\sqrt{d}) \le 2d + \delta^2$, which holds when $\delta \in \Omega(d^{1/4})$. Thus, mixtures of spherical Gaussians can be separated provided their centers are separated by more than $d^{\frac{1}{4}}$. One can actually separate Gaussians where the centers are much closer. In Chapter 4, we will see an algorithm that separates a mixture of k spherical Gaussians whose centers are much closer.

Algorithm for separating points from two Gaussians

Calculate all pairwise distances between points. The cluster of smallest pairwise distances must come from a single Gaussian. Remove these points and repeat the process.

Fitting a single spherical Gaussian to data

Given a set of sample points, $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_n}$, in a d-dimensional space, we wish to find the spherical Gaussian that best fits the points. Let F be the unknown Gaussian with mean μ and variance σ^2 in every direction. The probability of picking these very points when sampling according to F is given by

$$c \exp \left(-\frac{(\mathbf{x_1} - \boldsymbol{\mu})^2 + (\mathbf{x_2} - \boldsymbol{\mu})^2 + \dots + (\mathbf{x_n} - \boldsymbol{\mu})^2}{2\sigma^2}\right)$$

where the normalizing constant c is the reciprocal of $\left[\int e^{-\frac{|\mathbf{x}-\boldsymbol{\mu}|^2}{2\sigma^2}}dx\right]^n$. In integrating from $-\infty$ to ∞ , one could shift the origin to $\boldsymbol{\mu}$ and thus c is $\left[\int e^{-\frac{|\mathbf{x}|^2}{2\sigma^2}}dx\right]^{-n}$ and is independent of $\boldsymbol{\mu}$.

The Maximum Likelihood Estimator (MLE) of F, given the samples $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_n}$, is the F that maximizes the above probability.

Lemma 2.9 Let $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ be a set of n points in d-space. Then $(\mathbf{x}_1 - \boldsymbol{\mu})^2 + (\mathbf{x}_2 - \boldsymbol{\mu})^2 + \dots + (\mathbf{x}_n - \boldsymbol{\mu})^2$ is minimized when $\boldsymbol{\mu}$ is the centroid of the points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, namely $\boldsymbol{\mu} = \frac{1}{n}(\mathbf{x}_1 + \mathbf{x}_2 + \dots + \mathbf{x}_n)$.

Proof: Setting the derivative of $(\mathbf{x}_1 - \boldsymbol{\mu})^2 + (\mathbf{x}_2 - \boldsymbol{\mu})^2 + \cdots + (\mathbf{x}_n - \boldsymbol{\mu})^2$ to zero yields

$$-2\left(\mathbf{x}_{1}-\boldsymbol{\mu}\right)-2\left(\mathbf{x}_{2}-\boldsymbol{\mu}\right)-\cdots-2\left(\mathbf{x}_{d}-\boldsymbol{\mu}\right)=0.$$

Solving for μ gives $\mu = \frac{1}{n}(\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_n)$.

In the maximum likelihood estimate for F, μ is set to the centroid. Next we show that σ is set to the standard deviation of the sample. Substitute $\nu = \frac{1}{2\sigma^2}$ and $a = (\mathbf{x}_1 - \boldsymbol{\mu})^2 + (\mathbf{x}_2 - \boldsymbol{\mu})^2 + \dots + (\mathbf{x}_n - \boldsymbol{\mu})^2$ into the formula for the probability of picking the points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$. This gives

$$\frac{e^{-a\nu}}{\left[\int\limits_x e^{-|\mathbf{x}|^2\nu} dx\right]^n}.$$

Now, **a** is fixed and ν is to be determined. Taking logs, the expression to maximize is

$$-a\nu - n \ln \left[\int_{\mathbf{x}} e^{-\nu |\mathbf{x}|^2} dx \right].$$

To find the maximum, differentiate with respect to ν , set the derivative to zero, and solve for σ . The derivative is

$$-a + n \frac{\int_{\mathbf{x}} |\mathbf{x}|^2 e^{-\nu |\mathbf{x}|^2} dx}{\int_{\mathbf{x}} e^{-\nu |\mathbf{x}|^2} dx}.$$

Setting $\mathbf{y} = \sqrt{\nu}\mathbf{x}$ in the derivative, yields

$$-a + \frac{n}{\nu} \frac{\int_{\mathbf{y}} \mathbf{y}^2 e^{-\mathbf{y}^2} dy}{\int_{\mathbf{y}} e^{-\mathbf{y}^2} dy}.$$

Since the ratio of the two integrals is the expected distance squared of a d-dimensional spherical Gaussian of standard deviation $\frac{1}{\sqrt{2}}$ to its center, and this is known to be $\frac{d}{2}$, we get $-a + \frac{nd}{2\nu}$. Substituting σ^2 for $\frac{1}{2\nu}$ gives $-a + nd\sigma^2$. Setting $-a + nd\sigma^2 = 0$ shows that the maximum occurs when $\sigma = \frac{\sqrt{a}}{\sqrt{nd}}$. Note that this quantity is the square root of the average coordinate distance squared of the samples to their mean, which is the standard deviation of the sample. Thus, we get the following lemma.

Lemma 2.10 The maximum likelihood spherical Gaussian for a set of samples is the one with center equal to the sample mean and standard deviation equal to the standard deviation of the sample.

Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ be a sample of points generated by a Gaussian probability distribution. $\boldsymbol{\mu} = \frac{1}{n}(\mathbf{x}_1 + \mathbf{x}_2 + \dots + \mathbf{x}_n)$ is an unbiased estimator of the expected value of the distribution. However, if in estimating the variance from the sample set, we use the estimate of the expected value rather than the true expected value, we will not get an unbiased estimate of the variance since the sample mean is not independent of the sample set. One should use $\boldsymbol{\mu} = \frac{1}{n-1}(\mathbf{x}_1 + \mathbf{x}_2 + \dots + \mathbf{x}_n)$ when estimating the variance. See appendix.

2.7 Random Projection and the Johnson-Lindenstrauss Theorem

Many high-dimensional problems such as the nearest neighbor problem can be sped up by projecting the data to a random lower-dimensional subspace and solving the problem there. This technique requires that the projected distances have the same ordering as the original distances. If one chooses a random k-dimensional subspace, then indeed all the projected distances in the k-dimensional space are approximately within a known scale factor of the distances in the d-dimensional space. We first show that for one distance pair, the probability of its projection being badly represented is exponentially small in k. Then we use the union bound to argue that failure does not happen for any pair.

Project a fixed (not random) unit length vector \mathbf{v} in d-dimensional space onto a random k-dimensional space. By the Pythagoras theorem, the length squared of a vector is the sum of the squares of its components. Thus, we would expect the squared length of the projection to be $\frac{k}{d}$. The following theorem asserts that the squared length of the projection is very close to this quantity.

Theorem 2.11 (The Random Projection Theorem): Let \mathbf{v} be a fixed unit length vector in a d-dimensional space and let W be a random k-dimensional subspace. Let \mathbf{w} be the projection of \mathbf{v} onto W. For any $0 \le \varepsilon \le 1$, $Prob\left(\left||\mathbf{w}|^2 - \frac{k}{d}\right| \ge \varepsilon \frac{k}{d}\right) \le 4e^{-\frac{k\varepsilon^2}{64}}$.

Proof: A random subspace is generated by selecting a set of basis vectors. Working with such a set of dependent vectors is difficult. However, projecting a fixed vector onto a random subspace is the same as projecting a random vector onto a fixed subspace. That is, the probability distribution of \mathbf{w} in the theorem is the same as the probability distribution of the vector obtained by taking a random unit length vector \mathbf{z} and projecting it onto the fixed subspace U spanned by its first k coordinate vectors. This is because one can rotate the coordinate system so that a set of basis vectors for W are the first k coordinate axes.

Let $\tilde{\mathbf{z}}$ be the projection of \mathbf{z} onto U. We will prove that $|\tilde{\mathbf{z}}|^2 \approx \frac{k}{d}$. Now $||\tilde{\mathbf{z}}|^2 - \frac{k}{d}|$ is greater than or equal to $\varepsilon \frac{k}{d}$ if either $|\tilde{\mathbf{z}}|^2 \leq (1 - \varepsilon) \frac{k}{d}$ or $|\tilde{\mathbf{z}}|^2 \geq (1 - \varepsilon) \frac{k}{d}$. Let $\beta = 1 - \varepsilon$. We will prove that $\operatorname{Prob}\left(|\tilde{\mathbf{z}}|^2 < \beta \frac{k}{d}\right) \leq 2e^{-\frac{k\varepsilon^2}{4}}$. The other case is similar and is omitted. Together they imply $\operatorname{Prob}\left(||\mathbf{w}|^2 - \frac{k}{d}| \geq \varepsilon \frac{k}{d}\right) \leq 4e^{-\frac{k\varepsilon^2}{64}}$.

Pick a random vector \mathbf{z} of length one by picking independent Gaussian random variables x_1, x_2, \dots, x_d , each with mean zero and variance one. Let $\mathbf{x} = (x_1, x_2, \dots, x_d)$ and take $\mathbf{z} = \mathbf{x}/|\mathbf{x}|$. This yields a random vector \mathbf{z} of length one.

$$\operatorname{Prob}\left[|\tilde{\mathbf{z}}|^{2} < \beta \frac{k}{d}\right] = \operatorname{Prob}\left[|\tilde{\mathbf{z}}|^{2} \le \beta \frac{k}{d}|\mathbf{z}|^{2}\right]$$

$$= \operatorname{Prob}\left[x_{1}^{2} + x_{2}^{2} + \dots + x_{k}^{2} < \beta \frac{k}{d}\left(x_{1}^{2} + x_{2}^{2} + \dots + x_{d}^{2}\right)\right]$$

$$= \operatorname{Prob}\left[\beta k\left(x_{1}^{2} + x_{2}^{2} + \dots + x_{d}^{2}\right) - d\left(x_{1}^{2} + x_{2}^{2} + \dots + x_{k}^{2}\right) > 0\right].$$

If $k\varepsilon^2 < 64$, then $4e^{-\frac{k\varepsilon^2}{64}} > 1$, so the probability upper bound asserted in the theorem is greater than one and there is nothing to prove. So assume that $k\varepsilon^2 \geq 64$ which implies $\varepsilon \geq \frac{8}{\sqrt{k}}$. Define $c = \varepsilon \sqrt{k}/4$ and since $\varepsilon \geq \frac{8}{\sqrt{k}}$, it follows that $c \geq 2$.

Now if $\beta k \left(x_1^2 + x_2^2 + \dots + x_d^2\right) - d\left(x_1^2 + x_2^2 + \dots + x_k^2\right) > 0$, then one of the following inequalities must hold with $c = \varepsilon \sqrt{k}/4$:

$$\beta k(x_1^2 + x_2^2 + \dots + x_d^2) > \beta k(\sqrt{d-1} + c)^2$$
 (2.6)

$$d(x_1^2 + x_2^2 + \dots + x_k^2) < \beta k(\sqrt{d-1} + c)^2.$$
(2.7)

Using Lemma 2.8 we will prove that the probability of each of (2.6) and (2.7) is at most $\frac{4}{c^2}e^{-\frac{c^2}{4}} = \frac{64}{k\varepsilon^2}e^{-\frac{k\varepsilon^2}{64}} \le e^{-k\varepsilon^2/64}$ so that the probability of at least one of (2.6) or (2.7) is less than or equal to $2e^{-\frac{k\varepsilon^2}{64}}$ which proves the theorem. Lemma 2.8 implies

$$(x_1^2 + x_2^2 + \dots + x_d^2)^2 \ge (\sqrt{d-1} + c)^2$$

with probability less than or equal to $\frac{4}{c^2}e^{-c^2/4} \le e^{-k\varepsilon^2/64}$ from which (2.6) follows. For (2.7), from Lemma 2.8,

$$Prob(d(x_1^2 + x_2^2 + \dots + x_k^2) < d(\sqrt{k-1} - c)^2)$$

with probability less than or equal to $\frac{4}{c^2}e^{-c^2/4} \le e^{-k\varepsilon^2/64}$. Since $\beta k < d$, $\beta k(\sqrt{d-1}-c)^2 \le d(\sqrt{k-1}-c)^2$ and thus

$$\text{Prob}\left(d(x_1^2 + x_2^2 + \dots + x_k^2) < \beta k(\sqrt{d-1} - c)^2\right)$$

$$\leq \text{Prob}\left(d(x_1^2 + x_2^2 + \dots + x_k^2) < d(\sqrt{k-1} - c)^2\right)$$

$$< e^{-k\varepsilon^2/64}$$

completing the proof of Theorem 2.11.

The Random Projection Theorem enables us to argue, using the union bound, that the projection to order $\log n$ dimensions preserves all relative pairwise distances between a set of n points. This is the content of the Johnson-Lindenstrauss Lemma.

Theorem 2.12 (Johnson-Lindenstrauss Lemma): For any $0 < \varepsilon < 1$ and any integer n, let k be an integer such that

$$k \ge \frac{64 \ln n}{\varepsilon^2}.$$

For any set P of n points in \mathbb{R}^d , a random projection f mapping $f: \mathbb{R}^d \to \mathbb{R}^k$ has the property that for all \mathbf{u} and \mathbf{v} in P,

$$(1-\varepsilon)\frac{k}{d}|\mathbf{u}-\mathbf{v}|^2 \le |f(\mathbf{u})-f(\mathbf{v})|^2 \le (1+\varepsilon)\frac{k}{d}|\mathbf{u}-\mathbf{v}|^2$$

with probability at least 9/10.

Proof: Let S be a random k-dimensional subspace and let $f(\mathbf{u})$ be the projection of \mathbf{u} onto S multiplied by the scalar $\sqrt{\frac{d}{k}}$. Applying the Random Projection Theorem 2.11, for any fixed \mathbf{u} and \mathbf{v} , the probability that $||f(\mathbf{u}) - f(\mathbf{v})||^2$ is outside the range

$$\left[(1 - \varepsilon) \frac{k}{\beta} |\mathbf{u} - \mathbf{v}|^2, (1 + \varepsilon) \frac{k}{\beta} |\mathbf{u} - \mathbf{v}|^2 \right]$$

is at most

$$e^{-\frac{k\varepsilon^2}{16}} = e^{-4\ln n} = \frac{1}{n^4}.$$

By the union bound the probability that any pair has a large distortion is less than $\binom{n}{2} \times \frac{1}{n^4} \leq \frac{1}{n}$.

Remark: It is important to note that the conclusion of Theorem 2.12 is asserted for all \mathbf{u} and \mathbf{v} in P, not just for most \mathbf{u} and \mathbf{v} . The weaker assertion for most \mathbf{u} and \mathbf{v} is not that useful, since we do not know which \mathbf{v} would end up being the closest point to \mathbf{u} and an assertion for most may not cover the particular \mathbf{v} . A remarkable aspect of the theorem is that the number of dimensions in the projection is only dependent logarithmically on n. Since k is often much less than d, this is called a dimension reduction technique.

For the nearest neighbor problem, if the database has n_1 points and n_2 queries are expected during the lifetime, then take $n = n_1 + n_2$ and project the database to a random k-dimensional space, where $k \geq \frac{64 \ln n}{\varepsilon^2}$. On receiving a query, project the query to the same subspace and compute nearby database points. The theorem says that this will yield the right answer whatever the query with high probability. Note that the exponentially small in k probability in Theorem 2.11 was useful here in making k only dependent on $\log n$, rather than n.

2.8 Bibliographic Notes

The word vector model was introduced by Salton [SWY75]. Taylor series remainder material can be found in Whittaker and Watson 1990, pp. 95-96. There is vast literature on Gaussian distribution, its properties, drawing samples according to it, etc. The reader can choose the level and depth according to his/her background. For Chernoff bounds and their applications, see [MU05] or [MR95b]. The proof here and the application to heavy-tailed distributions is simplified from [Kan09]. The original proof of the Random Projection Theorem by Johnson and Lindenstrauss was complicated. Several authors used Gaussians to simplify the proof, see [Vem04] for details and applications of the theorem. The proof here is due to Das Gupta and Gupta [DG99].

The SVD based algorithm for identifying the space spanned by centers of spherical Gaussians is from Vempala and Wang [VW02]. The paper handles more complex densities besides spherical Gaussians, but the restricted case of spherical Gaussians contains the key ideas.

2.9 Exercises

Exercise 2.1 Assume you have 100 million documents each represented by a vector in the word vector model. How would you represent the documents so that given a query with a small number of words you could efficiently find the documents with the highest dot product with the query vector? Given the number of documents you do not have time to look at every document.

Exercise 2.2 Let x and y be independent random variables with uniform distribution in [0,1]. What is the expected value E(x)? $E(x^2)$? E(x-y)? E(xy)? and $E((x-y)^2)$?

Solution:
$$\frac{1}{2}$$
, $\frac{1}{3}$, $\frac{0}{4}$, $E\left[(x-y)^2\right] = E\left(x^2\right) - 2E\left(xy\right) + E\left(y^2\right) = \frac{1}{3} - 2 \times \frac{1}{2} + \frac{1}{3} = \frac{1}{6}$.

Exercise 2.3 What is the distribution of the distance between two points chosen uniformly at random in the interval [0,1]? In the unit square? In the unit cube in 100 dimensions? Give a qualitative answer.

Exercise 2.4 What is the expected distance between two points selected at random inside a d-dimensional unit cube? For two points selected at random inside a d-dimensional unit sphere? What is the cosine of the angle between them?

Exercise 2.5 Consider two random 0-1 vectors in high dimension. What is the angle between them? What is the probability that the angle is less than 45?

Exercise 2.6 Place two unit-radius spheres in d-dimensions, one at $(-2,0,0,\ldots,0)$ and the other at $(2,0,0,\ldots,0)$. Give an upper bound on the probability that a random line through the origin will intersect the spheres.

Solution: One could estimate by a computer program that randomly generated a line and tested if the line intersected the spheres. To generate a random line, generate a random vector (a_1, a_2, \dots, a_d) and let the line be the set of points $\left(x_1, \frac{a_2}{a_1}x_1, \frac{a_3}{a_1}x_1, \dots, \frac{a_d}{a_1}x_1\right)$. Ask if this set of points intersects the sphere $(x_1 - 2)^2 + x_2^2 + \dots + x_d^2 = 1$. If the components of the vector are selected uniformly at random over the range [0,1], the direction of the line will not be uniformly distributed. One needs to generate the components as Gaussians to get a spherical distribution. For many applications, selecting the coordinates of the vector uniformly from [0,1] may not matter. In fact we might be able to use

$$a_i = \begin{cases} 1 & \frac{1}{4} \\ 0 & \frac{1}{2} \\ 1 & \frac{1}{4} \end{cases}$$

Asking if the line intersects the sphere is equivalent to asking if there exists an x_1 such that

$$(x_1 - 2)^2 + \left(\frac{a_2}{a_1}x_1\right)^2 + \left(\frac{a_3}{a_1}x_1\right)^2 + \dots + \left(\frac{a_d}{a_1}x_1\right)^2 = 1$$

This simplifies to

$$(a_1^2 + a_2^2 + \dots + a_d^2) x_1^2 - 4a_1^2 x_1 + 3a_1^2 = 0$$

Applying the $b^2 - 4ac$ test for the existence of a root of the above quadratic equation, there is a solution provided $16a_1^2 \ge 12$ or $a_1^2 \ge \frac{3}{4}$. Use the fact that most of the mass is concentrated about the equator to derive a bound on the probability of this.

As a check in two dimensions this requires that $a_1 \ge \sqrt{3}a_2$. We see from the picture below that this is correct.

INSERT FIGURE

$$\sqrt{3}$$

At tangency $a_1^2 + a_2^2 = 3$ and $(2 - a_1)^2 + a_2^2 = 1$ or $a_1 = \frac{3}{2}$ and $a_2 = \frac{\sqrt{3}}{2}$. That is $a_1 = \sqrt{3}a_2$.

Exercise 2.7 Generate a 1,000 points at vertices of a 1,000-dimensional cube. Select two points i and j at random and find a path from i to j by the following algorithm. Start at i and go to a point k differing from i in only one coordinate so that dist (i,k) and dist (j,k) are both less than dist (i,j). Then continue the path by the same algorithm from k to j. What is the expected length of the path?

Exercise 2.8 (Overlap of spheres) Let x be a random sample from the unit sphere in d-dimensions with the origin as center.

- 1. What is the mean of the random variable x? The mean, denoted $E(\mathbf{x})$, is the vector, whose i^{th} component is $E(x_i)$.
- 2. What is the component-wise variance of \mathbf{x} ?
- 3. Show that for any unit length vector \mathbf{u} , the variance of the real-valued random variable $\mathbf{u}^T \cdot \mathbf{x}$ is $\sum_{i=1}^d u_i^2 E(x_i^2)$. Using this, compute the variance and standard deviation of $\mathbf{u}^T \mathbf{x}$.
- 4. Given two spheres in d-space, both of radius one whose centers are distance a apart, show that the volume of their intersection is at most

$$\frac{4e^{-\frac{a^2(d-1)}{8}}}{a\sqrt{d-1}}$$

times the volume of each sphere.

Hint: Relate the volume of the intersection to the volume of a cap, then, use Lemma 2.2.

5. From (4), conclude that if the inter-center separation of the two spheres of radius r is $\Omega(r/\sqrt{d})$, then they share very small mass. Theoretically, at this separation, given randomly generated points from the two distributions, one inside each sphere,

it is possible to tell which sphere contains which point, i.e., classify them into two clusters so that each cluster is exactly the set of points generated from one sphere. The actual classification requires an efficient algorithm to achive this. Note that the inter-center separation required here goes to zero as d gets larger, provided the radius of the spheres remains the same. So, it is easier to tell apart spheres (of the same radii) in higher dimensions.

Solution:

- 1. $E(X_i) = 0$ for all i, so E(X) = 0.
- 2. $\operatorname{Var}(X_i) = E(X_i^2) = \frac{1}{d}E(|X|^2)$ by symmetry. Let V(d) denote the volume of the unit sphere and A(d) denoting the surface area of the sphere of radius one. The infinitesimal volume of an annulus of width dr at radius rhas volume $A(d)r^{d-1}dr$. So we have

$$E(|X|^2) = \frac{1}{V(d)} \int_{r=0}^{1} A(d)r^{d-1}r^2 dr = \frac{A(d)}{V(d)(d+2)} = \frac{d}{d+2}.$$

Thus, $Var(X_i) = \frac{1}{d+2}$.

3. The proof is by induction on d. It is clear for d=1.

 $\operatorname{Var}(\sum_{i} u_i X_i) = E((\sum_{i} u_i X_i)^2)$, since the mean is 0. Now,

$$E((\sum_{i} u_{i}X_{i})^{2}) = E(\sum_{i} u_{i}^{2}X_{i}^{2}) + 2E(\sum_{i \neq j} u_{i}u_{j}X_{i}X_{j})$$

If the X_i had been independent, then the second term would be zero. But they are obviously not. So we take each section of the sphere cut by a hyperplane of the form X_1 =constant, first integrate over this section, then integrate over all sections. In probability notation, this is taking the "conditional expectation" conditioned on (each value of) X_1 and then taking the expectation over all values of X_1 . Doing this, we get

$$E(\sum_{i \neq j} u_i u_j X_i X_j) = E \sum_{i \geq 2} u_1 X_1 u_i X_i + E \sum_{i \neq j; i, j \geq 2} u_i u_j X_i X_j$$

$$= E_{X_1} \left(u_1 X_1 E_{X_2, X_3, \dots, X_d} \left(\sum_{i \geq 2} u_i X_i | X_1 \right) \right) + E_{X_1} \left(E_{X_2, X_3, \dots, X_d} \left(\sum_{i \neq j; i, j \geq 2} u_i X_i u_j X_j | X_1 \right) \right)$$

[Notation: $E(Y|X_1)$ is some function f of X_1 ; it is really short-hand for writing $f(a) = E(Y|X_1 = a)$.]

Now, for every fixed value of X_1 , $E(X_i|X_1) = 0$ for $i \ge 2$, so the first term is zero. Since a section of the sphere is just a d-1sphere, the second term is zero by induction on d.

- 4. Looking at the picture, by symmetry, we see that the volume of the intersection of the two spheres is just twice the volume of the section of the first sphere given by: $\{x: |x| \leq 1; x_1 \geq a/2\}$ if we assume without loss of generality that the center of the second sphere is at $(a, 0, 0, \dots 0)$.
- 5. Simple.
- 6. If a spherical Gaussian has standard deviation σ in each direction, then its radius (really the square root of the average squared distance from the mean) is $\sqrt{d}\sigma$. Its projection on any line is again a Gaussian with standard deviation σ (as we show in Chapter 4 (or 5)??). Let a>0 and let the centers be **0** and $(a,0,0,\ldots 0)$ without loss of generality. To find the shared mass, we can use the projection onto the x_1 axis and integrate to get that the shared mass is

$$\int_{x=-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} \operatorname{Min}\left(e^{-x^2/2\sigma}, e^{-(x-a)^2/2\sigma}\right).$$

We bound this by using

$$\int_{x=-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} \operatorname{Min}\left(e^{-x^{2}/2\sigma}, e^{-(x-a)^{2}/2\sigma}\right)
\leq \int_{x=-\infty}^{a/2} \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-a)^{2}/2\sigma} dx + \int_{x=a/2}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} e^{-x^{2}/2\sigma} dx
= 2 \int_{x=a/2}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} e^{-x^{2}/2\sigma} dx \leq 2 \int_{x=a/2}^{\infty} \frac{2x}{a\sqrt{2\pi}\sigma} e^{-x^{2}/2\sigma} dx
\leq \frac{2}{a} e^{\frac{-a^{2}}{8\sigma}}$$

where in the last step, we are able to integrate xe^{-cx^2} in closed form.

So again, as soon as the inter-center separation goes beyond a few standard deviations, the shared mass goes down exponentially.

Exercise 2.9 Derive an upper bound on $\int_{x=\alpha}^{\infty} e^{-x^2} dx$ where α is a positive real. Discuss for what values of α this is a good bound. Hint: Use $e^{-x^2} \leq \frac{x}{\alpha} e^{-x^2}$ for $x \geq \alpha$.

Exercise 2.10 What is the formula for the incremental unit of area in using polar coordinates to integrate the area of a circle that lies in a 2-dimensional cone whose vertex is at the center of the circle? What is the formula for the integral? What is the value of the integral if the cone is 36°?

Exercise 2.11 For what value of d is the volume, V(d), of a d-dimensional unit sphere maximum?

Hint: Consider the ratio $\frac{V(d)}{V(d-1)}$ for odd and even values of d.

Solution: The maximum is at d=5 where the volume is 5.26. Calculate the ratio V(d)/V(d+1). The ratio can be expressed as $\frac{d+1}{\sqrt{\pi}d}\frac{\Gamma\left(\frac{d+1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}$ and is monotonically increasing. At d=5 the ratio becomes greater than one. One may need to break the problem into two for even d and odd d.

Exercise 2.12 How does the volume of a sphere of radius two behave as the dimension of the space increases? What if the radius was larger than two but a constant independent of d? What function of d would the radius need to be for a sphere of radius r to have approximately constant volume as the dimension increases?

Solution: Assume d is even and use Sterling approximation for $\Gamma\left(\frac{d}{2}\right)$. Then the volume is given by $\frac{\frac{d}{2}}{\left(\frac{d}{2e}\right)^{\frac{d}{2}}\sqrt{\pi d}}r^d$. Thus, r must equal some constant times \sqrt{d} .

Exercise 2.13

- 1. What is the volume of a sphere of radius r in d-dimensions?
- 2. What is the surface area of a sphere of radius r in d-dimensions?
- 3. What is the relationship between the volume and the surface area of a sphere of radius r in d-dimensions?
- 4. Why does the relationship determined in (3) hold?

Exercise 2.14 Consider vertices of a d-dimensional cube of width two centered at the origin. Vertices are the points $(\pm 1, \pm 1, \ldots, \pm 1)$. Place a unit-radius sphere at each vertex. Each sphere fits in a cube of width two and, thus, no two spheres intersect. Show that the probability that a point of the cube picked at random will fall into one of the 2^d unit-radius spheres, centered at the vertices of the cube, goes to 0 as d tends to infinity.

Exercise 2.15 Consider the power law probability density

$$p(x) = \frac{c}{\mathit{Max}(1, x^2)}$$

over the nonnegative real line.

- 1. Determine the constant c.
- 2. For a nonnegative random variable x with this density, does E(x) exist? How about $E(x^2)$?

Exercise 2.16 Consider d-space and the following density over the positive orthant:

$$p(\mathbf{x}) = \frac{c}{Max(1, |\mathbf{x}|^{\alpha})}.$$

Show that $\alpha > d$ is necessary for this to be a proper density function. Show that $\alpha > d+1$ is a necessary condition for a (vector-valued) random variable \mathbf{x} with this density to have an expected value $E(|\mathbf{x}|)$. What condition do you need if we want $E(|\mathbf{x}|^2)$ to exist?

Exercise 2.17 Consider the upper hemisphere of a unit-radius sphere in d-dimensions. What is the height of the maximum volume cylinder that can be placed entirely inside the hemisphere? As you increase the height of the cylinder, you need to reduce the cylinder's radius so that it will lie entirely within the hemisphere.

Exercise 2.18 What is the volume of a radius r cylinder of height h in d-dimensions?

Solution: $2.18 \ h(d-1)r^{d-2}$.

Exercise 2.19 For a 1,000-dimensional unit-radius sphere centered at the origin, what fraction of the volume of the upper hemisphere is above the plane $x_1 = 0.1$? Above the plane $x_1 = 0.01$?

Exercise 2.20 Almost all of the volume of a sphere in high dimensions lies in a narrow slice of the sphere at the equator. However, the narrow slice is determined by the point on the surface of the sphere that is designated the North Pole. Explain how this can be true if several different locations are selected for the North Pole.

Exercise 2.21 Explain how the volume of a sphere in high dimensions can simultaneously be in a narrow slice at the equator and also be concentrated in a narrow annulus at the surface of the sphere.

Exercise 2.22 How large must ε be for 99% of the volume of a d-dimensional unit-radius sphere to lie in the shell of ε -thickness at the surface of the sphere?

Exercise 2.23

- 1. Write a computer program that generates n points uniformly distributed over the surface of a unit-radius d-dimensional sphere.
- 2. Generate 200 points on the surface of a sphere in 50 dimensions.
- 3. Create several random lines through the origin and project the points onto each line. Plot the distribution of points on each line.
- 4. What does your result from (3) say about the surface area of the sphere in relation to the lines, i.e., where is the surface area concentrated relative to each line?

Exercise 2.24 If one generates points in d-dimensions with each coordinate a unit variance Gaussian, the points will approximately lie on the surface of a sphere of radius \sqrt{d} . What is the distribution when the points are projected onto a random line through the origin?

Exercise 2.25 Project the surface area of a sphere of radius \sqrt{d} in d-dimensions onto a line through the center. For d equal 2 and 3, derive an explicit formula for how the projected surface area changes as we move along the line. For large d, argue (intuitively) that the projected surface area should behave like a Gaussian.

Solution: Instead of a sphere in d-dimensions consider generating points at random where each coordinate of a point is independent and distributed according to a unit variance Gaussian. The set of points generated will lie in a thin annulus of width O(1) at radius \sqrt{d} . We will use this annulus as a good approximation to a sphere of radius \sqrt{d} . If we now project this annulus onto the first coordinate axis, we get a unit variance Gaussian. Thus the surface area of a d-dimensional sphere of radius \sqrt{d} projected onto a line through the origin gives rise to a unit variance Gaussian. Thus, almost all the surface area of a radius \sqrt{d} sphere in d-dimensions lies in a band of width three about the equator.

Exercise 2.26 Generate 500 points uniformly at random on the surface of a unit-radius sphere in 50 dimensions. Then randomly generate five additional points. For each of the five new points calculate a narrow band at the equator assuming the point was the North Pole. How many of the 500 points are in each band corresponding to one of the five equators? How many of the points are in all five bands?

Exercise 2.27 We have claimed that a randomly generated point on a sphere lies near the equator of the sphere independent of the point selected for the North Pole. Is the same claim true for a randomly generated point on a cube? To test this claim, randomly generate ten ± 1 valued vectors in 128 dimensions. Think of these ten vectors as ten choices for the North Pole. Then generate some additional ± 1 valued vectors. To how many of the original vectors is each of the new vectors close to being perpendicular, that is how many of the equators is each new vectors close to.

Exercise 2.28 Consider a slice of a 100-dimensional sphere that lies between two parallel planes each equidistant from the equator and perpendicular to the line from the North to South Pole. What percentage of the distance from the center of the sphere to the poles must the planes be to contain 95% of the surface area?

Exercise 2.29 Place n points at random on a d-dimensional unit radius sphere. Assume d is large. Pick a random vector and let it define two parallel hyperplanes on opposite sides of the origin that are equal distance from the origin. How far apart can the hyperplanes be moved and still have no points between them?

Solution: If we project the surface area of a sphere of radius \sqrt{d} onto a line through the origin, we get a Gaussian with variance one. Thus, for large d, a sphere of radius d has all its surface area in a band of width approximately 6. If the sphere was of unit radius, the band would be of width $6/\sqrt{d}$.

Exercise 2.30 Consider two random vectors in a high-dimensional space. Assume the vectors have been normalized so that their lengths are one and thus the points lie on a unit sphere. Assume one of the vectors is the North pole. Prove that the ratio of the area of a cone, with axis at the North Pole of fixed angle say 45° to the area of a hemisphere, goes to zero as the dimension increases. Thus, the probability that the angle between two random vectors is at most 45° goes to zero. How does this relate to the result that most of the volume is near the equator?

Solution: For a vector to be within a 45 ° degree cone whose axis is at the North pole, it must be within 45 ° degrees of the North pole in each dimension. That is it must lie within a "square" cone containing the circular cone. The probability that in a given dimension a randomly choose vector is within 45 ° degrees of North is 1/2. Thus, the probability goes to zero as the dimension increases. Thus, with probability one, two randomly chosen vectors are at least 45 ° degree apart in direction and their dot product, assuming unit length vectors, is at most $\frac{\sqrt{2}}{2}$. This says that two vectors selected at random are close to orthogonal and are distance $\sqrt{2}$ apart.

Exercise 2.31 Project the vertices of a high-dimensional cube onto a line from (0, 0, ..., 0) to (1, 1, ..., 1). Argue that the "density" of the number of projected points (per unit distance) varies roughly as a Gaussian with variance O(1) with the mid-point of the line as center.

Solution: The projection can be thought of as taking the dot product with the unit vector $(1/\sqrt{d}, 1/\sqrt{d}, \dots, 1/\sqrt{d})$ along the line. By the Central Limit Theorem, this dot product minus its mean should behave as the Gaussian. Variance of $\sum_{i=1}^{d} (x_i - \frac{1}{2}) \frac{1}{\sqrt{d}}$ (for independent 0-1 variables x_i) is the sum of the variances which is clearly O(1).

Exercise 2.32 Draw a 3-dimensional cube and illustrate the equator as defined in Section 2.3.

Exercise 2.33

- 1. What is the surface area of a unit cube in d-dimensions?
- 2. Is the surface area of a unit cube concentrated close to the equator as is the case with the sphere?

Exercise 2.34 Consider the simplex

$$S = \{ \mathbf{x} \mid x_i \ge 0, 1 \le i \le d; \ \sum_{i=1}^{d} x_i \le 1 \}.$$

For a random point \mathbf{x} picked with uniform density from S, find $E(x_1 + x_2 + \cdots + x_d)$. Find the centroid of S.

Exercise 2.35 How would you sample uniformly at random from the parallelepiped

$$P = \{ \mathbf{x} \mid \mathbf{0} \le A\mathbf{x} \le \mathbf{1} \},$$

where A is a given nonsingular matrix? How about from the simplex

$$\{ \mathbf{x} \mid 0 \le (A\mathbf{x})_1 \le (A\mathbf{x})_2 \dots \le (A\mathbf{x})_d \le 1 \} ?$$

Your algorithms must run in polynomial time.

Exercise 2.36 Randomly generate a 100 points on the surface of a sphere in 3-dimensions and in 100-dimensions. Create a histogram of all distances between the pairs of points in both cases.

Exercise 2.37 We have claimed that in high dimensions a unit variance Gaussian centered at the origin has essentially zero probability mass in a unit-radius sphere centered at the origin since the unit-radius sphere has no volume. Explain what happens if the Gaussian has an extremely small variance and has no probability mass outside the unit-radius sphere? How small must the variance be in terms of d for this to happen?

Exercise 2.38 Consider two unit-radius spheres in d-dimensions whose centers are distance δ apart where δ is a constant independent of d. Let \mathbf{x} be a random point on the surface of the first sphere and \mathbf{y} a random point on the surface of the second sphere. Prove that the probability that $|\mathbf{x} - \mathbf{y}|^2$ is more than $2 + \delta^2 + a$ falls off exponentially with a.

Exercise 2.39 The Cauchy distribution in one dimension is $Prob(x) = \frac{1}{c+x^2}$. What would happen if one tried to extend the distribution to higher dimensions by the formula $Prob(r) = \frac{1}{1+r^2}$ where r is the distance from the origin? What happens when you try to determine a normalization constant c?

Exercise 2.40 Where do points generated by a heavy tailed, high-dimensional distribution lie? For the Gaussian distribution, points lie in an annulus because the probability distribution falls off quickly as the volume increases.

Exercise 2.41 Pick a point x uniformly at random from the following set in d-space:

$$K = \{ \mathbf{x} | x_1^4 + x_2^4 + \dots + x_d^4 \le 1 \}.$$

- 1. Show that the probability that $x_1^4 + x_2^4 + \cdots + x_d^4 \leq \frac{1}{2}$ is $\frac{1}{2^{d/4}}$.
- 2. Show that with high probability, $x_1^4 + x_2^4 + \cdots + x_d^4 \ge 1 O(1/d)$.
- 3. Show that with high probability, $|x_1| \leq O(1/d^{1/4})$.

Solution: Let $U(d) = \text{Volume} K_d$ which is the solid K defined earlier. We have

Volume
$$(K \cap \{\mathbf{x} | x_1 \ge \alpha\}) = \int_{t=\alpha}^{1} \text{Volume} ((x_2, x_3, \dots, x_d) | x_2^4 + x_3^4 + \dots + x_d^4 \le 1 - t^4) dt$$

$$= \int_{t=\alpha}^{1} U(d-1)(1-t^4)^{(d-1)/4} dt$$

$$\le U(d-1) \int_{t=\alpha}^{1} \frac{t^3}{\alpha^3} (1-t^4)^{(d-1)/4} \dots \text{integrable}$$

Also

$$\int_{t=0}^{1} U(d-1)(1-t^4)^{(d-1)/4} dt \ge U(d-1) \int_{t=0}^{1/d^{1/4}} (1-t^4)^{(d-1)/2} \ge U(d-1)e^{-1/4}.$$

Compare to get ratio. So, conclude that

$$Prob(|x_1| \ge \frac{c}{d^{1/4}}) \le \frac{1}{c^3}e^{-c^4/4}.$$

Exercise 2.42 Suppose there is an object moving at constant velocity along a straight line. You receive the gps coordinates corrupted by Gaussian noise every minute. How do you estimate the current position?

Exercise 2.43 Generate ten values by a Gaussian probability distribution with zero mean and variance one. What is the center determined by averaging the points? What is the variance? In estimating the variance use both the real center and the estimated center. When using the estimated center to estimate the variance, use both n = 10 and n = 9. How do the three estimates compare?

Exercise 2.44 Suppose you want to estimate the (unknown) center of a Gaussian in d-space which has variance one in each direction. Show that $O(\log d/\varepsilon^2)$ random samples from the Gaussian are sufficient to get an estimate $\tilde{\mu}$ of the true center μ so that with probability at least 99/100, we have

$$|\mu - \tilde{\mu}|_{\infty} \le \varepsilon.$$

How many samples are sufficient to ensure that

$$|\mu - \tilde{\mu}| \le \varepsilon$$
?

Exercise 2.45 Let G be a d-dimensional spherical Gaussian with variance $\frac{1}{2}$ centered at the origin. Derive the expected squared distance to the origin.

Exercise 2.46 Show that the maximum of $f(t) = (\sqrt{1 - 2t\beta k})^{(d-k)} (\sqrt{1 - 2t(\beta k - d)})^k$ is attained at $t = \frac{1-\beta}{2\beta(d-k\beta)}$.

Hint: Maximize the logarithm of f(t) by differentiating.

Exercise 2.47 Generate 20 points uniformly at random on a 1000-dimensional sphere of radius 100. Calculate the distance between each pair of points. Then project the data onto subspaces of dimension k=100, 50, 10, 5, 4, 3, 2, 1 and calculate the sum of squared error between $\frac{k}{d}$ times the original distances and the new pair wise distances for each of the above values of k.

Exercise 2.48 You are given two sets, P and Q, of n points each in n-dimensional space. Your task is to find the closest pair of points, one each from P and Q, i.e., find \mathbf{x} in P and \mathbf{y} in Q such that $|\mathbf{x} - \mathbf{y}|$ is minimum.

- 1. Show that this can be done in time $O(n^3)$.
- 2. Show how to do this with relative error 0.1% in time $O(n^2 \ln n)$, i.e., you must find a pair $\mathbf{x} \in P$, $\mathbf{y} \in Q$ so that the distance between them is, at most, 1.001 times the minimum possible distance. If the minimum distance is 0, you must find $\mathbf{x} = \mathbf{y}$.

Solution: Use the random projection theorem. Project P, Q to a random $O(\ln n)$ dimensional space (which preserves all pairwise distances) and compute all pairwise distances in that space.

Exercise 2.49 Given n data points in d-space, find a subset of k data points whose vector sum has the smallest length. You can try all $\binom{n}{k}$ subsets, compute each vector sum in time O(kd) for a total time of $O\left(\binom{n}{k}kd\right)$. Show that we can replace d in the expression above by $O(k \ln n)$, if we settle for an answer with relative error .02%.

Solution: We want a random projection that will preserve the lengths of all $\binom{n}{k}$ sums of k-subsets. For this, it suffices to project to $O(\ln(n^k)) = O(k \ln n)$ dimensions.

Exercise 2.50 Create a list of the five most important things that you learned about high dimensions.

Exercise 2.51 Write a short essay whose purpose is to excite a college freshman to learn about high dimensions.

3 Random Graphs

Large graphs appear in many contexts such as the World Wide Web, the internet, social networks, journal citations and other places. What is different about the modern study of large graphs from traditional graph theory and graph algorithms is that here one seeks statistical properties of these very large graphs rather than an exact answer to questions. This is perhaps akin to the switch physics made in the late 19^{th} century in going from mechanics to statistical mechanics. Just as the physicists did, one formulates clean abstract models of graphs that are not completely realistic in every situation, but admit a very nice mathematical development that can guide what really happens in practical situations. Perhaps the most important such model is the G(n,p) model of a random graph. In this chapter, we study several random graph models and the properties of the random graphs generated by these models.

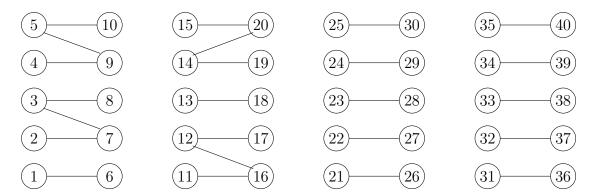
3.1 The G(n, p) Model

One of the earliest models of a random graph is the G(n,p) model due to Erdös and Rényi . The model has two parameters n and p. Here n is the number of vertices of the graph and p is the edge probability. For each pair of distinct vertices, v and w, the edge (v,w) is present with probability p. The presence of each edge is statistically independent of all other edges. The graph-valued random variable with these parameters is denoted by G(n,p). When we refer to "the graph G(n,p)", we mean one realization of the random variable. In many cases, p will be a function of n such as p=d/n for some constant d. In this case, the expected degree of a vertex of the graph is $d\frac{n-1}{n} \approx d$. The interesting thing about the G(n,p) model is that even though edges are chosen independently with no "collusion", certain global properties of the graph emerge from the independent choices. For small p, with p=d/n, d<1, each connected component in the graph is small. For d>1, there is a giant component consisting of $\Theta(n)$ vertices. Indeed, many large realworld graphs with constant average degree have a giant component. This is perhaps the most important global property.

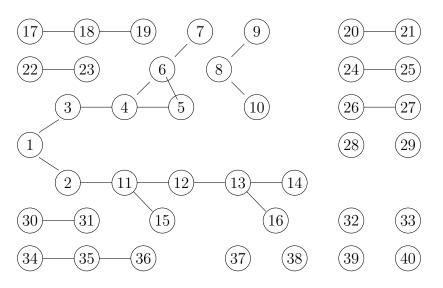
3.1.1 Degree Distribution

One of the simplest quantities to observe in a real graph is the number of vertices of given degree called the vertex degree distribution. It is also very simple to study these distributions in G(n,p) since the degree of each vertex is the sum of n-1 independent random variables which results in a binomial distribution. Since we will be dealing with graphs where n, the number of vertices, is large, from here on we often replace n-1 by n to simplify formulas.

Example: In $G(n, \frac{1}{2})$, each vertex is of degree close to n/2. In fact, for any $\varepsilon > 0$, the degree of each vertex almost surely is within $1 \pm \varepsilon$ times n/2. To see this, note that the



A graph with 40 vertices and 24 edges



A randomly generated G(n, p) graph with 40 vertices and 24 edges

Figure 3.1: Two graphs each with 40 vertices and 24 edges. The second graph was randomly generated using the G(n,p) model with p=1.2/n. A graph similar to the top graph is almost surely not going to be randomly generated in the G(n,p) model where as a graph similar to the lower graph will almost surely occur. Note that the lower graph consists of a giant component along with a number of small components that are trees.

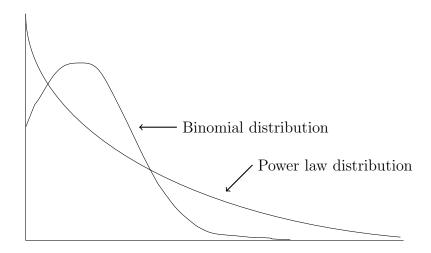


Figure 3.2: Illustration of the binomial and the power law distributions

probability that a vertex is of degree k is

$$\operatorname{Prob}(k) = \binom{n-1}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{n-k} \approx \binom{n}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{n-k} = \frac{1}{2^n} \binom{n}{k}.$$

This probability distribution has a mean of m=n/2 and variance $\sigma^2=n/4$. Near the mean, the binomial distribution is well approximated by the normal distribution $\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\frac{(k-m)^2}{\sigma^2}}$ or $\frac{1}{\sqrt{\pi n/2}}e^{-\frac{(k-n/2)^2}{n/2}}$. See appendix. The standard deviation of the normal distribution is $\frac{\sqrt{n}}{2}$ and essentially all of the probability mass is within an additive term $\pm c\sqrt{n}$ of n/2 for some constant c and thus is certainly within a multiplicative factor of $1\pm\varepsilon$ of n/2 for sufficiently large n. We will prove this later in more generality using Chernoff bounds.

The degree distribution of G(n, p) for general p is also binomial. Since p is the probability of an edge being present, the expected degree of a vertex is d = pn. The actual degree distribution is given by

Prob(vertex is degree
$$k$$
) = $\binom{n-1}{k} p^k (1-p)^{n-k-1} \approx \binom{n}{k} p^k (1-p)^{n-k}$.

The quantity $\binom{n-1}{k}$ is the number of ways of choosing k edges, out of the possible n-1 edges, and $p^k(1-p)^{n-k-1}$ is the probability that the k selected edges are present and the remaining n-k-1 are not. Since n is large, replacing n-1 by n does not cause much error.

The binomial distribution falls off exponentially fast as one moves away from the mean. However, the degree distributions of graphs that appear in many applications do not exhibit such sharp drops. Rather the degree distributions are much broader. This is often referred to as having a "heavy tail". The term tail refers to values of a random variable

far away from its mean, usually measured in number of standard deviations. Thus, although the G(n, p) model is important mathematically, more complex models are needed to represent real world graphs.

Consider an airline route graph. The graph has a wide range of degrees, from degree one or two for a small city to degree 100 or more for a major hub. The degree distribution is not binomial. Many large graphs that arise in various applications appear to have power law degree distributions. A power law degree distribution is one in which the frequency of a vertex having a given degree decreases as a power of the degree as in

Number(degree k vertices) =
$$c\frac{n}{k^r}$$
,

for some small positive real r often just slightly less than three. Later, we shall consider a random graph model giving rise to such degree distributions.

The following theorem claims that the degree distribution of the random graph G(n, p) is tightly concentrated about its expected value. That is, the probability that the degree of a vertex differs from its expected degree, np, by more than $c\sqrt{np}$ drops off exponentially fast with c.

Theorem 3.1 Let v be a vertex of the random graph G(n, p). For c > 0

$$Prob\left(\left|np-deg\left(v\right)\right| \geq c\sqrt{np}\right) \leq 4 \max\left(e^{-c^{2}/16}, e^{-c\sqrt{np}/12}\right).$$

Proof: deg(v) is the sum of n-1 independent Bernoulli random variables. So the theorem follows by Chernoff bounds, Lemma 2.6.

Suppose we want to assert that with high probability each vertex has a degree close to its expected degree. Clearly these events are not independent. But, we can assert using the union bound that

Prob (
$$\exists$$
 vertex v such that $|np - \deg(v)| \ge c\sqrt{np}$)
 $\le 4n \max\left(e^{-c^2/16}, e^{-c\sqrt{np}/12}\right)$.

In order to say that every vertex almost surely has degree within $\pm \varepsilon np$ of np, replace c by $\varepsilon \sqrt{np}$ in the above formula. The first element of the max is the larger and is $e^{-\varepsilon^2 np/16}$. For $ne^{-\varepsilon^2 np/16}$ to be o(1) requires p be at least $\Omega(\ln n/(n\varepsilon^2))$. When p goes below $\ln n/n$, for example, when p = d/n with $d \in O(1)$, the argument is no longer valid.

Corollary 3.2 If $p \in \Omega(\ln n/(n\varepsilon^2))$, then almost surely, every vertex has degree $(1\pm\varepsilon)np$.

In G(n, p), when p is a constant, the expected degree of vertices increases with n. For example, in $G\left(n, \frac{1}{2}\right)$, the expected degree of a vertex is n/2. In many real applications, we will be concerned with G(n, p) where p = d/n, for d a constant, i.e., graphs whose expected degree is a constant d independent of n. Holding d = np constant as n goes to infinity, the binomial distribution

$$\operatorname{Prob}(k) = \binom{n}{k} p^k (1-p)^{n-k}$$

approaches the Poisson distribution

$$Prob(k) = \frac{(np)^k}{k!}e^{-np} = \frac{d^k}{k!}e^{-d}.$$

To see this, assume k = o(n) use the approximations $n - k \cong n$, $\binom{n}{k} \cong \frac{n^k}{k!}$, and $\left(1 - \frac{1}{n}\right)^{n-k} \cong e^{-1}$ to approximate the binomial distribution by

$$\lim_{n \to \infty} \binom{n}{k} p^k (1-p)^{n-k} = \frac{n^k}{k!} \left(\frac{d}{n}\right)^k (1-\frac{d}{n})^{n-k} = \frac{d^k}{k!} e^{-d}.$$

Note that for d equal a constant independent of n, the probability falls off rapidly for k > d and is essentially zero for all but some finite number of values of k. This justifies the k = o(n) assumption and thus the Poisson distribution is a good approximation.

Example: In $G(n, \frac{1}{n})$ many vertices are of degree one but not all. Some are of degree zero and some are of degree greater than one. In fact, it is highly likely that there is a vertex of degree $\Omega(\log n/\log\log n)$. The probability that a given vertex is of degree k is

$$\operatorname{Prob}(k) = \binom{n}{k} \left(\frac{1}{n}\right)^k \left(1 - \frac{1}{n}\right)^{n-k} \approx \frac{e^{-1}}{k!}.$$

If $k = \log n / \log \log n$,

$$\log k^k = k \log k \cong \frac{\log n}{\log \log n} (\log \log n - \log \log \log n) \cong \log n$$

and thus $k^k \cong n$. Since $k! \leq k^k \cong n$, the probability that a vertex has degree $k = \log n/\log\log n$ is at least $\frac{1}{k!}e^{-1} \geq \frac{1}{en}$. If the degrees of vertices were independent random variables, then this would be enough to argue that there would be a vertex of degree $\log n/\log\log n$ with probability at least $1 - \left(1 - \frac{1}{en}\right)^n = 1 - e^{-\frac{1}{e}} \cong 0.31$. But the degrees are not quite independent since when an edge is added to the graph it affects the degree of two vertices. This is a minor technical point which one can get around.

3.1.2 Existence of Triangles in G(n, d/n)

What is the expected number of triangles in $G\left(n, \frac{d}{n}\right)$, when d is a constant? As the number of vertices increases one might expect the number of triangles to increase but this is not the case. Although the number of triples of vertices grows as n^3 , the probability of an edge between two specific vertices decreases linearly with n. Thus, the probability of all three edges between the pairs of vertices in a triple of vertices being present goes down as n^{-3} , exactly canceling the rate of grow of triples.

A random graph with n vertices and edge probability d/n has an expected number of triangles that is independent of n, namely $d^3/6$. There are $\binom{n}{3}$ triples of vertices. Each triple has probability $\left(\frac{d}{n}\right)^3$ of being a triangle. Even though the existence of triangles are not statistically independent events, by linearity of expectation, which does not assume independence of the variables, the expected value of a sum of random variables is the sum of the expected values. Thus, the expected number of triangles is

$$E ext{ (number of triangles)} = {n \choose 3} \left(\frac{d}{n}\right)^3 = \frac{d^3}{6}.$$

Even though on average there are $\frac{d^3}{6}$ triangles per graph, this does not mean that with high probability a graph has a triangle. Maybe half of the graphs have $\frac{d^3}{3}$ triangles and the other half have none for an average of $\frac{d^3}{6}$ triangles. Then with probability 1/2, a graph selected at random would have no triangle. If 1/n of the graphs had $\frac{nd^3}{6}$ triangles and the remaining graphs had no triangles, then as n goes to infinity, the probability that a graph had a triangle would go to zero.

We wish to assert that with some nonzero probability, there is at least one triangle in G(n,p) when $p=\frac{d}{n}$. It is conceivable that a small fraction of the graphs have a large number of triangles and the remaining graphs have no triangles so that the expected number of triangles works out to $d^3/6$. A second moment argument rules out such scenarios. Calculate $E(x^2)$, where x is the number of triangles. Write x as $x=\sum_{ijk}\Delta_{ijk}$, where Δ_{ijk} is the indicator variable of the triangle i,j,k being present, i.e., all three edges (i,j),(j,k), and (k,i) being present. By expanding the squared term we get

$$E(x^2) = E\left(\sum_{i,j,k} \Delta_{ijk}\right)^2 = E\sum_{i,j,k,i',j',k'} \Delta_{ijk} \Delta_{i'j'k'}.$$

Split the above sum into three parts. In Part 1, i, j, k and i', j', k' share at most one vertex and hence the triangles share no edge. In this case, Δ_{ijk} and $\Delta_{i'j'k'}$ are independent and

$$E\sum_{i,j,k,i',j',k'} \Delta_{ijk} \Delta_{i'j'k'} = E\left(\sum_{i,j,k} \Delta_{ijk}\right) E\left(\sum_{i',j',k'} \Delta_{i'j'k'}\right) = E^2(x).$$



Two triangles of Part 1



Two triangles of Part 2

Figure 3.3: The triangles in Part 1 and Part 2 of the second moment argument for the existence of triangles in $G(n, \frac{d}{n})$

In Part 2, i, j, k and i', j', k' share two vertices and hence one edge. See Figure 3.3. So four vertices and five edges are involved overall. There are at most $\binom{n}{4} \in O(n^4)$, 4-vertex subsets and two ways to partition the four vertices into two triangles with a common edge. The probability of all five edges in the two triangles being present is p^5 , so this part sums to $O(n^4p^5) = O(d^5/n) \in o(1)$. In Part 3, i, j, k and i', j', k' are the same sets. The contribution of this part of the summation to $E(x^2)$ is $\binom{n}{3}p^3 = \frac{d^3}{6}$. Thus,

$$E(x^2) \le E^2(x) + \frac{d^3}{6} + o(1)$$

which implies

$$Var(x) = E(x^2) - E^2(x) \le \frac{d^3}{6} + o(1).$$

Using Chebyshev inequality,

$$\operatorname{Prob}(x = 0) \le \operatorname{Prob}\left(|x - E(x)| \ge \frac{d^3}{6}\right) \le \frac{\operatorname{Var}(x)}{d^6/36} \le \frac{6}{d^3} + o(1).$$

Thus, for $d > \sqrt[3]{6} \cong 1.8$, $\operatorname{Prob}(x=0) < 1$ and G(n,p) has a triangle with nonzero probability.

3.1.3 Phase Transitions

Many properties of random graphs undergo structural changes as the edge probability passes some threshold value. This phenomenon is similar to the abrupt phase transitions in physics as the temperature or pressure increases. Some examples of this are the abrupt appearance of cycles in G(n,p) when p reaches 1/n and the disappearance of isolated vertices when p reaches $\frac{\log n}{n}$. The most important of these transitions is the emergence of a giant component, a connected component of size $\Theta(n)$, which happens at d=1.

For these and many other properties of random graphs, a threshold exists where an abrupt transition from not having the property to having the property occurs. If there exists a function p(n) such that when $\lim_{n\to\infty}\frac{p_1(n)}{p(n)}=0$, $G(n,p_1(n))$ almost surely does not

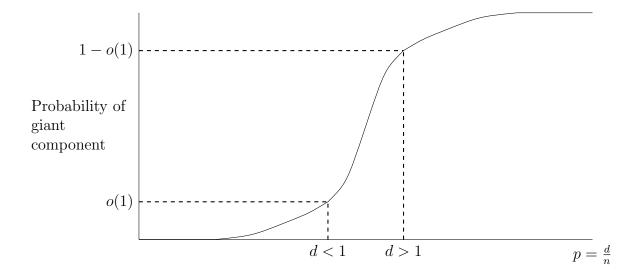


Figure 3.4: Probability of a property goes abruptly from 0 to 1

have the property and when $\lim_{n\to\infty}\frac{p_2(n)}{p(n)}=\infty$, $G\left(n,p_2\left(n\right)\right)$ almost surely has the property, then we say that a phase transition occurs and $p\left(n\right)$ is the threshold. Recall that G(n,p) "almost surely does not have the property" means that the probability that it has the property goes to zero in the limit as n goes to infinity. We shall soon see that every monotone property has a threshold. This is true not only for monotone properties of $G\left(n,p\right)$, but for monotone properties of any combinatorial structure. If for $cp\left(n\right)$, c<1, the graph almost surely does not have the property and for $cp\left(n\right)$, c>1, the graph almost surely has the property, we say that $p\left(n\right)$ is a sharp threshold. The existence of a giant component has a sharp threshold at 1/n. We will prove this later.

In establishing phase transitions for various properties, we often use a variable x(n) to denote the number of occurrences of some item in a random graph. Thus, x(n) is a nonnegative integer valued random variable. By showing that the expected value of x(n) goes to zero as n goes to infinity, we conclude that a graph picked at random almost surely has no occurrence of the item. This follows from Markov's inequality that states for a nonnegative random variable x that $\operatorname{Prob}(x \geq a) \leq \frac{1}{a}E(x)$, which implies that the probability that $x(n) \geq 1$ is at most E(x(n)). That is, when the expected number of occurrences of an item in a graph goes to zero, the probability that the number of occurrences of the item is one or more in a randomly selected graph goes to zero. This is called the first moment method.

However, when the expected value of x(n) goes to infinity, we cannot conclude that a graph picked at random will likely have a copy, since the items may all appear on a small fraction of the graphs. We resort to a technique called the *second moment method*. It is a simple idea based on the Chebyshev inequality.

No items	At least one occurrence of item in 10% graphs
$E(x) \ge 0.1$	For 10% of graphs $x \ge 1$

Figure 3.5: If the expected number of graphs in which an item occurs did not go to zero, then $E\left(x\right)$, the expected number of items per graph, could not be zero. Suppose 10% of the graphs had at least one occurrence of the item. Then the expected number of occurrences per graph must be at least 0.1. Thus, $E\left(x\right)=0$ implies the probability that a graph has an occurrence of the item goes to zero. However, the other direction needs more work. If $E\left(x\right)$ were not zero, a second moment argument is needed to conclude that the probability that a graph had an occurrence of the item was nonzero since there could be a large number of occurrences concentrated on a vanishingly small fraction of all graphs. The second moment argument claims that for a nonnegative random variable x with $E\left(x\right)>0$, if $\operatorname{Var}(x)$ is $o(E^{2}\left(x\right))$ or alternatively if $E\left(x^{2}\right)\leq E^{2}\left(x\right)\left(1+o(1)\right)$, then almost surely x>0.

Theorem 3.3 (Second Moment method) Let x = x(n) be a random variable with E(x) > 0. If

$$Var(x) = o[E^2(x)],$$

then x is almost surely greater than zero.

Proof: By Chebyshev inequality

$$\operatorname{Prob}(x \le 0) \le \operatorname{Prob}\left[|x - E(x)| \ge E(x)\right] \le \frac{\operatorname{Var}(x)}{E^2(x)} \to 0.$$

Corollary 3.4 Let x be a random variable with E(x) > 0. If

$$E(x^2) \le E^2(x)(1 + o(1))$$

then x is almost surely greater than zero.

Proof: If $E(x^2) \le E^2(x)(1 + o(1))$ then

$$Var(x) = E(x^2) - E^2(x) \le E^2(x)o(1) = o(E^2(x)).$$

Threshold for graph diameter two

We now present the first example of a phase transition for a property. This means that slightly increasing the edge probability p near the threshold takes us from almost surely not having the property to almost surely having it. The property is that of a random graph having diameter less than or equal to two. The diameter of a graph is the maximum length of the shortest path between a pair of nodes. When $p = c\sqrt{\frac{\ln n}{n}}$, for $c < \sqrt{2}$, the graph almost surely has diameter greater than two and for $c > \sqrt{2}$, the graph almost surely has diameter less than or equal to two.

Theorem 3.5 The property that G(n,p) has diameter two has a sharp threshold at $p = \sqrt{2}\sqrt{\frac{\ln n}{n}}$.

Proof: If G has diameter greater than two, then there exists a pair of nonadjacent vertices i and j such that no other vertex of G is adjacent to both i and j. This motivates calling such a pair bad.

Introduce a set of indicator random variables x_{ij} , one for each pair (i, j) with i < j, where x_{ij} is 1 if and only if the pair (i, j) is bad. Let

$$x = \sum_{i < j} x_{ij}$$

be the number of bad pairs of vertices. [Putting i < j in the sum ensures each pair (i, j) is counted only once.] A graph has diameter two if and only if it has no bad pair, i.e., x = 0. Thus, if $\lim_{n \to \infty} E(x) = 0$, then for large n almost surely a graph has no bad pairs and hence has diameter at most two. See Figure 3.5.

The probability that a given vertex is adjacent to both vertices in a pair of vertices (i, j) is p^2 and hence the probability that the vertex is not adjacent to both vertices is $1 - p^2$. The probability that no vertex is adjacent to the pair (i, j) is $(1 - p^2)^{n-2}$ and the probability that i and j are not adjacent is 1 - p. Since there are $\binom{n}{2}$ pairs of vertices, the expected number of bad pairs is

$$E(x) = \binom{n}{2} (1-p) (1-p^2)^{n-2}.$$

Setting $p = c\sqrt{\frac{\ln n}{n}}$,

$$E(x) \cong \frac{1}{2}n^2 \left(1 - c\sqrt{\frac{\ln n}{n}}\right) \left(1 - c^2 \frac{\ln n}{n}\right)^n$$
$$\cong \frac{1}{2}n^2 e^{-c^2 \ln n}$$
$$\cong \frac{1}{2}n^{2-c^2}$$

and for $c > \sqrt{2}$, $\lim_{n \to \infty} E\left(x\right) \to 0$. Thus, for $p = c\sqrt{\frac{\ln n}{n}}$ with $c > \sqrt{2}$, $G\left(n, p\right)$ almost surely has no bad pairs and hence has diameter at most two.

Next consider the case where $c < \sqrt{2}$. Here $\lim_{n \to \infty} E(x) \to \infty$. We appeal to a second moment argument to claim that almost surely a graph has a bad pair and thus has diameter greater than two.

$$E(x^{2}) = E\left(\sum_{i < j} x_{ij}\right)^{2} = E\left(\sum_{i < j} x_{ij} \sum_{k < l} x_{kl}\right) = E\left(\sum_{\substack{i < j \\ k < l}} x_{ij} x_{kl}\right) = \sum_{\substack{i < j \\ k < l}} E\left(x_{ij} x_{kl}\right)$$

The summation can be partitioned into three summations depending on the number of distinct indices among i, j, k, and l. Call this number a.

$$E(x^{2}) = \sum_{i < j} E(x_{ij}x_{kl}) + \sum_{i < j} E(x_{ij}x_{ik}) + \sum_{i < j} E(x_{ij}^{2})$$

$$a = 4$$

$$a = 3$$

$$a = 2$$

$$(3.1)$$

If i and j are distinct from k and l, then by independence $E(x_{ij}x_{kl}) = E(x_{ij}) E(x_{kl})$. So, the first sum is

$$\sum_{\substack{i < j \\ k < l}} E(x_{ij})E(x_{kl}) \le \left(\sum_{i < j} E(x_{ij})\right)^2 = E^2(x) \cong n^{4-2c^2}.$$

For the second summation observe that if $x_{ij}x_{ik} = 1$ then both pairs (i, j) and (i, k) are bad. Both pairs (i, j) and (i, k) being bad implies that for every vertex u not equal to i, j, or k, either there is no edge between i and u or there is an edge (i, u) and both edges (j, u) and (k, u) are absent. The probability of this event for one u is

$$1 - p + p(1 - p)^2 = 1 - 2p^2 + p^3 \approx 1 - 2p^2.$$

Thus, the probability for all u is $(1-2p^2)^n$. Substituting $c\sqrt{\frac{\ln n}{n}}$ for p yields

$$\left(1 - \frac{2c^2 \ln n}{n}\right)^n \cong e^{-2c^2 \ln n} = n^{-2c^2},$$

which is an upper bound on $E(x_{ij}x_{kl})$ for one i, j, k, and l with a = 3. Summing over all distinct triples yields n^{3-2c^2} for the second summation in (3.1).

For the third summation, since the value of x_{ij} is zero or one, $E\left(x_{ij}^2\right) = E\left(x_{ij}\right)$. Thus

$$\sum_{ij} E\left(x_{ij}^2\right) = E\left(x\right).$$

Hence $E\left(x^2\right) \leq n^{4-2c^2} + n^{3-2c^2} + n^{2-c^2}$ and $E\left(x\right) \cong n^{2-c^2}$ from which it follows that $E\left(x^2\right) \leq E^2\left(x\right)\left(1+o(1)\right)$. By a second moment argument, Corollary 3.4, a graph almost surely has at least one bad pair of vertices and thus has diameter greater than two. Therefore the property that the diameter of G(n,p) is less than or equal to two has a sharp threshold at $p = \sqrt{2}\sqrt{\frac{\ln n}{n}}$

Disappearance of Isolated Vertices

The disappearance of isolated vertices in G(n,p) has a sharp threshold of $\frac{\ln n}{n}$. At this point the giant component has absorbed all the small components and with the disappearance of isolated vertices the graph becomes connected.

Theorem 3.6 The disappearance of isolated vertices in G(n,p) has a sharp threshold of $\frac{\ln n}{n}$.

Proof: Let x be the number of isolated vertices in G(n,p). Then

$$E(x) = n(1-p)^{n-1}$$
.

Since we believe the threshold to be $\frac{\ln n}{n}$, consider $p = c \frac{\ln n}{n}$. Then

$$\lim_{n \to \infty} E(x) = \lim_{n \to \infty} n \left(1 - \frac{c \ln n}{n}\right)^n = \lim_{n \to \infty} n e^{-c \ln n} = \lim_{n \to \infty} n^{1-c}.$$

If c > 1, the expected number of isolated vertices, goes to zero. If c < 1, the expected number of isolated vertices goes to infinity. If the expected number of isolated vertices goes to zero, then it follows that almost all graphs have no isolated vertices. On the other hand, if the expected number of isolated vertices goes to infinity, a second moment argument is needed to show that almost all graphs have an isolated vertex and that the isolated vertices are not bunched on some vanishingly small set of graphs with almost all graphs having none.

Write $x = x_1 + x_2 + \cdots + x_n$ where x_i is the indicator variable indicating whether vertex i is an isolated vertex. Then $E\left(x^2\right) = \sum_{i=1}^n E\left(x_i^2\right) + \sum_{i\neq j} E\left(x_ix_j\right)$. Since x_i equals 0 or 1, $x_i^2 = x_i$ and the first sum has value $E\left(x\right)$. Since all elements in the second sum are equal

$$E(x^{2}) = E(x) + n(n-1) E(x_{1}x_{2})$$

= $E(x) + n(n-1) (1-p)^{2(n-1)-1}$.

The minus one in the exponent 2(n-1)-1 avoids counting the edge from vertex 1 to 2 twice. Now

$$\frac{E(x^2)}{E^2(x)} = \frac{n(1-p)^{n-1} + n(n-1)(1-p)^{2(n-1)-1}}{n^2(1-p)^{2(n-1)}}$$
$$= \frac{1}{n(1-p)^{n-1}} + \frac{1}{1-p} - \frac{1}{n(1-p)}.$$

For $p = c \frac{\ln n}{n}$ and c < 1, $\lim_{n \to \infty} E(x) = \infty$ and

$$\lim_{n \to \infty} \frac{E(x^2)}{E^2(x)} = \lim_{n \to \infty} \left[\frac{1}{n^{1-c}} + \frac{1}{1 - c\frac{\ln n}{n}} - \frac{1}{n - c\ln n} \right] = 1 + o(1).$$

By the second moment method, Corollary 3.4, the probability that x=0 goes to zero implying that almost all graphs have an isolated vertex. Thus, $\frac{\ln n}{n}$ is a sharp threshold for the disappearance of isolated vertices. For $p=c\frac{\ln n}{n}$, when c>1 there almost surely are no isolated vertices and when c<1 there almost surely are isolated vertices.

Threshold for Graph Connectivity

As p increases from p=0, small components form. At p=1/n a giant component emerges and swallows up smaller components starting with the larger components and ending up swallowing isolated vertices forming a single connected component at $p=\frac{\ln n}{n}$ at which point the graph becomes connected. We begin our development with a technical lemma.

Lemma 3.7 The expected number of connected components of size k in G(n, p) is at most

$$\binom{n}{k} k^{k-2} p^{k-1} (1-p)^{kn-k^2}.$$

Proof: The probability that k vertices form a connected component consists of the product of two probabilities. The first is the probability that the k vertices are connected and the second is the probability that there are no edges out of the component to the remainder of the graph. The first probability is at most the sum over all spanning trees of the k vertices, that the edges of the spanning tree are all in. The "at most" is because G(n,p) may contain more than one spanning tree on these nodes and in this case the union bound is higher than the actual probability. There are k^{k-2} spanning trees on k nodes. See appendix. The probability of all the k-1 edges of one spanning tree being in is p^{k-1} and the probability that there are no edges connecting the k vertices to the remainder of the graph is $(1-p)^{k(n-k)}$. Thus, the probability of one particular set of k vertices forming a connected component is at most $k^{k-2}p^{k-1}(1-p)^{kn-k^2}$.

Theorem 3.8 Let $p = c \frac{\ln n}{n}$. For c > 1/2, almost surely there are only isolated vertices and a giant component. For c > 1, almost surely the graph is connected.

Proof: We prove that almost surely for c > 1/2, there is no connected component with k vertices for any k, $2 \le k \le n/2$. This proves the first statement of the theorem since if there are two or more components which are not isolated vertices, one of them must have size between 2 and n/2. The second statement that for c > 1 the graph is connected then follows from the fact that isolated vertices disappear at c = 1 (Theorem 3.6).

We now show that for $p=c\frac{\ln n}{n}$, the expected number of components of size $k, 1 < k \le n/2$, is less than n^{1-2c} and thus for c>1/2 there are no components except for isolated vertices and the giant component. Let x_k be the number of connected components of size k. Substitute $p=c\frac{\ln n}{n}$ into $\binom{n}{k}k^{k-2}p^{k-1}\left(1-p\right)^{kn-k^2}$ and simplify using $\binom{n}{k} \le (en/k)^k$, $1-p \le e^{-p}, \ k-1 < k$, and $x=e^{\ln x}$ to get

$$E(x_k) \le \exp\left(\ln n + k + k \ln \ln n - 2 \ln k + k \ln c - ck \ln n + ck^2 \frac{\ln n}{n}\right).$$

It is good to keep in mind that the leading terms here for large k are the last two and in fact at k = n, they cancel each other so that our argument does not prove the fallacious statement (for $c \ge 1$) that there is no connected component of size n, since there is. Let

$$f(k) = \ln n + k + k \ln \ln n - 2 \ln k + k \ln c - ck \ln n + ck^{2} \frac{\ln n}{n}.$$

Differentiating with respect to k,

$$f'(k) = 1 + \ln \ln n - \frac{2}{k} + \ln c - c \ln n + \frac{2ck \ln n}{n}$$

and

$$f''(k) = \frac{2}{k^2} + \frac{2c \ln n}{n} > 0,$$

so the function f(k) attains its maximum over the range [2, n/2] at one of the extreme points 2 or n/2. At k=2, $f(2)\approx (1-2c)\ln n$ and at k=n/2, $f(n/2)\approx -c\frac{n}{4}\ln n$. So f(k) is maximum at k=2. For k=2, $x_k=e^{f(k)}$ is approximately $e^{(1-2c)\ln n}=n^{1-2c}$ and is geometrically falling as k increases from 2. At some point x_k starts to increase but never gets above $n^{-\frac{c}{4}n}$. Thus, the expected sum of the number of components of size k, for $2 \le k \le n/2$ is

$$E\left(\sum_{k=2}^{n/2} x_k\right) \in O(n^{1-2c}).$$

This expected number goes to zero for c > 1/2 and the first-moment method implies that almost surely there are no components of size between 2 and n/2. This completes the proof of Theorem 3.8.

Threshold for $O(\ln n)$ Diameter

We now show that within a constant factor of the threshold for graph connectivity, not only is the graph connected, but its diameter is $O(\ln n)$. That is, for $p \in \Omega(\ln n/n)$, the diameter of G(n, p) is $O(\ln n)$.

Consider a particular vertex v. Let S_i be the set of vertices at distance i from v. We argue that as i grows, $|S_1| + |S_2| + \cdots + |S_i|$ grows by a constant factor up to a size of n/1000. This implies that in $O(\ln n)$ steps, at least n/1000 vertices are connected to v. Then it is a simple argument that a pair of n/1000 sized subsets connected to two different vertices v and w have an edge between them.

Lemma 3.9 Consider G(n, p) for sufficiently large n with $p = c \ln n/n$ for any c > 0. Let S_i be the set of vertices at distance i from some fixed vertex v. If $|S_1| + |S_2| + \cdots + |S_i| \le n/1000$, then

$$Prob(|S_{i+1}| < 2(|S_1| + |S_2| + \dots + |S_i|)) \le e^{-10|S_i|}.$$

Proof: Let $|S_i| = k$, so $|S_1| + |S_2| + \cdots + |S_{i-1}| \le \frac{k}{2}$. For each vertex u not in $(S_1 \cup S_2 \cup \ldots \cup S_i)$, the probability that u is not in S_{i+1} is $(1-p)^k$ and these events are independent. So, $|S_{i+1}|$ is the sum of $n - (|S_1| + |S_2| + \cdots + |S_{i-1}| + |S_i|)$ independent Bernoulli random variables, each with probability of

$$1 - (1 - p)^k \ge 1 - e^{-ck \ln n/n}$$

of being one. Let $\alpha = \frac{k}{n}$. Thus,

$$E(|S_{i+1}|) \ge \left(n - \frac{3k}{2}\right) (1 - e^{-c\alpha \ln n}).$$

Subtracting 200k from each side and using the inequality $n-\frac{3}{2}k\geq \frac{n}{2}$

$$E(|S_{i+1}|) - 200k \ge \frac{n}{2}(1 - e^{-c\alpha \ln n} - 400\alpha).$$

Let $f(\alpha) = 1 - e^{-c\alpha \ln n} - 400\alpha$. By differentiation $f''(\alpha) \leq 0$, so f is concave. So the minimum value of f over the interval [0, 1/1000] is attained at one of the end points. It is easy to check that both f(0) and f(1/1000) are greater than or equal to zero for sufficiently large n. Thus f is nonnegative throughout the interval proving that $E(|S_{i+1}|) \geq 200|S_i|$. The lemma follows from Chernoff bounds (Lemma 2.6).

Theorem 3.10 For $p \ge c \ln n/n$, where c is a sufficiently large constant, almost surely, G(n,p) has diameter $O(\ln n)$.

Proof: By Corollary 3.2, almost surely, the degree of every vertex is $\Omega(np) = \Omega(\ln n)$, which is at least $20 \ln n$ for c sufficiently large. Assume this holds.

If for $i = 1, 2, ..., |S_{i+1}| \ge 2(|S_1| + |S_2| + ... + |S_i|)$ until $|S_1| + |S_2| + ... + |S_i| \ge n/1000$, then in $O(\ln n)$ steps, S_i grows to size n/1000. By Lemma 3.9 and a union bound the

probability that this does not happen is at most $\sum_{k=20\ln n}^{n/1000} e^{-10k} \le 1/n^4$. Now consider any other vertex w. We wish to find a short $O(\ln n)$ length path between v and w. By the same argument as above, we also have that the number of vertices at distance $O(\ln n)$ from w is at least n/1000. To complete the argument, either these two sets intersect in which case, we have found a path from v to w of length $O(\ln n)$ or they do not intersect. In the latter case, with high probability there is some edge between them. For a pair of disjoint sets of size at least n/1000, the probability that none of the possible $n^2/10^6$ or more edges between them is present is at most $(1-p)^{n^2/10^6} = e^{-\Omega(n\ln n)}$. There are at most 2^{2n} pairs of such sets and so the probability that there is some such pair with no edges is $e^{-\Omega(n\ln n)+O(n)} \to 0$. Note that there is no conditioning problem since we are arguing this for every pair of such sets. Think of whether such an argument made for just the n subsets of vertices which are vertices at distance at most $O(\ln n)$ from a specific vertex would work.

Emergence of Cycles

Another threshold property is the emergence of cycles in G(n, p) when p becomes asymptotically equivalent to 1/n.

Theorem 3.11 The threshold for the existence of cycles in G(n, p) is p = 1/n.

Proof: Let x be the number of cycles in G(n,p). To form a cycle of length k, the vertices can be selected in $\binom{n}{k}$ ways. Given the k vertices of the cycle, they can be ordered by arbitrarily selecting a first vertex, then a second vertex in one of k-1 ways, a third in one of k-2 ways, etc. Since a cycle and its reversal are the same cycle, divide by 2. Thus, there are $\binom{n}{k} \frac{(k-1)!}{2}$ cycles of length k and

$$E(x) = \sum_{k=3}^{n} {n \choose k} \frac{(k-1)!}{2} p^k \le \sum_{k=3}^{n} \frac{n^k}{2k} p^k \le \sum_{k=3}^{n} (np)^k.$$

When p is asymptotically less than 1/n, $\lim_{n\to\infty} np = 0$ and $\lim_{n\to\infty} \sum_{k=3}^n (np)^k = 0$. Thus, E(x) = 0 and a graph almost surely has no cycles by the first moment method. A second moment argument can be used to show that for p = d/n, d > 1, a graph will have a cycle with probability tending to one.

The argument above does not yield a sharp threshold since we argued that $E(x) \to 0$ only under the assumption that $np \to 0$. For a sharp threshold we need $E(x) \to 0$ for p = d/n, d < 1.

Now, consider what happens in more detail when p = d/n, d a constant.

$$E(x) = \sum_{k=3}^{n} \binom{n}{k} \frac{(k-1)!}{2} p^{k}$$

$$= \frac{1}{2} \sum_{k=3}^{n} \frac{n(n-1)\cdots(n-k+1)}{k!} (k-1)! p^{k}$$

$$= \frac{1}{2} \sum_{k=3}^{n} \frac{n(n-1)\cdots(n-k+1)}{n^{k}} \frac{d^{k}}{k}.$$

 $E\left(x\right)$ converges if d<1 and diverges if $d\geq1$. If d<1, $E\left(x\right)\leq\frac{1}{2}\sum_{k=3}^{n}\frac{d^{k}}{k}$ and $\lim_{n\to\infty}E\left(x\right)$ equals a constant. If d=1, $E\left(x\right)=\frac{1}{2}\sum_{k=3}^{n}\frac{n(n-1)\cdots(n-k+1)}{n^{k}}\frac{1}{k}$. Consider only the first $\log n$ terms of the sum.

$$E(x) \ge \frac{1}{2} \sum_{k=3}^{\log n} \frac{n(n-1)\cdots(n-k+1)}{n^k} \frac{1}{k} \ge \frac{1}{4} \sum_{k=3}^{\log n} \frac{1}{k}$$

Then in the limit as n goes to infinity

$$\lim_{n \to \infty} E(x) \ge \lim_{n \to \infty} \frac{1}{4} \sum_{k=3}^{\log n} \frac{1}{k} \ge \lim_{n \to \infty} (\log \log n) = \infty.$$

For p = d/n, d < 1, E(x) converges to a nonzero constant and with some nonzero probability, graphs will have a constant number of cycles independent of the size of the graph. For d > 1, they will have an unbounded number of cycles increasing with n.

Property	Threshold
cycles	1/n
giant component	1/n
giant component + isolated vertices	$\frac{1}{2} \frac{\ln n}{n}$
connectivity, disappearance of isolated vertices	$\frac{\ln n}{n}$
diameter two	$\sqrt{\frac{2 \ln n}{n}}$

3.1.4 Phase Transitions for Monotone Properties

For many graph properties such as connectivity, having no isolated vertices, having a cycle, etc., the probability of a graph having the property increases as edges are added to the graph. Such a property is called an increasing property. Q is an *increasing property* of G if when a graph G has the property any graph obtained by adding edges to G must

also have the property. Here, we will show that any increasing property in fact has a threshold although not necessarily a sharp one.

The notion of increasing property is defined in terms of adding edges. Lemma 3.12 proves that if Q is an increasing property, then increasing p in G(n,p) increases the probability of the property Q.

Lemma 3.12 If Q is an increasing property and $0 \le p \le q \le 1$, then the probability that G(n,p) has property Q is less than or equal to the probability that G(n,q) has property Q.

Proof: For this proof, we use an interesting relationship between G(n,p) and G(n,q). Generate G(n,q) as follows. First generate G(n,p). Recall that this means generating a graph on n vertices with edge probabilities p. Then independently generate another graph $G\left(n,\frac{q-p}{1-p}\right)$ and take the union by putting in an edge if either of the two graphs has the edge. Call the resulting graph H. The graph H has the same distribution as G(n,q). This follows since the probability that an edge is in H is $p+(1-p)\frac{q-p}{1-p}=q$ and clearly the edges of H are independent. The lemma follows since whenever G(n,p) has the property Q, H also has the property Q.

We now introduce a notion called "replication". An m-fold replication of G(n, p) is a random graph obtained as follows. Generate m independent copies of G(n, p). Include an edge in the m-fold replication graph if and only if the edge is in one of the m copies of G(n, p). The resulting random graph has the same distribution as G(n, q), where, $q = 1 - (1-p)^m$ since the probability that a particular edge is not in the m-fold replication is the product of probabilities that it is not in any of the m copies of G(n, p). If the m-fold replication of G(n, p) does not have property Q, then none of the m copies of G(n, p) has the property. The converse is not true because, even if no copy has the property, their union may have it. Thus, the probability that G(n, q) does not have property Q is less than or equal to the probability that none of the m copies of G(n, p) has property Q. Since the copies are independent, the probability that no copy has the property is just the product of the m individual probabilities. Thus

$$\operatorname{Prob}\left(G(n,q) \text{ does not have } Q\right) \leq \left(\operatorname{Prob}(G(n,p) \text{ does not have } Q)\right)^m.$$

Now $q = 1 - (1 - p)^m \le 1 - (1 - mp) = mp$ and since Q is an increasing property

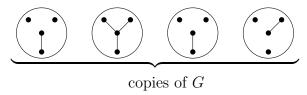
$$\operatorname{Prob}\left(G(n,q) \text{ has property } Q\right) \leq \operatorname{Prob}\left(G(n,mp) \text{ has } Q\right)$$

or

$$\operatorname{Prob}\left(G(n,mp) \text{ does not have } Q\right) \leq \operatorname{Prob}\left(G(n,q) \text{ does not have } Q\right).$$

Combining the above inequalities yields

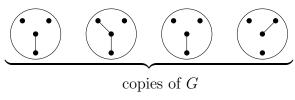
$$\operatorname{Prob}\left(G(n,mp) \text{ does not have } Q\right) \leq \left(\operatorname{Prob}\left(G(n,p) \text{ does not have } Q\right)\right)^m.$$



If any graph has three or more edges then the m-fold replication has three or more edges



The m-fold replication H



Even if no graph has three or more edges, the m-fold replication might have three or more edges



The m-fold replication H

Figure 3.6: The property that G has three or more edges is an increasing property. Let H be the m-fold replication of G. If any copy of G has three or more edges, H has three or more edges. However, H can have three or more edges even if no copy of G has three or more edges.

For any $\varepsilon > 0$, let m be an integer such that $(1 - \varepsilon)^m < \varepsilon$. For each value of n, let $p_0(n)$ be the largest value of p such that the probability G(n,p) has the property Q is less than or equal to ε . Similarly for each value of n, let $p_1(n)$ be the largest value of p such that the probability G(n,p) has the property Q is less than or equal to $1 - \varepsilon$. We now show that any increasing property Q has a threshold. That is, for any $\varepsilon > 0$ and any n the probability G(n,p) has property Q goes from ε to $1 - \varepsilon$ within a multiplicative factor m of p.

Theorem 3.13 For any $\varepsilon > 0$ and any n, the probability G(n,p) has property Q goes from ε to $1 - \varepsilon$ within a multiplicative factor m of p.

Proof: We need to prove that $p_1(n) \leq mp_0(n)$ where p_0 and p_1 are as defined above. The probability that $G(n, p_0(n))$ has Q is less than or equal to ε and thus that it does not have Q is greater than or equal to $1 - \varepsilon$. Let H be the m-fold replication of $G(n, p_0(n))$. Then H = G(n, q(n)) where $q(n) \leq 1 - (1 - p_0(n))^m \leq mp_0(n)$. If H does not have property Q then none of the m copies of $G(n, p_0(n))$ has the property. Since the copies are independent, the probability that no copy has Q is the product of the m individual probabilities. Thus

$$\operatorname{Prob}(H \text{ does not have } Q) \leq (1 - \varepsilon)^m \leq \varepsilon$$

by the definition of m and thus $Prob(H \text{ has } Q) \geq 1 - \varepsilon$

But for each n, $p_1(n)$ is the smallest value of p such that $G(n, p_1(n))$ has the property Q with probability greater than or equal to $1 - \varepsilon$. Since H = G(n, q(n)), where $q(n) \le mp_0(n)$, it follows that $p_1(n) \le mp_0(n)$.

3.1.5 Phase Transitions for CNF-sat

Phase transitions occur not only in random graphs, but in other random structures as well. An important example is that of satisfiability for a Boolean formula in conjunctive normal form.

Generate a random CNF formula f with n variables, m clauses, and k literals per clause. Here, n is going to infinity, m is a function of n, and k is to be thought of as a fixed constant. A reasonable value to think of is k=3. A literal is a variable or its negation. Unsatisfiability is an increasing property since adding more clauses preserves unsatisfiability. By arguments similar to the last section, there is a phase transition, i.e., a function m(n) such that if $m_1(n)$ is o(m(n)), a random formula with $m_1(n)$ clauses is almost surely satisfiable and for $m_2(n)$ with $m_2(n)/m(n) \to \infty$, almost surely, the formula is unsatisfiable. It has been conjectured that there is a constant r_k (independent of n) such that $r_k n$ is a sharp threshold.

Here we derive upper and lower bounds on r_k . It is relatively easy to get an upper bound on r_k . A fixed truth assignment satisfies a random k clause with probability $1 - \frac{1}{2^k}$. Of the 2^k truth assignments to the k variables in the clause only one fails to satisfy the clause. Thus with probability $\frac{1}{2^k}$ the clause is not satisfied and with probability $1 - \frac{1}{2^k}$ the clause is satisfied. Let m = cn. Now, cn independent clauses are all satisfied by the fixed assignment with probability $\left(1 - \frac{1}{2^k}\right)^{cn}$. Since there are 2^n truth assignments, the expected number of satisfying assignments for a formula with cn clauses is $2^n \left(1 - \frac{1}{2^k}\right)^{cn}$. If $c = 2^k \ln 2$, the expected number of satisfying assignments is

$$2^n \left(1 - \frac{1}{2^k}\right)^{n2^k \ln 2}$$
.

 $\left(1-\frac{1}{2^k}\right)^{2^k}$ is at most 1/e and approaches 1/e in the limit. Thus

$$2^{n} \left(1 - \frac{1}{2^{k}}\right)^{n2^{k} \ln 2} \le 2^{n} e^{-n \ln 2} = 2^{n} 2^{-n} = 1.$$

For $c > 2^k \ln 2$, the expected number of satisfying assignments goes to zero as $n \to \infty$. Here the expectation is over the choice of clauses which is random, not the choice of a truth assignment. From the first moment method, it follows that a random formula with cn clauses is almost surely not satisfiable. Thus, $r_k \le 2^k \ln 2$.

The other direction, showing a lower bound for r_k , is not that easy. From now on, we focus only on the case k = 3. The statements and algorithms given here can be extended

to $k \geq 4$, but with different constants. It turns out that the second moment method cannot be directly applied to get a lower bound on r_3 because the variance is too high. A simple algorithm called the Smallest Clause Heuristic (abbreviated SC) yields a satisfying assignment with probability tending to one if $c < \frac{2}{3}$, proving that $r_3 \geq \frac{2}{3}$. Other, more difficult to analyze algorithms, push the lower bound on r_3 higher.

The Smallest Clause Heuristic repeatedly executes the following. Assign true to a random literal in a random smallest length clause. Pick at random a 1-literal clause if one exists and set that literal to true. If there is no 1-literal clause, pick a 2-literal clause, select one of its two literals and set the literal to true. Otherwise, pick a 3-literal clause and a literal in it and set the literal to true. If we encounter a 0-length clause, then we have failed to find a satisfying assignment; otherwise, we have found one.

A related heuristic called the Unit Clause Heuristic selects a random clause with one literal, if there is one and sets the literal in it to true. Otherwise, it picks a random as yet unset literal and sets it to true. The "pure literal" heuristic sets a random "pure literal", a literal whose negation does not occur in any clause, to true, if there are any pure literals, otherwise it sets a random literal to true.

When a literal w is set to true, all clauses containing w are deleted since they are satisfied and \bar{w} is deleted from any clause containing \bar{w} . If a clause is reduced to length zero (no literals), then the algorithm has failed to find a satisfying assignment to the formula. The formula may in fact be satisfiable, but the algorithm has failed.

Example: Consider a 3-CNF formula with n variables and cn clauses. With n variables there are 2n literals since a variable and its complement are distinct literals. The expected number of times a literal occurs is calculated as follows. Each clause has three literals. Thus, each of the 2n different literals occurs $\frac{(3cn)}{2n} = \frac{3}{2}c$ times on average. Suppose c = 5. Then each literal appears 7.5 times on average. If one sets a literal to true, one would expect to satisfy 7.5 clauses. However, this process is not repeatable since after setting a literal to true there is conditioning so that the formula is no longer random.

Theorem 3.14 If the number of clauses in a random 3-CNF formula grows as cn where c is a constant less than 2/3, then with probability 1 - o(1), the Shortest Clause Heuristic finds a satisfying assignment.

The proof of this theorem will take the rest of this section. A general impediment to proving that simple algorithms work for random instances of many problems is conditioning. At the start, the input is random and has properties enjoyed by random instances. But as the algorithm is executed, the data is no longer random, it is conditioned on the steps of the algorithm so far. In the case of SC and other heuristics for finding a satisfying assignment for a Boolean formula, the argument to deal with conditioning is relatively simple.

We supply some intuition before going to the proof. Imagine maintaining a queue of 1 and 2-clauses. A 3-clause enters the queue when one of its literals is set to false and it becomes a 2-clause. SC always picks a 1 or 2-clause if there is one and sets one of its literals to true. At any step when the total number of 1 and 2-clauses is positive, one of the clauses is removed from the queue. Consider the "arrival rate" (the expected number of arrivals) into the queue. For a particular clause to arrive into the queue at time t (to become a 2-clause at time t), it must contain the negation of the literal being set to true at time t. It can contain any two other literals not yet set at time t. The number of such clauses is $\binom{n-t}{2}2^2$. So, the probability that a particular clause arrives in the queue at time t is at most

$$\frac{\binom{n-t}{2}2^2}{\binom{n}{3}2^3} \le \frac{3}{2(n-2)}.$$

Since there are cn clauses in total, the arrival rate is $\frac{3c}{2}$, which for c < 2/3 is a constant strictly less than one. The arrivals into the queue of different clauses occur independently (Lemma 3.15), the queue has arrival rate strictly less than one, and the queue looses one or more clauses whenever it is nonempty. This implies that the queue never has too many clauses in it. A slightly more complicated argument will show that no clause remains as a 1 or 2-clause for $\Omega(\ln n)$ steps (Lemma 3.16). This implies that the probability of two contradictory 1-length clauses, which is a precursor to a 0-length clause, is very small.

Lemma 3.15 Let T_i be the first time that clause i turns into a 2-clause. (T_i is say ∞ if clause i gets satisfied before turning into a 2-clause.) Then, T_i are mutually independent and for any t,

$$Prob(T_i = t) \le \frac{3}{2(n-2)}.$$

Proof: For the proof, we generate the clauses in a different way. The important thing is that the new method of generation, called the method of "deferred decisions" results in the same distribution of input formulae as the original. The method of deferred decisions is tied in with the SC algorithm and works as follows. At any time, the length of each clause (number of literals) is all that we know; we have not yet picked which literals are in each clause. At the start, every clause has length three and SC picks one of the clauses uniformly at random. Now, SC wants to pick one of the three literals in that clause to set to true, but we do not know which literals are in the clause. At this point, we pick uniformly at random one of the 2n possible literals – say for illustration we picked \bar{x}_{102} . We "put" that literal (\bar{x}_{102} in the example) in that clause and set the literal to true (so we set x_{102} = FALSE in the example). We must also deal with occurrences of that literal or its negation in all other clauses, but again, we do not know which clauses have such an occurrence. We decide that now. For each clause, independently, with probability 3/n, include the variable x_{102} or \bar{x}_{102} in the clause and if included, with probability 1/2, include the literal \bar{x}_{102} in the clause and with the other 1/2 probability include its negation, namely, x_{102} . In either case, we decrease the (residual) length of the clause by 1. For the algorithm, if we included the literal (\bar{x}_{102}) in the clause, we delete the clause, since now it is satisfied and we do not care what the other literals in it are. If we included the negation of the literal, namely x_{102} in the example, then we delete just that occurrence, and decrease the length of the clause by one.

At general stage do the following: Suppose the fates of i variables have already been decided and n-i are left to be decided. We have the residual length of each clause. Among the clauses which are not yet satisfied, choose a random shortest length clause. Among the n-i variables left, pick one uniformly at random, then pick it or its negation as the new literal. Include this literal in the picked clause (it is now satisfied and for the algorithm, delete it). For each other clause do the following: if its residual length is l, decide with probability l/(n-i) to include the new variable in the clause and if so with probability 1/2 each, include it or its negation. Then, decrease l by 1.

Why does this yield the same distribution as the original one? First observe that the order in which the variables are picked by the method of deferred decisions is independent of the clauses, it is just a random permutation of the n variables. Look at any one clause. For a clause, we decide in order whether each variable or its negation is in the clause. So for a particular clause and a particular triple i, j, k with i < j < k, the probability that the clause contains the i^{th} , the j^{th} and k^{th} literal (or their negations) in the order determined by deferred decisions is:

$$(1 - \frac{3}{n}) (1 - \frac{3}{n-1}) \cdots (1 - \frac{3}{n-i+2}) \frac{3}{n-i+1}$$

$$(1 - \frac{2}{n-i}) (1 - \frac{2}{n-i-1}) \cdots (1 - \frac{2}{n-j+2}) \frac{2}{n-j+1}$$

$$(1 - \frac{1}{n-j}) (1 - \frac{1}{n-j-1}) \cdots (1 - \frac{1}{n-k+2}) \frac{1}{n-k+1} = \frac{3}{n(n-1)(n-2)},$$

where, the $(1 - \cdots)$ factors are for not picking the current variable (or negation) to be included and the others are for including the current variable or is negation. Independence among clauses simply follows from the fact that we have never let the occurrence or nonoccurrence of any variable in any clause to influence our decisions on other clauses.

Now, we prove the lemma by appealing to the method of deferred decisions to generate the formula. $T_i = t$ if and only if the method of deferred decisions does not put the current literal at steps $1, 2, \ldots, t-1$ into the i th clause, but puts the negation of the literal at step t into it. Thus, the probability is precisely

$$\frac{1}{2} \left(1 - \frac{3}{n} \right) \left(1 - \frac{3}{n-1} \right) \cdots \left(1 - \frac{3}{n-t+2} \right) \frac{3}{n-t+1} \le \frac{3}{2(n-2)},$$

as claimed. Clearly the T_i are independent since again deferred decisions deals with different clauses independently.

Lemma 3.16 With probability 1 - o(1), no clause remains a 2 or 1-clause for $\Omega(\ln n)$ steps. I.e., once a 3-clause becomes a 2-clause, it is either satisfied or reduced to a 0-clause in $O(\ln n)$ steps.

Proof: Without loss of generality, again focus on Clause 1. Suppose it first becomes a 2-clause at step s_1 and remains a 2 or 1-clause until step s. Suppose $s - s_1 \ge c_2 \ln n$. Let r be the last time before s when there are no 2 or 1-clauses at all. Since at time 0, there are no 2 or 1-clauses, r is well-defined. We have $s - r \ge c_2 \ln n$. In the interval r to s, at each step, there is at least one 2 or 1-clause. Since SC always decreases the total number of 1 and 2-clauses by one whenever it is positive, we must have generated at least s - r new 2-clauses between r and s. Now define an indicator random variable for each 3-clause which has value one if the clause turns into a 2-clause between r and s. By Lemma 3.15 these variables are independent and the probability that a particular 3-clause turns into a 2-clause at a time t is at most 3/(2(n-2)). Summing over t between r and s, we get:

Prob (a 3-clause turns into a 2-clause during
$$[r, s]$$
) $\leq \frac{3(s-r)}{2(n-2)}$.

Since there are cn clauses in all, the expected sum of the indicator random variables is $cn\frac{3(s-r)}{2(n-2)} \approx \frac{3c(s-r)}{2}$. Note that 3c/2 < 1, which implies the arrival rate into the queue of 2 and 1-clauses is a constant strictly less than one. Using Chernoff bounds, the probability that more than s-r clauses turn into 2-clauses between r and s is at most $o(1/n^5)$. This is for one choice of a clause, one choice of s_1 and one choice each of r and s within $O(\ln n)$ of s_1 . Applying the union bound over $O(n^3)$ choices of clauses, O(n) choices of s_1 and $O(\ln n)^2$ choices of r and s, we get that the probability that any clause remains a 2 or 1-clause for $O(\ln n)$ steps is o(1).

Now suppose SC terminates in failure. Then at some point t, we have two clauses of the form w and \bar{w} . Let t_1 be the first time either of these two clauses became a 2-clause. We have $t - t_1 \in O(\ln n)$. Clearly until time t, neither of these two clauses is picked by SC. So, the literals which are set to true during this period are chosen independent of these clauses. Say the two clauses were w + x + y and $\bar{w} + u + v$ at the start. x, y, u, and v must all be negations of literals set to true during steps t_1 to t. So, there are only $O\left((\ln n)^4\right)$ choices for x, y, u, and v. There are O(n) choices of w, $O(n^2)$ choices of which two clauses of the input become these w and \bar{w} , and n choices for t_1 . Thus, there are $O\left(n^4(\ln n)^4\right)$ choices for these clauses. The probability of these choices is therefore $O\left(n^4(\ln n)^4/n^6\right) = o(1)$ as required.

3.1.6 The Emerging Graph

Returning to the G(n,p) graph model, consider G(n,p) as p grows. Starting with p=0, the graph has n vertices and no edges. As p increases and edges are added, a forest of trees emerges. For $p \in o(1/n)$ the graph is a forest of trees. We showed this by proving that for such p, almost surely, there are no cycles. When p becomes asymptotically equal to 1/n, cycles appear, but each component is either a tree or is unicyclic, i.e. the component contains at most one cycle, with no component having more than $\log n$ vertices. The number of components containing a single cycle is a constant independent of n. Thus, the graph consists of a forest of trees plus a few components that have a single cycle with

no component having more than $\log n$ vertices.

At p equal 1/n, a phase transition occurs in which a giant component emerges. The transition consists of a double jump. At p=1/n, components of $n^{2/3}$ vertices emerge, which are almost surely trees. Then at p=d/n, d>1, a true giant component emerges that has a number of vertices proportional to n. As p increases further, all non isolated vertices are absorbed into the giant component and at $p=\frac{1}{2}\frac{\ln n}{n}$ the graph consists only of isolated vertices plus a giant component. At $p=\frac{\ln n}{n}$ the graph becomes completely connected. By p=1/n, the graph is not only connected but is sufficiently dense that it has a clique of size $(2-\varepsilon)\log n$ for any $\varepsilon>0$. We prove many of these facts in this chapter.

The region p = d/n, d a constant, $d \le 1$.

Let x_m be the number of components of G that are trees with at least m vertices. Now

$$E(x_m) = \sum_{k=m}^{n} {n \choose k} k^{k-2} p^{k-1} (1-p)^{\binom{k}{2}-(k-1)} (1-p)^{k(n-k)}.$$

Recall the justification for a similar formula for connected components from the section on the threshold for graph connectivity. Given k vertices there are k^{k-2} possible ways to form a tree. Each of the k-1 edges of the tree is present with probability p. Each of the other $\binom{k}{2} - (k-1)$ edges among the k vertices of the tree is absent with probability 1-p and each of the k (n-k) edges from the k vertices of the tree to the remaining n-k vertices of the graph is absent with probability 1-p.

We now make a series of approximations to derive a formula for $E(x_m)$ assuming again that p = d/n with $d \le 1$.

$$(1-p)^{\binom{k}{2}-(k-1)+k(n-k)} = (1-p)^{-\frac{3}{2}k+1+(n-\frac{k}{2})k}$$

$$\cong \theta(1) \left[\left(1-\frac{d}{n}\right)^{n-\frac{k}{2}} \right]^k \cong \theta(1) \left[e^{\frac{kd}{2n}} e^{-d} \right]^k$$

Since $0 \le k \le n$, the term $\left(1 - \frac{d}{n}\right)^{-\frac{3}{2}k+1}$ is bounded above and below by a constant. In the limit as n goes to infinity, at k = 0, $\left(1 - \frac{d}{n}\right)^{-\frac{3}{2}k+1} = 1$ and at k = n, $\left(1 - \frac{d}{n}\right)^{-\frac{3}{2}k+1} = e^{\frac{3}{2}d}$. Thus $\left(1 - \frac{d}{n}\right)^{-\frac{3}{2}k+1}$ is $\theta(1)$ and it was replaced in the above equation by the $\theta(1)$ term.

Since $k! \cong \frac{k^{k+\frac{1}{2}}}{e^k}$, write $\binom{n}{k} = \frac{n(n-1)\cdots(n-k)}{k!} \cong \frac{n(n-1)\cdots(n-k)}{k^{k+\frac{1}{2}}} e^k$. Substituting into $E\left(x_m\right)$ (using the abbreviation \cong here to mean within a constant factor),

$$E(x_m) \cong \sum_{k=m}^n \frac{n(n-1)\cdots(n-k)}{k^{k+\frac{1}{2}}} e^k k^{k-2} \left(\frac{d}{n}\right)^{k-1} \left(\frac{e^{\frac{kd}{2n}}}{e^d}\right)^k$$
$$\cong \frac{n}{d} \sum_{k=m}^n \frac{n(n-1)\cdots(n-k)}{n^k} \frac{1}{k^{\frac{5}{2}}} \left[e^{\frac{dk}{2n}} de^{1-d}\right]^k.$$

Using $1 - \frac{x}{n} \le e^{-x/n}$,

$$\frac{n(n-1)\cdots(n-k)}{n^k} = \left(1 - \frac{1}{n}\right)\left(1 - \frac{2}{n}\right)\cdots\left(1 - \frac{k}{n}\right) \le \prod_{i=1}^k e^{-\frac{i}{n}} = e^{-\frac{k(k+1)}{2n}} \le e^{-\frac{k^2}{2n}}.$$

Thus,

$$E(x_m) \le \frac{1}{d} \frac{n}{k^2} e^{-\frac{k^2}{2n}} e^{\frac{dk^2}{2n}} (de^{1-d})^k.$$

Now for $d \le 1$, $\frac{1}{d}e^{\frac{(d-1)k^2}{2n}}$ is O(1). Thus,

$$E(x_m) = 0 \left(\sum_{k=m}^{n} \frac{n}{k^{\frac{5}{2}}} \left(de^{1-d} \right)^k \right).$$
 (3.2)

Theorem 3.17 In G(n,p) with $p \leq 1/n$, the tree components are almost surely of size $O(\log n)$.

Proof: From the discussion above, the expected number of components of G that are trees with at least m vertices is $E(x_m) \cong \sum_{k=m}^n \frac{n}{k^{5/2}} \left(de^{1-d}\right)^k$. For d < 1, it follows that $0 < de^{1-d} < 1$. To see this, let $f(d) = de^{1-d}$ where f(0) = 0, f(1) = 1, and $f' \neq 0$ for 0 < d < 1. Let $c = de^{1-d}$. Since c < 1, the summation is bounded by a constant times its first term., Thus, $E(x_m) = \theta(1) \frac{n}{m^{5/2}} c^m$ and if m grows asymptotically faster than $\log n$, c^m is smaller than 1/n and $E(x_m)$ goes to zero. Thus, for p < 1/n, all components that are trees have size $O(\log n)$.

For p = 1/n there is a phase transition in which a tree of size $n^{2/3}$ appears.

Theorem 3.18 For p = 1/n, the maximum size of a tree component is almost surely $O(n^{2/3})$. Also, for some constant c>0, the expected number of tree components of size at least $cn^{2/3}$ tends to a positive real.

Proof: For p = 1/n, $de^{1-d} = 1$ and from (3.2), the expected number of trees with at least m vertices is $\theta(1) n \sum_{k=m}^{n} \frac{1}{k^{5/2}}$. The sum, $\sum_{k=m}^{n} \frac{1}{k^{5/2}}$, is very close to $\int_{k=m}^{n} k^{-5/2} dk$ which is $(2/3)(m^{-3/2} - n^{-3/2}) = O(m^{-3/2})$. Thus, the expected number of trees of size at least m is less than or equal to $O(1) \frac{n}{m^{3/2}}$.

If m grows as a function of n and is asymptotically larger than $n^{2/3}$, then, $m^{3/2}$ is asymptotically greater than n and the expected number of trees of size at least m goes to zero. Thus, with high probability, there are no such components, proving the first statement. The second statement follows from the same calculation.

We have shown that for tree components, the maximum size component for p < 1/n is $\log n$ and for p = 1/n is order $n^{2/3}$. When $p \le 1/n$, almost all vertices are in trees (Theorem 3.11) and hence the maximum size tree is actually the maximum size component.

3.1.7 The Giant Component

When one looks at the connected components of large graphs that appear in various contexts, one observes that there is often one very large component. One example is a graph formed from a data base of protean interactions² where vertices correspond to proteins and edges correspond to pairs of proteins that interact. By an interaction one means two amino acid chains that bind to each other for a function. The graph has 2735 vertices and 3602 edges. At the time we looked at the data base, the associated graph had the number of components of various sizes shown in Table 1. There are a number of small components but only one component of size greater than 16 and that is a giant component of size 1851. As more proteins are added to the data base the giant component will grow even larger and eventually swallow up all the smaller components.

Size of component	1	2	3	4	5	6	7	8	9	10	11	12		15	16	• • •	1851
Number of components	48	179	50	25	14	6	4	6	1	1	1	0	0	0	1	0	1

Table 1: Size of components in the graph implicit in the database of interacting proteins.

The existence of a giant component is not unique to the graph produced from the protein data set. Take any data set that one can convert to a graph and it is likely that the graph will have a giant component provided that the ratio of edges to vertices is a small number greater than one. Table 2 gives two other examples. This phenomenon of the existence of a giant component in many real world graphs deserves study.

ftp://ftp.cs.rochester.edu/pub/u/joel/papers.lst

Vertices are papers and edges mean that two papers shared an author.

1	2	3	4	5	6	7	8	14	27488
2712	549	129	51	16	12	8	3	1	1

http://www.gutenberg.org/etext/3202

Vertices represent words and edges connect words that are synonyms of one another

	1	2	3	4	5	14	16	18	48	117	125	128	30242
Ì	7	1	1	1	0	1	1	1	1	1	1	1	1

Table 2: Size of components in two graphs constructed from data sets.

²Science 1999 July 30 Vol. 285 No. 5428 pp751-753.

Consider the random graph G(n, p) where p equals d/n, d a constant independent of n. Note that the expected degree of each vertex is d (actually it is d(n-1)/n which is very close to d for large n). Many large graphs have constant average degree, so this is an important range.

