GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

CROSS-VALIDATION

GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

K-NEAREST NEIGHBORS

I. CLASSIFICATION WITH K-NEAREST NEIGHBORS
II. DISTANCE MEASURES
III. THE CURSE OF DIMENSIONALITY

CLASSIFICATION WITH KNN

	continuous	*categorical*
supervised	???	???
unsupervised	???	???

	continuous	*categorical*
supervised	regression	classification
unsupervised	dimension reduction	clustering

- Sounds scary, but we work with it every day!
- Here is some 5-dimensional data:

Fisher's *Iris* Data

Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	*I. setosa*
4.9	3.0	1.4	0.2	*I. setosa*
4.7	3.2	1.3	0.2	*I. setosa*
4.6	3.1	1.5	0.2	*I. setosa*
5.0	3.6	1.4	0.2	*I. setosa*
5.4	3.9	1.7	0.4	*I. setosa*
4.6	3.4	1.4	0.3	*I. setosa*
5.0	3.4	1.5	0.2	*I. setosa*

- Sounds scary, but we work with it every day!

- Here are four features with a target we are trying to build a predictor for:

Target

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4.6	3.1	1.5	0.2	*I. setosa*
5.0	3.6	1.4	0.2	*I. setosa*
5.4	3.9	1.7	0.4	*I. setosa*

- Sounds scary, but we work with it every day!

- Here are four features with a target we are trying to build a predictor for:

```
data =
  [((5.1, 3.5, 1.4, 0.2), 0),
   ((4.9, 3.0, 1.4, 0.2), 0),
   ((4.7, 3.2, 1.3, 0.2), 0),
   ...
  ]
```

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Here's (part of) an example dataset:

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independent variables

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4.6	3.4	1.4	0.3	*I. setosa*
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class labels *(categorical)*

independent variables

Q: What does “supervised” mean?

Q: What does "supervised" mean?

A: We know the labels.

```
Welcome to R! Thu Feb 28 13:07:25 2013
> summary(iris)
  Sepal.Length    Sepal.Width     Petal.Length    Petal.Width   
 Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100  
 1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300  
 Median :5.800   Median :3.000   Median :4.350   Median :1.300  
 Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199  
 3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800  
 Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500  
       Species  
 setosa    :50  
 versicolor:50  
 virginica :50  
```

Q: How does a classification problem work?

Q: How does a classification problem work?

A: Data in, predicted labels out.

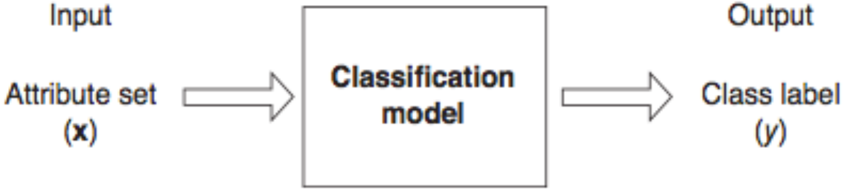
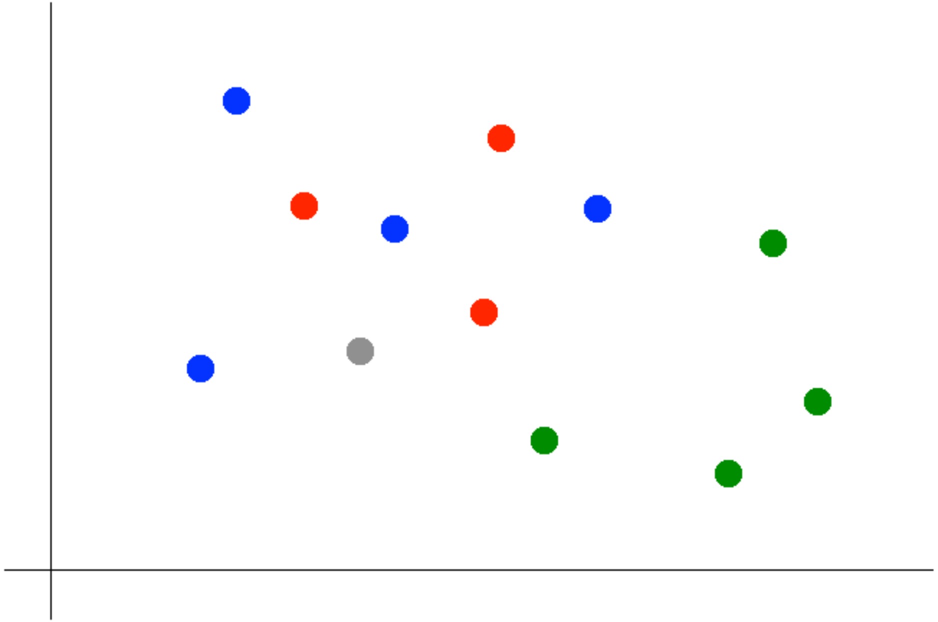


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

source: http://www-users.cs.umn.edu/~kumar/dmbook/ch4.pdf

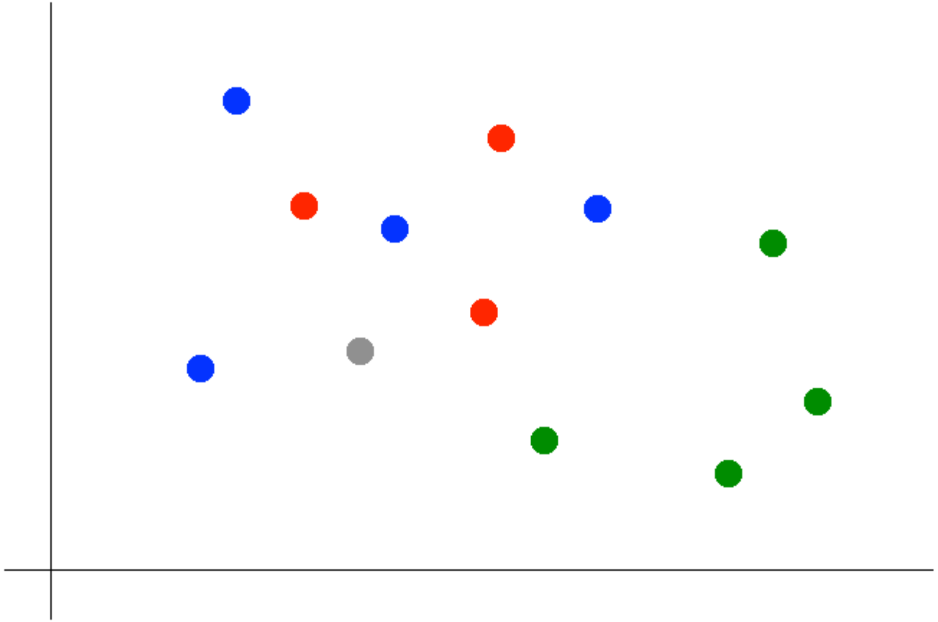
Suppose we want to predict the color of the grey dot.



Suppose we want to predict the color of the grey dot.

QUESTION:

What are the features?
What are the labels?