If d < 1, almost surely, each connected component of the graph is of size $O(\log n)$. At d = 1, the graph may have larger components, in fact, the expected number of components of size at least $\Omega(n^{2/3})$ is greater than one. This does not imply that almost surely there is such a component since the components may be concentrated on a small fraction of the graphs. For d > 1, the seminal result in random graph theory says that there is a unique giant component of size $\Omega(n)$ and all other components are of size $O(\log n)$. The overall process involves a phase transition at d = 1 where the sizes of the connected components grow from $O(\log n)$ with the emergence of the giant component that is of size $\Omega(n)$. The process involves a "double jump" where the size of components go from $O(\log n)$ to a number of components of size $\Omega(n)$ to a unique giant component of size $\Omega(n)$. More detailed studies are needed to see what happens at the critical point d = 1, i.e., when $d = 1 \pm o(1)$. Finally, note that we already showed that for $p \ge \frac{\log n}{n}$, the graph consists of a single connected component.

To compute the size of a connected component of G(n,p), do a breadth first search of a component starting from an arbitrary vertex and generate an edge only when the search process needs to know if the edge exists. Start at an arbitrary vertex and mark it discovered and unexplored. At a general step, select a discovered, but unexplored vertex v and explore it as follows. For each undiscovered vertex u, independently decide with probability p = d/n whether the edge (v, u) is in and if it is, mark u discovered and unexplored. After this, mark v explored. Discovered but unexplored vertices are called the frontier. The algorithm has found the entire connected component when the frontier becomes empty.

For each vertex u, other than the start vertex, the probability that u is undiscovered after the first i steps is precisely $(1 - \frac{d}{n})^i$. Let z_i be the number of vertices discovered in the first i steps of the search. The distribution of z_i is Binomial $\left(n - 1, 1 - \left(1 - \frac{d}{n}\right)^i\right)$.

Write
$$1 - \left(1 - \frac{d}{n}\right)^i$$
 as
$$1 - \left(1 - \frac{d}{n}\right)^{\frac{n}{d}} \frac{d}{n}i \approx 1 - e^{-\frac{d}{n}i}.$$

Thus, the expected value of z_i is $s \approx n \left(1 - e^{-\frac{d}{n}i}\right)$. At each unit of time, a vertex is marked as explored removing it from the frontier. Thus the expected size of the frontier after i steps of the search is

$$s - i = n \left(1 - e^{-\frac{d}{n}i} \right) - i$$

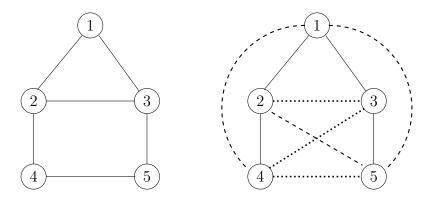


Figure 3.7: A graph (left) and the breadth first search of the graph (right). At vertex 1 the algorithm queried all edges. The solid edges are real edges, the dashed edges are edges that were queried but do not exist. At vertex 2 the algorithm queried all possible edges to vertices not yet discovered. The algorithm does not query whether the edge (2,3) exists since vertex 3 has already been discovered when the algorithm is at vertex 2. Potential edges not queried are illustrated with dotted edges

and the normalized expected size of the frontier is

$$\frac{s-i}{n} = 1 - e^{-\frac{d}{n}i} - \frac{i}{n}.$$

Replacing $\frac{i}{n}$ by x yields $f(x) = 1 - e^{-dx} - x$ where $f(x) = \frac{s-i}{n}$ is the normalized size of the frontier and x is the normalized time.

The search process stops when the frontier becomes empty. Initially, the expected size of the frontier grows as (d-1)i. As the fraction of discovered vertices increases, the expected rate of growth of newly discovered vertices decreases since many of the vertices adjacent to the vertex currently being searched have already been discovered. Once $\frac{d-1}{d}n$ vertices have been discovered, the growth of newly discovered vertices slows to one at each step. Eventually for d > 1, the growth of discovering new vertices drops below one per step and the frontier starts to shrink. For d < 1, (d-1)i, the expected size of the frontier is negative. The rate of growth is less than one even at the start.

Examining the expected normalized size of the frontier, $f(x) = 1 - e^{-dx} - x$, the second derivative of f(x) is always negative and thus f(x) is concave. The function f(x) is zero at x=0 and negative at x=1. Also f'(0) > 0. Thus, f(x) has a unique root Θ in (0,1] and is positive between x=0 and $x=\Theta$. For $x>\Theta$, f(x) is negative. For d=1, f(x) has a double root at x=0 and is negative for x>0.

Assume d > 1. The actual size of the frontier is a random variable. What is the probability that the actual size of the frontier will differ from the expected size of the frontier by a sufficient amount so that the actual size of the frontier is zero? To answer this, we need to understand the distribution of the number of discovered vertices after i steps.

d	Θ
1.2	0.311
1.4	0.512
1.6	0.642
1.8	0.732
2.0	0.799

Table 3: The normalized size Θ of the giant component in $G\left(n,\frac{d}{n}\right)$ for various values of the expected degree d.

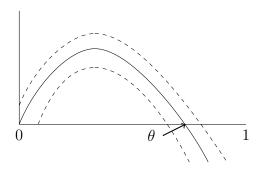


Figure 3.8: The solid curve is the expected size of the frontier. The two dashed curves indicate the range of possible values for the actual size of the frontier.

For small i, the probability that a vertex has been discovered is $1 - (1 - (d/n))^i \approx id/n$ and the binomial distribution for the number of discovered vertices, binomial $(n, \frac{id}{n})$, is well approximated by the Poisson distribution with the same mean id. The probability that a total of k vertices have been discovered in i steps is approximately $e^{-di} \frac{(di)^k}{k!}$. For a connected component to have exactly i vertices, the frontier must drop to zero for the first time at step i. A necessary condition is that exactly i vertices must have been discovered in the first i steps. The probability of this approximately equals

$$e^{-di} \frac{(di)^i}{i!} = e^{-di} \frac{d^i i^i}{i^i} e^i = e^{-(d-1)i} d^i = e^{-(d-1-\ln d)i}.$$

Note that for d > 1, $\ln d \le d - 1$ and hence $d - 1 - \ln d > 0$. Thus, this probability drops off exponentially with i. For $i > c \ln n$ and sufficiently large c, the probability that the breadth first search starting from a particular vertex terminates with a component of size i is o(1/n) as long as the Poisson approximation is valid. In the range of this approximation, the probability that breadth first search started from any vertex terminates with i vertices is o(1). Intuitively, if the component has not stopped growing within $\Omega(\ln n)$ steps, it is likely to continue to grow until it becomes much larger and the expected value of the size of the frontier again becomes small. While the expected value of the frontier is large the probability that the actual size will differ from the expected size sufficiently for the actual size of the frontier to be zero is vanishingly small.

For a small number i of steps, the probability distribution of the size of the set of discovered vertices at time i is $p(k) = e^{-di} \frac{(di)^k}{k!}$ and has expected value di. Thus, the expected size of the frontier is (d-1)i. For the frontier to be empty would require that the size of the set of discovered vertices be smaller than its expected value by (d-1)i. That is, the size of the set of discovered vertices would need to be di - (d-1)i = i. The probability of this is

$$e^{-di}\frac{(di)^i}{i!} = e^{-di}\frac{d^ii^i}{i^i}e^i = e^{-(d-1)i}d^i = e^{-(d-1-\ln d)i}$$

which drops off exponentially fast with i provided d > 1. Since $d - 1 - \ln d$ is some constant c > 0, the probability is e^{-ci} which for $i = \ln n$ is $e^{-c \ln n} = \frac{1}{n^c}$. Thus, with high probability, the largest small component in the graph is of size at most $\ln n$.

Illustration 3.1.

As the number i of steps becomes $\Omega(n)$, the approximation $\left(1-\frac{d}{n}\right)^i \approx 1-(id/n)$ is no longer valid. If i/n is near the point Θ at which the expected value of the size of the frontier is again zero, the expected value of the frontier increases linearly with $|i-\Theta n|$. For the actual frontier to be zero would require that the number of discovered vertices z_i deviates from its expected value by an amount proportional to the distance i is from Θn . For values of i near Θn , the binomial distribution for the number of discovered vertices can be approximated by a Gaussian distribution. The Gaussian distribution falls off exponentially fast with the square of the distance from its mean. Thus, for the frontier to be zero, the value of $k = |\Theta n - i|$ must be small. The distribution falls off proportional to $e^{-\frac{k^2}{\sigma^2}}$ where σ is the standard deviation which is proportional to \sqrt{n} . Thus, to have nonvanishing probability, k must be at most $O\left(\sqrt{n}\right)$. This implies that the giant component is in the range $\left[\Theta n - O\left(\sqrt{n}\right),\Theta n + O\left(\sqrt{n}\right)\right]$. Thus, either the component is small, $O\left(\log n\right)$, or it is the giant component in the range $\left[\Theta n - O\left(\sqrt{n}\right),\Theta n + O\left(\sqrt{n}\right)\right]$.

It is also the case that there is a unique giant component. The intuition for this is that if there were two large components, each of size $\Omega(n^{2/3})$ say, then there are $\Omega(n^{4/3})$ possible interconnections between them and the probability that they are all absent is small as we will prove.

We now prove that for d < 1, almost surely, no connected component is of size $\Omega(\ln n)$ and that for d > 1, no connected component is of size between $\Omega(\ln n)$ and O(n). To prove the existence of a giant component of size $\omega(n)$ when d > 1, we revisit our calculation of the number of connected components of each size k and argue that a constant fraction of vertices do not belong to components of size $O(\log n)$. Thus, there must be a giant component. Finally we argue that there is only one component of size greater than $n^{2/3}$.

Theorem 3.19 Let p=d/n with d < 1. The probability that G(n,p) has a component of size more than $\frac{4 \ln n}{(1-d)^2}$ is at most 1/n.

Proof: There is a connected component of size at least k containing a particular vertex v only if the breadth first search started at v has a nonempty frontier at all times up to k. Let z_k be the number of discovered vertices after k steps. Then the probability that v is in a connected component of size greater than or equal to k is less than or equal to $\operatorname{Prob}(z_k > k)$. Now z_k has distribution $\operatorname{Binomial}(n-1,1-(1-(d/n))^k)$. Since $(1-(d/n))^k \geq 1-(dk/n)$, the mean of $\operatorname{Binomial}(n,\frac{dk}{n})$ has mean dk, the mean of z_k is at most dk where d < 1. By a Chernoff bound, the probability that z_k is greater than k is at most e^{-k} . If $k \geq c \ln n$ for a suitably large c, then this probability is at most $1/n^2$. This bound is for a single vertex v. Multiplying by n for the union bound completes the proof.

Thus, when d < 1 almost surely there is no component of size larger than $\log n$. We now show that when d > 1 there is a gap in the size of components. That is, there is no component of size between $\log n$ and some constant times n and exactly one giant component of size a constant times n.

Theorem 3.20 Let p=d/n with d > 1.

- 1. There exist constants c_1 and c_2 such that the probability that there is a connected component of size between $c_1 \log n$ and $c_2 n$ is at most 1/n.
- 2. The number of vertices in components of size $O(\ln n)$ is at most cn in the limit for some c < 1. Thus, with probability 1 o(1), there is a connected component of size $\Omega(n)$.
- 3. The probability that there are two or more connected components, each of size more than $n^{2/3}$, is at most 1/n.
- **Proof:** (1) If a particular vertex v is in a connected component of size k, then the frontier of the breadth first search process started at v becomes empty for the first time at time k implying that $z_k = k$. Now z_k has distribution Binomial $(n-1, 1-(1-(d/n))^k)$. Provided $k < \frac{n}{d}$, $(1-\frac{d}{n})^k \le 1-\frac{kd}{n}$. Thus, $E(z_k) \ge kd$. Then by a Chernoff bound $\operatorname{Prob}(z_k = k) \le e^{-\Omega(k)}$. If k is greater than $c \ln n$ for some sufficiently large c, then $z_k = k$ with probability at most $1/n^3$ and this along with a union bound gives (1).
- (2) We prove that the number of vertices in components of size $O(\ln n)$ is at most cn in the limit for some c < 1. This by (1) implies that with high probability, there is a component of size $\Omega(n)$. Let x_k be the number of components of size k in G(n, p) for $k \in O(\ln n)$. Calculate the second moment of x_k as follows. For a subset of vertices S, "S is a cc" if the vertices of S form all of a connected component. Here $\mathbf{1}$ is used to denote

the indicator function of an event.

$$E(x_k^2) = E\left(\sum_{|S|=k} \mathbf{1}(S \text{ is a cc})\right)^2 = \sum_{\substack{|S|=k \ |T|=k}} E\left[\mathbf{1}(S \text{ is a cc}) \ \mathbf{1}(T \text{ is a cc})\right].$$

If S and T are not identical, but intersect, then both S and T cannot be connected components since they have a vertex in common. Such terms contribute zero. Thus, assume that S and T are either disjoint or identical. The terms from identical S and T together contribute $E(x_k)$. For disjoint S and T,

$$\operatorname{Prob}(S \text{ and } T \text{ are each a cc}) \leq \operatorname{Prob}(S \text{ is a cc})\operatorname{Prob}(T \text{ is a cc})(1-p)^{-k^2}.$$

In Prob(S is a cc), we stipulate that there be no edges from S to outside S and in Prob(T is a cc), we stipulate that there be no edges from T to outside T. The $(1-p)^{-k^2}$ arises since the absence of the k^2 edges from S to T was counted twice. Now

$$E(x_k^2) \le E(x_k) + (1-p)^{-k^2} \sum_{\substack{|S|=k\\|T|=k}} \operatorname{Prob}(S \text{ is a cc}) \operatorname{Prob}(T \text{ is a cc})$$

$$\le n + \frac{1}{1-pk^2} \Big(\sum_{|S|=k} \operatorname{Prob}(S \text{ is a cc}) \Big) \Big(\sum_{|T|=k} \operatorname{Prob}(T \text{ is a cc}) \Big)$$

$$\le n + (1+2\frac{dk^2}{n}) E^2(x_k)$$

implying

$$Var(x_k) = E(x_k^2) - E^2(x_k) \le n + \frac{2dk^2}{n}E^2(x_k).$$
(3.3)

Let $a = \left(1 + \frac{(\ln n)^2}{\sqrt{n}}\right) E(x_k) + n^{3/4}$. Then from Chebyshev inequality,

$$\operatorname{Prob}(x_k \ge a) \le \frac{\operatorname{Var}(x_k)}{a^2}.$$

Now $a^2 \ge n^{3/2} + \frac{(\ln n)^4}{n} E^2(x_k)$. Thus

$$\operatorname{Prob}\left(x_k \ge \left(1 + \frac{(\ln n)^2}{\sqrt{n}}\right) E(x_k) + n^{3/4}\right) \le \frac{\operatorname{Var}(x_k)}{n^{3/2} + \frac{(\ln n)^4}{n} E^2(X_k)} = o(1/\ln n).$$

Thus, with probability 1 - o(1),

$$\forall k \in O(\log n), \ x_k \le n^{3/4} + \left(1 + \frac{(\ln n)^2}{\sqrt{n}}\right) E(x_k).$$

From Lemma 3.7 using $k^2/n = O((\ln n)^2/n) = o(1)$,

$$E(x_k) \le \binom{n}{k} k^{k-2} \frac{d^{k-1}}{n^{k-1}} e^{-dk + d\frac{k^2}{n}} \le (1 + o(1)) \frac{n}{k! d} k^{k-2} d^k e^{k(-d + \frac{dk}{n})}.$$

Thus, with probability 1 - o(1), the number of vertices in connected components of size $O(\ln n)$, which is $\sum_{k=1}^{O(\ln n)} kx_k$, is at most

$$O(n^{3/4}(\ln n)^2) + (1 + o(1))\frac{n}{d}\sum_{k=1}^{\infty} \frac{k^{k-1}}{k!}(e^{-d}d)^k = (1 + o(1))\frac{n}{d}\sum_{k=1}^{\infty} \frac{k^{k-1}}{k!}(e^{-\rho}\rho)^k,$$

where, ρ is the unique value in (0,1) for which $\rho e^{-\rho} = de^{-d}$. Using Calculus, one can show that there is such a ρ . Now it is known that

$$\sum_{k=1}^{\infty} \frac{k^{k-1}}{k!} (e^{-\rho}\rho)^k = \rho,$$

however, these is no elementary proof of this surprising identity. Thus the number of vertices in all components of size $O(\ln n)$ is at most $\frac{n}{p}\rho$. This completes the proof of existence of the giant component. We now also give a more elementary proof that the number of vertices in all components of size $O(\ln n)$ is strictly less than n which suffices to establish the existence of a giant component. We show that $\sum_{k=1}^{\infty} \frac{k^{k-1}}{k!} (e^{-d}d)^k < 1$ which suffices. It is easy to check that $e^{-d}d < e^{-1}$. So, $\sum_{k=1}^{\infty} \frac{k^{k-1}}{k!} (e^{-d}d)^k \leq \sum_{k=1}^{\infty} \frac{k^{k-1}}{k!} e^{-k}$. Compute the values of the summand for k up to 10 and numerically bound their sum. For $k \geq 11$, use Stirling inequality to get $\frac{k^{k-1}}{k!} e^{-k} \leq \frac{1}{\sqrt{2\pi}k^{3/2}}$ and $\sum_{k=11}^{\infty} \frac{1}{k^{3/2}} \leq \int_{x=10}^{\infty} \frac{1}{x^{3/2}} dx = \frac{2}{\sqrt{10}}$. Adding the two parts gives the result.

The number of vertices in connected components of size k_0 or more is at most $cn \int_{k_0}^{O(\ln n)} x^{-3/2} dx$ which yields the last statement of (2).

(3) Suppose a pair of vertices u and v belong to two different connected components, each of size at least $n^{2/3}$. With high probability, they should have merged into one component producing a contradiction. First, run the breadth first search process starting at v for $\frac{1}{2}n^{2/3}$ steps. Since v is in a connected component of size $n^{2/3}$, there are $\Omega(n^{2/3})$ frontier vertices. (The expected size of the frontier continues to grow until some constant times n and the actual size does not differ significantly from the expected size. The size of the component also grows linearly with n. Thus, the frontier is of size $n^{\frac{2}{3}}$. See Exercise 3.52.) Further by the assumption, u does not belong to the connected component. Now temporarily stop the breadth first search tree of v and begin a breadth first search tree starting at u, again for $\frac{1}{2}n^{2/3}$ steps. It is important to understand that this change of order of building G(n,p) does not change the resulting graph. We can choose edges in any order since the order does not affect independence or conditioning. The breadth first search tree from u also will have $\Omega(n^{2/3})$ frontier vertices with high probability. Now grow the u tree further. The probability that none of the edges between the two frontier sets is encountered is $(1-p)^{\Omega(n^{4/3})} \leq e^{-\Omega(dn^{1/3})}$ which converges to zero. So almost surely, one of the edges is encountered and u and v end up in the same connected component. This argument shows for a particular pair of vertices u and v, the probability that they belong to different large connected components is very small. Now use the union bound to conclude that this does not happen for any of the $\binom{n}{2}$ pairs of vertices. The details are left to the reader.

Another method of proof that a giant component does form, i.e., essentially (2) of the Theorem 3.20 using Branching Processes is given in the next section.

3.2 Branching Processes

A branching process is a method for creating a random tree. Starting with the root node, each node has a probability distribution for the number of its children. The root of the tree denotes a parent and its descendants are the children with their descendants being the grand children. We call the children of the root the first generation, their children the second generation, and so on. Branching processes have obvious applications in population studies but also in exploring a connected component in a random graph.

We analyze a simple case of a branching process where the distribution of the number of children of each node is the same for every node in the tree. The basic question asked is what is the probability that the tree is finite, i.e., the probability that the branching process dies out? This is called the "extinction probability".

In the initial steps of a breadth first search in G(n,p) with $p=\frac{d}{n}$, the number of undiscovered nodes is approximately n. With this approximation, the distribution of the number of children of each node is binomial $(n,\frac{d}{n})$ and is the same for every node. This allows the use of the theory of branching processes to study the distribution of small components in G(n,p) whose sizes are $O(\log n)$ where the approximation that the number of undiscovered nodes is n remains valid.

The event that the branching process tree is finite corresponds to a small component of size $O(\ln n)$ in the G(n,p) model and the event that the branching process tree does not become extinct corresponds to a giant component. The theory gives the probability of extinction as well as the expected size of the components conditioned on extinction. Not surprisingly, the expected size of components conditioned on extinction is O(1). This says that in $G(n, \frac{d}{n})$, with d > 1, there is one giant component of size O(n), the rest of the components are $O(\ln n)$ in size and in fact, the expected size of the small components is O(1).

An important tool in our analysis of branching processes is the generating function. The generating function for a nonnegative integer valued random variable y, where p_i is the probability that y equals i, is $f(x) = \sum_{i=0}^{\infty} p_i x^i$. The reader not familiar with generating functions should consult the appendix.

Let the random variable z_j be the number of children in the j^{th} generation and let $f_j(x)$ be the generating function for z_j . Then $f_1(x) = f(x)$ is the generating function for

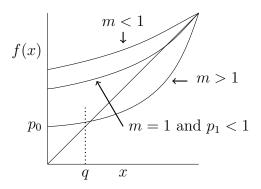


Figure 3.9: Illustration of root of equation f(x) = x in the interval [0,1].

the first generation. The generating function for the 2^{nd} generation is $f_2 = f(f(x))$. In general, the generating function for the $j+1^{st}$ generation is given by $f_{j+1}(x) = f_j(f(x))$. To see this, observe two things. First, the generating function for the sum of two identically distributed integer valued random variables x_1 and x_2 is the square of their generating function

$$f^{2}(x) = p_{0}^{2} + (p_{0}p_{1} + p_{1}p_{0}) x + (p_{0}p_{2} + p_{1}p_{1} + p_{2}p_{0}) x^{2} + \cdots$$

For $x_1 + x_2$ to have value zero, both x_1 and x_2 must have value zero, for $x_1 + x_2$ to have value one, exactly one of x_1 or x_2 must have value zero and the other have value one, and so on. In general, the generating function for the sum of i independent random variables, each with generating function f(x), is $f^i(x)$. The second observation is that the coefficient of x^i in $f_j(x)$ is the probability of there being i children in the j^{th} generation. If there are i children in the j^{th} generation $(z_j = i)$, the number of children in the $j + 1^{st}$ generation is the sum of i independent random variables each with generating function f(x). Thus the generating function for the $j + 1^{st}$ generation, given i children in the j^{th} , generation is $f^i(x)$. The generating function for the $j + 1^{st}$ generation is given by

$$f_{j+1}(x) = \sum_{i=0}^{\infty} \operatorname{Prob}(z_j = i) f^i(x).$$

If $f_j(x) = a_0 + a_1 x + \cdots$, then f_{j+1} is obtained by substituting $f^i(x)$ for x_i in $f_j(x)$.

Since f(x) and its iterates, f_2, f_3, \ldots , are all polynomials in x with nonnegative coefficients, f(x) and its iterates are all monotonically increasing and convex on the unit interval. Since the probabilities of the number of children of a node sum to one, if $p_0 < 1$, some coefficient of x to a power other than zero in f(x) is nonzero and f(x) is strictly increasing.

We now focus on roots of the equation f(x) = x in the interval [0,1]. The value x = 1 is always a root of the equation f(x) = x since $f(1) = \sum_{i=0}^{\infty} p_i = 1$. When is there a smaller

nonnegative root? The derivative of f(x) at x = 1 is $f'(1) = p_1 + 2p_2 + 3p_3 + \cdots$. Let m = f'(1). Thus, m is the expected number of children of a node. If m > 1, one might expect the tree to grow forever, since each node at time j is expected to have more than one child. But this does not imply that the probability of extinction is zero. In fact, if $p_0 > 0$, then with positive probability, the root will have no children and the process will become extinct right away. Recall that for $G(n, \frac{d}{n})$, the expected number of children is d, so the parameter m plays the role of d.

If m < 1, then the slope of f(x) at x = 1 is less than one. This fact along with convexity of f(x) implies that for $x \in [0,1)$, f(x) > x.

If m = 1 and $p_1 < 1$, then once again convexity implies that f(x) > x for $x \in [0, 1)$ and there is no root of f(x) in the interval [0, 1). If m = 1 and $p_1 = 1$, then f(x) is the straight line f(x) = x.

If m > 1, then the slope of f(x) is greater than the slope of x at x = 1. This fact, along with convexity of f(x), implies f(x) = x has a unique root in [0,1). When $p_0 = 0$, the root is at x = 0.

Let q be the smallest nonnegative root of the equation f(x) = x. For m < 1 and for m=1 and $p_0 < 1$, q equals one and for m > 1, q is strictly less than one. We shall see that the value of q is the extinction probability of the branching process and that 1-q is the immortality probability. That is, q is the probability that for some j, the number of children, z_j , in the j^{th} generation is zero. To see this, note that for m > 1, $\lim_{j \to \infty} f_j(x) = q$ for 0 < x < 1. Figure 3.10 illustrates the proof which is given in Lemma 3.21. Similarly note that when m < 1 or m = 1 with $p_0 < 1$, $f_j(x)$ approaches one as j approaches infinity.

Lemma 3.21 Assume m > 1. Let q be the unique root of f(x)=x in [0,1). In the limit as j goes to infinity, $f_i(x) = q$ for x in [0,1).

Proof: If $0 \le x \le q$, then $x < f(x) \le f(q)$ and iterating this inequality

$$x < f_1(x) < f_2(x) < \dots < f_j(x) < f(q) = q.$$

Clearly the sequence converges and it must converge to a fixed point where f(x) = x. Similarly, if $q \le x < 1$, then $f(q) \le f(x) < x$ and iterating this inequality

$$x > f_1(x) > f_2(x) > \dots > f_j(x) > f(q) = q$$

In the limit as j goes to infinity $f_j(x) = q$ for all $x, 0 \le x < 1$.

Recall that $f_j(x)$ is the generating function $\sum_{i=0}^{\infty} \operatorname{Prob}(z_j = i) x^i$. The fact that in the limit the generating function equals the constant q and is not a function of x says

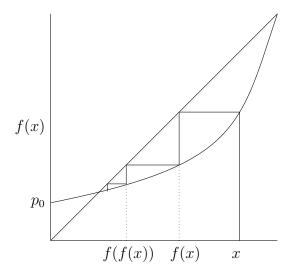


Figure 3.10: Illustration of convergence of the sequence of iterations $f_1(x), f_2(x), \ldots$ to q.

that $\operatorname{Prob}(z_j = 0) = q$ and $\operatorname{Prob}(z_j = i) = 0$ for all finite nonzero values of i. The remaining probability is the probability of a nonfinite component. Thus, when m > 1, q is the extinction probability and 1-q is the probability that z_j grows without bound, i.e., immortality.

Theorem 3.22 Consider a tree generated by a branching process. Let f(x) be the generating function for the number of children at each node..

- 1. If the expected number of children of each node is less than or equal to one, then the probability of extinction is one unless the probability of exactly one child is one.
- 2. If the expected number of children of each node is greater than one, then the probability of extinction is the unique solution to f(x) = x in [0, 1).

Proof: Let p_i be the probability of i children at each node. Then $f(x) = p_0 + p_1 x + p_2 x^2 + \cdots$ is the generating function for the number of children at each node and $f'(1) = p_1 + 2p_2 + 3p_3 + \cdots$ is the slope of f(x) at x = 1. Observe that f'(1) is also the expected number of children at each node.

Since the expected number of children at each node is the slope of f(x) at x = 1, if the expected number of children is less than or equal to one, the slope of f(x) at x = 1 is less than or equal to one and the unique root of f(x) = x in (0,1] is at x = 1 unless $p_1 = 1$ in which case f(x) = x and the tree is an infinite degree one chain. Thus if $p_1 \neq 1$ the probability of extinction is one. If the slope of f(x) at x = 1 is greater than one, then the probability of extinction is the unique solution to f(x) = x in [0,1).

A branching process with m < 1 or m=1 and $p_1 < 1$ dies out with probability one. If m=1 and $p_1 = 1$, then the branching process consists of an infinite chain with no fan out.

If m > 1 then it will die out with some probability less than one unless $p_0 = 0$ in which case it cannot die out since a node always has at least one descendent.

Note that the branching process corresponds to finding the size of a component in an infinite graph. In a finite graph, the probability distribution of descendants is not a constant as more and more vertices of the graph get discovered.

The simple branching process defined here either dies out or goes to infinity. In biological systems there are other factors since processes often go to stable populations. One possibility is that the probability distribution for the number of descendants of a child depends on the total population of the current generation.

Expected size of extinct families

We now consider the expected size of an extinct family and show that it is finite provided that $m \neq 1$. Note that at extinction, the size must be finite. However, the expected size at extinction could conceivably be infinite if the probability of dying out did not decay fast enough. To see this, let x be an integer valued random variable. Let p_i be the probability that x = i. If $\sum_{i=1}^{\infty} p_i = 1$, then with probability one, x will be finite.

However, the expected value of x may be infinite. That is, $\sum_{i=0}^{\infty} i p_i = \infty$. For example, if

for i > 0, $p_i = \frac{6}{\pi} \frac{1}{i^2}$, then $\sum_{i=1}^{\infty} p_i = 1$, but $\sum_{i=1}^{\infty} i p_i = \infty$. The value of the random variable x is always finite but its expected value is infinite. This does not happen in a branching process except in the special case where the slope m = f'(1) equals one and $p_1 \neq 1$

Lemma 3.23 If the slope m = f'(1) does not equal one, then the expected size of an extinct family is finite. If the slope m=1 and $p_1 = 1$, then the tree is an infinite degree one chain and there are no extinct families. If m=1 and $p_1 < 1$, then the expected size of the extinct family is infinite.

Proof: Let z_i be the random variable denoting the size of the i^{th} generation and let q be the probability of extinction. The probability of extinction for a tree with k children in the first generation is q^k since each of the k children has an extinction probability of q. Note that the expected size of z_1 , the first generation, over extinct trees will be smaller than the expected size of z_1 over all trees since when the root node has a larger number of children than average, the tree is more likely to be infinite.

By Bayes rule

$$P(z_1 = k | \text{extinction}) = P(z_1 = k) \frac{P(\text{extinction}|z_1 = k)}{P(\text{extinction})} = p_k \frac{q^k}{q} = p_k q^{k-1}.$$

Knowing the probability distribution of z_1 given extinction, allows us to calculate the expected size of z_1 given extinction.

$$E\left(z_{1}|extinction\right) = \sum_{k=0}^{\infty} k p_{k} q^{k-1} = f'\left(q\right)$$

We now prove using independence that the expected size of the i^{th} generation given extinction is

$$E(z_i|\text{extinction}) = (f'(q))^i$$
.

For i=2, z_2 is the sum of z_1 independent random variables, each independent of the random variable z_1 . So, $E(z_2|z_1=j)=E(\text{ sum of } j \text{ copies of } z_1)=jE(z_1)$. Summing over all values of j

$$E(z_2) = \sum_{j=1}^{\infty} E(z_2|z_1 = j) \operatorname{Prob}(z_1 = j) = \sum_{j=1}^{\infty} j E(z_1) \operatorname{Prob}(z_1 = j)$$
$$= E(z_1) \sum_{j=1}^{\infty} j \operatorname{Prob}(z_1 = j) = E^2(z_1).$$

Since $E(z_1|\text{extinction}) = f'(q)$, $E(z_2|\text{extinction}) = (f'(q))^2$. Similarly, $E(z_i|\text{extinction}) = (f'(q))^i$. The expected size of the tree is the sum of the expected sizes of each generation. That is,

Expected size of tree given extinction
$$= \sum_{i=0}^{\infty} E\left(\left(z_{i} | \text{extinction}\right)\right) = \sum_{i=0}^{\infty} \left(f'\left(q\right)\right)^{i} = \frac{1}{1 - f'\left(q\right)}.$$

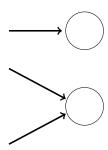
Thus, the expected size of an extinct family is finite since f'(q) < 1 provided $m \neq 1$.

The fact that f'(q) < 1 is illustrated in Figure 3.9. If m < 1, then q = 1 and f'(q) = m is less than one. If m > 1, then $q \in [0, 1)$ and again f'(q) < 1 since q is the solution to f(x) = x and f'(q) must be less than one for the curve f(x) to cross the line x. Thus, for m < 1 or m > 1, f'(q) < 1 and the expected tree size of $\frac{1}{1 - f'(q)}$ is finite. For m = 1 and $p_1 < 1$, one has q = 1 and thus f'(q) = 1 and the formula for the expected size of the tree diverges.

3.3 Nonuniform and Growth Models of Random Graphs

3.3.1 Nonuniform Models

So far we have considered the random graph G(n, p) in which all vertices have the same expected degree and showed that the degree is concentrated close to its expectation. However, large graphs occurring in the real world tend to have power law degree



Consider a graph in which half of the vertices are degree one and half are degree two. If a vertex is selected at random it is equally likely to be degree one or degree two. However, if we select an edge at random and walk to its endpoint, it is twice as likely to be degree two as degree one. In many graph algorithms, a vertex is reached by randomly selecting an edge and traversing the edge to reach an endpoint. In this case, the probability of reaching a degree i vertex is proportional to $i\lambda_i$ where λ_i is the fraction of vertices that are degree i.

Figure 3.11: Probability of encountering a degree d vertex when following a path in a graph

distributions. For a power law degree distribution, the number f(d) of vertices of degree d plotted as a function of d satisfies $f(d) \leq c/d^{\alpha}$, where α , the exponent of d, and c are constants.

To generate such graphs, we stipulate that there are f(d) vertices of degree d and choose uniformly at random from the set of graphs with this degree distribution. Clearly in this model the graph edges are not independent and this makes these random graphs harder to understand. But the question of when phase transitions occur in random graphs with arbitrary degree distributions is still of interest. In this section, we consider when a random graph with a nonuniform degree distribution has a giant component.

3.3.2 Giant Component in Random Graphs with Given Degree Distribution

Molloy and Reed address the issue of when a random graph with a nonuniform degree distribution has a giant component. Let λ_i be the fraction of vertices of degree i. There will be a giant component if and only $\sum_{i=0}^{\infty} i(i-2)\lambda_i > 0$.

To see intuitively that this is the correct formula, consider exploring a component of a graph starting from a given seed vertex. Degree zero vertices do not occur except in the case where the vertex is the seed. If a degree one vertex is encountered, then that terminates the expansion along the edge into the vertex. Thus, we do not want to encounter too many degree one vertices. A degree two vertex is neutral in that we come in one edge and go out the other. There is no net increase in the frontier. Vertices of degree i greater than two increase the frontier by i-2 edges. The vertex is entered by one of its edges and thus there are i-1 edges to new vertices in the frontier for a net gain of i-2. The $i\lambda_i$ in i (i-2) λ_i is proportional to the probability of reaching a degree i vertex and the i-2 accounts for the increase or decrease in size of the frontier when a degree i vertex is reached.

Example: Consider applying the Molloy Reed conditions to the G(n,p) model. The

summation $\sum_{i=0}^{n} i(i-2)p_i$ gives value zero precisely when p=1/n, the point at which the phase transition occurs. At p=1/n, the average degree of each vertex is one and there are n/2 edges. However, the actual degree distribution of the vertices is binomial where the probability that a vertex is of degree i is given by $p_i = \binom{n}{i} p^i (1-p)^{n-i}$. We now show that $\lim_{n\to\infty} \sum_{i=0}^n i(i-2)p_i = 0$ for $p_i = \binom{n}{i} p^i (1-p)^{n-i}$ when p=1/n.

$$\lim_{n \to \infty} \sum_{i=0}^{n} i(i-2) \binom{n}{i} \left(\frac{1}{n}\right)^{i} (1-\frac{1}{n})^{n-i}$$

$$= \lim_{n \to \infty} \sum_{i=0}^{n} i(i-2) \frac{n(n-1) \cdots (n-i+1)}{i! n^{i}} \left(1-\frac{1}{n}\right)^{n-i}$$

$$= \frac{1}{e} \lim_{n \to \infty} \sum_{i=0}^{n} i(i-2) \frac{n(n-1) \cdots (n-i+1)}{i! n^{i}} \left(\frac{n}{n-1}\right)^{i}$$

$$\leq \sum_{i=0}^{\infty} \frac{i(i-2)}{i!}$$

To see that $\sum_{i=0}^{\infty} \frac{i(i-2)}{i!} = 0$ note that

$$\sum_{i=0}^{\infty} \frac{i}{i!} = \sum_{i=1}^{\infty} \frac{i}{i!} = \sum_{i=1}^{\infty} \frac{1}{(i-1)!} = \sum_{i=0}^{\infty} \frac{1}{i!}$$

and

$$\sum_{i=0}^{\infty} \frac{i^2}{i!} = \sum_{i=1}^{\infty} \frac{i^2}{i!} = \sum_{i=1}^{\infty} \frac{i}{(i-1)!} = \sum_{i=0}^{\infty} \frac{i+1}{i!} = \sum_{i=0}^{\infty} \frac{i}{i!} + \sum_{i=0}^{\infty} \frac{1}{i!} = 2\sum_{i=0}^{\infty} \frac{1}{i!}.$$

Thus

$$\sum_{i=0}^{\infty} \frac{i(i-2)}{i!} = \sum_{i=0}^{\infty} \frac{i^2}{i!} - 2\sum_{i=0}^{\infty} \frac{i}{i!} = 0.$$

3.4 Growth Models

3.4.1 Growth Model Without Preferential Attachment

Many graphs that arise in the outside world started as small graphs that grew over time. In considering a model for such graphs there are many ways in which to select the vertices for attaching a new edge. One is to select two vertices uniformly at random from the set of existing vertices. Another is to select two vertices with probability proportional to their degree. This latter method is referred to as preferential attachment. A variant of this method would be to add a new vertex at each unit of time and with probability δ add an edge where one end of the edge is the new vertex and the other end is a vertex selected with probability proportional to its degree.

Consider a growth model for a random graph without preferential attachment. Start with zero vertices at time zero. At each unit of time a new vertex is created and with probability δ , two vertices chosen at random are joined by an edge. The two vertices may already have an edge between them. In this case, we will add another edge. So, the resulting structure is a multi-graph, rather then a graph. But since at time t, there are t vertices and in expectation only $O(\delta t)$ edges where there are t^2 pairs of vertices, it is very unlikely that there will be multiple edges.

The degree distribution for this growth model is calculated as follows. The number of vertices of degree k at time t is a random variable. Let $d_k(t)$ be the expectation of the number of vertices of degree k at time t. The number of isolated vertices increases by one at each unit of time and decreases by the number of isolated vertices, b(t), that are picked to be end points of the new edge. If an edge is added at time t, b(t) can take on values 0,1, or 2. Taking expectations,

$$d_0(t+1) = d_0(t) + 1 - E(b(t)).$$

Now b(t) is the sum of two 0-1 valued random variables whose values are the number of degree zero vertices picked for each end point of the new edge. Even though the two random variables are not independent, the expectation of b(t) is the sum of the expectations of the two variables and is $2\delta \frac{d_0(t)}{t}$. Thus,

$$d_0(t+1) = d_0(t) + 1 - 2\delta \frac{d_0(t)}{t}.$$

The number of degree k vertices increases whenever a new edge is added to a degree k-1 vertex and decreases when a new edge is added to a degree k vertex. Reasoning as above,

$$d_k(t+1) = d_k(t) + 2\delta \frac{d_{k-1}(t)}{t} - 2\delta \frac{d_k(t)}{t}.$$
(3.4)

Note that this formula, as others in this section, is not quite precise. For example, the same vertex may be picked twice, so that the new edge is a self-loop. For k << t, this problem contributes a miniscule error. Restricting k to be a fixed constant and letting $t \to \infty$ in this section avoids these problems. Assume that the above equations are exactly valid. Clearly, $d_0(1) = 1$ and $d_1(1) = d_2(1) = \cdots = 0$. By induction on t, there is a unique solution to Equation 3.4, since given $d_k(t)$ for all k, the equation determines all $d_k(t+1)$ for all k. There is a solution of the form $d_k(t) = p_k t$, where p_k depends only on k and not on t, provided k is fixed and $t \to \infty$. Again, this is not precisely true, $d_1(1) = 0$ and $d_1(2) > 0$ clearly contradict the existence of a solution of the form $d_1(t) = p_1 t$.

Set
$$d_k(t) = p_k t$$
. Then,
$$(t+1) p_0 = p_0 t + 1 - 2\delta \frac{p_0 t}{t}$$

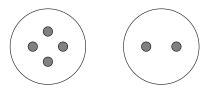


Figure 3.12: In selecting a component at random, each of the two components is equally likely to be selected. In selecting the component containing a random vertex, the larger component is twice as likely to be selected.

$$p_0 = 1 - 2\delta p_0$$
$$p_0 = \frac{1}{1 + 2\delta}$$

and

$$(t+1) p_k = p_k t + 2\delta \frac{p_{k-1}t}{t} - 2\delta \frac{p_k t}{t}$$
$$p_k = 2\delta p_{k-1} - 2\delta p_k$$

$$p_{k} = \frac{2\delta}{1 + 2\delta} p_{k-1}$$

$$= \left(\frac{2\delta}{1 + 2\delta}\right)^{k} p_{0}$$

$$= \frac{1}{1 + 2\delta} \left(\frac{2\delta}{1 + 2\delta}\right)^{k}.$$
(3.5)

Thus, the model gives rise to a graph with a degree distribution that falls off exponentially fast with degree.

The generating function for component size

Let $n_k(t)$ be the expected number of components of size k at time t. Then $n_k(t)$ is proportional to the probability that a randomly picked component is of size k. This is not the same as picking the component containing a randomly selected vertex (see Figure 3.12). Indeed the probability that the size of the component containing a randomly picked vertex is k is proportional to $kn_k(t)$. We will show that there is a solution for $n_k(t)$ of the form $a_k t$ where a_k is a constant independent of t. After showing this, we focus on the generating function g(x) for the numbers $ka_k(t)$ and use the generating function g(x) to find the threshold for giant components.

Consider $n_1(t)$, the expected number of isolated vertices at time t. At each unit of time, an isolated vertex is added to the graph and an expected $\frac{2\delta n_1(t)}{t}$ many isolated

vertices are chosen for attachment and thereby leave the set of isolated vertices. Thus

$$n_1(t+1) = n_1(t) + 1 - 2\delta \frac{n_1(t)}{t}.$$

For k > 1, $n_k(t)$ increases when two smaller components whose sizes sum to k are joined by an edge and decreases when a vertex in a component of size k is chosen for attachment. The probability that a vertex selected at random will be in a size k component is $\frac{kn_k(t)}{t}$. Thus

$$n_k(t+1) = n_k(t) + \delta \sum_{j=1}^{k-1} \frac{j n_j(t)}{t} \frac{(k-j) n_{k-j}(t)}{t} - 2\delta \frac{k n_k(t)}{t}.$$

To be precise one needs to consider the actual number of components of various sizes, rather than the expected numbers. Also, if both vertices at the end of the edge are in the same k-vertex component, then $n_k(t)$ does not go down as claimed. These small inaccuracies can be ignored.

Consider solutions of the form $n_k(t) = a_k t$. Solving for a_k yields $a_1 = \frac{1}{1+2\delta}$ and $a_k = \frac{\delta}{1+2k\delta} \sum_{j=1}^{k-1} j(k-j) a_j a_{k-j}$. The quantity a_k is proportional to the probability that a component selected at random is of size k but is not actually a probability. The quantity ka_k , however, is the probability that a randomly chosen vertex is in a component of size k. Thus, $\sum_{k=0}^{\infty} ka_k$ is the probability that a randomly chosen vertex is in a finite size component where finite here means a constant independent of t where t is growing to infinity. The sum $\sum_{k=0}^{\infty} ka_k$ may be less than 1, in which case, there are nonfinite size components whose sizes are growing with t.

Consider the generating function g(x) for the distribution of component sizes where the coefficient of x^k is the probability that a vertex chosen at random is in a component of size k.

$$g(x) = \sum_{k=1}^{\infty} k a_k x^k$$

Now, $g(1) = \sum_{k=0}^{\infty} ka_k$ is the probability that a randomly chosen vertex is in a finite sized component. For $\delta = 0$, this is clearly one, since all vertices are in components of size one. On the other hand, for $\delta = 1$, the vertex created at time one has expected degree $\log n$, so it is in a nonfinite size component. This implies that for $\delta = 1$, g(1) < 1 and there is a nonfinite size component. Assuming continuity, there is a $\delta_{critical}$ above which g(1) < 1. From the formula for the $a_i's$, we derive the differential equation

$$g = -2\delta x g' + 2\delta x g g' + x$$

and then use the equation for g to determine the value of δ at which the phase transition for the appearance of a nonfinite sized component occurs.

Derivation of g(x)

From

$$a_1 = \frac{1}{1 + 2\delta}$$

and

$$a_k = \frac{\delta}{1 + 2k\delta} \sum_{j=1}^{k-1} j(k-j) a_j a_{k-j}$$

derive the equations

$$a_1(1+2\delta) - 1 = 0$$

and

$$a_k (1 + 2k\delta) = \delta \sum_{j=1}^{k-1} j(k-j)a_j a_{k-j}$$

for $k \geq 2$. The generating function is formed by multiplying the k^{th} equation by kx^k and summing over all k. This gives

$$-x + \sum_{k=1}^{\infty} k a_k x^k + 2\delta x \sum_{k=1}^{\infty} a_k k^2 x^{k-1} = \delta \sum_{k=1}^{\infty} k x^k \sum_{j=1}^{k-1} j(k-j) a_j a_{k-j}.$$

Note that

$$g(x) = \sum_{k=1}^{\infty} k a_k x^k$$
 and $g'(x) = \sum_{k=1}^{\infty} a_k k^2 x^{k-1}$.

Thus

$$-x + g(x) + 2\delta x g'(x) = \delta \sum_{k=1}^{\infty} k x^k \sum_{j=1}^{k-1} j(k-j) a_j a_{k-j}.$$

Working with the right hand side

$$\delta \sum_{k=1}^{\infty} kx^k \sum_{j=1}^{k-1} j(k-j) a_j a_{k-j} = \delta x \sum_{k=1}^{\infty} \sum_{j=1}^{k-1} j(k-j) (j+k-j) x^{k-1} a_j a_{k-j}.$$

Now breaking the j + k - j into two sums gives

$$\delta x \sum_{k=1}^{\infty} \sum_{j=1}^{k-1} j^2 a_j x^{j-1} (k-j) a_{k-j} x^{k-j} + \delta x \sum_{k=1}^{\infty} \sum_{j=1}^{k-1} j a_j x^j (k-j)^2 a_{k-j} x^{k-j-1}.$$

Notice that the second sum is obtained from the first by substituting k-j for j and that both terms are $\delta x g' g$. Thus

$$-x + g(x) + 2\delta x g'(x) = 2\delta x g'(x)g(x).$$

Hence

$$g' = \frac{1}{2\delta} \frac{1 - \frac{g}{x}}{1 - g}.$$

Phase transition for nonfinite components

The generating function g(x) contains information about the finite components of the graph. A finite component is a component of size $1, 2, \ldots$ which does not depend on t. Observe that $g(1) = \sum_{k=0}^{\infty} ka_k$ and hence g(1) is the probability that a randomly chosen vertex will belong to a component of finite size. If g(1) = 1 there are no nonfinite components. When $g(1) \neq 1$, then 1 - g(1) is the expected fraction of the vertices that are in nonfinite components. Potentially, there could be many such nonfinite components. But an argument similar to Part (4) of Theorem 3.20 concludes that two fairly large components would merge into one. Suppose there are two connected components at time t, each of size at least, say, $t^{4/5}$. Consider the earliest created $\frac{1}{2}t^{4/5}$ vertices in each part. These vertices must have lived for at least $\frac{1}{2}t^{4/5}$ time after creation. At each time, the probability of an edge forming between two such vertices, one in each component is at least $\delta\Omega(t^{-2/5})$ and so the probability that no such edge formed is at most $(1 - \delta t^{-2/5})^{t^{4/5}/2} \leq e^{-\Omega(\delta t^{2/5})} \to 0$. So with high probability, such components would have merged into one. But this still leaves open the possibility of many components of size t^{ε} , $(\ln t)^2$, or some other slowly growing function of t.

We now calculate the value of δ at which the phase transition for a nonfinite component occurs. Recall that the generating function for g(x) satisfies

$$g'(x) = \frac{1}{2\delta} \frac{1 - \frac{g(x)}{x}}{1 - g(x)}.$$

If δ is greater than some $\delta_{critical}$, then $g(1) \neq 1$. In this case the above formula simplifies with 1 - g(1) canceling from the numerator and denominator, leaving just $1/(2\delta)$. Since ka_k is the probability that a randomly chosen vertex is in a component of size k, the average size of the finite components is $g'(1) = \sum_{k=1}^{\infty} k^2 a_k$. Now, g'(1) is given by

$$g'(1) = \frac{1}{2\delta} \tag{3.6}$$

for all δ greater than $\delta_{critical}$. If δ is less than $\delta_{critical}$, then all vertices are in finite components. In this case g(1) = 1 and both the numerator and the denominator approach zero. Appling L'Hopital's rule

$$\lim_{x \to 1} g'(x) = \frac{1}{2\delta} \left. \frac{\frac{xg'(x) - g(x)}{x^2}}{\frac{x^2}{g'(x)}} \right|_{x=1}$$

or

$$(g'(1))^2 = \frac{1}{2\delta}(g'(1) - g(1)).$$

The quadratic $(g'(1))^2 - \frac{1}{2\delta}g'(1) + \frac{1}{2\delta}g(1) = 0$ has solutions

$$g'(1) = \frac{\frac{1}{2\delta} \pm \sqrt{\frac{1}{4\delta^2} - \frac{4}{2\delta}}}{2} = \frac{1 \pm \sqrt{1 - 8\delta}}{4\delta}.$$
 (3.7)

The two solutions given by (3.7) become complex for $\delta > 1/8$ and thus can be valid only for $0 \le \delta \le 1/8$. For $\delta > 1/8$, the only solution is $g'(1) = \frac{1}{2\delta}$ and a nonfinite component exists. As δ is decreased, at $\delta = 1/8$ there is a singular point where for $\delta < 1/8$ there are three possible solutions, one from (3.6) which implies a giant component and two from (3.7) which imply no giant component. To determine which one of the three solutions is valid, consider the limit as $\delta \to 0$. In the limit all components are of size one since there are no edges. Only (3.7) with the minus sign gives the correct solution

$$g'(1) = \frac{1 - \sqrt{1 - 8\delta}}{4\delta} = \frac{1 - \left(1 - \frac{1}{2}8\delta - \frac{1}{4}64\delta^2 + \cdots\right)}{4\delta} = 1 + 4\delta + \cdots = 1.$$

In the absence of any nonanalytic behavior in the equation for g'(x) in the region $0 \le \delta < 1/8$, we conclude that (3.7) with the minus sign is the correct solution for $0 \le \delta < 1/8$ and hence the critical value of δ for the phase transition is 1/8. As we shall see this is different from the static case.

As the value of δ is increased, the average size of the finite components increase from one to

$$\left. \frac{1 - \sqrt{1 - 8\delta}}{4\delta} \right|_{\delta = 1/8} = 2$$

when δ reaches the critical value of 1/8. At $\delta = 1/8$, the average size of the finite components jumps to $\frac{1}{2\delta}|_{\delta=1/8} = 4$ and then decreases as $\frac{1}{2\delta}$ as the giant component swallows up the finite components starting with the larger components.

Comparison to static random graph

Consider a static random graph with the same degree distribution as the graph in the growth model. Again let p_k be the probability of a vertex being of degree k. From (3.5)

$$p_k = \frac{(2\delta)^k}{(1+2\delta)^{k+1}} \ .$$

Recall the Molloy Reed analysis of random graphs with given degree distributions which asserts that there is a phase transition at $\sum_{i=0}^{\infty} i(i-2)p_i = 0$. Using this, it is easy to see that a phase transition occurs for $\delta = 1/4$. For $\delta = 1/4$,

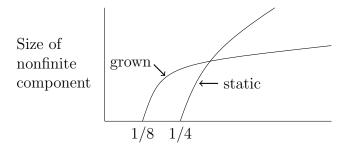


Figure 3.13: Figure obtained by integrating g'.

$$p_k = \frac{(2\delta)^k}{(1+2\delta)^{k+1}} = \frac{\left(\frac{1}{2}\right)^k}{\left(1+\frac{1}{2}\right)^{k+1}} = \frac{\left(\frac{1}{2}\right)^k}{\frac{3}{2}\left(\frac{3}{2}\right)^k} = \frac{2}{3}\left(\frac{1}{3}\right)^k$$

and

$$\sum_{i=0}^{\infty} i(i-2)\frac{2}{3} \left(\frac{1}{3}\right)^i = \frac{2}{3} \sum_{i=0}^{\infty} i^2 \left(\frac{1}{3}\right)^i - \frac{4}{3} \sum_{i=0}^{\infty} i \left(\frac{1}{3}\right)^i = \frac{2}{3} \times \frac{3}{2} - \frac{4}{3} \times \frac{3}{4} = 0.$$

Recall that
$$1 + a + a^2 + \dots = \frac{1}{1-a}$$
, $a + 2a^2 + 3a^3 + \dots = \frac{a}{(1-a)^2}$, and $a + 4a^2 + 9a^3 + \dots = \frac{a(1+a)}{(1-a)^3}$.

See references at end of the section for calculating the size S_{static} of the giant component in the static graph. The result is

$$S_{static} = \begin{cases} 0 & \delta \leq \frac{1}{4} \\ 1 - \frac{1}{\delta + \sqrt{\delta^2 + 2\delta}} & \delta > \frac{1}{4} \end{cases}$$

3.4.2 A Growth Model With Preferential Attachment

Consider a growth model with preferential attachment. At each time unit, a vertex is added to the graph. Then with probability δ an edge is attached to the new vertex and to a vertex selected at random with probability proportional to its degree.

Let $d_i(t)$ be the expected degree of the i^{th} vertex at time t. The sum of the degrees of all vertices at time t is $2\delta t$ and thus the probability that an edge is connected to vertex i at time t is $\frac{d_i(t)}{2\delta t}$. The degree of vertex i is governed by the equation

$$\frac{\partial}{\partial t}d_i(t) = \delta \frac{d_i(t)}{2\delta t} = \frac{d_i(t)}{2t}$$

where δ is the probability that an edge is added at time t and $\frac{d_i(t)}{2\delta t}$ is the probability that the vertex i is selected for the end point of the edge.

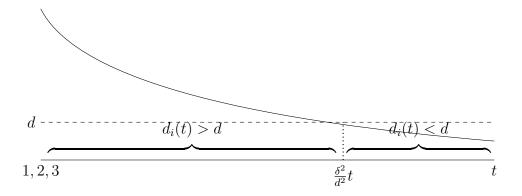


Figure 3.14: Illustration of degree of i^{th} vertex at time t. At time t, vertices numbered 1 to $\frac{\delta^2}{d^2}t$ have degrees greater than d.

The two in the denominator governs the solution which is of the form $at^{\frac{1}{2}}$. The value of a is determined by the initial condition $d_i(t) = \delta$ at t = i. Thus, $\delta = ai^{\frac{1}{2}}$ or $a = \delta i^{-\frac{1}{2}}$. Hence $d_i(t) = \delta \sqrt{\frac{t}{i}}$.

Next, we determine the probability distribution of vertex degrees. Now $d_i(t)$ is less than d provided $i > \frac{\delta^2}{d^2}t$. The fraction of the t vertices at time t for which $i > \frac{\delta^2}{d^2}t$ and thus that the degree is less than d is $1 - \frac{\delta^2}{d^2}$. Hence, the probability that a vertex has degree less than d is $1 - \frac{\delta^2}{d^2}$. The probability density P(d) satisfies

$$\int_{0}^{d} P(d)\partial d = \text{Prob}(degree < d) = 1 - \frac{\delta^{2}}{d^{2}}$$

and can be obtained from the derivative of Prob(degree < d).

$$P(d) = \frac{\partial}{\partial d} \left(1 - \frac{\delta^2}{d^2} \right) = 2 \frac{\delta^2}{d^3},$$

a power law distribution.

3.5 Small World Graphs

In the 1960's, Stanley Milgram carried out an experiment that indicated that any two individuals in the United States were connected by a short sequence of acquaintances. Milgram would ask a source individual, say in Nebraska, to start a letter on its journey to a target individual in Massachusetts. The Nebraska individual would be given basic information about the target including his address and occupation and asked to send the letter to someone he knew on a first name basis who was closer to the target individual in order to transmit the letter to the target in as few steps as possible. Each person receiving the letter would be given the same instructions. In successful experiments it would take

on average five to six steps for a letter to reach its target. This research generated the phrase "six degrees of separation" along with substantial research in social science on the inter connections between people. Surprisingly there was no work on how to find the short paths using only local information.

In many situations, phenomena are modeled by graphs whose edges can be partitioned into local and long distance. We adopt a simple model of a directed graph due to Kleinberg having local and long distance edges. Consider a 2-dimensional $n \times n$ grid where each vertex is connected to the four adjacent vertices. In addition to these local edges, there is one long distance edge out of each vertex. The probability that the long distance edge from vertex u terminates at $v, v \neq u$, is a function of the distance d(u, v) from u to v. Here distance is measured by the shortest path consisting only of local grid edges. The probability is proportional to $1/d^{r}(u,v)$ for some constant r. This gives a one parameter family of random graphs. For r equal zero, $1/d^0(u,v)=1$ for all u and v and thus the end of the long distance edge at u is uniformly distributed over all vertices v independent of distance. As r increases the expected length of the long distance edge decreases. As r approaches infinity, there are no long distance edges and thus no paths shorter than that of the lattice path. What is interesting is that for r less than two, there are always short paths but no local algorithm to find them. A local algorithm is an algorithm that is only allowed to remember the source, the destination and its current location and can query the graph to find the long-distance edge at the current location. Based on this information, it decides the next vertex on the path.

The difficulty is that for r < 2, the end points of the long distance edges tend to be uniformly distributed over the vertices of the grid and it is unlikely on a short path to encounter a long distance edge whose end point is close to the destination. When r equals two, there are short paths and the simple algorithm that always selects the edge that takes you closest to the destination will find a short path. For r greater than two, again there is no local algorithm to find a short path; indeed, we will show that with high probability, there are no short paths at all.

The probability that the long distance edge from u goes to v is proportional to $d^{-r}(u,v)$. Note that the constant of proportionality will vary with the vertex u depending on where u is relative to the border of the $n \times n$ grid. However, the number of vertices at distance exactly k from u is at most 4k and for $k \leq n/2$ is at least 2k. Let $c_r(u) = \sum_v d^{-r}(u,v)$ be the normalizing constant. It is the inverse of the constant of proportionality.

For r > 2 the normalizing constant $c_r(u)$ is lower bounded by

$$c_r(u) = \sum_v d^{-r}(u, v) \ge \sum_{k=1}^{n/2} (2k)k^{-r} = 2\sum_{k=1}^{n/2} k^{1-r}.$$

Since r > 2 the summation converges to a constant and $c_r(u) \ge \theta(1)$.

r < 2 The ends of long distance edges tend to be uniformly distributed. Short paths exist but a polylog length path is unlikely to encounter a long distance edge whose end point is close to the destination.

r=2 Selecting the edge with end point closest to the destination finds a short path.

r > 2 The lengths of long distance edges tend to be short so the probability of encountering a sufficiently long, long-distance edge is too low.

Figure 3.15: Effects of different values of r on the expected length of long distance edges and the ability to find short paths.

For r=2 the normalizing constant $c_r(u)$ is upper bounded by

$$c_r(u) = \sum_v d^{-r}(u, v) \le \sum_{k=1}^{2n} (4k)k^{-2} \le 4\sum_{k=1}^{2n} \frac{1}{k} = \theta(\ln n).$$

For r < 2, the normalizing constant $c_r(u)$ is lower bounded by

$$c_r(u) = \sum_{v} d^{-r}(u, v) \ge \sum_{k=1}^{n/2} (2k)k^{-r} \ge \sum_{k=n/4}^{n/2} k^{1-r} \ge \frac{n}{4}\theta(n^{1-r}) = \theta(n^{2-r}).$$

No short paths exist for the r > 2 case.

For at least one half of the pairs of vertices, the distance between the vertices is greater than or equal to n/4. For points s and t that are far apart, there almost surely is no short path. We first show that the expected number of edges of length greater than $n^{\frac{r+2}{2r}}$ goes to zero and thus by the first moment method, almost surely there are no such edges. Thus, if s and t are distance n/4 or more apart, any path between them must have at least $\frac{1}{4}n/n^{\frac{r+2}{2r}} = \frac{1}{4}n^{\frac{r-2}{2r}}$ edges and so there is no polylog length path.

To see that the expected number of edges of length greater than $n^{\frac{r+2}{2r}}$ goes to zero, note that the probability of an edge from u to v is proportional to $d^{-r}(u,v)$ where the constant of proportionality is upper bounded by a constant. Thus, the probability that an edge is of length greater than or equal to $n^{\frac{r+2}{2r}}$ is bounded by $\Theta\left(\left(n^{\frac{r+2}{2r}}\right)^{-r}\right) = \Theta\left(n^{-(\frac{r+2}{2})}\right)$. Since there are n^2 edges, the expected number of edges of length at least $n^{\frac{r+2}{2r}}$ is at most $\Theta\left(n^2n^{-\frac{(r+2)}{2}}\right) = \Theta\left(n^{\frac{2-r}{2}}\right)$ which for r>2 goes to zero. Thus, almost surely, there are no such edges.

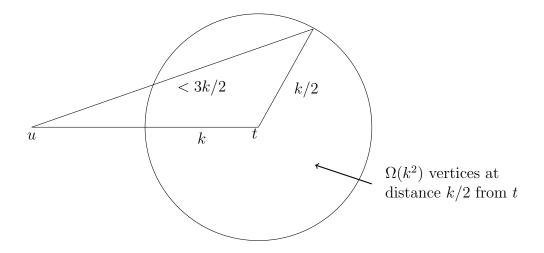


Figure 3.16: Small worlds.

An algorithm for the r = 2 case

For r=2, the local algorithm that selects the edge that ends closest to the destination t finds a polylog length path. Suppose at some point, the algorithm is at a vertex u at distance k from t. Then within an expected $O(\ln n)$ steps, the algorithm reaches a point at distance at most k/2. The reason is that there are $\Omega(k^2)$ vertices at distance at most k/2 from t. Each of these vertices is at distance at most k+k/2=O(k) from u. (See Figure 3.16.) The probability that the long-distance edge from u goes to one of these vertices is at least

$$\Omega(k^2k^{-r}/(\ln n)) = \Omega(1/\ln n).$$

(Recall that the normalizing constant is upper bounded by $\Theta(\ln n)$ and hence the constant of proportionality is $\Omega(1/\ln n)$.)

Consider $\Omega((\ln n)^2)$ steps of the path from u. The long-distance edges from the points visited at these steps are chosen independently and each has probability $\Omega(1/\ln n)$ of reaching within k/2 of t. The probability that none of them does is

$$(1 - \Omega(1/\ln n))^{c(\ln n)^2} = O(e^{-n}) = O(1/n)$$

for a suitable choice of constants. Thus the distance to t is halved every $O((\ln n)^2)$ steps and the algorithm reaches t in an expected $O((\ln n)^3)$ steps.

Local algorithm cannot find short paths for the r < 2 case

We now prove for r < 2 that no local polylog time algorithm exists for finding a short path. To illustrate the proof, we first describe it for the special case r = 0 and then give

the proof for the case r < 2.

When r = 0, all vertices are equally likely to be the end point of a long distance edge. Thus, the probability of a long distance edge hitting one of the n vertices that are within distance \sqrt{n} of the destination is 1/n. Along a path of length \sqrt{n} , the probability that we do not encounter such an edge is $(1 - 1/n)^{\sqrt{n}}$. Now

$$\lim_{n\to\infty} \left(1 - \frac{1}{n}\right)^{\sqrt{n}} = \lim_{n\to\infty} \left(1 - \frac{1}{n}\right)^{n\frac{1}{\sqrt{n}}} = \lim_{n\to\infty} e^{-\frac{1}{\sqrt{n}}} = 1$$

Since with probability 1/2 our starting point is at distance at least n/4 from the destination and in \sqrt{n} steps we will not encounter an edge taking us to within distance \sqrt{n} of the destination, at least half of the time the path length will be at least \sqrt{n} . Thus the expected time is at least $\frac{1}{2}\sqrt{n}$ and hence not in polylog time.

For the general r < 2 case, we show that a local algorithm cannot find paths of length $O(n^{(2-r)/4})$. Let $\delta = (2-r)/4$ and suppose the algorithm finds a path with at most n^{δ} edges. There must be a long-distance edge on the path which terminates within distance n^{δ} of t; otherwise, the path would end in n^{δ} grid edges and would be too long. There are $O(n^{2\delta})$ vertices within distance n^{δ} of t and the probability that the long distance edge from one vertex of the path ends at one of these vetices is at most $n^{2\delta}\left(\frac{1}{n^{2-r}}\right) = n^{(r-2)/2}$. To see this, recall that the lower bound on the normalizing constant is $\theta(n^{2-r})$ and hence an upper bound on the probability of a long distance edge hitting v is $\theta\left(\frac{1}{n^{2-r}}\right)$ independent of where v is. Thus, the probability that the long distance edge from one of the n^{δ} vertices on the path hits any one of the $n^{2\delta}$ vertices within distance n^{δ} of t is $n^{2\delta}\frac{1}{n^{2-r}}=n^{\frac{r-2}{2}}$. The probability that this happens for any one of the n^{δ} vertices on the path is at most $n^{\frac{r-2}{2}}$ and $n^{\frac{r-2}{2}}$ and $n^{\frac{r-2}{4}}$ and $n^{\frac{r-$

Short paths exist for r < 2

Finally we show for r > 2 that there are $O(\ln n)$ paths between s and t. The proof is similar to the proof of Theorem 3.10 showing $O(\ln n)$ diameter for G(n,p) with $p \in \Omega(\ln n/n)$, so we do not give all the details here. We give the proof only for the case when r = 0.

For a particular vertex v, let S_i denote the set of vertices at distance i from v. Using only local edges, we have for $i \in O(\sqrt{\ln n})$ that $|S_i| \in \Omega(\ln n)$. For later i, we argue a constant factor growth in the size of S_i as in Theorem 3.10. As long as $|S_1| + |S_2| + \cdots + |S_i| \le n^2/2$, for each of the $n^2/2$ or more vertices outside, the probability that it is not in S_{i+1} is $(1-\frac{1}{n})^{|S_i|} \le 1-\frac{|S_i|}{2n}$ since the long-distance edge from each vertex of S_i chooses a long-distance neighbor at random. So, the expected size of S_{i+1} is at least $|S_i|/4$ and using Chernoff, we get constant factor growth up to $n^2/2$. Thus, for any two vertices v and v, the number of vertices at distance $O(\ln n)$ from each is at least $n^2/2$. Any two

sets of cardinality at least $n^2/2$ must intersect giving us a $O(\ln n)$ length path from v to w.

3.6 Bibliographic Notes

The G(n,p) rabdom graph model is from Erdös Rényi [ER60]. Among the books written on properties of random graphs a reader may wish to consult Palmer [Pal85], Jansen, Luczak and Rucinski [JLR00], or Bolobas [Bol01]. Material on phase transitions can be found in [BT87]. The work on phase transitions for CNF was started by Chao and Franco [CF86]. Further work was done in [AM05] [FS96], [AP03], [Fri99] and others. The proof here that the SC algorithm produces a solution when the number of clauses is cN, $c < \frac{2}{3}$ is from [Chv92].

For material on the giant component consult [Kar90] or [JKLP93]. Material on branching process can be found in [AN72]. The phase transition for giant components in random graphs with given degree distributions is from Molloy and Reed [MR95a].

There are numerous papers on growth models. The material in this chapter was based primarily on [CHK⁺] and [BA]. The material on small world is based on Kleinberg [Kle00] which follows earlier work by Watts and Strogatz [WS98a].

3.7 Exercises

Exercise 3.1 Search the World Wide Web to find some real world graphs in machine readable form and compute their degree distributions. Describe what you find.

Exercise 3.2 Find the average degree of some large real world graphs.

Exercise 3.3 In G(n,p) the probability of a vertex having degree k is $\binom{n}{k}p^k(1-p)^{n-k}$. Show by direct calculation that the expected degree is np. Where is the mode of the binomial distribution? [Mode is the point at which the probability is maximum.] Compute directly the variance of the distribution.

Exercise 3.4

- 1. Plot the degree distribution for G(1000, 0.003).
- 2. Plot the degree distribution for G(1000, 0.030).

Exercise 3.5 In $G(n, \frac{1}{n})$ what is the probability that there is a vertex of degree $\log n$? Give an exact formula; also derive simple approximations.

Exercise 3.6 In example of Section 3.1.1 we showed that if the degrees in $G(n, \frac{1}{n})$ were independent that there would almost surely be a vertex of degree $\log n/\log\log n$. However the degrees are not independent. Show how to overcome this difficulty.

Exercise 3.7 Let f(n) be a function that is asymptotically less than n. Some such functions are 1/n, a constant d, $\log n$ or $n^{\frac{1}{3}}$. Show that

$$\lim_{n \to \infty} \left(1 + \frac{f(n)}{n} \right)^n = e^{f(n)}.$$

Exercise 3.8 Simplify $\left(1 - \frac{1}{n}\right)^{n \log n}$

Exercise 3.9 Prove that $1 + x \le e^x$ for all real x. For what values of x is the approximation $1 + x = e^x$ good?

Exercise 3.10 Generate a graph $G\left(n, \frac{d}{n}\right)$ with n = 1000 and d = 2, 3, and 6. Count the number of triangles in each graph. Try the experiment with n = 100.

Exercise 3.11 What is the expected number of squares (4-cycles) in $G(n, \frac{d}{n})$? What is the expected number of 4-cliques in $G(n, \frac{d}{n})$?

Exercise 3.12 What is the expected number of paths of length 3, 4, $\log \log n$, $\log n$ in $G(n, \frac{d}{n})$? What is the expected number of paths of length g(n) where g(n) is some very slow growing function of n?

Exercise 3.13 Consider generating a random graph by flipping two coins, one with probability p_1 of heads and the other with probability p_2 of heads. Add the edge to the graph if either coin comes down heads. What is the value of p for the generated G(n, p) graph.

Exercise 3.14 The Sudoku game consists of a 9×9 array of squares. The array is partitioned into nine 3×3 squares. Each small square should be filled with an integer between 1 and 9 so that each row, each column, and each 3×3 square contains exactly one copy of each integer. Initially the board has some of the small squares filled in in such a way that there is exactly one way to complete the assignments of integers to squares. Some simple rules can be developed to fill in the remaining squares such as if the row and column containing a square already contain a copy of every integer except one, that integer should be placed in the square.

Start with a 9×9 array of squares with each square containing a number between 1 and 9 such that no row, column, or 3×3 square has two copies of an integer.

- 1. How many integers can you randomly erase and there still be only one way to correctly fill in the board?
- 2. Develop a set of simple rules for filling in squares such as if a row does not contain a given integer and if every column except one in which the square in the row is blank contains the integer, then place the integer in the remaining blank entry in the row. How many integers can you randomly erase and your rules will still completely fill in the board?

Exercise 3.15 Generalize the Sudoku game for arrays of size $n^2 \times n^2$. Develop a simple set of rules for completing the game. An example of a rule is: If the a row does not contain a given integer and if every column except one in which the square in the row is blank contains the integer, then place the integer in the remaining blank entry in the row. Start with a legitimate completed array and erase k entries at random.

- 1. Is there a threshold for the integer k such that if only k entries of the array are erased, your set of rules will find a solution?
- 2. Experimentally determine k for some large value of n.

Exercise 3.16 Complete the second moment argument of Theorem 3.11 to show that for $p = \frac{d}{n}$, d > 1, a graph almost surely has a cycle.

Exercise 3.17 Let x_i , $1 \le i \le n$, be a set of indicator variables with identical probability distributions. Let $x = \sum_{i=1}^{n} x_i$ and suppose $E(x) \to \infty$. Show that if the x_i are statistically independent then $Prob(x = 0) \to 0$.

Exercise 3.18 How many isolated vertices are in G(n,p) for $p = \frac{1}{2} \frac{\ln n}{n}$?

Exercise 3.19 Theorem (??) shows that for some c > 0 and $p = c \ln n/n$, G(n, p) has diameter $O(\log n)$. Tighten the argument to pin down (as low a) value (as possible) for c.

Exercise 3.20 Let G(n,p) be a random graph and let x be the random variable denoting the number of unordered pairs of nonadjacent vertices (u,v) such that no other vertex of G is adjacent to both u and v. Prove that if $\lim_{n\to\infty} E(x) = 0$, then for large n there are almost no disconnected graphs i.e. $Prob(x=0) \to 1$ and hence Prob(G is connected) $\to 1$. Actually the graph becomes connected long before this condition is true.

Exercise 3.21 Draw a tree with 10 vertices and label each vertex with a unique integer from 1 to 10. Construct the Prüfer sequence (see Appendix) for the tree. Given the Prüfer sequence recreate the tree.

Exercise 3.22 Construct the tree corresponding to the following Prüfer sequences (see Appendix)

- 1. 113663(1,2),(1,3),(1,4),(3,5),(3,6),(6,7), and (6,8)
- 2. 552833226

See also Kirchhoff's theorem in Wikipedia on the number of spanning trees in a graph for interesting material.

Exercise 3.23 Find a data base in machine readable form that can be viewed as a graph. What is the expected number of edges? If the graph were a G(n,p) graph what would the value of p be? Find the number of components of various sizes. Examine the small components and see if any have cycles.

Exercise 3.24 Randomly generate G(50, p) for several values of p. Start with $p = \frac{1}{50}$.

- 1. For what value of p do cycles first appear?
- 2. For what value of p do isolated vertices disappear and the graphs become connected?

Exercise 3.25 Suppose $p = \frac{1}{3n}$. Then, we showed that almost surely there are no cycles of length 10.

- 1. Use the second moment method to show that almost surely, there is a path of length 10.
- 2. What goes wrong if we try to modify the argument that almost surely there are no cycles of length 10 to show that there is no path of length 10?

Exercise 3.26 What is diameter of G(n,p) for various values of p?

Exercise 3.27 In the proof that every monotone property has a threshold we defined an m-fold replication of G(n, p), where we took the union of m copies of G(n, p). Give an example to show that even if no copy has a property Q, the union may.

Exercise 3.28 Consider a model of a random subset N(n,p) of integers $\{1,2,\ldots n\}$ where, N(n,p) is the set obtained by independently at random including each of $\{1,2,\ldots n\}$ into the set with probability p. Define what an "increasing property" of N(n,p) means. Prove that every increasing property of N(n,p) has a threshold.

Exercise 3.29 What is the threshold for N(n, p) to contain

- 1. a perfect square,
- 2. a perfect cube,
- 3. an even number,
- 4. three numbers such that x + y = z?

Exercise 3.30 Modify the proof that every monotone property has a threshold for G(n, p) to apply to the 3-CNF satisfiability problem.

Exercise 3.31 In a square $n \times n$ grid, each of the $O(n^2)$ edges is randomly chosen to be present with probability p and absent with probability 1-p. Consider the increasing property that there is a path from the bottom left corner to the top right corner. Show that p = 1/2 is a threshold for the property. [Harder: Show that it is actually a sharp threshold.]

Exercise 3.32 The threshold property seems to be related to uniform distributions. What if we considered other distributions? Consider a model where i is selected with probability $\frac{c(n)}{i}$. Is there a threshold for perfect squares? Is there a threshold for arithmetic progressions?

Exercise 3.33 Explain why the property that N(n, p) contains the integer 1 has a threshold. What is the threshold?

Exercise 3.34 Consider G(n, p).

- 1. Where is phase transition for 3-colorability? Hint: For p = d/n, with d < 1, G(n,p) is acyclic, so it is bipartite and hence 2-colorable. When $pn \to \infty$, the expected number of triangles goes to infinity. Show that almost surely, there is a triangle? What does this do for 2-colorability?
- 2. What about 4-colorability?

Exercise 3.35 Experimentally play with the following problem. For $G(n, \frac{1}{2})$, for what value of k is there a vertex cover (a set of k vertices such that one end of each edge is in the set)?

Exercise 3.36 Is there a condition such that any property satisfying the condition has a sharp threshold? For example, is monotonicity such a condition?

Exercise 3.37

- 1. List five increasing properties of G(n, p).
- 2. List five nonincreasing properties.

Exercise 3.38 Birthday problem: What is the number of integers that must be drawn with replacement from a set of n integers so that some integer almost surely will be selected twice?

Exercise 3.39 Suppose the graph of a social network has 10,000 vertices. You have a program that starting from a random seed produces a community. In running the algorithm you find thousands of communities and wonder how many communities are there in the graph. Finally when you find the 10,000th community it is a duplicate. It is the same community as one found earlier.

- 1. Use the birthday problem to derive a lower bound on the number of communities.
- 2. Why do you only get a lower bound and not a good estimate?

Exercise 3.40 Evaluate $\left(1-\frac{1}{2^k}\right)^{2^k}$ for k=3, 5, and 7. How close is it to 1/e?

Exercise 3.41 Consider a random process for generating a Boolean function f in conjunctive normal form where each of c clauses is generated by placing each of n variables in the clause with probability p and complementing the variable with probability 1/2. What is the distribution of clause sizes for various p such as p = 3/n, 1/2, other values? Experimentally determine the threshold value of p for p to cease to be satisfied.

Exercise 3.42 For a random 3-CNF formula with n variables and cn clauses, what is the expected number of satisfying assignments?

Exercise 3.43 Which of the following variants of the SC algorithm admit a theorem like Theorem 3.15? (i) Among all clauses of least length, pick the first one in the order in which they appear in the formula. (ii) Set the literal appearing in most clauses (of any length) to 1.

Exercise 3.44 Suppose we have a queue of jobs serviced by one server. There is a total of n jobs in the system. At time t, each remaining job independently decided to join the queue to be serviced with probability p = d/n, where, d < 1 is a constant. Each job has a processing time of 1 and at each time, the server services one job if the queue is non-empty. Show that with high probability, no job waits more than $\Omega(\ln n)$ time to be serviced once it joins the queue.

- **Solution:** Just imitate the proof in the text for CNF. If some job stays in queue for $\Omega(\ln n)$ steps until, say, step s, there is a last time before s, say, step r when the queue is empty. $s r \in \Omega(\ln n)$ and s r jobs must have joined the queue during the period r to s; the probability of this is $O(1/n^3)$. Now use union bound over all s.
- Exercise 3.45 Consider graph 3-colorability. Randomly generate the edges of a graph and compute the number of solutions and the number of connected components of the solution set as a function of the number of edges generated. What happens?
- Exercise 3.46 Randomly generate clauses for a Boolean formula in CNF. Compute the number of solutions and the number of connected components of the solution set as a function of the number of clauses generated. What happens?
- Exercise 3.47 Construct an example of a formula which is satisfiable, but the SC heuristic fails to find a satisfying assignment.
- **Exercise 3.48** In G(n,p), let x_k be the number of connected components of size k. Using x_k , write down the probability that a randomly chosen vertex is in a connected component of size k. Also write down the expected size of the connected component a randomly chosen vertex is in.
- **Exercise 3.49** Let S be the expected number of vertices discovered as a function of the number of steps t in a breadth first search of $G\left(n, \frac{d}{n}\right)$. Write a differential equation using expected values for the size of S. Show that the solution is $S = d\left(1 \frac{S}{n}\right)$. Show that the normalized size f of the frontier is $f\left(x\right) = 1 e^{-dx} x$ where $x = \frac{t}{n}$ is the normalized time.
- **Exercise 3.50** Prove that the expected value of the size of the frontier increases linearly with i for i in the neighborhood of Θ .
- Exercise 3.51 Consider the binomial distribution binomial $\left[n, 1 \left(1 \frac{d}{n}\right)^i\right]$ for d > 1. Prove that as $n \to \infty$, the distribution goes to zero for all i except for i in the two ranges $[0, c_1 \log n]$ and $[\Theta - c_2 \sqrt{n}, \Theta + c_2 \sqrt{n}]$.
- **Exercise 3.52** What is the value of $x_{max} = \arg \max F(x) = 1 e^{-dx} x$? What is the value of $f(x_{max})$? Where does the expected value of the frontier of a breadth search in $G(n, \frac{d}{n})$ occur as a function of n.
- **Solution:** 3.52 $\frac{d}{dx}f(x) = de^{dx} 1$. Solving $de^{dx} 1 = 0$ yields $x = \frac{\ln d}{d}$. Thus $f(\frac{\ln d}{d}) = 1 e^{-\ln d} \frac{\ln d}{d} = 1 \frac{1 + \ln d}{d}$. Thus the maximum of the expected value of the frontier occurs at some constant between 0 and 1 times n. The size of the frontier at this point is some constant times n.

Exercise 3.53 Suppose one "hides" a clique of size k in a random graph $G\left(n, \frac{1}{2}\right)$; i.e., in the random graph, choose some subset S of k vertices and put in the missing edges to make S a clique. We are then presented with the modified graph and are asked to find S. The larger S is, the easier it should be to find. In fact, if k is more than $c\sqrt{n \ln n}$, then the clique leaves a "telltale" sign and we can identify S as just the k vertices of largest degree. Prove this statement by appealing to the Theorem 3.1. It remains a puzzling open problem to do this when k is smaller, say, $O(n^{1/3})$.

Exercise 3.54 The clique problem in a graph is to find the maximal size clique. This problem is known to be NP-hard and so a polynomial time algorithm is thought unlikely. We can ask the corresponding question about random graphs. For example, in $G(n, \frac{1}{2})$, we shall see that almost surely there is a clique of size $(2 - \varepsilon) \log n$ for any $\varepsilon > 0$. But it is not known how to find one in polynomial time.

- 1. Show that in $G(n, \frac{1}{2})$, there are almost surely no cliques of size $(2 + \varepsilon) \log_2 n$.
- 2. Use the second moment method to show that in $G(n, \frac{1}{2})$, there are almost surely cliques of size $(2 \varepsilon) \log_2 n$.
- 3. Show that for any $\varepsilon > 0$ a clique of size $(2 \varepsilon) \log n$ can be found in $G(n, \frac{1}{2})$ in time $n^{O(\ln n)}$.
- 4. Give an $O(n^2)$ algorithm for finding a clique of size $\Omega(\log n)$ in G(n, 1/2). (Hint use a greedy algorithm.) Apply your algorithm to $G(1000, \frac{1}{2})$. What size clique do you find?
- 5. An independent set of vertices in a graph is a set of vertices no two of which are connected by an edge. Give a polynomial time algorithm for finding an independent set in $G\left(n, \frac{1}{2}\right)$ of size $\Omega\left(\log n\right)$.

Exercise 3.55 If y and z are independent (nonnegative) random variables, then the generating function of the sum y + z is the product of the generating function of y and z. Show that this follows from $E(x^{y+z}) = E(x^y x^z) = E(x^y) E(x^z)$.

Exercise 3.56 Consider the branching process when m>1 with q as the root of the equation f(x)=x. Prove that $\lim_{j\to\infty} f_j(x)=q$ for 0< x<1.

Exercise 3.57 We showed that $\lim_{j\to\infty} f_j(x) = q$ for 0 < x < 1 for the generating function f of a branching process when m > 1. In the limit this implies $Prob(z_j = 0) = q$ and $Prob(z_j = i) = 0$ for all nonzero finite values of i. Shouldn't the probabilities add up to 1? Why is this not a contradiction?

Exercise 3.58 Try to create a probability distribution which varies with the current population in which future generations neither die out nor grow to infinity.

Exercise 3.59 Show that for a branching process with number of children distributed as $Binomial(n - c_1 n^{2/3}, \frac{d}{n})$, where d is a constant strictly greater than 1, the root of the generating function f(x) in (0,1) is at most a constant strictly less than 1. In other words, it cannot for example be greater than 1 - (1/n).

Exercise 3.60 For p asymptotically greater than $\frac{1}{n}$ show that $\sum_{i=0}^{\infty} i(i-2)\lambda_i > 0$.

Exercise 3.61 The global clustering coefficient of a graph is defined as follows. Let d_v be the degree of vertex v and let e_v be the number of edges connecting vertices adjacent to vertex v. The global clustering coefficient c is given by

$$c = \sum_{v} \frac{2e_v}{d_v(d_v - 1)}$$

In a social network, for example, it measures what fraction of pairs of friends of each person are themselves friends. If many are, the clustering coefficient is high. What is c for a random graph with $p = \frac{d}{n}$? For a denser graph? Compare this value to that for some social network.

Solution: (of Exercise 3.61): For a random graph G(n, p) the clustering coefficient is p. Thus, for $G(n, \frac{d}{n})$ the coefficient is zero. For $G(n, \frac{1}{2})$ the clustering coefficient is $\frac{1}{2}$.

Exercise 3.62 Consider a structured graph such as a grid or cycle and gradually add edges or reroute edges at random. Let L be the average distance between all pairs of vertices in a graph and let C be the ratio of triangles to connected sets of three vertices. Plot L and C as a function of the randomness introduced.

Exercise 3.63 Consider an $n \times n$ grid in the plane. Prove that for any vertex u there are at least 2k vertices at distance k for $1 \le k \le n/2$.

Exercise 3.64 Show that in a small-world graph with $r \le 2$ that there exist short paths with high probability. [We showed this for r = 0 in the text.]

Exercise 3.65 Suppose we change the small worlds graph as follows: we still have a $n \times n$ grid each vertex has one long-distance edge to a (uniformly) randomly chosen vertex. [These are exactly like the long-distance edges for r = 0.] But the grid edges are not present; instead, we have some other graph with the property that for each vertex, there are $\Theta(t^2)$ vertices at distance t from the vertex for $t \leq n$. Show that almost surely the diameter is $O(\ln n)$.

Solution: Just imitate the proof for small-world graphs. The only place in the proof using local grid edges is at the start to argue that at distance $O(\sqrt{\ln n})$, there are $O \ln n$) vertices. Replace this argument by the assumption here.

Exercise 3.66 Given an n node directed graph with two random edges from each node. For two vertices s and t chosen at random, prove that there exists a short path from s to t with high probability.

Solution: The proof probably looks at growth of size of set of nodes reachable in m steps. $S_0 = 1$ $S_1 = 2$ $S_i = \left(1 - \frac{S_{i-1}}{n}\right) 2 + S_{i-1} = S_{i-1} + 2 - \frac{2S_{i-1}}{n}$.

Exercise 3.67 How does the diameter of a graph consisting of a cycle change as one adds a few random long distance edges? This question explores how much randomness is needed to get a small world.

Exercise 3.68 Ideas and diseases spread rapidly in small world graphs. What about spread of social contagion? A disease needs only one contact and with some probability transfers. Social contagion needs several contacts. How many vertices must one start with to spread social contagion if the spread of contagion requires two adjacent vertices?

Exercise 3.69 How many edges are needed to disconnect a small world graph? By disconnect we mean at least two pieces each of reasonable size. Is this connected to the emergence of a giant component?

Exercise 3.70 In the small world model, would it help if the algorithm could look at edges at any node at a cost of one for each node looked at?

Exercise 3.71 Consider the $n \times n$ grid in the section on small world graphs. If the probability of an edges from vertex u to vertex v is proportional to $d^{-r}(u,v)$ show that the constant of proportionality $c_r(u)$ is

$$\begin{array}{ll} \theta(n^{2-r}) & for \ r > 2 \\ \theta(\ln n) & for \ r = 2 \\ \theta(1) & for \ r < 2 \end{array}$$

Exercise 3.72 In the $n \times n$ grid prove that for at least half of the pairs of vertices, the distance between the vertices is greater than or equal to n/4

4 Singular Value Decomposition (SVD)

The singular value decomposition of a matrix A is the factorization of A into the product of three matrices $A = UDV^T$ where the columns of U and V are orthonormal and the matrix D is diagonal with positive real entries. The SVD is useful in many tasks. Here we mention two examples. First, the rank of a matrix A can be read off from its SVD. This is useful when the elements of the matrix are real numbers that have been rounded to some finite precision. Before the entries were rounded the matrix may have been of low rank but the rounding converted the matrix to full rank. The original rank can be determined by the number of diagonal elements of D not exceedingly close to zero. Second, for a square and invertible matrix A, the inverse of A is $VD^{-1}U^T$.

To gain insight into the SVD, treat the rows of an $n \times d$ matrix A as n points in a d-dimensional space and consider the problem of finding the best k-dimensional subspace with respect to the set of points. Here best means minimize the sum of the squares of the perpendicular distances of the points to the subspace. We begin with a special case of the problem where the subspace is 1-dimensional, a line through the origin. We will see later that the best-fitting k-dimensional subspace can be found by k applications of the best fitting line algorithm. Finding the best fitting line through the origin with respect to a set of points $\{\mathbf{x_i}|1 \le i \le n\}$ in the plane means minimizing the sum of the squared distances of the points to the line. Here distance is measured perpendicular to the line. The problem is called the best least squares fit.

In the best least squares fit, one is minimizing the distance to a subspace. An alternative problem is to find the function that best fits some data. Here one variable y is a function of the variables x_1, x_2, \ldots, x_d and one wishes to minimize the vertical distance, i.e., distance in the y direction, to the subspace of the x_i rather than minimize the perpendicular distance to the subspace being fit to the data.

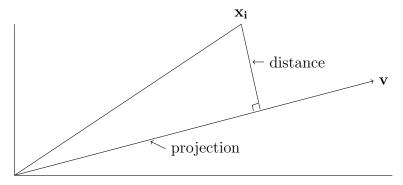


Figure 4.1: The projection of the point $\mathbf{x_i}$ onto the line through the origin in the direction of \mathbf{v}

Returning to the best least squares fit problem, consider projecting a point x_i onto a

line through the origin. Then

$$x_{i1}^2 + x_{i2}^2 + \dots + x_{id}^2 = (\text{length of projection})^2 + (\text{distance of point to line})^2$$
.

See Figure 4.1. Thus

(distance of point to line)² =
$$x_{i1}^2 + x_{i2}^2 + \cdots + x_{id}^2 - (\text{length of projection})^2$$
.

To minimize the sum of the squares of the distances to the line, one could minimize $\sum_{i=1}^{n} (x_{i1}^2 + x_{i2}^2 + \cdots + x_{id}^2)$ minus the sum of the squares of the lengths of the projections of

the points to the line. However, $\sum_{i=1}^{n} (x_{i1}^2 + x_{i2}^2 + \cdots + x_{id}^2)$ is a constant (independent of the line), so minimizing the sum of the squares of the distances is equivalent to maximizing the sum of the squares of the lengths of the projections onto the line. Similarly for best-fit subspaces, we could maximize the sum of the squared lengths of the projections onto the subspace instead of minimizing the sum of squared distances to the subspace.

4.1 Singular Vectors

We now define the *singular vectors* of an $n \times d$ matrix A. Consider the rows of A as n points in a d-dimensional space. Consider the best fit line through the origin. Let \mathbf{v} be a unit vector along this line. The length of the projection of $\mathbf{a_i}$, the i^{th} row of A, onto \mathbf{v} is $|\mathbf{a_i} \cdot \mathbf{v}|$. From this we see that the sum of length squared of the projections is $|A\mathbf{v}|^2$. The best fit line is the one maximizing $|A\mathbf{v}|^2$ and hence minimizing the sum of the squared distances of the points to the line.

With this in mind, define the *first singular vector*, $\mathbf{v_1}$, of A, which is a column vector, as the best fit line through the origin for the n points in d-space that are the rows of A. Thus

$$\mathbf{v_1} = \arg\max_{|\mathbf{v}|=1} |A\mathbf{v}|.$$

The value $\sigma_1(A) = |A\mathbf{v_1}|$ is called the *first singular value* of A. Note that σ_1^2 is the sum of the squares of the projections of the points to the line determined by $\mathbf{v_1}$.

The greedy approach to find the best fit 2-dimensional subspace for a matrix A, takes $\mathbf{v_1}$ as the first basis vector for the 2-dimensional subspace and finds the best 2-dimensional subspace containing $\mathbf{v_1}$. The fact that we are using the sum of squared distances helps. For every 2-dimensional subspace containing $\mathbf{v_1}$, the sum of squared lengths of the projections onto the subspace equals the sum of squared projections onto $\mathbf{v_1}$ plus the sum of squared projections along a vector perpendicular to $\mathbf{v_1}$ in the subspace. Thus, instead of looking for the best 2-dimensional subspace containing $\mathbf{v_1}$, look for a unit vector, call it $\mathbf{v_2}$, perpendicular to $\mathbf{v_1}$ that maximizes $|A\mathbf{v}|^2$ among all such unit vectors. Using the same greedy strategy to find the best three and higher dimensional subspaces, defines $\mathbf{v_3}, \mathbf{v_4}, \ldots$ in a similar manner. This is captured in the following definitions. There is no

apriori guarantee that the greedy algorithm gives the best fit. But, in fact, the greedy algorithm does work and yields the best-fit subspaces of every dimension.

The second singular vector, $\mathbf{v_2}$, is defined by the best fit line perpendicular to $\mathbf{v_1}$

$$\mathbf{v_2} = \underset{\mathbf{v} \perp \mathbf{v_1}, |\mathbf{v}| = 1}{\arg \max} |A\mathbf{v}|.$$

The value $\sigma_2(A) = |A\mathbf{v_2}|$ is called the second singular value of A. The third singular vector $\mathbf{v_3}$ is defined similarly by

$$\mathbf{v_3} = \underset{\mathbf{v} \perp \mathbf{v_1}, \mathbf{v_2}, |\mathbf{v}| = 1}{\arg \max} |A\mathbf{v}|$$

and so on. The process stops when we have found

$$v_1, v_2, \dots, v_r$$

as singular vectors and

$$\underset{\substack{\mathbf{v} \perp \mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r} \\ |\mathbf{v}| = 1}}{\arg \max} |A\mathbf{v}| = 0.$$

If instead of finding $\mathbf{v_1}$ that maximized $|A\mathbf{v}|$ and then the best fit 2-dimensional subspace containing $\mathbf{v_1}$, we had found the best fit 2-dimensional subspace, we might have done better. This is not the case. We now give a simple proof that the greedy algorithm indeed finds the best subspaces of every dimension.

Theorem 4.1 Let A be an $n \times d$ matrix where $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$ are the singular vectors defined above. For $1 \leq k \leq r$, let V_k be the subspace spanned by $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_k}$. Then for each k, V_k is the best-fit k-dimensional subspace for A.

Proof: The statement is obviously true for k = 1. For k = 2, let W be a best-fit 2-dimensional subspace for A. For any basis $\mathbf{w_1}, \mathbf{w_2}$ of W, $|A\mathbf{w_1}|^2 + |A\mathbf{w_2}|^2$ is the sum of squared lengths of the projections of the rows of A onto W. Now, choose a basis $\mathbf{w_1}, \mathbf{w_2}$ of W so that $\mathbf{w_2}$ is perpendicular to $\mathbf{v_1}$. If $\mathbf{v_1}$ is perpendicular to W, any unit vector in W will do as $\mathbf{w_2}$. If not, choose $\mathbf{w_2}$ to be the unit vector in W perpendicular to the projection of $\mathbf{v_1}$ onto W. Since $\mathbf{v_1}$ was chosen to maximize $|A\mathbf{v_1}|^2$, it follows that $|A\mathbf{w_1}|^2 \leq |A\mathbf{v_1}|^2$. Since $\mathbf{v_2}$ was chosen to maximize $|A\mathbf{v_2}|^2$ over all \mathbf{v} perpendicular to $\mathbf{v_1}$, $|A\mathbf{w_2}|^2 \leq |A\mathbf{v_2}|^2$. Thus

$$|A\mathbf{w_1}|^2 + |A\mathbf{w_2}|^2 \le |A\mathbf{v_1}|^2 + |A\mathbf{v_2}|^2.$$

Hence, V_2 is at least as good as W and so is a best-fit 2-dimensional subspace.

For general k, proceed by induction. By the induction hypothesis, V_{k-1} is a best-fit k-1 dimensional subspace. Suppose W is a best-fit k-dimensional subspace. Choose a basis $\mathbf{w_1}, \mathbf{w_2}, \dots, \mathbf{w_k}$ of W so that $\mathbf{w_k}$ is perpendicular to $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_{k-1}}$. Then

$$|A\mathbf{w_1}|^2 + |A\mathbf{w_2}|^2 + \dots + |A\mathbf{w_k}|^2 \le |A\mathbf{v_1}|^2 + |A\mathbf{v_2}|^2 + \dots + |A\mathbf{v_{k-1}}|^2 + |A\mathbf{w_k}|^2$$

since V_{k-1} is an optimal k-1 dimensional subspace. Since $\mathbf{w_k}$ is perpendicular to $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_{k-1}}$, by the definition of $\mathbf{v_k}, |A\mathbf{w_k}|^2 \leq |A\mathbf{v_k}|^2$. Thus

$$|A\mathbf{w_1}|^2 + |A\mathbf{w_2}|^2 + \dots + |A\mathbf{w_{k-1}}|^2 + |A\mathbf{w_k}|^2 \le |A\mathbf{v_1}|^2 + |A\mathbf{v_2}|^2 + \dots + |A\mathbf{v_{k-1}}|^2 + |A\mathbf{v_k}|^2$$

proving that V_k is at least as good as W and hence is optimal.

Note that the *n*-vector $A\mathbf{v_i}$ is really a list of lengths (with signs) of the projections of the rows of A onto $\mathbf{v_i}$. Think of $|A\mathbf{v_i}| = \sigma_i(A)$ as the "component" of the matrix A along $\mathbf{v_i}$. For this interpretation to make sense, it should be true that adding up the squares of the components of A along each of the $\mathbf{v_i}$ gives the square of the "whole content of the matrix A". This is indeed the case and is the matrix analogy of decomposing a vector into its components along orthogonal directions.

Consider one row, say $\mathbf{a_j}$, of A. Since $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$ span the space of all rows of A, $\mathbf{a_j} \cdot \mathbf{v} = 0$ for all \mathbf{v} perpendicular to $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$. Thus, for each row $\mathbf{a_j}$, $\sum_{i=1}^r (\mathbf{a_j} \cdot \mathbf{v_i})^2 = |\mathbf{a_j}|^2$. Summing over all rows j,

$$\sum_{j=1}^{n} |\mathbf{a_j}|^2 = \sum_{j=1}^{n} \sum_{i=1}^{r} (\mathbf{a_j} \cdot \mathbf{v_i})^2 = \sum_{i=1}^{r} \sum_{j=1}^{n} (\mathbf{a_j} \cdot \mathbf{v_i})^2 = \sum_{i=1}^{r} |A\mathbf{v_i}|^2 = \sum_{i=1}^{r} \sigma_i^2(A).$$

But $\sum_{j=1}^{n} |\mathbf{a_j}|^2 = \sum_{j=1}^{n} \sum_{k=1}^{d} a_{jk}^2$, the sum of squares of all the entries of A. Thus, the sum of squares of the singular values of A is indeed the square of the "whole content of A", i.e., the sum of squares of all the entries. There is an important norm associated with this quantity, the Frobenius norm of A, denoted $||A||_F$ defined as

$$||A||_F = \sqrt{\sum_{j,k} a_{jk}^2}.$$

Lemma 4.2 For any matrix A, the sum of squares of the singular values equals the Frobenius norm. That is, $\sum \sigma_i^2(A) = ||A||_F^2$.

Proof: By the preceding discussion.

A matrix A can be described fully by how it transforms the vectors $\mathbf{v_i}$. Every vector \mathbf{v} can be written as a linear combination of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_r}$ and a vector perpendicular to all the $\mathbf{v_i}$. Now, $A\mathbf{v}$ is the same linear combination of $A\mathbf{v_1}, A\mathbf{v_2}, \ldots, A\mathbf{v_r}$ as \mathbf{v} is of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_r}$. So the $A\mathbf{v_1}, A\mathbf{v_2}, \ldots, A\mathbf{v_r}$ form a fundamental set of vectors associated with A. We normalize them to length one by

$$\mathbf{u_i} = \frac{1}{\sigma_i(A)} A \mathbf{v_i}.$$

The vectors $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_r}$ are called the *left singular vectors* of A. The $\mathbf{v_i}$ are called the *right singular vectors*. The SVD theorem (Theorem 4.5) will fully explain the reason for these terms.

Clearly, the right singular vectors are orthogonal by definition. We now show that the left singular vectors are also orthogonal and that $A = \sum_{i=1}^{r} \sigma_i \mathbf{u_i v_i^T}$.

Theorem 4.3 Let A be a rank r matrix. The left singular vectors of A, $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_r}$, are orthogonal.

Proof: The proof is by induction on r. For r = 1, there is only one $\mathbf{u_i}$ so the theorem is trivially true. For the inductive part consider the matrix

$$B = A - \sigma_1 \mathbf{u_1} \mathbf{v_1}^T.$$

The implied algorithm in the definition of singular value decomposition applied to B is identical to a run of the algorithm on A for its second and later singular vectors and singular values. To see this, first observe that $B\mathbf{v_1} = A\mathbf{v_1} - \sigma_1\mathbf{u_1}\mathbf{v_1^T}\mathbf{v_1} = 0$. It then follows that the first right singular vector, call it \mathbf{z} , of B will be perpendicular to $\mathbf{v_1}$ since if it had a component $\mathbf{z_1}$ along $\mathbf{v_1}$, then, $\left|B_{|\mathbf{z}-\mathbf{z_1}|}\right| = \frac{|B\mathbf{z}|}{|\mathbf{z}-\mathbf{z_1}|} > |B\mathbf{z}|$, contradicting the arg max definition of z. But for any \mathbf{v} perpendicular to $\mathbf{v_1}$, $B\mathbf{v} = A\mathbf{v}$. Thus, the top singular vector of B is indeed a second singular vector of A. Repeating this argument shows that a run of the algorithm on B is the same as a run on A for its second and later singular vectors. This is left as an exercise.

Thus, there is a run of the algorithm that finds that B has right singular vectors $\mathbf{v_2}, \mathbf{v_3}, \ldots, \mathbf{v_r}$ and corresponding left singular vectors $\mathbf{u_2}, \mathbf{u_3}, \ldots, \mathbf{u_r}$. By the induction hypothesis, $\mathbf{u_2}, \mathbf{u_3}, \ldots, \mathbf{u_r}$ are orthogonal.

It remains to prove that $\mathbf{u_1}$ is orthogonal to the other $\mathbf{u_i}$. Suppose not and for some $i \geq 2$, $\mathbf{u_1}^T \mathbf{u_i} \neq 0$. Without loss of generality assume that $\mathbf{u_1}^T \mathbf{u_i} > 0$. The proof is symmetric for the case where $\mathbf{u_1}^T \mathbf{u_i} < 0$. Now, for infinitesimally small $\varepsilon > 0$, the vector

$$A\left(\frac{\mathbf{v}_1 + \varepsilon \mathbf{v_i}}{|\mathbf{v_1} + \varepsilon \mathbf{v_i}|}\right) = \frac{\sigma_1 \mathbf{u_1} + \varepsilon \sigma_i \mathbf{u_i}}{\sqrt{1 + \varepsilon^2}}$$

has length at least as large as its component along $\mathbf{u_1}$ which is

$$\mathbf{u_1^T}(\frac{\sigma_1\mathbf{u_1} + \varepsilon\sigma_i\mathbf{u_i}}{\sqrt{1 + \varepsilon^2}}) = \left(\sigma_1 + \varepsilon\sigma_i\mathbf{u_1^T}\mathbf{u_i}\right)\left(1 - \frac{\varepsilon^2}{2} + O\left(\varepsilon^4\right)\right) = \sigma_1 + \varepsilon\sigma_i\mathbf{u_1^T}\mathbf{u_i} - O\left(\varepsilon^2\right) > \sigma_1$$

a contradiction. Thus, $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_r}$ are orthogonal.

4.2 Singular Value Decomposition (SVD)

Let A be an $n \times d$ matrix with singular vectors $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$ and corresponding singular values $\sigma_1, \sigma_2, \dots, \sigma_r$. Then $\mathbf{u_i} = \frac{1}{\sigma_i} A \mathbf{v_i}$, for $i = 1, 2, \dots, r$, are the left singular vectors and by Theorem 4.5, A can be decomposed into a sum of rank one matrices as

$$A = \sum_{i=1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T.$$

We first prove a simple lemma stating that two matrices A and B are identical if $A\mathbf{v} = B\mathbf{v}$ for all \mathbf{v} . The lemma states that in the abstract, a matrix A can be viewed as a transformation that maps vector \mathbf{v} onto $A\mathbf{v}$.

Lemma 4.4 Matrices A and B are identical if and only if for all vectors \mathbf{v} , $A\mathbf{v} = B\mathbf{v}$.

Proof: Clearly, if A = B then $A\mathbf{v} = B\mathbf{v}$ for all \mathbf{v} . For the converse, suppose that $A\mathbf{v} = B\mathbf{v}$ for all \mathbf{v} . Let $\mathbf{e_i}$ be the vector that is all zeros except for the i^{th} component which has value 1. Now $A\mathbf{e_i}$ is the i^{th} column of A and thus A = B if for each i, $A\mathbf{e_i} = B\mathbf{e_i}$.

Theorem 4.5 Let A be an $n \times d$ matrix with right singular vectors $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$, left singular vectors $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_r}$, and corresponding singular values $\sigma_1, \sigma_2, \dots, \sigma_r$. Then

$$A = \sum_{i=1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T.$$

Proof: For each singular vector $\mathbf{v_j}$, $A\mathbf{v_j} = \sum_{i=1}^r \sigma_i \mathbf{u_i} \mathbf{v_i}^T \mathbf{v_j}$. Since any vector \mathbf{v} can be expressed as a linear combination of the singular vectors plus a vector perpendicular to the $\mathbf{v_i}$, $A\mathbf{v} = \sum_{i=1}^r \sigma_i \mathbf{u_i} \mathbf{v_i}^T \mathbf{v}$ and by Lemma 4.4, $A = \sum_{i=1}^r \sigma_i \mathbf{u_i} \mathbf{v_i}^T$.

The decomposition is called the *singular value decomposition*, SVD, of A. In matrix notation $A = UDV^T$ where the columns of U and V consist of the left and right singular vectors, respectively, and D is a diagonal matrix whose diagonal entries are the singular values of A.

For any matrix A, the sequence of singular values is unique and if the singular values are all distinct, then the sequence of singular vectors is unique also. However, when some set of singular values are equal, the corresponding singular vectors span some subspace. Any set of orthonormal vectors spanning this subspace can be used as the singular vectors.

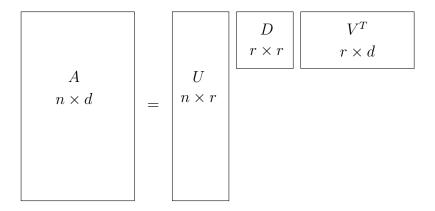


Figure 4.2: The SVD decomposition of an $n \times d$ matrix.

4.3 Best Rank k Approximations

There are two important matrix norms, the Frobenius norm denoted $||A||_F$ and the 2-norm denoted $||A||_2$. The 2-norm of the matrix A is given by

$$\max_{|\mathbf{v}|=1}\,|A\mathbf{v}|$$

and thus equals the largest singular value of the matrix.

Let A be an $n \times d$ matrix and think of the rows of A as n points in d-dimensional space. The Frobenius norm of A is the square root of the sum of the squared distance of the points to the origin. The 2-norm is the square root of the sum of squared distances to the origin along the direction that maximizes this quantity.

Let

$$A = \sum_{i=1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T$$

be the SVD of A. For $k \in \{1, 2, \dots, r\}$, let

$$A_k = \sum_{i=1}^k \sigma_i \mathbf{u_i} \mathbf{v_i}^T$$

be the sum truncated after k terms. It is clear that A_k has rank k. Furthermore, A_k is the best rank k approximation to A when the error is measured in either the 2-norm or the Frobenius norm.

Lemma 4.6 The rows of A_k are the projections of the rows of A onto the subspace V_k spanned by the first k singular vectors of A.

Proof: Let **a** be an arbitrary row vector. Since the $\mathbf{v_i}$ are orthonormal, the projection of the vector a onto V_k is given by $\sum_{i=1}^k (\mathbf{a} \cdot \mathbf{v_i}) \mathbf{v_i}^T$. Thus, the matrix whose rows are the projections of the rows of A onto V_k is given by $\sum_{i=1}^k A \mathbf{v_i} \mathbf{v_i}^T$. This last expression simplifies to

$$\sum_{i=1}^{k} A \mathbf{v_i} \mathbf{v_i}^T = \sum_{i=1}^{k} \sigma_i \mathbf{u_i} \mathbf{v_i}^T = A_k.$$

The matrix A_k is the best rank k approximation to A in both the Frobenius and the 2-norm. First we show that the matrix A_k is the best rank k approximation to A in the Frobenius norm.

Theorem 4.7 For any matrix B of rank at most k

$$||A - A_k||_F \le ||A - B||_F$$

Proof: Let B minimize $||A - B||_F^2$ among all rank k or less matrices. Let V be the space spanned by the rows of B. The dimension of V is at most k. Since B minimizes $||A - B||_F^2$, it must be that each row of B is the projection of the corresponding row of A onto V, otherwise replacing the row of B with the projection of the corresponding row of A onto V does not change V and hence the rank of B but would reduce $||A - B||_F^2$. Since each row of B is the projection of the corresponding row of A, it follows that $||A - B||_F^2$ is the sum of squared distances of rows of A to any k-dimensional subspace, it follows that $||A - A_k||_F \le ||A - B||_F$.

Next we tackle the 2-norm. We first show that the square of the 2-norm of $A - A_k$ is the square of the $(k+1)^{st}$ singular value of A,

Lemma 4.8 $||A - A_k||_2^2 = \sigma_{k+1}^2$.

Proof: Let $A = \sum_{i=1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T$ be the singular value decomposition of A. Then $A_k = \sum_{i=1}^{k} \sigma_i \mathbf{u_i} \mathbf{v_i}^T$ and $A - A_k = \sum_{i=k+1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T$. Let \mathbf{v} be the top singular vector of $A - A_k$.