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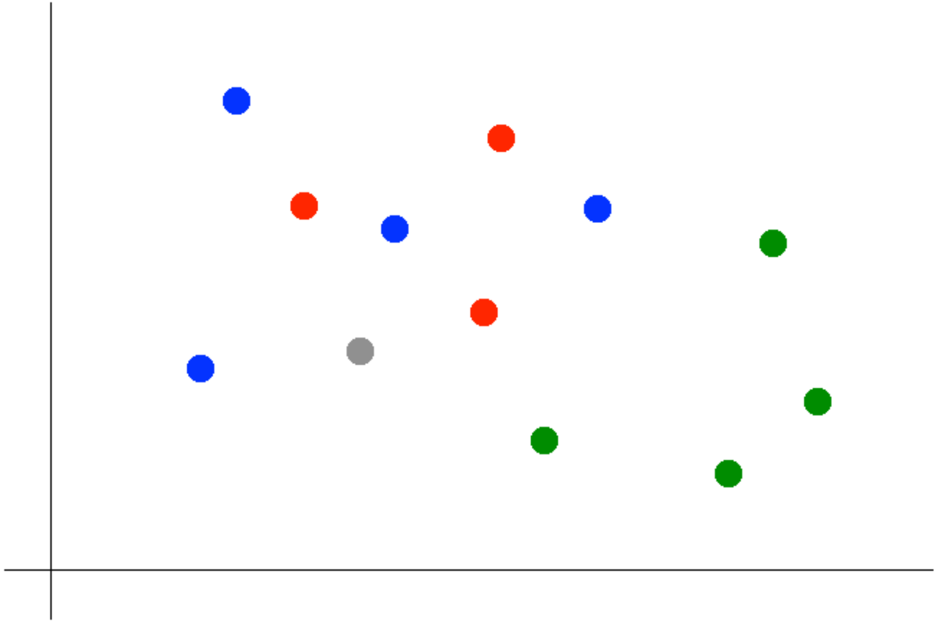
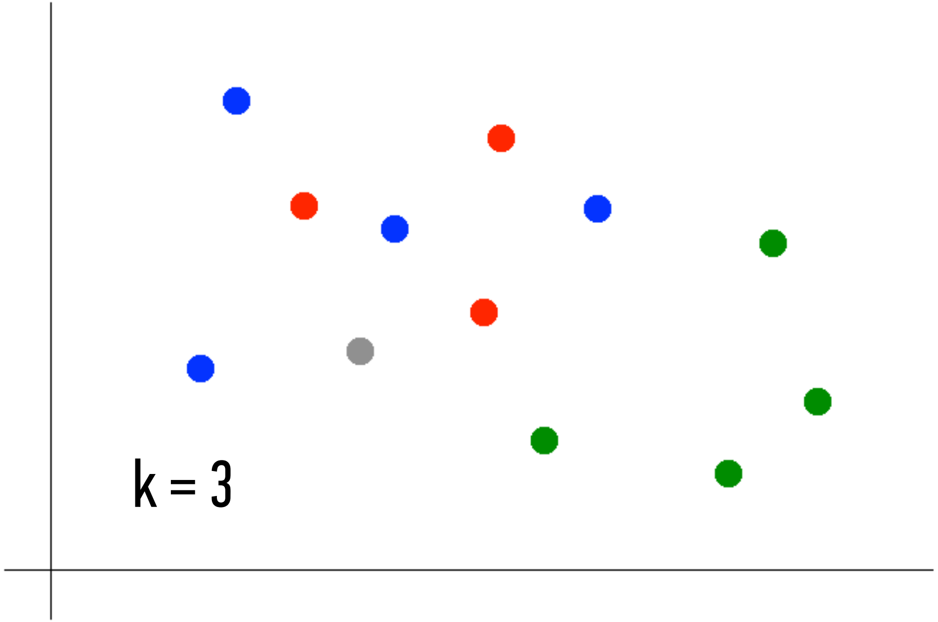


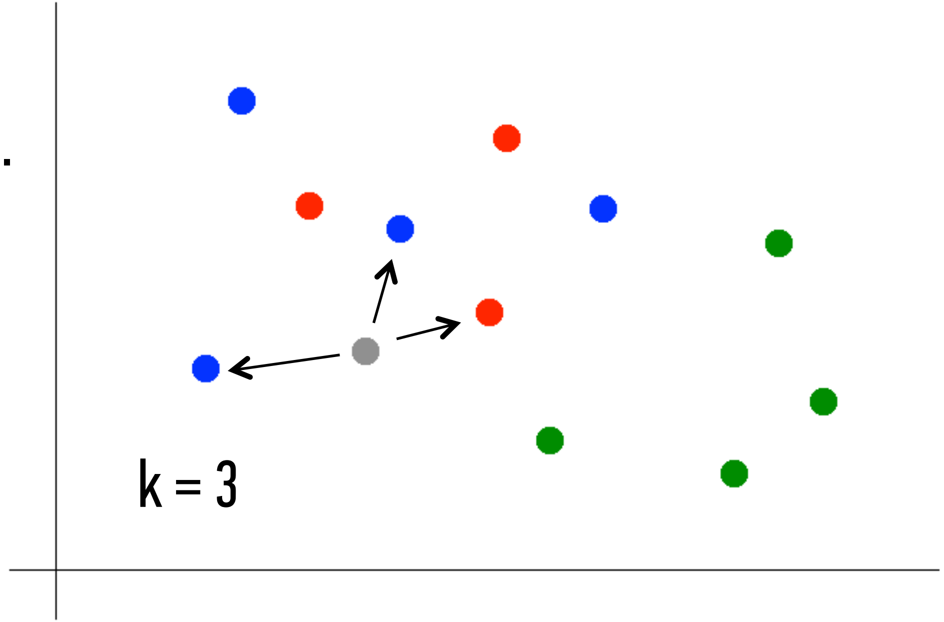
Suppose we want to predict the color of the grey dot.

1) Pick a value for k.



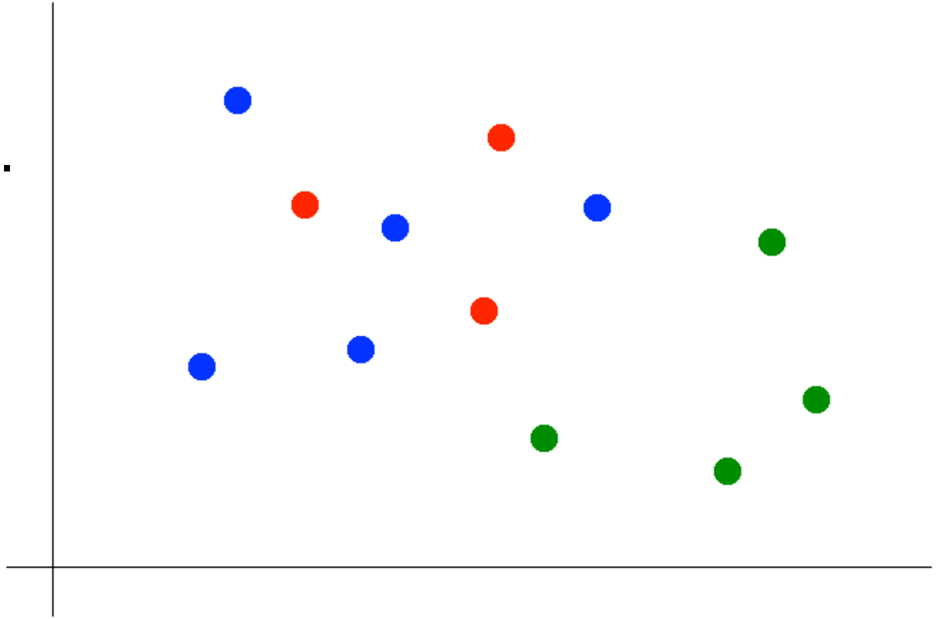
Suppose we want to predict the color of the grey dot.

1) Pick a value for k.
2) Find colors of k nearest neighbors.



Suppose we want to predict the color of the grey dot.

1) Pick a value for k.
2) Find colors of k nearest neighbors.
3) Assign the most common color to the grey dot.

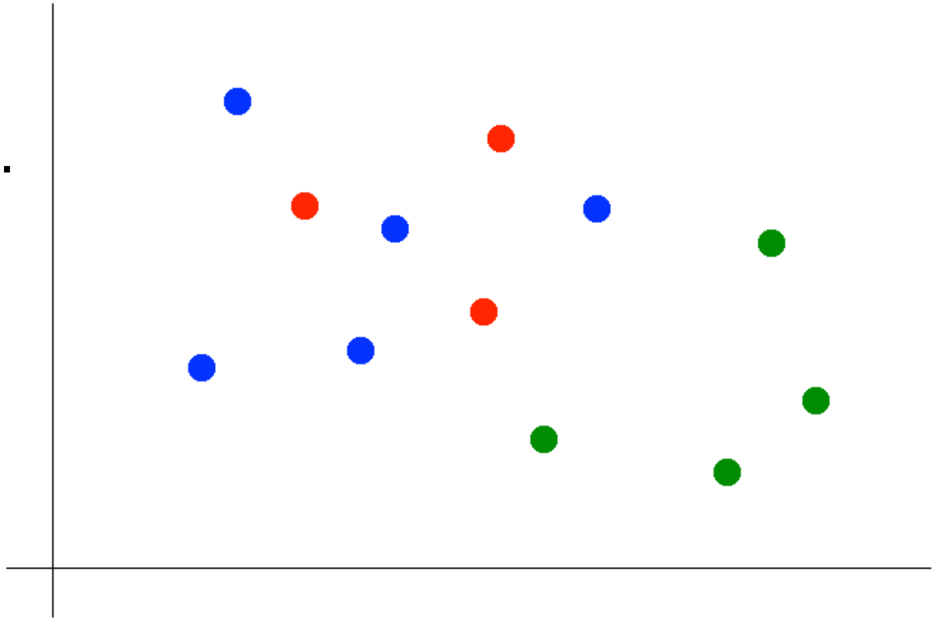


Suppose we want to predict the color of the grey dot.

1) Pick a value for k.
2) Find colors of k nearest neighbors.
3) Assign the most common color to the grey dot.