Express \mathbf{v} as a linear combination of $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$. That is, write $\mathbf{v} = \sum_{i=1}^r \alpha_i \mathbf{v_i}$. Then

$$|(A - A_k)\mathbf{v}| = \left| \sum_{i=k+1}^r \sigma_i \mathbf{u_i} \mathbf{v_i}^T \sum_{j=1}^r \alpha_j \mathbf{v_j} \right| = \left| \sum_{i=k+1}^r \alpha_i \sigma_i \mathbf{u_i} \mathbf{v_i}^T \mathbf{v_i} \right|$$
$$= \left| \sum_{i=k+1}^r \alpha_i \sigma_i \mathbf{u_i} \right| = \sqrt{\sum_{i=k+1}^r \alpha_i^2 \sigma_i^2}.$$

The **v** maximizing this last quantity, subject to the constraint that $|\mathbf{v}|^2 = \sum_{i=1}^{\tau} \alpha_i^2 = 1$, occurs when $\alpha_{k+1} = 1$ and the rest of the α_i are 0. Thus, $||A - A_k||_2^2 = \sigma_{k+1}^2$ proving the lemma.

Finally, we prove that A_k is the best rank k 2-norm approximation to A.

Theorem 4.9 Let A be an $n \times d$ matrix. For any matrix B of rank at most k

$$||A - A_k||_2 \le ||A - B||_2$$

Proof: If A is of rank k or less, the theorem is obviously true since $||A - A_k||_2 = 0$. Thus assume that A is of rank greater than k. By Lemma 4.8, $||A - A_k||_2^2 = \sigma_{k+1}^2$. Now suppose there is some matrix B of rank at most k such that B is a better 2-norm approximation to A than A_k . That is, $||A - B||_2 < \sigma_{k+1}$. The null space of B, Null (B), (the set of vectors \mathbf{v} such that $B\mathbf{v} = 0$) has dimension at least d - k. Let $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_{k+1}}$ be the first k+1 singular vectors of A. By a dimension argument, it follows that there exists a $\mathbf{z} \neq 0$ in

$$\text{Null}(B) \cap \text{Span}\{\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_{k+1}}\}.$$

Scale **z** so that $|\mathbf{z}| = 1$. We now show that for this vector **z**, which lies in the space of the first k+1 singular vectors of A, that $(A-B)\mathbf{z} \geq \sigma_{k+1}$. Hence the 2-norm of A-B is at least σ_{k+1} contradicting the assumption that $||A-B||_2 < \sigma_{k+1}$. First

$$||A - B||_2^2 \ge |(A - B)\mathbf{z}|^2$$
.

Since $B\mathbf{z} = 0$,

$$||A - B||_2^2 \ge |A\mathbf{z}|^2.$$

Since \mathbf{z} is in the Span $\{\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_{k+1}}\}$

$$|A\mathbf{z}|^2 = \left| \sum_{i=1}^n \sigma_i \mathbf{u_i} \mathbf{v_i}^T \mathbf{z} \right|^2 = \sum_{i=1}^n \sigma_i^2 \left(\mathbf{v_i}^T \mathbf{z} \right)^2 = \sum_{i=1}^{k+1} \sigma_i^2 \left(\mathbf{v_i}^T \mathbf{z} \right)^2 \ge \sigma_{k+1}^2 \sum_{i=1}^{k+1} \left(\mathbf{v_i}^T \mathbf{z} \right)^2 = \sigma_{k+1}^2.$$

It follows that

$$||A - B||_2^2 \ge \sigma_{k+1}^2$$

contradicting the assumption that $||A - B||_2 < \sigma_{k+1}$. This proves the theorem.

4.4 Power Method for Computing the Singular Value Decomposition

Computing the singular value decomposition is an important branch of numerical analysis in which there have been many sophisticated developments over a long period of time. Here we present an "in-principle" method to establish that the approximate SVD of a matrix A can be computed in polynomial time. The reader is referred to numerical

analysis texts for more details. The method we present, called the Power Method, is conceptually simple. The word power refers to taking high powers of the matrix $B = AA^T$. If the SVD of A is $\sum_i \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, then by direct multiplication

$$B = AA^{T} = \left(\sum_{i} \sigma_{i} \mathbf{u}_{i} \mathbf{v}_{i}^{T}\right) \left(\sum_{j} \sigma_{j} \mathbf{v}_{j} \mathbf{u}_{j}^{T}\right)$$
$$= \sum_{i,j} \sigma_{i} \sigma_{j} \mathbf{u}_{i} \mathbf{v}_{i}^{T} \mathbf{v}_{j} \mathbf{u}_{j}^{T} = \sum_{i,j} \sigma_{i} \sigma_{j} \mathbf{u}_{i} (\mathbf{v}_{i}^{T} \cdot \mathbf{v}_{j}) \mathbf{u}_{j}^{T}$$
$$= \sum_{i} \sigma_{i}^{2} \mathbf{u}_{i} \mathbf{u}_{i}^{T},$$

since $\mathbf{v_i}^T \mathbf{v_j}$ is the dot product of the two vectors and is zero unless i = j. [Caution: $\mathbf{u_i u_j}^T$ is a matrix and is not zero even for $i \neq j$.] Using the same kind of calculation,

$$B^k = \sum_i \sigma_i^{2k} \mathbf{u_i} \mathbf{u_i}^T.$$

As k increases, for $i>1,\,\sigma_i^{2k}/\sigma_1^{2k}$ goes to zero and B^k is approximately equal to

$$\sigma_1^{2k} \mathbf{u_1} \mathbf{u_1}^T$$

provided that for each i > 1, $\sigma_i(A) < \sigma_1(A)$.

This suggests a way of finding σ_1 and $\mathbf{u_1}$, by successively powering B. But there are two issues. First, if there is a significant gap between the first and second singular values of a matrix, then the above argument applies and the power method will quickly converge to the first left singular vector. Suppose there is no significant gap. In the extreme case, there may be ties for the top singular value. Then the above argument does not work. We overcome this problem in Theorem 4.11 below which states that even with ties, the power method converges to some vector in the span of those singular vectors corresponding to the "nearly highest" singular values.

A second issue is that computing B^k costs k matrix multiplications when done in a straight-forward manner or $O(\log k)$ when done by successive squaring. Instead we compute

$$B^k \mathbf{x}$$

where \mathbf{x} is a random unit length vector. Each increase in k requires a matrix-vector product which takes time proportional to the number of nonzero entries in B. Further saving may be achieved by writing

$$B^k \mathbf{x} = AA^T \left(B^{k-1} \mathbf{x} \right).$$

Now the cost is proportional to the number of nonzero entries in A. Since $B^k \mathbf{x} \approx \sigma_1^{2k} \mathbf{u_1} (\mathbf{u}_1^T \cdot \mathbf{x})$ is a scalar multiple of $\mathbf{u_1}$, $\mathbf{u_1}$ can be recovered from $B^k \mathbf{x}$ by normalization.

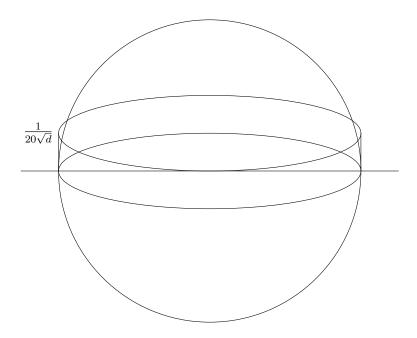


Figure 4.3: The volume of the cylinder of height $\frac{1}{20\sqrt{d}}$ is an upper bound on the volume of the hemisphere below $x_1 = \frac{1}{20\sqrt{d}}$

We start with a technical Lemma needed in the proof of the theorem.

Lemma 4.10 Let $(x_1, x_2, ..., x_d)$ be a unit d-dimensional vector picked at random. The probability that $|x_1| \ge \frac{1}{20\sqrt{d}}$ is at least 9/10.

Proof: We first show that for a vector \mathbf{v} picked at random with $|\mathbf{v}| \leq 1$, the probability that $v_1 \geq \frac{1}{20\sqrt{d}}$ is at least 9/10. Then we let $\mathbf{x} = \mathbf{v}/|\mathbf{v}|$. This can only increase the value of v_1 , so the result follows.

Let $\alpha = \frac{1}{20\sqrt{d}}$. The probability that $|v_1| \geq \alpha$ equals one minus the probability that $|v_1| \leq \alpha$. The probability that $|v_1| \leq \alpha$ is equal to the fraction of the volume of the unit sphere with $|v_1| \leq \alpha$. To get an upper bound on the volume of the sphere with $|v_1| \leq \alpha$, consider twice the volume of the unit radius cylinder of height α . The volume of the portion of the sphere with $|v_1| \leq \alpha$ is less than or equal to $2\alpha A(d-1)$ and

$$\operatorname{Prob}(|v_1| \le \alpha) \le \frac{2\alpha A(d-1)}{V(d)}$$

Now the volume of the unit radius sphere is at least twice the volume of the cylinder of height $\frac{1}{\sqrt{d-1}}$ and radius $\sqrt{1-\frac{1}{d-1}}$ or

$$V(d) \ge \frac{2}{\sqrt{d-1}}V(d-1)(1-\frac{1}{d-1})^{\frac{d-2}{2}}$$

Using $(1-x)^a \ge 1-ax$

$$V(d) \ge \frac{2}{\sqrt{d-1}}A(d-1)(1 - \frac{d-2}{2}\frac{1}{d-1}) \ge \frac{V(d-1)}{\sqrt{d-1}}$$

and

$$Prob(|v_1| \le \alpha) \le \frac{2\alpha V(d-1)}{\frac{1}{\sqrt{d-1}}V(d-1)} \le \frac{\sqrt{d-1}}{10\sqrt{d}} \le \frac{1}{10}.$$

Thus the probability that $v_1 \ge \frac{1}{20\sqrt{d}}$ is at least 9/10.

Theorem 4.11 Let A be an $n \times d$ matrix and \mathbf{x} a random unit length vector. Let V be the space spanned by the left singular vectors of A corresponding to singular values greater than $(1 - \varepsilon) \sigma_1$. Let k be $\Omega\left(\frac{\ln(n/\varepsilon)}{\varepsilon}\right)$. Let \mathbf{w} be unit vector after k iterations of the power method, namely,

$$\mathbf{w} = \frac{\left(AA^T\right)^k \mathbf{x}}{\left| \left(AA^T\right)^k \mathbf{x} \right|}.$$

The probability that \mathbf{w} has a component of at least ϵ perpendicular to V is at most 1/10.

Proof: Let

$$A = \sum_{i=1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T$$

be the SVD of A. If the rank of A is less than n, then complete $\{\mathbf{u_1}, \mathbf{u_2}, \dots \mathbf{u_r}\}$ into a basis $\{\mathbf{u_1}, \mathbf{u_2}, \dots \mathbf{u_n}\}$ of n-space. Write \mathbf{x} in the basis of the $\mathbf{u_i}'s$ as

$$\mathbf{x} = \sum_{i=1}^{n} c_i \mathbf{u_i}.$$

Since $(AA^T)^k = \sum_{i=1}^n \sigma_i^{2k} \mathbf{u_i} \mathbf{u_i}^T$, it follows that $(AA^T)^k \mathbf{x} = \sum_{i=1}^n \sigma_i^{2k} c_i \mathbf{u_i}$. For a random unit length vector \mathbf{x} picked independent of A, the $\mathbf{u_i}$ are fixed vectors and picking \mathbf{x} at random is equivalent to picking random c_i . From Lemma 4.10, $|c_1| \geq \frac{1}{20\sqrt{n}}$ with probability at least 9/10.

Suppose that $\sigma_1, \sigma_2, \ldots, \sigma_m$ are the singular values of A that are greater than or equal to $(1 - \varepsilon) \sigma_1$ and that $\sigma_{m+1}, \ldots, \sigma_n$ are the singular values that are less than $(1 - \varepsilon) \sigma_1$. Now

$$|(AA^T)^k \mathbf{x}|^2 = \left| \sum_{i=1}^n \sigma_i^{2k} c_i \mathbf{u_i} \right|^2 = \sum_{i=1}^n \sigma_i^{4k} c_i^2 \ge \sigma_1^{4k} c_1^2 \ge \frac{1}{400n} \sigma_1^{4k},$$

with probability at least 9/10. Here we used the fact that a sum of positive quantities is at least as large as its first element and the first element is greater than or equal to

 $\frac{1}{400n}\sigma_1^{4k}$ with probability at least 9/10.

The component of $|(AA^T)^k \mathbf{x}|^2$ perpendicular to the space V is

$$\sum_{i=m+1}^{n} \sigma_i^{4k} c_i^2 \le (1-\varepsilon)^{4k} \sigma_1^{4k} \sum_{i=m+1}^{n} c_i^2 \le (1-\varepsilon)^{4k} \sigma_1^{4k},$$

since $\sum_{i=1}^{n} c_i^2 = |\mathbf{x}| = 1$. Thus, the component of **w** perpendicular to V is at most

$$\frac{(1-\varepsilon)^{2k}\sigma_1^{2k}}{\frac{1}{20\sqrt{n}}\sigma_1^{2k}} = O(\sqrt{n}(1-\varepsilon)^{2k}) = O(\sqrt{n}e^{-2\varepsilon k}) = O\left(\sqrt{n}e^{-\Omega(\ln(n/\varepsilon))}\right) = O(\varepsilon)$$

as desired.

4.5 Applications of Singular Value Decomposition

4.5.1 Principal Component Analysis

The traditional use of SVD is in Principal Component Analysis (PCA). PCA is illustrated by an example - customer-product data where there are n customers buying dproducts. Let matrix A with elements a_{ij} represent the probability of customer i purchasing product j (or the amount or utility of product j to customer i). One hypothesizes that there are really only k underlying basic factors like age, income, family size, etc. that determine a customer's purchase behavior. An individual customer's behavior is determined by some weighted combination of these underlying factors. That is, a customer's purchase behavior can be characterized by a k-dimensional vector where k is much smaller that n and d. The components of the vector are weights for each of the basic factors. Associated with each basic factor is a vector of probabilities, each component of which is the probability of purchasing a given product by someone whose behavior depends only on that factor. More abstractly, A is an $n \times d$ matrix that can be expressed as the product of two matrices U and V where U is an $n \times k$ matrix expressing the factor weights for each customer and V is a $k \times d$ matrix expressing the purchase probabilities of products that correspond to that factor. One twist is that A may not be exactly equal to UV, but close to it since there may be noise or random perturbations.

Taking the best rank k approximation A_k from SVD (as described above) gives us such a U, V. In this traditional setting, one assumed that A was available fully and we wished to find U, V to identify the basic factors or in some applications to "denoise" A (if we think of A - UV as noise). Now imagine that n and d are very large, on the order of thousands or even millions, there is probably little one could do to estimate or even store A. In this setting, we may assume that we are given just given a few elements of A and wish to estimate A. If A was an arbitrary matrix of size $n \times d$, this would require $\Omega(nd)$ pieces of information and cannot be done with a few entries. But again hypothesize that A was a small rank matrix with added noise. If now we also assume that the given entries

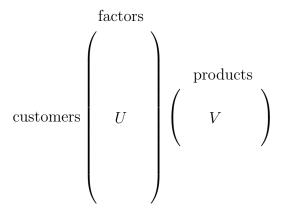


Figure 4.4: Customer-product data

are randomly drawn according to some known distribution, then there is a possibility that SVD can be used to estimate the whole of A. This area is called collaborative filtering and one of its uses is to target an ad to a customer based on one or two purchases. We will not be able to describe it here.

4.5.2 Clustering a Mixture of Spherical Gaussians

It is relatively easy to cluster points in two or three dimensions. However, clustering is not so easy in higher dimensions. Many problems have high-dimensional data and clustering problems are no exception. Clustering problems tend to be NP-hard, so we do not have polynomial time algorithms to solve them. For this reason, the application of stochastic models of input data to clustering problems has become important.

Mixture models are a very important class of stochastic models. A mixture is a probability density or distribution that is the weighted sum of simple component probability densities. It is of the form $w_1p_1 + w_2p_2 + \cdots + w_kp_k$ where p_1, p_2, \ldots, p_k are the basic densities and w_1, w_2, \ldots, w_k are positive real numbers called weights that add up to one. Clearly, $w_1p_1 + w_2p_2 + \cdots + w_kp_k$ is a probability density, it integrates to one.

The model fitting problem is to fit a mixture of k basic densities to n samples, each sample drawn according to the same mixture distribution. The class of basic densities is known, but the component weights of the mixture are not. Here, we deal with the case where the basic densities are all spherical Gaussians. The samples are generated by picking an integer i from the set $\{1, 2, ..., k\}$ with probabilities $w_1, w_2, ..., w_k$, respectively. Then, picking a sample according to p_i and repeating the process n times. This process generates n samples according to the mixture where the set of samples is naturally partitioned into k sets, each set corresponding to one p_i .

The model-fitting problem consists of two sub problems. The first sub problem is to

cluster the sample into k subsets where each subset was picked according to one component density. The second sub problem is to fit a distribution to each subset. We discuss only the clustering problem here. The problem of fitting a single Gaussian to a set of data points was discussed in Section 2.6 of Chapter 2.

If the component Gaussians in the mixture have their centers very close together, then the clustering problem is unresolvable. In the limiting case where a pair of component densities are the same, there is no way to distinguish between them. What condition on the inter-center separation will guarantee unambiguous clustering? First, by looking at 1-dimensional examples, it is clear that this separation should be measured in units of the standard deviation, since the density is a function of the number of standard deviation from the mean. In one dimension, if two Gaussians have inter-center separation at least ten times the maximum of their standard deviations, then they hardly overlap. What is the analog of this statement in higher dimensions?

For a d-dimensional spherical Gaussian, with standard deviation σ in each direction³, it is easy to see that the expected distance squared from the center is $d\sigma^2$. Define the radius r of the Gaussian to be the square root of the average distance squared from the center; so r is $\sqrt{d}\sigma$. If the inter-center separation between two spherical Gaussians, both of radius r is at least $2r = 2\sqrt{d}\sigma$, then it is easy to see that the densities hardly overlap. But this separation requirement grows with d and is too large to be useful in many cases. For a way out of such a strong requirement, imagine projecting the two Gaussians onto the 1-dimensional line joining their centers. The projection is also a Gaussian with the same standard deviation as shown in the following lemma.

Lemma 4.12 Suppose p is a d-dimensional spherical Gaussian with centre μ and standard deviation σ . The density of p projected onto an arbitrary k-dimensional subspace V is a spherical Gaussian with the same standard deviation.

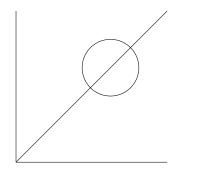
Proof: Since p is spherical, the projection is independent of the k-dimensional subspace. Pick V to be the subspace spanned by the first k coordinate vectors. For a point $\mathbf{x} = (x_1, x_2, \dots, x_d)$, we will use the notation $\mathbf{x}' = (x_1, x_2, \dots x_k)$ and $\mathbf{x}'' = (x_{k+1}, x_{k+2}, \dots, x_n)$. The density of the projected Gaussian at the point (x_1, x_2, \dots, x_k) is

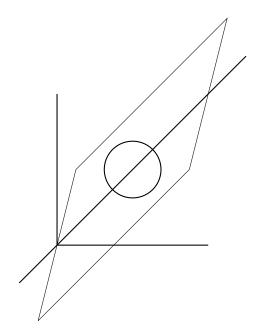
$$ce^{-\frac{|\mathbf{x}'-\mu'|^2}{2\sigma^2}} \int_{\mathbf{x}''} e^{-\frac{|\mathbf{x}''-\mu''|^2}{2\sigma^2}} d\mathbf{x}'' = c'e^{-\frac{|\mathbf{x}'-\mu'|^2}{2\sigma^2}}.$$

This clearly implies the lemma.

Once projected onto the line joining the two centers, the two Gaussians are just 1-dimensional Gaussians with standard deviation σ and so a separation distance of a certain

³Since a spherical Gaussian has the same standard deviation in every direction, we call it the standard deviation of the Gaussian.





- 1. Best fit 1-dimension subspace to a spherical Gaussian is the line through its center and the origin.
- 2. Any k-dimensional subspace containing the line is a best fit k-dimensional subspace for the Gaussian.
- 3. The best fit k-dimensional subspace for k Gaussians is the subspace containing their centers.
 - 1. Best fit 1-dimension subspace to a spherical Gaussian is the line through its center and the origin.
 - 2. Any k-dimensional subspace containing the line is a best fit k-dimensional subspace for the Gaussian.
 - 3. The best fit k-dimensional subspace for k Gaussians is the subspace containing their centers.

Figure 4.5: Best fit subspace to a spherical Gaussian.

number of σ (independent of d) should suffice. This leads to the question of how to find the space spanned by the two centers from the samples. More generally, if there are k Gaussians, how does one find the k-dimensional subspace spanned by the k centers? A simple argument shows that the best-fit k-dimensional subspace to the data points gives the answer.

We now show that the top k singular vectors produced by the SVD span the space of the k centers. First, we extend the notion of best fit to probability distributions. Then we show that for a single spherical Gaussian, the best fit 1-dimensional subspace is the line though the center of the Gaussian and the origin. Next, we show that the best fit k-dimensional subspace for a single Gaussian is any k-dimensional subspace containing the line through the Gaussian's center and the origin. Finally, for k spherical Gaussians, the best fit k-dimensional subspace is the subspace containing their centers. Thus, the

SVD finds the subspace that contains the centers.

Recall that for a set of points, the best-fit line is the line passing through the origin which minimizes the sum of squared distances to the points. We extend this definition to probability densities instead of a set of points.

Definition 4.1: If p is a probability density in d space, the best fit line for p is the line l passing through the origin that minimizes the expected squared (perpendicular) distance to the line, namely,

$$\int \operatorname{dist}\left(\mathbf{x},l\right)^{2} p\left(\mathbf{x}\right) d\mathbf{x}.$$

Recall that a k-dimensional subspace is the best-fit subspace if the sum of squared distances to it is minimized or equivalently, the sum of squared lengths of projections onto it is maximized. This was defined for a set of points, but again it can be extended to a density as above.

Definition 4.2: If p is a probability density in d-space and V is a subspace, then the expected squared perpendicular distance of V to p, denoted f(V, p), is given by

$$f(V, p) = \int \operatorname{dist}^{2}(\mathbf{x}, V) p(\mathbf{x}) d\mathbf{x},$$

where $\operatorname{dist}(\mathbf{x}, V)$ denotes the perpendicular distance from the point \mathbf{x} to the subspace V.

For the uniform density on the unit circle centered at the origin, it is easy to see that any line passing through the origin is a best fit line for the probability distribution.

Lemma 4.13 Let the probability density p be a spherical Gaussian with center $\mu \neq 0$. The best fit 1-dimensional subspace is the line passing through μ and the origin.

Proof: For a randomly chosen x (according to p) and a fixed unit length vector \mathbf{v} ,

$$E\left[\left(\mathbf{v}^{T}\mathbf{x}\right)^{2}\right] = E\left[\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)+\mathbf{v}^{T}\boldsymbol{\mu}\right)^{2}\right]$$

$$= E\left[\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right)^{2}+2\left(\mathbf{v}^{T}\boldsymbol{\mu}\right)\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right)+\left(\mathbf{v}^{T}\boldsymbol{\mu}\right)^{2}\right]$$

$$= E\left[\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right)^{2}\right]+2\left(\mathbf{v}^{T}\boldsymbol{\mu}\right)E\left[\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right]+\left(\mathbf{v}^{T}\boldsymbol{\mu}\right)^{2}$$

$$= E\left[\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right)^{2}\right]+\left(\mathbf{v}^{T}\boldsymbol{\mu}\right)^{2}$$

$$= \sigma^{2}+\left(\mathbf{v}^{T}\boldsymbol{\mu}\right)^{2}$$

since $E\left[\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right)^{2}\right]$ is the variance in the direction \mathbf{v} and $E\left(\mathbf{v}^{T}\left(\mathbf{x}-\boldsymbol{\mu}\right)\right)=0$. The lemma follows from the fact that the best fit line \mathbf{v} is the one that maximizes $\left(\mathbf{v}^{T}\mathbf{u}\right)^{2}$ which is maximized when \mathbf{v} is aligned with the center $\boldsymbol{\mu}$.

Lemma 4.14 For a spherical Gaussian with center μ , a k-dimensional subspace is a best fit subspace if and only if it contains μ .

Proof: By symmetry, every k-dimensional subspace through μ has the same sum of distances squared to the density. Now by the SVD procedure, we know that the best-fit k-dimensional subspace contains the best fit line, i.e., contains μ . Thus, the lemma follows.

This immediately leads to the following theorem.

Theorem 4.15 If p is a mixture of k spherical Gaussians whose centers span a k-dimensional subspace, then the best fit k-dimensional subspace is the one containing the centers.

Proof: Let p be the mixture $w_1p_1+w_2p_2+\cdots+w_kp_k$. Let V be any subspace of dimension k or less. Then, the expected squared perpendicular distance of V to p is

$$f(V, p) = \int \operatorname{dist}^{2}(\mathbf{x}, V) p(\mathbf{x}) d\mathbf{x}$$

$$= \sum_{i=1}^{k} w_{i} \int \operatorname{dist}^{2}(\mathbf{x}, V) p_{i}(\mathbf{x}) d\mathbf{x}$$

$$\geq \sum_{i=1}^{k} w_{i} (\text{ distance squared of } p_{i} \text{ to its best fit } k\text{-dimensional subspace}).$$

Choose V to be the space spanned by the centers of the densities p_i . By Lemma ?? the last inequality becomes an equality proving the theorem.

For an infinite set of points drawn according to the mixture, the k-dimensional SVD subspace gives exactly the space of the centers. In reality, we have only a large number of samples drawn according to the mixture. However, it is intuitively clear that as the number of samples increases, the set of sample points approximates the probability density and so the SVD subspace of the sample is close to the space spanned by the centers. The details of how close it gets as a function of the number of samples are technical and we do not carry this out here.

4.5.3 An Application of SVD to a Discrete Optimization Problem

In the last example, SVD was used as a dimension reduction technique. It found a k-dimensional subspace (the space of centers) of a d-dimensional space and made the Gaussian clustering problem easier by projecting the data to the subspace. Here, instead of fitting a model to data, we have an optimization problem. Again applying dimension reduction to the data makes the problem easier. The use of SVD to solve discrete optimization problems is a relatively new subject with many applications. We start with

an important NP-hard problem, the Maximum Cut Problem for a directed graph G(V, E).

The Maximum Cut Problem is to partition the node set V of a directed graph into two subsets S and \bar{S} so that the number of edges from S to \bar{S} is maximized. Let A be the adjacency matrix of the graph. With each vertex i, associate an indicator variable x_i . The variable x_i will be set to 1 for $i \in S$ and 0 for $i \in \bar{S}$. The vector $\mathbf{x} = (x_1, x_2, \dots, x_n)$ is unknown and we are trying to find it (or equivalently the cut), so as to maximize the number of edges across the cut. The number of edges across the cut is precisely

$$\sum_{i,j} x_i (1 - x_j) a_{ij}.$$

Thus, the Maximum Cut Problem can be posed as the optimization problem

Maximize
$$\sum_{i,j} x_i (1 - x_j) a_{ij}$$
 subject to $x_i \in \{0, 1\}$.

In matrix notation,

$$\sum_{i,j} x_i (1 - x_j) a_{ij} = \mathbf{x}^T A (\mathbf{1} - \mathbf{x}),$$

where $\mathbf{1}$ denotes the vector of all 1's . So, the problem can be restated as

Maximize
$$\mathbf{x}^T A(\mathbf{1} - \mathbf{x})$$
 subject to $x_i \in \{0, 1\}.$ (4.1)

The SVD is used to solve this problem approximately by computing the SVD of A and replacing A by $A_k = \sum_{i=1}^k \sigma_i \mathbf{u_i} \mathbf{v_i}^T$ in (4.1) to get

Maximize
$$\mathbf{x}^T A_k(\mathbf{1} - \mathbf{x})$$
 subject to $x_i \in \{0, 1\}.$ (4.2)

Note that the matrix A_k is no longer a 0-1 adjacency matrix.

We will show that:

- 1. For each 0-1 vector \mathbf{x} , $\mathbf{x}^T A_k (\mathbf{1} \mathbf{x})$ and $\mathbf{x}^T A (\mathbf{1} \mathbf{x})$ differ by at most $\frac{n^2}{\sqrt{k+1}}$. Thus, the maxima in (4.1) and (4.2) differ by at most this amount.
- 2. A near optimal **x** for (4.2) can be found by exploiting the low rank of A_k , which by Item 1 is near optimal for (4.1) where near optimal means with additive error of at most $\frac{n^2}{\sqrt{k+1}}$.

First, we prove Item 1. Since \mathbf{x} and $\mathbf{1} - \mathbf{x}$ are 0-1 *n*-vectors, each has length at most \sqrt{n} . By the definition of the 2-norm, $|(A - A_k)(\mathbf{1} - \mathbf{x})| \leq \sqrt{n}||A - A_k||_2$. Now since $\mathbf{x}^T(A - A_k)(\mathbf{1} - \mathbf{x})$ is the dot product of the vector \mathbf{x} with the vector $(A - A_k)(\mathbf{1} - \mathbf{x})$,

$$|\mathbf{x}^T(A - A_k)(\mathbf{1} - \mathbf{x})| \le n||A - A_k||_2.$$

By Lemma 4.8, $||A - A_k||_2 = \sigma_{k+1}(A)$. The inequalities,

$$(k+1)\sigma_{k+1}^2 \le \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_{k+1}^2 \le ||A||_F^2 = \sum_{i,j} a_{ij}^2 \le n^2$$

imply that $\sigma_{k+1}^2 \leq \frac{n^2}{k+1}$ and hence $||A - A_k||_2 \leq \frac{n}{\sqrt{k+1}}$ proving Item 1.

Next we focus on Item 2. It is instructive to look at the special case when k=1 and A is approximated by the rank one matrix A_1 . An even more special case when the left and right singular vectors \mathbf{u} and \mathbf{v} are required to be identical is already NP-hard to solve exactly because it subsumes the problem of whether for a set of n integers, $\{a_1, a_2, \ldots, a_n\}$, there is a partition into two subsets whose sums are equal. So, we look for algorithms that solve the Maximum Cut Problem approximately.

For Item 2, we want to maximize $\sum_{i=1}^k \sigma_i(\mathbf{x}^T \mathbf{u_i})(\mathbf{v_i}^T(\mathbf{1} - \mathbf{x}))$ over 0-1 vectors \mathbf{x} . A piece of notation will be useful. For any $S \subseteq \{1, 2, \dots n\}$, write $\mathbf{u_i}(S)$ for the sum of coordinates of the vector $\mathbf{u_i}$ corresponding to elements in the set S and also for $\mathbf{v_i}$. That is, $\mathbf{u}_i(S) = \sum_{i \in S} u_{ij}$. We maximize $\sum_{i=1}^k \sigma_i \mathbf{u_i}(S) \mathbf{v_i}(\bar{S})$ by dynamic programming.

Näively, we seem to need to compute for each subset S of $\{1, 2, ..., n\}$, the 2kdimensional vector $\mathbf{w}(S) = (\mathbf{u_1}(S), \mathbf{v_1}(\bar{S}), \mathbf{u_2}(S), \mathbf{v_2}(\bar{S}), \dots, \mathbf{u_k}(S), \mathbf{v_k}(\bar{S}))$. But this would take exponential (in n) time. Instead, we will approximate the $\mathbf{w}(S)$ to granularity δ , where, $\delta = O(\sqrt{n}/\sqrt{k})$; i.e., we will replace each $\mathbf{u_i}(S)$ and $\mathbf{v_i}(\bar{S})$ by their nearest integer multiple of δ . Since $|\mathbf{u_i}|, |\mathbf{v_i}| = 1$, we have $|\mathbf{u_i}(S)|, |\mathbf{v_i}(\bar{S})| \leq \sqrt{n}$ and so the set R of possible (approximate) values of each coordinate of $\mathbf{w}(S)$ has only $O(\sqrt{k})$ elements. Let R^{2k} be the set of possible values of the 2k-dimensional vector $\mathbf{w}(S)$ (with rounded to integer multiples of δ). We only need to know for each of the $O(\sqrt{k})^{2k}$ elements of R^{2k} whether or not there is some subset S whose \mathbf{w} is (approximated by) that element. [Then, we can find $\sigma_i \mathbf{u_i}(S) \mathbf{v_i}(\bar{S})$ approximately for each element for which there is an S and take the best of these. Later, we bound the error of this process. We do this by Dynamic Programming. We will consider subsets of S of $\{1, 2, \ldots, j\}$ for $j = 1, 2, \ldots, n$. Suppose we know already the elements of R^{2k} for which there is a subset S of $\{1, 2, \dots, j\}$ with $\mathbf{w}(S)$ (approximately) that element. We want to do this for all $S' \subseteq \{1, 2, \dots, j+1\}$. Each $S \subseteq \{1, 2, ..., j\}$ leads to two $S' : S \cup \{j+1\}$ and S. For each, we can clearly find the (approximate) $\mathbf{w}(S')$ easily from $\mathbf{w}(S)$. This completes the inductive step. [We do not get exponential (in n) growth, since we never need to keep track of more than $O(k)^{2k}$ records.] What is the error caused by approximating $\mathbf{w}(S)$? The error is at most

$$O(k \sigma_1 \operatorname{Max}_i(|\mathbf{u_i}(S)|, |\mathbf{v_i}(\bar{S})|)\delta) \in O(n^2/\sqrt{k}).$$

It is not difficult to show that the running time of the algorithm is $O(nk^k)$. The running time is exponential in k, but polynomial in n. We summarize what we have accomplished.

Theorem 4.16 Given a directed graph G(V, E), a cut of size at least the maximum cut minus $O\left(\frac{n^2}{\sqrt{k}}\right)$ can be computed in time k^k times a polynomial in n.

It would be quite a surprise to have an algorithm that actually achieves the same accuracy in time polynomial in n and k because this would give an exact max cut in polynomial time.

4.5.4 SVD as a Compression Algorithm

Suppose A is the pixel intensity matrix of a large image. The entry a_{ij} gives the intensity of the ij^{th} pixel. If A is $n \times n$, the transmission of A requires transmitting $O(n^2)$ real numbers. Instead, one could send A_k , that is, the top k singular values $\sigma_1, \sigma_2, \ldots, \sigma_k$ along with the left and right singular vectors $\mathbf{u_1}, \mathbf{u_2}, \ldots, \mathbf{u_k}$, and $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_k}$. This would require sending O(kn) real numbers instead of $O(n^2)$ real numbers. If k is much smaller than n, this results in savings. For many images, a k much smaller than n can be used to reconstruct the image provided that a very low resolution version of the image is sufficient. Thus, one could use SVD as a compression method.

It turns out that in a more sophisticated approach, for certain classes of pictures one could use a fixed basis so that the top (say) hundred singular vectors are sufficient to represent any picture approximately. This means that the space spanned by the top hundred singular vectors is not too different from the space spanned by the top two hundred singular vectors of a given matrix in that class. Compressing these matrices by this standard basis can save substantially since the standard basis is transmitted only once and a matrix is transmitted by sending the top several hundred singular values for the standard basis.

4.5.5 Spectral Decomposition

Let B be a square matrix. If the vector \mathbf{x} and scalar λ are such that $B\mathbf{x} = \lambda \mathbf{x}$, then \mathbf{x} is an eigenvector of the matrix B and λ is the corresponding eigenvalue. We present here a spectral decomposition theorem for the special case where B is of the form $B = AA^T$ for some (possibly rectangular) matrix A. If A is a real valued matrix, then B is symmetric and positive definite. That is, $\mathbf{x}^T B\mathbf{x} > 0$ for all nonzero vectors \mathbf{x} . The spectral decomposition theorem holds more generally and the interested reader should consult a linear algebra book.

Theorem 4.17 (Spectral Decomposition) If $B = AA^T$ then $B = \sum_i \sigma_i^2 u_i u_i^T$ where $A = \sum_i \sigma_i u_i v_i^T$ is the singular valued decomposition of A.

Proof:

$$B = AA^{T} = \left(\sum_{i} \sigma_{i} \mathbf{u_{i}} \mathbf{v_{i}}^{T}\right) \left(\sum_{j} \sigma_{j} \mathbf{u_{j}} v_{j}^{T}\right)^{T}$$
$$= \sum_{i} \sum_{j} \sigma_{i} \sigma_{j} \mathbf{u_{i}} \mathbf{v_{i}}^{T} \mathbf{v_{j}} \mathbf{u_{j}}^{T}$$
$$= \sum_{i} \sigma_{i}^{2} \mathbf{u_{i}} \mathbf{u_{i}}^{T}.$$

When the σ_i are all distinct, the $\mathbf{u_i}$ are the eigenvectors of B and the σ_i^2 are the corresponding eigenvalues. If the σ_i are not distinct, then any vector that is a linear combination of those $\mathbf{u_i}$ with the same eigenvalue is an eigenvector of B.

4.5.6 Singular Vectors and ranking documents

An important task for a document collection is to rank the documents. Recall the term-document vector representation from Chapter 2. A näive method would be to rank in order of the total length of the document (which is the sum of the components of its term-document vector). Clearly, this is not a good measure in many cases. This näive method attaches equal weight to each term and takes the projection (dot product) term-document vector in the direction of the all 1 vector. Is there a better weighting of terms, i.e., a better projection direction which would measure the intrinsic relevance of the document to the collection? A good candidate is the best-fit direction for the collection of term-document vectors, namely the top (left) singular vector of the term-document matrix. An intuitive reason for this is that this direction has the maximum sum of squared projections of the collection and so can be thought of as a synthetic term-document vector best representing the document collection.

Ranking in order of the projection of each document's term vector along the best fit direction has a nice interpretation in terms of the power method. For this, we consider a different example - that of web with hypertext links. The World Wide Web can be represented by a directed graph whose nodes correspond to web pages and directed edges to hypertext links between pages. Some web pages, called *authorities*, are the most prominent sources for information on a given topic. Other pages called *hubs*, are ones that identify the authorities on a topic. Authority pages are pointed to by many hub pages and hub pages point to many authorities. One is led to what seems like a circular definition: a hub is a page that points to many authorities and an authority is a page that is pointed to by many hubs.

One would like to assign hub weights and authority weights to each node of the web. If there are n nodes, the hub weights form a n-dimensional vector \mathbf{u} and the authority weights form a n-dimensional vector \mathbf{v} . Suppose A is the adjacency matrix representing

the directed graph: a_{ij} is 1 if there is a hypertext link from page i to page j and 0 otherwise. Given hub vector \mathbf{u} , the authority vector \mathbf{v} could be computed by the formula

$$\mathbf{v}_j = \sum_{i=1}^d u_i a_{ij}$$

since the right hand side is the sum of the hub weights of all the nodes that point to node j. In matrix terms,

$$\mathbf{v} = A^T \mathbf{u}$$
.

Similarly, given an authority vector \mathbf{v} , the hub vector \mathbf{u} could be computed by $\mathbf{u} = A\mathbf{v}$. Of course, at the start, we have neither vector. But the above suggests a power iteration. Start with any \mathbf{v} . Set $\mathbf{u} = A\mathbf{v}$; then set $\mathbf{v} = A^T\mathbf{u}$ and repeat the process. We know from the power method that this converges to the left and right singular vectors. So after sufficiently many iterations, we may use the left vector \mathbf{u} as hub weights vector and project each column of A onto this direction and rank columns (authorities) in order of this projection. But the projections just form the vector $A^T\mathbf{u}$ which equals \mathbf{v} . So we can just rank by order of v_i .

This is the basis of an algorithm called the HITS algorithm which was one of the early proposals for ranking web pages.

A different ranking called *page rank* is widely used. It is based on a random walk on the grap described above. (We will study Random Walks in detail in Chapter 5 and the reader may postpone reading this application until then.)

A random walk on the web goes from web page i to a randomly chosen neighbor of it. so if p_{ij} is the probability of going from i to j, then p_{ij} is just 1/ (number of hypertext links from i). Represent the p_{ij} in a matrix P. This matrix is called the *transition probability matrix* of the random walk. Represent the probabilities of being in each state at time t by the components of a row vector $\mathbf{p}(t)$. The probability of being in state j at time t is given by the equation

$$p_j(t) = \sum_{i} p_i(t-1) p_{ij}.$$

Then

$$\mathbf{p}\left(t\right) = \mathbf{p}\left(t-1\right)P$$

and thus

$$\mathbf{p}\left(t\right) = \mathbf{p}\left(0\right)P^{t}.$$

The probability vector $\mathbf{p}(t)$ is computed by computing P to the power t. It turns out that under some conditions, the random walk has a steady state probability vector that we can think of as $\mathbf{p}(\infty)$. It has turned out to be very useful to rank pages in decreasing order of $p_j(\infty)$ in essence saying that the web pages with the highest steady state probabilities are the most important.

In the above explanation, the random walk goes from page i to one of the web pages pointed to by i, picked uniformly at random. Modern technics for ranking pages are more complex. A more sophisticated random walk is used for several reasons. First, a web page might not contain any links and thus there is nowhere for the walk to go. Second, a page that has no in links will never be reached. Even if every node had at least one in link and one out link, the graph might not be strongly connected and the walk would eventually end up in some strongly connected component of the graph. Another difficulty occurs when the graph is periodic, that is, the greatest common divisor of all cycle lengths of the graph is greater than one. In this case, the random walk does not converge to a stationary probability distribution but rather oscillates between some set of probability distributions. We will consider this topic further in Chapter 5.

4.6 Bibliographic Notes

Singular value decomposition is fundamental to numerical analysis and linear algebra. There are many texts on these subjects and the interested reader may want to study these. A good reference is [GvL96]. The material on clustering a mixture of Gaussians in Section 4.5.2 is from [VW02]. Modeling data with a mixture of Gaussians is a standard tool in statistics. Several well-known heuristics like the expectation-minimization algorithm are used to learn (fit) the mixture model to data. Recently, in theoretical computer science, there has been modest progress on provable polynomial-time algorithms for learning mixtures. Some references are [DS07], [AK], [AM05], [MV10]. The application to the discrete optimization problem is from [FK99]. The section on ranking documents/webpages is from two influential papers, one on hubs and authorities by Jon Kleinberg [Kle99] and the other on pagerank by Page, Brin, Motwani and Winograd [BMPW98].

4.7 Exercises

Exercise 4.1 (Best fit functions versus best least squares fit) In many experiments one collects the value of a parameter at various instances of time. Let y_i be the value of the parameter y at time x_i . Suppose we wish to construct the best linear approximation to the data in the sense that we wish to minimize the mean square error. Here error is measured vertically rather than perpendicular to the line. Develop formulas for m and b to minimize the mean square error of the points $\{(x_i, y_i) | 1 \le i \le n\}$ to the line y = mx + b.

Exercise 4.2 Given five observed parameters, height, weight, age, income, and blood pressure of n people, how would one find the best least squares fit subspace of the form

$$a_1 \left(height \right) + a_2 \left(weight \right) + a_3 \left(age \right) + a_4 \left(income \right) + a_5 \left(blood \ pressure \right) = 0$$

Here a_1, a_2, \ldots, a_5 are the unknown parameters. If there is a good best fit 4-dimensional subspace, then one can think of the points as lying close to a 4-dimensional sheet rather than points lying in 5-dimensions. Why is it better to use the perpendicular distance to the subspace rather than vertical distance where vertical distance to the subspace is measured along the coordinate axis corresponding to one of the unknowns?

Exercise 4.3 What is the best fit line for each of the following set of points?

- 1. $\{(0,1),(1,0)\}$
- $2. \{(0,1),(2,0)\}$
- 3. The rows of the matrix

$$\left(\begin{array}{cc}
17 & 4 \\
-2 & 26 \\
11 & 7
\end{array}\right)$$

Exercise 4.4 Let A be a square $n \times n$ matrix whose rows are orthonormal. Prove that the columns of A are orthonormal.

Exercise 4.5 Suppose A is a $n \times n$ matrix with block diagonal structure with k equal size blocks where all entries of the i^{th} block are a_i with $a_1 > a_2 > \cdots > a_k > 0$. Show that A has exactly k nonzero singular vectors $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_k}$ where $\mathbf{v_i}$ has the value $(\frac{k}{n})^{1/2}$ in the coordinates corresponding to the i^{th} block and 0 elsewhere. In other words, the singular vectors exactly identify the blocks of the diagonal. What happens if $a_1 = a_2 = \cdots = a_k$? In the case where the a_i are equal, what is the structure of the set of all possible singular vectors?

Hint: By symmetry, the top singular vector's components must be constant in each block.

Exercise 4.6 Prove that the left singular vectors of A are the right singular vectors of A^T .

Exercise 4.7 Interpret the right and left singular vectors for the document term matrix.

Exercise 4.8 Verify that the sum of rank one matrices $\sum_{i=1}^{r} \sigma_i \mathbf{u_i} \mathbf{v_i}^T$ can be written as UDV^T , where the $\mathbf{u_i}$ are the columns of U and $\mathbf{v_i}$ are the columns of V. To do this, first verify that for any two matrices P and Q, we have

$$PQ = \sum_{i} \mathbf{p_i} \mathbf{q_i}^T$$

where $\mathbf{p_i}$ is the i^{th} column of P and $\mathbf{q_i}$ is the i^{th} column of Q.

Exercise 4.9

- 1. Show that the rank of A is r where r is the miminum i such that $\underset{|\mathbf{v}|=1}{\operatorname{arg max}} |A|\mathbf{v}| = 0.$
- 2. Show that $\left|\mathbf{u}_{1}^{T}A\right| = \max_{\left|\mathbf{u}\right|=1} \left|\mathbf{u}^{T}A\right| = \sigma_{1}$.

Hint: Use SVD.

Exercise 4.10 If $\sigma_1, \sigma_2, \ldots, \sigma_r$ are the singular values of A and $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r$ are the corresponding right singular vectors, show that

1.
$$A^T A = \sum_{i=1}^r \sigma_i^2 \mathbf{v_i} \mathbf{v_i}^T$$

- 2. $\mathbf{v}_1, \mathbf{v}_2, \dots \mathbf{v}_r$ are eigenvectors of $A^T A$.
- 3. Assuming that the set of eigenvectors of a matrix is unique, conclude that the set of singular values of the matrix is unique.

See the appendix for the definition of eigenvectors.

Exercise 4.11 Let A be a matrix. Given an algorithm for finding

$$\mathbf{v_1} = \underset{|\mathbf{v}|=1}{\operatorname{arg\,max}} |A\mathbf{v}|$$

describe an algorithm to find the SVD of A.

Exercise 4.12 Compute the singular valued decomposition of the matrix

$$A = \left(\begin{array}{cc} 1 & 2 \\ 3 & 4 \end{array}\right)$$

Exercise 4.13 Write a program to implement the power method for computing the first singular vector of a matrix. Apply your program to the matrix

$$A = \begin{pmatrix} 1 & 2 & 3 & \cdots & 9 & 10 \\ 2 & 3 & 4 & \cdots & 10 & 0 \\ \vdots & \vdots & \vdots & & & \vdots \\ 9 & 10 & 0 & \cdots & 0 & 0 \\ 10 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

Exercise 4.14 Modify the power method to find the first four singular vectors of a matrix A as follows. Randomly select four vectors and find an orthonormal basis for the space spanned by the four vectors. Then multiple each of the basis vectors times A and find a new orthonormal basis for the space spanned by the resulting four vectors. Apply your method to find the first four singular vectors of matrix A of Exercise 4.13

Exercise 4.15 Let A be a real valued matrix. Prove that $B = AA^T$ is positive definite.

Exercise 4.16 Prove that the eigenvalues of a symmetric real valued matrix are real.

Exercise 4.17 Suppose A is a square invertible matrix and the SVD of A is $A = \sum_{i} \sigma_{i} u_{i} v_{i}^{T}$. Prove that the inverse of A is $\sum_{i} \frac{1}{\sigma_{i}} v_{i} u_{i}^{T}$.

Exercise 4.18 Suppose A is square, but not necessarily invertible and has SVD $A = \sum_{i=1}^{r} \sigma_{i} u_{i} v_{i}^{T}$. Let $B = \sum_{i=1}^{r} \frac{1}{\sigma_{i}} v_{i} u_{i}^{T}$. Show that $B\mathbf{x} = \mathbf{x}$ for all \mathbf{x} in the span of the right singular vectors of A. For this reason B is sometimes called the pseudo inverse of A and can play the role of A^{-1} in many applications.

Exercise 4.19

- 1. For any matrix A, show that $\sigma_k \leq \frac{||A||_F}{\sqrt{k}}$.
- 2. Prove that there exists a matrix B of rank at most k such that $||A B||_2 \leq \frac{||A||_F}{\sqrt{k}}$.
- 3. Can the 2-norm on the left hand side in (b) be replaced by Frobenius norm?

Exercise 4.20 Suppose an $n \times d$ matrix A is given and you are allowed to preprocess A. Then you are given a number of d-dimensional vectors $\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_m}$ and for each of these vectors you must find the vector $A\mathbf{x_i}$ approximately, in the sense that you must find a vector $\mathbf{u_i}$ satisfying $|\mathbf{u_i} - A\mathbf{x_i}| \leq \varepsilon ||A||_F |\mathbf{x_i}|$. Here $\varepsilon > 0$ is a given error bound. Describe an algorithm that accomplishes this in time $O\left(\frac{d+n}{\varepsilon^2}\right)$ per $\mathbf{x_i}$ not counting the preprocessing time.

Exercise 4.21 (Constrained Least Squares Problem using SVD) Given A, b, and m, use the SVD algorithm to find a vector \mathbf{x} with $|\mathbf{x}| < m$ minimizing $|A\mathbf{x} - \mathbf{b}|$. This problem is a learning exercise for the advanced student. For hints/solution consult Golub and van Loan, Chapter 12.

Exercise 4.22 (Document-Term Matrices): Suppose we have a $m \times n$ document-term matrix where each row corresponds to a document where the rows have been normalized to length one. Define the "similarity" between two such documents by their dot product.

- 1. Consider a "synthetic" document whose sum of squared similarities with all documents in the matrix is as high as possible. What is this synthetic document and how would you find it?
- 2. How does the synthetic document in (1) differ from the center of gravity?
- 3. Building on (1), given a positive integer k, find a set of k synthetic documents such that the sum of squares of the mk similarities between each document in the matrix and each synthetic document is maximized. To avoid the trivial solution of selecting k copies of the document in (1), require the k synthetic documents to be orthogonal to each other. Relate these synthetic documents to singular vectors.
- 4. Suppose that the documents can be partitioned into k subsets (often called clusters), where documents in the same cluster are similar and documents in different clusters are not very similar. Consider the computational problem of isolating the clusters. This is a hard problem in general. But assume that the terms can also be partitioned into k clusters so that for i ≠ j, no term in the ith cluster occurs in a document in the jth cluster. If we knew the clusters and arranged the rows and columns in them to be contiguous, then the matrix would be a block-diagonal matrix. Of course the clusters are not known. By a "block" of the document-term matrix, we mean a submatrix with rows corresponding to the ith cluster of documents and columns corresponding to the ith cluster of terms. We can also partition any n vector into blocks. Show that any right singular vector of the matrix must have the property that each of its blocks is a right singular vector of the corresponding block of the document-term matrix.
- 5. Suppose now that the singular values of all the blocks are distinct (also across blocks). Show how to solve the clustering problem.

Hint: (4) Use the fact that the right singular vectors must be eigenvectors of A^TA . Show that A^TA is also block-diagonal and use properties of eigenvectors.

Exercise 4.23 Generate a number of samples according to a mixture of 1-dimensional Gaussians. See what happens as the centers get closer. Alternatively, see what happens when the centers are fixed and the standard deviation is increased.

Exercise 4.24 Show that maximizing $\mathbf{x}^T \mathbf{u} \mathbf{u}^T (\mathbf{1} - \mathbf{x})$ subject to $x_i \in \{0, 1\}$ is equivalent to partitioning the coordinates of \mathbf{u} into two subsets where the sum of the elements in both subsets are equal.

Exercise 4.25 Read in a photo and convert to a matrix. Perform a singular value decomposition of the matrix. Reconstruct the photo using only 10%, 25%, 50% of the singular values.

- 1. Print the reconstructed photo. How good is the quality of the reconstructed photo?
- 2. What percent of the Forbenius norm is captured in each case?

Hint: If you use Matlab, the command to read a photo is imread. The types of files that can be read are given by imformats. To print the file use imwrite. Print using jpeg format. To access the file afterwards you may need to add the file extension .jpg. The command imread will read the file in uint8 and you will need to convert to double for the SVD code. Afterwards you will need to convert back to uint8 to write the file. If the photo is a color photo you will get three matrices for the three colors used.

Exercise 4.26 Find a collection of something such as photgraphs, drawings, or charts and try the SVD compression technique on it. How well does the reconstruction work?

Exercise 4.27 Create a set of 100, 100×100 matrices of random numbers between 0 and 1 such that each entry is highly correlated with the adjacency entries. Find the SVD of A. What fraction of the Frobenius norm of A is captured by the top 100 singular vectors? How many singular vectors are required to capture 95% of the Frobenius norm?

Exercise 4.28 Create a 100×100 matrix A of random numbers between 0 and 1 such that each entry is highly correlated with the adjacency entries and find the first 100 vectors for a single basis that is reasonably good for all 100 matrices. How does one do this? What fraction of the Frobenius norm of a new matrix is captured by the basis?

Exercise 4.29 Show that the running time for the maximum cut algorithm in Section ?? can be carried out in time $O(n^3 + poly(n)k^k)$, where poly is some polynomial.

Exercise 4.30 Let $x_1, x_2, ..., x_n$ be n points in d-dimensional space and let X be the $n \times d$ matrix whose rows are the n points. Suppose we know only the matrix D of pairwise distances between points and not the coordinates of the points themselves. The x_{ij} are not unique since any translation, rotation, or reflection of the coordinate system leaves the distances invariant. Fix the origin of the coordinate system so that the centroid of the set of points is at the origin.

1. Show that the elements of X^TX are given by

$$x_i^T x_j = -\frac{1}{2} \left[d_{ij}^2 - \frac{1}{n} \sum_{j=1}^n d_{ij}^2 - \frac{1}{n} \sum_{i=1}^n d_{ij}^2 + \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^n d_{ij}^2 \right].$$

2. Describe an algorithm for determining the matrix X whose rows are the x_i .

Solution: (1) Since the centroid of the set of points is at the origin of the coordinate axes, $\sum_{i=1}^{n} x_{ij} = 0$. Write

$$d_{ij}^2 = (x_i - x_j)^T (x_i - x_j) = x_i^T x_i + x_j^T x_j - 2x_i^T x_j$$
(4.3)

Then

$$\frac{1}{n}\sum_{i=1}^{n}d_{ij}^{2} = \frac{1}{n}\sum_{i=1}^{n}x_{i}^{T}x_{i} + x_{j}^{T}x_{j}$$

$$(4.4)$$

Since $\frac{1}{n} \sum_{i=1}^{n} x_j^T x_j = x_j^T x_j$ and $\frac{1}{n} \left(\sum_{i=1}^{n} x_i^T \right) x_j = 0$. Similarly

$$\frac{1}{n}\sum_{j=1}^{n}d_{ij}^{2} = \frac{1}{n}\sum_{j=1}^{n}x_{j}^{T}x_{j} + x_{i}^{T}x_{i}$$

$$\tag{4.5}$$

Summing (4.4) over j gives

$$\frac{1}{n} \sum_{j=1}^{n} \sum_{i=1}^{n} d_{ij}^{2} = \sum_{i=1}^{n} x_{i}^{T} x_{i} + \sum_{j=1}^{n} x_{j}^{T} x_{j} = 2 \sum_{i=1}^{n} x_{i}^{T} x_{i}$$

$$(4.6)$$

Rearranging (4.3) and substituting for $x_i^T x_i$ and $x_i^T x_j$ from (4.3) and (4.4) yields

$$x_i^T x_j = -\frac{1}{2} \left(d_{ij}^2 - x_i^T x_i - x_j^T x_j \right) = -\frac{1}{2} \left(d_{ij}^2 - \frac{1}{n} \sum_{j=1}^n d_{ij}^2 - \frac{1}{n} \sum_{i=1}^n d_{ij}^2 + \frac{2}{n} \sum_{i=1}^n x_i^T x_i \right)$$

Finally substituting (4.6) yields

$$x_i^T x_j = -\frac{1}{2} \left(d_{ij}^2 - x_i^T x_i - x_j^T x_j \right) = -\frac{1}{2} \left(d_{ij}^2 - \frac{1}{n} \sum_{i=1}^n d_{ij}^2 - \frac{1}{n} \sum_{i=1}^n d_{ij}^2 + \frac{1}{n^2} \sum_{i=1}^n \sum_{i=1}^n d_{ij}^2 \right)$$

Note that is D is the matrix of pairwise squared distances, then $\frac{1}{n}\sum_{k=1}^{n}d_{ij}^2$, $\frac{1}{n}\sum_{i=1}^{n}d_{ij}^2$, and $\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}d_{ij}^2$ are the averages of the square of the elements of the i^{th} row, the square of the elements of the j^{th} column and all squared distances respectively.

(2) Having constructed X^TX we can use an eigenvalue decomposition to determine the coordinate matrix X. Clearly X^TX is symmetric and if the distances come from a set of n points in a d-dimensional space X^TX will be positive definite and of rank d. Thus we can decompose X^TX as $X^TX = V^T\sigma V$ where the first d eigenvalues are positive and the remainder are zero. Since the $X^TX = V^T\sigma^{\frac{1}{2}}\sigma^{\frac{1}{2}}V$ and thus the coordinates are given by $X = V^T\sigma^{\frac{1}{2}}$

Exercise 4.31

1. Consider the pairwise distance matrix for twenty US cities given below. Use the algorithm of Exercise 2 to place the cities on a map of the US.

2. Suppose you had airline distances for 50 cities around the world. Could you use these distances to construct a world map?

	В	В	\mathbf{C}	D	D	Η	${ m L}$	Μ	M	${ m M}$
	O	U	Η	A	\mathbf{E}	O	A	${ m E}$	I	I
	\mathbf{S}	\mathbf{F}	I	${ m L}$	N	U		\mathbf{M}	A	M
Boston	-	400	851	1551	1769	1605	2596	1137	1255	1123
Buffalo	400	-	454	1198	1370	1286	2198	803	1181	731
Chicago	851	454	-	803	920	940	1745	482	1188	355
Dallas	1551	1198	803	-	663	225	1240	420	1111	862
Denver	1769	1370	920	663	-	879	831	879	1726	700
Houston	1605	1286	940	225	879	-	1374	484	968	1056
Los Angeles	2596	2198	1745	1240	831	1374	-	1603	2339	1524
Memphis	1137	803	482	420	879	484	1603	-	872	699
Miami	1255	1181	1188	1111	1726	968	2339	872	-	1511
Minneapolis	1123	731	355	862	700	1056	1524	699	1511	-
New York	188	292	713	1374	1631	1420	2451	957	1092	1018
Omaha	1282	883	432	586	488	794	1315	529	1397	290
Philadelphia	271	279	666	1299	1579	1341	2394	881	1019	985
Phoenix	2300	1906	1453	887	586	1017	357	1263	1982	1280
Pittsburgh	483	178	410	1070	1320	1137	2136	660	1010	743
Saint Louis	1038	662	262	547	796	679	1589	240	1061	466
Salt Lake City	2099	1699	1260	999	371	1200	579	1250	2089	987
San Francisco	2699	2300	1858	1483	949	1645	347	1802	2594	1584
Seattle	2493	2117	1737	1681	1021	1891	959	1867	2734	1395
Washington D.C.	393	292	597	1185	1494	1220	2300	765	923	934

	N	Ο	Р	Р	Р	S	S	S	S	D
	Y	${ m M}$	Н	Н	I	\mathbf{t}	${ m L}$	F	\mathbf{E}	\mathbf{C}
		A	I	O	${ m T}$	${ m L}$	\mathbf{C}		A	
Boston	188	1282	271	2300	483	1038	2099	2699	2493	393
Buffalo	292	883	279	1906	178	662	1699	2300	2117	292
Chicago	713	432	666	1453	410	262	1260	1858	1737	597
Dallas	1374	586	1299	887	1070	547	999	1483	1681	1185
Denver	1631	488	1579	586	1320	796	371	949	1021	1494
Houston	1420	794	1341	1017	1137	679	1200	1645	1891	1220
Los Angeles	2451	1315	2394	357	2136	1589	579	347	959	2300
Memphis	957	529	881	1263	660	240	1250	1802	1867	765
Miami	1092	1397	1019	1982	1010	1061	2089	2594	2734	923
Minneapolis	1018	290	985	1280	743	466	987	1584	1395	934
New York	-	1144	83	2145	317	875	1972	2571	2408	205
Omaha	1144	-	1094	1036	836	354	833	1429	1369	1014
Philadelphia	83	1094	-	2083	259	811	1925	2523	2380	123
Phoenix	2145	1036	2083	-	1828	1272	504	653	1114	1963
Pittsburgh	317	836	259	1828	-	559	1668	2264	2138	192
Saint Louis	875	354	811	1272	559	-	1162	1744	1724	712
Salt Lake City	1972	833	1925	504	1668	1162	-	600	701	1848
San Francisco	2571	1429	2523	653	2264	1744	600	-	678	2442
Seattle	2408	1369	2380	1114	2138	1724	701	678	-	2329
Washington D.C.	250	1014	123	1983	192	712	1848	2442	2329	-

References

Hubs and Authorities Golub and Van Loan Clustering Gaussians

5 Markov Chains

The study of Markov chains is a classical subject with many applications such as Markov Chain Monte Carlo techniques for integrating multivariate probability distributions over complex volumes. An important recent application is in defining the pagerank of pages on the World Wide Web by their stationary probabilities.

A Markov chain has a finite set of states. For each pair x and y of states, there is a probability p_{xy} of going from state x to state y where for each x, $\sum_y p_{xy} = 1$. A random walk in the Markov chain consists of a sequence of states starting at some state x_0 . In state x, the next state y is selected randomly with probability p_{xy} . The starting probability distribution puts a mass of one on the start state x_0 and zero on every other state. More generally, one could start with any probability distribution \mathbf{p} , where \mathbf{p} is a row vector with non-negative components summing to one, with p_i being the probability of starting in state i. The probability of being at state j at time t+1 is the sum over each state i of being at i at time i and taking the transition from i to i. Let $\mathbf{p}^{(t)}$ be a row vector with a component for each state specifying the probability mass of the state at time i and let i and let i be the row vector of probabilities at time i and i and i and i at time i and i at time i and let i and i at time i and

$$\mathbf{p^{(t)}}P = \mathbf{p^{(t+1)}}.$$

Many real-world situations can be modeled as Markov chains. At any time, the only information about the chain is the current state, not how the chain got there. At the next unit of time the state is a random variable whose distribution depends only on the current state. A gambler's assets can be modeled as a Markov chain where the current state is the amount of money the gambler has on hand. The model would only be valid if the next state does not depend on past states, only on the current one. Human speech has been modeled as a Markov chain, where the state represents either the last syllable (or the last several syllables) uttered. The reader may consult sources on Markov chains for other examples; our discussion here focuses on the theory behind them.

A Markov chain can be represented by a directed graph with a vertex representing each state and an edge labeled p_{ij} from vertex i to vertex j if $p_{ij} > 0$. We say that the Markov chain is *strongly connected* if there is a directed path from each vertex to every other vertex. The matrix P of the p_{ij} is called the *transition probability matrix* of the chain.

A fundamental property of a Markov chain is that in the limit the long-term average probability of being in a particular state is independent of the start state or an initial probability distribution over states provided that the directed graph is strongly connected. This is the Fundamental Theorem of Markov chains which we now prove.

5.1 Stationary Distribution

Suppose after t steps of the random walk, the probability distribution is $\mathbf{p^{(t)}}$. Define the long-term probability distribution $\mathbf{a^{(t)}}$ by

$$\mathbf{a^{(t)}} = \frac{1}{t} \left(\mathbf{p^{(0)}} + \mathbf{p^{(1)}} + \dots + \mathbf{p^{(t-1)}} \right).$$

The next theorem proves that the long-term probability distribution of a strongly connected Markov chain converges to a unique probability vector. This does not mean that the probability distribution of the random walk converges. This would require an additional condition called aperiodic.

Theorem 5.1 (Fundamental Theorem of Markov chains) If the Markov chain is strongly connected, there is a unique probability vector $\boldsymbol{\pi}$ satisfying $\boldsymbol{\pi}P = \boldsymbol{\pi}$. Moreover, for any starting distribution, $\lim_{t\to\infty} \mathbf{a}^{(t)}$ exists and equals $\boldsymbol{\pi}$.

Proof:

$$\mathbf{a}^{(t)}P - \mathbf{a}^{(t)} = \frac{1}{t} \left[\mathbf{p}^{(0)}P + \mathbf{p}^{(1)}P + \dots + \mathbf{p}^{(t-1)}P \right] - \frac{1}{t} \left[\mathbf{p}^{(0)} + \mathbf{p}^{(1)} + \dots + \mathbf{p}^{(t-1)} \right]$$

$$= \frac{1}{t} \left[\mathbf{p}^{(1)} + \mathbf{p}^{(2)} + \dots + \mathbf{p}^{(t)} \right] - \frac{1}{t} \left[\mathbf{p}^{(0)} + \mathbf{p}^{(1)} + \dots + \mathbf{p}^{(t-1)} \right]$$

$$= \frac{1}{t} \left(\mathbf{p}^{(t)} - \mathbf{p}^{(0)} \right).$$

Thus, $\mathbf{b^{(t)}} = \mathbf{a^{(t)}}P - \mathbf{a^{(t)}}$ satisfies $|\mathbf{b^{(t)}}| \leq \frac{2}{t} \to 0$, as $t \to \infty$. Letting A be the $n \times (n+1)$ matrix [P-I], $\mathbf{1}$] obtained by augmenting the matrix P-I with an additional column of ones. Then $\mathbf{a^{(t)}}A = [\mathbf{b^{(t)}}]$, $\mathbf{1}$]. The matrix A has rank n since each row sum in P is 1 and hence row sums in P-I are all 0. Thus $A\begin{pmatrix} \mathbf{1} \\ 0 \end{pmatrix} = 0$. If the rank of A is less than n, there is a vector \mathbf{w} perpendicular to $\mathbf{1}$ and scalar α so that $(P-I)\mathbf{w} = \alpha \mathbf{1}$ or $P\mathbf{w} - \alpha \mathbf{1} = \mathbf{w}$. If $\alpha > 0$, then for the i with maximum value of w_i , $\mathbf{w}w_i$ is a convex combination of some w_j , all at most w_i minus α , a contradiction. Similarly for $\alpha < 0$. So assume $\alpha = 0$. For the i with maximum w_i , if for some j, $p_{ij} > 0$, then $w_j = w_i$. Otherwise, $(P\mathbf{w})_i$ would be less than w_i . Now suppose S is the set of k with w_k equal to the maximum value. \bar{S} is not empty since $\sum_k w_k = 0$. Connectedness implies that there exist $k \in S, l \in \bar{S}$ with $p_{kl} > 0$, which is a contradiction. So A has rank n and the $n \times n$ submatrix B of A consisting of all its columns except the first is invertible. Let $\mathbf{c}^{(\mathbf{t})}$ be obtained from $\mathbf{b}^{(\mathbf{t})}$ by removing the first entry. Then, $\mathbf{a}^{(\mathbf{t})} = [\mathbf{c}^{(\mathbf{t})}]$, $1 \in \mathbb{N}$

The vector $\boldsymbol{\pi}$ is called the *stationary probability distribution* of the Markov chain. The equations $\boldsymbol{\pi}P = \boldsymbol{\pi}$ expanded say that for every i,

$$\sum_{i} \pi_{j} p_{ji} = \pi_{i}.$$

Thus, executing one step of the Markov Chain starting with the distribution π results in the same distribution. Of course the same conclusion holds for any number of steps. Hence the name stationary distribution, sometimes called the steady state distribution.

5.2 Electrical Networks and Random Walks

In the next few sections, we study a special class of Markov chains derived from electrical networks. These include Markov chains on undirected graphs where one of the edges incident to the current vertex is chosen uniformly at random and the walk proceeds to the vertex at the other end of the edge. There are nice analogies between such Markov chains and certain electrical quantities.

An electrical network is a connected, undirected graph in which each edge xy has a resistance $r_{xy} > 0$. In what follows, it is easier to deal with conductance defined as the reciprocal of resistance, $c_{xy} = \frac{1}{r_{xy}}$, rather then resistance. Associated with an electrical network is a Markov chain on the underlying graph defined by assigning a probability $p_{xy} = \frac{c_{xy}}{c_y}$ to the edge (x, y) incident to a vertex, where the normalizing constant c_x equals $\sum_y c_{xy}$. Note that although c_{xy} equals c_{yx} , the probabilities p_{xy} and p_{yx} may not be equal due to the required normalization so that the probabilities at each vertex sum to one. Thus, the matrix P may not be symmetric. We shall soon see that there is a relationship between current flowing in an electrical network and a random walk on the underlying graph.

Denote by P the matrix whose xy^{th} entry p_{xy} is the probability of a transition from x to y. The matrix P is called the transition probability matrix. Suppose a random walk starts at a vertex x_0 . At the start, the probability mass is one at x_0 and zero at all other vertices. At time one, for each vertex y, the probability of being at y is the probability, p_{x_0y} , of going from x_0 to y.

If the underlying electrical network is connected, then the Markov chain is strongly connected and has a stationary probability distribution. We claim that the stationary probability is given by $f_x = \frac{c_x}{c}$ where $c = \sum_x c_x$. By Theorem 5.1, it suffices to check that

$$\mathbf{f}P = \mathbf{f}:$$

$$(\mathbf{f}P)_x = \sum_y \frac{c_y}{c} \frac{c_{yx}}{c_y} = \sum_y \frac{c_{xy}}{c} = \frac{c_x}{c} = f_x.$$

Note that if each edge has resistance one, then the value of $c_x = \sum_y c_{xy}$ is d_x where d_x is the degree of x. In this case, $c = \sum_x c_x$ equals 2m where m is the total number of edges and the stationary probability is $\frac{1}{2m}(d_1, d_2, \ldots, d_n)$. This means that for undirected graphs, the stationary probability of each vertex is proportional to its degree and if the walk starts with the stationary distribution, every edge is traversed in each direction with

the same probability of $\frac{1}{2m}$.

A random walk associated with an electrical network has the important property that given the stationary probability \mathbf{f} , the probability $f_x p_{xy}$ of traversing the edge xy from vertex x to vertex y is the same as the probability $f_y p_{yx}$ of traversing the edge in the reverse direction from vertex y to vertex x. This follows from the manner in which probabilities were assigned and the fact that the conductance c_{xy} equals c_{yx} .

$$f_x p_{xy} = \frac{c_x}{c} \frac{c_{xy}}{c_x} = \frac{c_{xy}}{c} = \frac{c_{yx}}{c} = \frac{c_y}{c} \frac{c_{yx}}{c_y} = f_y p_{yx}.$$

Harmonic functions

Harmonic functions are useful in developing the relationship between electrical networks and random walks on undirected graphs. Given an undirected graph, designate a nonempty set of vertices as boundary vertices and the remaining vertices as interior vertices. A harmonic function g on the vertices is one in which the value of the function at the boundary vertices is fixed to some boundary condition and the value of g at any interior vertex x is a weighted average of the values at all the adjacent vertices g, where the weights g_{xy} sum to one over all g. Thus, if $g_x = \sum_{y} g_y p_{xy}$ at every interior vertex g,

then g is harmonic. From the fact that $\mathbf{f}P = \mathbf{f}$, it follows that the function $g_x = \frac{f_x}{c_x}$ is harmonic:

$$g_x = \frac{f_x}{c_x} = \frac{1}{c_x} \sum_y f_y p_{yx} = \frac{1}{c_x} \sum_y f_y \frac{c_{yx}}{c_y}$$
$$= \frac{1}{c_x} \sum_y f_y \frac{c_{xy}}{c_y} = \sum_y \frac{f_y}{c_y} \frac{c_{xy}}{c_x} = \sum_y g_y p_{xy}.$$

A harmonic function on a connected graph takes on its maximum and minimum on the boundary. Suppose not. Let S be the set of interior vertices at which the maximum value is attained. Since S contains no boundary vertices, \bar{S} is nonempty. Connectedness implies that there is at least one edge (x,y) with $x \in S$ and $y \in \bar{S}$. But then the value of the function at x is the average of the value at its neighbors, all of which are less than or equal to the value at x and the value at y is strictly less, a contradiction. The proof for the minimum value is identical.

There is at most one harmonic function satisfying a given set of equations and boundary conditions. For suppose there were two solutions f(x) and g(x). The difference of two solutions is itself harmonic. Since h(x) = f(x) - g(x) is harmonic and has value zero on the boundary, by the maximum principle it has value zero everywhere. Thus f(x) = g(x).

The analogy between electrical networks and random walks

There are important connections between random walks on undirected graphs and electrical networks. Choose two vertices a and b. For reference purposes let the voltage

 v_b equal zero. Attach a current source between a and b so that the voltage v_a equals one. Fixing the voltages at v_a and v_b induces voltages at all other vertices along with a current flow through the edges of the network. The analogy between electrical networks and random walks is the following. Having fixed the voltages at the vertices a and b, the voltage at an arbitrary vertex x equals the probability of a random walk starting at x reaching a before reaching b. If the voltage v_a is adjusted so that the current flowing into vertex a is one, then the current flowing through an edge is the net frequency in which a random walk from a to b traverses the edge.

Probabilistic interpretation of voltages

Before showing that the voltage at an arbitrary vertex x equals the probability of a random walk from x reaching a before reaching b, we first show that the voltages form a harmonic function. Let x and y be adjacent vertices and let i_{xy} be the current flowing through the edge from x to y. By Ohm's law,

$$i_{xy} = \frac{v_x - v_y}{r_{xy}} = (v_x - v_y)c_{xy}.$$

By Kirchoff's Law the currents flowing out of each vertex sum to zero.

$$\sum_{y} i_{xy} = 0$$

Replacing currents in the above sum by the voltage difference times the conductance yields

$$\sum_{y} (v_x - v_y)c_{xy} = 0$$

or

$$v_x \sum_y c_{xy} = \sum_y v_y c_{xy}.$$

Observing that $\sum_{y} c_{xy} = c_x$ and that $p_{xy} = \frac{c_{xy}}{c_x}$, yields $v_x c_x = \sum_{y} v_y p_{xy} c_x$. Hence, $v_x = \sum_{y} v_y p_{xy}$. Thus, the voltage at each vertex x is a weighted average of the voltages at the adjacent vertices. Hence the voltages are harmonic.

Now let p_x be the probability that a random walk starting at vertex x reaches a before b. Clearly $p_a = 1$ and $p_b = 0$. Since $v_a = 1$ and $v_b = 0$, it follows that $p_a = v_a$ and $p_b = v_b$. Furthermore, the probability of the walk reaching a from x before reaching b is the sum over all y adjacent to x of the probability of the walk going from x to y and then reaching a from y before reaching b. That is

$$p_x = \sum_y p_{xy} p_y.$$

Hence, p_x is the same harmonic function as the voltage function v_x and \mathbf{v} and \mathbf{p} satisfy the same boundary conditions (a and b form the boundary). Thus, they are identical functions. The probability of a walk starting at x reaching a before reaching b is the voltage v_x .

Probabilistic interpretation of current

In a moment we will set the current into the network at a to have some value which we will equate with one random walk. We will then show that the current i_{xy} is the net frequency with which a random walk from a to b goes through the edge xy before reaching b. Let u_x be the expected number of visits to vertex x on a walk from a to b before reaching b. Clearly $u_b = 0$. Since every time the walk visits x, x not equal to a, it must come to x from some vertex y, the number of visits to x before reaching b is the sum over all y of the number of visits u_y to y before reaching b times the probability p_{yx} of going from y to x. Thus

$$u_x = \sum_{y} u_y p_{yx} = \sum_{y} u_y \frac{c_x p_{xy}}{c_y}$$

and hence $\frac{u_x}{c_x} = \sum_y \frac{u_y}{c_y} p_{xy}$. It follows that $\frac{u_x}{c_x}$ is harmonic (with a and b as the boundary).

Now, $\frac{u_b}{c_b} = 0$. Setting the current into a to one, fixed the value of v_a . Adjust the current into a so that v_a equals $\frac{u_a}{c_a}$. Since $\frac{u_x}{c_x}$ and v_x satisfy the same harmonic conditions, they are the same harmonic function. Let the current into a correspond to one walk. Note that if our walk starts at a and ends at b, the expected value of the difference between the number of times the walk leaves a and enters a must be one and thus the amount of current into a corresponds to one walk.

Next we need to show that the current i_{xy} is the net frequency with which a random walk traverses edge xy.

$$i_{xy} = (v_x - v_y)c_{xy} = \left(\frac{u_x}{c_x} - \frac{u_y}{c_y}\right)c_{xy} = u_x\frac{c_{xy}}{c_x} - u_y\frac{c_{xy}}{c_y} = u_xp_{xy} - u_yp_{yx}$$

The quantity $u_x p_{xy}$ is the expected number of times the edge xy is traversed from x to y and the quantity $u_y p_{yx}$ is the expected number of times the edge xy is traversed from y to x. Thus, the current i_{xy} is the expected net number of traversals of the edge xy from x to y.

Effective Resistance and Escape Probability

Set $v_a = 1$ and $v_b = 0$. Let i_a be the current flowing into the network at vertex a and out at vertex b. Define the effective resistance r_{eff} between a and b to be $r_{eff} = \frac{v_a}{i_a}$ and the effective conductance c_{eff} to be $c_{eff} = \frac{1}{r_{eff}}$. Define the escape probability, p_{escape} , to be the probability that a random walk starting at a reaches b before returning to a. We now show that the escape probability is $\frac{c_{eff}}{c}$.

$$i_a = \sum_{y} (v_a - v_y) c_{ay}$$

Since $v_a = 1$,

$$i_a = \sum_y (1 - v_y) \frac{c_{ay}}{c_a} c_a$$

$$= c_a \left[\sum_y \frac{c_{ay}}{c_a} - \sum_y v_y \frac{c_{ay}}{c_a} \right]$$

$$= c_a \left[1 - \sum_y p_{ay} v_y \right].$$

For each y adjacent to the vertex a, p_{ay} is the probability of the walk going from vertex a to vertex y. v_y is the probability of a walk starting at y going to a before reaching b, as was just argued. Thus, $\sum_y p_{ay} v_y$ is the probability of a walk starting at a returning to a before reaching b and $1 - \sum_y p_{ay} v_y$ is the probability of a walk starting at a reaching b before returning to a. Thus $i_a = c_a p_{escape}$. Since $v_a = 1$ and $c_{eff} = \frac{i_a}{v_a}$, it follows that $c_{eff} = i_a$. Thus $c_{eff} = c_a p_{escape}$ and hence $p_{escape} = \frac{c_{eff}}{c_a}$.

For a finite graph the escape probability will always be nonzero. Now consider an infinite graph such as a lattice and a random walk starting at some vertex a. Form a series of finite graphs by merging all vertices at distance d or greater from a into a single vertex b for larger and larger values of d. The limit of p_{escape} as d goes to infinity is the probability that the random walk will never return to a. If $p_{escape} \to 0$, then eventually any random walk will return to a. If $p_{escape} \to q$ where q > 0, then a fraction of the walks never return. Thus, the escape probability terminology.

5.3 Random Walks on Undirected Graphs

We now focus our discussion on random walks on undirected graphs with uniform edge weights. At each vertex, the random walk is equally likely to take any edge. This corresponds to an electrical network in which all edge resistances are one. Assume the graph is connected. If it is not, the analysis below can be applied to each connected component separately. We consider questions such as what is the expected time for a random walk starting at a vertex x to reach a target vertex y, what is the expected time until the random walk returns to the vertex it started at, and what is the expected time to reach every vertex?

Hitting time

The hitting time h_{xy} , sometimes called discovery time, is the expected time of a random walk starting at vertex x to reach vertex y. Sometimes a more general definition is given where the hitting time is the expected time to reach a vertex y from a start vertex

selected at random from some given probability distribution.

One interesting fact is that adding edges to a graph may either increase or decrease h_{xy} depending on the particular situation. An edge can shorten the distance from x to y thereby decreasing h_{xy} or the edge could increase the probability of a random walk going to some far off portion of the graph thereby increasing h_{xy} . Another interesting fact is that hitting time is not symmetric. The expected time to reach a vertex y from a vertex x in an undirected graph may be radically different from the time to reach x from y.

We start with two technical lemmas. The first lemma states that the expected time to traverse a chain of n vertices is $\Theta(n^2)$.

Lemma 5.2 The expected time for a random walk starting at one end of a chain of n vertices to reach the other end is $\Theta(n^2)$.

Proof: Consider walking from vertex 1 to vertex n in a graph consisting of a single path of n vertices. Let h_{ij} , i < j, be the hitting time of reaching j starting from i. Now $h_{12} = 1$ and

$$h_{i,i+1} = \frac{1}{2} \times 1 + \frac{1}{2} (1 + h_{i-1,i} + h_{i,i+1}) \quad 2 \le i \le n-1.$$

Solving for $h_{i,i+1}$ yields the recurrence

$$h_{i,i+1} = 2 + h_{i-1,i}.$$

Solving the recurrence yields

$$h_{i,i+1} = 2i - 1.$$

To get from 1 to n, go from 1 to 2, 2 to 3, etc. Thus

$$h_{1,n} = \sum_{i=1}^{n-1} h_{i,i+1} = \sum_{i=1}^{n-1} (2i - 1)$$

$$= 2 \sum_{i=1}^{n-1} i - \sum_{i=1}^{n-1} 1$$

$$= 2 \frac{n(n-1)}{2} - (n-1)$$

$$= (n-1)^{2}.$$

The next lemma shows that the expected time spent at vertex i by a random walk from vertex 1 to vertex n in a chain of n vertices is 2(i-1) for $2 \le i \le n-1$.

Lemma 5.3 Consider a random walk from vertex 1 to vertex n in a chain of n vertices. Let t(i) be the expected time spent at vertex i. Then

$$t(i) = \begin{cases} n-1 & i=1\\ 2(n-i) & 2 \le i \le n-1\\ 1 & i=n. \end{cases}$$

Proof: Now t(n) = 1 since the walk stops when it reaches vertex n. Half of the time when the walk is at vertex n-1 it goes to vertex n. Thus t(n-1) = 2. For $3 \le i \le n-1$, $t(i) = \frac{1}{2}[t(i-1) + t(i+1)]$ and t(1) and t(2) satisfy $t(1) = \frac{1}{2}t(2) + 1$ and $t(2) = t(1) + \frac{1}{2}t(3)$. Solving for t(i+1) for $1 \le i \le n-1$ yields

$$t(i+1) = 2t(i) - t(i-1)$$

which has solution t(i) = 2(n-i) for $3 \le i \le n-1$. Then solving for t(2) and t(1) yields t(2) = 2(n-2) and t(1) = n-1. Thus, the total time spent at vertices is

$$n-1+2(1+2+\cdots+n-2)+1=n-1+(n-1)(n-2)+1=(n-1)^2+1$$

which is one more than h_{1n} and thus is correct.

Next we show that adding edges to a graph might either increase or decrease the hitting time h_{xy} . Consider the graph consisting of a single path of n vertices. Add edges to this graph to get the graph in Figure 5.1 consisting of a clique of size n/2 connected to a path of n/2 vertices. Then add still more edges to get a clique of size n. Let x be the vertex at the midpoint of the original path and let y be the other endpoint of the path consisting of n/2 vertices as shown in Figure 5.1. In the first graph consisting of a single path of length n, $h_{xy} = \Theta(n^2)$. In the second graph consisting of a clique of size n/2 along with a path of length n/2, $h_{xy} = \Theta(n^3)$. To see this latter statement, note that starting at x, the walk will go down the chain towards y and return to x n times on average before reaching y for the first time. Each time the walk in the chain returns to x, with probability (n-1)/n it enters the clique and thus on average enters the clique $\Theta(n)$ times before starting down the chain again. Each time it enters the clique, it spends $\Theta(n)$ time in the clique before returning to x. Thus, each time the path returns to x from the chain it spends $\Theta(n^2)$ time in the clique before starting down the chain towards y for a total expected time that is $\Theta(n^3)$ before reaching y. In the third graph, which is the clique of size n, $h_{xy} = \Theta(n)$. Thus, adding edges first increased h_{xy} from n^2 to n^3 and then decreased it to n.

Hitting time is not symmetric even in the case of undirected graphs. In the graph of Figure 5.1, the expected time, h_{xy} , of a random walk from x to y, where x is the vertex of attachment and y is the other end vertex of the chain, is $\Theta(n^3)$. However, h_{yx} is $\Theta(n^2)$.

Next we ask what is the maximum that the hitting time could be. We first show that if vertices x and y are connected by an edge, then the expected time, h_{xy} , of a random walk from x to y plus the expected time, h_{yx} , from y to x is at most twice the number of edges.

Lemma 5.4 If vertices x and y are connected by an edge, then $h_{xy} + h_{yx} \le 2m$ where m is the number of edges in the graph.

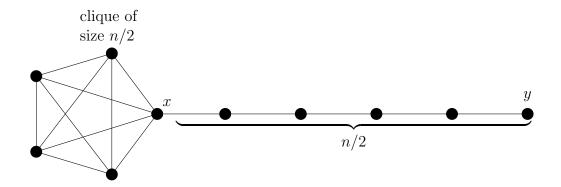


Figure 5.1: Illustration that adding edges to a graph can either increase or decrease hitting time.

Proof: In a random walk on an undirected graph starting in the steady state, the probability of traversing any edge in either direction is 1/(2m). This is because for any edge (u, v), the probability of being at u (in the steady state) is $d_u/(2m)$ and the probability of selecting the edge (u, v) is $1/d_u$. Hence, the probability of traversing the edge (u, v) is 1/(2m) implying that the expected time between traversals of the edge (x, y) from x to y is 2m. Thus, if we traverse edge (x, y), the expected time to traverse a path from y back to x and then traverse the edge (x, y) again is 2m. But since a random walk is a memory less process, we can drop the condition that we started by traversing the edge (x, y). Hence the expected time from y to x and back to y is at most 2m. Note that the path went from y to x and then may have returned to x several times before going through the edge (x, y). Thus, the less than or equal sign in the statement of the lemma since the path have gone from y to x to y without going through the edge (x, y).

Notice that the proof relied on the fact that there was an edge from x to y and thus the theorem is not necessarily true for arbitrary x and y. When x and y are not connected by an edge consider a path from x to y. The path is of length at most n. Consider the time it takes to reach each vertex on the path in the order they appear. Since the vertices on the path are connected by edges, the expected time to reach the next vertex on the path is at most twice the number of edges in the graph by the above theorem. Thus, the total expected time is $\Theta(n^3)$. This result is asymptotically tight since the bound is met by the graph of Figure 5.1 consisting of a clique of size n/2 and a path of length n/2.

Commute time

The commute time, commute (x, y), is the expected time of a random walk starting at x reaching y and then returning to x. Think of going from home to office and returning home.

Theorem 5.5 Given an undirected graph, consider the electrical network where each edge of the graph is replaced by a one ohm resistor. Given vertices x and y, the commute time,

commute(x, y), equals $2mr_{xy}$ where r_{xy} is the effective resistance from x to y and m is the number of edges in the graph.

Proof: Insert at each vertex i a current equal to the degree d_i of vertex i. The total current inserted is 2m where m is the number of edges. Extract from a specific vertex j all of this 2m current. Let v_{ij} be the voltage difference from i to j. The current into i divides into the d_i resistors at node i. The current in each resistor is proportional to the voltage across it. Let k be a vertex adjacent to i. Then the current through the resistor between i and k is $v_{ij} - v_{kj}$, the voltage drop across the resister. The sum of the currents out of i through the resisters must equal d_i , the current injected into i.

$$d_i = \sum_{\substack{k \text{ adj} \\ \text{to } i}} \left(v_{ij} - v_{kj} \right)$$

Noting that v_{ij} does not depend on k, write

$$d_i = d_i v_{ij} - \sum_{\substack{k \text{ adj} \\ \text{to } i}} v_{kj}.$$

Solving for v_{ij}

$$v_{ij} = 1 + \sum_{\substack{k \text{ adj} \\ \text{to } i}} \frac{1}{d_i} v_{kj} = \sum_{\substack{k \text{ adj} \\ \text{to } i}} \frac{1}{d_i} (1 + v_{kj}). \tag{5.1}$$

Now the expected time from i to j is the average time over all paths from i to k adjacent to i and then on from k to j. This is given by

$$h_{ij} = \sum_{\substack{k \text{ adj} \\ \text{to } i}} \frac{1}{d_i} (1 + h_{kj}). \tag{5.2}$$

Subtracting (5.2) from (5.1), gives $v_{ij} - h_{ij} = \sum_{\substack{k \text{ adj} \\ \text{to } i}} \frac{1}{d_i} (v_{kj} - h_{kj})$. Thus, the function $v_{ij} - h_{ij}$

is harmonic. Designate vertex j as the only exterior vertex. The value of $v_{ij} - h_{ij}$ at j, namely $v_{jj} - h_{jj}$, is zero, since both v_{jj} and h_{jj} are zero. So the function $v_{ij} - h_{ij}$ must be zero everywhere. Thus, the voltage v_{ij} equals the expected time h_{ij} from i to j.

To complete the proof, note that $h_{ij} = v_{ij}$ is the voltage from i to j when currents are inserted at all nodes in the graph and extracted at node j. If the current is extracted from i instead of j, then the voltages change and $v_{ji} = h_{ji}$ in the new setup. Finally, reverse all currents in this latter step. The voltages change again and for the new voltages $-v_{ji} = h_{ji}$. Since $-v_{ji} = v_{ij}$, we get $h_{ji} = v_{ij}$.

Thus, when a current is inserted at each node equal to the degree of the node and the current is extracted from j, the voltage v_{ij} in this set up equals h_{ij} . When we extract the current from i instead of j and then reverse all currents, the voltage v_{ij} in this new set up equals h_{ji} . Now, superpose both situations (i.e., add all the currents and voltages). By linearity, for the resulting v_{ij} , $v_{ij} = h_{ij} + h_{ji}$. All currents cancel except the 2m amps injected at i and withdrawn at j. Thus, $2mr_{ij} = v_{ij} = h_{ij} + h_{ji} = \text{commute}(i, j)$. Thus, commute $(i, j) = 2mr_{ij}$.

Note that Lemma 5.4 also follows from Theorem 5.5 since the effective resistance r_{uv} is less than or equal to 1 when u and v are connected by an edge.

Corollary 5.6 For any n vertex graph and for any vertices x and y, the commute time, commute(x, y), is less than or equal to n^3 .

Proof: By Theorem 5.5 the commute time is given by the formula commute $(x, y) = 2mr_{xy}$ where m is the number of edges. In an n vertex graph there exists a path from x to y of length at most n. This implies $r_{xy} \leq n$ since the resistance can not be greater than that of any path from x to y. Since the number of edges is at most $\binom{n}{2}$

commute
$$(x,y) = 2mr_{xy} \le 2\binom{n}{2}n \cong n^3$$
.

Again adding edges to a graph may increase or decrease the commute time. To see this, consider the graph consisting of a chain of n vertices, the graph of Figure 5.1, and the clique on n vertices.

Cover times

The $cover\ time\ cover(x,G)$ is the expected time of a random walk starting at vertex x in the graph G to reach each vertex at least once. We write cover(x) when G is understood. The cover time of an undirected graph G, denoted cover(G), is

$$cover(G) = \max_{x} cover(x, G).$$

For cover time of an undirected graph, increasing the number of edges in the graph may increase or decrease the cover time depending on the situation. Again consider three graphs, a chain of length n which has cover time $\Theta(n^2)$, the graph in Figure 5.1 which has cover time $\Theta(n^3)$, and the complete graph on n vertices which has cover time $\Theta(n \log n)$. Adding edges to the chain of length n to create the graph in Figure 5.1 increases the cover time from n^2 to n^3 and then adding even more edges to obtain the complete graph reduces the cover time to $n \log n$.

Note: The cover time of a clique is $n \log n$ since that is the time to select every integer out of n integers with high probability, drawing integers at random. This is called the coupon collector problem. The cover time for a straight line is $\Theta(n^2)$ since it is the same as the hitting time. For the graph in Figure 5.1, the cover time is $\Theta(n^3)$ since one takes the maximum over all start states and $\operatorname{cover}(x,G) = \Theta(n^3)$.

Theorem 5.7 Let G be a connected graph with n vertices and m edges. The time for a random walk to cover all vertices of the graph G is bounded above by 2m(n-1).

Proof: Consider a depth first search (dfs) of the graph G starting from vertex z and let T be the resulting dfs spanning tree of G. The dfs covers every vertex. Consider the expected time to cover every vertex in the order visited by the depth first search. Clearly this bounds the cover time of G starting from vertex z.

$$cover(z, G) \le \sum_{(x,y) \in T} h_{xy}.$$

If (x, y) is an edge in T, then x and y are adjacent and thus Lemma 5.4 implies $h_{xy} \leq 2m$. Since there are n-1 edges in the dfs tree and each edge is traversed twice, once in each direction, $\operatorname{cover}(z) \leq 2m(n-1)$. Since this holds for all starting vertices z, $\operatorname{cover}(G) \leq 2m(n-1)$

The theorem gives the correct answer of n^3 for the n/2 clique with the n/2 tail. It gives an upper bound of n^3 for the n-clique where the actual cover time is $n \log n$.

Let r_{xy} be the effective resistance from x to y. Define the resistance r(G) of a graph G by $r(G) = \max_{x,y}(r_{xy})$.

Theorem 5.8 Let G be an undirected graph with m edges. Then the cover time for G is bounded by the following inequality

$$mr(G) \le cover(G) \le 2e^3 mr(G) \ln n + n$$

where e=2.71 is Euler's constant and r(G) is the resistance of G.

Proof: By definition $r(G) = \max_{x,y}(r_{xy})$. Let u and v be the vertices of G for which r_{xy} is maximum. Then $r(G) = r_{uv}$. By Theorem 5.5, commute $(u,v) = 2mr_{uv}$. Hence $mr_{uv} = \frac{1}{2}\text{commute}(u,v)$. Clearly the commute time from u to v and back to u is less than twice the $\max(h_{uv}, h_{vu})$ and $\max(h_{uv}, h_{vu})$ is clearly less than the cover time of G. Putting these facts together

$$mr(G) = mr_{uv} = \frac{1}{2} \text{commute}(u, v) \le \max(h_{uv}, h_{vu}) \le \text{cover}(G).$$

For the second inequality in the theorem, by Theorem 5.5, for any x and y commute(x, y) equals $2mr_{xy}$ implying $h_{xy} \leq 2mr(G)$. By the Markov inequality, since the expected value

of h_{xy} is less than 2mr(G), the probability that y is not reached from x in $2mr(G)e^3$ steps is at most $\frac{1}{e^3}$. Thus, the probability that a vertex y has not been reached in $2e^3mr(G)\log n$ steps is at most $\frac{1}{e^3}^{\ln n} = \frac{1}{n^3}$ because a random walk of length $2e^3mr(G)\log n$ is a sequence of $\log n$ independent random walks, each of length $2e^3mr(G)$. Suppose after a walk of $2e^3mr(G)\log n$ steps, vertices v_1,v_2,\ldots,v_l where not reached. Walk until v_1 is reached, then v_2 , etc. By Corollary 5.6 the expected time for each of these is n^3 , but since each happens only with probability $1/n^3$, we effectively take O(1) time per v_i , for a total time of at most n.

Return time

The *return time* is the expected time of a walk starting at x returning to x. We explore this quantity later.

5.4 Random Walks in Euclidean Space

Many physical processes such as Brownian motion are modeled by random walks. Random walks in Euclidean d-space consisting of fixed length steps parallel to the coordinate axes are really random walks on a d-dimensional lattice and are a special case of random walks on graphs. In a random walk on a graph, at each time unit an edge from the current vertex is selected at random and the walk proceeds to the adjacent vertex. We begin by studying random walks on lattices.

Random walks on lattices

We now apply the analogy between random walks and current to lattices. Consider a random walk on a finite segment $-n, \ldots, -1, 0, 1, 2, \ldots, n$ of a one dimensional lattice starting from the origin. Is the walk certain to return to the origin or is there some probability that it will escape, i.e., reach the boundary before returning? The probability of reaching the boundary before returning to the origin is called the escape probability. We shall be interested in this quantity as n goes to infinity.

Convert the lattice to an electrical network by replacing each edge with a one ohm resister. Then the probability of a walk starting at the origin reaching n or -n before returning to the origin is the escape probability given by

$$p_{escape} = \frac{c_{eff}}{c_a}$$

where c_{eff} is the effective conductance between the origin and the boundary points and c_a is the sum of the conductance's at the origin. In a d-dimensional lattice, $c_a = 2d$ assuming that the resistors have value one. For the d-dimensional lattice

$$p_{escape} = \frac{1}{2d \ r_{eff}}$$

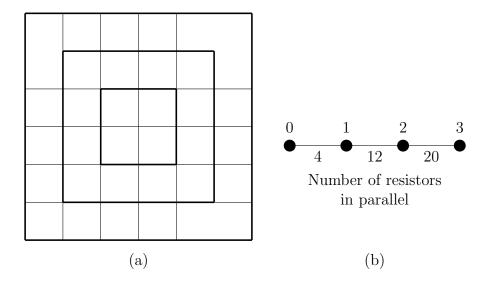


Figure 5.2: 2-dimensional lattice along with the linear network resulting from shorting resistors on the concentric squares about the origin.

In one dimension, the electrical network is just two series connections of n one ohm resistors connected in parallel. So, r_{eff} goes to infinity and the escape probability goes to zero as n goes to infinity. Thus, the walk in the unbounded one dimensional lattice will return to the origin with probability one.

Two dimensions

For the 2-dimensional lattice, consider a larger and larger square about the origin for the boundary as shown in Figure 5.2a and consider the limit of r_{eff} as the squares get larger. Shorting the resistors on each square can only reduce r_{eff} . Shorting the resistors results in the linear network shown in Figure 5.2b. As the paths get longer, the number of resistors in parallel also increases. So the resistor between node i and i+1 is really made up of O(i) unit resistors in parallel. The effective resistance of O(i) resistors in parallel is 1/O(i). Thus,

$$r_{eff} \ge \frac{1}{4} + \frac{1}{12} + \frac{1}{20} + \dots = \frac{1}{4} (1 + \frac{1}{3} + \frac{1}{5} + \dots) = \Theta(\ln n).$$

Since the lower bound on the effective resistance goes to infinity, the escape probability goes to zero for the 2-dimensional lattice.

Three dimensions

In three dimensions, the resistance along any path to infinity grows to infinity but the number of paths in parallel also grows to infinity. It turns out that r_{eff} remains finite and thus there is a nonzero escape probability.

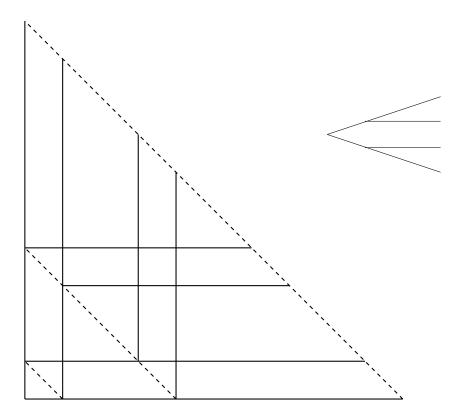


Figure 5.3: Paths in a 2-dimensional lattice obtained from the 3-dimensional construction applied in 2-dimensions.

The construction used in three dimensions is easier to explain first in two dimensions. Draw dotted diagonal lines at $x + y = 2^n - 1$. Consider two paths that start at the origin. One goes up and the other goes to the right. Each time a path encounters a dotted diagonal line, split the path into two, one which goes right and the other up. Where two paths cross, split the vertex into two, keeping the paths separate. By a symmetry argument, splitting the vertex does not change the resistance of the network. Remove all resistors except those on these paths. The resistance of the original network is less than that of the tree produced by this process since removing a resistor is equivalent to increasing its resistance to infinity.

The distances between splits increase and are 1, 2, 4, etc. At each split the number of paths in parallel doubles. Thus, the resistance to infinity in this two dimensional example is

$$\frac{1}{2} + \frac{1}{4}2 + \frac{1}{8}4 + \dots = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \dots = \infty.$$

In the analogous three dimensional construction, paths go up, to the right, and out of the plane of the paper. The paths split three ways at planes given by $x + y + z = 2^n - 1$.

Each time the paths split the number of parallel segments triple. Segments of the paths between splits are of length 1, 2, 4, etc. and the resistance of the segments are equal to the lengths. The resistance out to infinity for the tree is

$$\frac{1}{3} + \frac{1}{9}2 + \frac{1}{27}4 + \dots = \frac{1}{3}\left(1 + \frac{2}{3} + \frac{4}{9} + \dots\right) = \frac{1}{3}\frac{1}{1 - \frac{2}{3}} = 1$$

The resistance of the three dimensional lattice is less. Thus, in three dimensions the escape probability is nonzero. The upper bound on r_{eff} gives the lower bound

$$p_{escape} = \frac{1}{2d} \frac{1}{r_{eff}} \ge \frac{1}{6}.$$

A lower bound on r_{eff} gives an upper bound on p_{escape} . To get the upper bound on p_{escape} , short all resistors on surfaces of boxes at distances 1, 2, 3,, etc. Then

$$r_{eff} \ge \frac{1}{6} \left[1 + \frac{1}{9} + \frac{1}{25} + \cdots \right] \ge \frac{1.23}{6} \ge 0.2$$

This gives

$$p_{escape} = \frac{1}{2d} \frac{1}{r_{eff}} \ge \frac{5}{6}.$$

5.5 Random Walks on Directed Graphs

A major application of random walks on directed graphs comes from trying to establish the importance of pages on the World Wide Web. One way to do this would be to take a random walk on the web and rank pages according to their stationary probability. However, several situations occur in random walks on directed graphs that did not arise with undirected graphs. One difficulty occurs if there is a node with no out edges. In this case, the directed graph is not strongly connected and so Markov chain is not strongly connected either even though the underlying undirected graph may be connected. When the walk encounters this node the walk disappears. Another difficulty is that a node or a strongly connected component with no in edges is never reached. One way to resolve these difficulties is to introduce a random restart condition. At each step, with some probability r, jump to a node selected uniformly at random and with probability 1-r select an edge at random and follow it. If a node has no out edges, the value of r for that node is set to one. This has the effect of converting the graph to a strongly connected graph so that the stationary probabilities exist.

5.6 Finite Markov Processes

A Markov process is a random process in which the probability distribution for the future behavior depends only on the current state, not on how the process arrived at the current state. Markov processes are equivalent mathematically to random walks on directed graphs but the literature on the two topics developed separately with different terminology. Since much of the terminology of Markov processes appears in the literature on random walks, we introduce the terminology here to acquaint the reader with it.

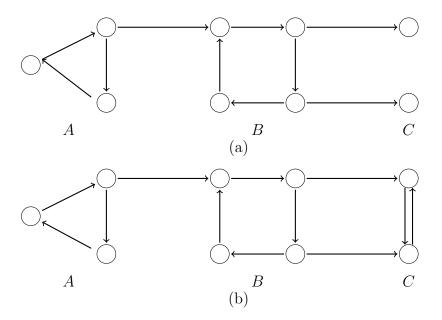


Figure 5.4: (a) A directed graph with nodes with no out out edges and a strongly connected component A with no in edges.

(b) A directed graph with three strongly connected components.

In a Markov process, nodes of the underlying graph are referred to as states. A state is persistent if it has the property that should the state ever be reached, the random process will return to it with probability one. This means that the state is in a strongly connected component with no out edges. Consider the directed graph in Figure 5.4b with three strongly connected components A, B, and C. Starting from any node in A there is a nonzero probability of eventually reaching any node in A. However, the probability of returning to a node in A is less than one and thus nodes in A and similarly nodes in B are not persistent. From any node in C, the walk will return with probability one to that node eventually since there is no way of leaving component C. Thus, nodes in C are persistent.

A state is *periodic* if it is contained only in cycles in which the greatest common divisor (gcd) of the cycle lengths is greater than one. A Markov process is *irreducible* if it consists of a single strongly connected component. An *ergodic* state is one that is aperiodic and persistent. A Markov process is *ergodic* if all states are ergodic. In graph theory this corresponds to a single strongly connected component that is aperiodic.

Page rank and hitting time

The page rank of a node in a directed graph is the stationary probability of the node. We assume some restart value, say r = 0.15, is used. The restart ensures that the graph is strongly connected. The page rank of a page is the fractional frequency with which the

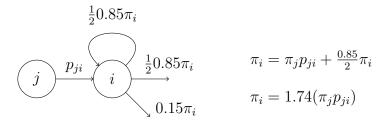


Figure 5.5: Impact on page rank of adding a self loop

page will be visited over a long period of time. If the page rank is p, then the expected time between visits or return time is 1/p. Notice that one can increase the pagerank of a page by reducing the return time and this can be done by creating short cycles.

Consider a node i with a single edge in from node j and a single edge out. The stationary probability π satisfies $\pi P = \pi$, and thus

$$\pi_i = \pi_j p_{ji}$$
.

Adding a self-loop at i, results in a new equation

$$= pi_i = \pi_j p_{ji} + \frac{1}{2}\pi_i$$

or

$$\pi_i = 2 \ \pi_j p_{ji}$$
.

Of course, π_j would have changed too, but ignoring this for now, pagerank is doubled by the addition of a self-loop. Adding k self loops, results in the equation

$$\pi_i = \pi_j p_{ji} + \frac{k}{k+1} \pi_i,$$

and again ignoring the change in π_j , we now have $\pi_i = (k+1)\pi_j p_{ji}$. What prevents one from increasing the page rank of a page arbitrarily? The answer is the restart. We neglected the 0.15 probability that is taken off for the random restart. With the restart taken into account, the equation for π_i when there is no self-loop is

$$\pi_i = 0.85\pi_i p_{ii}$$

whereas, with k self-loops, the equation is

$$\pi_i = 0.85\pi_j p_{ji} + 0.85 \frac{k}{k+1} \pi_i.$$

Adding a single loop only increases pagerank by a factor of 1.74 and adding k loops increases it by at most a factor of 6.67 for arbitrarily large k.

Hitting time

Related to page rank is a quantity called hitting time. Hitting time is closely related to return time and thus to the reciprocal of page rank. One way to return to a node v is by a path in the graph from v back to v. Another way is to start on a path that encounters a restart, followed by a path from the random restart node to v. The time to reach v after a restart is the hitting time. Thus, return time is clearly less than the expected time until a restart plus hitting time. The fastest one could return would be if there were only paths of length two since self loops are ignored in calculating page rank. If v is the restart value, then the loop would be traversed with at most probability v + (1 - r)v = (2 - r)v one restarts and then hits v. Thus, the return time is at least v is a least v in the return time is at least v in the return time. Combining these two bounds yields

$$(1-r)^2 + (2-r) rE$$
 (hitting time) $\leq E$ (return time) $\leq E$ (hitting time)

The relationship between return time and hitting time can be used to see if a node has unusually high probability of short loops. However, there is no efficient way to compute hitting time for all nodes as there is for return time. For a single node v, one can compute hitting time by removing the edges out of the node v for which one is computing hitting time and then run the page rank algorithm for the new graph. The hitting time for v is the reciprocal of the page rank in the graph with the edges out of v removed. Since computing hitting time for each node requires removal of a different set of edges, the algorithm only gives the hitting time for one node at a time. Since one is probably only interested in the hitting time of nodes with low hitting time, an alternative would be to use a random walk to estimate the hitting time of low hitting time nodes.

Spam

Suppose one has a web page and would like to increase its page rank by creating some other web pages with pointers to the original page. The abstract problem is the following. We are given a directed graph G and a node v whose page rank we want to increase. We may add new nodes to the graph and add edges from v or from the new nodes to any nodes we want. We cannot add edges out of other nodes. We can also delete edges from v.

The page rank of v is the stationary probability for node v with random restarts. If we delete all existing edges out of v, create a new node u and edges (v, u) and (u, v), then the page rank will be increased since any time the random walk reaches v it will be captured in the loop $v \to u \to v$. A search engine can counter this strategy by more frequent random restarts.

A second method to increase page rank would be to create a star consisting of the node v at its center along with a large set of new nodes each with a directed edge to v. These new nodes will sometimes be chosen as the target of the random restart and hence

the nodes increase the probability of the random walk reaching v. This second method is countered by reducing the frequency of random restarts.

Notice that the first technique of capturing the random walk increases page rank but does not effect hitting time. One can negate the impact of someone capturing the random walk on page rank by increasing the frequency of random restarts. The second technique of creating a star increases page rank due to random restarts and decreases hitting time. One can check if the page rank is high and hitting time is low in which case the page rank is likely to have been artificially inflated by the page capturing the walk with short cycles.

Personalized page rank

In computing page rank, one uses a restart probability, typically 0.15, in which at each step, instead of taking a step in the graph, the walk goes to a node selected uniformly at random. In personalized page rank, instead of selecting a node uniformly at random, one selects a node according to a personalized probability distribution. Often the distribution has probability one for a single node and whenever the walk restarts it restarts at that node.

Algorithm for computing personalized page rank

First, consider the normal page rank. Let α be the restart probability with which the random walk jumps to an arbitrary node. With probability $1 - \alpha$ the random walk selects a node uniformly at random from the set of adjacent nodes. Let \mathbf{p} be a row vector denoting the page rank and let G be the adjacency matrix with rows normalized to sum to one. Then

$$\mathbf{p} = \frac{\alpha}{n} (1, 1, \dots, 1) + (1 - \alpha) \mathbf{p} G$$

$$\mathbf{p}[I - (1 - \alpha)G] = \frac{\alpha}{n}(1, 1, \dots, 1)$$

or

$$\mathbf{p} = \frac{\alpha}{n} (1, 1, \dots, 1) [I - (1 - \alpha) G]^{-1}.$$

Thus, in principle, \mathbf{p} can be found by computing the inverse of $[I - (1 - \alpha)G]^{-1}$. But this is far from practical since for the whole web one would be dealing with matrices with billions of rows and columns. A more practical procedure is to run the random walk and observe using the basics of the power method in Chapter 4 that the process converges to the solution \mathbf{p} .

For the personalized page rank, instead of restarting at an arbitrary vertex, the walk restarts at a designated vertex. More generally, it may restart in some specified neighborhood. Suppose the restart selects a vertex using the probability distribution s. Then, in

the above calculation replace the vector $\frac{1}{n}(1,1,\ldots,1)$ by the vector **s**. Again, the computation could be done by a random walk. But, we wish to do the random walk calculation for personalized pagerank quickly since it is to be performed repeatedly. With more care this can be done, though we do not describe it here.

5.7 Markov Chain Monte Carlo

The Markov Chain Monte Carlo method is a technique for sampling a multivariate probability distribution $p(\mathbf{x})$, where $\mathbf{x} = (x_1, x_2, \dots, x_d)$ is the set of variables. Given the probability distribution $p(\mathbf{x})$, one might wish to calculate the marginal distribution

$$p(x_1) = \sum_{x_2,\dots,x_d} p(x_1,\dots,x_d)$$

or the expectation of some function $f(\mathbf{x})$

$$E(f) = \sum_{x_1,...,x_d} f(x_1,...,x_d) p(x_1,...,x_d).$$

The difficulty is that both computations require a summation over an exponential number of values. If each x_i can take on a value from the set $\{1, 2, ..., n\}$ of values, then there are n^d possible values for \mathbf{x} . One could compute an approximate answer by generating a sample set of values for $\mathbf{x} = (x_1, ..., x_d)$ according to the distribution $p(x_1, ..., x_d)$. This is done by designing a Markov chain whose stationary probabilities are exactly $p(x_1, x_2, ..., x_d)$ and running the chain for a sufficiently large number of steps and averaging f over the states seen in the run. The number of steps must be large enough that we are close to the limit which is the stationary distribution. In the rest of this section, we will show that under some mild conditions, the number of steps needed grows only polynomially, though the total number of states grows exponentially with d.

For ease of explanation, assume that the variables take on values from some finite set. Create a directed graph with one node corresponding to each possible value of \mathbf{x} . A random walk on the the graph is designed so that the stationary probability of the walk is $p(\mathbf{x})$. The walk is designed by specifying the probability of the transition from one node to another in such a way as to achieve the desired stationary distribution. Two common techniques for designing the walks are the Metropolis-Hasting algorithm and Gibbs sampling. We will see that the sequence of nodes after a sufficient number of steps of the walk provides a good sample of the distribution. The number of steps the walk needs to take depends on its convergence rate to its stationary distribution. We will show that this rate is related to a natural quantity called the minimum escape probability (MEP).

We used $\mathbf{x} \in \mathbf{R}^d$ to emphasize that our distributions are multi-variate. From a Markov chain perspective, each value \mathbf{x} can take on is a state, i.e., a node of the graph on which

the random walk takes place. Henceforth, we will use the subscripts i, j, k, ... to denote states and will use p_i instead of $p(x_1, x_2, ..., x_d)$ to denote the probability of the state corresponding to a given set of values for the variables. Recall that in the Markov chain terminology, nodes of the graph are called states.

Recall the notation that $\mathbf{p^{(t)}}$ is the row vector of probabilities of the random walk being at each state (node of the graph) at time t. So, $\mathbf{p^{(t)}}$ has as many components as there are states and its i^{th} component, $p_i^{(t)}$, is the probability of being in state i at time t. Recall the long-term (t-step) average is

$$\mathbf{a}^{(t)} = \frac{1}{t} \left[\mathbf{p}^{(0)} + \mathbf{p}^{(1)} + \dots + \mathbf{p}^{(t-1)} \right].$$
 (5.3)

The expected value of the function f under the probability distribution p is $E(f) = \sum_i f_i p_i$. Our estimate of this quantity will be the average value of f at the states seen in a t step run. Call this estimate a. Clearly, the expected value of a is

$$E(a) = \sum_{i} f_i a_i^{(t)}.$$

The expectation here is with respect to the "coin tosses" of the algorithm, not with respect to the underlying distribution p. Letting f_{max} denote the maximum absolute value of f. It is easy to see that

$$\left| E(a) - \sum_{i} f_i p_i \right| \le f_{\text{max}} \sum_{i} |p_i - a_i^{(t)}| = f_{\text{max}} |\mathbf{p} - \mathbf{a}^{(t)}|_1$$
 (5.4)

where the quantity $|\mathbf{p} - \mathbf{a}^{(t)}|_1$ is the l_1 distance between the probability distributions \mathbf{p} and $\mathbf{a}^{(t)}$ and is often called the "total variation distance" between the distributions. We will build tools to upper bound $|\mathbf{p} - \mathbf{a}^{(t)}|_1$. Since \mathbf{p} is the steady state distribution, the t for which $|\mathbf{p} - \mathbf{a}^{(t)}|_1$ becomes small is determined by the rate of convergence of the Markov chain to its steady state.

The following proposition is often useful.

Proposition 5.9 For two probability distributions \mathbf{p} and \mathbf{q} , $|\mathbf{p} - \mathbf{q}|_1 = 2\sum_i (p_i - q_i)^+ = 2\sum_i (q_i - p_i)^+$.

The proof is left as an exercise (Exercise 5.34).

5.7.1 Time Reversibility

Definition: A Markov chain is said to be *time-reversible* if for the steady state probabilities π , $\pi_i p_{ij} = \pi_i p_{ji}$ for all i and j.

The phrase "time-reversible" comes from the following fact. For a time-reversible Markov chain started in the steady state, the probability of a path (sequence of states) is the same as its reversal. That is

$$\pi_{i_1} p_{i_1,i_2} p_{i_2,i_3} \cdots p_{i_{k-1},i_k} = \pi_{i_k} p_{i_k,i_{k-1}} p_{i_{k-1},i_{k-2}} \cdots p_{i_2,i_1}.$$

Given only the sequence of states seen, one cannot tell if time runs forward or backward, both having the same probability. More important is the fact that time reversibility simplifies the underlying mathematics as illustrated in the following lemma. The lemma states that if a probability distribution \mathbf{q} has the property that the probability of traversing each edge is the same in both directions, then the probability distribution must be the steady state distribution of the Markov chain. The lemma is used frequently.

Lemma 5.10 In a strongly connected Markov chain with transition probabilities p_{ij} , if a vector \mathbf{q} with non-negative components satisfies

$$q_i p_{ij} = q_i p_{ji}$$

for all i and j, then $q_i / \sum_k q_k$ is the stationary probability of node i.

Proof: Since the chain is strongly connected, there is a unique stationary probability vector $\boldsymbol{\pi}$ satisfying the equations $\boldsymbol{\pi}P = \boldsymbol{\pi}$ and $\sum_i \pi_i = 1$. Now $\mathbf{q}/\sum_k q_k$ satisfies these equations since $\sum_i q_i/\sum_k q_k = 1$ and for each fixed j, $\sum_i q_i p_{ij} = \sum_i q_j p_{ji} = q_j \sum_i p_{ji} = q_j$. Thus \mathbf{q} must be the steady state distribution.

5.7.2 Metropolis-Hasting Algorithm

Metropolis-Hasting algorithm is a general method to design a Markov chain whose stationary distribution is a given target distribution p. Start with a connected undirected graph G on the set of states. For example, if the states are the lattice points (x_1, x_2, \ldots, x_d) in \mathbf{R}^d with $\{x_i \in \{0, 1, 2, \ldots, n\}\}$, then G is the lattice graph with 2d coordinate edges at each interior vertex. In general, let r be the maximum degree of any node of G. The transitions of the Markov chain are defined as follows. At state i select neighbor j with probability $\frac{1}{r}$. Since the degree of i may be less than r, with some probability no edge is selected and the walk remains at i. If a neighbor j is selected and $p_j \geq p_i$, go to j. If $p_j < p_i$, go to j with probability p_j/p_i and stay at i with probability $1 - \frac{p_j}{p_i}$. Intuitively, this favors "heavier" states with higher p values. For i and j adjacent in G, $p_{ij} = \frac{1}{r} \min\left(1, \frac{p_j}{p_i}\right)$ and $p_{ii} = 1 - \sum_{j \neq i} p_{ij}$. Then

$$p_i p_{ij} = \frac{p_i}{r} \min\left(1, \frac{p_j}{p_i}\right) = \frac{1}{r} \min(p_i, p_j) = \frac{p_j}{d} \min\left(1, \frac{p_i}{p_j}\right) = p_j p_{ji}.$$

By Lemma 5.10, the stationary probabilities are $p(\mathbf{x})$ as desired.

$$p(a) = \frac{1}{2}$$

$$p(a) = \frac{1}{2}$$

$$p(b) = \frac{1}{4}$$

$$p(c) = \frac{1}{8}$$

$$p(d) = \frac{1}{8}$$

$$p(d) = \frac{1}{8}$$

$$p(d) = \frac{1}{8}$$

$$p(d) = \frac{1}{12}$$

$$p(d) = p(a)p(a \to a) + p(b)p(b \to a) + p(c)p(c \to a) + P(d)p(d \to a)$$

$$= \frac{1}{2} \cdot \frac{2}{3} + \frac{1}{4} \cdot \frac{1}{3} + \frac{1}{8} \cdot \frac{1}{3} = \frac{1}{4}$$

$$p(d) = p(a)p(a \to b) + p(b)p(b \to b) + p(c)p(c \to b)$$

$$= \frac{1}{2} \cdot \frac{1}{6} + \frac{1}{4} \cdot \frac{1}{2} + \frac{1}{8} \cdot \frac{1}{3} = \frac{1}{4}$$

$$p(d) = p(a)p(a \to d) + p(b)p(b \to c) + p(c)p(c \to d) + P(d)p(d \to c)$$

$$= \frac{1}{2} \cdot \frac{1}{12} + \frac{1}{4} \cdot \frac{1}{6} + \frac{1}{8} \cdot 0 + \frac{1}{8} \cdot \frac{1}{3} = \frac{1}{8}$$

$$p(d) = p(a)p(a \to d) + p(c)p(c \to d) + P(d)p(d \to d)$$

$$= \frac{1}{2} \cdot \frac{1}{12} + \frac{1}{8} \cdot \frac{1}{3} + \frac{1}{8} \cdot \frac{1}{3} = \frac{1}{8}$$

Figure 5.6: Using the Metropolis-Hasting algorithm to set probabilities for a random walk so that the stationary probability will be a desired probability.

Example: Consider the graph in Figure 5.6. Using the Metropolis-Hasting algorithm, assign transition probabilities so that the stationary probability of a random walk is $p(a) = \frac{1}{2}$, $p(b) = \frac{1}{4}$, $p(c) = \frac{1}{8}$, and $p(d) = \frac{1}{8}$. The maximum degree of any vertex is three so at a the probability of taking the edge (a,b) is $\frac{1}{3}\frac{1}{4}\frac{2}{1}$ or $\frac{1}{6}$. The probability of taking the edge (a,c) is $\frac{1}{3}\frac{1}{8}\frac{2}{1}$ or $\frac{1}{12}$ and of taking the edge (a,d) is $\frac{1}{3}\frac{1}{8}\frac{2}{1}$ or $\frac{1}{12}$. Thus the probability of staying at a is $\frac{2}{3}$. The probability of taking the edge from a to a is a and the probability of taking the edge from a to a is a and the probability of taking the edge from a to a is a and the probability of taking the edge from a to a is a and the probability of taking the edge from a to a is a and the probability of taking the edge from a to a is a. Thus the stationary probability of a is a and a is a a

5.7.3 Gibbs Sampling

Gibbs sampling is another Markov Chain Monte Carlo method to sample from a multivariate probability distribution. Let $p(\mathbf{x})$ be the target distribution where $\mathbf{x} = (x_1, \dots, x_d)$. Gibbs sampling consists of a random walk on a graph whose vertices correspond to the values of $\mathbf{x} = (x_1, \dots, x_d)$ and in which there is an edge from \mathbf{x} to \mathbf{y} if \mathbf{x} and \mathbf{y} differ in only one coordinate.

To generate samples of $\mathbf{x} = (x_1, \dots, x_d)$ with a target distribution $p(\mathbf{x})$, the Gibbs sampling algorithm repeats the following steps. One of the variables x_i is chosen to be updated. Its new value is chosen based on the marginal probability of x_i with the other variables fixed. There are two commonly used schemes to determine which x_i to update. One scheme is to choose x_i randomly, the other is to choose x_i by sequentially scanning from x_1 to x_d .

Suppose that \mathbf{x} and \mathbf{y} are two states that differ in only one coordinate x_i . Then, in the scheme where a coordinate is randomly chosen to modify, the probability $p_{\mathbf{x}\mathbf{y}}$ of going from \mathbf{x} to \mathbf{y} is

$$p_{\mathbf{x}\mathbf{y}} = \frac{1}{d}p(y_i|x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d).$$

The normalizing constant is 1/d since for a given value i the probability distribution of $p(y_i|x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d)$ sums to one, and thus summing i over the d-dimensions results in a value of d. Similarly,

$$p_{\mathbf{yx}} = \frac{1}{d}p(x_i|x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d).$$

Here use was made of the fact that for $j \neq i$, $x_j = y_j$.

It is simple to see that this chain is time reversible with stationary probability proportional to $p(\mathbf{x})$. Rewrite $p_{\mathbf{x}\mathbf{y}}$ as

$$p_{\mathbf{x}\mathbf{y}} = \frac{1}{d} \frac{p(y_i|x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d) p(x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d)}{p(x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d)}$$

$$= \frac{1}{d} \frac{p(x_1, x_2, \dots, x_{i-1}, y_i, x_{i+1}, \dots, x_d)}{p(x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d)}$$

$$= \frac{1}{d} \frac{p(\mathbf{y})}{p(x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d)}$$

again using $x_j = y_j$ for $j \neq i$. Similarly write

$$p_{\mathbf{y}\mathbf{x}} = \frac{1}{d} \frac{p(\mathbf{x})}{p(x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d)}$$

from which it follows that $p(\mathbf{x})p_{xy} = p(\mathbf{y})p_{yx}$. By Lemma 5.10 the stationary probability of the random walk is $p(\mathbf{x})$.

5.8 Convergence to Steady State

The Metropolis-Hasting algorithm and Gibbs sampling both involve a random walk. Initial states of the walk are highly dependent on the start state of the walk. An important question is how fast does the walk start to reflect the stationary probability of the

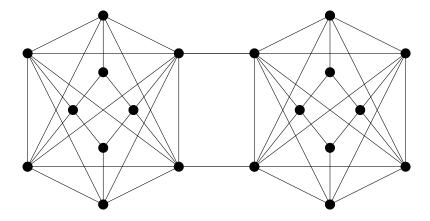


Figure 5.7: A constriction.

Markov process. If the convergence time was proportional to the number of states the algorithms would not be very useful, since as we remarked, the number of states can be exponentially large.

There are clear examples of connected chains that take a long time to converge. A chain with a constriction (see Figure 5.7) takes a long time to converge since the walk is unlikely to reach the narrow passage between the two halves, which are both reasonably big. The interesting thing is that a converse is also true. If there is no constriction, then the chain converges fast. We show this shortly.

A function is unimodal if it has a single maximum, i.e., it increases and then decreases. A unimodal function like the normal density has no constriction blocking a random walk from getting out of a large set, whereas a bimodal function can have a constriction. Interestingly, many common multivariate distributions as well as univariate probability distributions like the normal and exponential are unimodal and sampling according to these distributions can be done using the methods here.

A natural problem is estimating the probability of a convex region in d-space according to a normal distribution. Let R be the region defined by the inequality $x_1+x_2+\cdots+x_{d/2} \le x_{(d/2)+1}+\cdots+x_d$. Pick a sample according to the normal distribution and accept the sample if it satisfies the inequality. If not, reject the sample and retry until one gets a number of samples satisfying the inequality. Then the probability of the region is approximated by the fraction of the samples that satisfied the inequality. However, suppose R was the region $x_1 + x_2 + \cdots + x_{d-1} \le x_d$. The probability of this region is exponentially small in d and so rejection sampling runs into the problem that we need to pick exponentially many samples before we expect to accept even one sample. This second situation is typical. Imagine computing the probability of failure of a system. The object of design is to

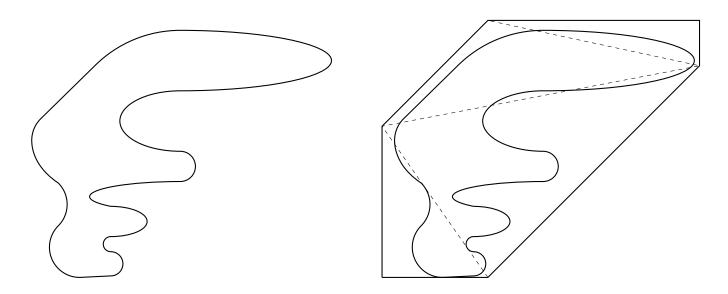


Figure 5.8: Area enclosed by curve.

make the system reliable, so the failure probability is likely to be very low and rejection sampling will take a long time to estimate the failure probability.

A similar problem is one of computing areas and volumes. First consider the problem of computing the area enclosed by the curve in Figure 5.8. One method would be to find a "nicer" enclosing shape. The picture on the right shows a convex polygon whose area we can compute in closed form by adding up the areas of the triangles. Throw darts at the larger shape, i.e., pick samples uniformly at random from the larger shape, and estimate the ratio of areas by the proportion of samples that land in the area enclosed by the curve.

Such methods fail in higher dimensions. For example, to compute the volume of a d-dimensional sphere by enclosing the sphere in a cube where the ratio of volume of the sphere to the cube is exponentially small, requires throwing exponentially many darts before getting any nonzero answer.

A different way to solve the problem of drawing a uniform random sample from a d-dimensional region is to put a grid on the region and do a random walk on the grid points. At each time, pick one of the 2d coordinate neighbors of the current grid point, each with probability 1/(2d), then go to the neighbor if it is still in the set; otherwise, stay put and repeat. This can be shown to lead to a polynomial time algorithm for drawing a uniform random sample from a bounded convex d-dimensional region. It turns out that this can be used to estimate volumes of such a region by immersing the region in a magnified copy of itself intersected with a nice object like a cube. We do not give the details here.

In general, there could be constrictions that prevent rapid convergence to the stationary probability. However, if the set is convex in any number of dimensions, then there are

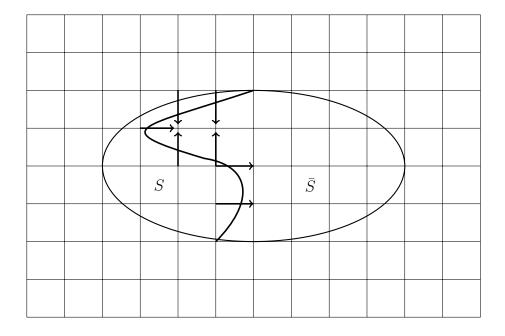


Figure 5.9: Each grid point in the ellipse is a state. The set of states in the ellipse is divided into two sets, S and \bar{S} , by the curve. The transitions from S to \bar{S} , which contribute to $\Phi(S)$, are marked with arrows.

no constrictions and there is rapid convergence although the proof of this is beyond the scope of this book.

Suppose \mathbf{q} is any probability distribution on the states. Execute one step of the Markov chain starting with distribution \mathbf{q} . Then the amount of probability that "flows" from i to j is $q_i p_{ji}$. If S and T are two possibly intersecting subsets of states, the total flow from S to T is $\sum_{i \in S, j \in T} q_i p_{ij}$. We use the notation

$$flow(i,j) = q_i p_{ij}$$

and

$$flow(S,T)) = \sum_{i \in S, j \in T} q_i p_{ij}.$$

We define below a combinatorial measure of constriction for a Markov chain, called the *minimum escape probability*, and relate this quantity to the rate of convergence to the stationarity probability.⁴

⁴In the Markov Chain literature, the word "conductance" is often used for minimum escape probability. Here, we have reserved the word conductance for the natural electrical quantity which is the reciprocal of resistance.

Definition: For a subset S of states of a Markov chain with stationary probabilities π , define $\Phi(S)$, the *escape probability of* S, by

$$\Phi(S) = \frac{\text{flow}(S, \bar{S})}{\pi(S)}.$$

The escape probability of S is the probability of taking a step from S to outside S conditioned on starting in S where the stationary probability at state i in S is proportional to its stationary probability, i.e., $\pi_i/\pi(S)$. The minimum escape probability MEP of the Markov chain, denoted Φ , is defined by

$$\Phi = \min_{\substack{S \\ \boldsymbol{\pi}(S) < 1/2}} \Phi(S).$$

The restriction to sets with $\pi \leq 1/2$ in the definition of ϕ is natural. One does not need to escape from big sets. Note that a constriction would mean a small Φ .

Definition: Fix an $\varepsilon > 0$. The ε -mixing time of a Markov chain is the minimum integer t such that for any starting distribution $\mathbf{p^{(0)}}$, the 1-norm distance between the t-step running average probability distribution $\mathbf{a^{(t)}}$ and the stationary distribution is at most ε .

The theorem below states that if the minimum escape probability Φ is large, then there is fast convergence of the running average probability. Intuitively, if Φ is large then the walk rapidly leaves any subset of states. Later we will see examples where the mixing time is much smaller than the cover time. That is, the number of steps before a random walk reaches a random state independent of its starting state is much smaller than the average number of steps needed to reach every state. We assume time reversibility, namely that $\pi_i p_{ij} = \pi_j p_{ji}$.

Theorem 5.11 The ε mixing time of a time-reversible Markov chain is

$$O\left(\frac{\ln(1/\pi_{min})}{\Phi^2\varepsilon^3}\right).$$

Proof: Recall that $\mathbf{a^{(t)}}$ is the long term average probability distribution. Let

$$t = \frac{c \ln(1/\pi_{\min})}{\Phi^2 \varepsilon^2},$$

for a suitable constant c. For convenience, let $\mathbf{a} = \mathbf{a^{(t)}}$. We need to show that $|\mathbf{a} - \boldsymbol{\pi}| \leq \varepsilon$.

Let v_i denote the ratio of the long term average probability at time t divided by the stationary probability. Thus $v_i = \frac{a_i}{\pi_i}$. Renumber states so that $v_1 \leq v_2 \leq \cdots$. Since

 $\mathbf{a}P$ is the probability vector after executing one step of the Markov chain starting with probabilities \mathbf{a} , $\mathbf{a} - \mathbf{a}P$ is the net loss of probability due to the step. Let k be any integer with $v_k > 1$. Let $A = \{1, 2, \dots, k\}$. The net loss of probability from the set A in one step is $\sum_{i=1}^k (a_i - (\mathbf{a}P)_i) \leq \frac{2}{t}$ as in the proof of Theorem 5.1.

Another way to reckon the net loss of probability from A is to take the difference of the probability flow from A to \bar{A} and the flow from \bar{A} to A. By time-reversibility, for i < j,

$$flow(i, j) - flow(j, i) = \pi_i p_{ij} v_i - \pi_j p_{ji} v_j = \pi_j p_{ji} (v_i - v_j) \ge 0,$$

Thus for any $l \ge k$, the flow from A to $\{k+1, k+2, \ldots, l\}$ minus the flow from $\{k+1, k+2, \ldots, l\}$ is non-negative. The net loss from A is at least

$$\sum_{\substack{i \le k \\ j > l}} \pi_j p_{ji} (v_i - v_j) \ge (v_k - v_{l+1}) \sum_{\substack{i \le k \\ j > l}} \pi_j p_{ji}.$$

Thus,

$$(v_k - v_{l+1}) \sum_{\substack{i \le k \\ i > l}} \pi_j p_{ji} \le \frac{2}{t}.$$

If $\pi(\{i|v_i \leq 1\}) \leq \varepsilon/2$, then

$$|\mathbf{a} - \boldsymbol{\pi}|_1 = 2 \sum_{\substack{i \ v_i \le 1}} (1 - v_i) \pi_i \le \varepsilon,$$

so we are done. Assume $\pi(\{i|v_i \leq 1\}) > \varepsilon/2$ so that $\pi(A) \geq \varepsilon \min(\pi(A), \pi(\bar{A}))/2$. Choose l to be the largest integer greater than or equal to k so that $\sum_{j=k+1}^{l} \pi_j \leq \varepsilon \Phi \pi(A)/2$. Since

$$\sum_{i=1}^{k} \sum_{j=k+1}^{l} \pi_j p_{ji} \le \sum_{j=k+1}^{l} \pi_j \le \varepsilon \Phi \pi(A)/2$$

by the definition of MEP,

$$\sum_{i \le k < j} \pi_j p_{ji} \ge \Phi \min(\pi(A), \pi(\bar{A})) \ge \varepsilon \Phi \pi(A).$$

Thus $\sum_{\substack{i \leq k \\ j > l}} \pi_j p_{ji} \geq \varepsilon \Phi \pi(A)/2$ and substituting into the above inequality gives

$$v_k - v_{l+1} \le \frac{8}{t\varepsilon\Phi\pi(A)}. (5.5)$$

Now, divide $\{1, 2, ...\}$ into groups as follows. The first group G_1 is $\{1\}$. In general, if the r^{th} group G_r begins with state k, the next group G_{r+1} begins with state l+1 where l is

as defined above. Let i_0 be the largest integer with $v_{i_0} > 1$. Stop with G_m , if G_{m+1} would begin with an $i > i_0$. If group G_r begins in i, define $u_r = v_i$. Let $\rho = 1 + \frac{\varepsilon \Phi}{2}$.

$$|\mathbf{a} - \boldsymbol{\pi}|_1 \le 2 \sum_{i=1}^{i_0} \pi_i(v_i - 1) \le \sum_{r=1}^m \pi(G_r)(u_r - 1) = \sum_{r=1}^m \pi(G_1 \cup G_2 \cup \ldots \cup G_r)(u_r - u_{r+1}),$$

where the analog of integration by parts (for sums) is used in the last step and used the convention that $u_{m+1} = 1$. Since $u_r - u_{r+1} \le 8/\varepsilon \Phi \pi(G_1 \cup \ldots \cup G_r)$, the sum is at most $8m/t\varepsilon \Phi$. Since $\pi_1 + \pi_2 + \cdots + \pi_{l+1} \ge \rho(\pi_1 + \pi_2 + \cdots + \pi_k)$,

$$m \le \ln_{\rho}(1/\pi_1) \le \ln(1/\pi_1)/(\rho - 1).$$

Thus $|\mathbf{a} - \boldsymbol{\pi}|_1 \leq O(\ln(1/\pi_{\min})/t\Phi^2\varepsilon^2) \leq \varepsilon$ for a suitable choice of c and this completes the proof.

5.8.1 Using Minimum Escape Probability to Prove Convergence

We now give some examples where Theorem 5.11 is used to bound the minimum escape probability and hence show rapid convergence. For the first example, consider a random walk on an undirected graph consisting of an n-vertex path with self-loops at the both ends. With the self loops, the stationary probability is a uniform $\frac{1}{n}$ over all vertices. The set with minimum escape probability consists of the first n/2 vertices, for which flow $(S, \bar{S}) = \pi_{n/2} p_{n/2, 1+n/2} = \Omega(\frac{1}{n})$ and $\pi(S) = \frac{1}{2}$. Thus

$$\Phi(S) = \frac{\text{flow}(S, \bar{S})}{\pi(S)} = 2\pi_{\frac{n}{2}} \ p_{\frac{n}{2}, \frac{n}{2} + 1} = \Omega(1/n).$$

By Theorem 5.11, for ε a constant such as 1/100, after $O(n^2 \log n)$ steps, $|\mathbf{a^{(t)}} - \boldsymbol{\pi}|_1 \le 1/100$. For this graph, the hitting time and the cover time are $O(n^2)$. In many interesting cases, the mixing time may be much smaller than the cover time. We will see such an example later.

For the second example, consider the $n \times n$ lattice in the plane where from each point there is a transition to each of the coordinate neighbors with probability $^1/_4$. At the boundary there are self-loops with probability 1-(number of neighbors)/4. It is easy to see that the chain is connected. Since $p_{ij} = p_{ji}$, the function $f_i = 1/n^2$ satisfies $f_i p_{ij} = f_j p_{ji}$ and by Lemma 5.10 is the stationary probability. Consider any subset S consisting of at most half the states. For at least half the states (x, y) in S, (each state is indexed by its x and y coordinate), either row x or column y intersects \bar{S} (Exercise 5.35). Each state in S adjacent to a state in \bar{S} contributes $\Omega(1/n^2)$ to the flow (S, \bar{S}) . Thus,

flow
$$(S, \bar{S}) = \sum_{i \in S} \sum_{j \notin S} \pi_i p_{ij} \ge \frac{\boldsymbol{\pi}(S)}{2} \frac{1}{n^2}$$

establishing that

$$\Phi = \frac{\text{flow}(S, \bar{S})}{\pi(S)} \ge \frac{1}{2n}.$$

By Theorem 5.11, after $O(n^2 \ln n/\varepsilon^2)$ steps, $|\mathbf{a^{(t)}} - \boldsymbol{\pi}|_1 \le 1/100$.

Next consider the $n \times n \times n \times n \times n$ grid in d-dimensions with a self-loop at each boundary point with probability 1 - (number of neighbors)/2d. The self loops make all π_i equal to n^{-d} . View the grid as an undirected graph and consider the random walk on this undirected graph. Since there are n^d states, the cover time is at least n^d and thus exponentially dependent on d. It is possible to show (Exercise 5.49) that MEP is $\Omega(1/dn)$. Since all π_i are equal to n^{-d} , the mixing time is $O(d^3n^2 \ln n/\varepsilon^2)$, which is polynomially bounded in n and d.

Next consider a random walk on a connected n vertex undirected graph where at each vertex all edges are equally likely. The stationary probability of a vertex equals the degree of the vertex divided by the sum of degrees which equals twice the number of edges. The sum of the vertex degrees is at most n^2 and thus, the steady state probability of each vertex is at least $\frac{1}{n^2}$. Since the degree of a vertex is at most n, the probability of each edge at a vertex is at least $\frac{1}{n}$. For any S,

flow
$$(S, \bar{S}) \ge \frac{1}{n^2} \frac{1}{n} = \frac{1}{n^3}$$
.

Thus the minimum escape probability is at least $\frac{1}{n^3}$. Since $\pi_{\min} \geq \frac{1}{n^2}$, $\ln \frac{1}{\pi_{\min}} = O(\ln n)$. Thus, the mixing time is $O(n^6(\ln n)/\varepsilon^2)$.

For our final example, consider the interval [-1,1]. Let δ be a "grid size" specified later and let G be the graph consisting of a path on the $\frac{2}{\delta}+1$ vertices $\{-1,-1+\delta,-1+2\delta,\ldots,1-\delta,1\}$ having self loops at the two ends. Let $\pi_x=ce^{-\alpha x^2}$ for $x\in\{-1,-1+\delta,-1+2\delta,\ldots,1-\delta,1\}$ where $\alpha>1$ and c has been adjusted so that $\sum_x \pi_x=1$.

We now describe a simple Markov chain with the π_x as its stationary probability and argue its fast convergence. With the Metropolis-Hastings' construction, the transition probabilities are

$$p_{x,x+\delta} = \frac{1}{2} \min \left(1, \frac{e^{-\alpha(x+\delta)^2}}{e^{-\alpha x^2}} \right) \text{ and } p_{x,x-\delta} = \frac{1}{2} \min \left(1, \frac{e^{-\alpha(x-\delta)^2}}{e^{-\alpha x^2}} \right).$$

Let S be any subset of states with $\pi(S) \leq \frac{1}{2}$. Consider the case when S is an interval

 $[k\delta, 1]$ for $k \geq 1$. It is easy to see that

$$\pi(S) \le \int_{x=(k-1)\delta}^{\infty} ce^{-\alpha x^2} dx$$

$$\le \int_{(k-1)\delta}^{\infty} \frac{x}{(k-1)\delta} ce^{-\alpha x^2} dx$$

$$= O\left(\frac{ce^{-\alpha((k-1)\delta)^2}}{\alpha(k-1)\delta}\right).$$

Now there is only one edge from S to \bar{S} and

flow
$$(S, \bar{S}) = \sum_{i \in S} \sum_{j \notin S} \pi_i p_{ij} = \pi_{k\delta} p_{k\delta, (k-1)\delta} = \min(ce^{-\alpha k^2 \delta^2}, ce^{-\alpha (k-1)^2 \delta^2}) = ce^{-\alpha k^2 \delta^2}.$$

Using $1 \le k \le 1/\delta$ and $\alpha \ge 1$, the minimum escape probability of S is

$$\Phi(S) = \frac{\text{flow}(S, \bar{S})}{\pi(S)} \ge ce^{-\alpha k^2 \delta^2} \frac{\alpha(k-1)\delta}{ce^{-\alpha((k-1)\delta)^2}}$$
$$\ge \Omega(\alpha(k-1)\delta e^{-\alpha\delta^2(2k-1)}) \ge \Omega(\delta e^{-O(\alpha\delta)}).$$

For $\delta < \frac{1}{\alpha}$, we have $\alpha \delta < 1$, so $e^{-O(\alpha \delta)} = \Omega(1)$, thus, $\Phi(S) \ge \Omega(\delta)$. Now, $\pi_{\min} \ge ce^{-\alpha} \ge e^{-1/\delta}$, so $\ln(1/\pi_{\min}) \le 1/\delta$.

If S is not an interval of the form [k,1] or [-1,k], then the situation is only better since there is more than one "boundary" point which contributes to flow (S,\bar{S}) . We do not present this argument here. By Theorem 5.11 in $\Omega(1/\delta^3\varepsilon^2)$ steps, a walk gets within ε of the steady state distribution.

In these examples, we have chosen simple probability distributions. The methods extend to more complex situations.

5.9 Bibliographic Notes

The material on the analogy between random walks on undirected graphs and electrical networks is from [DS84] as is the material on random walks in Euclidean space. Additional material on Markov Chains can be found in [MR95b], [MU05], and [per10]. For material on Markov Chain Monte Carlo methods see [Jer98] and [Liu01].

The use of Minimum Escape Probability (also called conductance) to prove convergence of Markov Chains is by Sinclair and Jerrum, [SJ] and Alon [Alo86]. A polynomial time bounded Markov Chain based method for estimating the volume of convex sets was developed by Dyer, Frieze and Kannan [DFK91].

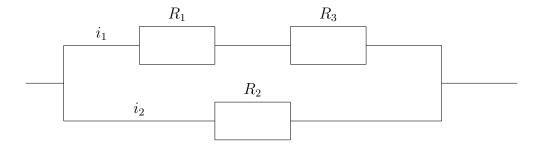


Figure 5.10: An electrical network of resistors.

5.10 Exercises

Exercise 5.1

- a Give an example of a graph, with cycles of more than one length, for which the greatest common divisor of all cycle lengths is three.
- b Prove that a graph is bipartite if and only if it has no odd length cycle.
- c Show that for the random walk on a bipartite graph (with any edge weights), the steady state probabilities do not exist.

Exercise 5.2

- (a) What is the set of possible harmonic functions on a graph if there are only interior vertices and no boundary vertices that supply the boundary condition?
- (b) Let q_x be the steady state probability of vertex x in a random walk on an undirected graph and let d_x be the degree of vertex x. Show that $\frac{q_x}{d_x}$ is a harmonic function.
- (c) If there are multiple harmonic functions when there are no boundary conditions why is the steady state probability of a random walk on an undirected graph unique?
- (d) What is the steady state probability of a random walk on an undirected graph?

Exercise 5.3 Consider the electrical resistive network in Figure 5.10 consisting of vertices connected by resistors. Kirchoff's law states that the currents at each node sum to zero. Ohm's law states that the voltage across a resistor equals the product of the resistance times the current through it. Using these laws calculate the effective resistance of the network.

Exercise 5.4 Given a graph consisting of a single path of five vertices numbered 1 to 5, what is the probability of reaching vertex 1 before vertex 5 when starting at vertex 4.

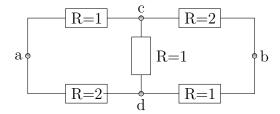


Figure 5.11: An electrical network of resistors.

Exercise 5.5 Consider the electrical network of Figure 5.11.

- (a) Set the voltage at a to one and at b to zero. What are the voltages at c and d?
- (b) What is the current in the edges a to c, a to d, c to d. c to b and d to b?
- (c) What is the effective resistance between a and b?
- (d) Convert the electrical network to a graph. What are the edge probabilities at each vertex?
- (e) What is the probability of a walk starting at c reaching a before b? a walk starting at d?
- (f) How frequently does a walk from a to b go through the edge from c to d?
- (g) What is the probability that a random walk starting at a will return to a before reaching b?

Exercise 5.6 Prove that the escape probability $p_{escape} = \frac{c_{eff}}{c_a}$ must be less than or equal to one.

Exercise 5.7 Prove that reducing the value of a resistor in a network cannot increase the effective resistance. Prove that increasing the value of a resistor cannot decrease the effective resistance.

Exercise 5.8 The energy dissipated by the resistance of edge xy in an electrical network is given by $i_{xy}^2 r_{xy}$. The total energy dissipation in the network is $E = \frac{1}{2} \sum_{x,y} i_{xy}^2 r_{xy}$ where the $\frac{1}{2}$ accounts for the fact that the dissipation in each edge is counted twice in the summation. Show that the actual current distribution is that distribution satisfying Ohm's law that minimizes energy dissipation.

Exercise 5.9 What is the hitting time h_{uv} for two adjacent vertices on a cycle of length n? What is the hitting time if the edge (u, v) is removed?

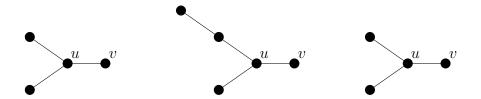


Figure 5.12: Three graphs

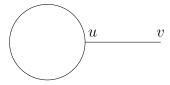


Figure 5.13: A graph consisting of a circle of edges along with a path of length m

Exercise 5.10 What is the hitting time h_{uv} for the three graphs if Figure 5.14.

Exercise 5.11 Consider the n node connected graph shown in Figure 5.13 consisting of an edge (u, v) plus a connected graph on n-1 vertices and some number of edges. Prove that $h_{uv} = 2m-1$ where m is the number of edges in the n-1 vertex subgraph.

Exercise 5.12 What is the most general solution to the difference equation t(i + 2) - 5t(i + 1) + 6t(i) = 0/ How many boundary conditions do you need to make the solution unique?

Exercise 5.13 Given the difference equation $a_k t(i+k) + at(i+k-1) + \cdots + a_1 t(i+1) + a_0 t(i) = 0$ the polynomial $a_k t^k + a_{k-i} t^{k-1} + \cdots + a_1 t + a_0 = 0$ is called the characteristic polynomial.

- (a) If the equation has a set of r distinct roots, what is the most general form of the solution?
- (b) If the roots of the characteristic polynomial are not unique what is the most general form of the solution?
- (c) What is the dimension of the solution spaced?
- (d) If the difference equation is not homogeneous and f(i) is a specific solution to the non homogeneous difference equation, what is the full set of solutions to the difference equation?

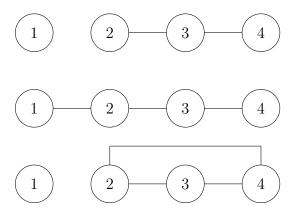


Figure 5.14: Three graph

Exercise 5.14 Consider the set of integers $\{1, 2, ..., n\}$. How many draws d with replacement are necessary so that every integer is drawn?

Exercise 5.15 Consider a random walk on a clique of size n. What is the expected number of steps before a given vertex is reached?

Exercise 5.16 Show that adding an edge can either increase or decrease hitting time by calculating h_{24} for the three graphs in figure 5.14.

Exercise 5.17 Show that adding an edge to a graph can either increase or decrease commute time.

Exercise 5.18 Prove that two independent random walks on a two dimensional lattice will hit with probability one.

Exercise 5.19 Consider the lattice in 2-dimensions. In each square add the two diagonal edges. What is the escape probability for the resulting graph?

Exercise 5.20 Determine by simulation the escape probability for the 3-dimensional lattice.

Exercise 5.21 What is the escape probability for a random walk starting at the root of a binary tree?

Exercise 5.22 Consider a random walk on the positive half line, that is the integers 1, 2, 3, At the origin, always move right one step. At all other integers move right with probability 2/3 and left with probability 1/3. What is the escape probability?

Exercise 5.23 What is the probability of returning to the start vertex on a random walk on an infinite planar graph?

Exercise 5.24 Create a model for a graph similar to a 3-dimensional lattice in the way that a planar graph is similar to a 2-dimensional lattice. What is probability of returning to the start vertex in your model?

Exercise 5.25 Consider a strongly connected directed graph. In the steady state calculate the flow through each edge of a random walk.

Exercise 5.26 Create a random directed graph with 200 nodes and roughly eight edges per node. Add k new nodes and calculate the page rank with and without directed edges from the k added nodes to node 1. How much does adding the k edges change the page rank of nodes for various values of k and restart frequency? How much does adding a loop at node 1 change the page rank? To do the experiment carefully one needs to consider the page rank of a node to which the star is attached. If it has low page rank its page rank is likely to increase a lot.

Exercise 5.27 Repeat the experiment in Exercise 5.26 for hitting time.

Exercise 5.28 Search engines ignore self loops in calculating page rank. Thus, to increase page rank one needs to resort to loops of length two. By how much can you increase the page rank of a page by adding a number of loops of length two?

Exercise 5.29 Can one increase the page rank of a node v in a directed graph by doing something some distance from v? The answer is yes if there is a long narrow chain of nodes into v with no edges leaving the chain. What if there is no such chain?

Exercise 5.30 Consider modifying personal page rank as follows. Start with the uniform restart distribution and calculate the steady state probabilities. Then run the personalized page rank algorithm using the steady state distribution calculated instead of the uniform distribution. Keep repeating until the process converges. That is, we get a steady state probability distribution such that if we use the steady state probability distribution for the restart distribution we will get the steady state probability distribution back. Does this process converge? What is the resulting distribution? What distribution do we get for the graph consisting of two vertices u and v with a single edge from u to v?

Exercise 5.31

- (a) What is the hitting time for a vertex in a complete directed graph with self loops?
- (b) What is the hitting time for a vertex in a directed cycle with n nodes?

Exercise 5.32 Using a web browser bring up a web page and look at the source html. How would you extract the url's of all hyperlinks on the page if you were doing a crawl of the web? With Internet Explorer click on "source" under "view" to access the html representation of the web page. With Firefox click on "page source" under "view".

Exercise 5.33 Sketch an algorithm to crawl the World Wide Web. There is a time delay between the time you seek a page and the time you get it. Thus, you cannot wait until the page arrives before starting another fetch. There are conventions that must be obeyed if one were to actually do a search. Sites specify information has to how long or which files can be searched. Do not attempt an actual search without guidance from a knowledgeable person.

Exercise 5.34 Prove Proposition 5.9 that for two probability distributions $\mathbf{p}, \mathbf{q}, |\mathbf{p} - \mathbf{q}|_1 = 2\sum_i (p_i - q_i)^+$.

Exercise 5.35 Suppose S is a subset of at most $n^2/2$ points in the $n \times n$ lattice. Show that

$$|\{(i,j) \in S : row \ i, \ col. \ j \subseteq S\}| \le |S|/2.$$

Exercise 5.36 Show that the steady state probabilities of the chain described in the Gibbs sampler is the correct p.

Exercise 5.37 A Markov chain is said to be symmetric if for all i and j, $p_{ij} = p_{ji}$. What is the steady state distribution of a connected aperiodic symmetric chain? Prove your answer.

Exercise 5.38 How would you integrate a multivariate polynomial distribution over some region?

Exercise 5.39 Given a time-reversible Markov chain, modify the chain as follows. At the current state, stay put (no move) with probability 1/2. With the other probability 1/2, move as in the old chain. Show that the new chain has the same steady state. What happens to the convergence time in this modification?

Exercise 5.40 Using the Metropolis-Hasting Algorithm create a Markov chain whose stationary probability is that given in the following table.

x_1x_2	00	01	02	10	11	12	20	21	22
Prob	1/16	1/8	1/16	1/8	1/4	1/8	1/16	1/8	1/16

Exercise 5.41 Let \mathbf{p} be a probability vector (nonnegative components adding up to 1) on the vertices of a connected, aperiodic graph. Set p_{ij} (the transition probability from i to j) to p_j for all $i \neq j$ which are adjacent in the graph. Show that the steady state probability vector for the chain is \mathbf{p} . Is running this chain an efficient way to sample according to a distribution close to \mathbf{p} ? Think, for example, of the graph G being the $n \times n \times n \times \cdots n$ grid.

Exercise 5.42 Construct the edge probability for a three state Markov chain so that the steady state probability is $(\frac{1}{2}, \frac{1}{3}, \frac{1}{6})$.

Exercise 5.43 Consider a three state Markov chain with steady state probability $(\frac{1}{2}, \frac{1}{3}, \frac{1}{6})$. Consider the Metropolis-Hastings algorithm with G the complete graph on these three nodes. What is the expected probability that we would actually make a move along a selected edge?

Exercise 5.44 Try Gibbs sampling on
$$p(x) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$
.

What happens? How does the Metropolis Hasting Algorithm do?

Exercise 5.45 Consider $p(\mathbf{x})$, where, $\mathbf{x} = (x_1, \dots, x_{100})$ and $p(\mathbf{0}) = \frac{1}{2}$, $p(\mathbf{x}) = \frac{1}{2^{100}}$ $x \neq 0$. How does Gibbs sampling behave?

Exercise 5.46 Construct an algorithm and compute the volume of a unit radius sphere in 20 dimensions by carrying out a random walk on a 20×20 grid with 0.1 spacing.

Exercise 5.47 Given a graph G and an integer k how would you generate a sequence of connected subgraphs S_1, S_2, \ldots of G of size k where S_i is generated with probability proportional to $2^{|E_i|}$ where E_i is the set of edges in S_i ?

Exercise 5.48 What is the mixing time for

- (a) a clique?
- (b) two cliques connected by a single edge?

Exercise 5.49 Show that for the $n \times n \times \cdots \times n$ grid in d space, MEP is $\Omega(1/dn)$. Hint: The argument is a generalization of the argument in Exercise 5.35. Argue that for any subset S containing at most 1/2 the grid points, for at least 1/2 the grid points in S, among the d coordinate lines through the point, at least one intersects \bar{S} .

6 Learning and VC-dimension

6.1 Learning

Learning algorithms are general purpose tools that solve problems often without detailed domain-specific knowledge. They have proven to be very effective in a large number of contexts. We start with an example. Suppose one wants an algorithm to distinguish among different types of motor vehicles such as cars, trucks, and tractors. Using domain knowledge one can create a set of features. Some examples of features are the number of wheels, the power of the engine, the number of doors, and the length of vehicle. If there are d features, each object can be represented as a d-dimensional vector, called the feature vector, with each component of the vector giving the value of one feature such as engine power, the number of doors, etc. Using domain knowledge one develops a set of rules to distinguish among different types of objects. A learning algorithm uses the feature vector representation of an object, which is assumed to be given by the domain "expert". Instead of having the domain expert develop a set of rules, the algorithm only asks the expert, called the teacher, to label each vector. In this example, the labels would be "car", "truck", and "tractor". The algorithm's task is to develop a set of rules that applied to the given vectors gives the same labels as the teacher. Each feature vector is called an example and the given set of labeled examples is called the training set. The task of the learner is to output a set of rules that correctly labels all training examples. Of course, for this limited task, one could output the rule "for each training example, use the teacher's label". But, we insist on Occam's razor principle that states that the rules output by the algorithm must be more succinct than the table of all labeled training examples. This is akin to developing a scientific theory to explain extensive observations. The theory must be more succinct than just a list of observations.

However, the general task of interest is not to be correct just on the training examples, but have the learnt rules correctly predict the labels of future examples. Intuitively, if the classifier is trained on sufficiently many training examples, then it seems likely that it would work well on the space of all examples. We will see later that the theory of Vapnik-Chervonenkis dimension (VC-dimension) confirms this intuition. In general, optimization techniques such as linear and convex programming, play an important role in learning algorithms. Throughout this chapter, we assume all the labels are binary. It is not difficult to see that the general problem of classifying into one of several types can be reduced to binary classification. Classifying into car or non-car, tractor or non-tractor, etc. will pin down the type of vehicle. So the teacher's labels are assumed to be +1 or -1. For an illustration, see Figure 6.1, where, examples are in 2-dimensions (there are two features) where those labeled -1 are unfilled circles and those labeled +1 are filled circles. The right hand picture illustrates a rule that the algorithm could come up with: the examples above the thick line are -1 and those below are +1.

The simplest rule in d-dimensional space is the generalization of a line in the plane,

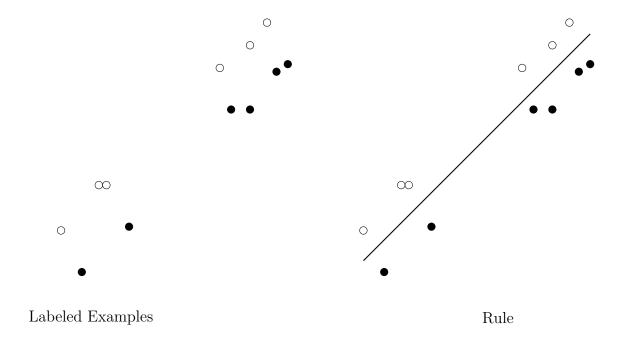


Figure 6.1: Training set and the rule that is learnt

namely, a half-space. Does a weighted sum of feature values exceed a threshold? Such a rule may be thought of as being implemented by a threshold gate that takes the feature values as inputs, computes their weighted sum and outputs yes or no depending on whether or not the sum is greater than the threshold. One could also look at a network of interconnected threshold gates called a neural net. Threshold gates are sometimes called perceptrons since one model of human perception is that it is done by a neural net in the brain.

6.2 Linear Separators, the Perceptron Algorithm, and Margins

The problem of learning a half-space or a linear separator consists of n labeled examples $\mathbf{a_1}, \mathbf{a_2}, \ldots, \mathbf{a_n}$ in d-dimensional space. The task is to find a d-dimensional vector \mathbf{w} , if one exists, and a threshold b such that

$$\mathbf{w} \cdot \mathbf{a_i} > b$$
 for each $\mathbf{a_i}$ labelled +1
 $\mathbf{w} \cdot \mathbf{a_i} < b$ for each $\mathbf{a_i}$ labelled -1. (6.1)

A vector-threshold pair, (\mathbf{w}, b) , satisfying the inequalities is called a linear separator.

The above formulation is a linear program (LP) in the unknowns \mathbf{w} and b that can be solved by a general purpose LP algorithm. Linear programming is solvable in polynomial time but a simpler algorithm called the perceptron learning algorithm can be much faster

when there is a feasible solution \mathbf{w} with a lot of wiggle room or margin, though it is not polynomial time bounded in general.

We begin by adding an extra coordinate to each \mathbf{a}_i and \mathbf{w} , writing $\hat{\mathbf{a}_i} = (\mathbf{a_i}, 1)$ and $\hat{\mathbf{w}} = (\mathbf{w}, -b)$. Suppose l_i is the ± 1 label on $\mathbf{a_i}$. Then, the inequalities in (6.1) can be rewritten as

$$(\hat{\mathbf{w}} \cdot \hat{\mathbf{a_i}})l_i > 0 \quad 1 \le i \le n.$$

Since the right hand side is zero, we may scale $\hat{\mathbf{a_i}}$ so that $|\hat{\mathbf{a_i}}| = 1$. Adding the extra coordinate increased the dimension by one but now the separator contains the origin. For simplicity of notation, in the rest of this section, we drop the hats and let $\mathbf{a_i}$ and \mathbf{w} stand for the corresponding $\hat{\mathbf{a_i}}$ and $\hat{\mathbf{w}}$.

The perceptron learning algorithm

The perceptron learning algorithm is simple and elegant. We wish to find a solution \mathbf{w} to

$$(\mathbf{w} \cdot \mathbf{a_i})l_i > 0 \qquad 1 \le i \le n \tag{6.2}$$

where $|\mathbf{a_i}| = 1$. Starting with $\mathbf{w} = l_1 \mathbf{a_1}$, pick any $\mathbf{a_i}$ with $(\mathbf{w} \cdot \mathbf{a_i}) l_i \leq 0$, and replace \mathbf{w} by $\mathbf{w} + l_i \mathbf{a_i}$. Repeat until $(\mathbf{w} \cdot \mathbf{a_i}) l_i > 0$ for all i.

The intuition behind the algorithm is that correcting \mathbf{w} by adding $\mathbf{a_i}l_i$ causes the new $(\mathbf{w} \cdot \mathbf{a_i})l_i$ to be higher by $\mathbf{a_i} \cdot \mathbf{a_i}l_i^2 = |\mathbf{a_i}|^2$. This is good for this $\mathbf{a_i}$. But this change may be bad for other $\mathbf{a_j}$. The proof below shows that this very simple process quickly yields a solution \mathbf{w} provided there exists a solution with a good margin.

Definition: For a solution \mathbf{w} to (6.2), where $|\mathbf{a_i}| = 1$ for all examples, the margin is defined to be the minimum distance of the hyperplane $\{\mathbf{x}|\mathbf{w}\cdot\mathbf{x}=0\}$ to any $\mathbf{a_i}$, namely, $\min_i \frac{(\mathbf{w}\cdot\mathbf{a_i})l_i}{|\mathbf{w}|}$.

If we did not require that all $|\mathbf{a_i}| = 1$ in (6.2), then one could artificially increase the margin by scaling up the $\mathbf{a_i}$. If we did not divide by $|\mathbf{w}|$ in the definition of margin, then again, one could artificially increase the margin by scaling \mathbf{w} up. The interesting thing is that the number of steps of the algorithm depends only upon the best margin any solution can achieve, not upon n or d. In practice, the perceptron learning algorithm works well.

Theorem 6.1 Suppose there is a solution \mathbf{w}^* to (6.2) with margin $\delta > 0$. Then, the perceptron learning algorithm finds some solution \mathbf{w} with $(\mathbf{w} \cdot \mathbf{a_i})l_i > 0$ for all i in at most $\frac{1}{\delta^2} - 1$ iterations.

Proof: Without loss of generality by scaling \mathbf{w}^* assume that $|\mathbf{w}^*| = 1$. Consider the cosine of the angle between the current vector \mathbf{w} and \mathbf{w}^* , that is, $\frac{\mathbf{w}^T \mathbf{w}^*}{|\mathbf{w}|}$. In each step of

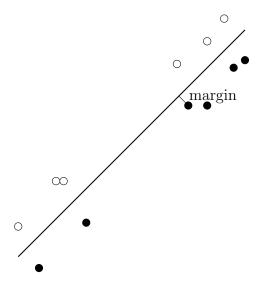


Figure 6.2: Margin of a linear separator.

the algorithm, the numerator of this fraction increases by at least δ because

$$(\mathbf{w} + \mathbf{a_i} l_i) \cdot \mathbf{w}^* = \mathbf{w} \cdot \mathbf{w}^* + l_i \mathbf{a_i} \cdot \mathbf{w}^* \ge \mathbf{w}^T \mathbf{w}^* + \delta.$$

On the other hand, the square of the denominator increases by at most one because

$$|\mathbf{w} + \mathbf{a_i} l_i|^2 = (\mathbf{w} + \mathbf{a_i} l_i) \cdot (\mathbf{w} + \mathbf{a_i} l_i) = |\mathbf{w}|^2 + 2(\mathbf{w} \cdot \mathbf{a_i})^T l_i + |\mathbf{a_i}|^2 l_i^2 \le |\mathbf{w}|^2 + 1$$

where, since $\mathbf{w}^T \mathbf{a_i} l_i \leq 0$, the cross term is non-positive.

After t iterations, $\mathbf{w} \cdot \mathbf{w}^* \geq (t+1)\delta$ since at the start $\mathbf{w} \cdot \mathbf{w}^* = l_1(\mathbf{a_1} \cdot \mathbf{w}^*) \geq \delta$ and at each iteration $\mathbf{w}^T \mathbf{w}^*$ increases by at least δ . Similarly after t iterations $|\mathbf{w}|^2 \leq t+1$ since at the start $|\mathbf{w}| = |\mathbf{a_1}| \leq 1$ and at each iteration $|\mathbf{w}|^2$ increases by at most one. Thus the cosine of the angle between \mathbf{w} and \mathbf{w}^* is at least $\frac{(t+1)\delta}{\sqrt{t+1}}$ and the cosine cannot exceed one. Therefore, the algorithm must stop before $\frac{1}{\delta^2} - 1$ iterations and at termination, $(\mathbf{w} \cdot \mathbf{a_i})l_i > 0$ for all i. This proves the theorem.

How strong is the assumption that there is a separator with margin at least δ ? Suppose for the moment, the $\mathbf{a_i}$ are picked from the uniform density on the surface of the unit hypersphere. We saw in Chapter 2 that for any fixed hyperplane passing through the origin, most of the mass of the unit sphere is within distance $O(1/\sqrt{d})$ of the hyperplane. So, the probability of one fixed hyperplane having a margin of more than c/\sqrt{d} is low. But this does not mean that there is no hyperplane with a larger margin. By the union bound, one can only assert that the probability of some hyperplane having a large margin times the number of hyperplanes which is infinite. Later we will see using VC-dimension arguments that indeed the probability of some hyperplane having a large margin is low if the examples are

selected at random from the hypersphere. So, the assumption of large margin separators existing may not be valid for the simplest random models. But intuitively, if what is to be learnt, like whether something is a car, is not very hard, then, with enough features in the model, there will not be many "near cars" that could be confused with cars nor many "near non-cars". In a real problem such as this, uniform density is not a valid assumption. In this case, there should be a large margin separator and the theorem would work.

The question arises as to how small margins can be. Suppose the examples $\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}$ were vectors with d coordinates, each coordinate a 0 or 1 and the decision rule for labeling the examples was the following.

If the first 1 coordinate of the example is odd, label the example +1. If the first 1 coordinate of the example is even, label the example -1.

This rule can be represented by the decision rule

$$(a_{i1}, a_{i2}, \dots, a_{in}) (1, -\frac{1}{2}, \frac{1}{4}, -\frac{1}{8}, \dots)^T = a_{i1} - \frac{1}{2}a_{i2} + \frac{1}{4}a_{i3} - \frac{1}{8}a_{i4} + \dots > 0.$$

However, the margin in this example can be exponentially small. Indeed, if for an example **a**, the first d/10 coordinates are all zero, then the margin is $O(2^{-d/10})$.

Maximizing the Margin

In this section, we present an algorithm to find the maximum margin separator. The margin of a solution \mathbf{w} to $(\mathbf{w}^T \mathbf{a_i}) l_i > 0$, $1 \le i \le n$, where $|\mathbf{a_i}| = 1$ is $\delta = \min_i \frac{l_i(\mathbf{w}^T \mathbf{a_i})}{|\mathbf{w}|}$. Since this is not a concave function of \mathbf{w} , it is difficult to deal with computationally.

Convex optimization techniques in general can only handle the maximization of concave functions or the minimization of convex functions over convex sets. However, by modifying the weight vector, one can convert the optimization problem to one with a concave objective function. Note that

$$l_i\left(\frac{\mathbf{w}^T \mathbf{a_i}}{|\mathbf{w}|\delta}\right) > 1$$

for all $\mathbf{a_i}$. Let $\mathbf{v} = \frac{\mathbf{w}}{\delta |\mathbf{w}|}$ be the modified weight vector. Then maximizing δ is equivalent to minimizing $|\mathbf{v}|$. So the optimization problem is

minimize
$$|\mathbf{v}|$$
 subject to $l_i(\mathbf{v}^T\mathbf{a_i}) > 1, \ \forall i.$

Although $|\mathbf{v}|$ is a convex function of the coordinates of \mathbf{v} , a better convex function to minimize is $|\mathbf{v}|^2$ since $|\mathbf{v}|^2$ is differentiable. So we reformulate the problem as:

Maximum Margin Problem:

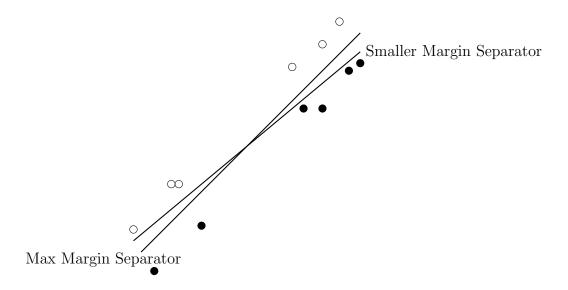


Figure 6.3: Separators with Different Margins

minimize
$$|\mathbf{v}|^2$$
 subject to $l_i(\mathbf{v}^T\mathbf{a_i}) \geq 1$.

This convex optimization problem has been much studied and algorithms that use the special structure of this problem solve it more efficiently than general convex optimization methods. We do not discuss these improvements here. An optimal solution \mathbf{v} to this problem has the following property. Let V be the space spanned by the examples $\mathbf{a_i}$ for which there is equality, namely for which $l_i(\mathbf{v}^T\mathbf{a_i})=1$. We claim that \mathbf{v} lies in V. If not, \mathbf{v} has a component orthogonal to V. Reducing this component infinitesimally does not violate any inequality, since, we are moving orthogonally to the exactly satisfied constraints; but it does decrease $|\mathbf{v}|$ contradicting the optimality. If V is full dimensional, then there are d independent examples for which equality holds. These d equations then have a unique solution and \mathbf{v} must be that solution. These examples are then called the *support vectors*. The d support vectors determine uniquely the maximum margin separator.

Linear Separators that classify most examples correctly

It may happen that there are linear separators for which almost all but a small fraction of examples are on the correct side. Going back to (6.2), ask if there is a **w** for which at least $(1-\varepsilon)n$ of the n inequalities in (6.2) are satisfied. Unfortunately, such problems are NP-hard and there are no good algorithms to solve them. A good way to think about this is that we suffer a "loss" of one for each misclassified point and would like to minimize the loss. But this loss function is discontinuous, it goes from 0 to 1 abruptly. However, with a nicer loss function it is possible to solve the problem. One possibility is to introduce slack variables y_i , $i = 1, 2, \ldots, n$, where y_i measures how badly the example $\mathbf{a_i}$ is classified. We

then include the slack variables in the objective function to be minimized:

minimize
$$|\mathbf{v}|^2 + c \sum_{i=1}^n y_i$$

subject to $(\mathbf{v} \cdot \mathbf{a_i}) l_i \ge 1 - y_i$
 $y_i \ge 0.$ $i = 1, 2, ..., n$ (6.3)

If for some i, $l_i(\mathbf{v} \cdot \mathbf{a_i}) \ge 1$, then set y_i to its lowest value, namely zero, since each y_i has a positive coefficient in the cost function. If, however, $l_i(\mathbf{v} \cdot \mathbf{a_i}) < 1$, then set $y_i = 1 - l_i(\mathbf{v} \cdot \mathbf{a_i})$, so y_i is just the amount of violation of this inequality. Thus, the objective function is trying to minimize a combination of the total violation as well as 1/margin. It is easy to see that this is the same as minimizing

$$|\mathbf{v}|^2 + c \sum_i (1 - l_i(\mathbf{v} \cdot \mathbf{a_i}))^+, ^5$$

subject to the constraints. The second term is the sum of the violations.

6.3 Nonlinear Separators, Support Vector Machines, and Kernels

There are problems where no linear separator exists but where there are nonlinear separators. For example, there may be a polynomial $p(\cdot)$ such that $p(\mathbf{a_i}) > 1$ for all +1 labeled examples and $p(\mathbf{a_i}) < 1$ for all -1 labeled examples. A simple instance of this is the unit square partitioned into four pieces where the top right and the bottom left pieces are the +1 region and the bottom right and the top left are the -1 region. For this, $x_1x_2 > 0$ for all +1 examples and $x_1x_2 < 0$ for all -1 examples. So, the polynomial $p(\cdot) = x_1x_2$ separates the regions. A more complicated instance is the checker-board pattern in Figure 6.4 with alternate +1 and -1 squares.

If we know that there is a polynomial p of degree⁶ at most D such that an example \mathbf{a} has label +1 if and only if $p(\mathbf{a}) > 0$, then the question arises as to how to find such a polynomial. Note that each d-tuple of integers (i_1, i_2, \ldots, i_d) with $i_1 + i_2 + \cdots + i_d \leq D$ leads to a distinct monomial, $x_1^{i_1} x_2^{i_2} \cdots x_d^{i_d}$. So, the number of monomials in the polynomial p is at most the number of ways of inserting d-1 dividers into a sequence of D + d - 1 positions which is $\binom{D+d-1}{d-1} \leq (D+d-1)^{d-1}$. Let $m = (D+d-1)^{d-1}$ be the upper bound on the number of monomials.

By letting the coefficients of the monomials be unknowns, we can formulate a linear program in m variables whose solution gives the required polynomial. Indeed, suppose

$${}^{5}x^{+} = \begin{cases} 0 & x \le 0 \\ x & \text{otherwise} \end{cases}$$

⁶The degree is the total degree. The degree of a monomial is the sum of the powers of each variable in the monomial and the degree of the polynomial is the maximum degree of its monomials.

-1	+1	-1	+1
+1	-1	+1	-1
-1	+1	-1	+1
+1	-1	+1	-1

Figure 6.4: The checker board pattern.

the polynomial p is

$$p(x_1, x_2, \dots, x_d) = \sum_{\substack{i_1, i_2, \dots, i_d \\ i_1 + i_2 + \dots + i_d \le D}} w_{i_1, i_2, \dots, i_d} x_1^{i_1} x_2^{i_2} \cdots x_d^{i_d}.$$

Then the statement $p(\mathbf{a_i}) > 0$ (recall $\mathbf{a_i}$ is a d-vector) is just a linear inequality in the $w_{i_1,i_2,...,i_d}$. One may try to solve such a linear program. But the exponential number of variables for even moderate values of D makes this approach infeasible. Nevertheless, this theoretical approach is useful. First, we clarify the discussion above with an example. Suppose d = 2 and D = 2. Then the possible (i_1, i_2) form the set $\{(1,0),(0,1),(2,0),(1,1),(0,2)\}$. We ought to include the pair (0,0); but it is convenient to have a separate constant term called b. So we write

$$p(x_1, x_2) = b + w_{10}x_1 + w_{01}x_2 + w_{11}x_1x_2 + w_{20}x_1^2 + w_{02}x_2^2.$$

Each example, $\mathbf{a_i}$, is a 2-vector, (a_{i1}, a_{i2}) . The linear program is

$$b + w_{1,0}a_{i1} + w_{01}a_{i2} + w_{11}a_{i1}a_{i2} + w_{20}a_{i1}^2 + w_{02}a_{i2}^2 > 0 \quad \text{if label of } i = +1 \\ b + w_{10}a_{i1} + w_{01}a_{i2} + w_{11}a_{i1}a_{i2} + w_{20}a_{i1}^2 + w_{02}a_{i2}^2 < 0 \quad \text{if label of } i = -1.$$

Note that we "pre-compute" $a_{i1}a_{i2}$, so this does not cause a nonlinearity. The linear inequalities have unknowns that are the **w**'s and b.

The approach above can be thought of as embedding the examples $\mathbf{a_i}$ that are in d-space into a m-dimensional space where there is one coordinate for each i_1, i_2, \ldots, i_d summing to at most D, except for $(0, 0, \ldots, 0)$, and if $\mathbf{a_i} = (x_1, x_2, \ldots, x_d)$, the coordinate is $x_1^{i_1} x_2^{i_2} \cdots x_d^{i_d}$. Call this embedding $\varphi(\mathbf{x})$. When d = D = 2, as in the above example, $\varphi(\mathbf{x}) = (x_1, x_2, x_1^2, x_1 x_2, x_2^2)$. If d = 3 and D = 2,

$$\varphi(\mathbf{x}) = (x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1^2, x_2^2, x_3^2),$$

and so on. We then try to find a m-dimensional vector \mathbf{w} such that the dot product of \mathbf{w} and $\varphi(\mathbf{a_i})$ is positive if the label is +1 and negative otherwise. Note that this \mathbf{w} is not

necessarily the φ of some vector in **d** space.

Instead of finding any \mathbf{w} , we want to find the \mathbf{w} maximizing the margin. As earlier, write this program as

$$\min |\mathbf{w}|^2$$
 subject to $(\mathbf{w}^T \boldsymbol{\varphi}(\mathbf{a_i})) l_i \geq 1$ for all i .

The major question is whether we can avoid having to explicitly compute the embedding φ and the vector \mathbf{w} . Indeed, we only need to have φ and \mathbf{w} implicitly. This is based on the simple, but crucial observation that any optimal solution \mathbf{w} to the convex program above is a linear combination of the $\varphi(\mathbf{a_i})$. If $\mathbf{w} = \sum_i y_i \varphi(\mathbf{a_i})$, then $\mathbf{w}^T \varphi(\mathbf{a_j})$ can be computed without actually knowing the $\varphi(\mathbf{a_i})$ but only the products $\varphi^T(\mathbf{a_i})\varphi(\mathbf{a_j})$.

Lemma 6.2 Any optimal solution \mathbf{w} to the convex program above is a linear combination of the $\varphi(\mathbf{a_i})$.

Proof: If **w** has a component perpendicular to all the $\varphi(\mathbf{a_i})$, simply zero out that component. This preserves all the inequalities since the $\mathbf{w}^T \varphi(\mathbf{a_i})$ do not change and decreases $|\mathbf{w}|^2$ contradicting the assumption that **w** is an optimal solution.

Assume that **w** is a linear combination of the $\varphi(\mathbf{a_i})$. Say $\mathbf{w} = \sum_i y_i \varphi(\mathbf{a_i})$, where the y_i are real variables. Note that then

$$|\mathbf{w}|^2 = \left(\sum_i y_i \boldsymbol{arphi}(\mathbf{a_i})\right)^T \left(\sum_j y_j \boldsymbol{arphi}(\mathbf{a_j})\right) = \sum_{i,j} y_i y_j \boldsymbol{arphi}(\mathbf{a_i})^T \boldsymbol{arphi}(\mathbf{a_j}).$$

Reformulate the convex program as

minimize
$$\sum_{i,j} y_i y_j \boldsymbol{\varphi}(\mathbf{a_i})^T \boldsymbol{\varphi}(\mathbf{a_j})$$
 (6.4)

subject to
$$l_i \left(\sum_j y_j \boldsymbol{\varphi}(\mathbf{a_j})^T \boldsymbol{\varphi}(\mathbf{a_i}) \right) \ge 1 \quad \forall i.$$
 (6.5)

It is important to notice that φ itself is not needed, only the dot products of $\varphi(\mathbf{a_i})$ and $\varphi(\mathbf{a_j})$ for all i and j including i = j. The Kernel matrix K defined as

$$k_{ij} = \boldsymbol{\varphi}(\mathbf{a_i})^T \boldsymbol{\varphi}(\mathbf{a_j}),$$

suffices since we can rewrite the convex program as

minimize
$$\sum_{ij} y_i y_j k_{ij}$$
 subject to $l_i \sum_j k_{ij} y_j \ge 1$. (6.6)

This convex program is called a *support vector machine* (SVM) though it is really not a machine. The advantage is that K has only n^2 entries instead of the $O(d^D)$ entries in each $\varphi(\mathbf{a_i})$. Instead of specifying $\varphi(\mathbf{a_i})$, we specify how to get K from the $\mathbf{a_i}$. The specification is usually in closed form. For example, the "Gaussian kernel" is given by:

$$k_{ij} = \boldsymbol{\varphi}(\mathbf{a_i})^T \boldsymbol{\varphi}(\mathbf{a_j}) = e^{-c|\mathbf{a_i} - \mathbf{a_j}|^2}.$$

We prove shortly that this is indeed a kernel function.

First, an important question arises. Given a matrix K, such as the above matrix for the Gaussian kernel, how do we know that it arises from an embedding φ as the pairwise dot products of the $\varphi(\mathbf{a_i})$? This is answered in the following lemma.

Lemma 6.3 A matrix K is a kernel matrix, i.e., there is an embedding φ such that $k_{ij} = \varphi(\mathbf{a_i})^T \varphi(\mathbf{a_j})$, if and only if K is positive semidefinite.

Proof: If K is positive semidefinite, then it can be expressed as $K = BB^T$. Define $\varphi(\mathbf{a_i})$ to be the i^{th} row of B. Then $k_{ij} = \varphi(\mathbf{a_i})^T \varphi(\mathbf{a_j})$. Conversely, if there is an embedding φ such that $k_{ij} = \varphi(\mathbf{a_i})^T \varphi(\mathbf{a_j})$, then using the $\varphi(\mathbf{a_i})$ for the rows of a matrix B, we have that $K = BB^T$ and so K is positive semidefinite.

Recall that a function of the form $\sum_{ij} y_i y_j k_{ij} = y^T K y$ is convex if and only if K is positive semidefinite. So the support vector machine problem is a convex program. We may use any positive semidefinite matrix as our kernel matrix.

We now give an important example of a kernel matrix. Consider a set of vectors $\mathbf{a_1}, \mathbf{a_2}, \ldots$ and let $k_{ij} = (\mathbf{a_i}^T \mathbf{a_j})^p$, where p is a positive integer. We prove that the matrix K with elements k_{ij} is positive semidefinite. Suppose \mathbf{u} is any n-vector. We must show that $\mathbf{u}^T K \mathbf{u} = \sum_{i:j} k_{ij} u_i u_j \geq 0$.

$$\sum_{ij} k_{ij} u_i u_j = \sum_{ij} u_i u_j (\mathbf{a_i}^T \mathbf{a_j})^p$$

$$= \sum_{ij} u_i u_j \left(\sum_k a_{ik} a_{jk} \right)^p$$

$$= \sum_{ij} u_i u_j \left(\sum_{k_1, k_2, \dots, k_p} a_{ik_1} a_{ik_2} \cdots a_{ik_p} a_{jk_1} \cdots a_{jk_p} \right) \text{ by expansion}^7.$$

Note that k_1, k_2, \ldots, k_p need not be distinct. Exchanging the summations and simplifying

$$\sum_{ij} u_i u_j \left(\sum_{k_1, k_2, \dots, k_p} a_{ik_1} a_{ik_2} \cdots a_{ik_p} a_{jk_1} \cdots a_{jk_p} \right) = \sum_{k_1, k_2, \dots, k_p} \sum_{ij} u_i u_j a_{ik_1} a_{ik_2} \cdots a_{ik_p} a_{jk_1} \cdots a_{jk_p}$$

$$= \sum_{k_1, k_2, \dots, k_p} \left(\sum_{i} u_i a_{ik_1} a_{ik_2} \cdots a_{ik_p} \right)^2.$$

The last term is a sum of squares and thus nonnegative proving that K is positive semidefinite.

From this, it is easy to see that for any set of vectors $\mathbf{a_1}, \mathbf{a_2}, \ldots$ and any c_1, c_2, \ldots greater than or equal to zero, the matrix K where k_{ij} has an absolutely convergent power series expansion $k_{ij} = \sum_{p=0}^{\infty} c_p (\mathbf{a_i} \cdot \mathbf{a_j})^p$ is positive semidefinite. For any \mathbf{u} ,

$$\mathbf{u}^T K \mathbf{u} = \sum_{ij} u_i k_{ij} u_j = \sum_{ij} u_i \left(\sum_{p=0}^{\infty} c_p (\mathbf{a_i}^T \mathbf{a_j})^p \right) u_j = \sum_{p=0}^{\infty} c_p \sum_{i,j} u_i u_j (\mathbf{a_i}^T \mathbf{a_j})^p \ge 0.$$

Lemma 6.4 For any set of vectors $\mathbf{a_1}, \mathbf{a_2}, \ldots$, the matrix K given by $k_{ij} = e^{-|\mathbf{a_i} - \mathbf{a_j}|^2/(2\sigma^2)}$ is positive semidefinite for any value of σ .

Proof:

$$e^{-|\mathbf{a_i} - \mathbf{a_j}|^2/2\sigma^2} = e^{-|\mathbf{a_i}|^2/2\sigma^2} e^{-|\mathbf{a_j}|^2/2\sigma^2} e^{-\mathbf{a_i}^T \mathbf{a_j}/\sigma^2} = \left(e^{-|\mathbf{a_i}|^2/2\sigma^2} e^{-|\mathbf{a_j}|^2/2\sigma^2}\right) \sum_{t=0}^{\infty} \left(\frac{(\mathbf{a_i}^T \mathbf{a_j})^t}{t!\sigma^{2t}}\right).$$

The matrix L given by $l_{ij} = \sum_{t=0}^{\infty} \left(\frac{(\mathbf{a_i}^T \mathbf{a_j})^t}{t!\sigma^{2t}} \right)$ is positive semidefinite. Now K can be written as DLD^T , where D is the diagonal matrix with $e^{-|\mathbf{a_i}|^2/2\sigma^2}$ as its $(i,i)^{th}$ entry. So K is positive semidefinite.

Example: (Use of the Gaussian Kernel) Consider a situation where examples are points in the plane on two juxtaposed curves, the solid curve and the dotted curve shown in Figure 6.5, where points on the first curve are labeled +1 and points on the second curve are labeled -1. Suppose examples are spaced δ apart on each curve and the minimum distance between the two curves is $\Delta >> \delta$. Clearly, there is no half-space in the plane that classifies the examples correctly. Since the curves intertwine a lot, intuitively, any polynomial which classifies them correctly must be of high degree. Consider the Gaussian kernel $e^{-|\mathbf{a_i}-\mathbf{a_j}|^2/\delta^2}$. For this kernel, the K has $k_{ij} \approx 1$ for adjacent points on the same

⁷Here a_{ik} denotes the k^{th} coordinate of the vector $\mathbf{a_i}$

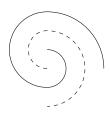


Figure 6.5: Two curves

curve and $k_{ij} \approx 0$ for all other pairs of points. Reorder the examples, first listing in order all examples on the solid curve, then on the dotted curve. K has the block form: $K = \begin{pmatrix} K_1 & 0 \\ 0 & K_2 \end{pmatrix}$, where K_1 and K_2 are both roughly the same size and are both block matrices with 1's on the diagonal and slightly smaller constants on the diagonals one off from the main diagonal and then exponentially falling off with distance from the diagonal.

The SVM is easily seen to be essentially of the form:

minimize
$$\mathbf{y_1}^T K_1 \mathbf{y_1} + \mathbf{y_2}^T K_2 \mathbf{y_2}$$

subject to $K_1 \mathbf{y_1} \ge 1$ and $K_2 \mathbf{y_2} \le -1$.

This separates into two programs, one for $\mathbf{y_1}$ and the other for $\mathbf{y_2}$. From the fact that $K_1 = K_2$, the solution will have $\mathbf{y_2} = -\mathbf{y_1}$. Further by the structure which is essentially the same everywhere except at the ends of the curves, the entries in $\mathbf{y_1}$ will all be essentially the same as will the entries in $\mathbf{y_2}$. Thus, the entries in $\mathbf{y_1}$ will be 1 everywhere and the entries in $\mathbf{y_2}$ will be -1 everywhere. Let l_i be the ± 1 labels for the points. The y_i values provide a nice simple classifier: $l_i y_i > 1$.

6.4 Strong and Weak Learning - Boosting

A strong learner is an algorithm that takes n labeled examples and produces a classifier that correctly labels each of the given examples. Since the learner is given the n examples with their labels and is responsible only for the given training examples, it seems a trivial task. Just store the examples and labels in a table and each time we are asked for the label of one of the examples, do a table look-up. By Occam's razor principle, the classifier produced by the learner should be considerably more concise than a table of the given examples. The time taken by the learner, and the length/complexity of the classifier output are both parameters by which we measure the learner. For now we focus on a different aspect. The word strong refers to the fact that the output classifier must label all the given examples correctly; no errors are allowed.

A weak learner is allowed to make mistakes. It is only required to get a strict majority, namely, a $(\frac{1}{2} + \gamma)$ fraction of the examples correct where γ is a positive real number. This seems very weak. But with a slight generalization of weak learning and using a technique

called boosting, strong learning can be accomplished with a weak learner.

Definition: (Weak learner): Suppose $U = \{\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}\}$ are n labeled examples. A weak learner is an algorithm that given the examples, their labels, and a nonnegative real weight w_i on each example $\mathbf{a_i}$ as input, produces a classifier that correctly labels a subset of examples with total weight at least $(\frac{1}{2} + \gamma) \sum_{i=1}^{n} w_i$.

A strong learner can be built by making $O(\log n)$ calls to a weak learner by a method called boosting. Boosting makes use of the intuitive notion that if an example was misclassified, one needs to pay more attention to it.

Boosting algorithm

Make the first call to the weak learner with all w_i set equal to 1.

At time t+1 multiply the weight of each example that was misclassified the previous time by $1+\varepsilon$. Leave the other weights as they are. Make a call to the weak learner.

After T steps, stop and output the following classifier:

Label each of the examples $\{a_1, a_2, \ldots, a_n\}$ by the label given to it by a majority of calls to the weak learner. Assume T is odd, so there is no tie for the majority.

Suppose m is the number of examples the final classifier gets wrong. Each of these m examples was misclassified at least T/2 times so each has weight at least $(1+\varepsilon)^{T/2}$. This says the total weight is at least $m(1+\varepsilon)^{T/2}$. On the other hand, at time t+1, we only increased the weight of examples misclassified the last time. By the property of weak learning, the total weight of misclassified examples is at most $f=(\frac{1}{2}-\gamma)$ of the total weight at time t. Let weight(t) be the total weight at time t. Then

$$\begin{split} \operatorname{weight}(t+1) &\leq \left[(1+\varepsilon)f + (1-f) \right] \times \operatorname{weight}(t) \\ &= (1+\varepsilon f) \times \operatorname{weight}(t) \\ &\leq (1+\frac{\varepsilon}{2} - \gamma \varepsilon) \times \operatorname{weight}(t). \end{split}$$

Thus since weight(0) = n,

$$m(1+\varepsilon)^{T/2} \leq \text{Total weight at end} \leq n(1+\frac{\varepsilon}{2}-\gamma\varepsilon)^T.$$

Example: Illustration of boosting

Learn x's from 0's. Items above or to the right of a line are classified as x's.

Weight of each example over time

Number of times misclassified

Taking logarithms

$$\ln m + \frac{T}{2}\ln(1+\varepsilon) \le \ln n + T\ln(1+\frac{\varepsilon}{2} - \gamma\varepsilon).$$

To a first order approximation, $\ln(1+\delta) \approx \delta$ for δ small. Make ε a small constant, say $\varepsilon = 0.01$. Then $\ln m \le \ln n - T\gamma\varepsilon$. Let $T = (1 + \ln n)/\gamma\varepsilon$. Then $\ln m \le -1$ and $m \le \frac{1}{e}$. Thus, the number of misclassified items, m, is less than one and hence must be zero.

6.5 Number of Examples Needed for Prediction: VC-Dimension Training and Prediction

Up to this point, we dealt only with training examples and focused on building a classifier that works correctly on them. Of course, the ultimate purpose is prediction of labels on future examples. In the car verses non-car example, we want our classifier to classify future feature vectors as car or non-car without human input. Clearly, we cannot expect the classifier to predict every example correctly. To measure how good the classifier is, we attach a probability distribution on the space of examples and measure the probability of misclassification. The reason for attaching a probability distribution is that we want the classifier to correctly classify likely examples but are not so concerned about examples that almost never arise.

A second question is how many training examples suffice so that as long as a classifier gets all the training examples correct (strong learner), the probability that it makes a

prediction error (measured with the same probability distribution as used to select training examples) of more than ε is less than δ ? Ideally, we would like this number to be sufficient whatever the unknown probability distribution is. The theory of VC-dimension will provide an answer to this.

A Sampling Motivation

The concept of VC-dimension is fundamental and is the backbone of learning theory. It is also useful in many other contexts. Our first motivation will be from a database example. Consider a database consisting of the salary and age of each employee in a company and a set of queries of the form: how many individuals between ages 35 and 45 have a salary between \$60,000 and \$70,000? Each employee is represented by a point in the plane where the coordinates are age and salary. The query asks how many data points fall within an axis-parallel rectangle. One might want to select a fixed sample of the data before queries arrive and estimate the number of points in a query rectangle based on the number of sample points in the rectangle. At first, such an estimate would not seem to work. Applying a union bound, the probability that there exists a rectangle that the sample fails to work for is at most the product of the probability that the sample fails for one particular rectangle times the number of possible rectangles. But, there are an infinite number of possible rectangles. So such a simple union bound argument does not give a finite upper bound on the probability that the sample fails to work for rectangles.

Define two axis-parallel rectangles to be equivalent if they contain the same data points. If there are n data points, only $O(n^4)$ of the 2^n subsets can correspond to the set of points in a rectangle. To see this, consider any rectangle R. If one of its sides does not pass through one of the n points that is inside the rectangle, then move the side parallel to itself until for the first time, it passes through one of the n points inside the rectangle. Clearly, the set of points in R and the new rectangle are the same since we did not "cross" any point. By a similar process, modify all four sides, so that there is at least one point on each side of the rectangle. Now, the number of rectangles with at least one point on each side is at most $O(n^4)$. The exponent four plays an important role; it will turn out to be the VC-dimension of axis-parallel rectangles.

Let U be a set of n points in the plane where each point corresponds to one employee's age and salary. Let $\varepsilon > 0$ be a given error parameter. Pick a random sample S of size s from U. When a query rectangle R arrives, estimate $|R \cap U|$ by the quantity $\frac{n}{s}|R \cap S|$. This is the number of employees in the sample within the ranges scaled up by $\frac{n}{s}$, since we picked a sample of size s out of s. We wish to assert that the fractional error is at most s for every rectangle s, i.e., that

$$\left| |R \cap U| - \frac{n}{s} |R \cap S| \right| \le \varepsilon n \text{ for every } R.$$

Of course, the assertion is not absolute, there is a small probability that the sample is atypical, for example picking no points from a rectangle R which has a lot of points. We

can only assert the above with high probability or that its negation holds with very low probability:

$$\operatorname{Prob}\left(\left||R \cap U| - \frac{n}{s}|R \cap S|\right| > \varepsilon n \text{ for some } R\right) \le \delta,\tag{6.7}$$

where $\delta > 0$ is another error parameter. Note that it is very important that our sample S be good for every possible query, since we do not know beforehand which queries will arise.

How many samples are necessary to ensure that (6.7) holds? Pick s samples uniformly at random from the n points in U. For one fixed R, the number of samples in R is a random variable which is the sum of s independent 0-1 random variables, each with probability $q = \frac{|R \cap U|}{n}$ of having value one. So, the distribution of $|R \cap S|$ is Binomial(s, q). Using Chernoff bounds, for $0 \le \varepsilon \le 1$:

$$\operatorname{Prob}\left(\left||R\cap U| - \frac{n}{s}|R\cap S|\right| > \varepsilon n\right) \le 2e^{-\varepsilon^2 s/(3q)} \le 2e^{-\varepsilon^2 s/3}.$$

Using the union bound and noting that there are only $O(n^4)$ possible sets $R \cap U$ yields

$$\operatorname{Prob}\left(\left||R\cap U|-\frac{n}{s}|R\cap S|\right|>\varepsilon n \text{ for some } R\right)\leq cn^4e^{-\varepsilon^2s/3}$$

for some sufficiently large c. Setting

$$s \ge \frac{3}{\varepsilon^2} \left(5 \ln n + \ln \frac{1}{\delta} \right)$$

ensures (6.7) when n is sufficiently large. In fact, we will see later that even the logarithmic dependence on n can be avoided. Indeed, we will see using VC-dimension that as long as s is at least a certain number depending upon the error ε and the VC-dimension of the set of shapes, (6.7) will hold.

In another situation, suppose we have an unknown probability distribution p over the plane and ask what is the probability mass p(R) of a query rectangle R? We might estimate the probability mass by first drawing a sample S of size s in s independent trials, each draw according to p, and wish to know how far the sample estimate $|S \cap R|/s$ is from the probability mass p(R). Again, we would like the estimate to be good for every rectangle. This is a more general problem than the first problem of estimating $|R \cap U|$. The first problem is the particular case when U consists of n points in the plane and the probability distribution p has value $\frac{1}{n}$ at each of n points. Then $\frac{1}{n}|R \cap U| = p(R)$.

There is no simple argument bounding the number of rectangles to $O(n^4)$ for the general problem. Moving the sides of the rectangle is no longer valid, since it could change the enclosed probability mass. Further, p could be a continuous distribution, where the analog of n would be infinite. So the argument above using the union bound would not solve the problem. The VC-dimension argument will yield the desired result for the more

general situation.

The question is also of interest for shapes other than rectangles. Indeed, half-spaces in d-dimensions is an important class of "shapes", since they correspond to threshold gates. A class of regions such as halfspaces or rectangles has a parameter called VC-dimension and we can bound the probability of the discrepancy between the sample estimate and the probability mass in terms of the VC-dimension of the shapes allowed. That is,

|prob mass - estimate|
$$< \varepsilon$$

with probability $1 - \delta$ where δ depends on ε and the VC-dimension.

In summary, we would like to create a sample of the data base without knowing which query we will face, knowing only the family of possible queries such as rectangles. We would like our sample to work well for every possible query from the class. With this motivation, we introduce VC-dimension and later relate it to learning.

6.6 Vapnik-Chervonenkis or VC-Dimension

A set system (U, \mathbb{S}) consists of a set U along with a collection \mathbb{S} of subsets of U. The set U may be finite or infinite. An example of a set system is the set $U = R^2$ of points in the plane, with \mathbb{S} being the collection of all axis-parallel rectangles.

Let (U, \mathbb{S}) be a set system. A subset $A \subseteq U$ is shattered by \mathbb{S} if each subset of A can be expressed as the intersection of an element of \mathbb{S} with A. The VC-dimension of the set system (U, \mathbb{S}) is the maximum size of any subset of U shattered by \mathbb{S} .

6.6.1 Examples of Set Systems and Their VC-Dimension

Rectangles with axis-parallel edges

There exist sets of four points that can be shattered by rectangles with axis-parallel edges. For example, four points at the vertices of a diamond. However, rectangles with axis-parallel edges cannot shatter any set of five points. To see this, find the minimum enclosing rectangle for the five points. For each edge there is at least one point that has stopped its movement. Identify one such point for each edge. The same point maybe identified as stopping two edges if it is at a corner of the minimum enclosing rectangle. If two or more points have stopped an edge, designate only one as having stopped the edge. Now, at most four points have been designated. Any rectangle enclosing the designated points must include the undesignated points. Thus, the subset of designated points cannot be expressed as the intersection of a rectangle with the five points. Therefore, the VC-dimension of axis-parallel rectangles is four.

Intervals of the reals

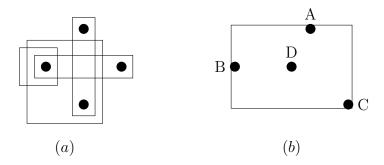


Figure 6.6: (a) shows a set of four points along with some of the rectangles that shatter them. Not every set of four points can be shattered as seen in (b). Any rectangle containing points A, B, and C must contain D. No set of five points can be shattered by rectangles with axis-parallel edges. No set of three collinear points can be shattered, since any rectangle that contains the two end points must also contain the middle point. More generally, since rectangles are convex, a set with one point inside the convex hull of the others cannot be shattered.

Intervals on the real line can shatter any set of two points but no set of three points since the subset of the first and last points cannot be isolated. Thus, the VC-dimension of intervals is two.

Pairs of intervals of the reals

There exists a set of size four that can be shattered but no set of size five since the subset of first, third, and last point cannot be isolated. Thus, the VC-dimension of pairs of intervals is four.

Convex polygons

Consider the system of all convex polygons in the plane. For any positive integer n, place n points on the unit circle. Any subset of the points are the vertices of a convex polygon. Clearly that polygon will not contain any of the points not in the subset. This shows that convex polygons can shatter arbitrarily large sets, so the VC-dimension is infinite.

Half spaces in d-dimensions

Define a half space to be the set of all points on one side of a hyper plane, i.e., a set of the form $\{\mathbf{x}|\mathbf{a}\cdot\mathbf{x}\geq a_0\}$. The VC-dimension of half spaces is d+1.

There exists a set of size d+1 that can be shattered by half spaces. Select the d

unit-coordinate vectors plus the origin to be the d+1 points. Suppose A is any subset of these d+1 points. Without loss of generality assume that the origin is in A. Take a 0-1 vector \mathbf{a} which has 1's precisely in the coordinates corresponding to vectors not in A. Then clearly A lies in the half-space $\mathbf{a} \cdot \mathbf{x} \leq 0$ and the complement of A lies in the complementary half-space.

To show that any set of d+2 points in d-dimensions cannot be shattered, we use the fact that in any set of d+2 points there are two disjoint subsets of points whose convex hulls intersect. Let convex(A) denote the convex hull of the set of points in A. Consider four points in 2-dimensions. If any three of the points lie on a straight line, then the mid point lies in the convex hull of the other two. Thus, assume that no three of the points lie on a straight line. Select three of the points. The three points must form a triangle. Extend the edges of the triangle to infinity. The three lines divide the plane into seven regions, one finite and six infinite. Place the fourth point in the plane. If the point is placed in the triangle, then it and the convex hull of the triangle intersect. If the fourth point lies in a two sided infinite region, the convex hull of the point plus the two opposite points of the triangle contains the third vertex of the triangle. If the fourth point is in a three sided region, the convex hull of the point plus the opposite vertex of the triangle intersects the convex hull of the other two points of the triangle. In higher dimensions the hyper planes in general position form a hyper tetrahedron. The infinite regions contain a vertex, edge, face, etc. of the finite region. Refer to the component of the finite region that meets an infinite region as a face of the tetrahedron. Let the points of the face be one subset and the remaining vertices of the tetrahedron plus a point in the infinite region be the other subset. The convex hulls of these two subsets intersect.

Theorem 6.5 (Radon): Any set $S \subseteq R^d$ with $|S| \ge d+2$, can be partitioned into two disjoint subsets A and B such that $convex(A) \cap convex(B) \ne \phi$.

Proof: We prove the theorem algebraically rather than geometrically. Without loss of generality, assume |S| = d+2. Form a $d \times (d+2)$ matrix with one column for each point of S. Call the matrix A. Add an extra row of all 1's to construct a $(d+1) \times (d+2)$ matrix B. Clearly, since the rank of this matrix is at most d+1, the columns are linearly dependent. Say $\mathbf{x} = (x_1, x_2, \dots, x_{d+2})$ is a nonzero vector with $B\mathbf{x} = 0$. Reorder the columns so that $x_1, x_2, \dots, x_s \geq 0$ and $x_{s+1}, x_{s+2}, \dots, x_{d+2} < 0$. Normalize x so $\sum_{i=1}^{s} |x_i| = 1$. Let $\mathbf{b_i}$ (respectively $\mathbf{a_i}$) be the i^{th} column of B (respectively A). Then, we have $\sum_{i=1}^{s} |x_i| \mathbf{b_i} = \sum_{i=s+1}^{d+2} |x_i| \mathbf{b_i}$ from which it follows that $\sum_{i=1}^{s} |x_i| \mathbf{a_i} = \sum_{i=s+1}^{d+2} |x_i| \mathbf{a_i}$ and $\sum_{i=1}^{s} |x_i| = \sum_{i=s+1}^{d+2} |x_i|$. Since $\sum_{i=1}^{s} |x_i| = 1$ and $\sum_{i=s+1}^{d+2} |x_i| = 1$ each side of $\sum_{i=1}^{s} |x_i| \mathbf{a_i} = \sum_{i=s+1}^{d+2} |x_i| \mathbf{a_i}$ is a convex combination of columns of A which proves the theorem. Thus, S can be partitioned into two sets, the first consisting of the first s points after the rearrangement and the second consisting of points s+1 through d+2. Their convex hulls intersect as required.

Radon's theorem immediately implies that half-spaces in d-dimensions do not shatter any set of d+2 points. Divide the set of d+2 points into sets A and B where $convex(A) \cap convex(B) \neq \phi$. Suppose that some half space separates A from B. Then the half space contains A and the complement of the half space contains B. This implies that the half space contains the convex hull of A and the complement of the half space contains the convex hull of B. Thus, $convex(A) \cap convex(B) = \emptyset$ a contradiction. Therefore, no set of d+2 points can be shattered by half planes in d-dimensions.

Spheres in d-dimensions

A sphere in d-dimensions is a set of points of the form $\{\mathbf{x} | |\mathbf{x} - \mathbf{x_0}| \leq r\}$. The VC-dimension of spheres is d+1. It is the same as that of half spaces. First, we prove that no set of d+2 points can be shattered by spheres. Suppose some set S with d+2 points can be shattered. Then for any partition A_1, A_2 of S, there are spheres B_1 and B_2 such that $B_1 \cap S = A_1$ and $B_2 \cap S = A_2$. Now B_1 and B_2 may intersect, but there is no point of S in their intersection. It is easy to see that there is a hyperplane with all of A_1 on one side and all of A_2 on the other and this implies that half spaces shatter S, a contradiction. Therefore no d+2 points can be shattered by hyperspheres.

It is also not difficult to see that the set of d+1 points consisting of the unit-coordinate vectors and the origin can be shattered by spheres. Suppose A is a subset of the d+1 points. Let a be the number of unit vectors in A. The center $\mathbf{a_0}$ of our sphere will be the sum of the vectors in A. For every unit vector in A, its distance to this center will be $\sqrt{|a|-1}$ and for every unit vector outside A, its distance to this center will be $\sqrt{|a|+1}$. The distance of the origin to the center is $\sqrt{|a|}$. Thus, we can choose the radius so that precisely the points in A are in the hypersphere.

Finite sets

The system of finite sets of real numbers can shatter any finite set of points on the reals and thus the VC-dimension of finite sets is infinite.

6.6.2 The Shatter Function

Consider a set system (U, \mathbb{S}) of finite VC-dimension d. For $n \leq d$ there exists a subset $A \subseteq U$, |A| = n, such that A can be shattered into 2^n pieces. This raises the question for |A| = n, n > d, as to what is the maximum number of subsets of A expressible as $S \cap A$ for $S \in \mathbb{S}$. We shall see that this maximum number is at most a polynomial in n with degree d.

The shatter function $\pi_{\mathbb{S}}(n)$ of a set system (U,\mathbb{S}) is the maximum number of subsets that can be defined by the intersection of sets in \mathbb{S} with some n element subset A of U.

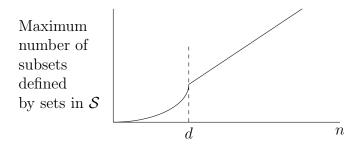


Figure 6.7: The shatter function for a set system of VC-dimension d

Thus

$$\pi_{\mathbb{S}}(n) = \max_{\substack{A \subseteq U \\ |A| = n}} |\{A \cap S | S \in \mathbb{S}\}|$$

For small values of n, $\pi_{\mathbb{S}}(n)$ will grow as 2^n . Once n equals the VC-dimension of \mathbb{S} , it grows more slowly. The definition of VC-dimension can clearly be reformulated as $\dim(\mathbb{S}) = \max\{n|\pi_{\mathbb{S}}(n) = 2^n\}$. Curiously, as we shall see, the growth of $\pi_{\mathbb{S}}(n)$ must be either polynomial or exponential in n. If the growth is exponential, then the VC-dimension of S is infinite.

Examples of set systems and their shatter function.

Example: Half spaces and circles in the plane have VC-dimension three. So, their shatter function is 2^n for n=1, 2, and 3. For n > 3, their shatter function grows as a polynomial in n. Axis-parallel rectangles have VC-dimension four and thus their shatter function is 2^n for n=1,2,3, and 4. For n > 4, their shatter function grows as a polynomial in n.

We already saw that for axis-parallel rectangles in the plane, there are at most $O(n^4)$ possible subsets of an n element set that arise as intersections with rectangles. The argument was that we can move the sides of the rectangle until each side is "blocked" by one point. We also saw that the VC-dimension of axis-parallel rectangles is four. We will see here that the two fours, one in the exponent of n and the other the VC-dimension, being equal is no accident. There is another four related to rectangles, that is, it takes four parameters to specify an axis-parallel rectangle. Although the VC-dimension of a collection of sets is often closely related to the number of free parameters, this latter four is a coincidence.

6.6.3 Shatter Function for Set Systems of Bounded VC-Dimension

We shall prove that for any set system (U, \mathbb{S}) of VC-dimension d that the quantity

$$\sum_{i=0}^{d} \binom{n}{i} = \binom{n}{0} + \binom{n}{1} + \dots + \binom{n}{d} \le 2n^d$$

bounds the shatter function $\pi_{\mathbb{S}}(n)$. That is, $\sum_{i=0}^{d} \binom{n}{i}$ bounds the number of subsets of any n point subset of U that can be expressed as the intersection with a set of \mathbb{S} . Thus, the shatter function $\pi_{\mathbb{S}}(n)$ is either 2^n if d is infinite or it is bounded by a polynomial of degree d.

Lemma 6.6 For any set system (U, \mathbb{S}) of VC-dimension at most d, $\pi_{\mathbb{S}}(n) \leq \sum_{i=0}^{d} {n \choose i}$ for all n.

Proof: The proof is by induction on d and n. The base case will handle all pairs (d, n) with either $n \leq d$ or d = 0. The general case (d, n) will use the inductive assumption on the cases (d-1, n-1) and (d, n-1).

For $n \leq d$, $\sum_{i=0}^{d} \binom{n}{i} = \sum_{i=0}^{n} \binom{n}{i} = 2^n$ and $\pi_{\mathbb{S}}(n) = 2^n$. For d = 0, a set system (U, \mathbb{S}) can have at most one set in \mathbb{S} since if there were two sets in \mathbb{S} there would exist a set A consisting of a single element that was contained in one of the sets but not in the other that could be shattered. If S contains only one set, then $\pi_{\mathbb{S}}(n) = 1$ for all n and for d = 0 $\sum_{i=0}^{d} \binom{n}{i} = 1$.

Consider the case for general d and n. Let A be a subset of U of size n such that $\pi_{\mathbb{S}}(n)$ subsets of A can be expressed as $A \cap S$ for S in \mathbb{S} . Without loss of generality, we may assume that U = A and replace each set $S \in \mathbb{S}$ by $S \cap A$ removing duplicate sets; i.e., if S_1 and S_2 in \mathbb{S} have $S_1 \cap A = S_2 \cap A$, keep only one of them. Now each set in \mathbb{S} corresponds to a subset of A and $\pi_{\mathbb{S}}(n) = |\mathbb{S}|$. Thus, to show $\pi_{\mathbb{S}}(n) \leq \sum_{i=0}^{d} \binom{n}{i}$, we only need to show $|\mathbb{S}| \leq \sum_{i=0}^{d} \binom{n}{i}$.

Remove some element u from the set A and from each set in \mathbb{S} . Consider the set system $\mathbb{S}_1 = (A - \{u\}, \{S - \{u\} | S \in \mathbb{S}\})$. For $S \subseteq A - \{u\}$, if exactly one of S and $S \cup \{u\}$ is in \mathbb{S} , then the set S contributes one set to both \mathbb{S} and \mathbb{S}_1 , whereas, if both S and $S \cup \{u\}$ are in \mathbb{S} , then they together contribute two sets to \mathbb{S} , but only one to \mathbb{S}_1 . Thus $|\mathbb{S}_1|$ is less than $|\mathbb{S}|$ by the number of pairs of sets in \mathbb{S} that differ only in the element S. To account for this difference, define another set system

$$\mathbb{S}_2 = (A - \{u\}, \{S | \text{both } S \text{ and } S \cup \{u\} \text{ are in } \mathbb{S}\}).$$

Then

$$|\mathbb{S}| = |\mathbb{S}_1| + |\mathbb{S}_2| = \pi_{\mathbb{S}_1}(n-1) + \pi_{\mathbb{S}_2}(n-1).$$

or

$$\pi_{\mathbb{S}}(n) = \pi_{\mathbb{S}_1}(n-1) + \pi_{\mathbb{S}_2}(n-1)$$

We make use of two facts

- (1) \mathbb{S}_1 has dimension at most d, and
- (2) \mathbb{S}_2 has dimension at most d-1.
- (1) follows because if \mathbb{S}_1 shatters a set of cardinality d+1, then \mathbb{S} also would shatter that set producing a contradiction. (2) follows because if \mathbb{S}_2 shattered a set $B \subseteq A \{u\}$ with $|B| \geq d$, then $B \cup \{u\}$ would be shattered by S where $|B \cup \{u\}| \geq d+1$, again producing a contradiction.

By the induction hypothesis applied to \mathbb{S}_1 , we have $|\mathbb{S}_1| = \pi_{\mathbb{S}_1} (n-1) \leq \sum_{i=0}^d \binom{n-1}{i}$. By the induction hypotheses applied to \mathbb{S}_2 , we have $|\mathbb{S}_2| = \pi_{\mathbb{S}_2} (n-1) \leq \sum_{i=0}^{d-1} \binom{n-1}{i}$. Since $\binom{n-1}{d-1} + \binom{n-1}{d} = \binom{n}{d}$ and $\binom{n-1}{0} = \binom{n}{0}$

$$\pi_{\mathbb{S}}(n) \leq \pi_{\mathbb{S}_{1}}(n-1) + \pi_{\mathbb{S}_{2}}(n-1)$$

$$\leq {\binom{n-1}{0}} + {\binom{n-1}{1}} + \dots + {\binom{n-1}{d}} + {\binom{n-1}{0}} + {\binom{n-1}{1}} + \dots + {\binom{n-1}{d-1}}$$

$$\leq {\binom{n-1}{0}} + \left[{\binom{n-1}{1}} + {\binom{n-1}{0}}\right] + \dots + \left[{\binom{n-1}{d}} + {\binom{n-1}{d-1}}\right]$$

$$\leq {\binom{n}{0}} + {\binom{n}{1}} + \dots + {\binom{n}{d}}.$$

6.6.4 Intersection Systems

Let (U, \mathbb{S}_1) and (U, \mathbb{S}_2) be two set systems on the same underlying set U. Define another set system, called the intersection system, $(U, \mathbb{S}_1 \cap \mathbb{S}_2)$, where $\mathbb{S}_1 \cap \mathbb{S}_2 = \{A \cap B | A \in \mathbb{S}_1; B \in \mathbb{S}_2\}$. In words, take the intersections of every set in \mathbb{S}_1 with every set in \mathbb{S}_2 . A simple example is $U = R^d$ and \mathbb{S}_1 and \mathbb{S}_2 are both the set of all half spaces. Then $\mathbb{S}_1 \cap \mathbb{S}_2$ consists of all sets defined by the intersection of two half spaces. This corresponds to taking the Boolean AND of the output of two threshold gates and is the most basic neural net besides a single gate. We can repeat this process and take the intersection of k half spaces. The following simple lemma helps us bound the growth of the shatter function as we do this.

Lemma 6.7 Suppose (U, \mathbb{S}_1) and (U, \mathbb{S}_2) are two set systems on the same set U. Then

$$\pi_{\mathbb{S}_1 \cap \mathbb{S}_2}(n) \le \pi_{\mathbb{S}_1}(n)\pi_{\mathbb{S}_2}(n).$$

Proof: The proof follows from the fact that for any $A \subseteq U$, the number of sets of the form $A \cap (S_1 \cap S_2)$ with $S_1 \in \mathbb{S}_1$ and $S_2 \in \mathbb{S}_2$ is at most the number of sets of the form $A \cap S_1$

times the number of sets of the form $A \cap S_2$ since for fixed S_1 , $|(A \cap S_1) \cap S_2| \leq |A \cap S_2|$.

6.7 The VC Theorem

Given a set system (U, \mathbb{S}) , the VC theorem proved in this section addresses the following question. For any probability distribution p on U, how many samples, each selected according to p, are required so that with high probability for every $S \in \mathbb{S}$, the fraction of samples in S is approximately p(S). It is important to note that one set of samples can estimate p(S) for every $S \in \mathbb{S}$. When $U = \mathbb{R}^d$ and \mathbb{S} is the set of half spaces, the sample must estimate p(S) for every one of the infinitely many half spaces.

First, we prove a simpler version of the theorem that only requires that the samples not miss any $S \in \mathbb{S}$ with $p(S) \geq \varepsilon$ for a fixed $\varepsilon > 0$. We start with two technical lemmas needed in the proof.

Lemma 6.8 If $y \ge x \ln x$, then $\frac{2y}{\ln y} \ge x$ provided x > 3.

Proof: First consider the situation where $y = x \ln x$. If $y = x \ln x$, then

$$\ln y = \ln x + \ln \ln x < 2 \ln x.$$

Thus $\frac{2y}{\ln y} \ge \frac{2x \ln x}{2 \ln x} \ge x$. Since $\frac{2y}{\ln y} \ge x$ when $y = x \ln x$ and since $\frac{2y}{\ln y}$ is a monotonically increasing function of y for $y \ge 3$, which is true when $x \ge 3$, it follows that $\frac{2y}{\ln y} \ge x$.

Lemma 6.9 If $z \geq 2$, then $5z \ln z \geq z \ln 16z$.

Proof: If $z \ge 2$, $\ln 16z = \ln z + 4 \ln 2 \le 5 \ln z$. Hence $5z \ln z \ge z \ln 16z$.

Theorem 6.10 (Simple version of Vapnik-Chervonenkis Theorem) Let (U, \mathbb{S}) be a set system with VC-dimension d and let p be a probability distribution on U. Let T be a set of m samples each picked from U according to p. For $\varepsilon \leq 1$ and $m \in \Omega\left(\frac{d}{\varepsilon}\log\frac{d}{\varepsilon}\right)$, the probability that there exists a set $S \in \mathbb{S}$ with $p(S) \geq \varepsilon$ for which $T \cap S = \emptyset$ is at most $2^{-\varepsilon m/4}$.

Proof: If one is concerned with only one set S with probability $p(S) \geq \varepsilon$ and picked m samples, then the probability that no sample lies in S is very small. However, \mathbb{S} may have infinitely many sets S. Thus a union bound over all possible S does not bound the probability that there exists a set in \mathbb{S} with no sample from T. A technique called "double sampling" is used to reduce the number of sets so that a union bound works.

First, we give an intuitive explanation of the technique. Rename T as T_1 . Say a particular set $S_0 \in \mathbb{S}$ with $p(S_0) \geq \varepsilon$ is missed by T_1 . Pick a second set T_2 of m samples independent of T_1 . With high probability, T_2 will have at least $\varepsilon m/2$ samples from the set

 S_0 . The first time we were "very unlucky" and missed S_0 completely, but the second-time we obtained samples from it. Instead of picking T_1 and then T_2 , pick $W = T_1 \cup T_2$, a random set of cardinality 2m and then pick a random subset of cardinality m out of W to be T_1 .