NOTE:

Our definition of "nearest" implicitly uses the *Euclidean distance function.*



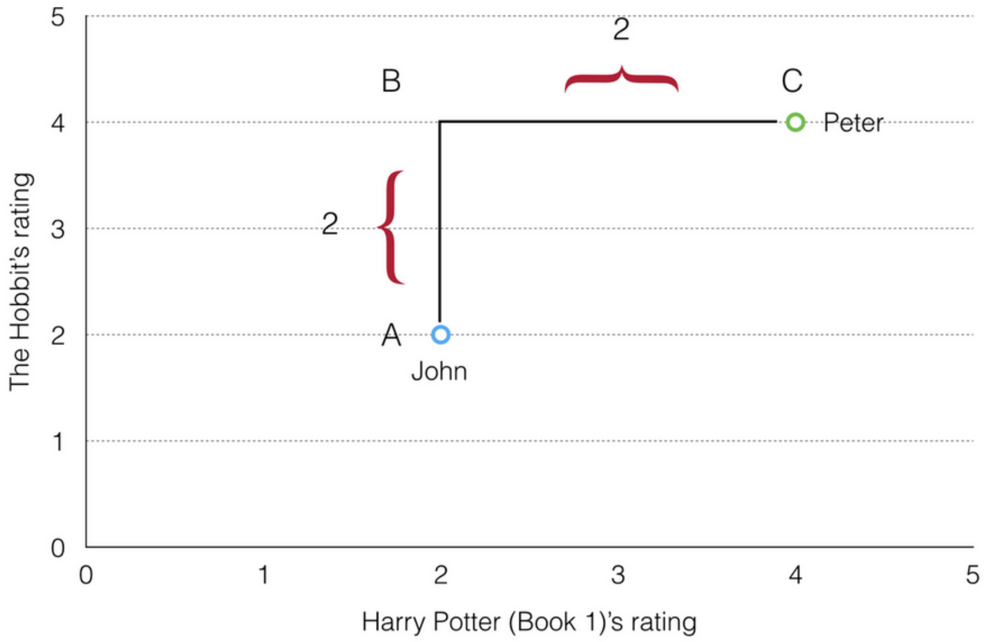
DISTANCE MEASURES

COMMON DISTANCE MEASURES

- Also known as “Taxicab Distance”.
- Here, two vectors X and Y are passed in. Each individual coordinate is compared.

Manhattan Distance

$$d(x,y)=\sum_{k=1}^{n}|x_k-y_k|$$



http://www.mickaellegal.com/blog/2014/1/30/how-to-build-a-recommender

Euclidean Distance

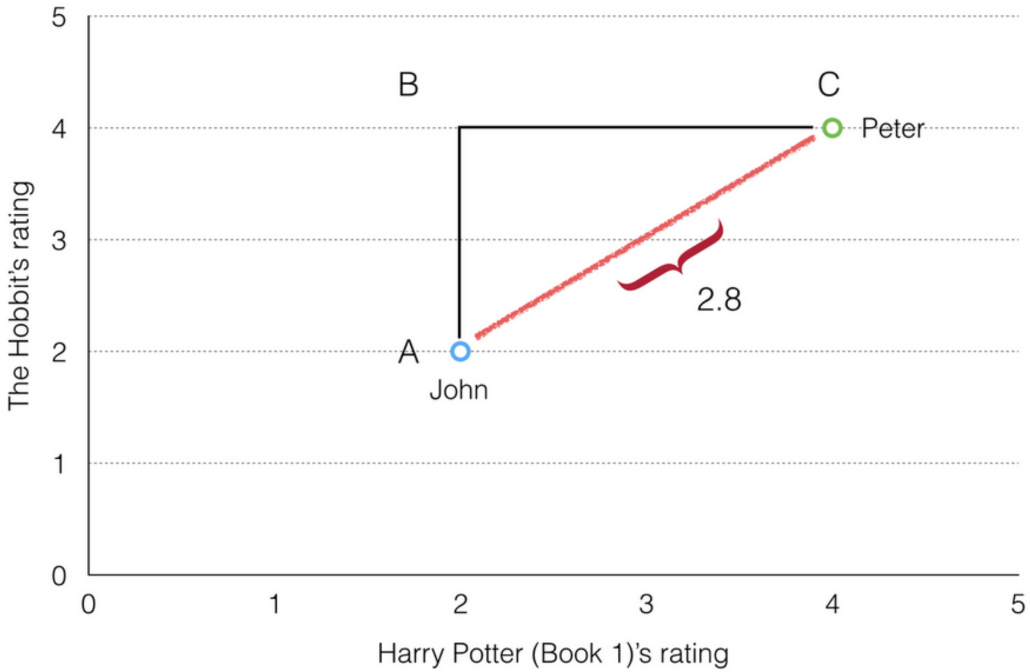
K-NEAREST NEIGHBORS

$$d(x,y) = \sqrt{\sum_{k=1}^{n} (x_k - y_k)^2}$$

- Make sure you understand how X and Y are defined:

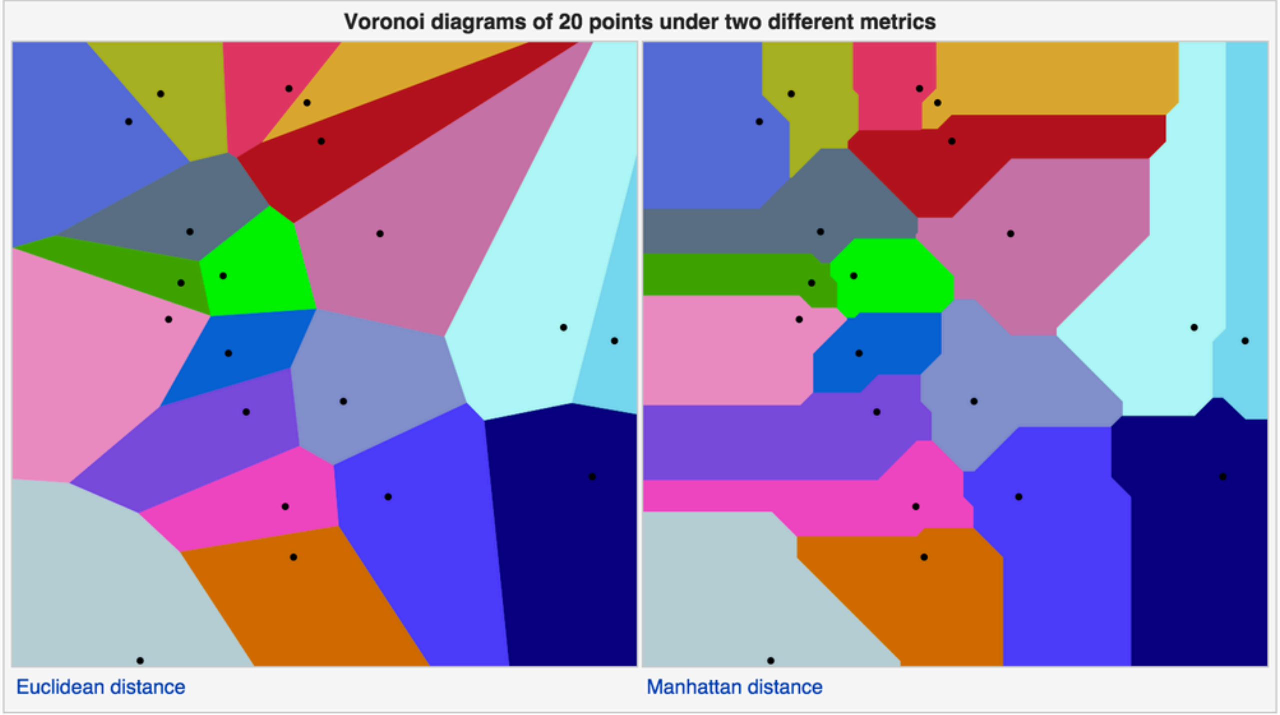
X = (1, 2, 3)
Y = (4, 5, 6)

d(X, Y) =
$(1 - 4)^2 + (2 - 5)^2 + (3 - 6)^2$



http://www.mickaellegal.com/blog/2014/1/30/how-to-build-a-recommender

- The regions that make up k-NN can be visualized using **Voronoi diagrams.**



https://en.wikipedia.org/wiki/Voronoi_diagram

Jaccard Distance

- Suppose A and B are sets of words in two different news articles.
- The Jaccard Distance between the news articles is the proportion of words they do not have in common.
- So, if two articles contained exactly the same words, the distance would be zero.

$$d_J(A,B) = 1 - J(A,B) = \frac{|A \cup B| - |A \cap B|}{|A \cup B|}.$$

http://www.mickaellegal.com/blog/2014/1/30/how-to-build-a-recommender

Hamming Distance

- Here, we have two bit strings X and Y.
- Each bit is either 0 or 1.
- So, if the bits are the same: |0-0| = |1–1| = 0.
- If the bits are different: |0-1|=|1-0|= 1.