The structure of the proof is as follows. Define two events E_1 and E_2 . Let E_1 be the event that there exists an S with $p(S) \ge \varepsilon$ and all points in T_1 miss S.

$$E_1 \qquad \exists S \in \mathbb{S} \text{ with } p(S) \geq \varepsilon, \ |S \cap T_1| = \emptyset$$

Let E_2 be the event that there exists an S with $p(S) \ge \varepsilon$, all points in T_1 miss S, and T_2 intersects S in at least $\varepsilon m/2$ points. That is,

$$E_2$$
 $\exists S \in \mathbb{S} \text{ with } p(S) \ge \varepsilon, \ |S \cap T_1| = \emptyset \text{ and } |S \cap T_2| \ge \frac{\varepsilon}{2}m.$

We wish to show that $\operatorname{Prob}(E_1)$ is very low. First we show that $\operatorname{Prob}(E_2|E_1) \geq 1/2$. Then by the double sampling technique we show that $\operatorname{Prob}(E_2)$ is very low. Since $\operatorname{Prob}(E_2) \geq \operatorname{Prob}(E_2|E_1)\operatorname{Prob}(E_1)$ this implies that $\operatorname{Prob}(E_1)$ is very low.

We now show that $\operatorname{Prob}(E_2/E_1) \geq 1/2$. Given E_1 there is a set S such that $S \cap T_1 = \emptyset$. For this one set S, the probability that $T_2 \cap S \leq \varepsilon m/2$ is at most 1/2 giving us $\operatorname{Prob}(E_2|E_1) \geq 1/2$.

 $\operatorname{Prob}(E_2)$ is bounded by the double sampling technique. Instead of picking T_1 and then T_2 , pick a set W of 2m samples. Then pick a subset of size m out of W without replacement to be T_1 and let $T_2 = W - T_1$. It is easy to see that the distribution of T_1 and T_2 obtained this way is the same as picking T_1 and T_2 directly.

The double sampling technique bounds the probability that m samples will miss S completely when another m samples will surely hit S. Now if E_2 occurs, then for some $S \in \mathbb{S}$, with $p(S) \geq \varepsilon$, we have both $|S \cap T_1| = 0$ and $|S \cap T_2| \geq \frac{\varepsilon}{2}m$. Since $|S \cap T_2| \geq \frac{\varepsilon}{2}m$ and $T_2 \subseteq W$, it follows that $|S \cap W| \geq \frac{\varepsilon}{2}m$. But if $|S \cap W| \geq \frac{\varepsilon}{2}m$ and T_1 is a random subset of cardinality m out of W, the probability that $|S \cap T_1| = 0$ is at most the probability of selecting m elements from the $2m - \frac{\varepsilon}{2}m$ elements other than the $\frac{\varepsilon}{2}m$ elements known to be in S. This probability is at most

$$\frac{\binom{2m-(\varepsilon/2)m}{m}}{\binom{2m}{m}} \le \frac{m(m-1)\cdots(m-\frac{\varepsilon}{2}m+1)}{(2m)(2m-1)\cdots(2m-\frac{\varepsilon}{2}m+1)} \le 2^{-\frac{\varepsilon m}{2}}.$$

This is the failure probability for just one S. The number of possible $W \cap S$ is at most $\pi_{\mathbb{S}}(2m)$ which from Lemma 6.6 is at most $(2m)^d$. Thus, by the union bound, the probability is at most $(2m)^d \, 2^{-\frac{\varepsilon m}{2}} \leq (2m)^d \, e^{-\frac{\varepsilon m}{2}}$. If $(2m)^d \leq e^{\frac{\varepsilon m}{4}}$, then the probability that T_1 does not intersect any S with $p(S) \geq \varepsilon$ is at most $e^{-\frac{\varepsilon m}{4}}$ and the theorem follows. To

insure that $(2m)^d \leq e^{\frac{\varepsilon m}{4}}$ requires that $d \ln (2m) \leq \frac{\varepsilon m}{4}$.

Finally we show that $m=40\frac{d}{\varepsilon}\ln\frac{d}{\varepsilon}$ implies $d\ln(2m)\leq\frac{\varepsilon m}{4}$ from which the result follows. If the sample size m is at least $m=40\frac{d}{\varepsilon}\ln\frac{d}{\varepsilon}$ then

$$m = 40\frac{d}{\varepsilon} \ln \frac{d}{\varepsilon} \ge 8 \left(5\frac{d}{\varepsilon}\right) \ln \frac{d}{\varepsilon} \ge 8\frac{d}{\varepsilon} \ln \left(16\frac{d}{\varepsilon}\right)$$

where the last inequality follows from Lemma 6.9 with $z = \frac{d}{\varepsilon}$. Hence $2m \ge 16\frac{d}{\varepsilon} \ln \left(16\frac{d}{\varepsilon}\right)$. By Lemma 6.8 with y = 2m and $x = 16\frac{d}{\varepsilon}$,

$$\frac{4m}{\ln(2m)} \ge 16\frac{d}{\varepsilon}$$

and hence $d \ln (2m) \leq \frac{\varepsilon m}{4}$ completing the proof.

Next we prove the general VC theorem. Whereas the special theorem asserted that with high probability for every S with $p(S) \geq \varepsilon$, our sample set T_1 has at least one element of S, the general theorem will assert that we can estimate p(S) for any set $S \in \mathbb{S}$ by $|T_1 \cap S|/|T_1|$ with an error of less than ε .

In the proof of the following theorem it will be useful to have a verbal description for certain events. For a set T_1 of samples and an $S \in \mathbb{S}$,

- 1. if $\left|\frac{|S\cap T_1|}{|T_1|} p(S)\right| > \varepsilon$, we say that " T_1 estimates p(S) badly", and
- 2. if $\left|\frac{|S\cap T_1|}{|T_1|} p(S)\right| \leq \frac{\varepsilon}{2}$, we say that " T_1 estimates S very well".

Theorem 6.11 (General version of the VC-Theorem) Let (U, S) be a set system with VC-dimension d and let p be any probability distribution on U. For any $\varepsilon \in [0,1]$, if $n = \Omega\left(\frac{d}{\varepsilon^2}\log(d/\varepsilon)\right)$, and T_1 is a set of n independent samples drawn from U according to p, then

$$Prob\left(\exists S \in \mathbb{S} : \left| \frac{|S \cap T_1|}{n} - p(S) \right| > \varepsilon \right) \le 2e^{-\varepsilon^2 n/6}.$$

Proof: Let E_1 be the event that there exists $S \in \mathbb{S}$ such that $\left|\frac{|S \cap T_1|}{|T_1|} - p(S)\right| \geq \varepsilon$. Pick an auxiliary sample T_2 of size $m = 4n/\varepsilon$ and define another event E_2 that says there is a set $S \in \mathbb{S}$ for which T_1 estimates p(S) badly, but T_2 estimates p(S) very well. We can again argue that $\text{Prob}(E_2) \geq (1/2)\text{Prob}(E_1)$. The idea of introducing E_2 is that it is the AND of two contradictory events, so its probability will be relatively easy to upper bound.

Again use double sampling. Pick a set W of cardinality n+m, then pick a random subset T_1 from W of cardinality m. Assume now that E_2 happens and for an $S_0 \in \mathbb{S}$, T_1 estimates $p(S_0)$ badly, but T_2 estimates $p(S_0)$ very well. We denote this event happening for S_0 by $E_2(S_0)$. Since T_2 estimates $p(S_0)$ very well it follows that $W = T_1 \cup T_2$ estimates

 $p(S_0)$ "moderately well" since T_2 is larger than T_1 and T_1 's corruption does not have much effect. More precisely,

$$|W \cap S_0| \ge |T_2 \cap S_0| \ge m \ p(S_0) - \frac{\varepsilon m}{2}$$

implies

$$\frac{|W \cap S_0|}{m+n} \ge \frac{m}{m+n} p(S_0) - \frac{\varepsilon}{2} \ge p(S_0) - \frac{n}{m+n} - \frac{\varepsilon}{2} \ge p(S_0) - \frac{3\varepsilon}{4}. \tag{6.8}$$

Also

$$|W \cap S_0| \le |T_2 \cap S_0| + |T_1| \le mp(S_0) + \frac{\varepsilon m}{2} + n$$

$$\frac{|W \cap S_0|}{m+n} \le \frac{m}{m+n} p(S_0) + \frac{\varepsilon}{2} + \frac{n}{m+n} \le p(S_0) + \frac{3\varepsilon}{4}.$$

Together these yield

$$\left| \frac{|W \cap S_0|}{m+n} - P(S_0) \right| \le \frac{3\varepsilon}{4}. \tag{6.9}$$

We know that T_1 estimates $p(S_0)$ badly. By the double sampling argument, T_1 is just a uniform random subset of W of cardinality n and W estimates $p(S_0)$ moderately well. We will use these facts along with the double sampling technique to show that the probability of E_2 cannot be big. For the moment, assume that T_1 is picked out of W with replacement. The probability that each trial picks an element of S_0 is $\frac{|W \cap S_0|}{m+n}$. Thus, the distribution of $|T_1 \cap S_0|$ is binomial $(n, \frac{|W \cap S_0|}{m+n})$. Since $\varepsilon \in [0, 1]$, from Chernoff bounds,

$$\operatorname{Prob}\left(\left||T_1 \cap S_0| - n\frac{|W \cap S_0|}{m+n}\right| > \frac{\varepsilon n}{4}\right) \le 2e^{-\varepsilon^2 n/3}.$$

Using (11.1) and the assumption that T_1 estimates $p(S_0)$ badly, under the event $E_2(S_0)$, $\left||T_1 \cap S_0| - n \frac{|W \cap S_0|}{m+n}|\right| > \frac{\varepsilon n}{4}$. By the above, we have the desired upper bound that $\operatorname{Prob}(E_2(S_0)) \leq 2e^{-\varepsilon^2 n/3}$. The bound is just for one S_0 . We need to apply the union bound over all possible S_0 . The only candidates for S_0 that need to be consider are sets of the form $S \cap W, S \in \mathbb{S}$ of which there are at most $\pi_{\mathbb{S}}(n+m)$ which is at most $(n+m)^d$. Since $m=\frac{4}{\varepsilon}n$, it follows that $(n+m)^d \leq (8n)^d/\varepsilon^d$. Now for $n \in \Omega\left(\frac{d}{\varepsilon^2}\ln(d/\varepsilon)\right)$, with a suitable constant, $\frac{\varepsilon^2 n}{6} \geq d\ln(8n/\varepsilon)$. Thus

$$\operatorname{Prob}(E_2(S_0))$$
 (for one S_0) × (number of possible S_0) $\leq 2e^{-\varepsilon^2 n/6}$

proving the theorem.

6.8 Priors and Bayesian Learning

Section to be written

6.9 Bibliographic Notes

Leslie Valiant formulated the Theory of Learning in a foundational paper- "A Theory of the learnable" [Val84]; this paper stipulates that the learning algorithm be measured on test examples drawn from the same probability distribution from which the training examples were drawn. The connection between Valiant's learning model and the more classical notion of Vapnik-Chervonekis dimension [VC71] was struck by Blumer, Ehrenfrucht, Hausler and Warmuth [BEHW]. Boosting was first introduced by Schapire [Sch90]. A general reference on Machine Learning is the book [Mit97] and a more theoretical introduction is given in [KV95]. [SS01] is a reference on Support Vector Machines and learning with kernels. The basic idea in boosting (of taking a weighted majority of several decisions, where the weights get updated based on past experience) has been used in Economics as well as other areas. A survey of many applications of this general method can be found in [Aro11]

6.10 Exercises

Exercise 6.1 (Boolean OR has a linear separator) Take as examples all the 2^d elements of $\{0,1\}^d$. Label the example by +1 if there is at least one coordinate with a +1 and label it by -1 if all its coordinates are 0. This is like taking the Boolean OR, except that the coordinates are the real numbers 0 and 1 rather than true or false. Show that there is a linear separator for the labeled examples. Show that we can achieve a margin of $\Omega(1/d)$ for this problem.

Exercise 6.2 Repeat Exercise 6.1 for the AND function.

Exercise 6.3 Repeat Exercise 6.1 for majority and minority functions.

Exercise 6.4 Show that the parity function, the Boolean function that is 1 if and only if an odd number of inputs is 1, cannot be represented as a threshold function.

Exercise 6.5 Suppose the starting w in the perceptron learning algorithm made an angle of 45° with the solution w^* whose margin is δ . Show that the number of iterations satisfies a smaller upper bound than $\frac{1}{\delta^2} - 1$ by a small modification to the proof of Theorem 6.1?

Exercise 6.6 The proof of Theorem 6.1 shows that for every w^* , with $l_i(w^* \cdot a_i) \geq \delta$ for i = 1, 2, ..., n, the cosine of the angle between w and w^* is at least $\sqrt{t+1}\delta$ after t iterations. What happens if there are multiple w^* , all satisfying $l_i(w^* \cdot a_i) \geq \delta$ for i = 1, 2, ..., n? Then, how can our one w make a small angle with all of these w^* ?

Exercise 6.7 Suppose the examples are points in d-space with 0,1 coordinates and the label is +1 if and only if the least i for which $x_i = 1$ is odd. Otherwise the example's label is -1. Show that the rule can be represented by the linear threshold function

$$(x_1, x_2, \dots, x_n) (1, -\frac{1}{2}, \frac{1}{4}, -\frac{1}{8}, \dots)^T = x_1 - \frac{1}{2}x_2 + \frac{1}{4}x_3 - \frac{1}{8}x_4 + \dots \ge 0$$

Exercise 6.8 (Hard) Can the problem of Exercise 6.7 be represented by any linear threshold function with margin at least 1/f(d) where f(d) is bounded above by a polynomial function of d? Prove your answer.

Exercise 6.9 Recall the definition of margin where the linear separator is required to correctly classify all examples with a margin of at least δ . Suppose this condition is relaxed to say that the linear separator classifies all examples correctly and has a margin of at least δ on all but an ϵ fraction of the examples. Consider the following modified version of the perceptron learning algorithm:

Start with $\mathbf{w} = (1, 0, 0, \dots, 0)$ Repeat until $(\mathbf{w} \cdot \mathbf{a_i})l_i > 0$ for all but at most a 2ϵ fraction of the examples Add to \mathbf{w} the average of all $\mathbf{a_i}l_i$ with $(\mathbf{w} \cdot \mathbf{a_i})l_i \leq 0$ Show that this is a "noise-tolerant" version of the algorithm. Namely, show that with the relaxed margin assumption, it correctly finds a linear separator that classifies all but at most a 2ϵ fraction correctly. Prove a bound on the number of steps the algorithm takes. What goes wrong if we use the old unmodified algorithm with the relaxed assumption?

Hint: Go over the proof of theorem 6.1 (convergence of perceptron learning algorithm) and adapt it. You only need to modify the argument that the numerator increases in every step.

Exercise 6.10 Let \mathbf{w} be the weight vector of a linear separator with margin δ and write $\mathbf{v} = \frac{\mathbf{w}}{\delta |\mathbf{w}|}$. Show that $|\mathbf{v}|$ and $|\mathbf{v}|^2$ are convex functions of the coordinates of \mathbf{w} . Find the gradient of $|\mathbf{v}|^2$ and show that it exists everywhere. How about the gradient of $|\mathbf{v}|$?

Exercise 6.11

1. Show that (6.3) can be reformulated as the unconstrained minimization of

$$|\mathbf{v}|^2 + c \sum_i (1 - l_i(\mathbf{v} \cdot \mathbf{a_i}))^+.$$

2. Show that x^+ is a convex function.

The function x^+ does not have a derivative at 0. The function $(x^+)^2$ is smoother (its first derivative at 0 exists) and it is better to minimize

$$|\mathbf{v}|^2 + c \sum_i ((1 - l_i(\mathbf{v} \cdot \mathbf{a_i}))^+)^2.$$

Exercise 6.12 Assume that the center of Figure 6.4 is (0,0) and the side of each small square is of length 1. Show that a point has label +1 if and only if

$$(x_1+1)x_1(x_1-1)(x_2+1)x_2(x_2-1) \ge 0.$$

Consider only examples which are interior to a small square.

Exercise 6.13 Consider a set of examples in 2-dimensions where any example inside the circle $x_1^2 + x_2^2 = 1$ is labeled +1 and any example outside the circle is labeled -1. Construct a function φ so that the examples are linearly separable in the space $\varphi(\mathbf{x})$.

Exercise 6.14 Label the points in the plane that are within the circle of radius one as +1 and label the points in the annulus of inner radius two and outer radius three as -1. Find a function φ mapping the points to a higher dimensional space where the two sets are linearly separable.

Exercise 6.15 Let p be a polynomial of degree D with d variables. Prove the the number of monomials in the polynomial p is at most

$$\sum_{i=0}^{D} \binom{d+i-1}{d-1}.$$

Then prove that $\sum_{i=0}^{D} {d+i-1 \choose d-1} \leq D(d+D)^{\min(d-1,D)}$.

Exercise 6.16 Produce a polynomial p(x,y) whose arguments x and y are real numbers and a set of real real numbers a_1, a_2, \ldots so that the matrix $K_{ij} = p(a_i, a_j)$ is not positive semidefinite.

Exercise 6.17 Make the proof that the majority of enough weak-learners in the boosting section is a strong learner rigorous by using inequalities instead of first order approximation. Prove that $T = \frac{3+\ln n}{\gamma \varepsilon} + \frac{1}{\varepsilon^2}$ will do for $\varepsilon < \gamma/8$

Exercise 6.18 (Experts picking stocks) Suppose there are n experts who are predicting whether one particular stock is going up or down at each of t time periods. There are only two outcomes at each time; up or down. Without knowing in advance their predictions or any other information, can you pick nearly as well as the best expert? Show that boosting can help predict within a factor of two of the best expert?

Exercise 6.19 Construction of the strong learner by boosting a weak learner required knowledge of the correct classification. After construction the strong learner, how does one apply the strong learner to classify new data where the correct classification is not available?

Exercise 6.20 What happens if in Section 6.5, instead of requiring

$$Prob\left(\left||R\cap U|-\frac{n}{s}|R\cap S|\right|\leq \varepsilon n \text{ for every } R\right)\geq 1-\delta,$$

one requires only:

$$Prob\left(\left|\left|R\cap U\right| - \frac{n}{s}\left|R\cap S\right|\right| \le \varepsilon n\right) \ge 1 - \delta, \text{ for every } R$$
?

Exercise 6.21 Given n points in the plane and a circle C_1 containing at least three points show that there exists a circle C_2 with two points on its circumference containing the same set of points as C_1 .

Exercise 6.22 Is the following statement true or false? Suppose we have n points in the plane and C_1 is a circle containing at least three points. There exists a circle C_2 with three points lying on the circle C_2 or two points lying on a diameter of C_2 and the set of points in C_2 is the same as the set of points in C_1 . Either give a counter example or a proof.

Exercise 6.23 Given n points in the plane define two circles as equivalent if they enclose the same set of points. Prove that there are only $O(n^3)$ equivalence classes of points defined by circles and thus only n^3 subsets out of the 2^n subsets can be enclosed by circles.

Exercise 6.24 Prove that the VC-dimension of circles is three?

Exercise 6.25 Consider a 3-dimensional space.

- 1. What is the VC-dimension of rectangular boxes with axis-parallel sides?
- 2. What is the VC-dimension of spheres?

Exercise 6.26 (Squares) Show that there is a set of three points which can be shattered by axis-parallel squares. Show that the system of axis-parallel squares cannot shatter any set of four points.

Solution: A square with axis parallel edges has VC-dimension three. To see this note, that a set of three points at the vertices of an equilateral triangle is easily shattered. No set of four points can be shattered. Consider a set of four points and let R be the minimum enclosing rectangle. Note we are using a rectangle not a square. If all four sides of the rectangle are constrained by three or fewer points then those points cannot be separated from the remaining points by any rectangle and hence by any square. Thus, assume all four points are necessary to restrain the edges. This implies that there is a point on the interior of each edge.

Let the points be a, b, c, and d. Let the edges containing a and c be at least as far apart as the edges containing b and d. A square containing a and c will contain at least one of b or d.

Exercise 6.27 Show that the VC-dimension of axis-aligned right triangles with the right angle in the lower left corner is four.

Exercise 6.28 Prove that the VC-dimension of 45°, 45°, 90° triangles with right angle in the lower left is four.

Exercise 6.29 Show that the VC-dimension of arbitrary right triangles is seven.

Exercise 6.30 What is the VC-dimension of triangles? Right triangles?

Exercise 6.31 Prove that the VC dimension of convex polygons is infinite.

Exercise 6.32 Create list of simple shapes for which we can calculate the VC-dimension and indicate the VC-dimension for each shape on your list.

Exercise 6.33 If a class contains only convex sets prove that it cannot shatter any set in which some point is in the convex hull of other points in the set.

Exercise 6.34 Prove that no set of six points can be shattered by squares in arbitrary position.

Exercise 6.35 (Square in general position) Show that the VC-dimension of (not necessarily axis-parallel) squares in the plane is 5.

Exercise 6.36 Show that the set of seven vertices of a regular septagon can be shattered by rotated rectangles.

Exercise 6.37 Prove that no set of eight points can be shattered by rotated rectangles.

Exercise 6.38 Show that the VC-dimension of (not necessarily axis-parallel) rectangles is 7.

Exercise 6.39 What is the VC-dimension for a corner? I.e. all points (x,y) such that for some (x_0, y_0) either

- 1. $(x x_0, y y_0) \ge (0, 0)$,
- 2. $(x_0 x, y y_0) \ge (0, 0)$,
- 3. $(x_0 x, y_0 y) \ge (0, 0)$, or
- 4. $(x-x_0, y_0-y) \ge (0,0)$.

Exercise 6.40 For large n, how should you place n points on the plane so that the maximum number of subsets of the n points are defined by rectangles? Can you achieve 4n subsets of size 2? Can you do better? What about size 3? What about size 10?

Exercise 6.41 For large n, how should you place n points on the plane so that the maximum number of subsets of the n points are defined by

- 1. half spaces?
- 2. circles?
- 3. axis-parallel rectangles?
- 4. some other simple shape of your choosing?

For each of the shapes how many subsets of size two, three, etc can you achieve?

Exercise 6.42 What is the shatter function for 2-dimensional half spaces? That is, given n points in the plane, how many subsets can be defined by half spaces?

Exercise 6.43 Intuitively define the most general form of a set system of VC-dimension one. Give an example of such a set system that can generate n subsets of an n element set.

Exercise 6.44 What does it mean to shatter the empty set? How many subsets does one get?

Exercise 6.45 (Hard) We proved that if the VC-dimension is small, then the shatter function is small as well. Can you prove some sort of converse to this?

Exercise 6.46 If $(U, \mathbb{S}_1), (U, \mathbb{S}_2), \dots, (U, \mathbb{S}_k)$ are k set systems on the same ground set U show that $\pi_{\mathbb{S}_1} \cap \mathbb{S}_2 \cap \dots \otimes_k (n) \leq \pi_{\mathbb{S}_1}(n) \pi_{\mathbb{S}_2}(n) \dots \pi_{\mathbb{S}_k}(n)$.

Exercise 6.47 In the proof of the simple version of Vapnik-Chervonenkis theorem we claimed if $p(S_0) \ge \varepsilon$ and we selected m elements of U for T that $Prob[|S_0 \cap T'| \ge \frac{\varepsilon}{2}m]$ was at least 1/2. Write out the details of the proof of this statement.

Exercise 6.48 Show that in the "double sampling" procedure, the probability of picking a pair of multi-sets T and T', each of cardinality m, by first picking T and then T' is the same as picking a W of cardinality 2m and then picking uniformly at random a subset T out of W of cardinality m and letting T' be W-T. For this exercise, assume that p, the underlying probability distribution is discrete.

Exercise 6.49 Randomly select n integers from the set $\{1, 2, ..., 2n\}$ without replacement. In the limit as n goes to infinity, what is the probability that you will not select any integer in the set $\{1, 2, ..., k\}$ for k a constant independent of n and for $k = \log n$?

References

weak learning Schapire

7 Algorithms for Massive Data Problems

Massive Data, Sampling

This chapter deals with massive data problems where the input data (a graph, a matrix or some other object) is too large to be stored in random access memory. One model for such problems is the streaming model, where the data can be seen only once. In the streaming model, the natural technique to deal with the massive data is sampling. Sampling is done "on the fly". As each piece of data is seen, based on a coin toss, one decides whether to include the data in the sample. Typically, the probability of including the data point in the sample may depend on its value. Models allowing multiple passes through the data are also useful; but the number of passes needs to be small. We always assume that random access memory (RAM) is limited, so the entire data cannot be stored in RAM.

To introduce the basic flavor of sampling on the fly, consider the following primitive. From a stream of n positive real numbers a_1, a_2, \ldots, a_n , draw a sample element a_i so that the probability of picking an element is proportional to its value. It is easy to see that the following sampling method works. Upon seeing a_1, a_2, \ldots, a_i , keep track of the sum $a = a_1 + a_2 + \cdots + a_i$ and a sample $a_j, j \leq i$, drawn with probability proportional to its value. On seeing a_{i+1} , replace the current sample by a_{i+1} with probability $\frac{a_{i+1}}{a+a_{i+1}}$ and update a.

7.1 Frequency Moments of Data Streams

An important class of problems concerns the frequency moments of data streams. Here a data stream a_1, a_2, \ldots, a_n of length n consists of symbols a_i from an alphabet of m possible symbols which for convenience we denote as $\{1, 2, \ldots, m\}$. Throughout this section, n, m, and a_i will have these meanings and s (for symbol) will denote a generic element of $\{1, 2, \ldots, m\}$. The frequency f_s of the symbol s is the number of occurrences of s in the stream. For a nonnegative integer p, the p^{th} frequency moment of the stream is

$$\sum_{s=1}^{m} f_s^p.$$

Note that the p=0 frequency moment corresponds to the number of distinct symbols occurring in the stream. The first frequency moment is just n, the length of the string. The second frequency moment, $\sum_{s} f_s^2$, is useful in computing the variance of the stream.

$$\frac{1}{m} \sum_{s=1}^{m} \left(f_s - \frac{n}{m} \right)^2 = \frac{1}{m} \sum_{s=1}^{m} \left(f_s^2 - 2 \frac{n}{m} f_s + \left(\frac{n}{m} \right)^2 \right) = \frac{1}{m} \sum_{s=1}^{m} f_s^2 - \frac{n^2}{m^2}$$

In the limit as p becomes large, $\left(\sum_{s=1}^{m} f_{s}^{p}\right)^{1/p}$ is the frequency of the most frequent element(s).

We will describe sampling based algorithms to compute these quantities for streaming data shortly. But first a note on the motivation for these various problems. The identity and frequency of the the most frequent item or more generally, items whose frequency exceeds a fraction of n, is clearly important in many applications. If the items are packets on a network with source destination addresses, the high frequency items identify the heavy bandwidth users. If the data is purchase records in a supermarket, the high frequency items are the best-selling items. Determining the number of distinct symbols is the abstract version of determining such things as the number of accounts, web users, or credit card holders. The second moment and variance are useful in networking as well as in database and other applications. Large amounts of network log data are generated by routers that can record for all the messages passing through them, the source address, destination address, and the number of packets. This massive data cannot be easily sorted or aggregated into totals for each source/destination. But it is important to know if some popular source-destination pairs have a lot of traffic for which the variance is the natural measure.

7.1.1 Number of Distinct Elements in a Data Stream

Consider a sequence a_1, a_2, \ldots, a_n of n elements, each a_i an integer in the range 1 to m where n and m are very large. Suppose we wish to determine the number of distinct a_i in the sequence. Each a_i might represent a credit card number extracted from a sequence of credit card transactions and we wish to determine how many distinct credit card accounts there are. The model is a data stream where symbols are seen one at a time. We first show that any deterministic algorithm that determines the number of distinct elements exactly must use at least m bits of memory.

Lower bound on memory for exact deterministic algorithm

Suppose we have seen the first $k \geq m$ symbols. The set of distinct symbols seen so far could be any of the 2^m subsets of $\{1, 2, ..., m\}$. Each subset must result in a different state for our algorithm and hence m bits of memory are required. To see this, suppose first that two different size subsets of distinct symbols lead to the same internal state. Then our algorithm would produce the same count of distinct symbols for both inputs, clearly an error for one of the input sequences. If two sequences with the same number of distinct elements but different subsets lead to the same state, then on next seeing a symbol that appeared in one sequence but not the other would result in subsets of different size and thus require different states.

Algorithm for the Number of distinct elements

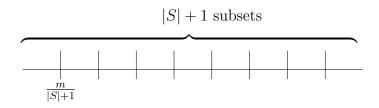


Figure 7.1: Estimating the size of S from the minimum element in S which has value approximately $\frac{m}{|S|+1}$. The elements of S partition the set $\{1,2,\ldots,m\}$ into |S|+1 subsets each of size approximately $\frac{m}{|S|+1}$.

Let a_1, a_2, \ldots, a_n be a sequence of elements where each $a_i \in \{1, 2, \ldots, m\}$. The number of distinct elements can be estimated with $O(\log m)$ space. Let $S \subseteq \{1, 2, \ldots, m\}$ be the set of elements that appear in the sequence. Suppose that the elements of S were selected uniformly at random from $\{1, 2, \ldots, m\}$. Let min denote the minimum element of S. Knowing the minimum element of S allows us to estimate the size of S. The elements of S partition the set $\{1, 2, \ldots, m\}$ into |S| + 1 subsets each of size approximately $\frac{m}{|S|+1}$. See Figure 7.1. Thus, the minimum element of S should have value close to $\frac{m}{|S|+1}$. Solving $min = \frac{m}{|S|+1}$ yields $|S| = \frac{m}{min} - 1$. Since we can determine min, this gives us an estimate of |S|.

The above analysis required that the elements of S were picked uniformly at random from $\{1, 2, ..., m\}$. This is generally not the case when we have a sequence $a_1, a_2, ..., a_n$ of elements from $\{1, 2, ..., m\}$. Clearly if the elements of S were obtained by selecting the |S| smallest elements of $\{1, 2, ..., m\}$, the above technique would give the wrong answer. If the elements are not picked uniformly at random, can we estimate the number of distinct elements? The way to solve this problem is to use a hash function h where

$$h: \{1, 2, \dots, m\} \to \{0, 1, 2, \dots, M-1\}$$

To count the number of distinct elements in the input, count the number of elements in the mapped set $\{h(a_1), h(a_2), \ldots\}$. The point being that $\{h(a_1), h(a_2), \ldots\}$ behaves like a random subset and so the above heuristic argument using the minimum to estimate the number of elements may apply. If we needed $h(a_1), h(a_2), \ldots$ to be completely independent, the space needed to store the hash function would too high. Fortunately, only 2-way independence is needed. We recall the formal definition of 2-way independence below. But first recall that a hash function is always chosen at random from a family of hash functions and phrases like "probability of collision" refer to the probability in the choice of hash function.

Universal Hash Functions

The set of hash functions

$$H = \{h \mid h : \{1, 2, \dots, m\} \rightarrow \{0, 1, 2, \dots, M - 1\}\}\$$

is 2-universal if for all x and y in $\{1, 2, \dots, m\}$, $x \neq y$, and for all z and w in $\{0, 1, 2, \dots, M-1\}$

Prob
$$[h(x) = z \text{ and } h(y) = w] = \frac{1}{M^2}$$

for a randomly chosen h. The concept of a 2-universal family of hash functions is that given x, h(x) is equally likely to be any element of $\{0, 1, 2, ..., M-1\}$ and for $x \neq y$, h(x) and h(y) are independent.

We now give an example of a 2-universal family of hash functions. For simplicity let M be a prime. For each pair of integers a and b in the range [0,M-1], define a hash function

$$h_{ab}(x) = ax + b \mod (M)$$

To store the hash function h_{ab} , store the two integers a and b. This requires only $O(\log M)$ space. To see that the family is 2-universal note that h(x) = z and h(y) = w if and only if

$$\left(\begin{array}{cc} x & 1 \\ y & 1 \end{array}\right) \left(\begin{array}{c} a \\ b \end{array}\right) = \left(\begin{array}{c} z \\ w \end{array}\right) \mod(M)$$

If $x \neq y$, the matrix $\begin{pmatrix} x & 1 \\ y & 1 \end{pmatrix}$ is invertible modulo M and there is only one solution for a and b. Thus, for a and b chosen uniformly at random, the probability of the equation holding is exactly $\frac{1}{M^2}$.

Analysis of distinct element counting algorithm

Let b_1, b_2, \ldots, b_d be the distinct values that appear in the input. Then $S = \{h(b_1), h(b_2), \ldots h(b_d)\}$ is a set of d random and 2-way independent values from the set $\{0, 1, 2, \ldots, M-1\}$. We now show that $\frac{M}{\min}$ is a good estimate for d, the number of distinct elements in the input, where $\min=\min(S)$.

Lemma 7.1 Assume M > 100d. With probability at least $\frac{2}{3}$, $\frac{d}{6} \leq \frac{M}{\min} \leq 6d$, where min is the smallest element of S.

Proof: First, we show that $Prob\left[\frac{M}{\min} > 6d\right] < \frac{1}{6}$.

$$\operatorname{Prob}\left[\frac{M}{\min} > 6d\right] = \operatorname{Prob}\left[\min < \frac{M}{6d}\right] = \operatorname{Prob}\left[\exists k \ h\left(b_{k}\right) < \frac{M}{6d}\right]$$

For $i = 1, 2, \dots, d$ define the indicator variable

$$z_i = \begin{cases} 1 & \text{if } h(b_i) < \frac{M}{6d} \\ 0 & \text{otherwise} \end{cases}$$

and let $z = \sum_{i=1}^{d} z_i$. If $h(b_i)$ is chosen randomly from $\{0, 1, 2, \dots, M-1\}$, then Prob $[z_i = 1] = \frac{1}{6d}$. Thus, $E(z_i) = \frac{1}{6d}$ and $E(z) = \frac{1}{6}$. Now

$$\operatorname{Prob}\left[\frac{M}{\min} > 6d\right] = \operatorname{Prob}\left[\min < \frac{M}{6d}\right]$$
$$= \operatorname{Prob}\left[\exists k \ h\left(b_{k}\right) < \frac{M}{6d}\right]$$
$$= \operatorname{Prob}\left(z \ge 1\right) = \operatorname{Prob}\left[z \ge 6E\left(z\right)\right].$$

By Markov's inequality $\operatorname{Prob}\left[z\geq6E\left(z\right)\right]\leq\frac{1}{6}.$

Finally, we show that Prob $\left[\frac{M}{\min} < \frac{d}{6}\right] < \frac{1}{6}$.

$$\operatorname{Prob}\left[\frac{M}{\min} < \frac{d}{6}\right] = \operatorname{Prob}\left[\min > \frac{6M}{d}\right] = \operatorname{Prob}\left[\forall k \ h\left(b_{k}\right) > \frac{6M}{d}\right]$$

For i = 1, 2, ..., d define the indicator variable

$$y_i = \begin{cases} 0 & \text{if } h(b_i) > \frac{6M}{d} \\ 1 & \text{otherwise} \end{cases}$$

and let $y = \sum_{i=1}^{d} y_i$. Now Prob $(y_i = 1) = \frac{6}{d}$, $E(y_i) = \frac{6}{d}$, and E(y) = 6. For 2-way independent random variables, the variance of their sum is the sum of their variances. So $Var(y) = dVar(y_1)$. Further, it is easy to see since y_1 is 0 or 1 that

$$Var(y_1) = E[(y_1 - E(y_1))^2] = E(y_1^2) - E^2(y_1) = E(y_1) - E^2(y_1) \le E(y_1).$$

Thus $Var(y) \leq E(y)$. Now by the Chebychev inequality,

$$\operatorname{Prob}\left[\frac{M}{\min} < \frac{d}{6}\right] = \operatorname{Prob}\left[\min > \frac{6M}{d}\right] = \operatorname{Prob}\left[\forall k \ h\left(b_{i}\right) > \frac{6M}{d}\right]$$
$$= \operatorname{Prob}\left(y = 0\right) \leq \operatorname{Prob}\left[|y - E\left(y\right)| \geq E\left(y\right)\right]$$
$$\leq \frac{\operatorname{Var}(y)}{E^{2}\left(y\right)} \leq \frac{1}{E\left(y\right)} \leq \frac{1}{6}$$

Since $\frac{M}{\min} > 6d$ with probability at most $\frac{1}{6}$ and $\frac{M}{\min} < \frac{d}{6}$ with probability at most $\frac{1}{6}$, $\frac{d}{6} \leq \frac{M}{\min} \leq 6d$ with probability at least $\frac{2}{3}$.

7.1.2 Counting the Number of Occurrences of a Given Element.

To count the number of occurrences of an element in a stream requires at most $\log n$ space where n is the length of the stream. Clearly, for any length stream that occurs in practice, we can afford $\log n$ space. For this reason, the following material may never be

used in practice, but the technique is interesting and may give insight into how to solve some other problem.

Consider a string of 0's and 1's of length n in which we wish to count the number of occurrences of 1's. Clearly if we had $\log n$ bits of memory we could keep track of the exact number of 1's. However, we can approximate the number with only $\log \log m$ bits.

Let m be the number of 1's that occur in the sequence. Keep a value k such that 2^k is approximately the number of occurrences m. Storing k requires only $\log \log n$ bits of memory. The algorithm works as follows. Start with k=0. For each occurrence of a 1, add one to k with probability $1/2^k$. At the end of the string, the quantity $2^k - 1$ is the estimate of m. To obtain a coin that comes down heads with probability $1/2^k$, flip a fair coin, one that comes down heads with probability 1/2, k times and report heads if the fair coin comes down heads in all k flips.

Given k, on average it will take 2^k ones before k is incremented. Thus, the expected number of 1's to produce the current value of k is $1+2+4+\cdots+2^{k-1}=2^k-1$.

7.1.3 Counting Frequent Elements

The Majority and Frequent Algorithms

First consider the very simple problem of n people voting. There are m candidates, $\{1,2,\ldots,m\}$. We want to determine if one candidate gets a majority vote and if so who. Formally, we are given a stream of integers a_1,a_2,\ldots,a_n , each a_i belonging to $\{1,2,\ldots,m\}$, and want to determine whether there is some $s \in \{1,2,\ldots,m\}$ which occurs more than n/2 times and if so which s. It is easy to see that to solve the problem exactly on read only once streaming data with a deterministic algorithm, requires $\Omega(n)$ space. Suppose n is even and the first n/2 items are all distinct and the last n/2 items are identical. After reading the first n/2 items, we need to remember exactly which elements of $\{1,2,\ldots,m\}$ have occurred. If for two different sets of elements occurring in the first half of the stream, the contents of the memory are the same, then a mistake would occur if the second half of the stream consists solely of an element in one set, but not the other. Thus, $\log_2\binom{m}{n/2}$ bits of memory, which if m > n is $\Omega(n)$, are needed.

The following is a simple low-space algorithm that always finds the majority vote if there is one. If there is no majority vote, the output may be arbitrary. That is, there may be "false positives", but no "false negatives".

Majority Algorithm

Store a_1 and initialized a counter to one. For each subsequent a_i , if a_i is the same as the currently stored item, increment the counter by one. If it differs, decrement the counter by one provided the counter is nonzero. If the counter is zero, then store a_i and set the counter to one.

To analyze the algorithm, it is convenient to view the decrement counter step as "eliminating" two items, the new one and the one that caused the last increment in the counter. It is easy to see that if there is a majority element s, it must be stored at the end. If not, each occurrence of s was eliminated; but each such elimination also causes another item to be eliminated and so for a majority item not to be stored at the end, we must have eliminated more than n items, a contradiction.

Next we modify the above algorithm so that not just the majority, but also items with frequency above some threshold are detected. We will also ensure (approximately) that there are no false positives as well as no false negatives. Indeed the algorithm below will find the frequency (number of occurrences) of each element of $\{1, 2, \ldots, m\}$ to within an additive term of $\frac{n}{k+1}$ using $O(k \log n)$ space by keeping k counters instead of just one counter.

Algorithm Frequent

Maintain a list of items being counted. Initially the list is empty. For each item, if it is the same as some item on the list, increment its counter by one. If it differs from all the items on the list, then if there are less than k items on the list, add the item to the list with its counter set to one. If there are already k items on the list decrement each of the current counters by one deleting an element from the list if its count becomes zero.

Theorem 7.2 At the end of Algorithm Frequent, for each $s \in \{1, 2, ..., m\}$, its counter on the list is at least the number of occurrences of s in the stream minus n/(k+1). In particular, if some s does not occur on the list, its counter is zero and the theorem asserts that it occurs fewer than n/(k+1) times in the stream.

Proof: View each decrement counter step as eliminating some items. An item is eliminated if it is the current a_i being read and there are already k symbols different from it on the list in which case it and k other items are simultaneously eliminated. Thus, the elimination of each occurrence of an $s \in \{1, 2, ..., m\}$ is really the elimination of k + 1 items. Thus, no more than n/(k+1) occurrences of any symbol can be eliminated. Now, it is clear that if an item is not eliminated, then it must still be on the list at the end. This proves the theorem.

Theorem 7.2 implies that we can compute the true relative frequency, the number of occurrences divided by n, of every $s \in \{1, 2, ..., m\}$ to within an additive term of $\frac{n}{k+1}$.

7.1.4 The Second Moment

This section focuses on computing the second moment of a stream with symbols from $\{1,2,\ldots,m\}$. Let f_s denote the number of occurrences of symbol s in the stream. The second moment of the stream is given by $\sum_{s=1}^m f_s^2$. To calculate the second moment, for each symbol s, $1 \le s \le m$, independently set a random variable x_s to ± 1 with probability 1/2. Maintain a sum by adding x_s to the sum each time the symbol s occurs in the stream. At the end of the stream, the sum will equal $\sum_{s=1}^m x_s f_s$. The expected value of the sum will be zero where the expectation is over the choosing of the ± 1 value for the x_s .

$$E\left(\sum_{s=1}^{m} x_s f_s\right) = 0.$$

Although the expected value of the sum is zero, its actual value is a random variable and the expected value of the square of the sum is given by

$$E\left(\sum_{s=1}^{m} x_s f_s\right)^2 = E\left(\sum_{s=1}^{m} x_s^2 f_s^2\right) + 2E\left(\sum_{s \neq t} x_s x_t f_s f_t\right) = \sum_{s=1}^{m} f_s^2,$$

The last equality follows since $E(x_sx_t) = 0$ for $s \neq t$. Thus

$$a = \left(\sum_{s=1}^{m} x_s f_s\right)^2$$

is an estimator of $\sum_{s=1}^{m} f_s^2$. One difficulty which we will come back to is that to store the x_i requires space m and we want to do the calculation in $\log m$ space.

How good this estimator is depends on its variance which we now compute.

$$Var\left(a\right) \le E\left(\sum_{s=1}^{m} x_s f_s\right)^4 = E\left(\sum_{1 \le s, t, u, v \le m} x_s x_t x_u x_v f_s f_t f_u f_v\right)$$

The first inequality is because the variance is at most the second moment and the second equality is by expansion. In the second sum, since the x_s are independent, if any one of s, u, t, or v is distinct from the others, then the expectation of the whole term is zero. Thus, we need to deal only with terms of the form $x_s^2 x_t^2$ for $t \neq s$ and terms of the form x_s^4 . Note that this does not need the full power of mutual independence of all the x_s , it only needs 4-way independence, that any four of the x_s' are mutually independent. In the above sum, there are four indices s, t, u, v and there are $\binom{4}{2}$ ways of choosing two of

them that have the same x value. Thus,

$$Var(a) \leq \binom{4}{2} E\left(\sum_{s=1}^{m} \sum_{t=s+1}^{m} x_s^2 x_t^2 f_s^2 f_t^2\right) + E\left(\sum_{s=1}^{m} x_s^4 f_s^4\right)$$

$$= 6 \sum_{s=1}^{m} \sum_{t=s+1}^{m} f_s^2 f_t^2 + \sum_{s=1}^{m} f_s^4$$

$$\leq 3 \left(\sum_{s=1}^{m} f_s^2\right)^2 + \left(\sum_{s=1}^{m} f_s^2\right)^2 = 4E^2(a).$$

The variance can be reduced by a factor of r by taking the average of r independent trials. With r independent trials the variance would be at most $\frac{4}{r}E^2(a)$, so to achieve relative error ε in the estimate of $\sum_{s=1}^{m} f_s^2$, we need $O(1/\varepsilon^2)$ independent trials.

We will briefly discuss the independent trials here, so as to understand exactly the amount of independence needed. Instead of computing a using the running sum $\sum_{s=1}^{m} x_s f_s$ for one random vector $x = (x_1, x_2, \ldots, x_m)$, we independently generate r m-vectors (x_1, x_2, \ldots, x_r) at the outset and compute r running sums

$$\sum_{s=1}^{m} x_{1s} f_s, \sum_{s=1}^{m} x_{2s} f_s, \dots, \sum_{s=1}^{m} x_{rs} f_s.$$

Let $a_1 = \left(\sum_{s=1}^m x_{1s} f_s\right)^2$, $a_2 = \left(\sum_{s=1}^m x_{2s} f_s\right)^2$, ..., $a_r = \left(\sum_{s=1}^m x_{rs} f_s\right)^2$. Our estimate is $\frac{1}{r}(a_1 + a_2 + \dots + a_r)$. The variance of this estimator is

$$\operatorname{Var}\left[\frac{1}{r}\left(a_{1}+a_{2}+\cdots+a_{r}\right)\right]=\frac{1}{r^{2}}\left[\operatorname{Var}\left(a_{1}\right)+\operatorname{Var}\left(a_{2}\right)+\cdots+\operatorname{Var}\left(a_{r}\right)\right]=\frac{1}{r}\operatorname{Var}\left(a_{1}\right),$$

where we have assumed that the a_1, a_2, \ldots, a_r are mutually independent. Now we compute the variance of a_1 as we have done for the variance of a. Note that this calculation assumes only 4-way independence between the coordinates of x_1 . We summarize the assumptions here for future reference:

To get an estimate of $\sum_{s=1}^{m} f_s^2$ within relative error ε with probability close to one, say at least 0.9999, it suffices to have $r = O(1/\varepsilon^2)$ vectors $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_r}$, each with m coordinates of ± 1 with

- 1. $E(\mathbf{x_s}\mathbf{x_t}) = 0$ for all s and t.
- 2. $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_r}$ are mutually independent. That is for any r vectors $\mathbf{v_1}, \mathbf{v_2}, \dots, \mathbf{v_r}$ with ± 1 coordinates, $\operatorname{Prob}(\mathbf{x_1} = \mathbf{v_1}, \ \mathbf{x_2} = \mathbf{v_2}, \ \dots, \ \mathbf{x_r} = \mathbf{v_r}) = \frac{1}{2^{mr}}$.

3. Any four coordinates of $\mathbf{x_1}$ are independent. Same for $\mathbf{x_2}, \mathbf{x_3}, \ldots$, and $\mathbf{x_r}$.

The only drawback with the algorithm as we have described it so far is that we need to keep the r vectors $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_r}$ in memory so that we can do the running sums. This is too space-expensive. We need to do the problem in space dependent upon the logarithm of the size of the alphabet m, not m itself. If ε is in $\Omega(1)$, then r is in O(1), so it is not the number of trials r which is the problem. It is the m.

In the next section, we will see that the computation can be done in $O(\log m)$ space by using pseudo-random vectors $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_r}$ instead of truly random ones. The pseudo-random vectors will satisfy (i), (ii), and (iii) and so they will suffice. This pseudo-randomness and limited independence has deep connections, so we will go into the connections as well.

Error-Correcting codes, polynomial interpolation and limited-way independence

Consider the problem of generating a random m-vector \mathbf{x} of ± 1 's so that any subset of four coordinates is mutually independent, i.e., for any distinct s, t, u, and v in $\{1, 2, \ldots, m\}$ and any a, b, c, and d in $\{-1, +1\}$,

Prob
$$(x_s = a, x_t = b, x_u = c, x_v = d) = \frac{1}{16}$$
.

We will see that such an n-dimensional vector may be generated from a truly random "seed" of only $O(\log m)$ mutually independent bits. Thus, we need only store the $\log m$ bits and can generate any of the m coordinates when needed. This allows us to store the 4-way independent random m-vector using only $\log m$ bits. The first fact needed for this is that for any k, there is a finite field F with exactly 2^k elements, each of which can be represented with k bits and arithmetic operations in the field can be carried out in $O(k^2)$ time. Here, k will be the ceiling of $\log_2 m$. We also assume another basic fact about polynomial interpolation which says that a polynomial of degree at most three is uniquely determined by its value over any field F at four points. More precisely, for any four distinct points $a_1, a_2, a_3, a_4 \in F$ and any four possibly not distinct values $b_1, b_2, b_3, b_4 \in F$, there is a unique polynomial $f(x) = f_0 + f_1 x + f_2 x^2 + f_3 x^3$ of degree at most three that with computations done over F, $f(a_1) = b_1$, $f(a_2) = b_2$, $f(a_3) = b_3$, and $f(a_4) = b_4$.

Now our definition of the pseudo-random \pm vector \mathbf{x} with 4-way independence is simple. Choose four elements f_0, f_1, f_2, f_3 at random from F and form the polynomial $f(s) = f_0 + f_1 s + f_2 s^2 + f_3 s^3$. This polynomial represents \mathbf{x} as follows. For $s = 1, 2, \ldots, m$, x_s is the leading bit of the k-bit representation of f(s). Thus, the m-dimensional vector \mathbf{x} requires only k bits where $k = \lceil \log m \rceil$.

Lemma 7.3 The x defined above have 4-way independence.

Proof: Assume that the elements of F are represented in binary using \pm instead of the traditional 0 and 1. Let s, t, u, and v be any four coordinates of \mathbf{x} and let α , β , γ , $\delta \in \{-1,1\}$. There are exactly 2^{k-1} elements of F whose leading bit is α and similarly for β , γ , and δ . So, there are exactly $2^{4(k-1)}$ 4-tuples of elements b_1 , b_2 , b_3 , $b_4 \in F$ so that the leading bit of b_1 is α , the leading bit of b_2 is β , the leading bit of b_3 is γ , and the leading bit of b_4 is δ . For each such b_1 , b_2 , b_3 , and b_4 , there is precisely one polynomial f so that

$$f(s) = b_1$$
, $f(t) = b_2$, $f(u) = b_3$, and $f(v) = b_4$

as we saw above. So, the probability that

$$x_s = \alpha$$
, $x_t = \beta$, $x_u = \gamma$, and $x_v = \delta$

is precisely
$$\frac{2^{4(k-1)}}{\text{total number of }f} = \frac{2^{4(k-1)}}{2^{4k}} = \frac{1}{16}$$
 as asserted.

The lemma states how to get one vector \mathbf{x} with 4-way independence. However, we need $r = O(1/\varepsilon^2)$ vectors. Also the vectors must be mutually independent. But this is easy, just choose r polynomials at the outset.

To implement the algorithm with low space, store only the polynomials in memory. This requires $4k = O(\log m)$ bits per polynomial for a total of $O(\log m/\varepsilon^2)$ bits. When a symbol s in the stream is read, compute $x_{1s}, x_{2s}, \ldots, x_{rs}$ and update the running sums. Note that x_{s1} is just the leading bit of the first polynomial evaluated at s; this calculation is in $O(\log m)$ time. Thus, we repeatedly compute the x_s from the "seeds", namely the coefficients of the polynomials.

This idea of polynomial interpolation is also used in other contexts. Error-correcting codes is an important example. Say we wish to transmit n bits over a channel which may introduce noise. One can introduce redundancy into the transmission so that some channel errors can be corrected. A simple way to do this is to view the n bits to be transmitted as coefficients of a polynomial f(x) of degree n-1. Now transmit f evaluated at points $1,2,3,\ldots,n+m$. At the receiving end, any n correct values will suffice to reconstruct the polynomial and the true message. So up to m errors can be tolerated. But even if the number of errors is at most m, it is not a simple matter to know which values are corrupted. We do not elaborate on this here.

7.2 Sketch of a Large Matrix

We will see how to find a good 2-norm approximation of an $m \times n$ matrix A, which is read from external memory, where m and n are large. The approximation consists of a sample of s columns and r rows of A along with an $s \times r$ multiplier matrix. The schematic diagram is given in Figure 7.2.

$$\begin{bmatrix} & & & \\$$

Figure 7.2: Schematic diagram of the approximation of A by a sample of s columns and r rows.

The crucial point is that a sampled row or column is drawn with probability proportional to the squared length of the row or column. One may recall that the top k singular vectors of the SVD of A, give a similar picture; but the SVD takes more time to compute, requires all of A to be stored in RAM, and does not have the property that the rows and columns are directly from A. However, the SVD does yield the best 2-norm approximation. Error bounds for our approximation are weaker.

We briefly touch upon two motivations for such a sketch. Suppose A is the document-term matrix of a large collection of documents. We are to "read" the collection at the outset and store a sketch so that later, when a query (represented by a vector with one entry per term) arrives, we can find its similarity to each document in the collection. Similarity is defined by the dot product. In Figure 7.2 it is clear that the matrix-vector product of a query with the right hand side can be done in time O(ns + sr + rm) which would be linear in n and m if s and r are O(1). To bound errors for this process, we need to show that the difference between A and the sketch of A has small 2-norm. Recall that the 2-norm $||A||_2$ of a matrix A is $\max_{|\mathbf{x}|=1} \mathbf{x}^T A \mathbf{x}$.

A second motivation comes from recommendation systems. Here A would be a customer-product matrix whose $(i,j)^{th}$ entry is the preference of customer i for product j. The objective is to collect a few sample entries of A and based on them, get an approximation to A so that we can make future recommendations. Our results say that a few sampled rows of A (all preferences of a few customers) and a few sampled columns (all customers' preferences for a few products) give a good approximation to A provided that the samples are drawn according to the length-squared distribution.

We first tackle a simpler problem, that of multiplying two matrices. The matrix multiplication also uses length squared sampling and is a building block to the sketch.

7.2.1 Matrix Multiplication Using Sampling

Suppose A is an $m \times n$ matrix and B is an $n \times p$ matrix and the product AB is desired. We show how to use sampling to get an approximate product faster than the traditional multiplication. Let A(:,k) denote the k^{th} column of A. A(:,k) is a $m \times 1$ matrix. Let B(k,:) be the k^{th} row of B. B(k,:) is a $1 \times n$ matrix. It is easy to see that

$$AB = \sum_{k=1}^{n} A(:,k)B(k,:).$$

Note that for each value of k, A(:,k)B(k,:) is an $m \times p$ matrix each element of which is a single product of elements of A and B. An obvious use of sampling suggests itself. Sample some values for k and compute A(:,k)B(k,:) for the sampled k's using their suitably scaled sum as the estimate of AB. It turns out that nonuniform sampling probabilities are useful. Define a random variable z that takes on values in $\{1,2,\ldots,n\}$. Let p_k denote the probability that z assumes the value k. The p_k are nonnegative and sum to one. Define an associated random matrix variable that has value

$$X = \frac{1}{p_k} A(:,k) B(k,:)$$

with probability p_k . Let E(X) denote the entry-wise expectation.

$$E(X) = \sum_{k=1}^{n} \text{Prob}(z = k) \frac{1}{p_k} A(:, k) B(k, :) = \sum_{k=1}^{n} A(:, k) B(k, :) = AB.$$

This explains the scaling by $\frac{1}{p_k}$ in X.

Define the variance of X as the sum of the variances of all its entries.

$$Var(X) = \sum_{i=1}^{m} \sum_{j=1}^{p} Var(x_{ij}) \le \sum_{ij} E(x_{ij}^2) \le \sum_{i,j} \sum_{k} p_k x_{ij}^2 = \sum_{ij} \sum_{k} p_k \frac{1}{p_k^2} a_{ik}^2 b_{kj}^2.$$

We can simplify the last term by exchanging the order of summations to get

$$\operatorname{Var}(X) \le \sum_{k} \frac{1}{p_k} \sum_{i} a_{ik}^2 \sum_{j} b_{kj}^2 = \sum_{k} \frac{1}{p_k} |A(:,k)|^2 |B(k,:)|^2.$$

If p_k is proportional to $|A(:,k)|^2$, i.e, $p_k = \frac{|A(:,k)|^2}{||A||_F^2}$, we get a simple bound for Var(X).

$$\operatorname{Var}(X) \le ||A||_F^2 \sum_{k} |B(k,:)|^2 = ||A||_F^2 ||B||_F^2.$$

Using probabilities that are proportional to length squared of columns of A turns out to be useful in other contexts as well and sampling according to them is called "length-squared sampling".

$$DD^{T} = \begin{pmatrix} & & d_{13} & & \\ & & & d_{24} \\ d_{31} & & & \\ & & d_{42} & & \end{pmatrix} \begin{pmatrix} & & d_{31} & & \\ & & & d_{42} \\ & & d_{24} & & \end{pmatrix} = \begin{pmatrix} d_{13}^{2} & & & \\ & d_{24}^{2} & & \\ & & d_{31}^{2} & \\ & & & d_{42}^{2} \end{pmatrix}$$

(a) Formation of DD^T

$$\begin{split} ADD^TB &= \left(\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ A(:,1) & A(:,2) & A(:,3) & A(:,4) \\ \downarrow & \downarrow & \downarrow & \downarrow \end{array}\right) \left(\begin{array}{c} d_{13}^2 \\ d_{13}^2 \\ d_{13}^2 \end{array}\right) \left(\begin{array}{c} \leftarrow B(1,:) \to \\ \leftarrow B(2,:) \to \\ \leftarrow B(3,:) \to \\ \leftarrow B(4,:) \to \end{array}\right) \\ &= \left(\begin{array}{c} d_{13}^2A(:,1), \ d_{24}^2A(:,2), \ d_{31}^2A(:,3), \ d_{42}^2A(:,4S) \ \right) \left(\begin{array}{c} \leftarrow B(1,:) \to \\ \leftarrow B(2,:) \to \\ \leftarrow B(2,:) \to \\ \leftarrow B(3,:) \to \\ \leftarrow B(3,:) \to \\ \leftarrow B(4,:) \to \end{array}\right) \\ &= d_{13}^2A(:,1)B(1,:) + d_{24}^2A(:,2)B(2,:) + d_{31}^2A(:,3)B(3,:) + d_{42}^2A(:,4)B(4,:) \end{split}$$

(b) Applying column selector matrix.

Figure 7.3: Illustration of column selector matrix

To reduce the variance, do s independent trials to pick k_1, k_2, \ldots, k_s . Then find the average of the corresponding X's. This is, $\frac{1}{s} \left(\frac{A(:,k_1)B(k_1,:)}{p_{k_1}} + \frac{A(:,k_2)B(k_2,:)}{p_{k_2}} + \cdots + \frac{A(:,k_s)B(k_s,:)}{p_{k_s}} \right)$, which can also be represented compactly as ADD^TB , where D is an $n \times s$ "column selector" matrix with $d_{k_i,i} = \frac{1}{\sqrt{sp_{k_i}}}$ for $i = 1, 2, \ldots, s$ and all other entries of D are zero. The k_i diagonal element of DD^T is $\frac{1}{sp_{k_i}}$. All other elements of DD^T are zero. Thus, ADD^TB consists of the weighted sum of the products of column k_i of A with row k_i of B.

Lemma 7.4 Suppose A is an $m \times n$ matrix and B is an $n \times p$ matrix. The product AB can be estimated by ADD^TB , where D is $n \times s$ and each column of D has precisely one nonzero entry. d_{ki} is picked to be the nonzero entry in column i with probability p_k proportional to $|A(:,k)|^2$ and if picked, it is set to $1/\sqrt{sp_k}$. The error is bounded by $E(||ADD^TB - AB||_F^2) \leq \frac{1}{s}||A||_F^2||B||_F^2$.

Proof: Taking the average of s independent samples divides the variance by s.

Computing ADD^TB in the order $(AD)(D^TB)$ can be done in O[s(mn + np + mp)] time by straight forward multiplication. Note that if $s \in O(1)$ and m = n = p, then this

time is big O of the number of entries in A and B and at worst quadratic in n.

An important special case is the multiplication A^TA where the length-squared distribution can be shown to be the optimal distribution. The variance of X defined above for this case is

$$\sum_{i,j} E(x_{ij}^2) - \sum_{ij} E^2(x_{ij}) = \sum_{k} \frac{1}{p_k} |A(:,k)|^4 - ||A^T A||_F^2.$$

The second term is independent of the p_k . The first term is minimized when the p_k are proportional to $|A(:,k)|^2$, hence length-squared distribution minimizes the variance of this estimator.

7.2.2 Approximating a Matrix with a Sample of Rows and Columns

Consider the following important problem. Suppose a large matrix A is read from external memory and a sketch of it is kept for further computation. A simple sketch idea would be to keep a random sample of rows and a random sample of columns of the matrix. With uniform random sampling, this can fail to be a good sketch. Consider the case where very few rows and columns of A are nonzero. A small sample will miss them, storing only zeros. This toy example can be made more subtle by making a few rows have very high absolute value entries compared to the rest. The sampling probabilities need to depend on the size of the entries. If we do length-squared sampling of both rows and columns, then we can get an approximation to A with a bound on the approximation error. Note that the sampling can be achieved in two passes through the matrix, the first to compute running sums of the length-squared of each row and column and the second pass to draw the sample. Only the sampled rows and columns, which is much smaller than the whole, need to be stored in RAM for further computations. The algorithm starts with:

- 1. Pick s columns of A using length-squared sampling. Let C (for columns) be the $m \times s$ matrix of the picked columns scaled by $1/\sqrt{s}$ (prob. of picked column). Write C = AD where D is a column selector matrix as in Lemma 7.4.
- 2. Pick r rows of A using length-squared sampling (here lengths are row lengths). Let R (for rows) be the $r \times n$ matrix of the picked rows scaled by $1/\sqrt{r}$ (prob. of picked row). Write $R = D_1 A$, where D_1 is a $r \times m$ row selector matrix.

We will approximate A by CUR, where U is a $s \times r$ multiplier matrix computed from C and R. Recall the schematic in Figure 7.2. We describe U assuming RR^T is invertible. Through the rest of this section, we make the assumption that RR^T is invertible. This case will convey the essential ideas. Also, note that since r in general will be much smaller than n and m, unless the matrix A is degenerate, it is likely that the r rows in the sample R will be linearly independent giving us invertibility of RR^T .

Before stating precisely what U is, we give some intuition. A first idea would be to approximate A by ADD^TI , where I is the $n \times n$ identity matrix. By Lemma 7.4, the

product ADD^TI approximates AI = A. Note that we would not multiply A and I by sampling; the use of Lemma 7.4 is simply a proof device here. Lemma 7.4 tells us that

$$E(||A - ADD^{T}I||_{F}^{2}) \le \frac{1}{s}||A||_{F}^{2}||I||_{F}^{2} = \frac{n}{s}||A||_{F}^{2}, \tag{7.1}$$

which is not very interesting since we want $s \ll n$. Instead of using the identity matrix which introduced the factor of $||I||_F^2 = n$, we will use an "identity-like" matrix based on R.

Lemma 7.5 If RR^T is invertible, then $R^T(RR^T)^{-1}R$ acts as the identity matrix on the row space of R. I.e., for every vector \mathbf{x} of the form $\mathbf{x} = R^T\mathbf{y}$ (this defines the row space of R), we have $R^T(RR^T)^{-1}R\mathbf{x} = \mathbf{x}$.

Proof: For $\mathbf{x} = R^T \mathbf{y}$, since RR^T is invertible

$$R^{T}(RR^{T})^{-1}R\mathbf{x} = R^{T}(RR^{T})^{-1}RR^{T}\mathbf{y} = R^{T}\mathbf{y} = \mathbf{x}$$

Go back to the starting idea of approximating A by ADD^TI . Now, instead of I, use $R^T(RR^T)^{-1}R$ which by the Lemma 7.5 acts as I on the row space of R. In analogy with that first idea, now we should get $\frac{r}{s}||A||_F^2$ instead of the $\frac{n}{s}||A||_F^2$ in the right hand side of (7.1). This is indeed what we rigorously argue below. Recall C = AD and define $U = D^TR^T(RR^T)^{-1}$, so as to make $CUR = ADD^T(R^T(RR^T)^{-1}R)$.

Lemma 7.6 Let $U = D^T R^T (RR^T)^{-1}$ (assuming RR^T is invertible). Then $CUR = ADD^T R^T (RR^T)^{-1} R$ and

$$E(||A - CUR||_2^2) \le \frac{4}{\sqrt{r}}||A||_F^2$$

provided $s \ge r^{3/2}$.

Proof: The first assertion is obvious. For the second assertion let $R^T(RR^T)^{-1}R = W$. Then $CUR = ADD^TW$. So,

$$||A - CUR||_2 < ||A - AW||_2 + ||AW - ADD^TW||_2$$

which implies that

$$||A - CUR||_2^2 \le 2||A - AW||_2^2 + 2||AW - ADD^TW||_2^2.$$

Thus,

$$E(||A - CUR||_2^2) \le 2 E(||A - AW||_2^2) + 2 E(||AW - ADD^TW||_2^2).$$
 (7.2)

To bound the second term of (7.2), pretend for the moment that we are trying to multiply A with W and use sampling as in the last section. The approximation to AW we get is ADD^TW and by Lemma (7.4),

$$E(||AW - ADD^TW||_2^2) \le E(||AW - ADD^TW||_F^2) \le \frac{1}{s}||A||_F^2||W||_F^2.$$

From Lemma 7.5, W acts like the identity on an r-dimensional space and $W\mathbf{z} = 0$ for any \mathbf{z} perpendicular to the row space of R. So, $||W||_F^2$, which is the sum of its squared singular values, is r and hence $E\left(||AW - ADD^TW||_2^2\right) \leq \frac{r}{s}||A||_F^2 \leq \frac{1}{\sqrt{r}}||A||_F^2$ since $s \geq r^{\frac{3}{2}}$.

Consider the first term, $E(||A - AW||_2^2)$ of (7.2). Recall that

$$||A - AW||_2 = \max_{|\mathbf{x}|=1} |(A - AW)\mathbf{x}|.$$

If **x** attains this maximum, **x** must be orthogonal to the row space of R, since by Lemma 7.5, for any vector **y** in the row space of R, W acts like the identity and so (A - AW)**y** would be **0**. For **x** orthogonal to rows of R, we have

$$|(A - AW)\mathbf{x}|^2 = |A\mathbf{x}|^2$$

$$= \mathbf{x}^T A^T A \mathbf{x}$$

$$= \mathbf{x}^T (A^T A - R^T R) \mathbf{x} \qquad \text{(since } R\mathbf{x} = 0\text{)}$$

$$\leq ||A^T A - A^T D_1^T D_1 A||_2 \qquad \text{(since } R = D_1 A\text{)}$$

$$\leq ||A^T A - A^T D_1^T D_1 A||_F.$$

We will use Lemma 7.4 again to bound this, since we are picking columns of A^T (same as rows of A) in picking R and we can view $A^TD_1^TD_1A$ as an approximation to the matrix multiplication A^TA . By Lemma 7.4, (noting that for any nonnegative random variable $X, E(X) \leq \sqrt{E(X^2)}$)

$$E(||A^TA - A^TD_1D_1^TA||_F) \le \frac{1}{\sqrt{r}}||A||_F^2$$

which implies that $E(||A - AW||_2^2) \leq \frac{1}{\sqrt{r}}||A||_F^2$. Substituting this into (7.2), proves the lemma.

7.3 Sketches of Documents

Suppose one wished to store all the web pages from the WWW. Since there are billions of web pages, one might store just a sketch of each page where a sketch is a few hundred bits that capture sufficient information to do whatever task one had in mind. A web page or a document is a sequence. We begin this section by showing how to sample a set and then how to convert the problem of sampling a sequence into a problem of sampling a set.

Consider subsets of size 1000 of the integers from 1 to 10^6 . Suppose one wished to compute the resemblance of two subsets A and B by the formula

resemblance
$$(A, B) = \frac{|A \cap B|}{|A \cup B|}$$

Suppose that instead of using the sets A and B, one sampled the sets and compared random subsets of size ten. How accurate would the estimate be? One way to sample would be to select ten elements uniformly at random from A and B. However, this method is unlikely to produce overlapping samples. Another way would be to select the ten smallest elements from each of A and B. If the sets A and B overlapped significantly one might expect the sets of ten smallest elements from each of A and B to also overlap. One difficulty that might arise is that the small integers might be used for some special purpose and appear in essentially all sets and thus distort the results. To overcome this potential problem, rename all elements using a random permutation.

Suppose two subsets of size 1000 overlapped by 900 elements. What would the overlap be of the 10 smallest elements from each subset? One would expect the nine smallest elements from the 900 common elements to be in each of the two subsets for an overlap of 90%. The resemblance (A, B) for the size ten sample would be 9/11=0.81.

Another method would be to select the elements equal to zero mod m for some integer m. If one samples mod m the size of the sample becomes a function of n. Sampling mod m allows us to also handle containment.

In another version of the problem one has a sequence rather than a set. Here one converts the sequence into a set by replacing the sequence by the set of all short subsequences of some length k. Corresponding to each sequence is a set of length k subsequences. If k is sufficiently large, then two sequences are highly unlikely to give rise to the same set of subsequences. Thus, we have converted the problem of sampling a sequence to that of sampling a set. Instead of storing all the subsequences, we need only store a small subset of the set of length k subsequences.

Suppose you wish to be able to determine if two web pages are minor modifications of one another or to determine if one is a fragment of the other. Extract the sequence of words occurring on the page. Then define the set of subsequences of k consecutive words from the sequence. Let S(D) be the set of all subsequences of length k occurring in document D. Define resemblance of A and B by

resemblance
$$(A, B) = \frac{|S(A) \cap S(B)|}{|S(A) \cup S(B)|}$$

And define containment as

containment
$$(A, B) = \frac{|S(A) \cap S(B)|}{|S(A)|}$$

Let W be a set of subsequences. Define $\min(W)$ to be the s smallest elements in W and define $\max(W)$ as the set of elements of w that are zero $\min(W)$.

Let π be a random permutation of all length k subsequences. Define F(A) to be the s smallest elements of A and V(A) to be the set mod m in the ordering defined by the permutation.

Then

$$\frac{F(A)\cap F(B)}{F(A)\cup F(B)}$$

and

$$\frac{|V(A) \cap V(B)|}{|V(A) \cup V(B)|}$$

are unbiased estimates of the resemblance of A and B. The value

$$\frac{|V(A) \cap V(B)|}{|V(A)|}$$

is an unbiased estimate of the containment of A in B.

7.4 Exercises

Algorithms for Massive Data Problems

Exercise 7.1 Given a stream of n positive real numbers a_1, a_2, \ldots, a_n , upon seeing a_1, a_2, \ldots, a_i keep track of the sum $a = a_1 + a_2 + \cdots + a_i$ and a sample a_j , $j \leq i$ drawn with probability proportional to its value. On reading a_{i+1} , with probability $\frac{a_{i+1}}{a+a_{i+1}}$ replace the current sample with a_{i+1} and update a. Prove that the algorithm selects an a_i from the stream with the probability of picking a_i being proportional to its value.

Exercise 7.2 Given a stream of symbols a_1, a_2, \ldots, a_n , give an algorithm that will select one symbol uniformly at random from the stream. How much memory does your algorithm require?

Exercise 7.3 Give an algorithm to select an a_i from a stream of symbols a_1, a_2, \ldots, a_n with probability proportional to a_i^2 .

Exercise 7.4 How would one pick a random word from a very large book where the probability of picking a word is proportional to the number of occurrences of the word in the book?

Exercise 7.5 For the streaming model give an algorithm to draw s independent samples each with the probability proportional to its value. Justify that your algorithm works correctly.

Frequency Moments of Data Streams
Number of Distinct Elements in a Data Stream
Lower bound on memory for exact deterministic algorithm
Algorithm for the Number of distinct elements
Universal Hash Functions

Exercise 7.6 Show that for a 2-universal hash family $Prob(h(x) = z) = \frac{1}{M+1}$ for all $x \in \{1, 2, ..., m\}$ and $z \in \{0, 1, 2, ..., M\}$.

Exercise 7.7 Let p be a prime. A set of hash functions

$$H = \{h | \{0, 1, \dots, p-1\} \rightarrow \{0, 1, \dots, p-1\}\}\$$

is 3-universal if for all u,v,w,x,y, and z in $\{0,1,\ldots,p-1\}$

$$Prob(h(x) = u, h(y) = v, h(z) = w) = \frac{1}{p^3}.$$

- (a) Is the set $\{h_{ab}(x) = ax + b \mod p | 0 \le a, b < p\}$ of hash functions 3-universal?
- (b) Give a 3-universal set of hash functions.

Exercise 7.8 Give an example of a set of hash functions that is not 2-universal.

Analysis of distinct element counting algorithm Counting the Number of Occurrences of a Given Element.

Exercise 7.9

- (a) What is the variance of the method in Section 7.1.2 of counting the number of occurrences of a 1 with log log n memory?
- **(b)** Can the algorithm be iterated to use only $\log \log \log n$ memory? What happens to the variance?

Exercise 7.10 Consider a coin that comes down heads with probability p. Prove that the expected number of flips before a head occurs is 1/p.

Exercise 7.11 Randomly generate a string $x_1x_2 \cdots x_n$ of 10^6 0's and 1's with probability 1/2 of x_i being a 1. Count the number of ones in the string and also estimate the number of ones by the approximate counting algorithm. Repeat the process for p=1/4, 1/8, and 1/16. How close is the approximation?

Counting Frequent Elements
The Majority and Frequent Algorithms
The Second Moment

Exercise 7.12 Construct an example in which the majority algorithm gives a false positive, i.e., stores a nonmajority element at the end.

Exercise 7.13 Construct examples where the frequent algorithm in fact does as badly as in the theorem, i.e., it "under counts" some item by n/(k+1).

Exercise 7.14 Recall basic statistics on how an average of independent trials cuts down variance and complete the argument for relative error ε estimate of $\sum_{s=1}^{m} f_s^2$.

Error-Correcting codes, polynomial interpolation and limited-way independence

Exercise 7.15 Let F be a field. Prove that for any four distinct points a_1, a_2, a_3 , and a_4 in F and any four (possibly not distinct) values b_1, b_2, b_3 , and b_4 in F, there is a unique polynomial $f(x) = f_0 + f_1 x + f_2 x^2 + f_3 x^3$ of degree at most three so that $f(a_1) = b_1$, $f(a_2) = b_2$, $f(a_3) = b_3$ $f(a_4) = b_4$ with all computations done over F.

Sketch of a Large Matrix

Exercise 7.16 Suppose we want to pick a row of a matrix at random where the probability of picking row i is proportional to the sum of squares of the entries of that row. How would we do this in the streaming model? Do not assume that the elements of the matrix are given in row order.

- (a) Do the problem when the matrix is given in column order.
- (b) Do the problem when the matrix is represented in sparse notation: it is just presented as a list of triples (i, j, a_{ij}) , in arbitrary order.

Matrix Multiplication Using Sampling

Exercise 7.17 Suppose A and B are two matrices. Show that $AB = \sum_{k=1}^{n} A(:,k)B(k,:)$.

Exercise 7.18 Generate two 100 by 100 matrices A and B with integer values between 1 and 100. Compute the product AB both directly and by sampling. Plot the difference in L_2 norm between the results as a function of the number of samples. In generating the matrices make sure that they are skewed. One method would be the following. First generate two 100 dimensional vectors a and b with integer values between 1 and 100. Next generate the i^{th} row of A with integer values between 1 and a_i and the i^{th} column of B with integer values between 1 and b_i .

Approximating a Matrix with a Sample of Rows and Columns

Exercise 7.19 Show that ADD^TB is exactly

$$\frac{1}{s} \left(\frac{A(:,k_1) B(k_1,:)}{p_{k_1}} + \frac{A(:,k_2) B(k_2,:)}{p_{k_2}} + \dots + \frac{A(:,k_s) B(k_s,:)}{p_{k_s}} \right)$$

Exercise 7.20 Suppose a_1, a_2, \ldots, a_m are nonnegative reals. Show that the minimum of $\sum_{k=1}^{m} \frac{a_k}{x_k}$ subject to the constraints $x_k \geq 0$ and $\sum_{k=1}^{m} x_k = 1$ is attained when the x_k are proportional to $\sqrt{a_k}$.

Sketches of Documents

Exercise 7.21 Consider random sequences of length n composed of the integers 0 through g. Represent a sequence by its set of length k-subsequences. What is the resemblance of the sets of length k-subsequences from two random sequences of length n for various values of k as n goes to infinity?

Exercise 7.22 What if the sequences in the Exercise 7.21 were not random? Suppose the sequences were strings of letters and that there was some nonzero probability of a given letter of the alphabet following another. Would the result get better or worse?

Exercise 7.23 Consider a random sequence of length 10,000 over an alphabet of size 100.

- (a) For k = 3 what is probability that two possible successor subsequences for a given subsequence are in the set of subsequences of the sequence?
- **(b)** For k = 5 what is the probability?

Exercise 7.24 How would you go about detecting plagiarism in term papers?

Exercise 7.25 (Finding duplicate web pages) Suppose you had one billion web pages and you wished to remove duplicates. How would you do this?

Exercise 7.26 Construct two sequences of 0's and 1's having the same set of subsequences of width w.

Exercise 7.27 Consider the following lyrics:

When you walk through the storm hold your head up high and don't be afraid of the dark. At the end of the storm there's a golden sky and the sweet silver song of the lark.

Walk on, through the wind, walk on through the rain though your dreams be tossed and blown. Walk on, walk on, with hope in your heart and you'll never walk alone, you'll never walk alone.

How large must k be to uniquely recover the lyric from the set of all subsequences of symbols of length k? Treat the blank as a symbol.

Exercise 7.28 Blast: Given a long sequence a, say 10⁹ and a shorter sequence b, say 10⁵, how do we find a position in a which is the start of a subsequence b' that is close to b? This problem can be solved by dynamic programming but not in reasonable time. Find a time efficient algorithm to solve this problem.

Hint: (Shingling approach) One possible approach would be to fix a small length, say seven, and consider the shingles of a and b of length seven. If a close approximation to b is a substring of a, then a number of shingles of b must be shingles of a. This should allows us to find the approximate location in a of the approximation of b. Some final algorithm should then be able to find the best match.

8 Clustering

8.1 Some Clustering Examples

Clustering comes up in many contexts. For example, one might want to cluster journal articles into clusters of articles on related topics. In doing this, one first represents a document by a vector. This can be done using the vector space model introduced in Chapter 2. Each document is represented as a vector with one component for each term giving the frequency of the term in the document. Alternatively, a document may be represented by a vector whose components correspond to documents in the collection and the i^{th} vector's j^{th} component is a 0 or 1 depending on whether the i^{th} document referenced the j^{th} document. Once one has represented the documents as vectors, the problem becomes one of clustering vectors.

Another context where clustering is important is the study of the evolution and growth of communities in social networks. Here one constructs a graph where nodes represent individuals and there is an edge from one node to another if the person corresponding to the first node sent an email or instant message to the person corresponding to the second node. A community is defined as a set of nodes where the frequency of messages within the set is higher than what one would expect if the set of nodes in the community were a random set. Clustering partitions the set of nodes of the graph into sets of nodes where the sets consist of nodes that send more messages to one another than one would expect by chance. Note that clustering generally asks for a strict partition into subsets although in reality in this case for instance, a node may well belong to several communities.

In these clustering problems, one defines either a similarity measure between pairs of objects or a distance measure (a notion of dissimilarity). One measure of similarity between two vectors \mathbf{a} and \mathbf{b} is the cosine of the angle between them:

$$\cos(\mathbf{a}, \mathbf{b}) = \frac{\mathbf{a}^T \mathbf{b}}{|\mathbf{a}| \, |\mathbf{b}|}$$

To get a distance measure, subtract the cosine similarity from one.

$$dist(\mathbf{a}, \mathbf{b}) = 1 - \cos(\mathbf{a}, \mathbf{b})$$

Another distance measure is the Euclidean distance. There is an obvious relationship between cosine similarity and Euclidean distance. If \mathbf{a} and \mathbf{b} are unit vectors, then

$$|\mathbf{a} - \mathbf{b}|^2 = (\mathbf{a} - \mathbf{b})^T (\mathbf{a} - \mathbf{b}) = |\mathbf{a}|^2 + |\mathbf{b}|^2 - 2\mathbf{a}^T \mathbf{b} = 2(1 - \cos(\mathbf{a}, \mathbf{b})).$$

In determining the distance function to use, it is useful to know something about the origin of the data. In problems where we have to cluster nodes of a graph, we may represent each node as a vector, namely, as the row of the adjacency matrix corresponding to the node. One notion of dissimilarity here is the square of the Euclidean distance. For 0-1

vectors, this measure is just the number of "uncommon" 1's, whereas, the dot product is the number of common 1's. In many situations one has a stochastic model of how the data was generated. An example is customer behavior. Suppose there are d products and n customers. A reasonable assumption is that each customer generates from a probability distribution, the basket of goods he or she buys. A basket specifies the amount of each good bought. One hypothesis is that there are only k types of customers, k << n. Each customer type is characterized by a probability density used by all customers of that type to generate their baskets of goods. The densities may all be Gaussians with different centers and covariance matrices. We are not given the probability densities, only the basket bought by each customer, which is observable. Our task is to cluster the customers into the k types. We may identify the customer with his or her basket which is a vector. One way to formulate the problem mathematically is via a clustering criterion which we then optimize. Some potential criteria are to partition the customers into k clusters so as to minimize

- 1. the sum of distances between all pairs of customers in the same cluster,
- 2. the sum of distances of all customers to their "cluster center" (any point in space may be designated as the cluster center), or
- 3. minimize the sum of squared distances to the cluster center.

The last criterion is called the k-means criterion and is widely used. A variant called the k-median criterion minimizes the sum of distances (not squared) to the cluster center. Another possibility, called the k-center criterion, is to minimize the maximum distance of any point to its cluster center.

The chosen criterion can affect the results. To illustrate, suppose we have data generated according to a equal weight mixture of k spherical Gaussian densities centered at $\mu_1, \mu_2, \ldots, \mu_k$, each with variance 1 in every direction. Then the density of the mixture is

$$F(\mathbf{x}) = \operatorname{Prob}[\mathbf{x}] = \frac{1}{k} \frac{1}{(2\pi)^{d/2}} \sum_{t=1}^{k} e^{-|\mathbf{x} - \boldsymbol{\mu_t}|^2}.$$

Denote by $\mu(\mathbf{x})$ the center nearest to \mathbf{x} . Since the exponential function falls off fast, we have the approximation

$$F(\mathbf{x}) \approx \frac{1}{k} \frac{1}{(2\pi)^{d/2}} e^{-|\mathbf{x} - \boldsymbol{\mu}(\mathbf{x})|^2}.$$

So, given a sample of points $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots \mathbf{x}^{(n)}$ drawn according to the mixture, the likelyhood of a particular $\mu_1, \mu_2, \dots, \mu_k$, namely, the (posterior) probability of generating the sample if $\mu_1, \mu_2, \dots, \mu_k$ were in fact the centers, is approximately

$$\frac{1}{k^n} \frac{1}{(2\pi)^{nd/2}} \prod_{i=1}^n e^{-|\mathbf{x}^{(i)} - \boldsymbol{\mu}(\mathbf{x}^{(i)})|^2} = c e^{-\sum_{i=1}^n |\mathbf{x}^{(i)} - \boldsymbol{\mu}(\mathbf{x}^{(i)})|^2}.$$

So, minimizing the sum of squared distances to cluster centers finds the maximum likelyhood $\mu_1, \mu_2, \ldots, \mu_k$ and this suggests the criterion: sum of distance squared to the cluster centers.

On the other hand, if the generating process had an exponential probability distribution, with the probability law

$$Prob\left[(x_1, x_2, \dots, x_d)\right] = \frac{1}{2} \prod_{i=1}^d e^{-|x_i - \mu_i|} = \frac{1}{2} e^{-\sum_{i=1}^d |x_i - \mu_i|} = \frac{1}{2} e^{-|\mathbf{x} - \boldsymbol{\mu}|}_1,$$

one would use the L_1 norm (not the L_2 or the square of the L_1) since the probability density decreases as the L_1 distance from the center. The intuition here is that the distance used to cluster data should be related to the actual distribution of the data.

The choice of whether to use a distance measure and cluster together points that are close or use a similarity measure and cluster together points with high similarity and what particular distance or similarity measure to use can be crucial to the application. However, there is not much theory on these choices; they are determined by empirical domain-specific knowledge. One general observation is worth making. Using distance squared instead of distance, "favors" outliers more since the square function magnifies large values, which means a small number of outliers may make a clustering look bad. On the other hand, distance squared has some mathematical advantages; see for example Corollary 8.3 which asserts that with the distance squared criterion, the centroid is the correct cluster center. The widely used k-means criterion is based on sum of squared distances.

In the formulations we have discussed so far, we have one number (eg. sum of distances squared to the cluster center) as the "measure of goodness" of a clustering and we try to optimize that number (to find the best clustering according to the measure). This approach does not always yield desired results, since often, it is hard to optimize exactly (most clustering problems are NP-hard). Often, there are polynomial time algorithms to find an approximately optimal solution. But such a solution may be far from the optimal (desired) clustering. We will in section (8.4) how to formalize some realistic conditions under which an approximate optimal solution indeed gives us a desired clustering as well. But first we see some simple algorithms for getting a good clustering according to some natural measures.

8.2 A Simple Greedy Algorithm for k-clustering

There are many algorithms for clustering high-dimensional data. We start with a simple one. Suppose we use the k-center criterion. The k-center criterion partitions the points into k clusters so as to minimize the maximum distance of any point to its cluster center. Call the maximum distance of any point to its cluster center the radius of the clustering. There is a k-clustering of radius r if and only if there are k spheres, each of radius r which together cover all the points. Below, we give a simple algorithm to find k spheres covering a set of points. The lemma following shows that this algorithm needs to

use a radius that is "off by a factor of at most two" from the optimal k-center solution.

The Greedy k-clustering Algorithm

Pick any data point to be the first cluster center. At time t, for t = 2, 3, ..., k, pick any data point that is not within distance r of an existing cluster center; make it the tth cluster center.

Lemma 8.1 If there is a k-clustering of radius $\frac{r}{2}$, then the above algorithm finds a k-clustering with radius at most r.

Proof: Suppose for contradiction that the algorithm using radius r fails to find a k-clustering. This means that after the algorithm chooses k centers, there is still at least one data point that is not in any sphere of radius r around a picked center. This is the only possible mode of failure. But then there are k + 1 data points, with each pair more than distance r apart. Clearly, no two such points can belong to the same cluster in any k-clustering of radius $\frac{r}{2}$ contradicting the hypothesis.

There are in general two variations of the clustering problem for each of the criteria. We could require that each cluster center be a data point or allow a cluster center to be any point in space. If we require each cluster center to be a data point, the problem can be solved in time $\binom{n}{k}$ times a polynomial in the length of the data. First, exhaustively enumerate all sets of k data points as the possible sets of k cluster centers, then associate each point to its nearest center and select the best clustering. No such naive enumeration procedure is available when cluster centers can be any point in space. But, for the k-means problem, Corollary 8.3 shows that once we have identified the data points that belong to a cluster, the best choice of cluster center is the centroid. Note that the centroid might not be a data point.

8.3 Lloyd's Algorithm for k-means Clustering

In k-means criterion, a set $A = \{\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}\}$ of n points in d-dimensions is partitioned into k-clusters, S_1, S_2, \dots, S_k , so as to minimize the sum of squared distances of each point to its cluster center. That is, A is partitioned into clusters, S_1, S_2, \dots, S_k , and a center is assigned to each cluster so as to minimize

$$d(S_1, S_2, \dots, S_k) = \sum_{j=1}^k \sum_{\mathbf{a_i} \in S_j} (\mathbf{c_j} - \mathbf{a_i})^2$$

where $\mathbf{c_i}$ is the center of cluster j.

Suppose we have already determined the clustering or the partitioning into S_1, S_2, \ldots, S_k . What are the best centers for the clusters? The following lemma shows that the answer is the centroids, the coordinatewise means, of the clusters.

Lemma 8.2 Let $\{a_1, a_2, \ldots, a_n\}$ be a set of points. The sum of the squared distances of the a_i to any point x equals the sum of the squared distances to the centroid plus the number of points times the squared distance from the point x to the centroid. That is,

$$\sum_{i} |\mathbf{a_i} - \mathbf{x}|^2 = \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2 + n |\mathbf{c} - \mathbf{x}|^2$$

where \mathbf{c} is the centroid of the set of points.

Proof:

$$\sum_{i} |\mathbf{a_i} - \mathbf{x}|^2 = \sum_{i} |\mathbf{a_i} - \mathbf{c} + \mathbf{c} - \mathbf{x}|^2$$
$$= \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2 + 2(\mathbf{c} - \mathbf{x}) \cdot \sum_{i} (\mathbf{a_i} - \mathbf{c}) + n |\mathbf{c} - \mathbf{x}|^2$$

Since **c** is the centroid, $\sum_{i} (\mathbf{a_i} - \mathbf{c}) = 0$. Thus, $\sum_{i} |\mathbf{a_i} - \mathbf{x}|^2 = \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2 + n \|\mathbf{c} - \mathbf{x}\|^2$

A corollary of Lemma 8.2 is that the centroid minimizes the sum of squared distances since the second term, $n \|\mathbf{c} - \mathbf{x}\|^2$, is always positive.

Corollary 8.3 Let $\{\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}\}$ be a set of points. The sum of squared distances of the $\mathbf{a_i}$ to a point \mathbf{x} is minimized when \mathbf{x} is the centroid, namely $\mathbf{x} = \frac{1}{n} \sum_{i} \mathbf{a_i}$.

Another expression for the sum of squared distances of a set of n points to their centroid is the sum of all pairwise distances squared divided by n. First, a simple notational issue. For a set of points $\{\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}\}$, $\sum_{i=1}^n \sum_{j=i+1}^n |\mathbf{a_i} - \mathbf{a_j}|^2$ counts the quantity $|\mathbf{a_i} - \mathbf{a_j}|^2$ once for each ordered pair (i, j), j > i. However, $\sum_{i,j} |\mathbf{a_i} - \mathbf{a_j}|^2$ counts each $|\mathbf{a_i} - \mathbf{a_j}|^2$ twice, so the later sum is twice the first sum.

Lemma 8.4 Let $\{\mathbf{a_1}, \mathbf{a_2}, \dots, \mathbf{a_n}\}$ be a set of points. The sum of the squared distances between all pairs of points equals the number of points times the sum of the squared distances of the points to the centroid of the points. That is, $\sum_i \sum_{j>i} |\mathbf{a_i} - \mathbf{a_j}|^2 = n \sum_i |\mathbf{a_i} - \mathbf{c}|^2$ where \mathbf{c} is the centroid of the set of points.

Proof: Lemma 8.2 states that for every \mathbf{x} ,

$$\sum_{i} |\mathbf{a_i} - \mathbf{x}|^2 = \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2 + n |\mathbf{c} - \mathbf{x}|^2.$$

Letting \mathbf{x} range over all $\mathbf{a_i}$ and summing the n equations yields

$$\sum_{i,j} |\mathbf{a_i} - \mathbf{a_j}|^2 = n \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2 + n \sum_{j} |\mathbf{c} - \mathbf{a_j}|^2$$
$$= 2n \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2.$$

Observing that

$$\sum_{i,j} |\mathbf{a_i} - \mathbf{a_j}|^2 = 2 \sum_{i} \sum_{j>i} |\mathbf{a_i} - \mathbf{a_j}|^2$$

yields the result that

$$\sum_{i} \sum_{j>i} |\mathbf{a_i} - \mathbf{a_j}|^2 = n \sum_{i} |\mathbf{a_i} - \mathbf{c}|^2.$$

The k-means clustering algorithm

A natural algorithm for k-means clustering is given below. There are two unspecified aspects of the algorithm. One is the set of starting centers and the other is the stopping condition.

k-means algorithm

Start with k centers.

Cluster each point with the center nearest to it.

Find the centroid of each cluster and replace the set of old centers with the centroids. Repeat the above two steps until the centers converge (according to some criterion).

The k-means algorithm always converges but possibly to a local minimum. To show convergence, we argue that the cost of the clustering, the sum of the squares of the distances of each point to its cluster center, always improves. Each iteration consists of two steps. First, consider the step which finds the centroid of each cluster and replaces the old centers with the new centers. By Corollary 8.3, this step improves the sum of internal cluster distances squared. The other step reclusters by assigning each point to its nearest cluster center, which also improves the internal cluster distances.

8.4 Meaningful Clustering via Singular Value Decomposition

Optimizing a criterion such as k—means is often not an end in itself. It is a means to finding a good (meaningful) clustering. How do we define a meaningful clustering? Here is a possible answer: an optimal clustering is meaningful if it is unique, in the sense that any other nearly optimal clustering agrees with it on most data points. We will formalize this below. But the bad news is that we will soon see that this is too much to ask for and many common data sets do not admit such a clustering. Luckily though, the discussion

will lead us to a weaker requirement which has the twin properties of being met by many data sets as well as admitting an efficient (SVD-based) algorithm to find the clustering. We start with some notation.

We denote by n the number of (data) points to be clustered; they are listed as the rows A_i of a $n \times d$ matrix A. A clustering (partition) of the data points is represented by a matrix of cluster centers C which is also a $n \times d$ matrix; the i th row of C is the center of the cluster that A_i belongs to. So C has only k distinct rows. We refer to A as the data and to C as the clustering.

Definition: The cost of the clustering C is the sum of distances squared to the cluster centers; so we have

$$cost(A, C) = ||A - C||_F^2.$$

The mean squared distance (MSD) of a clustering C is just cost(A, C)/n.

We will say two clusterings of A differ in s points if s is the minimum number of data points to be reassigned to get from one clustering to the other. [Note: a clustering is specified by just a partition; the cluster centers are just the centroids of data points in a cluster.] Here is the first attempt at defining when a clustering is meaningful:

A k- clustering C is meaningful if every k-clustering C' which differs from C in at least ϵn points has cost at least $(1 + \Omega(\epsilon)) \cos(C)$. [ϵ is a small constant.]

Claim 8.1 If C is meaningful under this definition, and each of its clusters has $\Omega(n)$ data points in it, then for any two cluster centers μ, μ' of C,

$$|\mu - \mu'|^2 \ge MSD(C) :$$

Proof: We will prove the claim by showing that if two cluster centers in C are too close, then we may move ϵn points from cluster to the other without increasing the cost by more than a factor of $(1 + O(\epsilon))$, thus contradicting the assumption that C is meaningful.

Let T be the cluster with cluster center μ . Project each data point $A_i \in T$, onto the line through μ, μ' and let d_i be the distance of the projected point to μ . Let T_1 be the subset of T whose projections land on the μ' side of μ and let $T_2 = T \setminus T_1$ be the points whose projections land on the other side. Since μ is the centroid of T, we have $\sum_{i \in T_1} d_i = \sum_{i \in T_2} d_i$. Since each $A_i \in T$ is closer to μ than to μ' , for $i \in T_1$, we have $d_i \leq |\mu - \mu'|/2$ and so $\sum_{i \in T_1} d_i \leq |T| |\mu - \mu'|/2$; hence also, $\sum_{i \in T_2} d_i \leq |T| |\mu - \mu'|/2$. So,

$$\sum_{i \in T} d_i \le |T||\mu - \mu'|.$$

Now from the assumption that $|T| \in \Omega(n)$, we have $|T| \ge 2\epsilon n$. So, the ϵn th smallest d_i is at most $\frac{|T|}{|T|-\epsilon n}|\mu-\mu'| \le 2|\mu-\mu'|$. We can now get a new clustering C' as follows: move the ϵn A_i in T with the smallest d_i to the cluster with μ' as center. Recompute centers. The recomputatation of the centers can only reduce the cost (as we saw in Corollary (8.3)). What about the move? The move can only add cost (distance squared) in the direction of the line joining μ, μ' and this extra cost is at most $4\epsilon n|\mu-\mu'|^2$. By the assumption that C is meaningful (under the proposed definition above), we must thus have $|\mu-\mu'|^2 \ge \text{MSD}(C)$ as claimed.

But we will now see that the condition that $|\mu - \mu'|^2 \ge \text{MSD}(C)$ is too strong for some common data sets. Consider two spherical Gaussians in d- space, each with variance 1 in each direction. Clearly if we have data generated from a (equal weight) mixture of the two, the "correct" 2-clustering one would seek is to split them into the Gaussians they were generated from with the actual centers of the Gaussians (or a very close point) as the cluster centers. But the MSD of this clustering is approximately d. So, by the Claim, for C to be meaningful, the centers must be $\Omega(d)$ apart. It is easy to see however that if the separation is $\Omega(\sqrt{\ln n})$, the clusters are distinct: the projection of each Gaussian to the line joining their centers is a 1 dimensional Gaussian of variance 1, so the probability that any data point lies more than a tenth of the way (in the projection) to the wrong center is at most $O(1/n^2)$, so by union bound, all data points have their distance to the wrong center at least 10 times the distance to the correct center, provided, we measure distances only in the projection. Since the variance is 1 in each direction, the Mean Squared Distance to the cluster center in each direction is only O(1). So, in this example, it would make more sense to require a inter-center separation of the maximum mean squared distance in any one direction to the cluster center. We will be able to achieve this in general.

Definition: Let A, C be the data and cluster centers matrices respectively. The *mean* squared distance in a direction (denoted MSDD(A, C)) is the maximum over all unit length vectors \mathbf{v} of the mean squared distance of data points to their cluster centers in the direction \mathbf{v} , namely,

$$MSDD(A, C) = \frac{1}{n} Max_{\mathbf{v}:|\mathbf{v}|=1} |(A - C)\mathbf{v}|^2 = \frac{1}{n} ||A - C||_2^2,$$

where, we have used the basic definition of the largest singular value to get the last expression.

Theorem 8.5 Suppose there exists a k-clustering C of data points A with (i) $\Omega(n)$ data points per cluster and (ii) distance at least $\Omega(\sqrt{MSDD(A,C)})$ between any two cluster centers. Then any clustering returned by the following simple algorithm (which we henceforth call the SVD clustering of A) differs from C is at most ϵn points (here, the hidden constants in Ω depend on ϵ .)

Find the SVD of A. Project data points to the space of the top k (right) singular vectors of A. Return a 2- approximate k-means clustering in the projection.

Remark: Note that if we did the approximate optimization in the whole space (without projecting), we will not succeed in general. In the example of the two spherical Gaussians above, for the correct clustering C, MSDD(A, C) = O(1). But if the inter-center separation is just O(1), then ϵn points of the first Gaussian may be put into the second at an added cost (where cost is distance squared in the whole space) of only O(n) as we argued, whereas, the cost of clustering C is O(nd).

⁸A 2-approximate clustering is one which has cost at most twice the optimal cost.

Remark: The Theorem also implies a sort of uniqueness of the clustering C, namely, that any other clustering satisfying both (i) and (ii) differs from C in at most $2\epsilon n$ points, as seen from the following: The Theorem applies to the other clustering as well, since it satisfies the hypothesis. So, it also differs from the SVD clustering in at most ϵn points. Thus, C and the other clustering cannot differ in more than $2\epsilon n$ points.

The proof of the Theorem will use the following two Lemmas, which illustrate the power of SVD. The first Lemma says that for any clustering C with $\Omega(n)$ points per cluster, the SVD clustering described in the Theorem finds cluster centers fairly close to the cluster centers in C, where, close is measured in terms of $\mathrm{MSDD}(A,C)$. The argument will be that one candidate clustering in the SVD projection is to just use the same centers as C (projected to the space) and if the SVD clustering does not have a cluster center close to a particular cluster of C, it ends up paying too high a penalty compared to this candidate clustering to be 2-optimal.

Lemma 8.6 Suppose A is the data matrix and C a clustering with $\Omega(n)$ points in each cluster. ⁹ Suppose C' is the SVD clustering (described in the Theorem) of A. Then for every cluster center μ of C, there is a cluster center of C' within distance $O(\sqrt{MSDD(A,C)})$.

Proof: Let $\alpha = \text{MSDD}(A, C)$. Let T be the set of data points in a cluster of C and suppose for contradiction that centroid μ of T has no cluster center of C' at distance $O(\sqrt{k\alpha})$. Let \bar{A}_i denote projection of A_i onto the SVD subspace; so the SVD clustering actually clusters points \bar{A}_i . Recall the notation that C'_i is the cluster center of C' closest to \bar{A}_i . The cost of a data point $A_i \in T$ in the SVD solution is

$$|\bar{A}_i - C_i'|^2 = |(\mu - C_i') - (\mu - \bar{A}_i)|^2 \ge \frac{1}{2}|\mu - C_i'|^2 - |\mu - \bar{A}_i|^2 \ge \Omega(\alpha) - |\mu - \bar{A}_i|^2,$$

where, we have used $|a-b|^2 \ge \frac{1}{2}|a|^2 - |b|^2$ for any two vectors a and b. Adding over all points in T, the cost of C' is at least $\Omega(n\alpha) - ||\bar{A} - C||_F^2$. Now, one way to cluster the points \bar{A}_i is to just use the same cluster centers as C; the cost of this clustering is $||\bar{A} - C||_F^2$. So the optimal clustering of points \bar{A}_i costs at most $||\bar{A} - C||_F^2$ and since the algorithm finds a 2-approximate clustering, the cost of the SVD clustering is at most $2||\bar{A} - C||_F^2$. So we get

$$2||\bar{A} - C||_F^2 \ge \Omega(n\alpha) - ||\bar{A} - C||_F^2 \quad \Longrightarrow \quad ||\bar{A} - C||_F^2 \ge \Omega(n\alpha).$$

We will prove that $\|\bar{A} - C\|_F^2 \le 5k\alpha n$ in Lemma 8.7. By (i), we have $k \in O(1)$, so $\|\bar{A} - C\|_F^2 = O(\alpha)$. So, we get a contradiction (with suitable choice of constants under the Ω .)

Note that in the Lemma below, the main inequality has Frobenius norm on the left hand side, but only operator norm on the right hand side. This makes it stronger than having either Frobenius norm on both sides or operator norm on both sides.

⁹Note that C is not assumed to satisfy condition (ii) of the Theorem.

Lemma 8.7 Suppose A is an $n \times d$ matrix and suppose C is an $n \times d$ rank k matrix. Let \bar{A} be the best rank k approximation to A found by SVD. Then, $||\bar{A} - C||_F^2 \leq 5k||A - C||_2^2$.

Proof: Let $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_k}$ be the top k singular vectors of A. Extend the set of the top k singular vectors to an orthonormal basis $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_p}$ of the vector space spanned by the rows of \bar{A} and C. Note that $p \leq 2k$ since \bar{A} is spanned by $\mathbf{u_1}, \mathbf{u_2}, \dots, \mathbf{u_k}$ and C is of rank at most k. Then,

$$||\bar{A} - C||_F^2 = \sum_{i=1}^k |(\bar{A} - C)\mathbf{u_i}|^2 + \sum_{i=k+1}^p |(\bar{A} - C)\mathbf{u_i}|^2.$$

Since $\{\mathbf{u_i}|1 \leq i \leq k\}$ are the top k singular vectors of A and since \bar{A} is the rank k approximation to A, for $1 \leq i \leq k$, $A\mathbf{u_i} = \bar{A}\mathbf{u_i}$ and thus $|(\bar{A} - C)\mathbf{u_i}|^2 = |(A - C)\mathbf{u_i}|^2$. For i > k, $\bar{A}\mathbf{u_i} = 0$, thus $|(\bar{A} - C)\mathbf{u_i}|^2 = |C\mathbf{u_i}|^2$. From this it follows that

$$\|\bar{A} - C\|_F^2 = \sum_{i=1}^k |(A - C)\mathbf{u_i}|^2 + \sum_{i=k+1}^p |C\mathbf{u_i}|^2$$

$$\leq k||A - C||_2^2 + \sum_{i=k+1}^p |A\mathbf{u_i} + (C - A)\mathbf{u_i}|^2$$

Using $|a+b|^2 \le 2|a|^2 + 2|b|^2$

$$\|\bar{A} - C\|_F^2 \le k||A - C||_2^2 + 2\sum_{i=k+1}^p |A\mathbf{u_i}|^2 + 2\sum_{i=k+1}^p |(C - A)\mathbf{u_i}|^2$$

$$\le k||A - C||_2^2 + 2(p - k - 1)\sigma_{k+1}^2(A) + 2(p - k - 1)||A - C||_2^2$$

Using $p \le 2k$ implies k > p - k - 1

$$\|\bar{A} - C\|_{E}^{2} \le k\|A - C\|_{2}^{2} + 2k\sigma_{k+1}^{2}(A) + 2k\|A - C\|_{2}^{2}. \tag{8.1}$$

As we saw in Chapter 4, for any rank k matrix B, $||A - B||_2 \ge \sigma_{k+1}(A)$ and so $\sigma_{k+1}(A) \le ||A - C||_2$ and plugging this in, we get the Lemma.

Proof: (of Theorem (8.5)) Let $\beta = \sqrt{\text{MSDD}(A, C)}$. We will use Lemma (8.6). To every cluster center μ of C, there is a cluster center ν of the SVD clustering within distance $O(\beta)$. Also, since, C satisfies (ii) of the Theorem, the mapping from μ to ν is 1-1. C and the SVD clustering differ on a data point A_i if the following happens: A_i belongs to cluster center μ of C whose closest cluster center in C' is ν , but \bar{A}_i (the projection of A_i

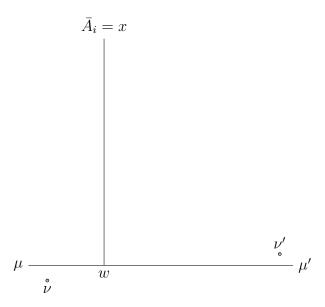


Figure 8.1: Illustration of the cost of a misclassified point.

onto the SVD subspace) has as its closest C' center some $\nu' \neq \nu$. Suppose μ' is the cluster center of C closest to ν' . (See Figure (8.1)). In this case, we have (with $x = \bar{A}_i$)

$$\begin{split} |x-\mu| &\geq |x-\nu| - |\nu-\mu| \geq |x-\nu'| - |\nu-\mu| \\ &\geq |x-\mu'| - |\nu'-\mu'| - |\nu-\mu| \geq |\mu-\mu'| - |\mu-x| - |\nu'-\mu'| - |\nu-\mu| \\ \text{So, } |x-\mu| &\geq \frac{1}{2} |\mu-\mu'| - O(\beta). \end{split}$$

Now, by making the hidden constant in condition (ii) of the Theorem large enough, we have that $|\bar{A}_i - \mu| \ge \frac{\beta}{\sqrt{\epsilon}}$. Suppose there are m such A_i (which are clustered differently in C, C'). Then, squaring the above and summing over them, we get $||\bar{A} - C||_F^2 \ge \frac{m\beta^2}{\epsilon}$. But on the other hand, by Lemma (8.7), we know that $||\bar{A} - C||_F^2 \le O(k||A - C||_2^2) = O(kn\beta^2)$. Also, by condition (i) of the Theorem, $k \in O(1)$, so $||\bar{A} - C||_F^2 = O(n\beta^2)$. This implies the conclusion of the Theorem that $m \le \epsilon n$.

8.5 Recursive Clustering based on Sparse Cuts

Going back to single criterion based optimization, the criteria considered earlier are "global optimality criteria" like minimizing the total sum of distances or sum of distances squared from the cluster center. The criteria were also made more definite by fixing k the number of clusters in advance although this can be relaxed by trying various k. But global criteria can sometimes mislead. Consider the example in Figure 8.2, where the 2-median criterion gives the 2-clustering B. But defining the similarity between two objects as either the inverse of the distance between them or some other inverse function of

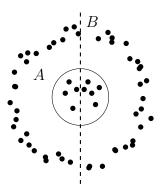


Figure 8.2: Example where 2-median clustering B illustrated by the dashed line is not natural.

the distance, the points in the inner circle have high similarity to other nearby points in the inner circle, whereas they have low similarity to all points of the outer circle, so the 2-clustering A is more natural.

In these contexts, we wish to divide the objects into clusters so that objects are in the same cluster as points that are highly similar and the total similarities between pairs of objects in different clusters is low. Just ensuring that the total sum of similarities among objects in one cluster is high is not sufficient since this permits the cluster to be comprised of two cliques (high pairwise similarities) that are disjoint and have no similarity between them. The cluster should really be split into two clusters. So, we stipulate that each cluster must be a natural cluster which cannot be split further, or in other words, there is no split of a cluster into two in which the total similarities between the two parts is low.

This suggests a recursive clustering procedure that starts with all objects in the same cluster. If there is some split into two subsets with low total similarity between the two parts, then split the cluster and repeat on each part until no further splits are possible. Unfortunately, if the similarities were uniformly spread, the split of any subset into two parts, one of which is a singleton will have low total similarity and this procedure will tend to subdivide the set into singletons or very small subsets which is not useful. The difficulty here is the following. Let $d_i = \sum_j a_{ij}$ be the total similarity of object i to all the others. Assume for the moment that the d_i are all roughly equal. Further, suppose

the others. Assume for the moment that the d_i are all roughly equal. Further, suppose that for any subset S of s objects (s small), the total similarity of objects in this subset to objects outside, namely $\sum_{i \in S} \sum_{j \in \bar{S}} a_{ij}$ is roughly sd_i . Then going by such totals will favor

small s, tending to decimate the set. Instead, it makes better sense to measure the total similarity of S to the rest of the set divided by s, i.e., the "per object" similarity to the outside. Note that this does not favor singletons being split off. But the division by s, the number of objects in S, only makes sense if the similarities were evenly spread. In the more general case, a better approach is to divide the sum of similarities between pairs of

objects where one is in S and the other is in \overline{S} by the sum of similarities between objects in S to all objects.

We now fix some notation for this section. Let A be the $n \times n$ matrix of pairwise similarities. A is a symmetric matrix; $a_{ij} = a_{ji}$. Let $d_i = \sum_k a_{ik}$ be the row sums of A. Also, let $d = \sum_i d_i$ be the sum of all similarities. We get another matrix P from A by normalizing all row sums to 1:

 $p_{ij} = \frac{a_{ij}}{d_i}.$

Note that P need not be symmetric. Now, we make a basic definition.