Hamming Distance

$$D_H = \sum_{i=1}^{k} |x_i - y_i|$$

$$x = y \Rightarrow D = 0$$

$$x \neq y \Rightarrow D = 1$$

X	Y	Distance
Male	Male	0
Male	Female	1

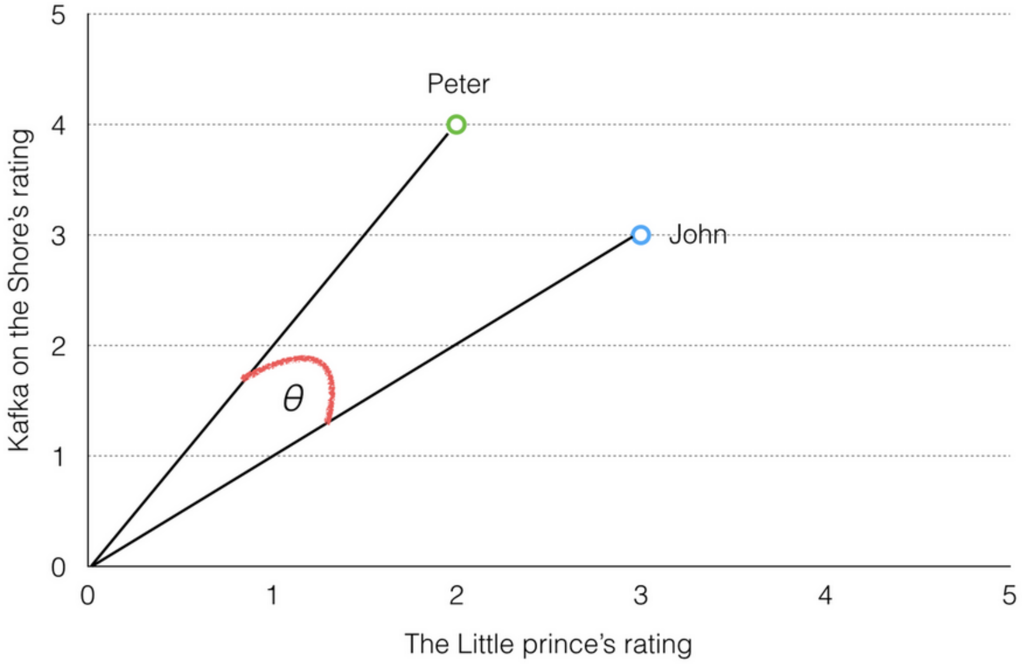
http://www.saedsayad.com/k_nearest_neighbors.htm

DISTANCES THAT SCALE

- Cosine Distance is popular because the magnitude of each vector is irrelevant.
- This is useful since biases in ratings are irrelevant.
- For example, suppose User 1 and User 2 both enjoy two books equally, but User 2 never gives 5. Then, User 1 and User 2 will have the same Cosine Distance.

Cosine Distance

$$cos(\theta) = \frac{x \cdot y}{||x|| * ||y||}$$



http://www.mickaellegal.com/blog/2014/1/30/how-to-build-a-recommender

- For some i, S_i is the standard deviation of the x_i and y_i over the sample set.
- This can alternatively be achieved by normalizing the features first then taking the standard Euclidean distance (subtract the mean and divide by the standard deviation): $\dfrac{x-\mu}{\sigma}$

Normalized Euclidean Distance

$$d(\vec{x}, \vec{y}) = \sqrt{\sum_{i=1}^{N} \frac{(x_i - y_i)^2}{s_i^2}},$$

Also see the Mahalanobis distance: https://en.wikipedia.org/wiki/Mahalanobis_distance

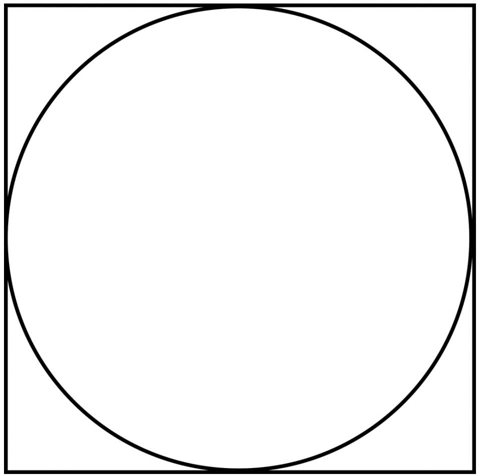
- **Neighbors are far apart with high dimensionality.**
- **Overfitting may easily occur.**
- Some features may require weighting.
- Some particular features may be correlated to others
- Many unknowns may result in poor Jaccard overlap
- Scaling problem with Euclidean distance, particularly with binary values
- Measurement error can affect result in unknown ways
- Calculation cost, since every data point must be compared

http://columbiadatascience.com/2012/10/18/week-7-hunch-com-recommendation-engines-svd-alternating-least-squares-convexity-filter-bubbles/