Definition: For a subset S of rows, define the sparsity $\Phi(S)$ of S to be the total similarity of all objects in S to all objects in \bar{S} divided by the total similarity of objects in S to all objects; in symbols:

$$\Phi(S) = \frac{\sum_{i \in S, j \in \bar{S}} a_{ij}}{\sum_{i \in S} d_i}.$$

Define the (overall) sparsity (denoted Φ) as 10 as the minimum of $\Phi(S)$ over all S with

$$\sum_{i \in S} d_i \le \frac{1}{2} \sum_{\text{all } j} d_j.$$

Sparsity measures the amount of similarity between a set and its complement, but divided by the total similarity of the set overall. The last restriction to sets of at most 1/2 the total similarities is natural.

These definitions are best understood using concepts from Markov Chains. Consider the Markov Chain with P as its transition probability matrix. [In Chapter 5, we had a matrix with its i, j th entry a_{ij} equal to the (electrical) conductance between nodes i and j and we normalized similarly. Here as there, P need not be symmetric, even though A is.] We will assume that the underlying graph (consisting of edges (i, j) with non-zero p_{ij}) is connected, so by Theorem (5.1), there are stationary probabilities π_i . As we did in Chapter 5, it is easy to check that the stationary probabilities π_i are proportional to d_i , namely, $\pi_i = \frac{d_i}{\sum_k d_k}$ by time-reversibility: $\frac{d_i}{d}p_{ij} = \frac{d_j}{d}p_{ji}$. Then, we see that what we have called the sparsity here is precisely the same as Minimum Escape Probability there.

If the sparsity of the whole set of objects is small, there is a sparse cut - (S_1, \bar{S}_1) , with low total similarity between S_1 and \bar{S}_1 (compared to the similarities of S_1 to all objects). So it makes sense to divide the set into S_1 and \bar{S}_1 . Then, clearly, it makes sense to recursively repeat this process. But one note of caution: how do we measure sparsity of a subset $S \subseteq S_1$, inside S_1 for the next step? There are two alternative definitions:

$$\frac{\text{Total similarity of } S \text{ to } S_1 \setminus S}{\text{Total similarity of } S \text{ to all } n \text{ objects}},$$

¹⁰The sparsity defined here is the same as Minimum Escape Probability we defined in Chapter 5 for Markov Chains; in the Markov Chain literature, it is often also called the conductance.

$$\frac{\text{Total similarity of } S \text{ to } S_1 \setminus S}{\text{Total similarity of } S \text{ to } S_1},$$

differing in the denominator. We will use the first one (which unlike the second) has the advantage that the weight (p_{ij}) of edges we remove to split into clusters (in this example, the edges between S and $S_1 \setminus S$) will be counted correctly.

The high-level description of the recursive clustering algorithm follows.

Recursive Clustering

If a set (of nodes) has a subset S with $\Phi(S) \leq \varepsilon$, split the set into two parts: S and the rest. Repeat in each part.

Here, ε is a real number between 0 and 1 and it is the desired lower bound on sparsity of each part when we finish. A single vertex has no proper partition and by definition, we take the sparsity of a single vertex to be 1.

Finding whether there is a set S with sparsity at most some value is NP-hard. We address this issue later. But first we show that the above scheme yields a clustering with a certain provable guarantee. Unfortunately what we can prove in this generality is rather weak compared to empirically observed behavior.

Theorem 8.8 Suppose we run the algorithm above with one modification: At the outset, keep aside each vertex with $d_i \leq \varepsilon d/n$ as a separate cluster. Then at termination, the total similarity over all edges (i,j) with i and j in different clusters is at most $O(\varepsilon \log(n/\varepsilon))$ times the total similarity of all edges. Also, at termination, each part has sparsity at least ε .

Proof: The initial cutting out of vertices with $d_i \leq \varepsilon d/n$ cuts out edges with total similarity at most εd . Suppose at some point, the algorithm is cutting up a subset S into two: W, R. Say W is the smaller set in the sense $\sum_{i \in W} d_i \leq \sum_{j \in R} d_j$. We "charge" the total similarity of all edges being cut $\sum_{i \in W, j \in R} a_{ij}$ to the vertices of W as follows: for $k \in W$, we add the charge $-\frac{d_k \sum_{i \in W, j \in R} a_{ij}}{\sum_{\ell \in W} d_\ell}$. Since we only make the cut when the sparsity is at most ε , the charge added to each $k \in W$ is a most εd_k . How many times is a vertex charged? It is only charged when it is in the smaller part of the cut. So between any two times it is charged, the size, measured by $\sum_{\ell \in \text{part containing } k} d_\ell$ is cut down by a factor of at least 2. Since the total d_i at the start is d and never goes below $\varepsilon d/n$ for any vertex which is involved in a cut, a vertex can be charged at most $O(\log(n/\varepsilon))$ times. Adding up the charges, we get the Theorem.

But determining whether a set has small sparsity and then finding a sparse cut are NP-hard problems, so the theorem cannot be implemented right away.

Luckily, eigenvalues and eigenvectors (which can be computed fast) give us an approximation to sparsity. The connection between eigenvalues and sparsity, known as Cheeger's inequality, is a deep one with applications to Markov chains among others. This can be

proved by the same method as we used for the proof of Theorem (5.11) of Chapter 5 on Markov Chains. Here, we will only state the result.

Suppose \mathbf{v} is the right eigen-vector of P corresponding to the second largest eigenvalue. Call S a level set of \mathbf{v} is there is some real number α such that $S = \{i : v_i \geq \alpha\}$. Then Cheeger's inequality says that there is a level set S of \mathbf{v} for which $\Phi(S) \leq 4\sqrt{\Phi}$; in other words, one of the level sets of \mathbf{v} has approximately the lowest sparsity (in the sense of square roots). Eigen-vectors can be found, and then the n level sets can be enumerated and we may take the one yielding the sparsest cut among those. We would cut along this cut and proceed recursively. Again, we do not work out the details here.

8.6 Kernel Methods

The k-means criteria cannot separate clusters that are not linearly separable in the input space. This is because, in the final clustering, each cluster is defined by the set of data points closest to a particular cluster center. Indeed, all the methods so far, including spectral methods, optimized a well-defined objective function and assumed that the problem was already well formulated, either in terms of distances or similarities. In this section, we discuss a method of altering the problem formulation so that we can get the desired clustering.

In the chapter on learning, we saw many examples that were not linearly separable in the original space, but were linearly separable when mapped to a higher dimensional space using a nonlinear function called a kernel. An analogous technique can be used in the case of clustering, but with two differences.

- 1. There may be any number k of clusters, whereas in learning, there were just two classes, the positive and negative examples.
- 2. There is unlabelled data, i.e., we are not given which cluster each data point belongs to, whereas in the case of learning each data point was labeled. The clustering situation is sometimes called "unsupervised" whereas the labeled learning situation is called "supervised", the reason being, one imagines a supervisor (human judgement) supplying the labels.

These two differences do not prevent the application of kernel methods to clustering. Indeed, here too, one could first embed the data in a different space using the Gaussian or other kernel and then run k-means in the embedded space. Again, one need not write down the whole embedding explicitly. But in the learning setting, since there were only two classes with a linear separator, we were able to write a convex program to find the normal of the separator. When there are k classes, there could be as many as $\binom{k}{2}$ hyperplanes separating pairs of classes, so the computational problem is harder and there is no simple convex program to solve the problem. However, we can still run the k-means algorithm in the embedded space. The centroid of a cluster is kept as the average of the data points in the cluster. Recall that we only know dot products, not distances in the

higher dimensional space, but we can use the relation $|x-y|^2 = x \cdot x + y \cdot y + 2x \cdot y$ to go from dot products to distances. We do not dwell on the details here.

There are situations where the data points, which are high-dimensional points, lie in a lower dimensional manifold. In such situations, a Gaussian kernel is useful. Say we are given a set of n points $S = \{\mathbf{s_1}, \mathbf{s_2}, \dots, \mathbf{s_n}\}$ in \mathbf{R}^d that we wish to cluster into k subsets. The Gaussian kernel uses an affinity measure that emphasizes closeness of points and drops off exponentially as the points get farther apart. We define the "affinity" between points i and j by

 $a_{ij} = \begin{cases} e^{-\frac{1}{2\sigma^2}} \|\mathbf{s_i} - \mathbf{s_j}\|^2 & i \neq j \\ 0 & i = j \end{cases}$

The affinity matrix gives a closeness measure for points. The measure drops off exponentially fast with distance and thus favors close points. Points farther apart have their closeness shrink to zero. We give two examples to illustrate briefly the use of Gaussian kernels. The first example is similar to Figure 8.2 of points on two concentric annuli. Suppose the annuli are close together, i.e., the distance between them is $\delta << 1$. Even if we used similarity between objects, rather than say the k-median criterion, it is not clear that we will get the right clusters; namely two separate circles. Instead, suppose the circles are sampled at a rate so that adjacent samples are separated by a distance $\varepsilon << \delta$. Define a Gaussian kernel with variance ε^2 . Then, if sample $\mathbf{s_1}$ is on Circle 1 and sample $\mathbf{s_2}$ is on Circle 2, $e^{-|\mathbf{s_1}-\mathbf{s_2}|^2/2\varepsilon^2} << 1$, so they are very likely to be put in separate clusters as desired.

Our second example has three curves. Suppose two points from two different curves are never closer than δ . Again, if we sample at a high enough rate, then every sample will have many other samples from the same curve close to it giving high similarity according to the Gaussian kernel, but no two samples from different curves will have high similarity. This example can be generalized to a situation where the points lie on different "sheets" or low dimensional manifolds.

WITH THE KERNAL METHOD ARE WE REALLY USING SINGLE LINK TO CLUSTER NOT K-MEANS? Answer: No, we do not specify what method exactly we use in the embedded space. Indeed, we could single linkage or k-means. In the idealized examples discussed either method should find the correct clustering.

Another data set The rows of y form two very tight clusters.

Two points near each other on the same circle will have a high affinity value, i.e., they will be close together in this metric. For the right sigma value, the two closest points, one from each circle, will be infinitely far apart. Thus, the affinity matrix is a band matrix, consisting of two blocks of data.

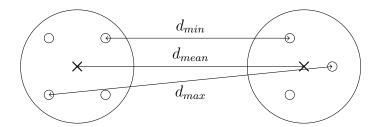


Figure 8.3: Illustration of minimum, maximum and mean distances for a set of points.

8.7 Agglomerative Clustering

Agglomerative clustering starts with each point in a separate cluster and then repeatedly merges the two closest clusters into one. There are various criteria to determine which two clusters are merged at any point. They are based on first defining a distance between two clusters in terms of the distance between points. Four possibilities are listed below:

1. Nearest neighbor - the distance between clusters C_i and C_j is the distance between the points in C_i and C_j that are closest.

$$d_{\min}\left(C_{i}, C_{j}\right) = \min_{\substack{x \in C_{i} \\ y \in C_{j}}} \left\|x - y\right\|$$

This measure basically builds the minimal cost spanning tree (with one node per cluster) for the data.

2. Farthest neighbor - the distance between clusters C_i and C_j is the distance between the points in C_i and C_j that are farthest apart.

$$d_{\max}\left(C_{i}, C_{j}\right) = \max_{\substack{x \in C_{i} \\ y \in C_{j}}} \left\|x - y\right\|$$

- 3. Mean the distance between two clusters is the distance between the centroids of the clusters.
- 4. Average the distance between two clusters is the average distance between points in the two clusters.

Agglomerative clustering in moderate and high dimensions often gives rise to a very unbalanced tree. This section gives some insight into the cause of this phenomenon. We begin by considering agglomerative clustering of 1-dimensional data. The 1-dimensional

case gives rise to a balanced tree.

Consider agglomerative clustering using nearest neighbor of n points on a line. Assume the distances between adjacent points are independent random variables and measure the distance between clusters by the distance of the nearest neighbors. Here it is easy to see that each cluster is always an interval. In this case, any two adjacent intervals are equally likely to be merged. The last merge will occur when the largest distance between two adjacent points is encountered. This is equally likely to be the distance between point i and point i + 1 for any $i, 1 \le i < n$. The height of the final merge tree will be one more than the maximum of the heights of the two subtrees. Let h(n) be the expected height of a merge tree with n leaves. Then

$$h(n) = 1 + \frac{1}{n} \sum_{i=1}^{n} \max \{h(i), h(n-i)\}$$

$$= 1 + \frac{2}{n} \sum_{i=\frac{n}{2}+1}^{n} h(i)$$

$$= 1 + \frac{2}{n} \sum_{i=\frac{n}{2}+1}^{n} h(i) + \frac{2}{n} \sum_{i=\frac{3}{4}n+1}^{n} h(i)$$

Since h(i) is monotonic, for $\frac{n}{2} < i \le \frac{3}{4}n$, bound h(i) by $h\left(\frac{3}{4}n\right)$ and for $\frac{3}{4}n < i \le n$, bound h(i) by h(n). Thus,

$$h(n) \le 1 + \frac{2}{n} \frac{n}{4} h\left(\frac{3n}{4}\right) + \frac{2}{n} \frac{n}{4} h(n)$$

$$\le 1 + \frac{1}{2} h\left(\frac{3n}{4}\right) + \frac{1}{2} h(n).$$

This recurrence has a solution $h(n) \leq b \log n$ for sufficiently large b. Thus, the merge tree has no long path and is bushy.

If the n points are in high dimension rather than constrained to a line, then the distance between any two points, rather than two adjacent points, can be the smallest distance. One can think of edges being added one at a time to the data to form a spanning tree. Only now we have an arbitrary tree rather than a straight line. The order in which the edges are added corresponds to the order in which the connected components are merged by the agglomerative algorithm. Two extreme cases of the spanning tree for the set of points are the straight line which gives a bushy agglomerative tree or a star which gives a skinny agglomerative tree of height n. Note there are two trees involved here, the spanning tree and the agglomerative tree.

The question is what is the shape of the spanning tree? If distance between components is nearest neighbor, the probability of an edge between two components is proportional to the size of the components. Thus, once a large component forms it will swallow up small components giving a more star like spanning tree and hence a tall skinny agglomerative tree. Notice the similarity to the G(n, p) problem.

If we defined distance between two clusters to be the maximum distance between any two points in the clusters, then we are more likely to get a bushy spanning tree and a skinny agglomerative tree. If all distances between points are independent and we have two clusters of size k and a singleton, the maximum distance between the points in the two clusters of size k is likely to give a larger distance than the maximum between the singleton and the k points in a cluster. Thus, the singleton will likely merge into one of the clusters before the two clusters will merge and in general small clusters will combine before larger ones, resulting in a bushy spanning tree and a skinny agglomerative tree.

8.8 Communities, Dense Submatrices

Represent n data points in d-space by the rows of an $n \times d$ matrix A. Assume that A has all nonnegative entries. Examples to keep in mind for this section are the document-term matrix and the customer-product matrix. We address the question of how to define and find efficiently a coherent large subset of rows. To this end, the matrix A can be represented by a bipartite graph. One side has a vertex for each row and the other side a vertex for each column. Between the vertex for row i and the vertex for column j, there is an edge with weight a_{ij} .

We want a subset S of row vertices and a subset T of column vertices so that A(S,T) defined as the sum of the entries in the S rows and T columns, i.e., $A(S,T) = \sum_{i \in S, j \in T} a_{ij}$ is high. This simple definition is not good since A(S,T) will be maximized by taking all rows and columns. We need a balancing criterion that ensures that A(S,T) is high relative to the sizes of S and T. One possibility is to maximize $\frac{A(S,T)}{|S||T|}$. This is not a good measure either, since it is maximized by the single edge of highest weight. The definition we use is the following. Let A be a matrix with nonnegative entries. For a subset S of rows and a subset T of columns, the density d(S,T) of S and T is $d(S,T) = \frac{A(S,T)}{\sqrt{|S||T|}}$. The density d(A) of A is defined as the maximum value of d(S,T) over all subsets of rows and columns. This definition applies to bipartite as well as non bipartite graphs.

In the case where A's rows and columns both represent the same set and a_{ij} is the similarity between object i and object j, the case S = T is clearly of interest. Here $d(S,S) = \frac{A(S,S)}{|S|}$. If A is an $n \times n$ 0-1 matrix, it can be thought of as the adjacency matrix of an undirected graph, and d(S,S) is the average degree of a vertex in S. The subgraph of maximum average degree in a graph can be found exactly by network flow techniques, as we will show in the next section. We do not know an efficient (polynomial-

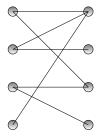


Figure 8.4: Example of a bipartite graph.

time) algorithm for finding d(A) exactly in general. However, we show that d(A) is within a $O(\log^2 n)$ factor of the top singular value of A assuming $|a_{ij}| \leq 1$ for all i and j. While this is a theoretical result, the gap may be much better than $O(\log^2 n)$ for many problems, making the singular value and singular vector quite useful. Also, S and T with $d(S,T) \geq \Omega(d(A)/\log^2 n)$ can be found algorithmically.

Theorem 8.9 Suppose A is a $n \times d$ matrix with entries between 0 and 1. Then

$$\sigma_1(A) \ge d(A) \ge \frac{c\sigma_1(A)}{\log n \log d}$$

for some constant c. Furthermore, subsets S and T satisfying $d(S,T) \ge \frac{c\sigma_1(A)}{\log n \log d}$ may be found from the top singular vector of A.

Proof: Let S and T be the subsets of rows and columns that achieve d(A) = d(S, T). Consider a n-vector \mathbf{u} which is $\frac{1}{\sqrt{|S|}}$ on S and 0 elsewhere and a d-vector \mathbf{v} which is $\frac{1}{\sqrt{|T|}}$ on T and 0 elsewhere. Then,

$$\sigma_1(A) \ge \sum_{ij} u_i v_j a_{ij} = d(S, T) = d(A)$$

proves the first inequality.

To prove the second inequality, express $\sigma_1(A)$ in terms of the first left and right singular vectors \mathbf{x} and \mathbf{y} .

$$\sigma_1(A) = \mathbf{x}^T A \mathbf{y} = \sum_{i,j} x_i a_{ij} y_j, \qquad |\mathbf{x}| = |\mathbf{y}| = 1.$$

Since the entries of A are nonnegative, the components of the first left and right singular vectors must be all positive, that is, $x_i \geq 0$ and $y_j \geq 0$ for all i and j. To bound $\sum_{i,j} \mathbf{x}_i a_{ij} \mathbf{y}_j$, break the summation into $O(\log n \log d)$ parts. Each part corresponds to a given α and β and consists of all i such that $\alpha \leq x_i < 2\alpha$ and all j such that $\beta \leq y_i < 2\beta$. The $\log n \log d$ parts are defined by breaking the rows into $\log n$ blocks with α equal to

 $\frac{1}{2}\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, 2\frac{1}{\sqrt{n}}, 4\frac{1}{\sqrt{n}}, \ldots, 1$ and by breaking the columns into $\log d$ blocks with β equal to $\frac{1}{2}\frac{1}{\sqrt{d}}, \frac{1}{\sqrt{d}}, \frac{2}{\sqrt{d}}, \frac{4}{\sqrt{d}}, \ldots, 1$. The i such that $x_i < \frac{1}{2\sqrt{n}}$ and the j such that $y_j < \frac{1}{2\sqrt{d}}$ will be ignored at a loss of at most $\frac{1}{4}\sigma_1(A)$.

Since
$$\sum_{i} x_i^2 = 1$$
, the set $S = \{i | \alpha \le x_i < 2\alpha\}$ has $|S| \le \frac{1}{\alpha^2}$ and similarly, $T = \{j | \beta \le y_j \le 2\beta\}$ has $|T| \le \frac{1}{\beta^2}$. Thus

$$\sum_{\substack{i \\ \alpha \le x_i \le 2\alpha}} \sum_{\substack{j \\ \beta \le y_j \le 2\beta}} x_i y_j a_{ij} \le 4\alpha\beta A(S,T) \le 4\alpha\beta d(S,T) \sqrt{|S||T|} \le 4d(S,T) \le 4d(A).$$

From this it follows that $\sigma_1(A) \leq 4d(A) \log n \log d$ or $d(A) \geq \frac{c\sigma_1(A)}{\log n \log d}$ proving the second inequality. Note that in many cases, the nonzero values of x_i and y_j (after zeroing out the low entries) will only go from $\frac{1}{2}\frac{1}{\sqrt{n}}$ to $\frac{c}{\sqrt{n}}$ for x_i and $\frac{1}{2}\frac{1}{\sqrt{d}}$ to $\frac{c}{\sqrt{d}}$ for y_j , since the singular vectors are likely to be balanced given that a_{ij} are all between 0 and 1. In this case, there will be O(1) groups only and the log factors disappear.

Another measure of density is based on similarities. Recall that the similarity between objects represented by vectors (rows of A) is defined by their dot products. Thus, similarities are entries of the matrix AA^T . Define the average cohesion f(S) of a set S of rows of A to be the sum of all pairwise dot products of rows in S divided by |S|. The average cohesion of A is the maximum over all subsets of rows of the average cohesion of the subset.

Since the singular values of AA^T are squares of singular values of A, we expect f(A) to be related to $\sigma_1(A)^2$ and $d(A)^2$. Indeed it is. We state the following without proof.

Lemma 8.10
$$d(A)^2 \le f(A) \le d(A) \log n$$
. Also, $\sigma_1(A)^2 \ge f(A) \ge \frac{c\sigma_1(A)^2}{\log n}$.

f(A) can be found exactly using flow techniques as we will see later.

In this section, we described how to find a large global community. There is another question, that of finding a small local community including a given vertex. We will visit this question in Section 8.10.

8.9 Flow Methods

We defined notions of dense submatrices in Section 8.6. Here, we show that finding an induced subgraph (subgraph on a subset of vertices) of a graph with maximum average degree can be done by network flow techniques. This is simply maximizing d(S, S) of Section 8.6 over all subsets S of the graph. First consider the problem of finding a subset of vertices such that the induced subgraph has average degree at least λ for some parameter λ . Then do a binary search on the value of λ until the maximum λ for which there exists a subgraph with average degree at least λ is found.

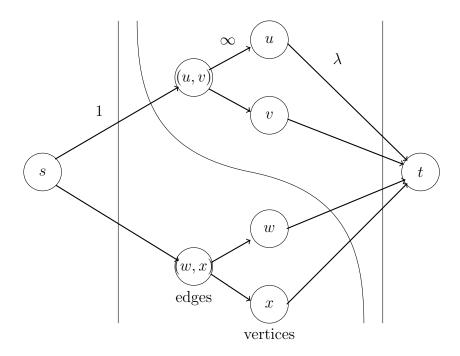


Figure 8.5: The directed graph H used by the flow technique to find a dense sugraph

Given a graph G in which one wants to find a dense subgraph, construct a directed graph H from the given graph and then carry out a flow computation on H. H has a node for each edge of the original graph, a node for each vertex of the original graph, plus two additional nodes s and t. There is a directed edge with cost one from s to each node corresponding to an edge of the original graph and a directed edge with infinite cost from each node corresponding to an edge of the original graph to the two nodes corresponding to the vertices the edge connects. Finally, there is a directed edge with cost λ from each node corresponding to a vertex of the original graph to t.

Notice there are three types of cut sets of the directed graph that have finite capacity. The first cuts all arcs from the source. It has capacity e, the number of edges of the original graph. The second cuts all edges into the sink. It has capacity λv , where v is the number of vertices of the original graph. The third cuts some arcs from s and some arcs into t. It partitions the set of vertices and the set of edges of the original graph into two blocks. The first block contains the source node s, a subset of the edges e_s , and a subset of the vertices v_s defined by the subset of edges. The first block must contain both end points of each edge in e_s ; otherwise an infinite arc will be in the cut. The second block contains t and the remaining edges and vertices. The edges in this second block either connect vertices in the second block or have one endpoint in each block. The cut set will cut some infinite arcs from edges not in e_s coming into vertices in v_s . However, these arcs are directed from nodes in the block containing t to nodes in the block containing s. Note that any finite cost cut that leaves an edge node connected to s must cut the two

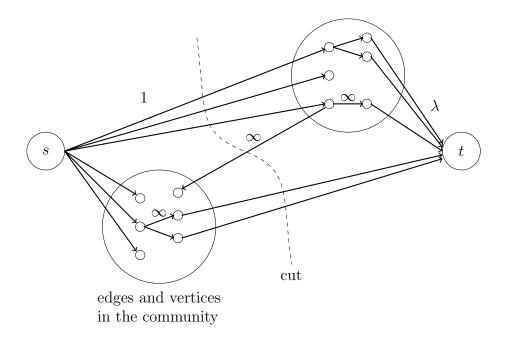


Figure 8.6: Cut in flow graph

related vertex nodes from t. Thus, there is a cut of cost $e - e_s + \lambda v_s$ where v_s and e_s are the vertices and edges of a subgraph. For this cut to be the minimal cut, the quantity $e - e_s + \lambda v_s$ must be minimal over all subsets of vertices of the original graph and the cost must be less than e and also less than λv .

If there is a subgraph with v_s vertices and e_s edges where the ratio $\frac{e_s}{v_s}$ is sufficiently large so that $\frac{e_S}{v_S} > \frac{e}{v}$, then for λ such that $\frac{e_S}{v_S} > \lambda > \frac{e}{v}$, $e_s - \lambda v_s > 0$ and $e - e_s + \lambda v_s < e$. Similarly $e < \lambda v$ and thus $e - e_s + \lambda v_s < \lambda v$. This implies that the cut $e - e_s + \lambda v_s$ is less than either e or λv and the flow algorithm will find a nontrivial cut and hence a proper subset. For different values of λ in the above range there maybe different nontrivial cuts.

Note that for a given density of edges, the number of edges grows as the square of the number of vertices and $\frac{e_s}{v_s}$ is less likely to exceed $\frac{e}{v}$ if v_S is small. Thus, the flow method works well in finding large subsets since it works with $\frac{e_S}{v_S}$. To find small communities one would need to use a method that worked with $\frac{e_S}{v_S^2}$ as the following example illustrates.

Example: Consider finding a dense subgraph of 1,000 vertices and 2,000 internal edges in a graph of 10^6 vertices and 6×10^6 edges. For concreteness, assume the graph was generated by the following process. First, a 1,000-vertex graph with 2,000 edges was generated as a random regular degree four graph. The 1,000-vertex graph was then augmented to have 10^6 vertices and edges were added at random until all vertices were of degree 12. Note that each vertex among the first 1,000 has four edges to other vertices among the first

1,000 and eight edges to other vertices. The graph on the 1,000 vertices is much denser than the whole graph in some sense. Although the subgraph induced by the 1,000 vertices has four edges per vertex and the full graph has twelve edges per vertex, the probability of two vertices of the 1,000 being connected by an edge is much higher than for the graph as a whole. The probability is given by the ratio of the actual number of edges connecting vertices among the 1,000 to the number of possible edges if the vertices formed a complete graph. $\frac{A(S,S)}{|S|^2}$?

$$p = \frac{e}{\left(\binom{v}{2}\right)} = \frac{2e}{v(v-1)}$$

For the 1,000 vertices, this number is $p = \frac{2 \times 2,000}{1,000 \times 999} \cong 4 \times 10^{-3}$. For the entire graph this number is $p = \frac{2 \times 6 \times 10^6}{10^6 \times 10^6} = 12 \times 10^{-6}$. This difference in probability of two vertices being connected should allow us to find the dense subgraph.

In our example, the cut of all arcs out of s is of cost 6×10^6 , the total number of edges in the graph, and the cut of all arcs into t is of cost λ times the number of vertices or $\lambda \times 10^6$. A cut separating the 1,000 vertices and 2,000 edges would have cost $6 \times 10^6 - 2,000 + \lambda \times 1,000$. This cut cannot be the minimum cut for any value of λ since $\frac{e_s}{v_s} = 2$ and $\frac{e}{v} = 6$, hence $\frac{e_s}{v_s} < \frac{e}{v}$. The point is that to find the 1,000 vertices, we have to maximize $A(S,S)/|S|^2$ rather than A(S,S)/|S|. Note that $A(S,S)/|S|^2$ penalizes large |S| much more and therefore can find the 1,000 node "dense" subgraph.

8.10 Linear Programming Formulation

It is difficult to formulate a clustering problem such as k-means as a linear or convex program. This is because variables are needed to determine which point is included in each cluster. The cluster centers depend on these variables. Finally, the distance to the cluster center is a nonlinear function. Problems where the cluster centers are restricted to be in a finite given set (possibly the set of points themselves) are easier to formulate. It is not difficult to see that for k-means, restricting the cluster centers to be one of the points only changes the sum of distance squared to the nearest cluster center by a factor of four. Since linear programming and convex programming formulations come only within constant factors, this is fine.

In this section, we are given a set of n points to be clustered and a set of m points (possibly the same set) which can serve as cluster centers. We are also given the distance d_{ij} between the i^{th} point and the j^{th} center. We are to open k of the potential centers, so as to minimize the sum of distances of the n points to their nearest cluster centers. We introduce 0-1 variables, x_{ij} , $1 \le i \le n$, $1 \le j \le m$, where $x_{ij} = 1$ if and only if the i^{th} point is assigned to the j^{th} center. We also have 0-1 variables, y_j , $1 \le j \le m$, where $y_j = 1$ if and only if the j^{th} point is chosen as a center. Then, we write the integer program:

Minimize $\sum_{ij} d_{ij} x_{ij}$ subject to

$$\sum_{j=1}^{m} y_j = k$$

$$\sum_{j=1}^{m} x_{ij} = 1 \quad \text{for } 1 \le i \le n$$

$$x_{ij} \le y_j \quad \text{for } 1 \le i \le n, \ 1 \le j \le m,$$

$$0 \le x_{ij}, \ y_i \le 1; \quad \text{integers.}$$

The first constraint ensures that exactly k centers are opened. The second ensures that each point is assigned to one center and the third ensures that we only assign points to open centers. Finally, since we are minimizing, the integer program will automatically assign each point to its nearest center. The integer constraints make the problem hard. A standard technique is to start by solving the corresponding linear programming after relaxing (discarding) the integer constraints. This may open fractional centers and may make fractional assignments. Again each i will be assigned to the nearest center to the extent it is open; then the residual to the next nearest center to the extent it is open, etc. until it is fully assigned. Rounding the fractions so as to get a near optimal solution can be done, but this is very involved and the subject of current research.

8.11 Finding a Local Cluster Without Examining the Whole graph

If one wishes to find the community containing a vertex v in a large graph with say a billion vertices, one would like to find the community in time proportional to the size of the community and independent of the size of the graph. Thus, we would like local methods that do not inspect the entire graph but only the neighborhood around the vertex v. We now give several such algorithms.

Breadth-First Search

The simplest method is to do a breadth first search starting at v. Clearly if there is a small connected component containing v, we will find it in time depending only on the size (number of edges) of the component. In a more subtle situation, each edge may have a weight that is the similarity between the two end points. If there is a small cluster C containing v, with each outgoing edge from C to \bar{C} having weight less than some ε , C could clearly also be found by breadth-first search in time proportional to the size of C. However, in general, it is unlikely that the cluster will have such obvious telltale signs of its boundary and one needs more complex techniques, some of which we describe now.

By max flow

Given a vertex v in a directed graph, we want to find a small set S of vertices whose boundary is a set of a few out going edges. Suppose we are looking for a set S whose boundary is of size at most b and whose cardinality is at most k. Clearly, if $\deg(v) < b$ then the problem is trivial, so assume $\deg(v) \ge b$.

Think of a flow problem where v is the source. Put a capacity of one on each edge of the graph. Create a new vertex that is the sink and add an edge of capacity α from each vertex of the original graph to the new sink vertex, where $\alpha = b/k$. If a community of size at most k with boundary at most k containing k exists, then there will be a cut of size at most k + b = 2b, since the cut will have k edges from the community to the sink and k edges from the community to the remainder of the graph. Conversely, if there is a cut of size at most k vertices since each vertex has an edge to the sink with capacity k. Thus, to come within a factor of two of the answer, all one needs to do is determine whether there is a cut of size at most k. If the flow algorithm can do more than k flow augmentations, then the maximum flow and hence the minimum cut is of size more than k. If not, the minimum cut is of size at most k.

In executing the flow algorithm one finds an augmenting path from source to sink and augments the flow. Each time a new vertex not seen before is reached, there is an edge to the sink and the flow can be augmented by α directly on the path from v to the new vertex to the sink. So the amount of work done is a function of b and k, not the total number of vertices in the graph.

Sparsity and Local communities

Suppose we want to find if a given vertex is in a local community. One natural definition of a local community is a locally smallest set whose sparsity is small. For a more formal description, recall some definitions from Section 8.4.5. Suppose P is a stochastic matrix (a matrix with nonnegative entries and row sums equal to one). In this context, P may be obtained from the adjacency matrix A of the graph by dividing each entry by its row sum. If the graph is undirected, A would have been symmetric. But we also allow directed graphs, where A is not necessarily symmetric. In any case, we can now forget A and just deal with P. We assume that P is time-reversible, namely, there is a vector π such that

$$\pi_i p_{ij} = \pi_j p_{ji}$$
.

If P came from an undirected graph, then setting π_i equal to the degree of vertex i, satisfies the above equation. Normalizing π to sum to one, gives the steady state probabilities, if they exist, for a random walk on the graph. One sees this by noting that $\pi_i p_{ij}$ is the probability of stepping from i to j starting with distribution π . Time reversibility implies that the flows from i to j and j to i are equal. Since the flow out of each node equals

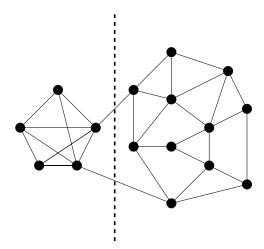


Figure 8.7: Example of a highly connected community of low sparsity.

the flow in when the probability distribution of being at a node is π , the distribution π is maintained and is the steady state distribution.

Recall the definition of sparsity, $\Phi(S) = \frac{\sum\limits_{i \in S, j \in \bar{S}} a_{ij}}{\sum\limits_{i \in S} d_i}$, from Section 8.4.5. One definition of a local community is a low sparsity subset S of vertices in which every proper subset T has high connectivity to the rest of S. The schematic picture is given in Figure 8.7

Say we have a subset S with at most half of the probability, with a small number of edges leaving S so that the sparsity is less than some number α . Further suppose that for any subset T of S where T has less than half the probability of S, the sparsity of T with respect to S is large, say β where $\beta > \alpha$. That is,

$$\Phi(S) \le \alpha;$$

$$\forall T \subseteq S \text{ with } \pi(T) \le \pi(S)/2, \sum_{i \in T; j \in S \setminus T} \pi_i p_{ij} \ge \beta$$
(8.2)

A condition like $\pi(T) \leq \pi(S)/2$ is needed since if T is most of S, then its sparsity with respect to S would be very low. Given a starting vertex v in S satisfying (8.2), we would like to discover S by a random walk. Finding S exactly is difficult. If the random walk started at a frontier vertex in S, it is intuitively clear that we cannot hope to discover S, since the random walk is likely to exit S soon. But if the walk starts in the interior of S will we at some stage discover S? We saw in Section 8.4.5 **DID WE? - Yes** that if the random wlak runs for a number of steps which is $O(1/\Phi^2)$, where Φ is the sparsity of the whole graph, then it would be close to the steady state π , i.e., by then, the probability would have spread not only over S, but also \bar{S} . This means that it would be difficult to identify S from long-term probabilities. But intuitively, it would seem that if the walk

ran for a number of steps that is at least $\Omega(1/\beta^2)$ and at most $O(1/\alpha)$, it should be close to the steady state on S alone. Since at most α mass escapes from S to \bar{S} in each step (as we will show formally below), most of the mass is still in S. This means, after $\Omega\left(\frac{1}{\beta^2}\right)$ steps, we should be able to discover S. The following theorem says that indeed for a large subset S_0 of S, where large is measured by π , if we start a random walk at a vertex in S_0 , then the intuition holds that after a certain number of steps, we approximately discover S as the set of vertices with high probability mass.

The theorem states that the probability of the Markov chain on \bar{S} overall is small and secondly, that on S, it is close to the steady state probabilities. A question in applying the theorem is how do we know S_0 ? Of course, we do not know S or S_0 . But by trying a number of starts at different vertices close to the given vertex v (whose local community we want), we are likely to find S. Note that we cannot guarantee that starting from v itself will do, since v may be a frontier vertex in S and random walks started at v will easily stray into \bar{S} . The intuition is that for starting vertices deep inside S, this cannot happen since the sparsity of S as a whole is low.

The theorem itself does not guarantee a fast algorithm with time dependent only on |S| rather than the total number of vertices. But we can use a truncation method. Instead of running the Markov chain on the whole graph, we keep track of the probability distribution at each step, except for vertices whose probability is below a threshold value ε . We set the probability of these vertices to zero. Thus, the number of vertices with nonzero probability, which is all we keep track of, is small. We do not prove this here.

Theorem 8.11 Let S be a subset of vertices satisfying (8.2) with $\alpha < O(\beta^2)$. Let $t_0 \in \Omega(1/\beta^2)$. There is a subset S_0 of S with $\pi(S_0) \ge \pi(S)/2$, so that the Markov chain with transition probability matrix P, started at any $i \in S_0$, after t_0 steps has

- 1. probability at most 0.1 of being in \bar{S} , and
- 2. the set S_i of vertices j in S for which the probability of being at j is at least $0.9\frac{\pi_j}{\pi(S)}$ satisfies $\pi(S_i) \geq 0.99\pi(S)$.

Proof: Let f(i,t) be the probability that at time t, the Markov chain starting at vertex i in S takes a step from a vertex in S to a vertex in \bar{S} . We would like to upper bound f(i,t). While this is difficult, observe that had the walk started in the steady state distribution π , then it would remain in the steady state distribution and so the probability that it would step from a vertex in S to a vertex in \bar{S} at time t is precisely $\sum_{i \in S} \sum_{j \in \bar{S}} \pi_i p_{ij} = \Phi(S)\pi(S)$.

By linearity, this probability is $\sum_{i \in S} \pi_i f(i, t)$, so we get

$$\sum_{i \in S} \pi_i f(i, t) = \Phi(S) \pi(S) \le \alpha \pi(S) \le \alpha$$

which implies that $\sum_{t=1}^{t_0} \sum_{i \in S} \pi_i f(i,t) \leq \alpha t_0 \pi(S) \leq \varepsilon_1 \pi(S)$ where $\varepsilon_1 \geq \alpha t_0$ is a small positive constant.

For $i \in S$, let f_i be the probability that when the chain is started at i, it steps into \bar{S} at least once within t_0 steps. Let $S_0 = \{i \in S | f_i \leq 2\varepsilon_1\}$. We first show that $\pi(S_0) \leq \pi(S)/2$. For $i \in S \setminus S_0$, $\frac{f_i}{2\varepsilon_1} > 1$. Thus the probability that the chain will have left S_0 is

$$\pi\left(S\backslash S_{0}\right) = \sum_{i\in S\backslash S_{0}} \pi_{i} \leq \frac{1}{2\varepsilon_{1}} \sum_{i\in S\backslash s_{0}} \pi_{i}f \leq \frac{1}{2\varepsilon_{1}} \sum_{i\in S\backslash s_{0}} \pi_{i}f_{i} + \frac{1}{2\varepsilon_{1}} \sum_{i\in S_{0}} \pi_{i}f_{i} \leq \frac{1}{2\varepsilon_{1}} \sum_{i\in S} \pi_{i}f_{i}$$

$$\leq \frac{1}{2\varepsilon_{1}} \sum_{i\in S} \sum_{t=1}^{t_{0}} \pi_{i}f(i,t) \leq \pi(S)/2$$

yielding $\pi(S \setminus S_0) \leq \pi(S)/2$, which implies that $\pi(S_0) \geq \pi(S)/2$. Clearly, this $S_0 = \{i \in S | f_i \leq 2\varepsilon_i\}$ satisfies (1) with a suitable choice of the ε_i constants.

Next, we show that the set S_i of vertices j in S for which the probability of being at j is at least $0.9 \frac{\pi_j}{\pi(S)}$ satisfies $\pi(S_i) \geq 0.99\pi(S)$. Assume the chain starts in some $i \in S_0$. For $j \in S$, let g_{ij} be the probability that we never step into \bar{S} and are at node j after t_0 steps. $\sum_{j \in S} g_{ij}$ is the probability that started at i, we do not step into \bar{S} . Since the probability that we step into \bar{S} is less than $\varepsilon \pi(S) < \varepsilon$, $\sum_{i \in S} g_{ij} \geq 1 - \varepsilon_1 \quad \forall i \in S_0$ (10.9.2)

In what follow replace A BY P and LC – (Yes done) AND ALSO WE NEED TO STATE WE ARE RESTRICTING A TO S SOMEHOW.—- the tilde is the restriction to S

We now get an upper bound on g_{ij} . Let \tilde{P} be the transition probability matrix of a Markov chain with states S. Define $\tilde{p}_{ii} = 1 - \sum_{j \neq i} p_{ij}$. That is, adjust the diagonal elements so that \tilde{P} has row sums equal to one. We see that \tilde{P} also satisfies the time-reversibility condition with the same vector π , now restricted to S. Further, the sparsity of \tilde{P} is at least β by (8.9.1). So, by Theorem ??? of Chapter 5 (Random Walks), $(\tilde{P}^t)_{ij} \approx \frac{\pi_j}{\pi(S)}$ in the sense that for all i, $\sum_{j \in S} \left| (\tilde{P})_{ij}^t - \frac{\pi_j}{\pi(S)} \right| \leq \varepsilon_2$ for a suitable constant ε_2 , which implies that the sum of the positive terms $\sum_{j \in S} \left((\tilde{P})_{ij}^t - \frac{\pi_j}{\pi(S)} \right)^+ \leq \varepsilon_2$ for all i. But, it is easy to see that $(\tilde{P}^t)_{ij}$ is greater than or equal to g_{ij} , since for every path of length t_0 in the chain, there is a corresponding path with product of \tilde{P} entries which is no less. Thus,

$$\sum_{i \in S} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right)^+ \le \varepsilon_2. \text{ But}$$

$$\sum_{j \in S} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right) = \sum_{j \in S} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right)^+ + \sum_{j \in S} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right)^-$$

and also from (8.9.2),

$$\sum_{i \in S} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right) \ge 1 - 2\varepsilon_1 - 1 = -2\varepsilon_1$$

So, $\sum_{j \in S} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right)^- \ge -\varepsilon_3$. Now, define BAD $_i = \{ j \in S : g_{ij} \le (1 - 300\varepsilon_3) \frac{\pi_j}{\pi(S)} \}$. So, for j in BAD $_i$, we have $(g_{ij} - (\pi_j/\pi(S))^- \le -300\varepsilon_3\pi_j/\pi(S)$. Thus,

$$\sum_{j \in \text{BAD}_i} \frac{\pi_j}{\pi(S)} \le -\frac{1}{300\varepsilon_3} \sum_{j \in \text{BAD}_i} \left(g_{ij} - \frac{\pi_j}{\pi(S)} \right)^- \le 0.01.$$

So, with $S_i = S \setminus BAD_i$, we get (ii), finishing the proof.

Modularity clustering

Another way to partition a graph into communities is based on the concept of modularity. The method is popular for small graphs. Consider the partition of the vertices of a graph into communities. The modularity of the partition is defined to be the fraction of edges that lie within communities minus the expected number of edges that lie within communities in a random graph with the same degree distribution. Let A be the adjacency matrix of a graph, m the total number of edges, d_v the degree of vertex v, and let i index the communities defined by a partition of the vertices. Then, the modularity is given by

$$Q = \frac{1}{2m} \sum_{i} \sum_{v,w \in i} a_{vw} - \sum_{i} \sum_{v,w \in i} \frac{d_v}{2m} \frac{d_w}{2m}$$

Let e_{ij} denote the fraction of the total set of edges that connect communities i and j and let a_i denote the fraction of edges with ends in community i. Then

$$e_{ij} = \frac{1}{2m} \sum_{\substack{v \in i \\ w \in j}} a_{vw}$$

and

$$a_i = \frac{1}{2m} \sum_{v \in i} d_v$$

Write

$$Q = \sum_{i} \sum_{v,w \in i} \left(\frac{1}{2m} a_{vw} - \frac{d_v}{2m} \frac{d_w}{2m} \right)$$
$$= \sum_{i} \left(e_{ij} - a_i^2 \right)$$

The algorithm for finding communities works as follows. Start with each vertex in a community. Repeatedly merge the pair of communities that maximizes the change in Q. This can be done in time $O\left(m\log^2 n\right)$ where n is the number of vertices in the graph and m is the number of edges where $m \geq n$. The algorithm works well on small graphs but is inefficient for graphs with even a few thousand vertices.

8.12 Statistical Clustering

8.13 Axioms for Clustering

Each clustering algorithm tries to optimize some criteria, like the sum of squared distances to the nearest cluster center, over all possible clustering's. We have seen many different optimization criteria in this chapter and many more are used. Now, we take a step back and ask what some desirable properties of a clustering criterion are and if there are criteria satisfying these properties. The first result we present is negative. We present three seemingly desirable properties of a measure, and then show that no measure satisfies them. Next we argue that these requirements are too stringent and under more reasonable requirements, a slightly modified form of the sum of Euclidean distance squared between all pairs of points inside the same cluster is indeed a measure satisfying the desired properties.

8.13.1 An Impossibility Result

Let A(d) denote the optimal clustering found by the clustering algorithm A using distance function d on a set S. The clusters of the clustering A(d) form a partition Γ of S.

The first desirable property of a clustering algorithm is scale invariance. A clustering algorithm A is scale invariant if for any $\alpha > 0$, $A(d) = A(\alpha d)$. That is, multiplying all distances by some scale factor does not change the optimal clustering. In general, there could be ties for what the algorithm returns; in that case, we adopt the convention that $A(d) = A(\alpha d)$ really means for any clustering returned by A on distance d, it can also be returned by A on distance d.

A clustering algorithm A is rich (full/complete) if for every partitioning Γ there exists a distance function d such that $A(d) = \Gamma$. That is, for any desired partitioning, we can find a set of distances so that the clustering algorithm returns the desired partitioning.

A clustering algorithm is *consistent* if increasing the distance between points in different clusters and reducing the distance between points in the same cluster does not change the clusters produced by the clustering algorithm.

If a clustering algorithm is consistent and $A(d) = \Gamma$, one can find a new distance function d' such that $A(d') = \Gamma$ where there are only two distances a and b. Here a is the distance between points within a cluster and b is the distance between points in

different clusters. By consistency, we can reduce all distances within clusters and increase all distances between clusters there by getting two distances a and b with a < b where a is the distance between points within a cluster and b is the distance between points in different clusters.

There exist natural clustering algorithms satisfying any two of the three axioms. The single link clustering algorithm starts with each point in a cluster by itself and then merges the two clusters that are closest. The process continues until some stopping condition is reached. One can view the process as the points being vertices of a graph and edges being labeled by the distances between vertices. One merges the two vertices that are closest and merges parallel edges taking the distance of the merged edge to be the minimum of the two distances.

Theorem 8.12

- 1. The single link clustering algorithm with the k-cluster stopping condition, stop when there are k clusters, satisfies scale-invariance and consistency. We do not get richness since we only get clustering's with k clusters.
- 2. The single link clustering algorithm with scale α stopping condition satisfies scale invariance and richness. The scale α stopping condition is to stop when the closest pair of clusters is of distance greater than or equal to αd_{max} where d_{max} is the maximum pair wise distance. Here we do not get consistency. If we select one distance between clusters and increase it significantly until it becomes d_{max} and in addition αd_{max} exceeds all other distances, the resulting clustering has just one cluster containing all of the points.
- 3. The single linkage with the distance r stopping condition, stop when the inter-cluster distances are all at least r, satisfies richness and consistency; but not scale invariance.

Proof: (1) Scale-invariance is easy to see. If one scales up all distances by a factor, then at each point in the algorithm, the same pair of clusters will be closest. The argument for consistency is more subtle. Since edges inside clusters of the optimal (final) clustering can only be decreased and since edges between clusters can only be increased, the edges that led to merges between any two clusters are less than any edge between the final clusters. Since the final number of clusters is fixed, these same edges will cause the same merges unless the merge has already occurred due to some other edge that was inside a final cluster having been shortened even more. No edge between two final clusters can cause a merge before all the above edges have been considered. At this time the final number of clusters has been reached and the process of merging has stopped.

(2) and (3) are straight forward.

Next, we show that no clustering algorithm can satisfy all three axioms. A distance function d, (a-b)-conforms to a partition Γ if all points in a cluster are within distance a of each other and all points in distinct clusters are at least distance b apart. For a clustering algorithm A, the pair of numbers (a,b) is said to force the partition Γ if all distances functions d that (a-b) conform to Γ have $A(d) = \Gamma$.

Associated with a clustering algorithm is a collection of allowable clustering's it can produce using different distance functions. We begin with a theorem stating that scale invariance and consistency imply that no allowable clustering can be a refinement of another allowable clustering.

Theorem 8.13 If a clustering algorithm satisfies scale-invariance and consistency, then no two clustering's, one of which is a refinement of the other, can both be optimal clustering's returned by the algorithm.

Proof: Suppose that the range of the clustering algorithm A contains two clustering's, Γ_0 and Γ_1 where Γ_0 is a refinement of Γ_1 . Modify the distance functions giving rise to Γ_0 and Γ_1 so that there are only two distinct distances a_0 and b_0 for Γ_0 and a_1 and b_1 for Γ_1 . Points within a cluster of Γ_0 are distance a_0 apart and points between clusters of Γ_0 are distance b_0 apart. The distances a_1 and b_1 play similar roles for Γ_1 .

Let a_2 be any number less than a_1 and choose ε such that $0 < \varepsilon < a_0 a_2 b_0^{-1}$. Let d be a new distance function where

$$d\left(i,j\right) = \left\{ \begin{array}{l} \varepsilon \text{ if } i \text{ and } j \text{ are in the same cluster of } \Gamma_0 \\ a_2 \text{ if } i \text{ and } j \text{ are in differnt clusers of } \Gamma_0 \text{ but the same cluster of } \Gamma_1 \\ b_1 \text{ if } i \text{ and } j \text{ are in different clusters of } \Gamma_1 \end{array} \right.$$

From $a_0 < b_0$ it follows that $a_0b_0^{-1} < 1$. Thus $\varepsilon < a_0a_2b_0^{-1} < a_2 < a_1$. Since both ε and a_2 are less than a_1 , it follows by consistency that $A(d) = \Gamma_1$. Let $\alpha = b_0a_2^{-1}$. Since $\varepsilon < a_0a_2b_0^{-1}$ and $a_2 < a_1 < b_1$, which implies $a_2^{-1} > a_1^{-1} > b_1^{-1}$, it follows that

$$\alpha d\left(i,j\right) = \left\{ \begin{array}{ll} b_0 a_2^{-1} \varepsilon < b_0 a_2^{-1} a_0 a_2 b_0^{-1} = a_0 & \text{if } i \text{ and } j \text{ are in the same cluster of } \Gamma_0 \\ b_0 a_2^{-1} a_2 = b_0 & \text{if } i \text{ and } j \text{ are in differnt clusers of } \Gamma_0 \\ b_0 a_2^{-1} b_1 > b_0 b_1^{-1} b_1 = b_0 & \text{if } i \text{ and } j \text{ are in different clusters of } \Gamma_1 \\ \end{array} \right.$$

Thus, by consistency $A(\alpha d) = \Gamma_0$. But by scale invariance $A(\alpha d) = A(d) = \Gamma_1$, a contradiction.

Corollary 8.14 For $n \geq 2$ there is no clustering function f that satisfies scale-invariance, richness, and consistency.

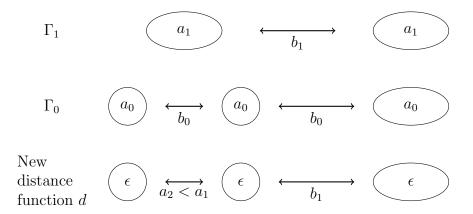


Figure 8.8: Illustration of the sets Γ_0 , Γ_1 , and those for the distance function d.

It turns out that any collection of clustering's in which no clustering is a refinement of any other clustering in the collection is the range of a clustering algorithm satisfying scale invariance and consistency. To demonstrate this, we use the sum of pairs clustering algorithm. Given a collection of clustering's, the *sum of pairs clustering* algorithm finds the clustering that minimizes the sum of all distances between points in the same cluster over all clustering's in the collection.

Theorem 8.15 Every collection of clustering's in which no clustering is the refinement of another is the range of a clustering algorithm A satisfying scale invariance and consistency.

Proof: We first show that the sum of pairs clustering algorithm satisfies scale invariance and consistency. Then we show that every collection of clustering's in which no cluster is a refinement of another can be achieved by a sum of pairs clustering algorithm.

Let A be the sum of pairs clustering algorithm. It is clear that A satisfies scale invariance since multiplying all distances by a constant, multiplies the total cost of each cluster by a constant and hence the minimum cost clustering is not changed.

To demonstrate that A satisfies consistency let d be a distance function and Γ the resulting clustering. Increasing the distance between pairs of points in different clusters of Γ does not affect the cost of Γ . If we reduce distances only between pairs of points in clusters of Γ then the cost of Γ is reduced as much or more than the cost of any other clustering. Hence Γ remains the lowest cost clustering.

Consider a collection of clustering's in which no cluster is a refinement of another. It remains to show that every clustering in the collection is in the range of A. In sum of pairs clustering, the minimum is over all clustering's in the collection. We now show for any clustering Γ how to assign distances between pairs of points so that A returns the desired



Figure 8.9: Illustration of the objection to the consistency axiom. Reducing distances between points in a cluster may suggest that the cluster be split into two.

clustering. For pairs of points in the same cluster assign a distance of $1/n^3$. For pairs of points in different clusters assign distance one. The cost of the clustering Γ is less than one. Any clustering that is not a refinement of Γ has cost at least one. Since there are no refinements of Γ in the collection it follows that Γ is the minimum cost clustering.

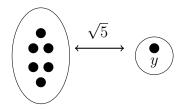
Note that one may question both the consistency axiom and the richness axiom. The following are two possible objections to the consistency axiom. Consider the two clusters in Figure 8.8. If one reduces the distance between points in cluster B, they might get an arrangement that should be three clusters instead of two.

The other objection, which applies to both the consistency and the richness axioms, is that they force many unrealizable distances to exist. For example, suppose the points were in Euclidean d space and distances were Euclidean. Then, there are only nd degrees of freedom. But the abstract distances used here have $O(n^2)$ degrees of freedom since the distances between the $O(n^2)$ pairs of points can be specified arbitrarily. Unless d is about n, the abstract distances are too general. The objection to richness is similar. If for n points in Euclidean d space, the clusters are formed by hyper planes (each cluster may be a Voronoi cell or some other polytope), then as we saw in the theory of VC dimensions (Section ??) there are only $\binom{n}{d}$ interesting hyper planes each defined by d of the n points. If k clusters are defined by bisecting hyper planes of pairs of points, there are only n^{dk^2} possible clustering's rather than the 2^n demanded by richness. If d and k are significantly less than n, then richness is not reasonable to demand. In the next section, we will see a possibility result to contrast with this impossibility theorem.

The k-means clustering algorithm is one of the most widely used clustering algorithms. We now show that any centroid based algorithm such as k-means does not satisfy the consistency axiom.

Theorem 8.16 A centroid based clustering such as k-means does not satisfy the consistency axiom.

Proof: The cost of a cluster is $\sum_{i} (\mathbf{x_i} - \mathbf{u})^2$, where u is the centroid. An alternative way to compute the cost of the cluster if the distances between pairs of points in the cluster are known is to compute $\frac{1}{n} \sum_{i \neq j} (\mathbf{x_i} - \mathbf{x_j})^2$ where n is the number of points in the cluster. For a proof see Lemma 8.3. Consider seven points, a point \mathbf{y} and two sets of three points each,



All interpoint distances of $\sqrt{2}$

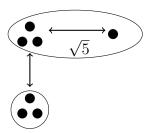


Figure 8.10: Example illustrating k-means does not satisfy the consistency axiom.

called X_0 and X_1 . Let the distance from \mathbf{y} to each point in $X_0 \cup X_1 \text{be}\sqrt{5}$ and let all other distances between pairs of points be $\sqrt{2}$. These distances are achieved by placing each point of X_0 and X_1 a distance one from the origin along a unique coordinate and placing \mathbf{y} at distance two from the origin along another coordinate. Consider a clustering with two clusters (see Figure 8.9). The cost depends only on how many points are grouped with \mathbf{y} . Let that number be m. The cost is

$$\frac{1}{m+1} \left[2 \binom{m}{2} + 5m \right] + \frac{2}{6-m} \binom{6-m}{2} = \frac{8m+5}{m+1}$$

which has its minimum at m = 0. That is, the point **y** is in a cluster by itself and all other points are in a second cluster.

If we now shrink the distances between points in X_0 and points in X_1 to zero, the optimal clustering changes. If the clusters were $X_0 \cup X_1$ and \mathbf{y} , then the distance would be $9 \times 2 = 18$ whereas if the clusters are $X_0 \cup \{\mathbf{y}\}$ and X_1 , the distance would be only $3 \times 5 = 15$. Thus, the optimal clustering is $X_0 \cup \{\mathbf{y}\}$ and X_1 . Hence k-means does not satisfy the consistency axiom since shrinking distances within clusters changes the optimal clustering.

5 Relaxing the axioms

Given that no clustering algorithm can satisfy scale invariance, richness, and consistency, one might want to relax the axioms in some way. Then one gets the following results.

- 1. Single linkage with a distance stopping condition satisfies a relaxed scale-invariance property that states that for $\alpha > 1$, then $f(\alpha d)$ is a refinement of f(d).
- 2. Define refinement consistency to be that shrinking distances within a cluster or expanding distances between clusters gives a refinement of the clustering. Single linkage with α stopping condition satisfies scale invariance, refinement consistency and richness except for the trivial clustering of all singletons.

8.13.2 A Satisfiable Set of Axioms

In this section, we propose a different set of axioms that are reasonable for distances between points in Euclidean space and show that the clustering measure, the sum of squared distances between all pairs of points in the same cluster, slightly modified, is consistent with the new axioms. We assume through the section that points are in Euclidean d-space. Our three new axioms follow.

We say that a clustering algorithm satisfies the *consistency condition* if, for the clustering produced by the algorithm on a set of points, moving a point so that its distance to any point in its own cluster is not increased and its distance to any point in a different cluster is not decreased, then the algorithm returns the same clustering after the move.

Remark: Although it is not needed in the sequel, it is easy to see that for an infinitesimal perturbation dx of x, the perturbation is consistent if and only if each point in the cluster containing x lies in the half space through x with dx as the normal and each point in a different cluster lies in the other half space.

An algorithm is *scale-invariant* if multiplying all distances by a positive constant does not change the clustering returned.

An algorithm has the *richness* property if for any set K of k distinct points in the ambient space, there is some placement of a set S of n points to be clustered so that the algorithm returns a clustering with the points in K as centers. So there are k clusters, each cluster consisting of all points of S closest to one particular point of K.

We will show that the following algorithm satisfies these three axioms.

Balanced k-means algorithm

Among all partitions of the input set of n points into k sets, each of size n/k, return the one that minimizes the sum of squared distances between all pairs of points in the same cluster.

Theorem 8.17 The balanced k-means algorithm satisfies the consistency condition, scale invariance, and the richness property.

Proof: Scale invariance is obvious. Richness is also easy to see. Just place n/k points of S to coincide with each point of K. To prove consistency, define the *cost* of a cluster T to be the sum of squared distances of all pairs of points in T.

Suppose S_1, S_2, \ldots, S_k is an optimal clustering of S according to the balanced k-means algorithm. Move a point $x \in S_1$ to z so that its distance to each point in S_1 is non increasing and its distance to each point in S_2, S_3, \ldots, S_k is non decreasing. Suppose T_1, T_2, \ldots, T_k is an optimal clustering after the move. Without loss of generality assume $z \in T_1$. Define $\tilde{T}_1 = (T_1 \setminus \{z\}) \cup \{x\}$ and $\tilde{S}_1 = (S_1 \setminus \{x\}) \cup \{z\}$. Note that $\tilde{T}_1, T_2, \ldots, T_k$ is a clustering before the move, although not necessarily an optimal clustering. Thus

$$\operatorname{cost}\left(\tilde{T}_{1}\right) + \operatorname{cost}\left(T_{2}\right) + \dots + \operatorname{cost}\left(T_{k}\right) \geq \operatorname{cost}\left(S_{1}\right) + \operatorname{cost}\left(S_{2}\right) + \dots + \operatorname{cost}\left(S_{k}\right).$$

If
$$cost(T_1) - cost(\tilde{T}_1) \ge cost(\tilde{S}_1) - cost(S_1)$$
 then

$$cost(T_1) + cost(T_2) + \cdots + cost(T_k) \ge cost(\tilde{S}_1) + cost(S_2) + \cdots + cost(S_k).$$

Since T_1, T_2, \ldots, T_k is an optimal clustering after the move, so also must be $\tilde{S}_1, S_2, \ldots, S_k$ proving the theorem.

It remains to show that $\cot(T_1) - \cot(\tilde{T}_1) \ge \cot(\tilde{S}_1) - \cot(S_1)$. Let u and v stand for elements other than x and z in S_1 and T_1 . The terms $|u-v|^2$ are common to T_1 and \tilde{T}_1 on the left hand side and cancel out. So too on the right hand side. So we need only prove

$$\sum_{u \in T_1} (|z - u|^2 - |x - u|^2) \ge \sum_{u \in S_1} (|z - u|^2 - |x - u|^2).$$

For $u \in S_1 \cap T_1$, the terms appear on both sides, and we may cancel them, so we are left to prove

$$\sum_{u \in T_1 \setminus S_1} (|z - u|^2 - |x - u|^2) \ge \sum_{u \in S_1 \setminus T_1} (|z - u|^2 - |x - u|^2)$$

which is true because by the movement of x to z, each term on the left hand side is non negative and each term on the right hand side is non positive.

8.14 Exercises

Clustering
Some Clustering Examples
A Simple Greedy Algorithm for k-clustering

Exercise 8.1 Construct examples where using distances instead of distance squared gives bad results for Gaussian densities. For example, pick samples from two 1-dimensional unit variance Gaussians, with their centers 10 units apart. Cluster these samples by trial and error into two clusters, first according to k-means and then according to the k-median criteria. The k-means clustering should essentially yield the centers of the Gaussians as cluster centers. What cluster centers do you get when you use the k-median criterion?

Exercise 8.2 Let v = (1,3). What is the L_1 norm of v? The L_2 norm? The square of the L_1 norm?

Exercise 8.3 Show that in 1-dimension, the center of a cluster that minimizes the sum of distances of data points to the center is in general not unique. Suppose we now require the center also to be a data point; then show that it is the median element (not the mean). Further in 1-dimension, show that if the center minimizes the sum of squared distances to the data points, then it is unique.

The k-means Clustering Algorithm Spectral Clustering Significance of a Given Clustering

Exercise 8.4 The simple greedy algorithm of Section 8.2 assumes that we know the clustering radius r. Suppose we do not. Describe how we might arrive at the correct r?

Exercise 8.5 For the k-median problem, show that there is at most a factor of two ratio between the optimal value when we either require all cluster centers to be data points or allow arbitrary points to be centers.

Exercise 8.6 For the k-means problem, show that there is at most a factor of four ratio between the optimal value when we either require all cluster centers to be data points or allow arbitrary points to be centers.

Exercise 8.7 Consider clustering points in the plane according to the k-median criterion, where cluster centers are required to be data points. Enumerated all possible clustering's and select the one with the minimum cost. The number of possible ways of labeling n points, each with a label from $\{1, 2, ..., k\}$ is k^n which is prohibitive. Show that we can find the optimal clustering in time at most a constant times $\binom{n}{k} + k^2$. Note that $\binom{n}{k} \leq n^k$ which is much smaller than k^n when k << n.

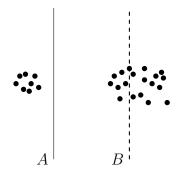


Figure 8.11: insert caption

Exercise 8.8 Suppose in the previous exercise, we allow any point in space (not necessarily data points) to be cluster centers. Show that the optimal clustering may be found in time at most a constant times n^{2k^2} .

Exercise 8.9 Corollary 8.3 shows that for a set of points $\{a_1, a_2, \ldots, a_n\}$, there is a unique point x, namely their centroid, which minimizes $\sum_{i=1}^{n} |a_i - x|^2$. Show examples where the x minimizing $\sum_{i=1}^{n} |a_i - x|$ is not unique. (Consider just points on the real line.) Show examples where the x defined as above are far apart from each other.

Exercise 8.10 Let $\{a_1, a_2, \ldots, a_n\}$ be a set of unit vectors in a cluster. Let $c = \frac{1}{n} \sum_{i=1}^{n} a_i$ be the cluster centroid. The centroid c is not in general a unit vector. Define the similarity between two points \mathbf{a}_i and \mathbf{a}_j as their dot product. Show that the average cluster similarity $\frac{1}{n^2} \sum_{i,j} a_i a_j^T$ is the same whether it is computed by averaging all pairs or computing the average similarity of each point with the centroid of the cluster.

Exercise 8.11 For some synthetic data estimate the number of local minima for k-means by using the birthday estimate. Is your estimate an unbaised estimate of the number? an upper bound? a lower bound? Why?

Exercise 8.12 Examine the example in Figure and discuss how to fix it. Optimizing according to the k-center or k-median criteria would seem to produce clustering B while clustering A seems more desirable.

Meaningful Clustering via SVD

Problems to be put in.

Recursive Clustering Based on the Second Eigenvector

Exercise 8.13 Prove that for any two vectors a and b, $|a-b|^2 \ge \frac{1}{2}|a|^2 - |b|^2$.

Exercise 8.14 Let A be an $n \times d$ data matrix, B its best rank k approximation, and C the optimal centers for k-means clustering of rows of A. How is it possible that $||A - B||_F^2 < ||A - C||_F^2$?

Exercise 8.15 Suppose S is a finite set of points in space with centroid μ . If a set T of points is added to S, show that the centroid of $S \cup T$ is at distance at most $\frac{|T|}{|S|+|T|}|m(T)-\mu|$ from μ .

Exercise 8.16 What happens if we relax this restriction, for example, if we allow for S, the entire set? textbfCLARIFY

Exercise 8.17 A stochastic matrix is a matrix with non negative entries in which each row sums to one. Show that for a stochastic matrix, the largest eigenvalue is one. Show that the eigenvalue has multiplicity one if and only if the corresponding Markov Chain is connected.

Exercise 8.18 Using time reversibility, prove that π is the left eigenvector of P with associated eigenvalue one, namely $\pi P = \pi$ (with π viewed as a row vector).

Exercise 8.19 Prove that
$$\Phi(S, \bar{S}) = \frac{\sum\limits_{i \in S; j \in \bar{S}} \pi_i p_{ij}}{\sum\limits_{i \in S} \pi_i}$$
.

Exercise 8.20 Show that if P is a stochastic matrix and π satisfies $\pi_i p_{ij} = \pi_j p_{ji}$, then for any left eigenvector \mathbf{v} of P, the vector \mathbf{u} with components $u_i = \frac{v_i}{\pi_i}$ is a right eigenvector with the same eigenvalue.

Exercise 8.21 Let D be the diagonal matrix with the vector π along its diagonal. Show that P and $D^{1/2}PD^{-1/2}$ are similar and have the same eigenvalues. Show that $D^{1/2}PD^{-1/2}$ is symmetric. WHY?—Time reversibility Hence its eigenvectors are orthogonal. Use this to show that if \mathbf{u} is a right eigenvector of P with eigenvalue less than 1, then $\sum_{i} u_i \pi_i = 0$.

Exercise 8.22 Consider a 0-1 matrix generated from a block probability matrix. Let p be the probability of a one for diagonal blocks and q be the probability of a one for off diagonal blocks. Given the ratio of p and q what is the ratio of first to second eigenvalue? Second given the ratio of first to second eigenvalue what is the stability given by the 95% test. **EXPAND**

Kernel Methods

Exercise 8.23 Give an example of a clustering problem where the clusters are not linearly separable in the original space, but are separable in a higher dimensional space.

Hint: Look at the example for Gaussian kernels in the chapter on learning.

Exercise 8.24 The Gaussian kernel maps points to a higher dimensional space. What is this mapping?

Agglomerative Clustering

Exercise 8.25 Agglomerative clustering requires that one calculate the distances between all pairs of points. If the number of points is a million or more, then this is impractical. One might try speeding up the agglomerative clustering algorithm by maintaining a 100 clusters at each unit of time. Start by randomly selecting a hundred points and place each point in a cluster by itself. Each time a pair of clusters is merged randomly select one of the remaining data points and create a new cluster containing that point. Suggest some other alternatives.

Tree shape
Communities, Dense Submatrices
Flow Methods
Linear Programming Formulation
Finding a Local Cluster Without Examining the Whole graph
Statistical Clustering

Exercise 8.26 Let A be the adjacency matrix of an undirected graph. Let $d(S, S) = \frac{A(S,S)}{|S|}$ be the density of the subgraph induced by the set of vertices S. Prove that d(S, S) is the average degree of a vertex in S.

Exercise 8.27 Suppose A is a matrix with non negative entries. Show that A(S,T)/(|S||T|) is maximized by the single edge with highest a_{ij} .

Exercise 8.28 Suppose A is a matrix with non negative entries and

$$\sigma_1(A) = \mathbf{x}^T A \mathbf{y} = \sum_{i,j} x_i a_{ij} y_j, \qquad |\mathbf{x}| = |\mathbf{y}| = 1.$$

Zero out all x_i less than $1/2\sqrt{n}$ and all y_j less than $1/2\sqrt{d}$. Show that the loss is no more than $1/4^{th}$ of $\sigma_1(A)$.

Exercise 8.29 Consider other measures of density such as $\frac{A(S,T)}{|S|^{\rho}|T|^{\rho}}$ for different values of ρ . Discuss the significance of the densest subgraph according to these measures.

Modularity

Exercise 8.30 Let A be the adjacency matrix of an undirected graph. Let M be the matrix whose ij^{th} element is $a_{ij} - \frac{d_i d_j}{2m}$. Partition the vertices into two groups S and \bar{S} . Let s be the indicator vector for the set S and let \bar{s} be the indicator variable for \bar{S} . Then $s^T M s$ is the number of edges in S above the expected number given the degree distribution and $s^T M \bar{s}$ is the number of edges from S to \bar{S} above the expected number given the degree distribution. Prove that if $s^T M s$ is positive $s^T M \bar{s}$ must be negative.

Axioms for Clustering An Impossibility Result A Satisfiable Set of Axioms

Exercise 8.31 Which of the three axioms, scale invariance, richness, and consistency are satisfied by the following clustering algorithms.

1.

2.

Exercise 8.32 (Research Problem): What are good measures of density that are also effectively computable? Is there empirical/theoretical evidence that some are better than others?

NOTES

Reference: A constant factor approximation algorithm for the k-median problem, Moses Charikar, Sudipto Guha, Eva Tardos and David Shmoys, in Proceedings of the 31st Annual ACM Symposium on Theory of Computing (1999),

invited to special issue of JCSS for STOC '99.

Lemma (8.7) is from Achlioptas and McSherry???

Lemma (8.6 is from Kannan, Vempala?????

Theorem (8.5) is an elementary version of a theorem from Amit Kumar and Kannan (FOCS 2010)

First Set of Axioms and Impossibility from Kleinberg Reference: Analysing the structure of large graphs, Ravi Kannan and V. Vinay, Manuscript (1999) Local

Clustering: Ref's Spielman, Teng; Anderson, Chung, Hopcroft,.. 10.4.2, Lemma 10.5 from Achlioptas and McSherry

(The proof here seems to be new.)

9 Graphical Models and Belief Propagation

A graphical model is a compact representation of a joint probability distribution. It consists of a graph, directed or undirected, whose vertices correspond to variables that take on values from some set. In this chapter we consider the case where the values the variables take on are finite, although graphical models are often used to represent probability distributions with continuous variables. The edges of the graph represent relationships or constraints between the variables.

The directed model represents a joint probability distribution over the variables that factors into a product of conditional probabilities.

$$p(x_1, x_2, \dots, x_n) = \prod_{i=1}^{n} p(x_i|\text{parents of } x_i)$$

The directed graphical model is called a Bayesian or belief network and appears frequently in the AI and the statistics literature. The undirected model, called a Markov Random Field, consists of an undirected graph and an associated probability distribution that factorizes into functions, each function associated with a clique of the graph. For example,

$$p(x_1, x_2, \cdots, x_n) = \frac{1}{Z} \prod_C \Psi_C(x_C)$$

where C is a clique of the graph and Ψ_C is a function defined on the variables x_C of the clique. A special case is the pair wise Markov Random Field where the probability distribution factors into functions of two variables and the edges of the graph correspond to constraints between pairs of variables. Here vertices are consider to be cliques of size one.

9.1 Bayesian Networks

A Bayesian network is a directed graph where vertices correspond to variables and a directed edge from y to x represents a conditional probability p(x/y). If a vertex x has edges into it from y_1, y_2, \dots, y_k , then the conditional probability is $p(x/y_1, y_2, \dots, y_k)$. The variable at a vertex with no in edges has an unconditional probability distribution. If the value of a variable at some vertex is known, then the variable is called *evidence*. An important property of a Bayesian network is that the joint probability is given by the product over all nodes of the conditional probability of the node conditioned on all its immediate predecessors.

In the example of Fig. 9.1, a patient is ill and sees a doctor. The doctor ascertains the symptoms of the patient and the possible causes such as whether the patient was in contact with farm animals, whether he had eaten certain foods, or whether the patient has an hereditary predisposition to any diseases. Using the above Bayesian network where the variables are true or false, the doctor may wish to determine one of two things. What

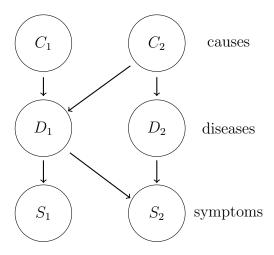


Figure 9.1: A Bayesian network

is the marginal probability of a given disease or what is the most likely set of diseases. In determining the most likely set of diseases, we are given a T or F assignment to the causes and symptoms and ask what assignment of T or F to the diseases maximizes the joint probability. This latter problem is called the maximum a posteriori probability (MAP).

Given the conditional probabilities and the probabilities $p(C_1)$ and $p(C_2)$ in Example 9.1, the joint probability $p(C_1, C_2, D_1, \cdots)$ can be computed easily for any combination of values of C_1, C_2, D_1, \cdots . We might wish to find that value of the variables of highest probability called the maximum a posteriori probability (MAP) or we might want one of the marginal probabilities $p(D_1)$ or $p(D_2)$. The obvious algorithms for these two problems require evaluating the probability $p(C_1, C_2, D_1, \cdots)$ over exponentially many input values or summing $p(C_1, C_2, D_1, \cdots)$ over exponentially many values of the variables other than those for which we want the marginal probability. In certain situations, when the joint probability distribution can be expressed as a product of factors, a belief propagation algorithm can solve the maximum a posteriori problem or compute all marginal probabilities quickly.

9.2 Markov Random Fields

A Markov Random Field consists of an undirected graph and an associated probability distribution that factorizes into functions, each function associated with a clique of the graph. For example

$$p(x) = \frac{1}{Z} \prod_{C} \Psi_{C}(x_{C})$$

where C is a clique of the graph and Ψ_C is a function defined on the variables x_C of the clique. A special case is the pairwise Markov Random Field consisting of an undirected graph where the vertices are associated with variables that take on values from some set. Associated with the edges are functions of the variables at the end points of the edge.

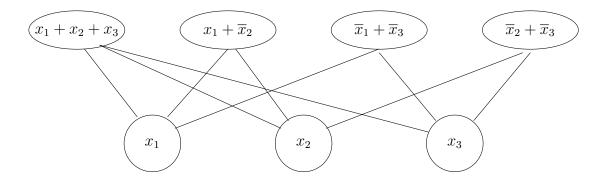


Figure 9.2: The factor graph for the function $(x_1, x_2, x_3) = (x_1 + x_2 + x_3)(x_1 + x_2)(x_1 + x_3)(x_2 + x_3)$.

Sometime the model is used to represent a joint probability distribution. Other times it is used as a representation for a combinatorial optimization problem.

When using this model to represent a joint probability distribution, it is often the case that some of the variables, y_i , are known quantities and there is a related unknown quantity, x_i , where x_i and y_i are related by a function $\phi_i(x_i, y_i)$. Since values for the y_i are known, the function $\phi_i(x_i, y_i)$ is written $\phi_i(x_i)$ and is called the evidence for x_i . In addition, certain pairs of x_i are related by a compatibility function $\Psi_{i,j}(x_i, x_j)$. The joint probability function is

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{ij} \psi_{ij}(x_i, x_j) \prod_i \varphi(x_i)$$

Often we want to compute marginal probabilities at each node x_i , $b\left(x_i\right) = \sum_{x_i} \mathbf{p}\left(x\right)$, called the *belief*. An alternative view of the pair wise Markov random field is as a combinatorial optimization problem. Here the goal is to find the assignment to the variables so as to maximize the function $\prod_{ij} \Psi_{ij}\left(x_i, x_j\right) \prod_i \varphi\left(x_i\right)$.

One application of this model is in image enhancement. The y_i are observed pixel values and the x_i are the unknown true values. The functions $\Psi_{ij}(x_i, x_j)$ may be constraints on the true values of adjacent pixels. The manner in which a function $\Psi_{ij}(x_i, x_j)$ can be used to enforce a constraint such as $x_i = x_j$ where x_i and x_j take on values 0 or 1 is to let $\Psi_{ij}(x_i, x_j)$ equal $|x_i - x_j|^{-\lambda}$ where λ is a sufficiently large positive constant. Then maximizing the product $\prod_{ij} \Psi_{ij}(x_i, x_j)$ requires setting x_i equal to x_j . Maximizing the function is the same as maximizing the logarithm of the function and this leads to a summation version of the problem where we wish to maximize $\sum_{ij} \log (\Psi_{ij}(x_i, x_j))$.

9.3 Factor Graphs

Factor graphs arise when we have a function f of a variable $\mathbf{x} = (x_1, x_2, \dots, x_n)$ where f can be expressed as $f(\mathbf{x}) = \prod_{\alpha} f_{\alpha}(x_{\alpha})$ where each factor depends only on some small number of variables x_{α} . Associate a bipartite graph with the product of factors where one set of vertices correspond to the factors and the other set to the variables. Place an edge between a variable and a factor if the factor contains that variable.

9.4 Tree Algorithms

Let $f(\mathbf{x})$ be a function that is a product of factors. When the factor graph is a tree there are efficient algorithms for solving certain problems. [With slight modifications, the algorithms presented can also solve the problems when the function is the sum of terms rather than a product of factors.]

The first problem is called marginalization and involves evaluating the sum of f() over all variables except one. In the case where f is a probability distribution the algorithm computes the marginal probabilities and thus the word marginalization. The second problem involves computing the assignment to the variables that maximizes the function f. When f is a probability distribution, this problem is the maximum a posteriori probability or MAP problem.

If the factor graph is a tree, then there exists an efficient algorithm for solving these problems. Note that there are four problems: the function f is either a product or a sum and we are either marginalizing or finding the maximizing assignment to the variables. All four problems are solved by essentially the same algorithm and we present the algorithm for the marginalization problem when f is a product.

Consider the following example where

$$f = x_1 (x_1 + x_2 + x_3) (x_3 + x_4 + x_5) x_4 x_5$$

and the variables take on values 0 or 1. In this case the factor graph is a tree as shown in Figure 9.3. Consider marginalizing f by computing

$$f(x_1) = \sum_{x_2 x_3 x_4 x_5} x_1 (x_1 + x_2 + x_3) (x_3 + x_4 + x_5) x_4 x_5,$$

One could move the summation over x_4 and x_5 in past the first two terms of the product and then sum over all values of x_4 and x_5 . Summing over x_4 and x_5 replaces the product of factors $(x_3 + x_4 + x_5) x_4 x_5$ by a single factor $x_3 + x_5$ in the formula and gives a new factor graph with the sub tree below the vertex 3 node replaced by a single factor node corresponding to $x_3 + x_5$ as shown. This corresponds to the following computation.

$$\sum_{x_2x_3x_4x_5} x_1 (x_1 + x_2 + x_3) (x_3 + x_4x_5) x_4x_5 = \sum_{x_2x_3} x_1 (x_1 + x_2 + x_3) \sum_{x_4x_5} (x_3 + x_4 + x_5) x_4x_5$$
$$= \sum_{x_2x_3} x_1 (x_1 + x_2 + x_3) (x_3 + x_4 + x_5) x_4x_5$$

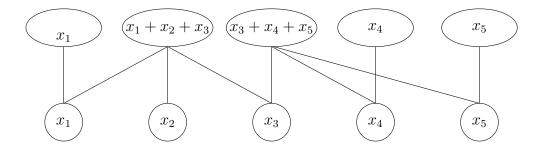


Figure 9.3: The factor graph for the function $f = x_1(x_1 + x_2 + x_3)(x_3 + x_4 + x_5)x_4x_5$.

Instead of modifying the tree one could instead send a message $x_3 + 2$ from vertex x_3 to the factor node $x_1 + x_2 + x_3$ indicating that summing over all variables in the sub tree below x_3 would result in a factor $x_3 + 2$. One advantage to passing messages rather than modifying the tree is that in computing all the marginal's $f_i(x_i)$, summing over all variables in a sub tree need only be done once and the result used in all marginal's requiring it.

The rules for calculating the messages are as follows. At each leaf node that is a variable, sum the variable over all of its possible values and send the sum up the edge to its parent. In this example, the leaf node corresponding to x_2 sends the message 1 since the variable x_2 takes on the values 0 and 1. For each leaf node that is a factor, send the one variable function associated with the node up to its parent. For each edge at an interior node, wait until all the other edges at the node have received a message. Then, for an interior variable node compute the product of all incoming messages, except for the one edge, and sum this product function over all assignments to the variables except for the variable of the node. Send the resulting function of one variable out along the remaining edge. For an interior factor node, compute the product of the factor function along with incoming messages on all edges except one and send the resulting function out along the remaining edge. The message from a variable node is the value of the sub tree below the node when all variables except for the variable at the node have been summed out.

If instead of computing marginal's one wanted the variable assignment that maximizes the function f, one would modify the above procedure by replacing the summation by a maximization operation. Obvious modifications handle the situation where $f(\mathbf{x})$ is a sum of products.

$$f\left(\mathbf{x}\right) = \sum_{x_1, \dots, x_n} f\left(\mathbf{x}\right)$$

9.5 Message Passing Algorithm

There are two message passing algorithms. The first is called *belief propagation* or *belief update* in which one marginalizes the variables by summing over them. The second

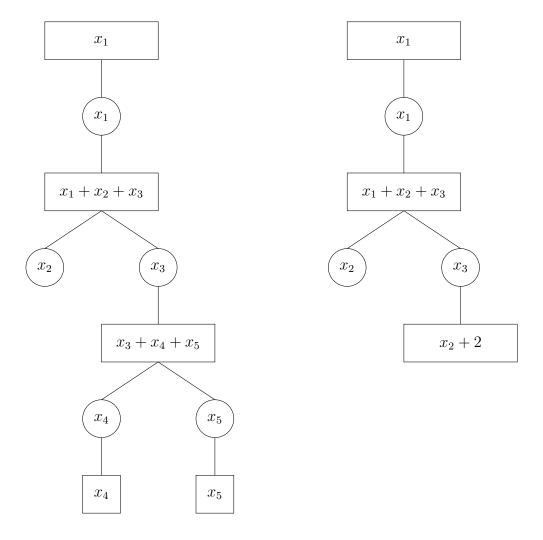


Figure 9.4: Moving the summation over x_4 and x_5 in and summing over x_4 and x_5 .

is called *belief revision* in which one maximizes over the values of the variables to obtain the maximum a posteriori, MAP, assignment.

The algorithms for computing the marginal's and for computing the MAP assignment on a tree send messages from the leaves and are guaranteed to provide the correct answers. However, there is no reason why one could not apply the message passing algorithms on an arbitrary factor graph. One would place an initial message on each edge and then update messages and hope that the process converges. Of course, there is no guarantee that even when the algorithms converge, that the values converge to the correct marginal probabilities or MAP assignment. A number of researchers have applied these message passing algorithms to a number of problems achieving good performance on graphs with cycles although a theoretical understanding of when and why these algorithms work well is still an active area of research.

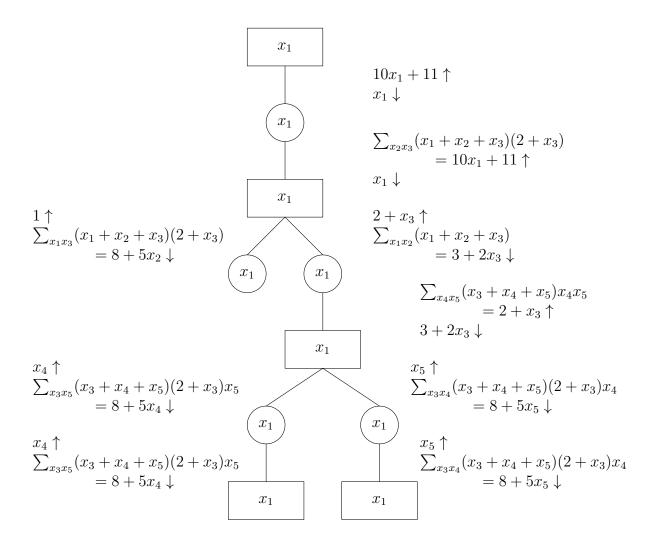


Figure 9.5: messages.

To illustrate the process, consider the pair wise Markov random field. We have an undirected graph where the vertices correspond to variables and edges have constraint functions. The edge from x to y has a constraint function $\Psi(x,y)$. Recall that a constraint such as x equals y is enforced by a function $|x-y|^{\lambda}$ where λ is a large positive number.

Suppose we want to find the assignment to the variables that maximizes $\prod_{x,y} \Psi_{xy}(x,y)$. Initially assign a message to each edge. The message from x to y is a vector with a component for each possible value of x. To determine the maximum value of the formula when the graph is a tree, select a node to be the root of the tree and if x is the variable at that node, component wise multiply the maximum value of each sub tree together to get a vector giving the maximum value of the entire tree for each value of x. In the graph case, at the vertex of variable x, we hope that the components of the message will converge so

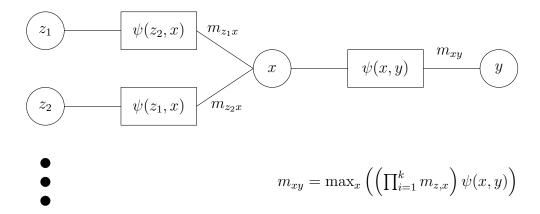


Figure 9.6: Message passing in an arbitrary graph.

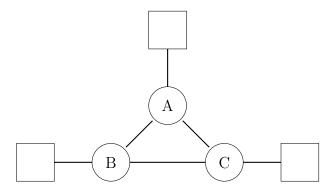
that when we multiply the messages together component wise we will get the maximum value for the graph for each value of x. However, because of cycles, this is not strictly true.

The process for updating messages is the following. Suppose that x gets messages from each of its adjacent vertices, z_1, z_2, \dots, z_k , **WHY z AND NOT x?**other than y. The message m_{z_ix} gives a value for each possible value of x. The messages along with the function $\Psi_{xy}(x,y)$ are multiplied together component wise and maximized over x to obtain the message $\mathbf{m}_{\mathbf{xy}}$ that provides a value for each possible value of y. Note that $\Psi_{xy}(x,y)$ is a matrix, not a vector. An analogous algorithm works for marginalization only the maximization is replaced by summation.

9.6 Graphs with a Single Cycle

The message passing algorithm gives the correct answers on trees and on certain other graphs. One such situation is graphs with a single cycle which we treat here. We switch from the marginalization problem to the MAP problem as the proof of correctness is simpler for the MAP problem. Consider the network in the Figure 9.7a below with a single cycle. The message passing scheme will multiply count some evidence. The local evidence at A will get passed around the loop and will come back to A. Thus, A will count the local evidence multiple times. If all evidence is multiply counted in equal amounts, then there is a possibility that all though the numerical values of the marginal probabilities (beliefs) are wrong, the algorithm still converges to the correct maximum a posteriori assignment.

Consider the unwrapped version of the graph in Figure 9.7b. The messages that the loopy version will eventually converge to, assuming convergence, are the same messages that occur in the unwrapped version provided that the nodes are sufficiently far in from the ends. The beliefs in the unwrapped version are correct for the unwrapped graph since it is a tree. The only question is, how similar are they to the true beliefs in the original network.



(a) A graph with a single cycle

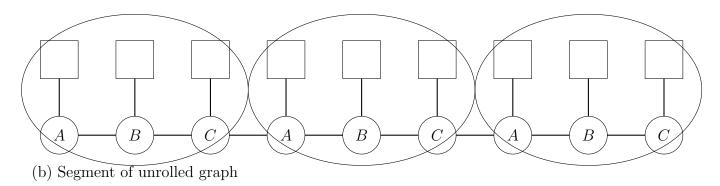


Figure 9.7: Unwrapping a graph with a single cycle

Write $p(A, B, C) = e^{\log p(A, B, C)} = e^{J(A, B, C)}$ where $J(A, B, C) = \log p(A, B, C)$. Then the probability for the unwrapped network is of the form $e^{kJ(A,B,C)+J'}$ where the J' is associated with vertices at the ends of the network where the beliefs have not yet stabilized and the kJ(A, B, C) comes from k inner copies of the cycle where the beliefs have stabilized. Note that the last copy of J in the unwrapped network shares an edge with J' and that edge has an associated Ψ . Thus, changing a variable in J has an impact on the value of J' through that Ψ . Since the algorithm maximizes $J_k = kJ(A, B, C) + J'$ in the unwrapped network for all k, it must maximize J(A, B, C). To see this, set the variables A, B, C, so that J_k is maximized. If J(A, B, C) is not maximized, then change A, B, A and C to maximize J(A, B, C). This increases J_k by some quantity that is proportional to k. However, two of the variables that appear in copies of J(A, B, C) also appear in J' and J' might decrease in value. As long as J' decreases by some finite amount, we can increase J_k by increasing k sufficiently. As long as all Ψ are nonzero, J' which is proportional to $\log \Psi$, can change by at most some finite amount. Hence, for a network with a single loop, assuming that the message passing algorithm converges, it converges to the maximum a posteriori assignment.

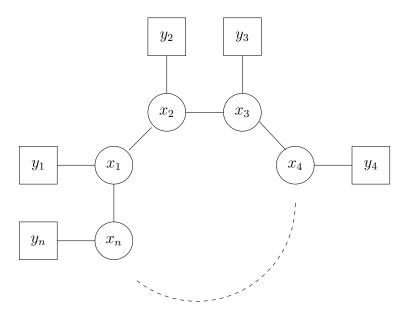


Figure 9.8: A Markov random field with a single loop.

9.7 Belief Update in Networks with a Single Loop

In the previous section we showed that when the message passing algorithm converges, it correctly solves the MAP problem for graphs with a single loop. The message passing algorithm can also be used to obtain the correct answer for the marginalization problem. Consider a network consisting of a single loop with variables x_1, x_2, \dots, x_n and evidence y_1, y_2, \dots, y_n as shown in Figure 9.8. The vectors $\mathbf{x_i}$ and y_i have one component for each value x_i can take on. To simplify the discussion assume the x_i take on values $1, 2, \dots, m$.

Let m_i be the message sent from vertex i to vertex i+1 mod n. At vertex i+1 each component of the message m_i is multiplied by the evidence y_{i+1} and the constraint function Ψ . This is done by forming a diagonal matrix D_{i+1} where the diagonal elements are the evidence and then forming a matrix M_i whose rs^{th} element is $\Psi(x_{i+1} = r, x_i = s)$. The message m_{i+1} is $M_iD_{i+1}m_i$. Multiplication by the diagonal matrix D_{i+1} multiplies the components of the message m_i by the associated evidence. Multiplication by the matrix M_i multiplies each component of the vector by the appropriate value of Ψ and sums over the values producing the vector which is the message m_{i+1} . Once the message has travelled around the loop, the new message m'_1 is given by

$$m_1' = M_n D_1 M_{n-1} D_n \cdots M_2 D_3 M_1 D_2 m_1$$

Let $M = M_n D_1 M_{n-1} D_n \cdots M_2 D_3 M_1 D_2 m_1$. Assuming that M's principle eigenvalue is unique, the message passing will converge to the principle vector of M. The rate of convergences depends on the ratio of the first and second eigenvalues.

An argument analogous to the above concerning the messages gong clockwise around the loop applies to messages moving counter clockwise around the loop. To obtain the estimate of the marginal probability $p(x_1)$, one multiples component wise the two messages arriving at x_1 along with the evidence y_1 . This estimate does not give the true marginal probability but the true marginal probability can be computed from the estimate and the rate of convergences by linear algebra.

9.8 Graphs with Multiple Loops

In a graph with multiple cycles, if the belief propagation algorithm converges it might converge to a local maximum rather than the global maximum. However, the local maximum has the property that changing the assignment of any subset of variables will not improve on the local maximum provided the graph induced by the variables consists of a set of trees and a single cycle.

Consider the 2-dimensional grid shown in Fig. 9.9. Assume that the propagation algorithm converges to a local maximum. Then one can arbitrarily change the values of any darkened variables in the figure and the assignment will not improve on the local maximum.

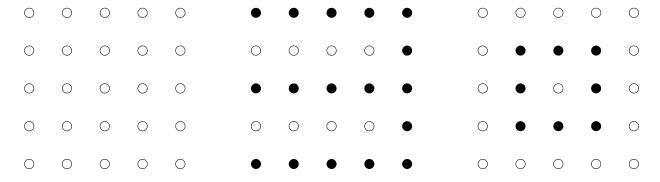


Figure 9.9: 2-dimensional grid with tree and single cycle assignment

Lemma 9.1 The belief propagation algorithm converges to an assignment such that changing the assignment of any subset of variables will not improve on the local maximum provided the graph induced by the variables whose values are changed consists of a set of trees and a single cycle.

Proof: Consider unfolding the graph to an infinite tree making duplicate copies of nodes to unroll cycles. The assignment in the tree is a global optimum. Now changing the values of any set of variables in the graph that correspond to a tree cannot increase the value of the product since we can identify the tree in the unwrapped version of the graph and there it cannot increase the product value since it is already optimal. The effect in the unwrapped version and the graph are the same since the neighbors of the tree vertices

are the same. Thus, if the belief propagation algorithm converges, it will converge to a maximum that cannot be improved on by changing a subset of variables for which the induced graph consists solely of trees.

This argument fails for cycles since we cannot identify the cycle in the unwrapped version of the graph. However, for a single cycle we can find an infinite path that corresponds to unwinding the cycle and use an argument similar to that in Section 9.6 for single cycle graphs. Note that the set of assignments which cannot improve on the local maximum is exponentially large.

9.9 Clustering by Message Passing

Clustering a set of vertices can be expressed as a problem of maximizing the sum of a set of terms and thus is a candidate for a message passing algorithm. Let c_{ij} be a variable that takes on values 0 or 1. The meaning of $c_{ij} = 1$ is that vertex i belongs in the cluster whose center is at vertex j. If s_{ij} is the similarity of i and j, the problem is to maximize the sum of the products $s_{ij}c_{ij}$ subject to the constraints that the values of the c_{ij} correspond to a legal clustering. That is,

$$\max_{c_{ij}} \left[\sum_{ij} s_{ij} c_{ij} - \lambda \sum_{i} \left| \left(\sum_{j} c_{ij} \right) - 1 \right| - \lambda \sum_{ij} c_{ij} \left(1 - c_{jj} \right) \right]$$

where λ is a large positive number. The large positive λ forces $\sum_{j} c_{ij} = 1$ and $\sum_{ij} c_{ij} (1 - c_{jj}) = 0$. The first constraint states that each vertex i is in exactly one cluster. The second constraint states that if j is the center for i, then j must be its own center.

Consider the graph corresponding to the clustering problem. The variable nodes correspond to the c_{ij} and the function nodes correspond to the constraints. There is an edge from a variable node to a function node if the variable appears in the function. Rather then draw the entire graph, we have drawn the neighborhood of a typical node. For variables c_{ij} there are two types of nodes depending on whether or not i=j. There are three types of function nodes.

For a variable node c_{ij} with $i \neq j$, such as c_{12} , assume that the message sent from the variable node to the function node $\lambda c_{12} (1 - c_{22})$ is $a_{12}c_{12}$ and the message sent to the summation function node is $b_{12}c_{12}$. Then the message from the summation node back to c_{12} is

$$\max_{c_{ij} \neq c_{12}} \left(\sum_{j \neq 2} b_{1j} c_{1j} - \lambda \left| \left(\sum_{j} c_{1j} \right) - 1 \right| \right)$$

The max is over all c_{1j} except for c_{12} . If λ is sufficiently large, the max forces exactly one c_{1j} to have value one. If $c_{12} = 0$, then exactly one c_{1j} , $j \neq 2$, would have value one

and the message would be $\max_{j\neq 2} b_{1j}$. If $c_{12} = 1$, then all c_{1j} , $j \neq 2$ would have value zero and the message would be zero. Combining these two cases into one, produces a message $(1 - c_{12}) \max_{j\neq 2} b_{1j}$. If the constant term is discarded, the message sent is $-c_{12} \max_{j\neq 2} b_{1j}$.

In order to calculate the message, d_{12} , from the function node λc_{12} ($c_{22} - 1$) to the variable node c_{12} , first calculate the message from the variable node c_{22} to the function node λc_{12} ($c_{22} - 1$). This requires calculating all messages into the variable node c_{22} . The message sent from the function node λc_{i2} ($c_{22} - 1$), $i \neq 2$, to the variable node c_{22} is a function of c_{22} . If $c_{22} = 0$, then $c_{i2} = 0$ and the message sent is $a_{i2}c_{i2} + \lambda c_{i2}$ ($c_{22} - 1$) = 0.

If $c_{22} = 1$ then c_{i2} can be either 0 or 1. Selecting c_{i2} to maximize $a_{i2}c_{i2} + \lambda c_{i2}$ ($c_{22} - 1$) results in the message max $\{a_{i2}, 0\}$. Thus, the message is max $\{a_{i2}, 0\}$ c_{22} . Since we send only the coefficient of c_{22} , the message is max $\{a_{i2}, 0\}$. We now know all messages into

Figure 9.10: Message passing

 c_{22} and thus can calculate the message from c_{22} to $\lambda c_{12} (1 - c_{22})$. This message is

$$s_{22}c_{22} - \left(\max_{j \neq 2} b_{2j}\right)c_{22} + \sum_{j \neq 1,2} \max\{0, a_{j2}\}c_{22}$$

Knowing the message from c_{22} to $c_{12}(1-c_{22})$ allows us to calculate the message from $c_{12}(1-c_{22})$ to c_{12} as follows. If $c_{12}=0$ then the message is

$$\max \left\{ 0, s_{22} - \max_{j \neq 2} b_{2j} + \sum_{j \neq 1, 2} \max \left\{ 0, a_{j2} \right\} \right\}.$$

If $c_{12} = 1$ then $c_{22} = 1$ and the message is $s_{22} - \max_{j \neq 2} b_{2j} + \sum_{j \neq 1,2} \max\{0, a_{j2}\}$. Let $A = s_{22} - \max_{j \neq 2} b_{2j} + \sum_{j \neq 1,2} \max\{0, a_{j2}\}$. Then the linear form is $[A - \max\{0, A\}] c_{12} + \min\{0, A\}$. Observing that $A - \max\{0, A\} = \min\{0, A\}$, the message is $\min\{0, A\}$. Thus

$$d_{12} = \min \left\{ 0, s_{22} - \max_{j \neq 2} b_{2j} + \sum_{j \neq 1, 2} \max \left\{ 0, a_{j2} \right\} \right\}.$$

Now we can equate messages. At c_{12}

$$a_{12} = s_{12} - \max_{j \neq 2} b_{1j}$$

and at c_{1i}

$$b_{1j} = s_{1j} + d_{1j}.$$

Eliminating b_{1j} yields

$$a_{12} = s_{12} - \max_{j \neq 2} \left\{ s_{1j} + d_{1j} \right\}.$$

This gives an equation for the a_{ij} 's in terms of the d_{ij} 's. Now

$$d_{12} = \min \left\{ 0, \underbrace{s_{22} - \max_{j \neq 2} b_{2j}}_{a_{22}} + \sum_{j \neq 1, 2} \max \left\{ 0, a_{j2} \right\} \right\} = \min \left\{ 0, a_{22} + \sum_{j \neq 1, 2} \max \left\{ 0, a_{j2} \right\} \right\}$$

At c_{22} the message sent from c_{22} to the summation node is

$$b_{22} = s_{22} + \sum_{j \neq 2} \max\{0, a_{j2}\}\$$

Now
$$b_{22} = s_{22} + d_{22}$$
, we get $d_{22} = \sum_{j \neq 2} \max\{0, a_{j2}\}$.

This gives us a pair of formulas, one for a_{12} in terms of d_{1j} and one for d_{12} in terms of a_{j2} which we can iterate until we get a fixed point.

Reference

Notes

- 1. Does the above process always converge?
- 2. If the process converges are all the constraints satisfied? Probably yes.
- 3. Note that the method does not use KL divergence.
- 4. For what types of d give good answers?

9.10 Maximum Weight Matching

We have seen that the belief propagation algorithm converges to the correct solution in trees and graphs with a single cycle. It also correctly converges for a number of other problems. Here we give one example, the maximum weight matching problem where there is a unique solution.

We apply the belief propagation algorithm to find the maximal weight matching (MWM) in a complete bipartite graph. We shall see that if the MWM in the bipartite graph is unique, then the belief propagation algorithm will converge to it.

Let $G = (V_1, V_2, E)$ be a complete bipartite graph where $V_1 = \{a_1, \dots, a_n\}$, $V_2 = \{b_1, \dots, b_n\}$, and $(a_i, b_j) \in E$, $1 \le i, j \le n$. Let $\pi = \{\pi(1), \dots, \pi(n)\}$ be a permutation of $\{1, \dots, n\}$. The collection of edges $\{(a_1, b_{\pi(1)}), \dots, (a_n, b_{\pi(n)})\}$ is called a matching which is denoted by π . Let w_{ij} be the weight associated with the edge (a_i, b_j) . The weight of the matching π is $w_{\pi} = \sum_{i=1}^{n} w_{i\pi(i)}$. The maximum weight matching π^* is

$$\pi^* = \arg\max_{\pi} \ w_{\pi}$$

The first step is to create a factor graph corresponding to the MWM problem. Each edge of the bipartite graph is represented by a variable c_{ij} which takes on the values zero or one. The value one means that the edge is present in the matching, the value zero means that the edge is not present in the matching. A set of constraints is used to force the set of edges to be a matching. The constraints are of the form $\sum_{j} c_{ij} = 1$ and $\sum_{i} c_{ij} = 1$. Any assignment of 0,1 to the variables c_{ij} that satisfies all of the constraints defines a matching. In addition, we have constraints for the weights of the edges.

We now construct a factor graph, a portion of which is shown in Fig. 9.10. Associated with the factor graph is a function $f(c_{11}, c_{12}, \cdots)$ consisting of a set of terms for each c_{ij} enforcing the constraints and summing the weights of the edges of the matching. The terms for c_{12} are

$$-\lambda \left| \left(\sum_{i} c_{i2} \right) - 1 \right| - \lambda \left| \left(\sum_{j} c_{1j} \right) - 1 \right| + w_{12}c_{12}$$

where λ is a large positive number used to enforce the constraints when we maximize the function. Finding the values of c_{11}, c_{12}, \cdots that maximize f finds the maximum weighted matching for the bipartite graph.

If the factor graph was a tree, then the message from a variable node x to its parent is a message g(x) that gives the maximum value for the sub tree for each value of x. To compute g(x), one sums all messages into the node x. For a constraint node, one sums all messages from sub trees and maximizes the sum over all variables except the variable of the parent node subject to the constraint. The message from a variable x consists of two pieces of information, the value p(x = 0) and the value p(x = 1). This information can be encoded into a linear function of x.

$$[p(x = 1) - p(x = 0)]x + p(x = 0)$$

Thus, the messages are of the form ax + b. To determine the MAP value of x once the algorithm converges, sum all messages into x and take the maximum over x=1 and x=0 to determine the value for x. Since the arg maximum of a linear form ax+b depends only on whether a is positive or negative and since maximizing the output of a constraint depends only on the coefficient of the variable, we can send messages consisting of just the variable coefficient.

To calculate the message to c_{12} from the constraint that node b_2 has exactly one neighbor, add all the messages that flow into the constraint node from the c_{i2} , $i \neq 1$ nodes and maximize subject to the constraint that exactly one variable has value one. If $c_{12} = 0$, then one of c_{i2} , $i \neq 1$, will have value one and the message is $\max_{i \neq 1} \alpha(i, 2)$. If $c_{12} = 1$, then the message is zero. Thus, we get

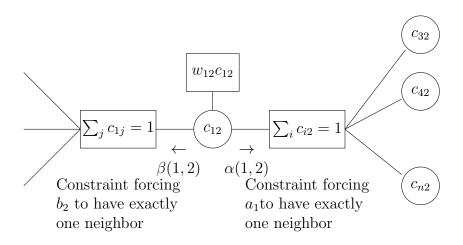


Figure 9.11: Portion of factor graph for the maximum weight matching problem.

$$-\max_{i\neq1}\alpha\left(i,2\right)x+\max_{i\neq1}\alpha\left(i,2\right)$$

and send the coefficient $-\max_{i\neq 1} \alpha(i,2)$. This means that the message from c_{12} to the other constraint node is $\beta(1,2) = w_{12} - \max_{i\neq 1} \alpha(i,2)$.

The alpha message is calculated in a similar fashion. If $c_{12} = 0$, then one of c_{1j} will have value one and the message is $\max_{j \neq 1} \beta(1, j)$. If $c_{12} = 1$, then the message is zero. Thus, the coefficient $-\max_{j \neq 1} \alpha(1, j)$ is sent. This means that $\alpha(1, 2) = w_{12} - \max_{j \neq 1} \alpha(1, j)$.

To prove convergence, we enroll the constraint graph to form a tree with a constraint node as the root. In the enrolled graph a variable node such as c_{12} will appear a number of times which depends on how deep a tree is built. Each occurrence of a variable such as c_{12} is deemed to be a distinct variable.

Lemma 9.2 If the tree obtained by unrolling the graph is of depth k, then the messages to the root are the same as the messages in the constraint graph after k-iterations.

Proof: Straight forward.

Define a matching in the tree to be a set of vertices so that there is exactly one variable node of the match adjacent to each constraint. Let Λ denote the vertices of the matching. Heavy circles represent the nodes of the above tree that are in the matching Λ .

Let Π be the vertices corresponding to maximum weight matching edges in the bipartite graph. Recall that vertices in the above tree correspond to edges in the bipartite graph. The vertices of Π are denoted by dotted circles in the above tree.

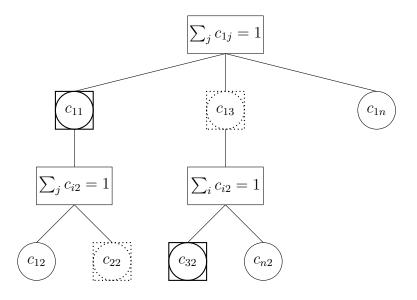


Figure 9.12: Tree for MWM problem.

Consider a set of trees where each tree has a root that corresponds to one of the constraints. If the constraint at each root is satisfied by the edge of the MWM, then we have found the MWM. Suppose that the matching at the root in one of the trees disagrees with the MWM. Then there is an alternating path of vertices of length 2k consisting of vertices corresponding to edges in Π and edges in Λ . Map this path onto the bipartite graph. In the bipartite graph the path will consist of a number of cycles plus a simple path. If k is large enough there will be a large number of cycles since no cycle can be of length more than 2n. Let m be the number of cycles. Then $m \geq \frac{2k}{2n} = \frac{k}{n}$.

Let π^* be the MWM in the bipartite graph. Take one of the cycles and use it as an alternating path to convert the MWM to another matching. Assuming that the MWM is unique and that the next closest matching is ε less, $W_{\pi^*} - W_{\pi} > \varepsilon$ where π is the new matching.

Consider the tree matching. Modify the tree matching by using the alternating path of all cycles and the left over simple path. The simple path is converted to a cycle by adding two edges. The cost of the two edges is at most $2w^*$ where w^* is the weight of the maximum weight edge. Each time we modify Λ by an alternating cycle, we increase the cost of the matching by at least ε . When we modify Λ by the left over simple path, we increase the cost of the tree matching by $\varepsilon - 2w^*$ since the two edges that were used to create a cycle in the bipartite graph are not used. Thus

weight of
$$\Lambda$$
 - weight of $\Lambda' \ge \frac{k}{n}\varepsilon - 2w*$

which must be negative since Λ' is optimal for the tree. However, if k is large enough this becomes positive, an impossibility since Λ' is the best possible. Since we have a

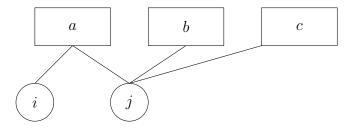


Figure 9.13: warning propagation

tree, there can be no cycles, as messages are passed up the tree, each sub tree is optimal and hence the total tree is optimal. Thus the message passing algorithm must find the maximum weight matching in the weighted complete bipartite graph assuming that the maximum weight matching is unique. Note that applying one of the cycles that makes up the alternating path decreased the bipartite graph match but increases the value of the tree. However, it does not give a higher tree matching, which is not possible since we already have the maximum tree matching. The reason for this is that the application of a single cycle does not result in a valid tree matching. One must apply the entire alternating path to go from one matching to another.

9.11 Warning Propagation

Significant progress has been made using methods similar to belief propagation in finding satisfying assignments for 3-CNF formulas. Thus, we include a section on a version of belief propagation, called warning propagation (wp), that is quite effective in finding assignments. Consider a factor graph for a SAT problem. Index the variables by i, j, and k and the factors by a, b, and c. Factor a sends a message m_{ai} to each variable i that appears in the factor a called a warning. The warning is 0 or 1 depending on whether or not factor a believes that the value assigned to i is required for a to be satisfied. A factor a determines the warning to send to variable i by examining all warnings received by other variables in factor a from factors containing them.