THE CURSE OF DIMENSIONALITY

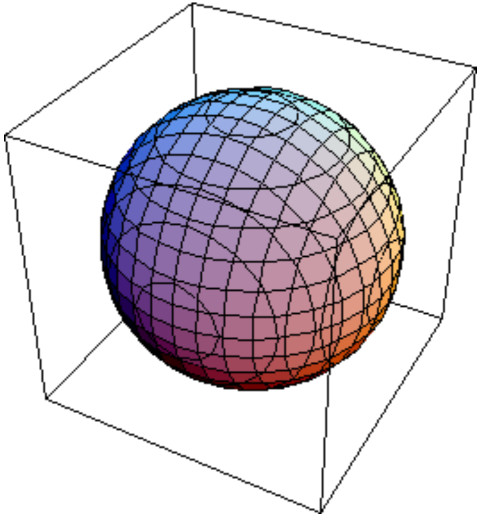
$$x^2 < R^2$$

1-dimensional



$$x^2 + y^2 < R^2$$

2-dimensional



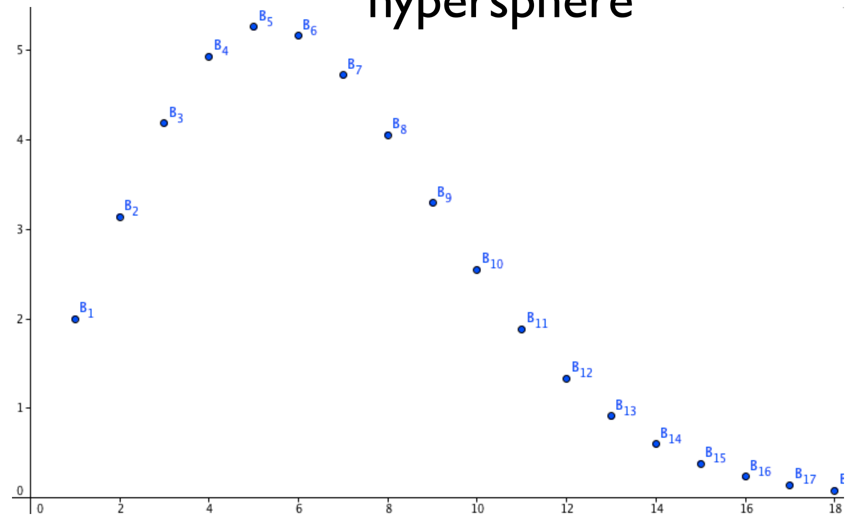
$$x^2 + y^2 + z^2 < R^2$$

3-dimensional

- As the number of dimensions increases with fixed radius, the hypersphere volume approaches zero.

Volume of n-dimensional hypersphere

Volume



Dimensions

$$V_1(R) = 2R,\ V_2(R) = \pi R^2, \text{ and } V_n(R) = \frac{2\pi R^2}{n} V_{n-2}(R),\ \text{for } n \geq 3.$$

Source: http://divisbyzero.com/2010/05/09/volumes-of-n-dimensional-balls/

- You may hear that most volume of an N-dimensional feature space is concentrated at the edges. To see this, define a hypersphere of radius 1:

$$x_1^2 + x_2^2 + \ldots + x_N^2 < 1$$

- Then, for $n = 100$, the point of equilibrium where all x are equal is $x = 0.1$, as follows:

$$N\overline{x}^2 = 1 \qquad \overline{x} = \sqrt{1/N}$$

- Hence, the edge of the "average" hypersphere is far away from the edge of the feature space.

Let's roughly estimate the effect of high dimensionality on k-NN. Doing this, we'll see that to hold a steady error rate, **exponentially more data is needed with each dimension added.**

- Suppose we have n features.
- Then, our "feature space" is n-dimensional.
- We will scale each feature to make it an n-dimensional unit cube, with a total volume of 1.

From Norvig & Russell, "Artificial Intelligence: A Modern Approach"

We will use k-NN with N data points.

- So, each neighborhood will require k/N fraction of the data points.
- On average, this is k/N of the total feature space.

To simplify calculations, suppose each neighborhood is an n-dimensional cube with side length b. Then:

$$b^n = k/N$$

Assuming the total feature space has sides 1, how is b affected by larger feature sets?

From Norvig & Russell, "Artificial Intelligence: A Modern Approach"

Knowing the total n-dimensional feature space has unit sides, how is the side length b of each neighborhood affected by more features?

$$b^n = k/N$$

Suppose $N = 1{,}000{,}000$ data points.
$k = 3$ nearest neighbors.

If $n = 3$ features, then $b \sim 0.01$.
If $n = 100$ features, then $b \sim 0.88$.

To encircle the 3 nearest neighbors, each neighborhood requires:

1% of feature space

88% of feature space!