For each variable j, sum the warnings from factors containing j that warn j to take value T and subtract the warnings that warn j to take value F. If the difference says that j should take value T or F and this value for variable j does not satisfy a, and this is true for all j, then a sends a warning to i that the value of variable i is critical for factor a.

Start the warning propagation algorithm by assigning 1 to a warning with probability 1/2. Iteratively update the warnings. If the warning propagation algorithm converges, then compute for each variable i the local field h_i and the contradiction number c_i . The local field h_i is the number of clauses containing the variable i that sent messages that i should take value T minus the number that sent messages that i should take value F.

The contradiction number c_i is 1 if variable i gets conflicting warnings and 0 otherwise. If the factor graph is a tree, the WP algorithm converges. If one of the warning messages is one, the problem is unsatisfiable; otherwise it is satisfiable.

9.12 Correlation Between Variables

In many situations one is interested in how the correlation between variables drops off with some measure of distance. Consider a factor graph for a 3-CNF formula. Measure the distance between two variables by the shortest path in the factor graph. One might ask the question if one variable is assigned the value true what is the percentage of satisfying assignments in which the second variable also is true. If the percentage is the same as when the first variable is assigned false, then we say that the two variables are uncorrelated. How difficult it is to solve a problem is likely to be related to how fast the correlation decreases with distance.

Another illustration of this concept is in counting the number of perfect matchings in a graph. One might ask what is the percentage of matching in which some edge is present and ask how correlated this percentage is with the presences or absence of edges at some distance d. One is interested in whether the correlation drops off with distance d. To illustrate this concept we consider the Ising model studied earlier in physics.

The Ising or ferromagnetic model is a pair wise random Markov field. The underlying graph, usually a lattice, assigns a value of ± 1 , called spin, to the variable at each vertex. The probability (Gibbs measure) of a given configuration of spins is proportional to $exp(\beta \sum_{(i,j)\in E} x_i x_j) = \prod_{(i,j)\in E} e^{\beta x_i x_j}$ where $x_i = \pm 1$ is the value associated with vertex i. Thus

$$p(x_1, x_2, \dots, x_n) = \frac{1}{Z} \prod_{(i,j) \in E} exp(\beta x_i x_j) = \frac{1}{Z} e^{\beta \sum_{(i,j) \in E} x_i x_j}$$

where Z is a normalization constant.

The value of the summation is simply the difference in the number of edges whose vertices have the same spin minus the number of edges whose vertices have opposite spin. The constant β is viewed as inverse temperature. High temperature corresponds to a low value of β . At low temperature, high β , adjacent vertices have identical spins where as at high temperature the spins of adjacent vertices are uncorrelated.

One question of interest is given the above probability distribution, what is the correlation between two variables, say x_i and x_j . To answer this question, we want to determine the $Prob(x_i = 1)$ as a function of $Prob(x_j = 1)$. If $Prob(x_i = 1) = \frac{1}{2}$ independent of the value of $Prob(x_j = 1)$, we say the values are uncorrelated.

Consider the special case where the graph G is a tree. In this case a phase transition

occurs at $\beta_0 = \frac{1}{2} \ln \frac{d+1}{d-1}$ where d is the degree of the tree. For a sufficiently tall tree and for $\beta > \beta_0$, the probability that the root has value +1 is bounded away from 1/2 and depends on whether the majority of leaves have value +1 or -1. For $\beta < \beta_0$ the probability that the root has value +1 is 1/2 independent of the values at the leaves of the tree.

Consider a height one tree of degree d. If i of the leaves have spin +1 and d-i have spin -1, then the probability of the root having spin +1 is proportional to

$$e^{i\beta - (d-i)\beta} = e^{(2i-d)\beta}.$$

If the probability of a leaf being +1 is p, then the probability of i leaves being +1 and d-i being -1 is

$$\begin{pmatrix} d \\ i \end{pmatrix} p^i (1-p)^{d-i}$$

Thus, the probability of the root being +1 is proportional to

$$A = \sum_{i=1}^{d} \binom{d}{i} p^{i} (1-p)^{d-i} e^{(2i-d)\beta} = e^{-d\beta} \sum_{i=1}^{d} \binom{d}{i} (pe^{2\beta})^{i} (1-p)^{d-i} = e^{-d\beta} \left[pe^{2\beta} + 1 - p \right]^{d}$$

and the probability of the root being -1 is proportional to

$$B = \sum_{i=1}^{d} \binom{d}{i} p^{i} (1-p)^{d-i} e^{-(2i-d)\beta} = e^{-d\beta} \sum_{i=1}^{d} \binom{d}{i} (p)^{i} \left[(1-p) e^{2\beta} \right]^{d-i} = e^{-d\beta} \left[p + (1-p) e^{2\beta} \right]^{d}.$$

The probability of the root being +1 is

$$q = \frac{A}{A+B} = \frac{\left[pe^{2\beta} + 1 - p\right]^d}{\left[pe^{2\beta} + 1 - p\right]^d + \left[p + (1 - p)e^{2\beta}\right]^d} = \frac{C}{D}$$

where

$$C = \left[pe^{2\beta} + 1 - p \right]^d$$

and

$$D = \left[pe^{2\beta} + 1 - p \right]^d + \left[p + (1-p)e^{2\beta} \right]^d.$$

At high temperature the probability q of the root of this height one tree being 1 is 1/2 independent of p. At low temperature q goes from low probability of 1 below p=1/2 to high probability of 1 above p=1/2.

Now consider a very tall tree. If the p is the probability that a root has value +1, we can iterate the formula for the height one tree and observe that at low temperature the probability of the root being one converges to some value. At high temperature, the probability of the root being one is 1/2 independent of p. At the phase transition, the slope

of q at p=1/2 is one.

Now the slope of the probability of the root being 1 with respect to the probability of a leaf being 1 in this height one tree is

$$\frac{\partial q}{\partial p} = \frac{D\frac{\partial C}{\partial p} - C\frac{\partial D}{\partial p}}{D^2}$$

Since the slope of the function q(p) at p=1/2 when the phase transition occurs is one, we can solve $\frac{\partial q}{\partial p} = 1$ for the value of β where the phase transition occurs. First, we show that $\frac{\partial D}{\partial p}\Big|_{p=\frac{1}{2}} = 0$.

$$D = \left[pe^{2\beta} + 1 - p \right]^d + \left[p + (1 - p) e^{2\beta} \right]^d$$

$$\frac{\partial D}{\partial p} = d \left[pe^{2\beta} + 1 - p \right]^{d-1} \left(e^{2\beta} - 1 \right) + d \left[p + (1 - p) e^{2\beta} \right]^{d-1} \left(1 - e^{2\beta} \right)$$

$$\frac{\partial D}{\partial p} \Big|_{p = \frac{1}{2}} = \frac{d}{2^{d-1}} \left[e^{2\beta} + 1 \right]^{d-1} \left(e^{2\beta} - 1 \right) + \frac{d}{2^{d-1}} \left[1 + e^{2\beta} \right]^{d-1} \left(1 - e^{2\beta} \right) = 0$$

Then

$$\frac{\partial q}{\partial p}\Big|_{p=\frac{1}{2}} = \frac{D\frac{\partial C}{\partial p} - C\frac{\partial D}{\partial p}}{D^2}\Big|_{p=\frac{1}{2}} = \frac{\frac{\partial C}{\partial p}}{D}\Big|_{p=\frac{1}{2}} = \frac{d\left[pe^{2\beta} + 1 - p\right]^{d-1}\left(e^{2\beta} - 1\right)}{\left[pe^{2\beta} + 1 - p\right]^d + \left[p + (1 - p)e^{2\beta}\right]^d}\Big|_{p=\frac{1}{2}} = \frac{d\left[\frac{1}{2}e^{2\beta} + \frac{1}{2}\right]^{d-1}\left(e^{2\beta} - 1\right)}{\left[\frac{1}{2}e^{2\beta} + \frac{1}{2}\right]^d + \left[\frac{1}{2} + \frac{1}{2}e^{2\beta}\right]^d} = \frac{d\left(e^{2\beta} - 1\right)}{1 + e^{2\beta}}$$

Setting

$$\frac{d\left(e^{2\beta} - 1\right)}{1 + e^{2\beta}} = 1$$

And solving for β yields

$$d\left(e^{2\beta} - 1\right) = 1 + e^{2\beta}$$
$$e^{2\beta} = \frac{d+1}{d-1}$$
$$\beta = \frac{1}{2} \ln \frac{d+1}{d-1}$$

Shape of q as a function of p. Figure caption

To complete the argument, we need to show that q is a monotonic function of p. To see this, write $q = \frac{1}{1+\frac{B}{A}}$. A is a monotonically increasing function of p and B is monotonically decreasing. From this it follows that q is monotonically increasing.

In the iteration going from p to q, we do not get the true marginal probabilities at each level since we ignored the effect of the portion of the tree above. However, when we

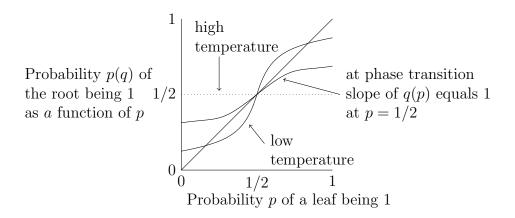


Figure 9.14: Shape of q as a function of p.

get to the root, we do get the true marginal for the root. To get the true marginal's for the interior nodes we need to send messages down from the root.

Note: The joint probability distribution for the tree is of the form $e^{\beta \sum\limits_{(ij)\in E} x_i x_j} = \prod\limits_{(i,j)\in E} e^{\beta x_i x_j}$.

Suppose x_1 has value 1 with probability p. Then define a function φ , called evidence, such that

$$\varphi(x_1) = \begin{cases} p & \text{for } x_1 = 1\\ 1 - p & \text{for } x_1 = -1 \end{cases}$$
$$= \left(p - \frac{1}{2}\right) x_1 + \frac{1}{2}$$

and multiply the joint probability function by φ . Note, however, that the marginal probability of x_1 is not p. In fact, it may be further from p after multiplying the conditional probability function by the function φ .

9.13 Exercises

Exercise 9.1 In the Ising model for a tree of degree one, a chain of vertices, is there a phase transition where the correlation between the value at the root and the value at the leaves becomes independent? Work out mathematical what happens.

Exercise 9.2 Consider an n by n grid of vertices with a variable at each vertex. Define the single loop and tree neighborhood (SLT) of an assignment r to the variables to be the set of all assignments that differ from the assignment r by changing the value of a set of variables whose induced graph is a set of trees plus possibly a single loop. Prove that any assignment to the variables is in the SLT neighborhood of an assignment v where v is in the SLT neighborhood of the optimal assignment.

Exercise 9.3 What happens in Exercise 9.2 if the graph is an n-clique? What if the underlying graph is regular degree d?

Exercise 9.4 Research question: How many solutions are required for 2-d grid so that every solution is in one of their SLT neighborhoods?

Exercise 9.5 For a Boolean function in CNF the marginal probability gives the number of satisfiable assignments with x_1 . NOT QUITE TRUE

How does one obtain the number of satisfying assignments for a 2-CNF formula? Not completely related to first sentence. FIX STATEMENT

References

"Factor graphs and the sum product algorithm"
Yair Weiss, "Belief propagation and revision in networks with loops" 1997

"On the optimality of solutions of the max-product belief propagation algorithm in arbitrary graphs" Yair Weiss and William T. Freeman

Brendan J. Frey and Delbert Dueck, "Clustering by passing messages between data points", Science 315 Feb 16, 2007 pp972-976.

Bethe free energy, Kikuchi approximations, and belief propogation algorithms, Jonathan S. Yedidia, William T. Freeman, and Yair Weiss 2001

Jonathan S. Yedidia, William T. Freeman, and Yair Weiss, Understanding Belief Propagation and its Generalizations. 2002

Frank R. Kschischang, Brendan J. Frey, and Hans-Andrea Loeliger, "Factor Graphs and the Sum-Product Algorithm, IEEE Transactions on Information Theory Vol 47:2 Feb 2001.

M. Mezard, G. Parisi, R. Zecchina, "Analytic and Algorithmic Solution of Random Satisfiability Problems, Science Vol 297 no 5582 pp812-815, 2002

A. Braunstein, M. Mezard, and R. Zecchina, "Survey propagation: an algorithm for satisfiability" 2004

Dimitris Achlioptas and Federico Ricci-Tersenghi, "On the solution-space geometry of random constraint satisfaction problems", STOC 2006

Bayati, Shah, and Sharma, "Max-product for maximum weight matching: convergence, correctness and LP duality. Good overview of field with references. Claims single cycle graphs rigorously analyzed

"Exact inference using the attenuated max-product algorithm", Brendan J. Frey and Ralf Koetter July 31, 2000

Notes on warning propagation taken from A. Braunstein, M. Mezard, and R. Zecchina, "Survey propagation: an algorithm for satisfiability" 2004

10 Other Topics

10.1 Rankings

Ranking is important. We rank movies, restaurants, students, web pages, and many other items. Ranking has become a multi-billion dollar industry as organizations try to raise the position of their web pages in the display of web pages returned by search engines to relevant queries. Search engines respond by trying to insure that the ranking of web pages they return for a query is independent of such activities. Developing a method of ranking that is not manipulative is an important task.

A ranking is a complete ordering in the sense that for every pair of items a and b, either a is preferred to b or b is preferred to a. Furthermore, a ranking is transitive in that a > b and b > c implies a > c.

One problem of interest in ranking is that of combining many individual rankings into one global ranking. However, merging ranked lists is nontrivial as the following example illustrates.

Example: Suppose there are three individuals who rank items a, b, and c as illustrated in the following table.

individual	first item	second item	third item
1	a	b	c
2	b	c	a
3	c	a	b

Suppose our algorithm tried to rank the items by first comparing a to b and then comparing b to c. In comparing a to b, two of the three individuals prefer a to b and thus we conclude a is preferable to b. In comparing b to c, again two of the three individuals prefer b to c and we conclude that b is preferable to c. Now by transitivity one would expect that the individuals would prefer a to c, but such is not the case, only one of the individuals prefers a to c and thus c is preferable to a. We come to the illogical conclusion that a is preferable to b, b is preferable to c, but c is preferable to a.

Suppose there are a number of individuals or voters and a set of candidates to be ranked. Each voter produces a ranked list of the candidates. From the set of ranked lists can one construct a single ranking of the candidates? Assume the method of producing a global ranking is required to satisfy the following three axioms.

Nondictatorship – The algorithm cannot always simply select one individual's ranking.

Unanimity – If every individual prefers a to b, then the global ranking must prefer a to b.

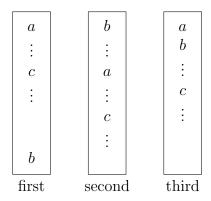


Figure 10.1: Rankings of v

Independent of irrelevant alternatives – If individuals modify their rankings but keep the order of a and b unchanged, then the global order of a and b should not change.

Arrow showed that no ranking algorithm exists satisfying the above axioms.

Theorem 10.1 (Arrow) Any algorithm for creating a global ranking of three or more elements that satisfies unanimity and independence of irrelevant alternatives is a dictatorship.

Proof: Let a, b, and c be distinct items. Consider a set of rankings in which each individual ranks b either first or last. Some individuals may rank b first and others may rank b last. For this set of rankings the global ranking must put b first or last. Suppose to the contrary that b is not first or last in the global ranking. Then there exist a and c where the global ranking puts a > b and b > c. By transitivity, the global ranking puts a > c. By independence of irrelevant alternatives, the global ranking would continue to rank a > b and b > c even if all individuals moved c above a since that would not change the relative order of a and b or the relative order of b and c. But then by unanimity, the global ranking would put c > a, a contradiction. We conclude that the global ranking puts b first or last.

Consider a set of rankings in which every individual ranks b last. By unanimity, the global ranking must also rank b last. Let the individuals, one by one, move b from bottom to top leaving the other rankings in place. By unanimity, b must eventually move from the bottom all the way to the top in the global ranking. When b first moves it must move all the way to the top by the previous argument. Let v be the first individual whose change causes the global ranking of b to change.

We now argue that v is a dictator. First we argue that v is a dictator for any pair ac not involving b. We will refer to three rankings of v (see Figure 10.1). The first ranking of v is the ranking prior to v moving b from the bottom to the top and the second is the

ranking just after v has moved b to the top. Choose any pair ac where a is above c in v's ranking. The third ranking of v is obtained by moving a above b so that a > b > c in v's ranking. By independence of irrelevant alternatives the global ranking after v has switched to the third ranking puts a > b since all individual ab votes are the same as just before v moved b to the top of his ranking. At that time the global ranking placed a > b. Similarly b > c in the global ranking since all individual bc votes are the same as just after v moved b to the top causing b to move to the top in the global ranking. By transitivity the global ranking must put a > c and thus the global ranking of a and c agrees with v.

Now note that all individuals except v can modify their rankings arbitrarily while leaving b in its extreme position and by independence of irrelevant alternatives, this does not affect the global ranking of a and b or of c and b. Thus, by transitivity this does not affect the global ranking of a and c. Next all individuals except v can move b to any position without affecting the global ranking of a and c.

At this point we have argued that independent of other individuals' rankings, the global ranking of a and c will agree with v's ranking. Now v can change its ranking arbitrarily, provided it maintains the order of a and c, and by independence of irrelevant alternatives the global ranking of a and c will not change and hence will agree with v. Thus, we conclude that for all a and c, the global ranking agrees with v independent of the other rankings except for the placement of b. But other rankings can move b without changing the global order of other elements. Thus, v is a dictator for the ranking of any pair of elements not involving b.

Note that v changed the relative order of a and b in the global ranking when it moved b from the bottom to the top in the previous argument. We will use this in a moment.

The individual v is also a dictator over every pair ab. Repeat the construction showing that v is a dictator for every pair ac not involving b only this time place c at the bottom. There must be an individual v_c who is a dictator for any pair such as ab not involving c. Since both v and v_c can affect the global ranking of a and b independent of each other, it must be that v_c is actually v. Thus, the global ranking agrees with v no matter how the other voters modify their rankings.

10.2 Hare System for Voting

One voting system would be to have everyone vote for their favorite candidate. If some candidate receives a majority of votes, he or she is declared the winner. If no candidate receives a majority of votes, the candidate with the fewest votes is dropped from the slate and the process is repeated.

The Hare system implements this method by asking each voter to rank all the candidates. Then one counts how many voters ranked each candidate as number one. If no

candidate receives a majority, the candidate with the fewest number one votes is dropped from each voters ranking. If the dropped candidate was number one on some voters list, then the number two candidate becomes that voter's number one choice. The process of counting the number one rankings is then repeated.

Although the Hare system is widely used it fails to satisfy Arrow' axioms as all voting systems must. Consider the following situation in which there are 21 voters that fall into four categories. Voters within a category rank individuals in the same order.

Category	Number of voters in category	Preference order
1	7	abcd
2	6	bacd
3	5	cbad
4	3	dcba

The Hare system would first eliminate d since d gets only three rank one votes. Then it would eliminate b since b gets only six rank one votes where as a gets seven and c gets eight. At this point a is declared the winner since a has thirteen votes to c's eight votes.

Now assume that Category 4 voters who prefer b to a move a up to first place. Then the election proceeds as follows. In round one, d is eliminated since it gets no rank 1 votes. Then c with five votes is eliminated and b is declared the winner with 11 votes. Note that by moving a up, category 4 voters were able to deny a the election and get b to win, who they prefer over a.

10.3 Compressed Sensing and Sparse Vectors

If one has a discrete time sequence \mathbf{x} of length n, the Nyquist theorem states that n coefficients in the frequency domain are needed to represent the signal \mathbf{x} . However, if the signal \mathbf{x} has only s nonzero elements, even though one does not know which elements they are, one can recover the signal by randomly selecting a small subset of the coefficients in the frequency domain. It turns out that one can reconstruct sparse signals with far fewer samples than one might suspect and an area called compressed sampling has emerged with important applications.

Motivation

Let A be an $n \times 2n$ matrix whose elements are generated by independent Gaussian processes. Let \mathbf{x} be a sparse random 2n-dimensional vector in which, say, at most five coordinates are nonzero. Multiply A times \mathbf{x} to get a vector \mathbf{b} . Forget the original \mathbf{x} and try to recover \mathbf{x} from the equation $A\mathbf{x} = \mathbf{b}$. Since A has 2n columns and only n rows,

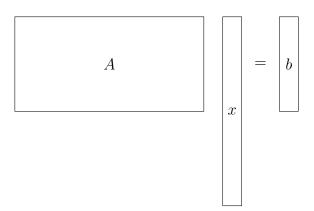


Figure 10.2: $A\mathbf{x} = \mathbf{b}$ has a vector space of solutions but possibly only one sparse solution.

one would expect that there would be an n-dimensional space of solutions. However, if the solution is required to be sparse, then it is unique.

This raises certain questions.

- 1. Why is the sparse solution unique?
- 2. How can one find the unique sparse solution?
- 3. What property of matrices leads to such a situation?
- 4. Are there physical problems that give rise to such phenomena?

10.3.1 Unique Reconstruction of a Sparse Vector

A vector is said to be s-sparse if it has at most s nonzero elements. Let \mathbf{x} be an n-dimensional s-sparse vector with s << n. Consider solving $A\mathbf{x} = \mathbf{b}$ for \mathbf{x} where A is an $m \times n$ matrix with m < n. The set of solutions to $A\mathbf{x} = \mathbf{b}$ is an affine space. However, if we restrict ourselves to sparse solutions, under certain conditions on A there is a unique s-sparse solution. Suppose that there were two s-sparse solutions, $\mathbf{x_1}$ and $\mathbf{x_2}$. Then $\mathbf{x_1} - \mathbf{x_2}$ would be a 2s-sparse solution to the homogeneous equation $A\mathbf{x} = \mathbf{0}$. A 2s-sparse solution to the homogeneous equation $A\mathbf{x} = \mathbf{0}$ requires that some 2s columns of A be linearly dependent. Unless A has 2s linearly dependent columns there can be only one s-sparse solution.

To find a sparse solution to $A\mathbf{x} = \mathbf{b}$, one would like to minimize the zero norm $\|\mathbf{x}\|_0$ over $\{\mathbf{x}|A\mathbf{x} = \mathbf{b}\}$. The difficulty is that this is a computationally hard problem. With no further hypotheses, it is NP-hard. With this in mind, we use the one norm as a proxy for the zero norm and minimize $\|\mathbf{x}\|_1$ over $\{\mathbf{x}|A\mathbf{x} = \mathbf{b}\}$. Although this problem appears to be nonlinear, it can be solved by linear programming by writing $\mathbf{x} = \mathbf{u} - \mathbf{v}$, $\mathbf{u} \geq 0$, and

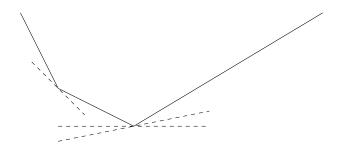


Figure 10.3: Some subgradients for a function that is not everywhere differentiable.

 $\mathbf{v} \geq 0$, and then minimizing the linear function $\sum_{i} u_i + \sum_{i} v_i$ subject to $A\mathbf{u} - A\mathbf{v} = \mathbf{b}$, $\mathbf{u} \geq 0$, and $\mathbf{v} \geq 0$.

Under what conditions will minimizing $\|\mathbf{x}\|_1$ over $\{\mathbf{x}|A\mathbf{x}=\mathbf{b}\}$ recover the s-sparse solution to $A\mathbf{x}=\mathbf{b}$? If $g(\mathbf{x})$ is a convex function, then any local minimum of g is a global minimum. If $g(\mathbf{x})$ is differentiable at its minimum, the gradient ∇g must be zero there. However, the 1-norm is not differentiable at its minimum. Thus, we introduce the concept of a subgradient of a convex function. Where the function is differentiable the subgradient is just the gradient. Where the function is not differentiable, the sub gradient is any line touching the function at the point that lies totally below the function. See Figure 10.3.

If a convex function g is not differentiable at some point $\mathbf{x_0}$, a subgradient ∇g at $\mathbf{x_0}$ satisfies $g(\mathbf{x_0} + \Delta \mathbf{x}) \geq g(\mathbf{x_0}) + (\nabla g)^T \Delta \mathbf{x}$. A point is a minimum for a convex function if there is a subgradient at that point with slope zero.

Consider the function $||x||_1$, where x is a real variable. For x < 0, the subgradient equals the gradient and has value -1. For x > 0, the subgradient equals the gradient and has value 1. At x = 0, the subgradient can be any value in the range [-1,1]. The following proposition generalizes this example to the 1-norm function in d-space.

Proposition 10.2 Let $g(\mathbf{x}) = ||\mathbf{x}||_1$ be the 1-norm function. The i^{th} component of a subgradient $\nabla g(\mathbf{x})$ at \mathbf{x} has value

- 1. -1 if $x_i < 0$,
- 2. 1 if $x_i > 0$,
- 3. is in [-1,1] if $x_i = 0$

To characterize the value of \mathbf{x} that minimizes $\|\mathbf{x}\|_1$ subject to $A\mathbf{x}=\mathbf{b}$, note that at the minimum $\mathbf{x_0}$, there can be no downhill direction consistent with the constraint $A\mathbf{x}=\mathbf{b}$.

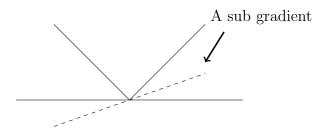


Figure 10.4: Illustration of a subgradient for $|\mathbf{x}|_1$ at $\mathbf{x}=0$

Thus, if $\Delta \mathbf{x}$ at $\mathbf{x_0}$ is such that $A\Delta \mathbf{x} = 0$, so that $A(\mathbf{x_0} + \Delta \mathbf{x}) = \mathbf{b}$, and ∇ is a subgradient for $\|\mathbf{x}\|_1$ at $\mathbf{x_0}$, it must be that $\nabla^T \Delta \mathbf{x} = 0$. That is, there is no downhill direction consistent with the constraint $A\mathbf{x} = \mathbf{b}$.

A sufficient but not necessary condition for $\mathbf{x_0}$ to be a minimum is that there exists some \mathbf{w} such that the sub gradient at $\mathbf{x_0}$ satisfies $\nabla = A^T \mathbf{w}$. Then for any $\Delta \mathbf{x}$ such that $A\Delta \mathbf{x} = 0$, we have $\nabla^T \Delta \mathbf{x} = \mathbf{w}^T A\Delta \mathbf{x} = \mathbf{w}^T \cdot \mathbf{0} = 0$. That is, for any direction consistent with the constraint $A\mathbf{x} = \mathbf{b}$, the subgradient is zero and hence $\mathbf{x_0}$ is a minimum.

10.3.2 The Exact Reconstruction Property

Theorem 10.3 below gives a condition that guarantees that a solution $\mathbf{x_0}$ to $A\mathbf{x} = \mathbf{b}$ is the unique minimum 1-norm solution to $A\mathbf{x} = \mathbf{b}$. This is a sufficient condition, but not necessary.

Theorem 10.3 Suppose $\mathbf{x_0}$ satisfies $A\mathbf{x_0} = \mathbf{b}$. If there is a subgradient ∇ to the 1-norm function at $\mathbf{x_0}$ for which

- 1. there exists a \mathbf{w} , $\nabla = A^T \mathbf{w}$,
- 2. the i^{th} component of ∇ equals the sign of the i^{th} component of $\mathbf{x_0}$ when the i^{th} component of $\mathbf{x_0}$ is not zero,
- 3. the i^{th} component of $\nabla \in (-1,1)$ when the i^{th} component of $\mathbf{x_0}$ is zero, and
- 4. the columns of A corresponding to nonzero components of $\mathbf{x_0}$ are linearly independent,

then $\mathbf{x_0}$ minimizes $\|\mathbf{x}\|_1$ subject to $A\mathbf{x}=\mathbf{b}$. Furthermore, these conditions imply that $\mathbf{x_0}$ is the unique minimum.

Proof: We first show that $\mathbf{x_0}$ minimizes $\|\mathbf{x}\|_1$. Suppose \mathbf{y} is another solution to $A\mathbf{x} = \mathbf{b}$. We need to show that $||y||_1 \ge ||x_0||_1$. Let $\mathbf{z} = \mathbf{y} - \mathbf{x_0}$. Then $A\mathbf{z} = A\mathbf{y} - A\mathbf{x_0} = \mathbf{0}$. Hence, $\nabla^T \mathbf{z} = (A^T \mathbf{w})^T \mathbf{z} = \mathbf{w}^T A \mathbf{z} = 0$. Now, since ∇ is a subgradient of the 1-norm function at x_0 ,

$$||\mathbf{y}||_1 = ||x_0 + z||_1 \ge ||\mathbf{x_0}||_1 + \nabla^T \cdot \mathbf{z} = ||\mathbf{x_0}||_1$$

and so we have that $||\mathbf{x}_0||_1$ minimizes $||\mathbf{x}||_1$ over all solutions to $A\mathbf{x} = \mathbf{b}$.

Suppose now $\tilde{\mathbf{x}}_0$ were another minimum. Then ∇ is also a subgradient at $\tilde{\mathbf{x}}_0$ as it is at \mathbf{x}_0 . To see this, for $\Delta \mathbf{x}$ such that $A\Delta \mathbf{x} = 0$.

$$\left\|\tilde{\mathbf{x}}_{0} + \Delta \mathbf{x}\right\|_{1} = \left\|\mathbf{x}_{0} + \underbrace{\tilde{\mathbf{x}}_{0} - \mathbf{x}_{0} + \Delta \mathbf{x}}_{\alpha}\right\|_{1} \ge \left\|\mathbf{x}_{0}\right\|_{1} + \nabla^{T} \left(\tilde{\mathbf{x}}_{0} - \mathbf{x}_{0} + \Delta \mathbf{x}\right).$$

The above equation follows from the definition of ∇ being a subgradient for the one norm function, $\|\mathbf{\|}_1$, at $\mathbf{x_0}$. Thus, $\|\mathbf{\tilde{x_0}} + \Delta \mathbf{x}\|_1 \ge \|\mathbf{x_0}\|_1 + \nabla^T (\mathbf{\tilde{x_0}} - \mathbf{x_0}) + \nabla^T \Delta \mathbf{x}$. But $\nabla^T (\mathbf{\tilde{x_0}} - \mathbf{x_0}) = \mathbf{w}^T A (\mathbf{\tilde{x_0}} - \mathbf{x_0}) = \mathbf{w}^T (\mathbf{b} - \mathbf{b}) = 0$. Hence, since $\mathbf{\tilde{x_0}}$ being a minimum means $\|\mathbf{\tilde{x_0}}\|_1 = \|\mathbf{x_0}\|_1$,

$$\|\tilde{\mathbf{x}}_{\mathbf{0}} + \Delta \mathbf{x}\|_{1} \ge \|\mathbf{x}_{\mathbf{0}}\|_{1} + \nabla^{T} \Delta \mathbf{x} = \|\tilde{\mathbf{x}}_{\mathbf{0}}\|_{1} + \nabla^{T} \Delta \mathbf{x}.$$

This implies that ∇ is a sub gradient at $\tilde{\mathbf{x}}_{\mathbf{0}}$.

Now, ∇ is a subgradient at both $\mathbf{x_0}$ and $\tilde{\mathbf{x}_0}$. By Lemma 10.2, we must have that $(\nabla)_i = \operatorname{sgn}[(x_0)_i] = \operatorname{sgn}[(\tilde{x}_0)_i]$, whenever either is nonzero and $|(\nabla)_i| < 1$, whenever either is 0. It follows that $\mathbf{x_0}$ and $\tilde{\mathbf{x}_0}$ have the same sparseness pattern. Since $A\mathbf{x_0} = \mathbf{b}$ and $A\tilde{\mathbf{x}_0} = \mathbf{b}$ and $\mathbf{x_0}$ and $\tilde{\mathbf{x}_0}$ are both nonzero on the same coordinates, and by (4) of the theorem, the columns of A corresponding to the nonzeros of $\mathbf{x_0}$ and $\tilde{\mathbf{x}_0}$ are independent, it must be that $\mathbf{x_0} = \tilde{\mathbf{x}_0}$.

10.3.3 Restricted Isometry Property

Next we introduce the restricted isometry property that plays a key role in exact reconstruction of sparse vectors. A matrix A satisfies the restricted isometry property, RIP, if there exists δ_s such that for any s-sparse \mathbf{x}

$$(1 - \delta_s) |\mathbf{x}|^2 \le |A\mathbf{x}|^2 \le (1 + \delta_s) |\mathbf{x}|^2 \tag{10.1}$$

Isometry is a mathematical concept; it refers to linear transformations that exactly preserve length such as rotations. So, if A is an $n \times n$ isometry, all its eigenvalues are 1 and it represents a coordinate system. Since a pair of orthogonal vectors are always orthogonal whatever coordinate system we choose, for an isometry A and two orthogonal vectors \mathbf{x} and \mathbf{y} , we have $\mathbf{x}^T A^T A \mathbf{y} = 0$. We will prove approximate versions of these properties for matrices A satisfying the restricted isometry property. The approximate versions will be used in the sequel.

A piece of notation will be useful. For a subset S of columns of A, let A_S denote the submatrix of A consisting of the columns of S.

Lemma 10.4 If A satisfies the restricted isometry property, then

- 1. For any subset S of columns with |S| = s, the singular values of A_S are all between $1 \delta_s$ and $1 + \delta_s$.
- 2. For any two orthogonal vectors \mathbf{x} and \mathbf{y} , with supports of size s_1 and s_2 respectively, $|\mathbf{x}^T A^T A \mathbf{y}| \leq 4|\mathbf{x}||\mathbf{y}|(\delta_{s_1} + \delta_{s_2})$.

Proof: Item 1 follows from the definition. To prove the second item, assume without loss of generality that $|\mathbf{x}| = |\mathbf{y}| = 1$. Since \mathbf{x} and \mathbf{y} are orthogonal, $|\mathbf{x} + \mathbf{y}|^2 = 2$. Consider $|A(\mathbf{x}+\mathbf{y})|^2$. This is between $2(1-\delta_{s_1}+\delta_{s_2})^2$ and $2(1+\delta_{s_1}+\delta_{s_2})^2$ by the restricted isometry property. Also $|A\mathbf{x}|^2$ is between $(1-\delta_{s_1})^2$ and $(1+\delta_{s_1})^2$ and $(1+\delta_{s_2})^2$. Since

$$2\mathbf{x}^T A^T A \mathbf{y} = (\mathbf{x} + \mathbf{y})^T A^T A (\mathbf{x} + \mathbf{y}) - \mathbf{x}^T A^T A \mathbf{x} - \mathbf{y}^T A^T A \mathbf{y}$$
$$= |A(\mathbf{x} + \mathbf{y})|^2 - |A\mathbf{x}|^2 - |A\mathbf{y}|^2,$$

it follows that

$$|2x^{T}A^{T}Ay| \leq 2(1 + \delta_{S_{1}} + \delta_{S_{2}})^{2} - (1 - \delta_{s_{1}})^{2} - (1 - \delta_{s_{2}})^{2}$$

$$4(\delta_{S_{1}} + \delta_{S_{2}}) - (\delta_{S_{1}} - \delta_{S_{2}})^{2}$$

$$\leq 4(\delta_{S_{1}} + \delta_{S_{2}})$$

Thus, for arbitrary \mathbf{x} and $\mathbf{y} |\mathbf{x}^T A^T A \mathbf{y}| \leq 4|\mathbf{x}||\mathbf{y}|(\delta_{s_1} + \delta_{s_2}).$

Theorem 10.5 Suppose A satisfies the restricted isometry property with

$$\delta_{s+1} \le \frac{1}{5\sqrt{s}}.$$

Suppose $\mathbf{x_0}$ has at most s nonzero coordinates and satisfies $A\mathbf{x} = \mathbf{b}$. Then, a subgradient $\nabla ||(\mathbf{x_0})||_1$ for the 1-norm function exists at $\mathbf{x_0}$ which satisfies the conditions of Theorem 10.3 and so $\mathbf{x_0}$ is the unique minimum 1-norm solution to $A\mathbf{x} = \mathbf{b}$.

Proof: Let

$$S = \{i | (\mathbf{x_0})_{\mathbf{i}} \neq 0\}$$

be the support of $\mathbf{x_0}$ and let $\bar{S} = \{i | (\mathbf{x_0})_i = \mathbf{0}\}$ be the complement set of coordinates. To find a subgradient \mathbf{u} at $\mathbf{x_0}$ satisfying Theorem 10.3, search for a \mathbf{w} such that $\mathbf{u} = A^T \mathbf{w}$ where for coordinates in which $\mathbf{x_0} \neq 0$, $\mathbf{u} = sgn(\mathbf{x_0})$ and for the remaining coordinates the 2-norm of \mathbf{u} is minimized. Solving for \mathbf{w} is a least squares problem. Let \mathbf{z} be the vector with support S, with $z_i = sgn(\mathbf{x_0})$ on S. Consider the vector \mathbf{w} defined by

$$\mathbf{w} = A_S \left(A_S^T A_S \right)^{-1} \mathbf{z}.$$

This happens to be the solution of the least squares problem, but we do not need this fact. We only state it to tell the reader how we came up with this expression. Note that A_S has independent columns from part (2) of Lemma 10.4, and so $A_S^T A_S$ is invertible. We

will prove that this **w** satisfies the conditions of Theorem 10.3. First, for coordinates in S, we have

$$(A^T \mathbf{w})_S = (A_S)^T A_S (A_S^T A_S)^{-1} \mathbf{z} = \mathbf{z}$$

as required.

For coordinates in \bar{S} , we have

$$(A^T \mathbf{w})_{\bar{S}} = (A_{\bar{S}})^T A_S (A_S^T A_S)^{-1} \mathbf{z}.$$

Now, the eigenvalues of $A_S^T A_S$, which are the squares of the singular values of A_S , are between $(1 - \delta_s)^2$ and $(1 + \delta_s)^2$. So $||(A_S^T A_S)^{-1}|| \le \frac{1}{(1 - \delta_S)^2}$. Letting $\mathbf{p} = (A_S^T A_S)^{-1} \mathbf{z}$, we have $|\mathbf{p}| \le \frac{\sqrt{s}}{(1 - \delta_S)^2}$. Write $A_s \mathbf{p}$ as $A \mathbf{q}$, where \mathbf{q} has all coordinates in \bar{S} equal to zero. Now, for $j \in \bar{S}$

$$(A^T \mathbf{w})_j = e_j^T A^T A \mathbf{q}$$

and part (2) of Lemma 10.4 gives $|u_j| \le 8\delta_{s+1}\sqrt{s} \le 1/2$ establishing that part (3) of Theorem 10.3 holds.

Gaussian matrices satisfy RIP — Prove (Exercise???)

10.4 Applications

10.4.1 Sparse Vector in Some Coordinate Basis

Consider $A\mathbf{x} = \mathbf{b}$ where A is a square $n \times n$ matrix. The vectors \mathbf{x} and \mathbf{b} can be considered as two representations of the same quantity. For example, the matrix A might be the Fourier transform, \mathbf{x} a discrete time sequence, and \mathbf{b} the frequency spectrum of \mathbf{x} . The quantity \mathbf{x} can be represented in the time domain by \mathbf{x} and in the frequency domain by its Fourier transform \mathbf{b} . In fact, any orthonormal matrix can be thought of as a transformation and there are many important transformations other than the Fourier transformation.

Consider a transformation A and a signal \mathbf{x} in some standard representation. Then $\mathbf{y} = A\mathbf{x}$ transforms the signal \mathbf{x} to another representation \mathbf{y} . If A spreads any sparse signal \mathbf{x} out so that the information contained in each coordinate in the standard basis is spread out to all coordinates in the second basis, then the two representations are said to be *incoherent*. A signal and its Fourier transform are one example of incoherent vectors. This suggests that if \mathbf{x} is sparse, only a few randomly selected coordinates of its Fourier transform are needed to reconstruct \mathbf{x} . In the next section we show that a signal cannot be too sparse in both its time domain and its frequency domain.

10.4.2 A Representation Cannot be Sparse in Both Time and Frequency Domains

We now show that there is an uncertainty principle that states that a time signal cannot be sparse in both the time domain and the frequency domain. If the signal is of

length n, then the product of the number of nonzero coordinates in the time domain and the number of nonzero coordinates in the frequency domain must be at least n. We first prove two technical lemmas.

Lemma 10.6 The arithmetic mean $\frac{a+b}{2}$ of two numbers a and b is greater than the geometric mean \sqrt{ab} of the two numbers.

Proof:

$$(a - b)^{2} \ge 0$$

$$a^{2} - 2ab + b^{2} \ge 0$$

$$a^{2} + 2ab + b^{2} \ge 4ab$$

$$(a + b)^{2} \ge 4ab$$

$$a + b \ge 2\sqrt{ab}$$

In dealing with the Fourier transform it is convenient for indices to run from 0 to n-1 rather than from 1 to n. Let $x_0, x_1, \ldots, x_{n-1}$ be a sequence and let $f_0, f_1, \ldots, f_{n-1}$ be its discrete Fourier transform. Let $i = \sqrt{-1}$. Then $f_j = \frac{1}{\sqrt{n}} \sum_{k=0}^{n-1} x_k e^{-\frac{2\pi i}{n}jk}, \quad j = 0, \ldots, n-1$. This can be written in matrix form $\mathbf{f} = Z\mathbf{x}$ where $z_{jk} = e^{-\frac{2\pi i}{n}jk}$.

$$\begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_{n-1} \end{pmatrix} = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ e^{-\frac{2\pi i}{n}} & e^{-\frac{2\pi i}{n}} 2 & \cdots & e^{-\frac{2\pi i}{n}} (n-1) \\ \vdots & \vdots & & \vdots \\ e^{-\frac{2\pi i}{n}} (n-1) & e^{-\frac{2\pi i}{n}} 2 (n-1) & \cdots & e^{-\frac{2\pi i}{n}} (n-1)^2 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix}$$

If some of the elements of \mathbf{x} are zero, delete the corresponding columns from the matrix. To maintain a square matrix, let n_x be the number of nonzero elements in \mathbf{x} and select n_x consecutive rows of Z. Normalize the columns of the resulting submatrix by dividing each element in a column by the column element in the first row. The resulting submatrix is a Vandermonde matrix that looks like

$$\left(\begin{array}{ccccc}
1 & 1 & 1 & 1 \\
a & b & c & d \\
a^2 & b^2 & c^2 & d^2 \\
a^3 & b^3 & c^3 & d^3
\end{array}\right)$$

which is nonsingular.

Lemma 10.7 If $x_0, x_1, \ldots, x_{n-1}$ has n_x nonzero elements, then $f_0, f_1, \ldots, f_{n-1}$ cannot have n_x consecutive zeros.

Proof: Let $i_1, i_2, \ldots, i_{n_x}$ be the indices of the nonzero elements of \mathbf{x} . Then the elements of the Fourier transform in the range $k = m + 1, m + 2, \ldots, m + n_x$ are

$$f_k = \frac{1}{\sqrt{n}} \sum_{i=1}^{n_x} x_{i_j} e^{\frac{-2\pi i}{n} k i_j}$$

Note the use of i as $\sqrt{-1}$ and the multiplication of the exponent by i_j to account for the actual location of the element in the sequence. Normally, if every element in the sequence was included, we would just multiply by the index of summation.

Convert the equation to matrix form by defining $z_{kj} = \frac{1}{\sqrt{n}} \exp(-\frac{2\pi i}{n}ki_j)$ and write $\mathbf{f} = Z\mathbf{x}$. Actually instead of \mathbf{x} , write the vector consisting of the nonzero elements of \mathbf{x} . By its definition, $\mathbf{x} \neq 0$. To prove the lemma we need to show that \mathbf{f} is nonzero. This will be true provided Z is nonsingular. If we rescale Z by dividing each column by its leading entry we get the Vandermonde determinant which is nonsingular.

Theorem 10.8 Let n_x be the number of nonzero elements in \mathbf{x} and let n_f be the number of nonzero elements in the Fourier transform of \mathbf{x} . Let n_x divide n. Then $n_x n_f \geq n$.

Proof: If \mathbf{x} has n_x nonzero elements, \mathbf{f} cannot have a consecutive block of n_x zeros. Since n_x divides n there are $\frac{n}{n_x}$ blocks each containing at least one nonzero element. Thus, the product of nonzero elements in \mathbf{x} and \mathbf{f} is at least n.

Fourier transform of spikes prove that above bound is tight

To show that the bound in Theorem 10.8 is tight we show that the Fourier transform of the sequence of length n consisting of \sqrt{n} ones, each one separated by $\sqrt{n}-1$ zeros, is the sequence itself. For example, the Fourier transform of the sequence 100100100 is 100100100. Thus, for this class of sequences, $n_x n_f = n$. The Fourier transform is $y_j = \frac{1}{\sqrt{n}} \sum_{k=0}^{n-1} z^{jk}$.

Theorem 10.9 Let $S(\sqrt{n}, \sqrt{n})$ be the sequence of 1's and 0's with \sqrt{n} 1's spaced \sqrt{n} apart. The Fourier transform of $S(\sqrt{n}, \sqrt{n})$ is itself.

Proof: Consider the columns $0, \sqrt{n}, 2\sqrt{n}, \dots, (\sqrt{n}-1)\sqrt{n}$. These are the columns for which $S(\sqrt{n}, \sqrt{n})$ has value 1. The element of the matrix Z in the row $j\sqrt{n}$ of column $k\sqrt{n}$, $0 \le k < \sqrt{n}$ is $z^{nkj} = 1$. Thus, for these rows Z times the vector $S(\sqrt{n}, \sqrt{n}) = \sqrt{n}$ and the $1/\sqrt{n}$ normalization yields $f_{j\sqrt{n}} = 1$.

For rows whose index is not of the form $j\sqrt{n}$, the row $b, b \neq j\sqrt{n}, j \in \{0, \sqrt{n}, \dots, \sqrt{n} - 1\}$, the elements in row b in the columns $0, \sqrt{n}, 2\sqrt{n}, \dots, (\sqrt{n} - 1)\sqrt{n}$ are $1, z^b, z^{2b}, \dots, z^{(\sqrt{n} - 1)b}$ and thus $f_b = \frac{1}{\sqrt{n}} \left(1 + z^b + z^{2b} \dots + z^{(\sqrt{n} - 1)b}\right) = \frac{1}{\sqrt{n}} \frac{z^{\sqrt{n}b} - 1}{z - 1} = 0$ since $z^{b\sqrt{n}} = 1$ and $z \neq 1$.

Figure 10.5: The matrix Z for n=9.

Uniqueness of l_1 optimization

Consider a redundant representation for a sequence. One such representation would be representing a sequence as the concatenation of two sequences, one specified by its coordinates and the other by its Fourier transform. Suppose some sequence could be represented as a sequence of coordinates and Fourier coefficients sparsely in two different ways. Then by subtraction, the zero sequence could be represented by a sparse sequence. The representation of the zero sequence cannot be solely coordinates or Fourier coefficients. If y is the coordinate sequence in the representation of the zero sequence, then the Fourier portion of the representation must represent -y. Thus y and its Fourier transform would have sparse representations contradicting $n_x n_f \geq n$. Notice that a factor of two comes in when we subtract the two representations.

Suppose two sparse signals had Fourier transforms that agreed in almost all of their coordinates. Then the difference would be a sparse signal with a sparse transform. This is not possible. Thus, if one selects $\log n$ elements of their transform these elements should distinguish between these two signals. Need argument that we distinguish between all signals.

10.4.3 Biological

There are many areas where linear systems arise in which a sparse solution is unique. One is in plant breading. Consider a breeder who has a number of apple trees and for each tree observes the strength of some desirable feature. He wishes to determine which genes are responsible for the feature so he can cross bread to obtain a tree which better expresses the desirable feature. This gives rise to a set of equations $A\mathbf{x} = \mathbf{b}$ where each row of the matrix A corresponds to a tree and each column to a position on the genone. See Figure 10.6). The vector \mathbf{b} corresponds to the strength of the desired feature in each tree. The solution \mathbf{x} tells us the position on the genone corresponding to the genes that

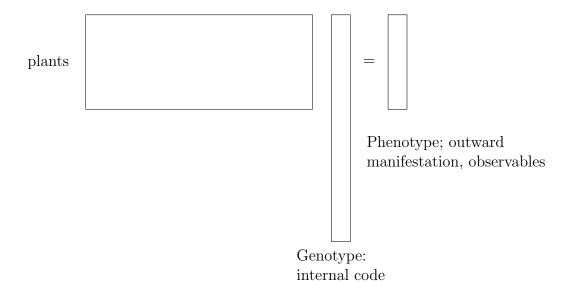


Figure 10.6: The system of linear equations used to find the internal code for some observable phenomenon.

account for the feature. It would be surprising if there were two small independent sets of genes that accounted for the desired feature. Thus, the matrix must have a property that allows only one sparse solution.

10.4.4 Finding Overlapping Cliques or Communities

Consider a graph that consists of several cliques. Suppose we can observe only low level information such as edges and we wish to identify the cliques. An instance of this problem is the task of identifying which of ten players belongs to which of two teams of five players each when one can only observe interactions between pairs of individuals. There is an interaction between two players if and only if they are on the same team. In this situation we have a matrix A with $\binom{10}{5}$ columns and $\binom{10}{2}$ rows. The columns represent possible teams and the rows represent pairs of individuals. Let **b** be the $\binom{10}{2}$ dimensional vector of observed interactions. Let \mathbf{x} be a solution to $A\mathbf{x} = \mathbf{b}$. There is a sparse solution \mathbf{x} where \mathbf{x} is all zeros except for the two 1's for 12345 and 678910 where the two teams are $\{1,2,3,4,5\}$ and $\{6,7,8,9,10\}$. The question is can we recover x from **b.** If the matrix A had satisfied the restricted isometry condition, then we could surely do this. Although A does not satisfy the restricted isometry condition which guarantees recover of all sparse vectors, we can recover the sparse vector in the case where the teams are non overlapping or almost non overlapping. If A satisfied the restricted isometry property we would minimize $\|\mathbf{x}\|_1$ subject to $A\mathbf{x} = \mathbf{b}$. Instead, we minimize $\|\mathbf{x}\|_1$ subject to $||A\mathbf{x} - \mathbf{b}||_{\infty} \le \varepsilon$ where we bound the largest error.

FINISH

10.4.5 Low Rank Matrices

Suppose we have a low rank matrix L that has been corrupted by noise. That is M = L + R. If the R is Gaussian, then principle component analysis will recover L from M. However, if L has been corrupted by several missing entries or several entries have a large noise added to them and they become outliers, then principle component analysis may be far off. However, if L is low rank and R is sparse, then we can recover L effectively from L + R. To do this we find the L and R that minimize $||L||_* + \lambda ||R||_1$. Here $||L||_*$ is the sum of the singular values of L. Notice that we do not need to know the rank of L or the elements that were corrupted. All we need is that the low rank matrix L is not sparse and that the sparse matrix R is not low rank. We leave the proof as an exercise.

An example where low rank matrices that have been corrupted might occur is aerial photographs of an intersection. Given a long sequence of such photographs, they will be the same except for cars and people. If each photo is converted to a vector and the vector used to make a column of a matrix, then the matrix will be low rank corrupted by the traffic. Finding the original low rank matrix will separate the cars and people from the back ground.

10.5 Exercises

Exercise 10.1 Select a method of combining individual rankings into a global ranking. Consider a set of rankings where each individual ranks b last. One by one move b from the bottom to the top leaving the other rankings in place. Determine v_b as in Theorem 10.1 where b_b is the ranking that causes b to move from the bottom to the top in the global ranking.

Exercise 10.2 Show that the three axioms: non dictator, unanimity, and independence of irrelevant alternatives are independent.

Exercise 10.3 Does the axiom of independence of irrelevant alternatives make sense? What if there were three rankings of five items. In the first two rankings, A is number one and B is number two. In the third ranking, B is number one and A is number five. one might compute an average score where a low score is good. A gets a score of 1+1+5=7 and B gets a score of 2+2+1=5 and B is ranked number one in the global raking. Now if the third ranker moves A up to the second position, A's score becomes 1+1+2=4 and the global ranking changes. Is there some alternative axiom to replace independence of irrelevant alternatives? **NEEDS WORK**

Exercise 10.4 Prove that the global ranking agrees with column v_b even if b is moved down through the column.

Exercise 10.5 Create a random 100 by 100 orthonormal matrix A and a sparse 100-dimensional vector \mathbf{b} . Compute $\mathbf{y} = A\mathbf{x}$. Randomly select a few coordinates of \mathbf{y} and reconstruct \mathbf{x} from the samples of \mathbf{y} using the minimization of 1-norm technique of Section 10.3.1. Did you get \mathbf{x} back?

Exercise 10.6 (maybe belongs in a different chapter) Let A be a low rank $n \times m$ matrix. Let r be the rank of A. Let \tilde{A} be A corrupted by Gaussian noise. Prove that the rank r SVD approximation to \tilde{A} minimizes $\left|A-\tilde{A}\right|_F^2$.

Exercise 10.7 Prove that minimizing $||x||_0$ subject to Ax = b is NP-complete.

Exercise 10.8 Generate 100×100 matrices of rank 20, 40, 60 80, and 100. In each matrix randomly delete 50, 100, 200, or 400 entries. In each case try to recover the original matrix. How well do you do?

Exercise 10.9 Repeat the previous exercise but instead of deleting elements, corrupt the elements by adding a reasonable size corruption to the randomly selected matrix entires.

Exercise 10.10 Compute the Fourier transform of the sequence 1000010000.

Exercise 10.11 What is the Fourier transform of a cyclic shift?

Exercise 10.12 The number n=6 is factorable but not a perfect square. What is Fourier transform of F(2,3)? Is the transform of 100100, 101010?

Exercise 10.13 Let Z be the n root of unity. Prove that $\{z^{bi}|0 \le i < n\} = \{z^i|0 \le i < n\}$ proved that b does not divide n.

Exercise 10.14 The Vandermonde determinant is of the form

$$\begin{pmatrix}
1 & 1 & 1 & 1 \\
a & b & c & d \\
a^2 & b^2 & c^2 & d^2 \\
a^3 & b^3 & c^3 & d^3
\end{pmatrix}$$

Show that if a, b, c, and d are distinct, then the Vandermonde determinant is nonsingular. **Hint**: Given value at each of n points, there is a unique polynomial that takes on the values at the points.

Exercise 10.15 Many problems can be formulated as finding \mathbf{x} satisfying $A\mathbf{x} = \mathbf{b} + \mathbf{r}$ where \mathbf{r} is some residual error. Discuss the advantages and disadvantages of each of the following three versions of the problem.

- 1. Set $\mathbf{r} = 0$ and find $\mathbf{x} = argmin \|\mathbf{x}\|_1$ satisfying $A\mathbf{x} = \mathbf{b}$
- 2. Lasso: find $\mathbf{x} = argmin(\|\mathbf{x}\|_1 + \alpha \|\mathbf{r}\|_2^2)$ satisfying $A\mathbf{x} = \mathbf{b}$
- 3. find \underline{x} =argmin $\|\mathbf{x}\|_1$ such that $\|\mathbf{r}\|_2 < \varepsilon$

Exercise 10.16 Create a graph of overlapping communities as follows. Let n=1,000. Partition the integers into ten blocks each of size 100. The first block is $\{1,2,\ldots,100\}$. The second is $\{100,101,\ldots,200\}$ and so on. Add edges to the graph so that the vertices in each block form a clique. Now randomly permute the indices and partition the sequence into ten blocks of 100 vertices each. Again add edges so that these new blocks are cliques. Randomly permute the indices a second time and repeat the process of adding edges. The result is a graph in which each vertex is in three cliques. Explain how to find the cliques given the graph.

Exercise 10.17 Repeat the above exercise but instead of adding edges to form cliques, use each block to form a G(100,p) graph. For how small a p can you recover the blocks? What if you add G(1,000,q) to the graph for some small value of q.

Exercise 10.18 Construct an $n \times m$ matrix A where each of the m columns is a 0-1 indicator vector with approximately 1/4 entries being 1. Then $B = AA^T$ is a symmetric matrix that can be viewed as the adjacency matrix of an n vertex graph. Some edges will have weight greater than one. The graph consists of a number of possibly over lapping cliques. Your task given B is to find the cliques by the following technique of finding a

0-1 vector in the column space of B by the following linear program for finding b and x.

$$b = argmin||b||_1$$

subject to

$$Bx = b$$

$$b_1 = 1$$

$$0 \le b_i \le 1 \quad 2 \le i \le n$$

Then subtract bb^T from B and repeat.

Exercise 10.19 Construct an example of a matrix A satisfying the following conditions

- 1. The columns of A are 0-1 vectors where the support of no two columns overlap by 50% or more.
- 2. No column's support is totally within the support of another column.
- 3. The minimum 1-norm vector in the column space of A is not a 0-1 vector.

Exercise 10.20 Let M = L + R where L is a low rank matrix corrupted by a sparse noise matrix R. Why can we not recover L from M if R is low rank or if L is sparse?

Exercise 10.21 LASSO Create exercise on LASSO min $(\|Ax - b\|^2 + \lambda \|x\|_1)$

References

Arrow's impossibility theorem – Wikipedia

John Geanakoplos, "Three brief proofs of Arrow's Impossibility Theorem" see http://bcn.boulder.co.us/government/approvalvote/altvote.html for Hare system

- 1. Xiaoye Jiang, Yuan Yao, and Leonidas J. Guibas, "Stable Identification of Cliques With Restricted Sensing"
 - 2. Emamnuel J. Candes, "Compressive Sampling"
 - 3. David L. Donoho and Philip B. Stark, "Uncertainty Principles and Signal Recovery"
- 4. David L. Donoho and Xiaoming Huo, ""Uncertainty Principles and Ideal Atomic Decomposition"
- 5. Emamnuel J. Candes and Michael B. Wakin, "An Introduction to Compressive Sampling"
- 6. Emamnuel J. Candes, Xiaodong Li, Yi Ma, and John Wright, "Robust Principal Component Analysis"

11 Appendix

11.1 Asymptotic Notation

We introduce the big O notation here. The motivating example is the analysis of running time of an algorithm. The running time (as a function of the input length n to the instance) may be a complicated function such as $5n^3 + 25n^2 \ln n - 6n + 22$. In asymptotic analysis, we are interested in the behavior as $n \to \infty$; here, the higher order term $5n^3$ dominates. Further, the coefficient 5 of $5n^3$ is not of interest since its value varies depending on the machine model and other specific factors. So we say that this function is $O(n^3)$. The big O notation applies to functions on the positive integers taking on positive real values.

Definition: For functions f, g from the natural numbers to the positive reals, f(n) is O(g(n)) if there exists a constant c > 0 such that for all $n, f(n) \le cg(n)$.

Thus $f(n) = 5n^3 + 25n^2 \ln n - 6n + 22$ is $O(n^3)$. The upper bound need not be tight. Not only is f(n) $O(n^3)$ but it is also $O(n^4)$. Note g(n) must be strictly greater than 0 for all n. Big O is an upper bound; loosely, the function f(n) here is bounded from above by n^3 .

To say that the function f(n) grows at least as fast as g(n), we use a notation called omega of n. We say f(n) is $\Omega(g(n))$ (for positive real valued f,g) if there exists a constant c>0 such that for all n, $f(n)\geq cg(n)$. If f(n) is both O(g(n)) and $\Omega(g(n))$, then f(n) is $\Theta(g(n))$. Thus theta of n is used when the two functions have the same asymptotic growth rate.

Many times we wish to bound the low order terms. To do this, we use a notation called little o of n. We say f(n) is o(g(n)) if $\lim_{n\to\infty}\frac{f(n)}{g(n)}=0$. Note that f(n) being O(g(n)) means that asymptotically f(n) does not grow faster than g(n) where as f(n) being o(g(n)) means that asymptotically f(n)/g(n) goes to zero. If $f(n)=2n+\sqrt{n}$ then f(n) is O(n) but in bounding the lower order term, we write f(n)=2n+o(n). Finally we write $f(n)\sim g(n)$ if $\lim_{n\to\infty}\frac{f(n)}{g(n)}=1$ and say f(n) is $\omega(g(n))$ if $\lim_{n\to\infty}\frac{f(n)}{g(n)}=\infty$. The difference between f(n) being $\Theta(g(n))$ and $f(n)\sim g(n)$ is that in the first case f(n) and g(n) may differ by a multiplicative constant factor.

$$f(n)$$
 is $O(g(n))$ if for all $n, f(n) \leq cg(n)$ for some constant $c > 0$

asymptotic lower bound

$$f(n)$$
 is $\Omega(g(n))$ if for all $n, f(n) \geq cg(n)$ for some constant $c > 0$

asymptotic equality

$$f(n)$$
 is $\Theta(g(n))$ if it is both $O(g(n))$ and $\Omega(g(n))$ for some constant $c>0$

$$f(n)$$
 is $o(g(n))$ if $\lim_{n\to\infty}\frac{f(n)}{g(n)}=0$

$$f(n) \sim g(n)$$
 if $\lim_{n \to \infty} \frac{f(n)}{g(n)} = 1$

$$f(n)$$
 is $\omega\left(g\left(n\right)\right)$ if $\lim_{n\to\infty}\frac{f(n)}{g(n)}=\infty$

Exercise 11.1 What is the difference between saying f(n) is $O(n^3)$ and f(n) is $o(n^3)$?

Solution: In the first case, f(n) grows no faster than n^3 . In the second case, f(n) asymptotically grows slower than n^3 .

Exercise 11.2 If $f(n) \sim g(n)$ what can we say about f(n) + g(n) and f(n) - g(n)?

Solution:
$$f(n) + g(n) \sim 2f(n)$$
 and $f(n) - g(n)$ is $o(f(n))$.

Exercise 11.3 What is the difference between \sim and Θ ?

Solution: For \sim , $\lim_{n\to\infty}\frac{f(n)}{g(n)}=1$ where as for Θ the limit goes to some constant but it might not be one.

Exercise 11.4 If f(n) is O(g(n)) does this imply that g(n) is $\Omega(f(n))$?

Solution: If f(n) is O(g(n)) then there exists c such that $f(n) \le cg(n)$ for sufficiently large n. Thus $g(n) \ge \frac{1}{c}f(n)$ and hence g(n) is $\Omega(g(n))$.

11.2 Useful Inequalities

 $1 + x \le e^x$ for all real x.

One often establishes an inequality such as $1 + x \le e^x$ by showing that the difference of the two sides, namely $e^x - (1 + x)$, is always positive. This can be done by taking derivatives. The first and second derivatives are $e^x - 1$ and e^x . Since e^x is always positive, $e^x - 1$ is monotonic and $e^x - (1 + x)$ is convex. Since $e^x - 1$ is monotonic it can be zero only once and is zero at x = 0. Thus $e^x - (1 + x)$ takes on its minimum at x = 0 where it is zero establishing the inequality.

$$(1-x)^n \ge 1 - nx$$
 for $0 \le x \le 1$

Let $g(x) = (1-x)^n - (1-nx)$. We establish $g(x) \ge 0$ for x in [0,1] by taking the derivative. $g'(x) = -n(1-x)^{n-1} + n = n[1-(1-x)^{n-1}] \ge 0$ for $0 \le x \le 1$. Thus, g takes on its minimum for x in [0,1] at x = 0 where g(0) = 0 proving the inequality.

$$(a+b)^2 \le 2a^2 + 2b^2$$

Since $(a+b)^2+(a-b)^2=2a^2+2b^2$ the inequality follows by subtracting $(a-b)^2$ from both sides of the equation. We can also prove the inequality by resorting to differentiation as in the previous examples: Wlg, assume $a\geq b$. Fix b. Let $f(a)=2a^2+2b^2-(a+b)^2$. Then $f'(a)=4a-2(a+b)=2(a-b)\geq 0$ for $a\geq b$. So the minimum of f(a) over $a\geq b$ is attained at a=b, where it is 0. So the inequality follows.

Triangle Inequality

For any two vectors \mathbf{a} and \mathbf{b} , $|\mathbf{a} + \mathbf{b}| \le |\mathbf{a}| + |\mathbf{b}|$.

 $|\mathbf{a} + \mathbf{b}|^2 = (\mathbf{a} + \mathbf{b}) \cdot (\mathbf{a} + \mathbf{b}) = |\mathbf{a}|^2 + |\mathbf{b}|^2 + 2\mathbf{a} \cdot \mathbf{b} \le |\mathbf{a}|^2 + |\mathbf{b}|^2 + 2|\mathbf{a}||\mathbf{b}| = (|\mathbf{a}| + |\mathbf{b}|)^2$ The inequality follows by taking square roots.

Stirling approximation

$$n! \cong \left(\frac{n}{e}\right)^n \sqrt{2\pi n} \qquad {2n \choose n} \cong \frac{1}{\sqrt{\pi n}} 2^{2n}$$
$$\sqrt{2\pi n} \frac{n^n}{e^n} < n! < \sqrt{2\pi n} \frac{n^n}{e^n} \left(1 + \frac{1}{12n - 1}\right)$$

We will prove the inequalities, except for constant factors, namely, we prove that

$$1.4 \left(\frac{n}{e}\right)^n \sqrt{n} \le n! \le e \left(\frac{n}{e}\right)^n \sqrt{n}.$$

Write $\ln(n!) = \ln 1 + \ln 2 + \cdots + \ln n$. Now this sum is approximately $\int_{x=1}^{n} \ln x \, dx$. [Recall this from Calculus and/or draw the picture; we will discuss approximations of sums by integrals in a later section.] Now, the indefinite $\int \ln x \, dx = (x \ln x - x)$ in closed form and plugging this in gives an approximation, but without the \sqrt{n} term. We need to do a little more work to get the \sqrt{n} . First note that $\ln x$ is a concave function by differentiating twice. This means that for any positive x_0 ,

$$\frac{\ln x_0 + \ln(x_0 + 1)}{2} \le \int_{x = x_0}^{x_0 + 1} \ln x \, dx,$$

since for $x \in [x_0, x_0 + 1]$, the curve $\ln x$ is always above the spline joining $(x_0, \ln x_0)$ and $(x_0 + 1, \ln(x_0 + 1))$. Thus,

$$\ln(n!) = \frac{\ln 1}{2} + \frac{\ln 1 + \ln 2}{2} + \frac{\ln 2 + \ln 3}{2} + \dots + \frac{\ln(n-1) + \ln n}{2} + \frac{\ln n}{2}$$

$$\leq \int_{x=1}^{n} \ln x \, dx + \frac{\ln n}{2} = [x \ln x - x]_{1}^{n} + \frac{\ln n}{2}$$

$$= n \ln n - n + 1 + \frac{\ln n}{2}.$$

Thus, $n! \leq n^n e^{-n} \sqrt{n}e$. For the lower bound on n!, we start with the fact that for any $x_0 \geq 1/2$:

$$\ln x_0 \ge \frac{1}{2} (\ln(x_0 + \rho) + \ln(x_0 - \rho)) \implies \ln x_0 \ge \int_{x = x_0 - 0.5}^{x_0 + .5} \ln x \, dx.$$

So, we get

$$\ln(n!) = \ln 2 + \ln 3 + \dots + \ln n \ge \int_{x=1.5}^{n+.5} \ln x \, dx,$$

from which we can derive a lower bound with a calculation.

Stirling approximation for the binomial coefficient

$$\binom{n}{k} \le \left(\frac{en}{k}\right)^k$$

We get this by using the Stirling approximation for k!:

$$\binom{n}{k} = \frac{n!}{(n-k)!k!} \le \frac{n^k}{k!} \cong \left(\frac{en}{k}\right)^k.$$

The gamma function

$$\Gamma(a) = \int_{0}^{\infty} x^{a-1} e^{-x} dx$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \quad \Gamma(1) = \Gamma(2) = 1, \text{ and for } n \ge 2, \quad \Gamma(n) = (n-1)\Gamma(n-1).$$

The last statement is proved by induction on n. It is easy to see that $\Gamma(1) = 1$. For $n \ge 2$, we will use integration by parts. Recall

Integration by parts

$$\int f(x) g'(x) dx = f(x) g(x) - \int f'(x) g(x) dx$$

Write $\Gamma(n) = \int_{x=0}^{\infty} f(x)g'(x) dx$, where, $f(x) = x^{n-1}$ and $g'(x) = e^{-x}$. Thus,

$$\Gamma(n) = [f(x)g(x)]_{x=0}^{\infty} + \int_{x=0}^{\infty} (n-1)x^{n-2}e^{-x} dx = (n-1)\Gamma(n-2),$$

as claimed.

Cauchy-Schwartz Inequality

$$\left(\sum_{i=1}^{n} x_i^2\right) \left(\sum_{i=1}^{n} y_i^2\right) \ge \left(\sum_{i=1}^{n} x_i y_i\right)^2$$

In vector form, $|\mathbf{x}||\mathbf{y}| \ge \mathbf{x}^T \mathbf{y}$, the inequality states that the dot product of two vectors is at most the product of their lengths. The Cauchy-Schwartz inequality is a special case of Hölder's inequality below with p = q = 2.

Young's inequality

For real numbers p and q where $\frac{1}{p} + \frac{1}{q} = 1$ and positive reals a and b,

$$ab \le \frac{a^p}{p} + \frac{b^q}{q}.$$

The right hand side of Young's inequality, $\frac{1}{p}a^p + \frac{1}{q}b^q$, is a convex combination of a^p and b^q since $\frac{1}{p}$ and $\frac{1}{q}$ sum to 1. Thus

$$\ln(\frac{a^p}{p} + \frac{b^q}{q}) \ge \frac{1}{p}\ln(a^p) + \frac{1}{q}\ln(b^q) = \ln(ab).$$

Since for $x \geq 0$, $\ln x$ is a monotone increasing function, the proof is complete.

Hölder's inequality

For any positive real numbers p and q with $\frac{1}{p} + \frac{1}{q} = 1$,

$$\sum_{i=1}^{n} |x_i y_i| \leq \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p} \left(\sum_{i=1}^{n} |y_i|^q\right)^{1/q}.$$

Let x_i' be $x_i / (\sum_{i=1}^n |x_i|^p)^{1/p}$ and $y_i' = y_i / (\sum_{i=1}^n |y_i|^q)^{1/q}$. Replace x_i by x_i' and y_i by y_i' . This does not change the inequality. Now $\sum_{i=1}^n |x_i'|^p = \sum_{i=1}^n |y_i'|^q = 1$, so it suffices to prove $\sum_{i=1}^n |x_i'y_i'| \le 1$. Apply Young's inequality to get $|x_i'y_i'| \le \frac{(x_i')^p}{p} + \frac{(y_i')^q}{q}$. Summing over i, the right hand side sums to $\frac{1}{p} + \frac{1}{q} = 1$ finishing the proof.

For a_1, a_2, \ldots, a_n real and k a positive integer,

$$(a_1 + a_2 + \dots + a_n)^k \le n^{k-1} (|a_1|^k + |a_2|^k + \dots + |a_n|^k).$$

Using Hölder's inequality with p = k and q = k/(k-1), we have

$$|a_1 + a_2 + \dots + a_n| \le |a_1 \cdot 1| + |a_2 \cdot 1| + \dots + |a_n \cdot 1| \le \left(\sum_{i=1}^n |a_i|^k\right)^{1/k} (1 + 1 + \dots + 1)^{(k-1)/k},$$

from which the current inequality follows.

Arithmetic and geometric means

The arithmetic mean of a set of nonnegative reals is at least their geometric mean. For $a_1, a_2, \ldots, a_n > 0$

$$\frac{1}{n} \sum_{i=1}^{n} a_i \ge \sqrt[n]{a_1 a_2 \cdots a_n}$$

Wlg, we may assume that $a_1 \geq a_2 \geq \ldots a_n$. We will reduce the proof to the case when all the a_i are equal; in that case, the inequality clearly holds with equality. Suppose $a_1 > a_2$. Let ε be a positive infinitesimal. Add ε to a_2 and subtract ε from a_1 (to get closer to the case when they are equal). The left hand side $\frac{1}{n} \sum_{i=1}^{n} a_i$ does not change. $(a_1 - \varepsilon)(a_2 + \varepsilon)a_3a_4 \cdots a_n = a_1a_2 \cdots a_n + \varepsilon(a_1 - a_2)a_3a_4 \cdots a_n + O(\varepsilon^2) > a_1a_2 \cdots a_n$ for small enough $\varepsilon > 0$. Thus, the change has increased $\sqrt[n]{a_1a_2 \cdots a_n}$. So if the inequality holds after the change, it must hold before. By continuing this process, we can make all the a_i equal.

Approximating sums by integrals

For monotonic decreasing f(x),

$$\int_{x=m}^{n+1} f(x)dx \le \sum_{i=m}^{n} f(i) \le \int_{x=m-1}^{n} f(x)dx.$$

See Fig. 11.1. Thus,

$$\int_{x-2}^{n+1} \frac{1}{x^2} dx \le \sum_{i=2}^{n} \frac{1}{i^2} = \frac{1}{4} + \frac{1}{9} + \dots + \frac{1}{n^2} \le \int_{x=1}^{n} \frac{1}{x^2} dx$$

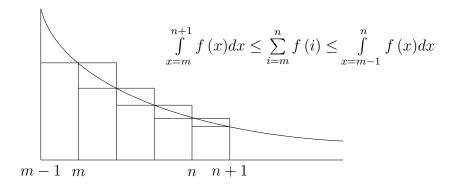


Figure 11.1: Approximating sums by integrals

and hence
$$\frac{3}{2} - \frac{1}{n+1} \le \sum_{i=1}^{n} \frac{1}{i^2} \le 2 - \frac{1}{n}$$
.

Jensen's Inequality

For any convex function f,

$$f\left(\frac{x_1+x_2}{2}\right) \leq \frac{1}{2} \left(f(x_1) + f(x_2)\right).$$

More generally for a convex function f,

$$f\left(\sum_{i=1}^{n} \alpha_i x_i\right) \le \sum_{i=1}^{n} \alpha_i f\left(x_i\right),$$

where $0 \le \alpha_i \le 1$ and $\sum_{i=1}^n \alpha_i = 1$. From this, it follows that for a random variable x,

$$E\left(f\left(x\right)\right) \geq f\left(E\left(x\right)\right)$$

for any convex function f.

Example: Let $f(x) = x^k$, k an even positive integer. Then, $f''(x) = k(k-1)x^{k-2}$ which is always nonnegative since k-2 is even. So f is convex. Thus

$$E(x) \leq \sqrt[k]{E(x^k)},$$

since $t^{\frac{1}{k}}$ is a monotone function of t. It is easy to see that this inequality does not necessarily hold when k is odd; indeed for odd k, x^k is not a convex function.

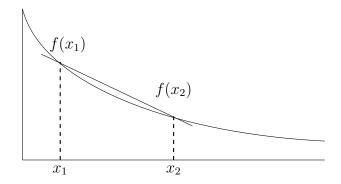


Figure 11.2: For a convex function f, $f\left(\frac{x_1+x_2}{2}\right) \leq \frac{1}{2}\left(f\left(x_1\right) + f\left(x_2\right)\right)$.

Tails of Gaussian

For bounding the tails of Gaussian densities, the following inequality is useful. The proof uses a trick which is used in many contexts.

For
$$t > 0$$
, $\int_{x=t}^{\infty} e^{-x^2} dx \le \frac{e^{-t^2}}{2t}$.

In proof, first write: $\int_{x=t}^{\infty} e^{-x^2} dx \leq \int_{x=t}^{\infty} \frac{x}{t} e^{-x^2} dx$, using the fact that $x \geq t$ in the range. Now the latter expression is integrable in closed form since $d(e^{-x^2}) = (-2x)e^{-x^2}$ and doing the integration, we get the claimed bound.

A similar trick can be used to get an upper bound on

$$\int_{x=\beta}^{1} (1-x^2)^{\alpha} dx,$$

where $\beta \in [0,1]$ and $\alpha > 0$. Just use $(1-x^2)^{\alpha} \le \frac{x}{\beta}(1-x^2)^{\alpha}$ over the range and integrate in closed form the last expression.

11.3 Sums of Series

Summations

$$\sum_{i=0}^{n} a^{i} = 1 + a + a^{2} + \dots = \frac{1 - a^{n+1}}{1 - a}$$

$$\sum_{i=0}^{\infty} a^{i} = 1 + a + a^{2} + \dots = \frac{1}{1 - a}, \quad |a| < 1$$

$$\sum_{i=0}^{\infty} i a^{i} = a + 2a^{2} + 3a^{3} + \dots = \frac{a}{(1 - a)^{2}}, \quad |a| < 1$$

$$\sum_{i=0}^{\infty} i^{2} a^{i} = a + 4a^{2} + 9a^{3} + \dots = \frac{a(1 + a)}{(1 - a)^{3}}, \quad |a| < 1$$

$$\sum_{i=1}^{n} i^{2} = \frac{n(n+1)}{2}$$

$$\sum_{i=1}^{n} i^{2} = \frac{n(n+1)(2n+1)}{6}$$

$$\sum_{i=1}^{\infty} \frac{1}{i^{2}} = \frac{\pi^{2}}{6}$$

We prove one equality.

$$\sum_{i=0}^{\infty} ia^i = a + 2a^2 + 3a^3 \dots = \frac{a}{(1-a)^2}, \text{ provided } |a| < 1.$$

Write $S = \sum_{i=0}^{\infty} ia^i$.

$$aS = \sum_{i=0}^{\infty} ia^{i+1} = \sum_{i=1}^{\infty} (i-1)a^{i}.$$

Thus,

$$S - aS = \sum_{i=1}^{\infty} ia^{i} - \sum_{i=1}^{\infty} (i-1)a^{i} = \sum_{i=1}^{\infty} a^{i} = \frac{a}{1-a},$$

from which the equality follows. The sum $\sum_{i}i^{2}a^{i}$ can also be done by an extension of this method (left to the reader). Using generating functions, we will see another proof of both these equalities by derivatives.

$$\sum_{i=1}^{\infty} \frac{1}{i} = 1 + \frac{1}{2} + \left(\frac{1}{3} + \frac{1}{4}\right) + \left(\frac{1}{5} + \frac{1}{6} + \frac{1}{7} + \frac{1}{8}\right) + \dots \ge 1 + \frac{1}{2} + \frac{1}{2} + \dots$$
 and thus diverges.

The summation $\sum_{i=1}^{n} \frac{1}{i}$ grows as $\ln n$, since, $\sum_{i=1}^{n} \frac{1}{i} \approx \int_{x=1}^{n} \frac{1}{x} dx$. In fact, $\lim_{i \to \infty} \left(\sum_{i=1}^{n} \frac{1}{i} - \ln(n) \right) = \gamma$ where $\gamma \cong 0.5772$ is Euler's constant. Thus $\sum_{i=1}^{n} \frac{1}{i} \cong \ln(n) + \gamma$ for large n.

BEGINNING OF NEW POSSIBLE OMIT A Technique

A sum of the form $\sum_{i=1}^{\infty} \frac{i}{2^i}$ can be rewritten in terms of sums of the form $\sum_{i=1}^{\infty} \frac{1}{2^i}$ where the j^{th} sum is multiplied by $\frac{1}{2^{j-1}}$.

$$\sum_{i=1}^{\infty} \frac{i}{2^i} = \frac{1}{2} + \frac{1}{4}2 + \frac{1}{8}3 + \cdots$$

$$= \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \cdots$$

$$+ \frac{1}{4} + \frac{1}{8} + \cdots$$

$$+ \frac{1}{8} + \cdots$$

$$= 1 + \frac{1}{2} + \frac{1}{4} + \cdots$$

$$= 2$$

For an alternative proof similar to that for the sum $\sum_{i} ia^{i}$, let $S = \sum_{i=0}^{\infty} \frac{i}{2^{i}}$. Then,

$$2S = \sum_{i=1}^{\infty} \frac{i}{2^{i-1}} = \sum_{i=0}^{\infty} \frac{i+1}{2^i}.$$

Subtracting S from 2S,

$$S = \sum_{i=0}^{\infty} \frac{1}{2^i} = 2.$$

END OF NEW POSSIBLE OMIT Exponentials and logs

$$e^{x} = 1 + x + \frac{x^{2}}{2!} + \frac{x^{3}}{3!} + \cdots$$

 $e = 2.7182$
 $\frac{1}{e} = 0.3679$

Setting x=1 in $e^x=1+x+\frac{x^2}{2!}+\frac{x^3}{3!}+\cdots$ yields $e=\sum_{i=0}^{\infty}\frac{1}{i!}$. By definition $\frac{d}{dx}e^x=e^x$. Thus, $\lim_{\Delta x\to 0}\frac{e^{x+\Delta x}-e^x}{\Delta x}=e^x$ or $\lim_{\Delta x\to 0}\frac{e^{\Delta x}-1}{\Delta x}=1$. Hence, $\lim_{\Delta x\to 0}\left(\frac{e^{\Delta x}-1}{\Delta x}-1\right)=0$ which implies $\lim_{\Delta x\to 0}\left(e^{\Delta x}-1-\Delta x\right)=0$ and thus $\lim_{\Delta x\to 0}\left((1+\Delta x)^{\frac{1}{\Delta x}}\right)=e$. From this is follows that $\lim_{n\to\infty}\left(1+\frac{1}{n}\right)^n$.

$$\lim_{n \to \infty} \left(1 + \frac{a}{n} \right)^n = e^a$$

$$\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 \cdot \dots \quad |x| < 1$$

The above expression with -x substituted for x gives rise to the approximations $\ln(1-x) < -x$ which also follows from $1-x \le e^{-x}$, since $\ln(1-x)$ is a monotone function for $x \in (0,1)$.

For 0 < x < 0.69, $\ln(1-x) > -x - x^2$.

Exercise 11.5 What is $\lim_{k\to\infty} \left(\frac{k-1}{k-2}\right)^{k-2}$.

Solution:
$$(1 - \frac{1}{k-2})^{k-2} = e$$
.

Exercise 11.6 $e^{-\frac{x^2}{2}}$ has value 1 at x=0 and drops off very fast as x increases. Suppose we wished to approximate $e^{-\frac{x^2}{2}}$ by a function f(x) where

$$f(x) = \begin{cases} 1 & |x| \le a \\ 0 & |x| > a \end{cases}.$$

What value of a should we use? What is the integral of the error between f(x) and $e^{-\frac{x^2}{2}}$?

Solution: $\int_{x=-\infty}^{\infty} e^{-\frac{x^2}{2}} dx = \sqrt{2\pi}.$ Thus if we select $a = \frac{1}{2}\sqrt{2\pi}$ or approximately 1.25 we will have $\int_{x=-\infty}^{\infty} f(x) dx = \sqrt{2\pi}.$ The error will be $4 \int_{x=-\infty}^{a} e^{-\frac{x^2}{2}} dx = 4 (0.1056) = 0.42$ out of an area of $\sqrt{2\pi} \cong 2.5$ or 17%.

BEGIN NEW POSSIBLE OMIT

Trigonometric identities

$$\sin(x \pm y) = \sin(x)\cos(y) \pm \cos(x)\sin(y)$$

$$cos(x \pm y) = cos(x) cos(y) \mp sin(x) sin(y)$$

$$\cos(2\theta) = \cos^2 \theta - \sin^2 \theta = 1 - 2\sin^2 \theta$$

$$\sin(2\theta) = 2\sin \theta \cos \theta$$

$$\sin^2 \frac{\theta}{2} = \frac{1}{2}(1 - \cos \theta)$$

$$\cos^2 \frac{\theta}{2} = \frac{1}{2}(1 + \cos \theta)$$

END OF NEW POSSIBLE OMIT

Gaussian and related Integrals

$$\int \frac{1}{a^2 + x^2} dx = \frac{1}{a} \tan^{-1} \frac{x}{a} \text{ thus } \int_{-\infty}^{\infty} \frac{1}{a^2 + x^2} dx = \frac{\pi}{a}$$

$$\int_{-\infty}^{\infty} e^{-\frac{a^2 x^2}{2}} dx = \frac{\sqrt{2\pi}}{a} \text{ thus } \frac{a}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{a^2 x^2}{2}} dx = 1$$

$$\int_{0}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$$
integration by parts reduces it to $\int xe^{-ax^2}.$

$$\int_{0}^{\infty} x^{2n} e^{-ax^{2}} dx = \frac{1 \cdot 3 \cdot 5 \cdot \cdot \cdot (2n-1)}{2^{n+1} a^{n}} \sqrt{\frac{\pi}{a}}$$

repeated integration by parts

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

To verify $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$, consider $\left(\int_{-\infty}^{\infty} e^{-x^2} dx\right)^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\left(x^2+y^2\right)} dx dy$. Let $x = r \cos \theta$ and $y = r \sin \theta$. The Jacobian of this transformation of variables is

$$J(r,\theta) = \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{vmatrix} = \begin{vmatrix} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{vmatrix} = r$$

Thus,

$$\left(\int_{-\infty}^{\infty} e^{-x^2} dx\right)^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\left(x^2 + y^2\right)} dx dy = \int_{0}^{\infty} \int_{0}^{2\pi} e^{-r^2} J\left(r, \theta\right) dr d\theta$$
$$= \int_{0}^{\infty} e^{-r^2} r dr \int_{0}^{2\pi} d\theta$$
$$= 2\pi \left[\frac{e^{-r^2}}{2}\right]_{0}^{\infty} = \pi$$

Thus
$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$
.

Binomial coefficients

$$\binom{n}{d} + \binom{n}{d+1} = \binom{n+1}{d+1}.$$

The number of ways of choosing k items from 2n equals the number of ways of choosing i items from the first n and choosing k-i items from the second n summed over all i, $0 \le i \le k$.

$$\sum_{i=0}^{k} \binom{n}{i} \binom{n}{k-i} = \binom{2n}{k}.$$

An alternative derivation is to equate the coefficients of

$$x^k$$
 in $(1+x)^n (1+x)^n = (1+x)^{2n}$.

Setting k = n in the above formula and observing that $\binom{n}{i} = \binom{n}{n-i}$ yields

$$\sum_{i=0}^{n} \binom{n}{i}^2 = \binom{2n}{n}$$

More generally $\sum_{i=0}^{k} {n_1 \choose i} {n_2 \choose k-i} = {n_1+n_2 \choose k}$ by a similar derivation.

11.4 Probability

Consider an experiment such as flipping a coin whose outcome is determined by chance. To talk about the outcome of a particular experiment, we introduce the notion of a random variable, a variable whose value is the outcome of the experiment. The set of possible outcomes is called the *sample space*. If the sample space is finite, we can assign a probability of occurrence to each outcome. In some situations where the sample space is infinite,

we can assign a probability of occurrence. The probability $p(i) = \frac{6}{\pi^2} \frac{1}{i^2}$ for i an integer greater than or equal to one is such an example. The function assigning the probabilities is called a *probability distribution function*.

In many situations, a probability distribution function does not exist. For example, the uniform probability on the interval [0,1]. What we can do instead is define a probability density function p(x) such that

$$Prob(a < x < b) = \int_{a}^{b} p(x)dx$$

If x is a continuous random variable for which a density function exists, then we can define the cumulative distribution function f(a) by

$$f(a) = \int_{-\infty}^{a} p(x)dx$$

which gives the probability that $x \leq a$.

11.4.1 Sample Space, Events, Independence

There may be more than one relevant random variable in a situation. For example, if we toss n coins, there are n random variables, x_1, x_2, \ldots, x_n , taking on values 0 and 1, a 1 for heads and a 0 for tails. The set of possible outcomes (the sample space) here is $\{0,1\}^n$. An *event* is a subset of the sample space. For example, the event, an odd number of heads, consists of all elements of $\{0,1\}^n$ with an odd number of 1's. For two events A and B, the conditional probability of A given that B has occurred is denoted by P(A|B). We have

$$P(A|B) = \frac{P(A \text{ and } B)}{P(B)}.$$

Events A and B are independent if P(A, B) = P(A)P(B) or equivalently, P(A|B) = P(A). Two random variables x and y are independent if for every possible set A of values of x and every possible set B of values of y, the events $x \in A$ and $y \in B$ are independent.

Example: Dependent variables: Consider two independent random variables x and y. The variables $\frac{x}{x+y}$ and $\frac{y}{x+y}$ are dependent since their sum is one. Since $\frac{y}{x+y} = 1 - \frac{x}{x+y}$ knowing the value of $\frac{x}{x+y}$ uniquely determines the value of $\frac{y}{x+y}$.

Example: x_1 , x_2 , and x_3 are independent random variables, each equal to zero with probability $\frac{1}{2}$. Let $S = x_1 + x_2 + x_3$ and let F be event that $S \in \{1, 2\}$. Conditioning on S, x_1 , x_2 , and x_3 are still each zero with probability $\frac{1}{2}$ but are no longer independent.

$$\frac{1}{4} = p(x_1 = 0|S)p(x_2 = 0|S) \neq p(x_1 = 0, x_2 = 0|S) = 1/6$$

Exercise 11.7 Select a, b, and c uniformly at random from [0,1]. The probability that b < a is 1/2. The probability that c < a is 1/2. However, the probability that both b and c are less than a is 1/3 not 1/4. Why is this? Note that the six possible permutations abc, acb, bac, cab, bca, and cba, are all equally likely. Assume that a, b, and c are drawn from the interval (0,1]. Given that b < a, what is the probability that c < a?

Solution: Even though b and c were drawn independently at random, the events b < a and c < a are not statistically independent.

A collection of n random variables x_1, x_2, \ldots, x_n are mutually independent if for all possible sets A_1, A_2, \ldots, A_n of values of x_1, x_2, \ldots, x_n , we have

$$P(x_1 \in A_1, x_2 \in A_2, \dots, x_n \in A_n) = P(x_1 \in A_1)P(x_2 \in A_2)\cdots P(x_n \in A_n).$$

This condition is much stronger than requiring only that each pair of the variables is independent. Indeed, consider the example of 2-universal hash functions we discussed in Chapter ??. Let M be a prime. For each pair of integers a and b in the range [0,M-1], define a hash function

$$h_{ab}(x) = ax + b \mod (M),$$

for $x \in \{0, 1, 2, ..., m\}$. Consider any two values z, w for the hash function and any two arguments x and y. We would have h(x) = z and h(y) = w if and only if

$$\left(\begin{array}{cc} x & 1 \\ y & 1 \end{array}\right) \left(\begin{array}{c} a \\ b \end{array}\right) = \left(\begin{array}{c} z \\ w \end{array}\right) \mod(M)$$

If $x \neq y$, the matrix $\begin{pmatrix} x & 1 \\ y & 1 \end{pmatrix}$ is invertible modulo M and there is only one solution for a and b. Thus, for a and b chosen uniformly at random, the probability of the equation holding is exactly $\frac{1}{M^2}$. This shows that given the values $h_{ab}(x)$ and $h_{ab}(y)$ at two distinct points x, y, a and b are uniquely determined. This implies that three arguments x, y, and u do not have independent values h(x), h(y), and h(u). Thus, h(x), h(y), and h(u) are pairwise independent, but not mutually independent.

Linearity of Expectation

Another important concept is that of the expectation of a random variable. The expected value of a random variable x is $E(x) = \sum_{x} xp(x)$ in the discrete case and $E(x) = \sum_{x} xp(x)$

 $\int_{-\infty}^{\infty} xp(x)dx$ in the continuous case. The expectation of a sum of random variables is equal to the sum of their expectations. The linearity of expectation follows directly from the definition and does not require independence.

Theorem 11.1
$$E(\sum x_i) = \sum E(x_i)$$

Proof:

$$E(x_1 + x_2) = \sum_{x_1} \sum_{x_2} (x_1 + x_2) p(x_1, x_2)$$

$$= \sum_{x_1} \sum_{x_2} x_1 p(x_1, x_2) + \sum_{x_1} \sum_{x_2} x_2 p(x_1, x_2)$$

$$= \sum_{x_1} x_1 p(x_1) + \sum_{x_2} x_2 p(x_2)$$

$$= E(x_1) + E(x_2)$$

Indicator variables

A useful tool is that of an indicator variable that takes on value 0 or 1 to indicate whether some quantity is present or not. For example, an indicator variable x_i might take on the value 0 or 1 to indicate if the integer i is in a set. The indicator variable is useful in determining the expected size of a subset. Given a random subset of the integers $\{1, 2, \ldots, n\}$, the expected size of the subset is the expected value of $x_1+x_2+\cdots+x_n$ where x_i is the indicator variable that takes on value 1 if i is in the subset. For another example suppose y_1, y_2, \ldots, y_n are independent real-valued random variables. We are interested in how many of them are greater than 10. Define x_i to be an indicator random variable for the event $y_i \geq 10$. The x_i are independent and we can use Chernoff bounds for the sum of the x_i .

Example: Define the indicator function $x_i = 1$ if the i^{th} integer in a permutation of n integers is i. What is expected number of fixed points?

$$E\left(\sum_{i=1}^{n} x_i\right) = \sum_{i=1}^{n} E(x_i) = n\frac{1}{n} = 1.$$
 .

Note that th x_i are not independent. But, linearity of expectation still applies.

Example: Suppose we want to determine the expected number of vertices in a random graph G(n, p) of degree d. The number of vertices of degree d is the sum of n indicator random variables, one for each vertex, telling us if that vertex has degree d or not. Thus the expectation is the sum of the expectations of the n indicator random variables and by symmetry, this is just n times the expectation of one of them.

11.4.2 Variance

In addition to the expected value of a random variable, another important parameter is the variance. The variance of a random variable is $\sigma^2 = E(x - E(x))^2$ and measures how close to the expected value the random variable is likely to be. The standard deviation σ is the square root of the variance. The units of σ are the same as those of x.

By linearity of expectation

$$\sigma^{2} = E(x - E(x))^{2} = E(x^{2}) - 2E(x)E(x) + E^{2}(x) = E(x^{2}) - E^{2}(x).$$

11.4.3 Covariance

The covariance measures the degree to which random variables are correlated. Let x and y be random variables. Define

$$cov(x, y) = E[(x - E(x))(y - E(y))] = E(xy) - E(x)E(y)$$

Covariance is related to variance:

$$var(x + y) = E[(x + y)^{2}] - E^{2}(x + y)$$

$$= E(x^{2}) - E^{2}(x) + E(y^{2}) - E^{2}(y) + 2E(xy) - 2E(x)E(y)$$

$$= var(x) + var(y) + 2cov(x, y)$$

11.4.4 Variance of Sum of Independent Random Variables

If x and y are independent, then E(xy) = E(x) E(y) and cov(x, y) = 0. In this case

$$var(x + y) = var(x) + var(y)$$
.

More generally, if x_1, x_2, \ldots, x_n are pairwise independent random variables, then

$$var(x_1 + x_2 + \dots + x_n) = var(x_1) + var(x_2) + \dots + var(x_n).$$

11.4.5 Sum of independent random variables, Central Limit Theorem

Let $s = x_1 + x_2 + \cdots + x_n$ be a sum of n independent random variables where each x_i has probability distribution

$$x_i = \left\{ \begin{array}{cc} 0 & \frac{1}{2} \\ 1 & \frac{1}{2} \end{array} \right..$$

The expected value of each x_i is 1/2 with variance $\sigma_i^2 = \left(\frac{1}{2} - 0\right)^2 \frac{1}{2} + \left(\frac{1}{2} - 1\right)^2 \frac{1}{2} = \frac{1}{4}$. The expected value of s is n/2 and since the variables are independent, the variance of the sum is the sum of the variances and hence is n/4. How concentrated s is around its mean depends on the standard deviation of s or $\frac{\sqrt{n}}{2}$. Thus, for n equal 100 the expected value of s is 50 with a standard deviation of 5 which is 10% of the mean. For n = 10,000 the expected value of s is 5,000 with a standard deviation of 50 which is 1% of the mean. Note that as n increases, the standard deviation increases, but the ratio of the standard deviation to the mean goes to zero. In fact, the central result of Probability Theory is the Central Limit Theorem (which we now state) quantifies this.

Theorem 11.2 Suppose x_i , i = 1, 2, ... is an (infinite) sequence of independent identically distributed random variables, each with mean μ and variance σ^2 . The distribution of the random variable

$$\frac{1}{\sqrt{n}}\left(x_1+x_2+\cdots+x_n-n\mu\right)$$

converges to the distribution of the Gaussian with mean 0 and variance σ^2 .

The variance of $x_1 + x_2 + \cdots + x_n$ thus behaves as $n\sigma^2$ which is what we expect since it is the sum of n independent random variables, each with variance σ^2 . We divide the sum $x_1 + x_2 + \cdots + x_n$ by \sqrt{n} to make the variance bounded (recall that limiting value has to be bounded for the limit to exist.)

11.4.6 Median

One often calculates the average value of a random variable or a set of items to get a feeling for the magnitude of the variable. If the probability distribution of the variable is Gaussian, or has a small variance this is reasonable. However, if there are outliers or if the probability is not concentrated about its expected value, then the average may be distorted by some outlier. An alternative to calculating the expected value is to calculate the median, the value for which half of the probability is above and half is below.

Exercise 11.8 Give examples of non-negative valued random variables with median >> mean. Can we have median << mean?

11.4.7Unbiased estimators

Consider n samples x_1, x_2, \ldots, x_n from a Gaussian distribution of mean μ and variance σ . For this distribution $m = \frac{x_1 + x_2 + \cdots + x_n}{n}$ is an unbiased estimator of μ . If μ is known then $\frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$ is an unbiased estimator of σ^2 . However, if μ is not known and we approximate μ by m, then $\frac{1}{n-1}\sum_{i=1}^{n}(x_i-m)^2$ turns out to be an unbiased estimator of σ^2 . This can be seen by a detailed calculation.

SUGGEST WE OMIT THE CALCULATION BELOW Note that m is not independent of the x_i and that $\frac{1}{n}\sum_{i=1}^{n}(x_i-m)^2 \leq \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$ since y = m minimizes $\frac{1}{n} \sum_{i=1}^{n} (x_i - y)^2$ and thus $\frac{1}{n} \sum_{i=1}^{n} (x_i - m)^2$ is likely to be a biased estimator.

To see that $s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - m)^2$ is an unbiased estimator of the variance σ^2 consider $E(s^2)$. In what follows note that x_1, x_2, \ldots, x_n and m are all random variables where as μ is not.

$$E(s^{2}) = \frac{1}{n-1}E\left(\sum_{i=1}^{n}(x_{i}-m)^{2}\right)$$

$$= \frac{1}{n-1}E\left(\sum_{i=1}^{n}x_{i}^{2}-2m\sum_{i=1}^{n}x_{i}+\sum_{i=1}^{n}m^{2}\right)$$

$$= \frac{1}{n-1}\left(\sum_{i=1}^{n}E(x_{i}^{2})-2nE(m^{2})+nE(m^{2})\right)$$

$$= \frac{1}{n-1}\left(\sum_{i=1}^{n}E(x_{i}^{2})-nE(m^{2})\right)$$

Now by definition, the variance of a random variable y is given by

$$Var(y) = E[(y - E(y))^{2}] = E(y^{2}) - (E(y))^{2}.$$

Using this formula

$$E(x_i^2) = Var(x_i) + (E(x_i))^2 = \sigma^2 + \mu^2$$

and

$$E(m^{2}) = Var(m) + (E(m))^{2}$$

$$= Var\left(\frac{1}{n}\sum_{i=1}^{n}x_{i}\right) + \mu^{2}$$

$$= \frac{1}{n^{2}}Var\left(\sum_{i=1}^{n}x_{i}\right) + \mu^{2}$$

$$= \frac{1}{n^{2}}\left(\sum_{i=1}^{n}Var(x_{i})\right) + \mu^{2}$$

$$= \frac{1}{n}\sigma^{2} + \mu^{2}$$

Substituting into the formula for $E(s^2)$ we get

$$E(s^{2}) = \frac{1}{n-1} \left[n(\sigma^{2} + \mu^{2}) - n\left(\frac{1}{n}\sigma^{2} + \mu^{2}\right) \right]$$
$$= \frac{1}{n-1} \left[(n-1)\sigma^{2} \right]$$
$$= \sigma^{2}$$

Thus
$$E(s^2) = \frac{1}{n-1} E\left(\sum_{i=1}^n (x_i - m)^2\right)$$
 is indeed unbiased.

END OF OMIT

Given a distribution, the sample mean $m = \frac{x_1 + x_2 + \dots + x_n}{n}$ is an unbiased estimator of the mean μ . To estimate the variance one can use $s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - m)^2$ or $s^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \mu)^2$ if the true mean μ is known. If the distribution is symmetric, the median is also an unbiased estimator of the mean.

11.4.8 Probability Distributions

John, Bernoulli trials and the calculations with the binomial are important.. But we have now at different places (for example when we do the new tail bounds proof) put in stuff about approximating binomial with the normal. So I am in two minds about leaving this in... Possible Omit??

Bernoulli trials and the binomial distribution

A Bernoulli trial has two possible outcomes, called success or failure, with probabilities p and 1-p, respectively. If there are n independent Bernoulli trials, the probability of exactly k successes is given by the binomial distribution

$$B(n,p) = \binom{n}{k} p^k (1-p)^{n-k}$$

The mean and variance of the binomial distribution B(n, p) are np and np(1-p) respectively.

The mean of the binomial distribution can be easily seen to be np, by just linearity of expectations. Also the variance can easily be seen to be np(1-p) by using the fact that the variance of a sum of independent random variables is the sum of their variances. But we will give different derivations to explain the technique for summing some combinatorial quantities that come up. To derive the mean for the binomial distribution, express the

mean as

$$m = \sum_{k=0}^{n} k \binom{n}{k} p^{k} (1-p)^{n-k}.$$

To evaluate the summation consider the formula $(p+q)^n = \sum_k \binom{n}{k} p^k q^{n-k}$. Taking derivatives of both sides with respect to p yields

$$n(p+q)^{n-1} = \frac{1}{p} \sum_{k} k \binom{n}{k} p^{k} q^{n-k}.$$

Setting q = 1 - p gives $n = \frac{1}{p} \sum_{k} k \binom{n}{k} p^k (1 - p)^{n-k}$ or $np = \sum_{k} k \binom{n}{k} p^k (1 - p)^{n-k}$. Thus, the mean for the binomial distribution is np.

To derive the variance for the binomial distribution, take the second derivative and again set q = 1 - p. This yields

$$n(n-1) = \frac{1}{p^2} \sum_{k} k(k-1) \binom{n}{k} p^k (1-p)^{n-k}.$$

Thus,

$$p^{2}n(n-1) = \sum_{k} k^{2} \binom{n}{k} p^{k} (1-p)^{n-k} - \sum_{k} k \binom{n}{k} p^{k} (1-p)^{n-k}$$

or

$$p^{2}n(n-1) + np = \sum_{k} k^{2} \binom{n}{k} p^{k} (1-p)^{n-k}.$$

Now

$$\sigma^{2} = \sum (np - k)^{2} {n \choose k} p^{k} (1 - p)^{n-k} = (np)^{2} - 2 (np)^{2} + \sum k^{2} {n \choose k} p^{k} (1 - p)^{n-k}$$

or

$$\sigma^2 = -(np)^2 + p^2 n (n-1) + np = np (1-p).$$

Thus, the variance of the binomial distribution is $\sigma^2 = np(1-p)$.

Let x_1 be the number of successes in n_1 trials and let x_2 be the number of successes in n_2 trials. Then the probability distribution of the sum of the successes, $x_1 + x_2$, is the same as the distribution of $x_1 + x_2$ successes in $n_1 + n_2$ trials. That is, if x_1 is distributed according to $B(n_1, p)$ and x_2 is $B(n_2, p)$, then $x_1 + x_2$ is $B(n_1 + n_2, p)$. To see this, let $p(x_1 = k) = \binom{n_1}{k} p^k (1-p)^{n_1-k}$ and $p(x_2 = k) = \binom{n_2}{k} p^k (1-p)^{n_2-k}$. Then

$$p(x_1 + x_2 = k) = \sum_{i=0}^{k} {n_1 \choose i} {n_2 \choose k-1} p^i p^{k-i} (1-p)^{n_1-i} (1-p)^{n_2-k+i}$$

$$= \sum_{i=0}^{k} {n_1 \choose i} {n_2 \choose k-1} p^k (1-p)^{n_1+n_2-k}$$

$$= {n_1 + n_2 \choose k} p^k (1-p)^{n_1+n_2-k}$$

Thus, $B(n_1, p) + B(n_2, p) = B(n_1 + n_2, p)$.

END OF POSSIBLE OMIT

Poisson distribution

The Poisson distribution describes the probability of k events happening in a unit of time if the average rate per unit of time is λ . Divide the unit of time into n segments. When n is large enough, each segment is sufficiently small so that the probability of two events happening in the same segment is negligible. The Poisson distribution gives the probability of k events happening in a unit of time and can be derived from the binomial distribution by taking the limit as $n \to \infty$.

Let
$$p = \frac{\lambda}{n}$$
. Then

Prob (k successes in a unit of time) =
$$\lim_{n \to \infty} \binom{n}{k} \left(\frac{\lambda}{n}\right)^k \left(1 - \frac{\lambda}{n}\right)^{n-k}$$

= $\lim_{n \to \infty} \frac{n(n-1)\cdots(n-k+1)}{k!} \left(\frac{\lambda}{n}\right)^k \left(1 - \frac{\lambda}{n}\right)^n \left(1 - \frac{\lambda}{n}\right)^{-k}$
= $\lim_{n \to \infty} \frac{\lambda^k}{k!} e^{-\lambda}$

In the limit as n goes to infinity the binomial distribution $p(k) = \binom{n}{k} p^k (1-p)^{n-k}$ becomes the Poisson distribution $p(k) = e^{-\lambda} \frac{\lambda^k}{k!}$. The mean and the variance of the Poisson distribution have value λ . If x and y are both Poisson random variables from distributions with means λ_1 and λ_2 respectively, then x + y is Poisson with mean $m_1 + m_2$. For large n and small p we can approximate the binomial distribution with the Poisson distribution.

The Gaussian or Normal distribution

In one dimension the normal distribution is

$$\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{1}{2}\frac{(x-m)^2}{\sigma^2}}$$

where m is the mean and σ^2 is the variance. The coefficient $\frac{1}{\sqrt{2\pi}\sigma}$ makes the integral of the distribution be one. If we measure distance in units of the standard deviation σ from the mean, then

$$\phi(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

Standard tables give values of the integral

$$\int_{0}^{t} \phi(x) dx$$

and from these values we can compute probability integrals for a normal distribution with mean m and variance σ^2 .

"In a normal distribution, a one-standard-deviation event occurs with a probability of one in three, a two-standard-deviation event occurs with a probability of one in twenty and a three-standard-deviation event occurs with a probability of one in a hundred. Based on a 250-business-day year, an eight-standard deviation event occurs once every three trillion years. Twenty-five-standard-deviation events should not happen"

David F. Swensen "Unconventional Success A Fundamental Approach to Personal Investment" in talking about the 1987 stock market crash.

Exercise 11.9 Given the distribution $\frac{1}{\sqrt{2\pi}3}e^{-\frac{1}{2}\left(\frac{x}{3}\right)^2}$ what is the probability that x > 1?

Solution: Substitute $y = \frac{x}{3}$. Then

$$\frac{1}{2\pi} \int_{\frac{1}{2}}^{\infty} e^{-\frac{1}{2}y^2} = \frac{1}{2} - \frac{1}{2\pi} \int_{0}^{\frac{1}{3}} e^{-\frac{1}{2}y^2} \cong \frac{1}{2} - 0.1293 \cong 0.3707$$

The binomial distribution with mean np and variance np(1-p) can be approximated by the normal distribution with mean np and variance np(1-p). The Central Limit Theorem tells us that there is such an approximation in the limit. The approximation is good if both np and n(1-p) are greater than 10 provided also k is not extreme. Thus

$$\binom{n}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{n-k} \cong \frac{1}{\sqrt{\pi n/2}} e^{-\frac{(n/2-k)^2}{\frac{1}{2}n}}.$$

This approximation is excellent provided k is $\Theta(n)$. The Poisson approximation

$$\binom{n}{k} p^k \left(1 - p\right)^k \cong e^{-np} \frac{(np)^k}{k!}$$

is off for central values and tail values even for p = 1/2. The approximation

$$\binom{n}{k} p^k (1-p)^{n-k} \cong \frac{1}{\sqrt{\pi pn}} e^{-\frac{(pn-k)^2}{pn}}$$

is good for p=1/2 but error for other values of p.

Product distributions in high dimensions

We now consider random variables which take on vector values $\mathbf{x} = (x_1, x_2, \dots, x_d)$. If the x_i are independent, we can express the joint probability distribution as the product of individual distributions:

$$p(\mathbf{x}) = p_1(x_1)p_2(x_2)\cdots p_n(x_n).$$

Such distributions are called product distributions. For example, define

$$p\left(x_{i}\right) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x_{i}^{2}}{2}}$$

and

$$p(x_1, x_2, \dots, x_d) = \prod_{i=1}^{d} p(x_i) = \frac{1}{(2\pi)^{\frac{d}{2}}} e^{-\frac{x_1^2 + x_2^2 + \dots + x_d^2}{2}}.$$

For a Gaussian distribution with the same variance in each dimension the resulting distribution p(x) is spherically symmetric. One can use any orthogonal vectors for the axes and get the same result. If instead of Gaussian the individual coordinates were Cauchy, then we would not get a spherically symmetric distribution. For example define

$$p\left(x_{i}\right) = \frac{1}{1 + x_{i}^{2}}$$

and

$$p(x) = \frac{1}{\pi^d} \frac{1}{(1+x_1^2)\cdots(1+x_d^2)}.$$

The distribution in d dimensions is not spherically symmetric. A symmetric distribution would be

$$p(x) = \frac{1}{\pi^d} \frac{1}{1 + (x_1^2 + x_2^2 + \dots + x_d^2)}.$$

If we generate a distribution in d-dimensions where each coordinate is $p(x_i) = \frac{1}{1+x_i^2}$ and coordinates are independent, how far off from spherical is the distribution? Consider a sphere of radius 1. The maximum probability on the sphere occurs at $x_1 = 1$, $x_2 = x_3 = \cdots = x_d = 0$ where the value is $\frac{1}{2\pi}$. The minimum occurs at $x_1 = x_2 = \cdots = x_d = \frac{1}{\sqrt{d}}$

where the value is $\frac{1}{\pi} \frac{1}{\left(1 + \frac{1}{d}\right)^d}$ which for large d approaches $\frac{1}{\pi e}$. Thus the ratio of maximum to minimum on the sphere is $\frac{e}{2} \cong 1.36$.

Rotation of coordinates

In general, rotation of coordinates does not preserve independence. Let

$$x, y = \begin{cases} 1 & \text{Prob } \frac{1}{2} \\ 0 & \text{Prob } \frac{1}{2} \end{cases}$$

Consider rotating the coordinates 30°. Then

$$x_1 = x \sin \theta + y \cos \theta$$

$$y_1 = -x \cos \theta + y \sin \theta$$

Given the value of x_1 , one can calculate both x and y and thus y_1 . Since, the value of x_1 uniquely determines the value of y_1 and they are not independent. However, for spherical Gaussian distributions rotation of axis does not lose independence.

Random Vectors with Dependent Coordinates

There are non-product distributions. The most commonly used is a non-spherical Gaussian. In a non-spherical Gaussian, the coordinates x_i of the random vector \mathbf{x} are not independent. There are non-zero correlations among them. These correlations define the Gaussian.

The variance-covariance matrix S of a d-dimensional Gaussian is an $d \times d$ matrix with S_{ij} equal to the covariance of x_i and x_j for $i \neq j$ and S_{ii} equal to the variance of x_i . It is easy to show that S must be positive semi-definite and barring trivial cases, positive definite. So S^{-1} exists. The probability density of the Gaussian is given by

$$F(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} \sqrt{\det(S)}} \exp\left(-\frac{1}{2} (\mathbf{x} - \mu)^T S^{-1} (\mathbf{x} - \mu)\right).$$

BEGIN POSSIBLE NEW OMIT

Exponential distribution

The probability density function for the exponential distribution is

$$p(x) = \begin{cases} \alpha e^{-\alpha x} & x \ge 0\\ 0 & x < 0 \end{cases}$$

Then $\int_{0}^{\infty} \alpha e^{-\alpha x} dx = -e^{-\alpha x}|_{0}^{\infty} = 1$. The mean and variances are given by

$$\int_{0}^{\infty} \alpha x e^{-\alpha x} dx = -\frac{e^{-\alpha x}}{\alpha} (\alpha x - 1) \Big|_{0}^{\infty} = \frac{1}{\alpha}$$

and

$$\int_{0}^{\infty} \left(\frac{1}{\alpha} - x\right)^{2} \alpha e^{-\alpha x} dx = \frac{1}{\alpha^{2}}$$

INSERT FIGURE

Generation of random numbers according to a given probability distribution

Suppose you wish to generate a random variable with probability density p(x) where p(x) is continuous. Let P(x) be the cumulative distribution function for x and let u be a random variable with uniform probability density over the interval [0,1]. Then the random variable $x = P^{-1}(u)$ has probability density p(x).

Example: For a Cauchy density function

$$P(x) = \int_{t=-\infty}^{x} \frac{1}{\pi} \frac{1}{1+t^2} dt = \frac{1}{2} + \frac{1}{\pi} \tan^{-1}(x).$$

Setting u = P(x) and solving for x yields $x = \tan\left(\pi\left(u - \frac{1}{2}\right)\right)$. The cumulative distribution function is given by

$$\frac{1}{2} + \int_{0}^{y} p(x) dx = \frac{1}{2} + \frac{2}{\pi} \int_{0}^{y} \frac{1}{1 + x^{2}} dx = \frac{1}{2} + \frac{1}{\pi} \tan^{-1}(y)$$

Thus, to generate a random number $x \ge 0$ with Cauchy distribution, generate $u, 0 \le u \le 1$, uniformly and calculate $\tan \left[\pi \left(u - \frac{1}{2}\right)\right]$. The value of x varies from $-\infty$ to ∞ with x = 0 for u = 1/2.

END OF NEW POSSIBLE OMIT

Maximum likelihood estimation MLE

Suppose the probability distribution of a random variable x depends on a parameter r. With slight abuse of notation (since r is a parameter rather than a random variable), we denote the probability distribution of x as p(x|r); this is the likelihood of observing x if r was in fact the parameter value. The job of the maximum likelihood estimator (MLE) to find the best r after observing values of the random variable x. The likelihood of r given the observed values of x, denoted L(r|x) is the probability of observing the observed value of x as a function of the parameter r. The maximum likelihood is the value of r that maximizes the function L(r|x).

Consider flipping a coin 100 times. Suppose we observe 62 heads and 38 tails. What is the most likely value of the probability of the coin to come down heads when the coin is

flipped? In this case, it is r = 0.62. The probability that we get 62 heads if the unknown probability of heads in one trial is r is

Prob(62 heads
$$|r| = {100 \choose 62} r^{62} (1-r)^{38}$$
.

This quantity is maximized when r = 0.62. To see this, take the logarithm which as a function of r is $\ln \binom{100}{62} + 62 \ln r + 38 \ln(1-r)$. Differentiating with respect to r, we see that the derivative is zero at r = 0.62 and the second derivative tells us this is a maximum. This r = 0.62 is called the maximum likelihood estimator of the probability of heads in a trial.

Bayes rule

Given a joint probability distribution P(A, B), Bayes Theorem relates the conditional probability of A given B to the conditional probability of B given A.

$$P(A|B) = \frac{P(B|A) P(A)}{P(B)}$$

Suppose we know the probability of A and want to know how this probability changes if we know that B has occurred. P(A) is called the prior probability. The conditional probability P(A|B) is called the posterior probability because it is the probability of A after we know that B has occurred.

BEGIN NEW POSSIBLE OMIT

The following example illustrates the use of Bayes theorem.

Example: Given two sets of red and black balls

	red	black
Set 1	40	60
Set 2	50	50

Randomly draw a ball from one of the sets. Suppose that it turns out to be red. What is the probability that we drew from Set 1?

Let A be the event that we drew from Set 1 and let B be the event that the ball drawn is red. Then P(A) = 0.5, P(B) = 90/200, and P(B|A) = 0.4. Thus $P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{0.4 \times 0.5}{0.45} = 0.44$.

END OF NEW POSSIBLE OMIT

The example below illustrates that if a situation is rare, a highly accurate test will often give the wrong answer.

Example: Let A be the event that a product is defective and let B be the event that a test says a product is defective. Let P(B|A) be the probability that the test says a product is defective assuming the product is defective and let $P(B|\overline{A})$ be the probability that the test says a product is defective if it is not actually defective.

What is the probability P(A|B) that the product is defective if the test say it is defective? Suppose P(A) = 0.001, P(B|A) = 0.99, and $P(B|\bar{A}) = 0.02$. Then

$$P(B) = P(B|A) P(A) + P(B|\bar{A}) P(\bar{A})$$

= 0.99 × 0.001 + 0.02 × 0.999
= 0.02087

and

$$P(A|B) = \frac{P(B|A) P(A)}{P(B)} \approx \frac{0.99 \times 0.001}{0.0210} = 0.0471$$

Even though the test fails to detect a defective product only 1% of the time when it is defective and claims that it is defective when it is not only 2% of the time, the test is correct only 4.7% of the time when it says a product is defective. This comes about because of the low frequencies of defective products.

Omit the following? It is a good example for them to have, but, perhaps, the students should work something like this out themselves? Perhaps make it an exercise?

Given two events A and B define the *joint probability distribution* which gives the probability of the two events happening together. The *marginal probability* of A is the just the probability of A and is obtained by summing columns in the example below.

P(A,B)	A=0	A=1
B=0	1/16	1/8
B=1	1/4	9/16

$$P(A) = (5/16, 11/16)$$

The conditional distribution P(A|B) is the probability distribution of A given the value of B. The conditional distribution is obtained by normalizing each row of the joint probability distribution to sum to one.

P(B A)	A = 0	A = 1
B=0	1/3	2/3
B=1	4/13	9/13

The words prior, a posteriori, and likelihood come from Bayes theorem.

a posteriori =
$$\frac{\text{likelihood} \times \text{prior}}{\text{normalizing constant}}$$
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Note that the a posteriori probability is the conditional probability of A given B. The conditional probability P(B|A) is called the likelihood.

Example: Consider rolling two dice A and B. What is the probability that the sum S will add to nine? Of the 36 possible outcomes, four sum to nine. Thus, the prior probability that the sum S=9 is 1/9. Once A is rolled we have new information. Assume A is 3. Then of the six possible outcomes for B only one results in a sum of 9 Thus the probability of a sum of 9 is now 1/6. The value 1/9 was the prior probability and the value 1/6 is the a posteriori probability. The likelihood that A will equal three given that the sum is nine is 1/4. By Bayes rule

$$P(S = 9/A = 3) = \frac{P(A = 3|S = 9) P(S = 9)}{P(A = 3)} = \frac{\frac{1}{4} \times \frac{1}{9}}{\frac{1}{6}} = \frac{1}{6}$$

With no knowledge of A the prior probability that S = 9 was 1/9. With the knowledge that A = 3, the a posteriori probability that S = 9 is 1/6.

John, See comment at the beginning. Perhaps Omit all of the following section on tail inequalities and instead put in the new tail inequalities section into chapter 2?

11.4.9 Tail Bounds

Markov's inequality

One can bound the probability that a nonnegative random variable exceeds a by the expected value of the variable divided by a.

Theorem 11.3 (Markov's inequality) Let x be a non negative random variable. Then

$$p(x \ge a) \le \frac{E(x)}{a}.$$

Proof:

$$E(x) = \int_{0}^{\infty} xp(x)dx = \int_{0}^{a} xp(x)dx + \int_{a}^{\infty} xp(x)dx \ge \int_{a}^{\infty} xp(x)dx$$
$$\ge \int_{a}^{\infty} ap(x)dx = a\int_{a}^{\infty} p(x)dx = ap(x \ge a)$$

Thus
$$p(x \ge a) \le \frac{E(x)}{a}$$

Corollary 9.XXX: Substituting $\alpha E(x)$ for a we get $p[x \ge \alpha E(x)] \le \frac{1}{\alpha}$

Exercise 11.10 Why cannot one prove an analogous type of theorem that states $p(x \le a) \le \frac{E(x)}{a}$?

Solution: The fact that there is no upper limit on the value of x prevents a theorem of this type. Select a value for E(x) and define a probability function for any $\varepsilon > 0$ by placing $1 - \varepsilon$ probability at zero and ε probability at $\frac{1}{e}E(x)$. Then for any a > 0, $p(x \le a)$ must be at least $1 - \varepsilon$. Pick ε so that $1 - \varepsilon > \frac{E(x)}{a}$.

Chebyshev's inequality

The Markov inequality bounds the tail of a distribution using only information about the mean. A better bound can be obtained by also using the variance.

Theorem 11.4 (Chebyshev's Inequality) Let x be a random variable with mean m and variance σ^2 . Then

$$p(|x - m| \ge a\sigma) \le \frac{1}{a^2}$$

Proof: $p(|x-m| \ge a\sigma) = p((x-m)^2 \ge a^2\sigma^2)$. Note that $(x-m)^2$ is a nonnegative random variable, so Markov's Inequality can be a applied to it giving us:

$$p((x-m)^2 \ge a^2\sigma^2) \le \frac{E((x-m)^2)}{a^2\sigma^2} = \frac{\sigma^2}{a^2\sigma^2} = \frac{1}{a^2}.$$

Thus,
$$p(|x - m| \ge a\sigma) \le \frac{1}{a^2}$$
.

Exercise 11.11 Compare the Markov and Chebyshev bounds for the following probability distributions

a)
$$p(x) = \begin{cases} 1 & x = 1 \\ 0 & otherwise \end{cases}$$

b) $p(x) = \begin{cases} 1/2 & 0 \le x \le 2 \\ 0 & otherwise \end{cases}$

11.4.10 Chernoff Bounds: Bounding of Large Deviations

Chebyshev's inequality bounds the probability that a random variable will deviate from its mean by more than a given amount. Chebyshev's inequality holds for any probability distribution. For some distributions we can get much tighter bounds. For example, the probability that a Gaussian random variable deviates from its mean falls off exponentially with the distance from the mean. Here we shall be concerned with the situation where we have a random variable that is the sum of n independent random variables. This is

another situation in which we can derive a tighter bound than that given by the Chebyshev inequality. We consider the case where the n independent variables are binomial but similar results can be shown for independent random variables from any distribution that has a finite variance.

Let x_1, x_2, \ldots, x_n be independent random variables where

$$x_i = \left\{ \begin{array}{ll} 0 & \text{Prob } 1 - p \\ 1 & \text{Prob} & p \end{array} \right..$$

Consider the sum $s = \sum_{i=1}^{n} x_i$. Here the expected value of each x_i is p and by linearity of expectation, the expected value of the sum is m=np. Theorem 9.1.XXX bounds the probability that the sum s exceeds $(1+\delta)m$.

Theorem 11.5 For any
$$\delta > 0$$
, $Prob[s > (1 + \delta)m] < \left[\frac{e^{\delta}}{(1+\delta)^{(1+\delta)}}\right]^m$

Proof: For any $\lambda > 0$, the function $e^{\lambda x}$ is monotone. So, $\text{Prob}[s > (1+\delta)m] = \text{Prob}[e^{\lambda s} > e^{\lambda(1+\delta)m}]$ $e^{\lambda x}$ is nonnegative for all x, so we can apply Markov's inequality to get

$$Prob[e^{\lambda s} > e^{\lambda(1+\delta)m}] < e^{-\lambda(1+\delta)m} E[e^{\lambda s}].$$

Since the x_i are independent

$$E\left(e^{\lambda s}\right) = E\left(e^{\lambda \sum_{i=1}^{n} x_i}\right) = E\left(\prod_{i=1}^{n} e^{\lambda x_i}\right) = \prod_{i=1}^{n} E\left(e^{\lambda x_i}\right)$$
$$= \prod_{i=1}^{n} \left(e^{\lambda p} + 1 - p\right) = \prod_{i=1}^{n} \left(p(e^{\lambda} - 1) + 1\right)$$

Using the inequality $1 + x < e^x$ with $x = p(e^{\lambda} - 1)$ yields

$$E\left(e^{\lambda s}\right) < \prod_{i=1}^{n} e^{p(e^{\lambda} - 1)}$$

Thus, for all $\lambda > 0$

$$Prob[s > (1 + \delta)m] \le Prob[e^{\lambda s} > e^{\lambda(1+\delta)m}]$$
$$\le e^{-\lambda(1+\delta)m} E[e^{\lambda s}] \le e^{-\lambda(1+\delta)m} \prod_{i=1}^{n} e^{p(e^{\lambda}-1)}$$

Setting $\lambda = \ln(1 + \delta)$

$$\operatorname{Prob}\left[s > (1+\delta)m\right] \leq \left(e^{-\ln(1+\delta)}\right)^{(1+\delta)m} \prod_{i=1}^{n} e^{p(e^{\ln(1+\delta)}-1)}$$

$$\leq \left(\frac{1}{1+\delta}\right)^{(1+\delta)m} \prod_{i=1}^{n} e^{p\delta}$$

$$\leq \left(\frac{1}{(1+\delta)}\right)^{(1+\delta)m} e^{np\delta}$$

$$\leq \left(\frac{e^{\delta}}{(1+\delta)^{(1+\delta)}}\right)^{m}$$

To simplify the bound of Theorem 11.4, observe that

$$(1+\delta)\ln(1+\delta) = \delta + \frac{\delta^2}{2} - \frac{\delta^3}{6} + \frac{\delta^4}{12} - \cdots$$

Therefore

$$(1+\delta)^{(1+\delta)} = e^{\delta + \frac{\delta^2}{2} - \frac{\delta^3}{6} + \frac{\delta^4}{12} - \cdots}$$

and hence

$$\frac{e^{\delta}}{(1+\delta)^{(1+\delta)}} = e^{-\frac{\delta^2}{2} + \frac{\delta^3}{6} - \cdots}.$$

Thus, the bound simplifies to

Prob
$$[s < (1+\delta) m] \le e^{-\frac{\delta^2}{2}m + \frac{\delta^3}{6}m - \cdots}$$

For small δ the probability drops exponentially with δ^2 .

When δ is large another simplification is possible. First

$$\operatorname{Prob}(s > (1+\delta) m) \le \left(\frac{e^{\delta}}{(1+\delta)^{(1+\delta)}}\right)^m \le \left(\frac{e}{1+\delta}\right)^{(1+\delta)m}$$

If $\delta > 2e-1$, substituting 2e-1 for δ in the denominator yields

$$Prob(s > (1 + \delta) m) \le 2^{-(1+\delta)m}$$
.

Theorem 9.1.XXX gives a bound on the probability of the sum being greater than the mean. We now bound the probability that the sum will be less than its mean.

Theorem 11.6 Let
$$0 < \gamma \le 1$$
, then $\Pr{ob[s < (1 - \gamma)m]} < \left[\frac{e^{-\gamma}}{(1 + \gamma)^{(1 + \gamma)}}\right]^m < e^{-\frac{\gamma^2 m}{2}}$

Proof: For any $\lambda > 0$

$$Prob[s < (1 - \gamma)m] = Prob[-s > -(1 - \gamma)m] = Prob[e^{-\lambda s} > e^{-\lambda(1 - \gamma)m}].$$

Applying Markov's inequality

$$\operatorname{Prob}(s < (1 - \gamma)m) < \frac{E(e^{-\lambda x})}{e^{-\lambda(1 - \gamma)m}} < \frac{\prod_{i=1}^{n} E(e^{-\lambda X_i})}{e^{-\lambda(1 - \gamma)m}}.$$

Now

$$E(e^{-\lambda x_i}) = pe^{-\lambda} + 1 - p = 1 + p(e^{-\lambda} - 1) + 1.$$

Thus,

Prob
$$(s < (1 - \gamma)m) < \frac{\prod_{i=1}^{n} [1 + p(e^{-\lambda} - 1)]}{e^{-\lambda(1 - \gamma)m}}$$

Since $1 + x < e^x$

$$\operatorname{Prob}[s < (1 - \gamma)m] < \frac{e^{np(e^{-\lambda} - 1)}}{e^{-\lambda(1 - \gamma)m}}$$

Set $\lambda = \ln \frac{1}{1-\gamma}$, then

$$\operatorname{Prob}[s < (1 - \gamma)m] < \frac{e^{np(1 - \gamma - 1)}}{(1 - \gamma)^{(1 - \gamma)m}}$$
$$\mathsf{i} \left[\frac{e^{-\gamma}}{(1 - \gamma)^{(1 - \gamma)}} \right]^m$$

But for $0 < \gamma \le 1$, $(1 - \gamma)^{(1 - \gamma)} > e^{-\gamma + \frac{\gamma^2}{2}}$. To see this note that

$$(1 - \gamma) \ln (1 - \gamma) = (1 - \gamma) \left(-\gamma - \frac{\gamma^2}{2} - \frac{\gamma^3}{3} - \cdots \right)$$

$$= -\gamma - \frac{\gamma^2}{2} - \frac{\gamma^3}{3} - \cdots + \gamma^2 + \frac{\gamma^3}{2} + \frac{\gamma^4}{3} + \cdots$$

$$= -\gamma + \left(\gamma^2 - \frac{\gamma^2}{2} \right) + \left(\frac{\gamma^3}{2} - \frac{\gamma^3}{3} \right) + \cdots$$

$$= -\gamma + \frac{\gamma^2}{2} + \frac{\gamma^3}{6} + \cdots$$

$$\geq -\gamma + \frac{\gamma^2}{2}$$

It then follows that

$$\operatorname{Prob}[s < (1 - \gamma)m]_{\mathsf{i}} \left[\frac{e^{-\gamma}}{(1 - \gamma)^{(1 - \gamma)}} \right]^m < e^{-\frac{m\gamma^2}{2}}$$

Exercise 11.12 (a) How large must δ be if we wish to have $Prob(s < (1 - \delta)m) < \varepsilon$? (b) If we wish to have $Prob(s > (1 + \delta)m) < \varepsilon$?

Solution:

11.4.11 Hoeffding's Inequality

Markov's inequality bounds the probability that a random variable exceeds some constant times its expected value. Chebyshev's inequality bounds the probability that a random variable exceeds its mean by some number of standard deviations. If we know more about the shape of the distribution, tighter bounds are possible. In particular, if a random variable is the sum of independent random variables with finite variance, then better bounds are possible.

Chernoff bounds the probability that a sum of binomial random variables deviates from its mean. Hoeffding (1963) extends this result to sums of bounded random variables.

Theorem 11.7 (Devroye et al p122)(Hoeffding(1963)).

Let $x_1, x_2, ..., x_n$ be independent bounded random variables such that each x_i falls in an interval $[a_i, b_i]$ with probability one. Let $S_n = \sum_{i=1}^n x_i$. For any $\varepsilon > 0$

$$Prob\left[\left(S_{n}-E\left(S_{n}\right)\right) \geq \varepsilon\right] \leq e^{-2\varepsilon^{2}/\sum_{i=1}^{n}\left(b_{i}-a_{i}\right)^{2}}$$
$$Prob\left[\left(S_{n}-E\left(S_{n}\right)\right) \leq \varepsilon\right] \leq e^{-2\varepsilon^{2}/\sum_{i=1}^{n}\left(b_{i}-a_{i}\right)^{2}}$$

Proof: See Devroye et al pp122-123

The result is further extended to martingale difference sequences. A sequence of random variables z_1, z_2, \ldots, z_n is called a martingale if $E(z_{i+1}|z_1, \ldots, z_i) = z_i$ with probability one.

Example: Let $S_n = \text{(number of heads)} - \text{(number of tails)}$. S_1, S_2, \dots, S_n is a martingale.

The Hoeffding Bound

In n trials each with probability p of success, what is the probability that the total number of successes x exceeds the expected number, pn, by more than ε . Hoeffding's bound states

$$\operatorname{Prob}\left(x - pn \ge \varepsilon\right) \le e^{-\frac{2\varepsilon^2}{n}}.$$

Thus, if $p = \frac{1}{2}$, the probability of exceeding 0.5n by more than say \sqrt{n} is less than e^{-2} . If $p = \frac{1}{n}$, the probability of exceeding 1 by $\log n$ is less than $e^{-\frac{2\log^2 n}{n}}$, which goes asymptotically to 1 and the bound provides no information.

Heavy tailed distributions

From an economic point of view if shelf space is expensive a retailer will only stock high demand items. However, if shelf space becomes free why not stock everything. Given a heavy tailed distribution, although items in tail sell almost zero copies there are such a large number of such items that they can add up to a constant fraction of all sales. One of the driving forces changing the world today is that the internet has made shelf space virtually free.

Exercise 11.13 What is the expected number of flips of a coin until a head is reached? Assume p is probability of a head on an individual flip. What is value if p=1/2?

Solution: Let q = 1 - p. The probability that the first head will occur on i^{th} flip is $q^{i-1}p$. Thus, the expected number of flips is given by

$$E = \sum_{i=1}^{\infty} q^{i-1}p = \frac{p}{q} \sum_{i=1}^{\infty} iq^{i} = \frac{p}{q} \frac{q}{(1-q)^{2}} = \frac{1}{p}$$

For p = 1/2 E = 2.

References

- 1. Bernard W. Lindgren, "Statistical theory," MacMillan Publishing Co. New York 1976 QA276 L74 S7 1976
- 2. Athanasios Papoulis, "Probability, Random Variables, and Stochastic Processes," McGraw-Hill 1965. QA273 P21 1984.
 - 3. Parzen p166

END OF OMIT - TAIL Inequalities

John, Eigenvalues/vectors are important and classic. It would be nice to cover some of them. I am not sure of which topics here to cover. One possibility to consider (though I am not clear that is the best option) is to substitute this subsection with a write-up "spectral-decomp.tex" I am enclosing (as per note at the beginning) which derives spectral decomposition and minimax from SVD, the point being then there is a single focus in our treatement of Lienar Algebra - namely SVD. We would then include that material as part of chapter 4, rather than the Appendix....What do you think?

11.5 Generating Functions

Given a sequence a_0, a_1, \ldots , consider the associated generating function $g(x) = \sum_{i=0}^{\infty} a_i x^i$.

The advantage of the generating function is that it captures the entire sequence in a closed form that can be manipulated as an entity. For example, if g(x) is the generating function for the sequence a_0, a_1, \ldots , then $x \frac{d}{dx} g(x)$ is the generating function for the sequence 0, $a_1, 2a_2, 3a_3, \ldots$ Also note that $x^2 g''(x) + xg'(x)$ is the generating function for the sequence for 0, $a_1, 4a_2, 9a_3, \ldots$

Example: The sequence $1, 1, \ldots$ is captured by the generating function $\sum_{i=0}^{\infty} x^i = \frac{1}{1-x}$. The sequence $0, 1, 2, 3, \ldots$ is captured by

$$\sum_{i=0}^{\infty} ix^i = \sum_{i=0}^{\infty} x \frac{d}{dx} x^i = x \frac{d}{dx} \sum_{i=0}^{\infty} x^i = x \frac{d}{dx} \frac{1}{1-x} = \frac{x}{(1-x)^2}.$$

Example: If A can be selected 0 or 1 times and B can be selected 0, 1, or 2 times and C can be selected 0, 1, 2, or 3 times, in how many ways can we select five objects. Consider the generating function for the number of ways to select objects. The generating function for the number of ways of selecting objects, selecting only A's is 1 + x, only B's is $(1 + x + x^2)$, and only C's is $(1 + x + x^2 + x^3)$. The generating function when selecting A's, B's, and C's is the product.

$$(1+x)(1+x+x^2)(1+x+x^2+x^3) = 1 + 3x + 5x^2 + 6x^3 + 5x^4 + 3x^5 + x^6$$

The coefficient of x^5 is 3 and hence we can select five objects in three ways: ABCCC, ABCCC, or BBCCC.

Example: Given a supply of pennies, nickels and dimes, in how many ways can one give 23 cents in change. Consider the generating function for the number of ways to provide i cents. The generating function for using only pennies, nickels and dimes are

$$(1+x+x^2+\cdots) (1+x^5+x^{10}+\cdots) (1+x^{10}+x^{20}+\cdots)$$

Thus, the generating function for the number of ways of making change using pennies, nickels, and dimes is

$$(1+x+x^{2}+\cdots)(1+x^{5}+x^{10}+\cdots)(1+x^{10}+x^{20}+\cdots) = 1+x+x^{2}+x^{3}+x^{4}+2x^{5}+2x^{6}+2x^{7}+2x^{8}+2x^{9}+4x^{10} +4x^{11}+4x^{12}+4x^{13}+4x^{14}+6x^{15}+6x^{16}+6x^{17}+6x^{18} +6x^{19}+9x^{20}+9x^{21}+9x^{22}+9x^{23}+\cdots$$

There are nine ways to give 23 cents change.

Products of generating functions

Let $f(x) = \sum_{i=0}^{\infty} p_i x^i$ be the generating function for an integer valued random variable where p_i is the probability that the random variable takes on value i. Let $g(x) = \sum_{i=0}^{\infty} q_i x^i$ be the generating function of an independent integer valued random variable where q_i is the probability that the random variable takes on the value i. Then the sum of these two

random variables has the generating function f(x)g(x), the product of the two generating functions. This is because the coefficient of x^i in the product f(x)g(x) is $\sum_{k=0}^{i} p_k q_{k-i}$ and this is clearly also the probability that the sum of the random variables is i. Repeating this, we get that the generating function of a sum of independent nonnegative integer valued random variables is the product of their generating functions.

11.5.1 Generating Functions for Sequences Defined by Recurrence Relationships

We now demonstrate a technique for producing the generating function for a sequence from a recurrence relationship defining the sequence. Consider the Fibonacci sequence

$$0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, \dots$$

defined by the recurrence relationship

$$f_0 = 0$$

 $f_1 = 1$
 $f_i = f_{i-1} + f_{i-2}$ $i \ge 2$

Multiply each side of the recurrence by x^i and sum from i equals two to infinity.

$$\sum_{i=2}^{\infty} f_i x^i = \sum_{i=2}^{\infty} f_{i-1} x^i + \sum_{i=2}^{\infty} f_{i-2} x^i$$

$$f_2 x^2 + f_3 x^3 + \dots = f_1 x^2 + f_2 x^3 + \dots + f_0 x^2 + f_1 x^3 + \dots$$

$$f_2 x^2 + f_3 x^3 + \dots = x \left(f_1 x + f_2 x^2 + \dots \right) + x^2 \left(f_0 + f_1 x + \dots \right)$$
(11.1)

Let

$$f(x) = \sum_{i=0}^{\infty} f_i x^i. \tag{11.2}$$

Substituting (11.2) into (11.1) yields

$$f(x) - 0 - x = x (f(x) - 0) + x^{2} f(x)$$

$$f(x) - x = x f(x) + x^{2} f(x)$$

$$f(x)(1 - x - x^{2}) = x$$

Thus $f(x) = \frac{x}{1-x-x^2}$ is the generating function for the Fibonacci sequence.

Note that generating functions are formal manipulations and do not necessarily converge outside some region of convergence. This explains why even though $f(x) = \sum_{i=0}^{\infty} f_i x^i = \frac{x}{1-x-x^2}$, for $f(x) = \sum_{i=0}^{\infty} f_i x^i$, $f(1) = \sum_{i=0}^{\infty} f_i = f_0 + f_1 + f_2 \cdots = \infty$, and for

$$f(x) = \frac{x}{1-x-x^2}, f(1) = \frac{1}{1-1-1} = -1.$$

Asymptotic behavior

To determine the asymptotic behavior of the Fibonacci sequence write

$$f(x) = \frac{x}{1 - x - x^2} = \frac{\frac{\sqrt{5}}{5}}{1 - \phi_1 x} + \frac{-\frac{\sqrt{5}}{5}}{1 - \phi_2 x}$$

where $\phi_1 = \frac{1+\sqrt{5}}{2}$ and $\phi_1 = \frac{1-\sqrt{5}}{2}$ are the two roots of the quadratic $1-x-x^2=0$.

Then

$$f(x) = \frac{\sqrt{5}}{5} \left[1 + \phi_1 x + (\phi_1 x)^2 + \dots - \left(1 + \phi_2 x + (\phi_2 x)^2 + \dots \right) \right]$$

Thus

$$f_n = \frac{\sqrt{5}}{5} \left(\phi_1^n - \phi_2^n \right).$$

Since $\phi_2 < 1$ and $\phi_1 > 1$, for large n, $f_n \cong \frac{\sqrt{5}}{5}\phi_1^n$. In fact, since $f_n = \frac{\sqrt{5}}{5}(\phi_1^n - \phi_2^n)$ is an integer and $\phi_2 < 1$, it must be the case that $f_n = \left\lfloor f_n + \frac{\sqrt{5}}{5}\phi_2^n \right\rfloor = \left\lfloor \frac{\sqrt{5}}{5}\phi_1^n \right\rfloor$ for all n.

Means and standard deviations of sequences

Generating functions are useful for calculating the mean and standard deviation of a sequence. Let z be an integral valued random variable where p_i is the probability that z equals i. The expected value of z is given by $m = \sum_{i=0}^{\infty} i p_i$. Let $p(x) = \sum_{i=0}^{\infty} p_i x^i$ be the generating function for the sequence p_1, p_2, \ldots The generating function for the sequence $p_1, 2p_2, 3p_3, \ldots$ is

$$x\frac{d}{dx}p(x) = \sum_{i=0}^{\infty} ip_i x^i.$$

Thus, the expected value of the random variable z is $m = xp'(x)|_{x=1} = p'(1)$ If p was not a probability function, the average would have been $\frac{p'(1)}{p(1)}$ since we would need to normalize the area under p to one.

The second moment of z can be derived from $g''(x) = \sum_{i=2}^{\infty} i(i-1)x^i p_i = \sum_{i=2}^{\infty} i^2 - \sum_{i=2}^{\infty} i p_i$. Thus the second moment of z is given by $\sum_{i=1}^{\infty} i^2 p_i = g''(1) + p_1 + \sum_{i=2}^{\infty} i p_i = g''(1) + g'(1) = e$.

11.5.2 Exponential Generating Function

Besides the ordinary generating function there are a number of other types of generating functions. One of these is the exponential generating function. Given a sequence a_0, a_1, \ldots , the associated exponential generating function is $g(x) = \sum_{i=0}^{\infty} a_i \frac{x^i}{i!}$.

Moment generating functions

The k^{th} moment of a random variable x around the point b is given by $E((x-b)^k)$. Usually the word moment is used to denote the moment around the value 0 or around the mean. In the following, we use moment to mean the moment about the origin.

The moment generating function of a random variable x is defined by

$$\Psi(t) = E(e^{tx}) = \int_{-\infty}^{\infty} e^{tx} p(x) dx$$

Replacing e^{tx} by its power series expansion $1 + tx + \frac{(tx)^2}{2!} \cdots$ gives

$$\Psi(t) = \int_{-\infty}^{\infty} \left(1 + tx + \frac{(tx)^2}{2!} + \cdots \right) p(x) dx$$

Thus, the k^{th} moment of x about the origin is k! times the coefficient of t^k in the power series expansion of the moment generating function. Thus, the moment generating function is the exponential generating function for the sequence of moments about the origin.

The moment generating function transforms the probability distribution p(x) into a function $\Psi(t)$ of t. Note $\Psi(0) = 1$ and is the area or integral of p(x). The moment generating function is closely related to the characteristic function which is obtained by replacing e^{tx} by e^{itx} in the above integral where $i = \sqrt{-1}$ and is related to the Fourier transform by replacing e^{tx} by e^{-itx} .

 $\Psi(t)$ is closely related to the Fourier transform and its properties are essentially the same. In particular, p(x) can be uniquely recovered by an inverse transform from $\Psi(t)$. More specifically, if all the moments m_i are finite and the sum $\sum_{i=0}^{\infty} \frac{m_i}{i!} t^i$ converges absolutely in a region around the origin then p(x) is uniquely determined.[2] **REFERENCE?**

The Gaussian probability distribution with zero mean and unit variance is given by $p(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}$. Its moments are given by

$$u_n = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^n e^{-\frac{x^2}{2}} dx$$
$$= \begin{cases} \frac{n!}{2^{\frac{n}{2}} (\frac{n}{2})!} & \text{n even} \\ 0 & \text{n odd} \end{cases}$$

To derive the above, use integration by parts to get $u_n = (n-1) u_{n-2}$ and combine this with $u_0 = 1$ and $u_1 = 0$. The steps are as follows. Let $u = e^{-\frac{x^2}{2}}$ and $v = x^{n-1}$. Then $u' = -xe^{-\frac{x^2}{2}}$ and $v' = (n-1) x^{n-2}$. Now $uv = \int u'v + \int uv'$ or

$$e^{-\frac{x^2}{2}}x^{n-1} = \int x^n e^{-\frac{x^2}{2}} dx + \int (n-1)x^{n-2} e^{-\frac{x^2}{2}} dx$$

From which

$$\int_{-\infty}^{\infty} x^n e^{-\frac{x^2}{2}} dx = (n-1) \int_{-\infty}^{\infty} x^{n-2} e^{-\frac{x^2}{2}} dx - e^{-\frac{x^2}{2}} x^{n-1}$$
$$\int_{-\infty}^{\infty} x^n e^{-\frac{x^2}{2}} dx = (n-1) \int_{-\infty}^{\infty} x^{n-2} e^{-\frac{x^2}{2}} dx$$

Thus $u_n = (n-1) u_{n-2}$.

The moment generating function is given by

$$g\left(s\right) = \sum_{n=0}^{\infty} \frac{u_n s^n}{n!} = \sum_{\substack{n=0 \ \text{argon}}}^{\infty} \frac{n!}{2^{\frac{n}{2}} \frac{n}{2}!} \frac{s^n}{n!} = \sum_{i=0}^{\infty} \frac{s^{2i}}{2^i i!} = \sum_{i=0}^{\infty} \frac{1}{i!} \left(\frac{s^2}{2}\right)^i = e^{\frac{s^2}{2}}$$

For the general Gaussian, the moment generating function is

$$q(s) = e^{su + \left(\frac{\sigma^2}{2}\right)s^2}$$

Thus, given two independent Gaussians with mean u_1 and u_2 and variances σ_1^2 and σ_2^2 , the product of their moment generating functions is

$$e^{s(u_1+u_2)+\left(\sigma_1^2+\sigma_2^2\right)s^2}.$$

the moment generating function for a Gaussian with mean $u_1 + u_2$ and variance $\sigma_1^2 + \sigma_2^2$. Thus, the convolution of two Gaussians is a Gaussian and the sum of two random variables that are both Gaussian is a Gaussian random variable.

Catalan numbers

Let c_n be the number of different strings of n pairs of balanced parentheses.

$$c_0 = 1$$

 $c_1 = 1$ ()
 $c_2 = 2$ (()) and ()()
 $c_3 = 5$ ()()(), ((())), ()(()), and (())()

Any string of i pairs of balanced parentheses is of the form (A)B where A and B are strings of j and i - j - 1 pairs of balanced parentheses, respectively. Thus

$$c_i = c_0 c_{i-1} + c_1 c_{i-2} + \dots + c_{i-1} c_0$$

Let $c(x) = \sum_{i=0}^{\infty} c_i x^i$ be the generating function for the $c_i's$. Then

$$c^{2}(x) = \left(\sum_{i=0}^{\infty} c_{i} x^{i}\right) \left(\sum_{i=0}^{\infty} c_{i} x^{i}\right) = c_{0}^{2} + (c_{0}c_{1} + c_{1}c_{0})x + (c_{0}c_{2} + c_{1}c_{1} + c_{2}c_{0})x^{2} + \cdots$$

Substituting c_i for $c_0c_{i-1} + c_1c_{i-2} + \cdots + c_{i-1}c_0$ in the above equation yields

$$c^{2}(x) = c_{1} + c_{2}x + c_{3}x^{2} + \cdots$$

Thus,

$$c_0 + xc^2(x) = c(x)$$

Substituting $c_0 = 1$ and solving the quadratic $xc^2(x) - c(x) + 1 = 0$ for c(x) gives

$$c(x) = \frac{1 - \sqrt{1 - 4x}}{2x}$$

Since c(0) = 1 we replaced the \pm sign with the minus sign. If we had used the plus sign, c(0) would be ∞ .

Since
$$(1+y)^{\frac{1}{2}} = 1 + \frac{1}{2}y - \left(\frac{1}{2}\right)\left(\frac{1}{2}\right)y^2 + \left(\frac{1}{2}\right)\left(\frac{1}{2}\right)y^3 - \cdots$$
, letting $y = -4x$ gives
$$(1-4x)^{\frac{1}{2}} = 1 - \frac{1}{2}4x + \frac{\frac{1}{2}(-\frac{1}{2})(4x)^2}{2!} - \frac{\frac{1}{2}\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)(4x)^3}{3!} + \cdots$$
$$= 1 - 2x - \frac{2^2x^2}{2!} - \frac{3 \cdot 2^3x^3}{3!} - \cdots - \frac{3 \cdot 5 \cdots (2n-3)2^nx^n}{n!}$$

Since
$$1 \cdot 3 \cdot 5 \cdots (2n-3) = \frac{(2n)!}{(2n-1)n!2^n}$$

$$(1-4x)^{\frac{1}{2}} = 1 - \sum_{n=1}^{\infty} \frac{(2n)!x^n}{(2n-1)n!n!}$$

Thus,

$$c(x) = \frac{1}{2x} \sum_{n=1}^{\infty} \frac{(2n)!}{(2n-1)n!n!} x^n = \sum_{n=1}^{\infty} \frac{(2n)(2n-1)(2n-2)!}{2(2n-1)n^2(n-1)!(n-1)!} x^{n-1}$$
$$= \sum_{n=1}^{\infty} \frac{(2n-2)!}{n(n-1)!(n-1)!} x^{n-1}$$

Substituting n = i + 1 yields

$$c(x) = \sum_{i=0}^{\infty} \frac{1}{i+1} {2i \choose i} x^{i}$$

Thus the Catalan numbers are given by

$$c_i = \frac{1}{i+1} \binom{2i}{i}$$

Alternative method to determine Catalan numbers

We derived the Catalan numbers using generating functions to illustrate the use of generating functions. The formula for the Catalan numbers can be derived more easily as follows. The number of strings of length 2n with equal numbers of left and right parentheses is $\binom{2n}{n}$. Each of these strings is a string of balanced parentheses unless there is a prefix with one more right parentheses than left. Consider such a string and flip all parentheses following this one, from right parentheses to left and vice versa. This results in a string of n-1 left parentheses and n+1 right parentheses of which there are $\binom{2n}{n-1}$. It turns out that there is a one-to-one correspondence between strings of length 2n with equal numbers of left and right parentheses that are not balanced and strings of length 2n with n-1 left parentheses and n+1 right parentheses.

We have already shown the correspondence from unbalanced strings of length 2n with equal numbers of parentheses to strings of length 2n with n-1 left parentheses. To see the correspondence the other way take any string of length 2n with n+1 right parentheses. Find the first position where there is one more right parentheses than left and flip all parentheses beyond this point. Clearly this results in an unbalanced string. Thus.

$$c_n = \binom{2n}{n} - \binom{2n}{n-1} = \frac{1}{n+1} \binom{2n}{n}$$

Exercise 11.14 A dice has six faces, each face of the dice having one of the numbers 1 though 6. The result of a role of the dice is the integer on the top face. Consider two roles of the dice. For each integer 1,2,3... in how many ways can it be the sum of two roles of the dice.

Solution:
$$(x + x^2 + x^3 + x^4 + x^5 + x^6)^2 = x^2 + 2x^3 + 3x^4 + 4x^5 + 5x^6 + 6x^7 + 5x^8 + 4x^9 + 3x^{10} + 2x^{11} + x^{12}$$

Exercise 11.15 If a(x) is the generating function for the sequence a_0, a_1, a_2, \ldots , for what sequence is a(x)(1-x) the generating function.

Solution:
$$a_0, a_1 - a_0, a_2 - a_1, \dots$$

Exercise 11.16 How many ways can one draw n a's and b's with an even number of a's.

Solution: The generating function for the number of multi sets of a's and b's with an even number of a's is $\frac{1}{1-x^2}\frac{1}{1-x}$ which by a partial fraction expansion is $\frac{1}{2}\frac{1}{(1-x)^2}+\frac{1}{4}\frac{1}{1-x}+\frac{1}{4}\frac{1}{1+x}$. The coefficient of x^n is $\frac{1}{2}(n+1)+\frac{1}{4}+(-1)^n\frac{1}{4}$. Thus, for example, for n=10 the value would be six.

Exercise 11.17 Find the generating function for the recurrence $a_i = 2a_{i-1} + i$ where $a_0 = 1$.

Solution: Multiply each side of the recurrence equation by x^i and sum. This gives

$$\sum_{i=1}^{\infty} a_i x^i = 2 \sum_{i=1}^{\infty} a_{i-1} x^i + \sum_{i=1}^{\infty} i x^i.$$

Let $g(x) = \sum_{i=0}^{\infty} a_i x^i$. Then $g(x) - 1 = 2xg(x) + \frac{x}{(1-x)^2}$ or

$$g(x) = \frac{x}{(1-2x)(1-x)^2} + \frac{1}{1-2x}$$

Wilf gives a different answer $\frac{1-2x+2x^2}{(1-x)^2(1-2x)} = \frac{-1}{(1-x)^2} + \frac{2}{1-2x}$ but ours appears correct

Exercise 11.18 Find a closed form for the generating function for the infinite sequence of prefect squares 1, 4, 9, 16, 25, ...

Solution: Take the derivative of $\frac{1}{1-x}$, multiply by x, take derivative and multiply by x again. The answer is $\frac{x(x+1)}{(1-x)^3}$.

Exercise 11.19 Given that $\frac{1}{1-x}$ is the generating function for the sequence $1, 1, \ldots$, for what sequence is $\frac{1}{1-2x}$ the generating function?

Solution: $\frac{1}{1-x} = 1 + x + x^2 + \cdots$. Thus $\frac{1}{1-2x} = 1 + 2x + 4x^2 + 8x^3 + \cdots$ is the generating function for $1, 2, 4, 8, \ldots$.

Exercise 11.20 Find a closed form for the exponential generating function for the infinite sequence of prefect squares 1, 4, 9, 16, 25, ...

Solution:
$$\sum_{i=0}^{\infty} \frac{i^2 x^i}{i!} = x (x+1) e^x$$

Exercise 11.21 The generating function for the Catalan numbers is $c(x) = \frac{1-\sqrt{1-4x}}{2x}$. Find an approximation for c_n by expanding $\sqrt{1-4x}$ by the binomial expression and using Sterling's approximation for n!.

Solution:
$$c_n = \frac{4^n}{n^{\frac{3}{2}}\sqrt{\pi}}$$
.

Exercise 11.22 Consider generating a random graph adding one edge at a time. Let N(i,t) be the number of components of size i at time t. MATERIAL COMMENTED OUT

$$\begin{split} N(1,1) &= n \\ N(1,t) &= 0 \quad t > 1 \\ N(i,t) &= N(i,t-1) + \sum \frac{j(i-j)}{n^2} N\left(j,t-1\right) N\left(i-j,t-1\right) - \frac{2i}{n} N\left(i\right) \end{split}$$

Compute N(i,t) for a number of values of i and t. What is the behavior? What is the sum of N(i,t) for fixed t and all i? Can you write a generating function for N(i,t)?

Solution: The sum of N(i,t) decreases over time presumably because a giant component forms.

Exercise 11.23 Show that C_n is the number of ways a convex polygon with n+2 vertices can be partitioned into triangles by adding edges between pairs of vertices.

Exercise 11.24 Show that C_n satisfies the recurrence relationship $C_{n+1} = \frac{2(2n+1)}{n+2}C_n$

References Herbert S. Wilf, "Generating functionology" QA353 G44 W67, book is on line.

Graham, Knuth and Patashnik, "Concrete mathematics: A foundation for Computer Science"

Also see C. L. Lui Chapter 2 on generating functions

For moment generating function applied to Gaussian see Grinstead p395.

Notes

See also material on Wigner's semi circular law - should I find this material

11.6 Eigenvalues and Eigenvectors

11.6.1 Eigenvalues and Eigenvectors

Let A be an n-by-n real matrix. The scalar λ is called an eigenvalue of A if there exists a nonzero vector x satisfying the equation $Ax = \lambda x$. The vector x is called the eigenvector of A associated with λ . The set of all eigenvectors associated with a given eigenvalue plus the zero vector form a subspace. The equation $Ax = \lambda x$ has a non trivial solution for x only if $\det(A - \lambda I) = 0$. The equation $\det(A - \lambda I) = 0$ is called the *characteristic* equation and has n not necessarily distinct roots.

Matrices A and B are said to be similar if there is an invertible matrix P such that $A = P^{-1}BP$. Similar matrices A and B can be thought of as representations of the same linear transformation expressed in different basis.

Theorem 11.8: If A and B are similar, then they have the same eigenvalues.

Proof: Let A and B be similar matrices. Then there exists an invertible matrix P such that $A = P^{-1}BP$. Thus

$$\det(A - \lambda I) = \det\left(P^{-1}BP - \lambda I\right) = \det\left(P^{-1}BP - P^{-1}\lambda IP\right)$$
$$= \det\left(P^{-1}(B - \lambda I)P\right)$$
$$= \det\left(P^{-1}\right) \det\left(B - \lambda I\right) \det\left(P\right)$$
$$= \det\left(P^{-1}P\right) \det\left(B - \lambda I\right) = \det\left(B - \lambda I\right)$$

Since A and B have the same characteristic equation they have the same eigenvalues.

Even though two similar matrices, A and B, have the same eigenvalues, their eigenvectors are in general different. We say that the matrix A is diagonalizable if A is similar to a diagonal matrix.

Theorem 11.9 A is diagonalizable if and only if it has n linearly independent eigenvectors.

Proof: (only if) Assume A is diagonalizable. Then there exists P and D such that $P^{-1}AP = D$. Thus AP = PD. Let the diagonal elements of D be $\lambda_1, \lambda_2, \ldots, \lambda_n$ and let p_1, p_2, \ldots, p_n be the columns of P. Then $AP = [Ap_1, Ap_2, \ldots, Ap_n]$ and $PD = [\lambda_1 p_1, \lambda_2 p_2, \ldots, \lambda_n p_n]$ and hence $Ap_i = \lambda_i p_i$. That is, the λ_i are the eigenvalues of A and the p_i are the corresponding eigenvectors. Since P is invertible, the p_i are linearly independent.

(if) Assume that A has n linearly independent eigenvectors p_1, p_2, \ldots, p_n with corresponding eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then $Ap_i = \lambda_i p_i$ and reversing the above steps

$$AP = [Ap_1, Ap_2, \dots, Ap_n] = [\lambda_1 p_1, \lambda_2 p_2, \dots \lambda_n p_n] = PD$$

and thus AP = DP. Since the p_i are linearly independent, P is invertible and we can write $A = P^{-1}DP$.

Note that the theorem implies that if A is diagonalizable and has eigenvalue λ with multiplicity k, then there are k linearly independent eigenvectors associated with λ .

A matrix P is orthogonal if it is invertible and $P^{-1} = P^{T}$. A matrix A is orthogonally diagonalizable if there exists an orthogonal matrix P such that $P^{-1}AP = D$ is diagonal. If A is orthogonally diagonalizable, then $A = PDP^{T}$. This implies that AP = PD and thus the columns of P are the eigenvectors of A and the diagonal elements of D are the corresponding eigenvalues.

11.6.2 Symmetric Matrices

For an arbitrary matrix some of the eigenvalues may be complex. However, for a symmetric matrix all eigenvalues will be real. The number of eigenvalues of an arbitrary matrix counting multiplicities equals the dimension of the matrix. The set of eigenvectors associated with a given eigenvalue form a vector space, although for a nonsymmetric matrix, the dimension of this space may be less than the multiplicity of the eigenvalue. Thus, a nonsymmetric matrix may not be diagonalizable. However, for a symmetric matrix the eigenvectors associated with a given eigenvalue form a vector space of dimension equal to the multiplicity of the eigenvalue. Thus, all symmetric matrices are diagonalizable. The above facts for symmetric matrices are summarized in the following theorem.

Theorem 11.10 (Real Spectral Theorem) Let A be a real symmetric matrix. Then

- 1. All eigenvalues are real
- 2. If λ is an eigenvalue with multiplicity k, then λ has k linearly independent eigenvectors.
 - 3. A is diagonalizable

Proof: Let λ be an eigenvalue of A with eigenvector x. Then $Ax = \lambda x$ and $x^cAx = \lambda x^cx$. (here the c superscript means conjugate.) Assume that x has been normalized so that $x^cx = 1$. Then

$$\lambda = x^c A x = (x^c A x)^{cc} = (x^c A x)^c = \lambda^c$$

and hence λ is real.

Since λ is real, a nontrivial solution x to $(A - \lambda) x = 0$ implies that there is a nontrivial solution x with real components.

Let x be an eigenvector of A having all real components associated with eigenvalues λ . Let P be a real symmetric matrix such that $Px = e_1$ where $e_1 = (1, 0, 0, \dots, 0)^T$ and $P^{-1} = P^T$. We will construct P shortly.

Since $Ax = \lambda x$, $PAP^Te_1 = \lambda e_1$. The condition $PAP^Te_1 = \lambda e_1$ plus symmetry implies that $PAP^T = \begin{pmatrix} \lambda & 0 \\ 0 & A' \end{pmatrix}$ where A' is n-1 by n-1 and symmetric. That A is diagonalizable follows by induction. Diagonalizable implies that an eigenvalue of multiplicity k has k linearly independent eigenvectors.

It remains to construct P. Let |x| = 1. Note that Ix = x and $(xx^T)x = x$. Thus $(I - xx^T)x = 0$. With this in mind let $P = I - \frac{2vv^T}{v^Tv}$ where $v = x - e_1$. Then $v^Tv = x^Tx - 2x_1 + 1 = 2(1 - x_1)$. Thus

$$Px = x - \frac{vv^Tx}{1 - x_1} = x - \frac{(x - e_1)(1 - x_1)}{1 - x_1} = e_1$$

Need to show that P is invertible.

$$PP^{T} = \left(I - 2\frac{vv^{T}}{v^{T}v}\right)\left(I - 2\frac{vv^{T}}{v^{T}v}\right)^{T} = I - 4\frac{vv^{T}}{v^{T}v} + 4\frac{vv^{T}vv^{T}}{v^{T}vv^{T}v} = I - 4\frac{vv^{T}}{v^{T}v} + 4\frac{vv^{T}}{v^{T}v} = I$$

Theorem 11.11 (The fundamental theorem of symmetric matrices) A is orthogonally diagonalizable iff A is symmetric.

Proof: (if) Assume A is orthogonally diagonalizable. Then there exists P such that $D = P^{-1}AP$. Since $P^{-1} = P^t$ we get

$$A = PDP^{-1} = PDP^t$$

which implies

$$A^t = (PDP)^T = PDP^t = A$$

and hence A is symmetric.

(only if) Find all eigenvalues of A and their multiplicity. If λ has multiplicity k find k linearly independent eigenvectors. (Needs Real Spectral Thm). Find orthonormal basis. Let these form columns of P. Then $P^{-1}AP = P^tAP = D$ will be diagonal. Note that a nonsymmetric matrix may not be diagonalizable, it may have eigenvalues that are not real, and the number of linearly independent eigenvectors corresponding to an eigenvalue

may be less than its multiplicity. For example, the matrix $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$ has eigenvalues

$$2, \frac{1}{2} + i\frac{\sqrt{3}}{2}$$
, and $\frac{1}{2} - i\frac{\sqrt{3}}{2}$. The matrix $\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$ has characteristic equation $(1 - \lambda)^2 = 0$ and

thus has eigenvalue 1 with multiplicity 2 but has only one linearly independent eigenvector associated with the eigenvalue 1, namely $x = c \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $c \neq 0$. Neither of these situations is possible for a symmetric matrix.

Extremal Properties of Eigenvalues 11.6.3

In this section we derive a min max characterization of eigenvalues that implies that the largest eigenvalue of a symmetric matrix A has a value equal to the maximum of $x^T A x$ over all vectors x of unit length. If A is a symmetric matrix there exists an orthogonal matrix P that diagonalizes A. Thus

$$P^TAP = D$$

where D is a diagonal matrix with the eigenvalues of A, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, on its diagonal. Rather than working with A we shall find it easier to work with the diagonal matrix D. This will be an important technique that will simplify many proofs.

Consider maximizing $x^T A x$ subject to the conditions

- (1) $\sum_{i} x_i^2 = 1$ (2) $r_i^T x = 0$

where the r_i are any set of nonzero vectors. We ask over all possible choices of s vectors what is the minimum value assumed by this maximum.

Theorem 11.12 (Min max theorem): For a symmetric matrix A, $\min_{\substack{r_1,\ldots,r_s \\ r_i \mid x}} \max_{\substack{x \\ r_i \mid x}} x^t A x = \lambda_{s+1}$ where the minimum is over all sets of s non zero vectors and the maximum is over all unit vectors x orthogonal to the s non zero vectors.

Proof: A is orthogonally diagonalizable. Let P satisfy $P^TP = I$ and $P^TAP = D$, D diagonal. Let $y = P^T x$. Then x = Py and

$$x^{T}Ax = y^{T}P^{T}APy = y^{T}Dy = \sum_{i=1}^{n} \lambda_{i}y_{i}^{2}$$

Since there is a one to one correspondence between unit \mathbf{x} and unit \mathbf{y} vectors, maximizing $x^T A x$ subject to $\sum x_i^2 = 1$ is equivalent to maximizing $\sum_{i=1}^n \lambda_i y_i^2$ subject to $\sum y_i^2 = 1$. Since $\lambda_1 \geq \lambda_i, 2 \leq i \leq n, \ y = (1, \ 0, \ \dots, \ 0)$ maximizes $\sum_{i=1}^n \lambda_i y_i^2$ at λ_1 . Then x = Py is the first column of P and is the first eigenvector of A. Similarly λ_n is the minimum value of $x^T A x$ subject to the same conditions.

Now consider maximizing $x^T A x$ subject to the conditions

$$(1) \sum x_i^2 = 1$$

(2)
$$r_i^T x = 0$$

where the r_i are any set of nonzero vectors. We ask over all possible choices of s vectors what is the minimum value assumed by this maximum.

$$\min_{r_1,\dots,r_s} \max_{r_i^t x = 0} x^t A x$$

As above, we may work with y. The conditions are

(1)
$$\sum_{i} y_i^2 = 1$$

(2) $q_i^T y = 0$ $q_i^T = r_i^T P$

Now consider any choice for the vectors r_1, r_2, \ldots, r_s . This gives a corresponding set of q_i . The y_i therefore satisfy s linear homogeneous equations. If we add $y_{s+2} = y_{s+3} = \cdots y_n = y_{s+3} = y_{s+3$ 0 we have n-1 homogeneous equations in n unknowns y_1, \ldots, y_n . There is at least one solution which can be normalized so that $\sum y_i^2 = 1$. With this choice of y

$$y^T D y = \sum \lambda_i y_i^2 \ge \lambda_{s+1}$$

since some coefficient greater than or equal to s+1 is nonzero. Thus, for any choice of r_i there will be a y such that

$$\max(y^T P^T A P y) \ge \lambda_{s+1}$$

and hence

$$\min \max(y^T P^T A P y) \ge \lambda_{s+1}$$

However, there is a set of s constraints for which the minimum is less than or equal to λ_{s+1} . Fix the relations to be $y_i = 0$ $1 \le i \le s$. There are s equations in n unknowns and for any y subject to these relations

$$y^T D y = \sum_{s+1}^n \lambda_i y_i^2 \le \lambda_{s+1}$$

Combining we get $\min \max y^T Dy = \lambda_{s+1}$.

The above theorem tells us that the maximum of $x^T A x$ subject to the constraint that $|x|^2 = 1$ is λ_1 . If we consider the problem of maximizing $x^T A x$ subject to the additional restriction that x is orthogonal to the first eigenvector. This is equivalent to maximizing $y^t P^t A P y$ subject to y being orthogonal to $(1,0,\ldots,0)$, i.e. the first component of y being 0. This maximum is clearly λ_2 and occurs for $y=(0,1,0,\ldots,0)$. The corresponding x is the second column of P or the second eigenvector of A.

Similarly we can find the maximum of $x^T A x$ for $p_1^T x = p_2^T x = \cdots p_s^T x = 0$. The value is λ_{s+1} and is obtained for $x = p_{s+1}^T$.

11.6.4 Eigenvalues of the Sum of Two Symmetric Matrices

The min max theorem is useful in proving many other results. The following theorem tells us how adding a matrix B to a matrix A changes the eigenvalues of A. The theorem is useful if we wish to determine the effect on the eigenvalues of A of a small perturbation.

Theorem 11.13 Let C=A+B. Let α_i,β_i , and γ_i denote the eigenvalues of A, B, and C respectively. Then $\alpha_s + \beta_1 \geq \gamma_s \geq \alpha_s + \beta_n$.

Proof: By the min max theorem we have

$$\gamma_s = \min \max(x^T C x)$$

where the maximum is taken over all x of unit length orthogonal to some set of s-1 linear relations and the minimum is over all sets of s-1 linear relations. Select any set of s-1 relations. Then

$$\gamma_s \le \max(x^T C x) = \max(x^T A x + x^T B x)$$

Let $P^TAP = D$. Let the s-1 relations to be satisfied be $p_i x = 0, 1 \le i \le s-1$. This implies that $e_i^T y = 0$. That is, the first s-1 components of y=0. Thus

$$\gamma_s \le \max(\sum_{i=s}^n \alpha_i y_i^2 + x^T B x).$$

However, for all x

$$\sum_{i=s}^{n} \alpha_i y_i^2 \le \alpha_s, \text{ and }$$

$$x^T B x < \beta_1$$

Therefore, $\gamma_s \leq \alpha_s + \beta_1$

Since A = C + (-B), an application of the result we have just proven gives $\alpha_s \le \gamma_s - \beta_n$. [The eigenvalues of -B are minus the eigenvalues of B and thus $-\beta_n$ is the largest eigenvalue.]

Hence $r_s \ge \alpha_s + \beta_n$ and combining inequalities yields $\alpha_s + \beta_1 \ge \gamma_s \ge \alpha_s + \beta_n$.

Lemma 11.14 Also $\gamma_{r+s-1} \leq \alpha_r + \beta_s$.

Proof: There is a set of r-1 relations such that over all x satisfying the r-1 relationships $\max(x^TAx) = \alpha_r$

And a set of s-1 relations such that over all x satisfying the s-1 relationships

$$\max(x^T B x) = \beta_r.$$

Consider all x satisfying the r + s - 2 relations. For any such x

$$x^T C x = x^T A x + x^T B x \le \alpha_r + \beta_s$$

and hence over all the x

$$\max(x_T C x) \le \alpha_s + \beta_r$$

Therefore, taking the minimum over all sets of r + s - 2 relations we get

$$\gamma_{r+s-1} = \min \max(x^T C x) \le \alpha_r + \beta_s + 1$$

11.6.5 Separator Theorem

Theorem 11.15 The eigenvalues $\lambda'_1, \lambda'_2, \ldots, \lambda'_{n-1}$ of the leading principal minor A_{n-1} of A separate the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A.

Proof: The set of values assumed by $x^T A_{n-1} x$ for all n-1 dimensional unit vectors x is the same as the values assumed by $x^T A x$ for all n dimensional unit vectors with $x_n = 0$. Hence,

$$\lambda_s' = \min \max(x^T A_n x)$$

Subject to $x^Tx = 1$, $x_n = 0$, and $p_i^Tx = 0$ $1 \le i \le s - 1$. Now the minimum is achieved for some set of s - 1 $p_i's$. For this set of $p_i's$, λ_s' is the maximum of x^TA_nx subject to the s conditions $x_n = 0$, $p_i^Tx = 0$ $1 \le i \le s - 1$. However, λ_{s+1} is the minimum value taken by the maximum subject to any s relations. Hence

$$\lambda_{s+1} \leq \lambda'_s$$
.

Now consider any s-1 p_i . Let $f_n(p_i) = \max x^T A x$ over all unit x satisfying p_i . Let $f_{n-1}(p_i) = \max x^T A x$ subject to the additional condition $x_n = 0$. Clearly

$$f_{n-1}(p_i) \le \min f_n(p_i)$$

And hence

$$\min f_{n-1}(p_i) \le \min f_n(p_i)$$

Therefore $\lambda_s' \leq \lambda_s$.

If we went with the idea of replacing the Eigenvalues and eigenvectors stuff with an SVD based proof, we could omit stuff up to this point. We should still keep Norms and what follows, I think.

11.6.6 Norms

Types of matrices

A set of vectors $\{x_1, \ldots, x_n\}$ is **orthogonal** if $x_i x_j^T = 0$ for $i \neq j$ and is **orthonormal** if in addition $|x_i| = 1$ for all i. A matrix A is **orthonormal** if $A^T A = I$. If A is a square orthonormal matrix, then rows as well as columns are orthogonal. (In other words, if A is square orthonormal, then A^T is also.) In the case of matrices over the complexes, the concept of an orthonormal matrix is replaced by that of a unitary matrix. A^* is the conjugate transpose of A if $a_{ij}^* = \bar{a}_{ji}$ where a_{ij}^* is the ij^{th} entry of A^* and \bar{a}^* is the complex conjugate of the ij^{th} element of A. A matrix A over the field of complex numbers is **unitary** if $AA^* = I$.

 $tr\left(AB\right) = tr\left(A^TB^T\right)$. Since $(AB)^T = B^TA^T$ the diagonal elements of AB and B^TA^T are the same.

Norms

A **norm** is a function satisfying the following three axioms.

 $(1) f(x) \ge 0,$

(2) $f(x+y) \le f(x) + f(y)$, and

(3) $f(\alpha x) = |\alpha| f(x)$.

A norm on a vector space provides a distance function where distance (x, y) = norm(x - y). An important class of norms for vectors is the *p*-norms defined by

$$|x|_p = (|x_1|^p + \dots + |x_n|^p)^{\frac{1}{p}}.$$

Important special cases are

$$|x|_1 = |x_1| + \dots + |x_n|$$

 $|x|_2 = \sqrt{|x_1|^2 + \dots + |x_n|^2}$
 $|x|_{\infty} = \max |x_i|.$

Exercise 11.25 Prove that the L_2 norm of $(a_1, a_2, ..., a_n)$ is less than or equal to the L_1 norm of $(a_1, a_2, ..., a_n)$.

Solution: We need to show that $\sqrt{\sum_{i=1}^n a_i^2} \leq \sum_{i=1}^n |a_i|$. The result follows immediately from squaring both sides of the inequality. $\sum_{i=1}^n a_i^2 \leq \sum_{i=1}^n a_i^2 + \sum_{i,j} |a_i| |a_j|$ $i \neq j$

Lemma 11.16 For any $1 \le p < q$, $|\mathbf{x}|_q \le |\mathbf{x}|_p$.

Proof: NEEDS WORK

$$|\mathbf{x}|_q^q = \sum_i |x_i|^q \le \left(\sum_i |x_i|^p\right)^{q/p}$$

Using the inequality that for any positive reals a_1, a_2, \ldots, a_n and any $\rho \in (0, 1)$, we have $(\sum_{i=1}^n a_i)^{\rho} \leq \sum_{i=1}^n a_i^{\rho}$, which is easily proved.

There are two important matrix norms, the p-norm

$$||A||_{P} = \max_{|x|=1} \, \|Ax\|_{p}$$

and the Frobenius norm

$$||A||_F = \sqrt{\sum_{ij} a_{ij}^2}.$$

Let a_i be the i^{th} column of A. Then $||A||_F^2 = \sum_i a_i^T a_i = tr(A^T A)$. A similar argument on the rows yields $||A||_F^2 = tr(AA^T)$. Thus $||A||_F^2 = tr(A^T A) = tr(AA^T)$.

The vector norm

$$|x|_2 = \sqrt{|x_1|^2 + \dots + |x_n|^2}$$

The matrix norm

$$\begin{aligned} ||A||_2 &= \max_{|x|=1} |Ax|_2 & ||A||_F &= \sqrt{\sum_{i,j} a_{ij}^2} \\ ||AB||_2 &\leq ||A||_2 ||B||_2 & ||AB_F|| &\leq ||A||_F ||B||_F \end{aligned}$$

If A is symmetric and rank k

$$||A||_2^2 \le ||A||_F^2 \le k ||A||_2^2$$

11.6.7 Important Norms and Their Properties

Lemma 11.17 $||AB||_2 \le ||A||_2 ||B||_2$

Proof: $||AB||_2 = \max_{|x|=1} |ABx|$. Let y be the value of x that achieves the maximum and let z = By. Then

$$||AB||_2 = |ABy| = |Az| = \left| A\frac{z}{|z|} \right| |z|$$

 $\mathrm{But}\ \left|A\frac{z}{|z|}\right| \leq \max_{|x|=1}|Ax| = ||A||_2 \ \mathrm{and}\ |z| \leq \max_{|x|=1}|Bx| = ||B||_2. \ \mathrm{Thus}\ ||AB||_2 \leq ||A||_2 ||B||_2.$

Let Q be an orthonormal matrix.

Lemma 11.18 *For all* x, |Qx| = |x|.

Proof:
$$|Qx|_2^2 = x^T Q^T Q x = x^T x = |x|_2^2$$
.

Lemma 11.19 $||QA||_2 = ||A||_2$

Proof: For all x, |Qx| = |x|. Replacing x by Ax, |QAx| = |Ax| and thus $\max_{|x|=1} |QAx| = \max_{|x|=1} |Ax|$

Lemma 11.20 $||AB||_F^2 \le ||A||_F^2 ||B||_F^2$

Proof: Let a_i be the i^{th} column of A and let b_j be the j^{th} column of B. By the Cauchy-Schwartz inequality $||a_i^Tb_j|| \le ||a_i|| ||b_j||$. Thus $||AB||_F^2 = \sum_i \sum_j |a_i^Tb_j|^2 \le \sum_i \sum_j ||a_i||^2 ||b_j||^2 = \sum_i ||a_i||^2 \sum_i ||b_j||^2 = ||A||_F^2 ||B||_F^2$

Lemma 11.21 $||QA||_F = ||A||_F$

Proof: Since $tr(A^TA) = tr(AA^T)$ we get **NEXT EQN NOT CLEAR**

$$||A||_F = \sqrt{tr(A^tA)} = \sqrt{tr\left(AQQ^TA^T\right)} = \sqrt{tr(Q^tA^tAQ)} = ||QA||_F$$

Since $||QA||_2 = ||A||_2$ and $||QA||_F = ||A||_F$ the 2-norm and the Frobenius norm of a matrix A equal the 2-norm and the Frobenius norm of their diagonal matrix $\Sigma = Q^T A Q$.

Lemma 11.22 For real, symmetric matrices $||A||_2^2 = \lambda_1^2$ and $||A||_F^2 = \lambda_1^2 + \lambda_2^2 + \dots + \lambda_n^2$

Proof: Follows immediately from the above remark.

If A is real and symmetric and of rank k then $||A||_2^2 \le ||A||_F^2 \le k ||A||_2^2$

Theorem 11.23 $||A||_2^2 \le ||A||_F^2 \le k ||A||_2^2$

Proof: It is obvious for diagonal matrices that $||D||_2^2 \leq ||D||_F^2 \leq k ||D||_2^2$. Let $D = Q^t A Q$ where Q is orthonormal. The result follows immediately since for Q orthonormal $||QA||_2 = ||A||_2$ and $||QA||_F = ||A||_F$.

Note: Real and symmetric are necessary for some of these theorems. This condi-

tion was needed to express $\Sigma = Q^T A Q$. For example, $A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix}$. $||A||_2 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix}$

2 $||A||_F = \sqrt{2n}$ but A is rank 2 and $||A||_F > 2 ||A||_2$ for n > 8.

Lemma 11.24 Let A be a symmetric matrix. Then $||A||_2 = \max_{|x|=1} |x^t Ax|$.

Proof: By definition, the 2-norm of A is $||A||_2 = \max_{|x|=1} |Ax|$. Thus,

$$||A||_2 = \max_{|x|=1} |Ax| = \max_{|x|=1} \sqrt{x^t A^t A x} = \sqrt{\lambda_1^2} = \lambda_1 = \max_{|x|=1} |x^t A x|$$

The two norm of a matrix A is greater than or equal to the 2-norm of any of its columns. Let A_u be a column of A.

Lemma 11.25 $|A_u| \leq ||A||_2$

Proof: Note $\lambda = \max_{|x|=1} |Ax|$. Let $x = e_u$ where a_u is row u. Then $|a_u| = |Ae_u| \le \max_{|x|=1} |Ax| = \lambda$. **DEFINE** e_u

Best rank k approximation

Let $A^{(k)}$ be the rank k approximation to A using the first k eigenvectors. Then

Theorem 11.26 $||A - A^{(k)}||_2 \le \min ||A - B||_2$ where the minimum is over all B of rank less than or equal to k.

Proof: Suppose there exists a B of rank k or less such that $||A - B||_2 < ||A - A^{(k)}||_2$. Then there exists a subspace W of rank n - k such that for all $w \in W$, Bw = 0. Thus Aw = (A - B)w and

$$|Aw|_2 = |(A - B)w|_2 \le ||A - B||_2 |w|_2 < ||A - A^{(k)}||_2 |w|_2 = \lambda_{k+1} |w|_2.$$

But for the k+1 dimensional subspace spanned by the first k+1 eigenvectors of A, $|Aw|_2 \ge \lambda_{k+1} |w|_2$. Since the sum of the dimensions of these two subspaces exceeds n, they must contain some $w \ne 0$ in common and thus we have a contradiction.

When we write $\lambda_1 = \min_{|x|=1} x^T A x$ we assume that the minimum value exists. One could imagine an infinite sequence of smaller and smaller values of λ_1 but the limit does not exist. That there is an x that gives the limiting value λ_1 . This point is critical in the next proof where let X be the matrix that minimizes $||A - S||_F$. One needs to argue that such a matrix does indeed exist and not the situation that there is an infinite sequence of matrices giving lower and lower values that approach some limit but no matrix actually achieves the limit.

Theorem 11.27 $||A - A^{(k)}||_F \le \min ||A - B||_F$ where the minimum is over all B of rank less than or equal to k.

Proof: Let X be the matrix that minimizes $||A - S||_F$. Then clearly $||A - X||_F \le ||A - A^{(k)}||_F \le (\lambda_{k+1}^2 + \lambda_{k+2}^2 + \dots + \lambda_n^2)$ since we can let $X = A^{(k)}$. We need to show that $||A - X||_F \ge (\lambda_{k+1}^2 + \lambda_{k+2}^2 + \dots + \lambda_n^2)$. Let $Q\Omega P^T$ be the singular value decomposition of X. Define $B = Q^T A P$ and write $A = QBP^T$. Then

$$\left|\left|A-X\right|\right|_{F}=\left|\left|Q\left(B-\Omega\right)P^{T}\right|\right|_{F}=\left|\left|B-\Omega\right|\right|_{F}.$$

Since X is rank k, Ω is a rank k diagonal matrix and we can partition it as

$$\Omega = \left(\begin{array}{cc} \Omega_k & 0 \\ 0 & 0 \end{array} \right)$$

Where Ω_k is a $k \times k$ diagonal matrix. Partition B in the same manner as Ω .

$$B = \left(\begin{array}{cc} B_{11} & B_{12} \\ B_{21} & B_{22} \end{array}\right).$$

Then

$$||A - X||_F = ||B_{11} - \Omega||_F + ||B_{12}||_F + ||B_{21}||_F + ||B_{22}||_F$$

We need to show that B_{12} and B_{21} must be zero. Otherwise there would exist a rank k matrix Y such that $||A - Y||_k < ||A - X||_k$, a contradiction. Define $Y = Q \begin{pmatrix} B_{11} & B_{12} \\ 0 & 0 \end{pmatrix} P^T$. Then $||A - Y||_F^2 = ||B_{22}||_F^2 \le ||B_{11} - \Omega||_F^2 + ||B_{22}||_F^2 = ||A - X||_F^2$.

It follows that $B_{11}=\Omega$ otherwise $||A-Z||_F^2<||A-X||_F^2$. Let B_{22} have singular value decomposition $B_{22}=U\Lambda V_1^T$. Then $||A-X||_F=||B_{22}||_F=||\Lambda||_F$. Let $U_2=\begin{pmatrix}I_k&0\\0&U_1\end{pmatrix}$ and $V_2=\begin{pmatrix}I_k&0\\0&V_1\end{pmatrix}$. Then $U_2^TQ^TAPV_2=\begin{pmatrix}\Omega_k&0\\0&\Lambda\end{pmatrix}$ or

$$A = QU_2 \begin{pmatrix} \Omega_k & 0 \\ 0 & \Lambda \end{pmatrix} (PV_2)^T$$

and hence the diagonal elements of Λ are eigenvalues of A. Thus $||A - X||_F = ||\Lambda|| \ge (\sigma_{k+1}^2 + \dots + \sigma_n^2)^{\frac{1}{2}}$. [\ge because we don't know which eigenvalues.] Therefore $||A - X||_F = (\sigma_{k+1}^2 + \dots + \sigma_n^2)^{\frac{1}{2}} = (A - A^{(k)})_F$.

11.6.8 Linear Algebra

ARE WE TALKING ABOUT EIGENVALUE OR SINGULAR VALUE?

Lemma 11.28 Let A be an $n \times n$ symmetric matrix. Then $det(A) = \lambda_1 \lambda_2 \cdots \lambda_n$

Proof: The det $(A - \lambda I)$ is a polynomial in λ of degree n. The coefficient of λ^n will be ± 1 depending on whether n is odd or even. Let the roots of this polynomial be $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then $\det(A - \lambda I) = (-1)^n \prod_{i=1}^n (\lambda - \lambda_i)$. Thus

$$\det(A) = \det(A - \lambda I)|_{\lambda=0} = (-1)^n \prod_{i=1}^n (\lambda - \lambda_i) \Big|_{\lambda=0} = \lambda_1 \lambda_2 \cdots \lambda_n$$

The trace of a matrix is defined to be the sum of its diagonal elements. That is, $trace(A) = a_{11} + a_{22} + \cdots + a_{nn}$.

Lemma 11.29 $trace(A) = \lambda_1 + \lambda_2 + \cdots + \lambda_n$

Proof: Consider the coefficient of λ^{n-1} in $\det(A - \lambda I) = (-1)^n \prod_{i=1}^n (\lambda - \lambda_i)$. Write $A - \lambda_i$

$$\lambda I = \begin{pmatrix} a_{11} - \lambda & a_{12} & \cdots \\ a_{21} & a_{22} - \lambda & \cdots \\ \vdots & \vdots & \vdots \end{pmatrix}.$$
 Calculate $\det(A - \lambda I)$ by expanding along the first row.

Each term in the expansion involves a determinant of size n-1 which is a polynomial in

 λ of deg n-2 except for the principal minor which is of deg n-1. Thus the term of deg n-1 comes from **ADD SENTENCE OF EXPLAINATION**

$$(a_{11}-\lambda)(a_{22}-\lambda)\cdots(a_{nn}-\lambda)$$

and has coefficient $(-1)^{n-1}(a_{11} + a_{22} + \cdots + a_{nn})$. Now $(-1)^n \prod_{i=1}^n (\lambda - \lambda_i) = (-1)^n (\lambda - \lambda_1)(\lambda - \lambda_2) \cdots (\lambda - \lambda_n) = (-1)^n [\lambda^n - (\lambda_1 + \lambda_2 + \cdots + \lambda_n)\lambda^{n-1} + \cdots]$ Therefore equating coefficients $\lambda_1 + \lambda_2 + \cdots + \lambda_n = a_{11} + a_{22} + \cdots + a_{nn} = trace(A)$

Note that $(trace(A))^2 \neq trace(A^2)$. For example $A = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$ has trace 3, $A^2 = \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}$ has trace $5 \neq 9$. However $trace(A^2) = \lambda_1^2 + \lambda_2^2 + \dots + \lambda_n^2$. To see this, observe that $A^2 = (V^T D V)^2 = V^T D^2 V$. Thus, the eigenvalues of A^2 are the squares of the eigenvalues for A.

Alternative proof that $trace(A) = \lambda_1 + \lambda_2 + \cdots + \lambda_n$.

Lemma 11.30 If A is $n \times m$ and B is a $m \times n$ matrix, then trace(AB) = trace(BA).

See Wikipedia algebra for good example. Then proof of Lemma

$$A = U\Sigma V$$

$$trace(A) = trace(U\Sigma V) = trace(UV\Sigma) = trace(\Sigma) = \lambda_1 + \lambda_2 + \dots + \lambda_n$$

$$trace(AB) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}b_{ji} = \sum_{j=1}^{n} \sum_{i=1}^{n} b_{ji}a_{ij} = trace(BA)$$

In addition used that U and V are orthogonal.

Example: An interesting example to talk about eigenvectors when this section is developed is given below. Consider a randomly generated graph with 1,000 vertices. 100 of them are designated as a cluster. All vertices are degree 8. Edges are added between pairs of vertices in the cluster until all vertices in the cluster are degree 6. There are 300 such edges. Then edges are added from vertices in the cluster to vertices outside the cluster until all cluster vertices are degree 8. This is an additional 200 edges. Finally edges are added to pairs of vertices outside the cluster until all vertices are degree 8. This is an additional 3,500 edges for a total of 4,000. The major eigenvector for the graph should have all coefficients equal.

Now consider the Markov process with two vertices A and B corresponding to vertices in the cluster and vertices outside the cluster. The transition probabilities are given by the matrix $m = \begin{bmatrix} 0.75 & 0.0278 \\ 0.25 & 0.9722 \end{bmatrix}$. This matrix has eigenvectors and eigenvalues given by $v = \begin{bmatrix} -0.7071 & -0.1105 \\ 0.7071 & -0.9939 \end{bmatrix}$ and $d = \begin{bmatrix} 0.7222 & 0 \\ 0 & 1.0000 \end{bmatrix}$.

Question: If we took a random walk how frequently would we be at vertices in the cluster? The major eigenvector says that a random walk will spend 10% of its time in vertices of the cluster. 1105/(1105+9939)=0.10

Wielandt-Hoffman Theorem

$$\sum_{i=1}^{n} (\lambda_i (A + E) - \lambda_i (A))^2 \le ||E||_F^2$$

Golub and Van Loan p395 refer to Wilkenson 1965 pp104-108 or Stewart and Sun 1991 pp189-191 for a proof.

Alternative statement of Wielandt-Hoffman Theorem

$$\sum_{i=1}^{n} (\sigma_i(A) - \sigma_i(B))^2 \le ||A - B||_F^2.$$

From the theorem it follows that $A^{(k)}$ is the best rank k approximation since

$$\sum_{i=1}^{n} (\sigma_i(A) - \sigma_i(B))^2 \ge \sum_{i=1}^{k} (\sigma_i(A) - \sigma_i(B))^2 + \sum_{i=k+1}^{n} \sigma_i^2 \ge \sum_{i=k+1}^{n} \sigma_i^2$$

Pseudo inverse

Let A be an $n \times m$ rank r matrix and let $A = U\Sigma V^T$ be the singular value decomposition of A. Let $\Sigma' = diag\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_1}, 0, \dots, 0\right)$ where $\sigma_1, \dots, \sigma_r$ are the singular values of A. Then $A' = V\Sigma'U^T$ is the pseudo inverse of A. It is the unique X that minimizes $\|AX - I\|_F$.

Spectrum of clique

The first eigenvalue of a clique is n-1 with u = (1, 1, ..., 1) being the associated eigenvector. All other eigenvectors must be orthogonal to u and hence their coordinates sum to zero. Write $K_n = U_n - I_n$ where K_n is a clique and U_n is the all ones square matrix. If x is an eigenvector orthogonal to u then $K_n x = \lambda x$. Hence $U_n x - I_n x = \lambda x$. But since x is orthogonal to u, $U_n x = 0$. Thus $\lambda = -1$. Thus the spectrum of a clique K_n is $(n-1,-1,\ldots,-1)$.

Second eigenvector – similar material in 4.4 p5

The second eigenvector plays an important role with respect to graphs. Note that it is not necessarily the eigenvector of A associated with the eigenvalue with second largest absolute value and that it is the smallest eigenvalue greater than zero for the Laplacian.

The second eigenvalue, λ_{ij} , is the second eigenvalue in the order $\lambda_1 \geq \lambda_2 \geq \cdots$. It may be the case that $|\lambda_n| > |\lambda_2|$.

Why is the second eigenvalue so important? Consider partitioning the vertices of a regular degree d graph G = (V, E) into two blocks of equal size so as to minimize the number of edges between the two blocks. Assign value +1 to the vertices in one block and -1 to the vertices in the other block. Let x be the vector whose components are the ± 1 values assigned to the vertices. If two vertices, i and j, are in the same block, then x_i and x_j are both +1 or both -1 and $(x_i-x_j)^2=0$. If vertices i and j are in different blocks then $(x_i-x_j)^2=4$. Thus, partitioning the vertices into two blocks so as to minimize the edges between vertices in different blocks is equivalent to finding a vector x with coordinates ± 1 of which half of its coordinates are +1 and half of which are -1 that minimizes

$$E_{cut} = \frac{1}{4} \sum_{ij \in E} (x_i - x_j)^2$$

Let A be the adjacency matrix of G. Then

$$x^{T}Ax = \sum_{ij} a_{ij}x_{i}x_{j} = 2\sum_{edges} x_{i}x_{j}$$

$$= 2 \times \left(\begin{array}{c} \text{number of edges} \\ \text{within components} \end{array} \right) - 2 \times \left(\begin{array}{c} \text{number of edges} \\ \text{between components} \end{array} \right)$$

$$= 2 \times \left(\begin{array}{c} \text{total number} \\ \text{of edges} \end{array} \right) - 4 \times \left(\begin{array}{c} \text{number of edges} \\ \text{between components} \end{array} \right)$$

Maximizing $x^T A x$ over all x whose coordinates are ± 1 and half of whose coordinates are +1 is equivalent to minimizing the number of edges between components.

Since finding such an x is computational difficult, replace the integer condition on the components of x and the condition that half of the components are positive and half of the components are negative with the conditions $\sum_{i=1}^{n} x_i^2 = 1$ and $\sum_{i=1}^{n} x_i = 0$. Then finding the optimal x gives us the second eigenvalue

$$\lambda_2 = \max_{x \perp v_1} \frac{x^T A x}{\sum x_i^2}$$

Actually we should use $\sum_{i=1}^{n} x_i^2 = n$ not $\sum_{i=1}^{n} x_i^2 = 1$. Thus $n\lambda_2$ must be greater than $2 \times \binom{\text{total number }}{\text{of edges}} - 4 \times \binom{\text{number of edges}}{\text{between components}}$ since the maximum is taken over a larger set of x. The fact that λ_2 gives us a bound on the minimum number of cross edges is what makes it so important.

Notes on chapter

$$\lambda_1$$
 is at least the average degree of G . Proof: $\lambda_1 = \min_{\dim(F)=n} \max_{x \in F} \frac{x^T A x}{x^T x}$. Since $x \neq 0$

dim(F) = n there is only one space and thus $\lambda_1 = \max_x \frac{x^T A x}{x^T x}$. Since for x = (1, 1, ..., 1), $\frac{x^T A x}{x^T x} = average \deg of A$, λ_1 is at least the average deg of A.

Clever proof in Alon, Krivelevich and Sudakov, "Finding a large hidden clique in a random graph", p595 second column in proof of prop 2.1

Archived original Chap 2.2

LEFT OVER MATERIAL Suppose you wished to distribute information efficiently with no centralized control. Which edge is the highest priority. It we could calculate both the first and second eigenvectors, then we could look at the coefficient of the second eigenvector. At a vertex the most important edge is the edge with the largest difference in the coefficient of the second eigenvector at its endpoints. Calculating both the first and second eigenvectors requires local algorithm for orthonormalization at each step.

Above paragraph seems to suggest that importance of an edge is determined by second eigenvector. Where did this idea come from?

Homework

Exercise 11.26 Show that if A is a symmetric matrix and λ_1 and λ_2 are distinct eigenvalues then their corresponding eigenvectors x_1 and x_2 are orthogonal. **Hint:**

Solution: Write

$$\lambda_1(x_1^t x_2) = (Ax_1)^t x_2$$

$$= (x_1^t A^t) x_2$$

$$= x_1^t (Ax_2) \quad \text{since A is symmetric}$$

$$= x_1^t (\lambda_2 x_2)$$

$$= \lambda_2 (x_1^t x_2)$$

Thus $(\lambda_1 - \lambda_2)x_1^t x_2 = 0$. Since λ_1 and λ_2 are distinct x_1 and x_2 must be orthogonal.

Exercise 11.27 Show that if the eigenvalues of a matrix are all distinct then the eigenvectors must be linearly independent.

Hint:

Solution: Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be n distinct eigenvalues with eigenvectors x_1, x_2, \ldots, x_n . Assume that the first m eigenvectors are linearly independent but the first m+1 are dependent. Then $x_{m+1} = c_1x_1 + c_2x_2 + \cdots + c_mx_m$ where the c_i 's are not all zero. Multiplying both sides by A gives

$$Ax_{m+1} = c_1 Ax_1 + c_2 Ax_2 + \dots + c_m Ax_m$$
$$\lambda_{m+1} x_{m+1} = c_1 \lambda_1 x_1 + c_2 \lambda_2 x_2 + \dots + c_m \lambda_m x_m$$

Multiply the earlier equation $(x_{m+1} = c_1x_1 + c_2x_2 + \cdots + c_nx_n)$ by λ_{m+1} yields

$$\lambda_{m+1} x_{m+1} = c_1 \lambda_{m+1} x_1 + c_2 \lambda_{m+1} x_2 + \dots + c_m \lambda_{m+1} x_m$$

Subtracting yields

$$c_1(\lambda_{m+1} - \lambda_1)x_1 + c_2(\lambda_{m+1} - \lambda_2)x_2 + \dots + c_m(\lambda_{m+1} - \lambda_m)x_m = 0$$

Since the eigenvalues are distinct and the first m eigenvectors are linearly independent, $c_i = 0$ $1 \le i \le m$. This contradicts that the assumption the x_{m+1} can be written as a linear combination of the first m eigenvectors. Hence all eigenvectors are linearly independent.

Exercise 11.28 Show that a matrix is rank k if and only if it has k nonzero eigenvalues and eigenvalue 0 of rank n-k.

Exercise 11.29 Prove that maximizing $\frac{x^T A x}{x^T x}$ is equivalent to maximizing $x^T A x$ subject to the condition that x be of unit length.

Exercise 11.30 Let A be a symmetric matrix with smallest eigenvalue λ_{\min} . Give a bound on the largest element of A^{-1} .

References

Larson/Edwards, "Elementary Linear Algebra," QA184 L335

Notes: Read Alon and Spencer p137-138 on eigenvalues and expanders

9.5.5 Distance between subspaces

Define the square of the distance between two subspaces by

$$dist^{2}(X_{1}, X_{2}) = ||X_{1} - X_{2}X_{2}^{T}X_{1}||_{F}^{2}$$

Since $X_1 - X_2 X_2^T X_1$ and $X_2 X_2^T X_1$ are orthogonal

$$||X_1||_F^2 = ||X_1 - X_2 X_2^T X_1||_F^2 + ||X_2 X_2^T X_1||_F^2$$

and hence

$$dist^{2}(X_{1}, X_{2}) = ||X_{1}||_{F}^{2} - ||X_{2}X_{2}^{T}X_{1}||_{F}^{2}.$$

Intuitively, the distance between X_1 and X_2 is the Frobenius norm of the component of X_1 not in the space spanned by the columns of X_2 .

If X_1 and X_2 are 1-dimensional unit length vectors, $dist^2(X_1, X_2)$ is the sin squared of the angle between the spaces.

Example: Consider two subspaces in four dimensions

$$X_{1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0\\ 0 & \frac{1}{\sqrt{3}}\\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}}\\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \qquad X_{2} = \begin{pmatrix} 1 & 0\\ 0 & 1\\ 0 & 0\\ 0 & 0 \end{pmatrix}$$

Here

$$dist^{2}\left(X_{1},X_{2}\right) = \left\| \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \right\|_{F}^{2} = \left\| \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \right\|_{F}^{2} = \frac{7}{6}$$

In essence, we projected each column vector of X_1 onto X_2 and computed the Frobenius norm of X_1 minus the projection. The Frobenius norm of each column is the sin squared of the angle between the original column of X_1 and the space spanned by the columns of X_2 .

11.7 Miscellaneous

TD-IDF

The term TD-IDF stands for (term frequency)*(inverse document frequency) and is a technique for weighting keywords from a document. Let

 w_{ik} be the weight of keyword k in document i

 n_k be the number of documents containing keyword k

 tf_{ik} be the number of occurrences of keyword k in document i.

Then $w_{ik} = tf_{ik} \log \frac{\text{number of doc}}{n_k}$. Sometimes the term frequency tf is normalized by the number of words in the document to prevent a bias towards long documents.

Log-concave

There has been considerable work in the case where the distributions are Gaussian or log-concave. f(x) is log-concave if $\ln(f(x))$ is concave. That is, if $\frac{d^2}{dx^2}\ln(f(x)) \leq 0$. For example, $\frac{d^2}{dx^2}\ln\left(e^{-x^2}\right) = -2$. Here we extend this work to distributions with heavy tails such as the Cauchy $\frac{1}{\pi(1+x^2)}$ which has infinite variance.

PCA

PCA applies SVD to X-E(X) where as LSI applies SVD to X itself.

Nonnegative matrix factorization (NMF)

NMF expresses X as YZ where the elements of Y and Z are non negative. Y is the set of factors extracted from X and Z indicates how they should be combined. The fact that the elements of Y are nonnegative may make them easier to interpret than the factors obtained from SVD.

Maximization

Maximize f = a + 2b subject to $a^2 + b^2 = 1$.

$$f = a + 2b = a + 2\sqrt{1 - a^2}$$

$$\frac{\partial f}{\partial a} = 1 - (1 - a^2)^{\frac{1}{2}} 2a = 0$$

$$\frac{2a}{\sqrt{1 - a^2}} = 1$$

$$4a^2 = 1 - a^2$$

$$a = \frac{1}{\sqrt{5}}$$

Should work out general situation for $\sum_{i=1}^{n} a_i x_i$

Exercise 11.31 We are given the probability distribution for two random vectors x and y and we wish to stretch space to maximize the expected distance between them. Thus we will multiply each coordinate by some quantity a_i . We restrict $\sum_{i=1}^d a_i^2 = d$. Thus, if we increase some coordinate by $a_i > 1$, some other coordinate must shrink. Given random vectors $x = (x_1, x_2, \ldots, x_d)$ and $y = (y_1, y_2, \ldots, y_d)$ how should we select a_i to maximize $E(|x-y|^2)$? The a_i stretch different coordinates. Assume

$$y_i = \left\{ \begin{array}{cc} 0 & \frac{1}{2} \\ 1 & \frac{1}{2} \end{array} \right.$$

and that x_i has some arbitrary distribution.

$$E(|x-y|^2) = E\sum_{i=1}^d [a_i^2 (x_i - y_i)^2] = \sum_{i=1}^d a_i^2 E(x_i^2 - 2x_i y_i + y_i^2)$$
$$= \sum_{i=1}^d a_i^2 E(x_i^2 - x_i + \frac{1}{2})$$

Since $E(x_i^2) = E(x_i)$ we get. Thus weighting the coordinates has no effect assuming $\sum_{i=1}^{d} a_i^2 = 1$. Why is this? Since $E(y_i) = \frac{1}{2}$.

 $E(|x-y|^2)$ is independent of the value of x_i hence its distribution.

What if
$$y_i = \begin{cases} 0 & \frac{3}{4} \\ 1 & \frac{1}{4} \end{cases}$$
 and $E(y_i) = \frac{1}{4}$. Then

$$E(|x-y|^2) = \sum_{i=1}^d a_i^2 E(x_i^2 - 2x_i y_i + y_i^2) = \sum_{i=1}^d a_i^2 E(x_i - \frac{1}{2}x_i + \frac{1}{4})$$
$$= \sum_{i=1}^d a_i^2 \left(\frac{1}{2}E(x_i) + \frac{1}{4}\right)$$

To maximize put all weight on the coordinate of x with highest probability of one. What if we used 1-norm instead of the two norm?

$$E(|x - y|) = E\sum_{i=1}^{d} a_i |x_i - y_i| = \sum_{i=1}^{d} a_i E|x_i - y_i| = \sum_{i=1}^{d} a_i b_i$$

where $b_i = E(x_i - y_i)$. If $\sum_{i=1}^{d} a_i^2 = 1$, then to maximize let $a_i = \frac{b_i}{b}$. Taking the dot product of a and b is maximized when both are in the same direction.

Lagrangian multipliers

Lagrangian multipliers are used to convert a constrained optimization problem into an unconstrained optimization. Suppose we wished to maximize a function f(x,y) subject to a constraint g(x,y) = c. If we walk along the constraint g(x,y) = c the value of f(x,y) might increase for a while and then start to decrease. At the point where f(x,y) stops increasing and starts to decrease, the contour line for f(x,y) is tangent to the curve of the constraint g(x,y) = c. Stated another way the gradient of f(x,y) and the gradient of g(x,y) are parallel.

By introducing a new variable λ we can express the condition by $\nabla_{xy} f = \lambda \nabla_{xy} g$ and g=c. These two conditions hold if and only if

$$\nabla_{xy\lambda} \left[f\left(x, y \right) + \lambda \left(g\left(x, y \right) - c \right) \right] = 0$$

(The partial with respect to λ establishes that g(x,y)=c.) We have converted the constrained optimization problem in variables x and y to an unconstrained problem with variables x, y, and λ .

Exercise 11.32 Maximize x+y subject to the constraint that $x^2 + y^2 = 1$.

Solution: Write $x + y + \lambda (x^2 + y^2 - 1)$ and take derivatives with respect to x, y and λ .

$$1 + 2\lambda x = 0$$

$$1 + 2\lambda y = 0$$

$$x^2 + y^2 - 1 = 0$$

From the first two equations x=y and substituting into the last equation $2y^2=1$ or $y=\pm\frac{\sqrt{2}}{2}$. Thus the extremes are at $[x,y]=\pm\left[\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}\right]$.

11.7.1 Variational Methods

References

Jordan, Ghahramani, Joakkola, Saul, "An introduction to Variational Methods for Graphical Models"

Expressing the log function as a minimization problem

The function ln(x) is concave and thus for a line λx with slope λ there is an intercept c such that $\lambda x + c$ is tangent to the curve ln(x) in exactly one point. The value of c is $-\ln \lambda - 1$. To see this, note that the slope of ln(x) is 1/x and this equals the slope of the

line ar $x = \frac{1}{\lambda}$. The value of c so that $\lambda x + c = \ln(x)$ at x = 1/2 is $c = \ln(\frac{1}{\lambda}) - 1 = -\ln \lambda - 1$.

Now for every λ and every x, $\ln(x) = \leq (\lambda x - \ln \lambda - 1)$ and for every x there is a λ such that equality holds. Thus

$$\ln\left(x\right) = \min_{\lambda} \left(\lambda x - \ln \lambda - 1\right)$$

The logistic function $f(x) = \frac{1}{1+e^{-x}}$ is not convex but we can transform it to a domain where the function is concave by taking the $\ln f(x)$.

$$g\left(x\right) = -\ln\left(1 + e^{-x}\right)$$

Thus we can bound the log logistic function with linear functions

$$g(x) = \min_{\lambda} \left\{ \lambda x - H(\lambda) \right\}$$

Taking exponential of both sides

$$f(x) = \min_{\lambda} \left\{ e^{\lambda x - H(\lambda)} \right\}.$$

Convex duality

A convex function f(x) can be represented via a conjugate or dual function as follows

$$f(x) = \min_{\lambda} (\lambda x - f^*(\lambda))$$

The conjugate function f * (x) is obtained from the dual expression

$$f^*(\lambda) = \min_{x} (\lambda x - f(x))$$

11.7.2 Hash Functions

Sources:

Randomized algoritms – Motwani and Raghavan pp213-221

Universal Hash Families

ADD PARAGRAPH ON MOTIVATION

Let $M = \{1, 2, ..., m\}$ and $N = \{1, 2, ..., n\}$ where $m \ge n$. A family of hash functions H where $h \in H$ maps $h : M \to N$ is said to be 2-universal if for all x and y in M, x = y, and for h chosen uniformly at random from H,

$$Prob\left[h\left(x\right) = h\left(y\right)\right] \le \frac{1}{n}$$

Note that if H is the set of all possible mappings from M to N, then H is 2-universal. In fact $Prob\left[h\left(x\right)=h\left(y\right)\right]=\frac{1}{n}$. The difficulty in letting H consist of all possible functions is that a random h from H has no short representation. What we want is a small set H where each $h \in H$ has a short representation and is easy to compute.

Note that for a 2-universal H, for any two elements x and y, h(x) and h(y) behave as independent random variables. For a random f and any set X the set $\{f(x) | x \in X\}$ is a set of independent random variables.

Example: The following set of variables is two independent but not truly independent since 001 never occurs.

X	у	Z
0	0	0
0	1	1
1	0	1
1	1	0

Construction of 2-universal hash function

Fix m and n and select a prime p > m. Let $f_{ab}(x) = ax + b \mod p$. Then the set of all f_{ab} for a and b in $\{0, 1, \ldots, p-1\}$ with $a \neq 0$ is a set of 2-universal hash functions. The only difficulty is that p > n. Thus, consider $h_{ab}(x) = f_{ab}(x) \mod n$.

11.7.3 Sperner's Lemma

Consider a triangulation of a 2-dimensional simplex. Let the vertices of the simplex be colored R, B, and G. If the vertices on each edge of the simplex are colored only with the two colors at the endpoints then the triangulation must have a triangle whose vertices are three different colors. In fact it must have an odd number of such vertices. A generalization of the lemma to higher dimensions also holds.

Create a graph whose vertices correspond to the triangles of the triangulation plus an additional vertex corresponding to the outside region. Connect two vertices of the graph by an edge if the triangles corresponding to the two vertices share a common edge that is color R and B. The edge of the original simplex must have an odd number of such triangular edges. Thus the outside vertex of the graph must be of odd degree. The graph must have an even number of odd degree vertices. Each odd vertex is of degree 0, 1, or 2. The vertices of odd degree, i.e. degree one, correspond to triangles which have all three colors.

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References

- [ABC⁺08] Reid Andersen, Christian Borgs, Jennifer T. Chayes, John E. Hopcroft, Vahab S. Mirrokni, and Shang-Hua Teng. Local computation of pagerank contributions. *Internet Mathematics*, 5(1):23–45, 2008.
- [AF] David Aldous and James Fill. Reversible Markov Chains and Random Walks on Graphs. http://www.stat.berkeley.edu/aldous/RWG/book.html.
- [AK] Sanjeev Arora and Ravindran Kannan. Learning mixtures of separated non-spherical gaussians. *Annals of Applied Probability*, 15(1A):6992.
- [Alo86] Noga Alon. Eigenvalues and expanders. Combinatorica, 6:83–96, 1986.
- [AM05] Dimitris Achlioptas and Frank McSherry. On spectral learning of mixtures of distributions. In *COLT*, pages 458–469, 2005.
- [AN72] Krishna Athreya and P. E. Ney. *Branching Processes*, volume 107. Springer, Berlin, 1972.
- [AP03] Dimitris Achlioptas and Yuval Peres. The threshold for random k-sat is 2^k (ln 2 o(k)). In STOC, pages 223–231, 2003.
- [Aro11] Multiplicative weights method: a meta-algorithm and its applications. *Theory of Computing journal to appear*, 2011.
- [AS08] Noga Alon and Joel H. Spencer. *The probabilistic method*. Wiley-Interscience Series in Discrete Mathematics and Optimization. John Wiley & Sons Inc., Hoboken, NJ, third edition, 2008. With an appendix on the life and work of Paul Erdős.
- [BA] Albert-Lszl Barabsi and Rka Albert. Emergence of scaling in random networks. *Science*, 286(5439).
- [BEHW] A. Blumer, A. Ehrenfeucht, D. Haussler, and M. K. Warmuth. Learnability and the vapnik-chervonenkis dimension. *Journal of the Association for Computing Machinary*.
- [BMPW98] Sergey Brin, Rajeev Motwani, Lawrence Page, and Terry Winograd. What can you do with a web in your pocket? *Data Engineering Bulletin*, 21:37–47, 1998.
- [Bol01] Béla Bollobás. Random Graphs. Cambridge University Press, 2001.
- [BT87] Béla Bollobás and Andrew Thomason. Threshold functions. *Combinatorica*, 7(1):35–38, 1987.

- [CF86] Ming-Te Chao and John V. Franco. Probabilistic analysis of two heuristics for the 3-satisfiability problem. SIAM J. Comput., 15(4):1106–1118, 1986.
- [CGTS99] Moses Charikar, Sudipto Guha, Éva Tardos, and David B. Shmoys. A constant-factor approximation algorithm for the k-median problem (extended abstract). In Proceedings of the thirty-first annual ACM symposium on Theory of computing, STOC '99, pages 1–10, New York, NY, USA, 1999. ACM.
- [CHK⁺] Duncan S. Callaway, John E. Hopcroft, Jon M. Kleinberg, M. E. J. Newman, and Steven H. Strogatz. Are randomly grown graphs really random?
- [Chv92] 33rd Annual Symposium on Foundations of Computer Science, 24-27 October 1992, Pittsburgh, Pennsylvania, USA. IEEE, 1992.
- [CLMW11] Emmanuel J. Candès, Xiaodong Li, Yi Ma, and John Wright. Robust principal component analysis? *J. ACM*, 58(3):11, 2011.
- [DFK91] Martin Dyer, Alan Frieze, and Ravindran Kannan. A random polynomial time algorithm for approximating the volume of convex bodies. *Journal of the Association for Computing Machinary*, 1991.
- [DFK+99] Petros Drineas, Alan M. Frieze, Ravi Kannan, Santosh Vempala, and V. Vinay. Clustering in large graphs and matrices. In SODA, pages 291–299, 1999.
- [DG99] Sanjoy Dasgupta and Anupam Gupta. An elementary proof of the johnson-lindenstrauss lemma. 99(006), 1999.
- [DS84] Peter G. Doyle and J. Laurie Snell. Random walks and electric networks, volume 22 of Carus Mathematical Monographs. Mathematical Association of America, Washington, DC, 1984.
- [DS07] Sanjoy Dasgupta and Leonard J. Schulman. A probabilistic analysis of em for mixtures of separated, spherical gaussians. *Journal of Machine Learning Research*, 8:203–226, 2007.
- [ER60] Paul Erdös and Alfred Rényi. On the evolution of random graphs. *Publication of the Mathematical Institute of the Hungarian Academy of Sciences*, 5:17–61, 1960.
- [FK99] Alan M. Frieze and Ravindan Kannan. Quick approximation to matrices and applications. *Combinatorica*, 19(2):175–220, 1999.
- [Fri99] Friedgut. Sharp thresholds of graph properties and the k-sat problem. *Journal* of the American Math. Soc., 12, no 4:1017–1054, 1999.
- [FS96] Alan M. Frieze and Stephen Suen. Analysis of two simple heuristics on a random instance of k-sat. *J. Algorithms*, 20(2):312–355, 1996.

- [GvL96] Gene H. Golub and Charles F. van Loan. *Matrix computations (3. ed.)*. Johns Hopkins University Press, 1996.
- [Jer98] Mark Jerrum. Mathematical foundations of the markov chain monte carlo method. In Dorit Hochbaum, editor, Approximation Algorithms for NP-hard Problems, 1998.
- [JKLP93] Svante Janson, Donald E. Knuth, Tomasz Luczak, and Boris Pittel. The birth of the giant component. *Random Struct. Algorithms*, 4(3):233–359, 1993.
- [JLR00] Svante Janson, Tomasz Ĺuczak, and Andrzej Ruciński. *Random Graphs*. John Wiley and Sons, Inc, 2000.
- [Kan09] Ravindran Kannan. A new probability inequality using typical moments and concentration results. In *FOCS*, pages 211–220, 2009.
- [Kar90] Richard M. Karp. The transitive closure of a random digraph. Random Structures and Algorithms, 1(1):73–94, 1990.
- [Kle99] Jon M. Kleinberg. Authoritative sources in a hyperlinked environment. *JOURNAL OF THE ACM*, 46(5):604–632, 1999.
- [Kle00] Jon M. Kleinberg. The small-world phenomenon: an algorithm perspective. In STOC, pages 163–170, 2000.
- [Kle02] Jon M. Kleinberg. An impossibility theorem for clustering. In *NIPS*, pages 446–453, 2002.
- [KV95] Michael Kearns and Umesh Vazirani. An introduction to Computational Learning Theory. MIT Press, 1995.
- [KV09] Ravi Kannan and Santosh Vempala. Spectral algorithms. Foundations and Trends in Theoretical Computer Science, 4(3-4):157–288, 2009.
- [Liu01] Jun Liu. Monte Carlo Strategies in Scientific Computing. Springer, 2001.
- [Mat10] Jiří Matoušek. Geometric discrepancy, volume 18 of Algorithms and Combinatorics. Springer-Verlag, Berlin, 2010. An illustrated guide, Revised paperback reprint of the 1999 original.
- [Mit97] Tom M. Mitchell. Machine Learning. McGraw-Hill, New York, 1997.
- [MR95a] Michael Molloy and Bruce A. Reed. A critical point for random graphs with a given degree sequence. *Random Struct. Algorithms*, 6(2/3):161–180, 1995.
- [MR95b] Rajeev Motwani and Prabhakar Raghavan. Randomized Algorithms. Cambridge University Press, 1995.

- [MR99] Rajeev Motwani and Prabhakar Raghavan. Randomized algorithms. In *Algorithms and theory of computation handbook*, pages 15–1–15–23. CRC, Boca Raton, FL, 1999.
- [MU05] Michael Mitzenmacher and Eli Upfal. Probability and computing randomized algorithms and probabilistic analysis. Cambridge University Press, 2005.
- [MV10] Ankur Moitra and Gregory Valiant. Settling the polynomial learnability of mixtures of gaussians. In *FOCS*, pages 93–102, 2010.
- [Pal85] Edgar M. Palmer. *Graphical evolution*. Wiley-Interscience Series in Discrete Mathematics. John Wiley & Sons Ltd., Chichester, 1985. An introduction to the theory of random graphs, A Wiley-Interscience Publication.
- [Par98] Beresford N. Parlett. The symmetric eigenvalue problem, volume 20 of Classics in Applied Mathematics. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1998. Corrected reprint of the 1980 original.
- [per10] Markov Chains and Mixing Times. American Mathematical Society, 2010.
- [Sch90] Rob Schapire. Strength of weak learnability. *Machine Learning*, 5:197–227, 1990.
- [SJ] Alistair Sinclair and Mark Jerrum. Approximate counting, uniform generation and rapidly mixing markov chains. *Information and Computation*.
- [Sly10] Allan Sly. Computational transition at the uniqueness threshold. In FOCS, pages 287-296, 2010.
- [SS01] Bernhard Scholkopf and Alexander J. Smola. Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond. MIT Press, Cambridge, MA, USA, 2001.
- [SWY75] G. Salton, A. Wong, and C. S. Yang. A vector space model for automatic indexing. *Commun. ACM*, 18:613–620, November 1975.
- [Val84] Leslie G. Valiant. A theory of the learnable. In STOC, pages 436–445, 1984.
- [VC71] V. Vapnik and A. Chervonenkis. On the uniform convergence of relative frequencies of events to their probabilities. *Theory of Probability and its* Applications, 16(2):264–280, 1971.
- [Vem04] Santosh Vempala. The Random Projection Method. DIMACS, 2004.
- [VW02] Santosh Vempala and Grant Wang. A spectral algorithm for learning mixtures of distributions. *Journal of Computer and System Sciences*, pages 113–123, 2002.

- [WS98a] D. J. Watts and S. H. Strogatz. Collective dynamics of 'small-world' networks. Nature, 393 (6684), 1998.
- [WS98b] Duncan J. Watts and Steven H. Strogatz. Collective dynamics of 'small-world' networks. *Nature*, 393, 1998.
- [WW96] E. T. Whittaker and G. N. Watson. A course of modern analysis. Cambridge Mathematical Library. Cambridge University Press, Cambridge, 1996. An introduction to the general theory of infinite processes and of analytic functions; with an account of the principal transcendental functions, Reprint of the fourth (1927) edition.