Data Mining and Analysis: Fundamental Concepts and Algorithms

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Chapter 6: High-dimensional Data

High-dimensional Space

Let $\mathbf{D}$ be a $n \times d$ data matrix. In data mining typically the data is very high dimensional. Understanding the nature of high-dimensional space, or *hyperspace*, is very important, especially because it does not behave like the more familiar geometry in two or three dimensions.

Hyper-rectangle: The data space is a d-dimensional *hyper-rectangle*

$$R_d = \prod_{j=1}^{d} \Big[\min(X_j), \max(X_j)\Big]$$

where $\min(X_j)$ and $max(X_j)$ specify the range of X_j.

Hypercube: Assume the data is centered, and let m denote the maximum attribute value

$$m = \max_{j=1}^{d} \max_{i=1}^{n} \Big\{ |x_{ij}| \Big\}$$

The data hyperspace can be represented as a *hypercube*, centered at $\mathbf{0}$, with all sides of length $l = 2m$, given as

$$H_d(l) = \Big\{ \mathbf{x} = (x_1, x_2, \ldots, x_d)^T \;\Big|\; \forall i,\; x_i \in [-l/2, l/2] \Big\}$$

The *unit hypercube* has all sides of length $l = 1$, and is denoted as $H_d(1)$.

Hypersphere

Assume that the data has been centered, so that $\boldsymbol{\mu} = \mathbf{0}$. Let r denote the largest magnitude among all points:

$$r = \max_i \left\{ \|\mathbf{x}_i\| \right\}$$

The data hyperspace can be represented as a d-dimensional *hyperball* centered at $\mathbf{0}$ with radius r, defined as

$$B_d(r) = \left\{ \mathbf{x} \mid \; \|\mathbf{x}\| \le r \right\}$$

$$\text{or } B_d(r) = \left\{ \mathbf{x} = (x_1, x_2, \dots, x_d) \;\middle|\; \sum_{j=1}^{d} x_j^2 \le r^2 \right\}$$

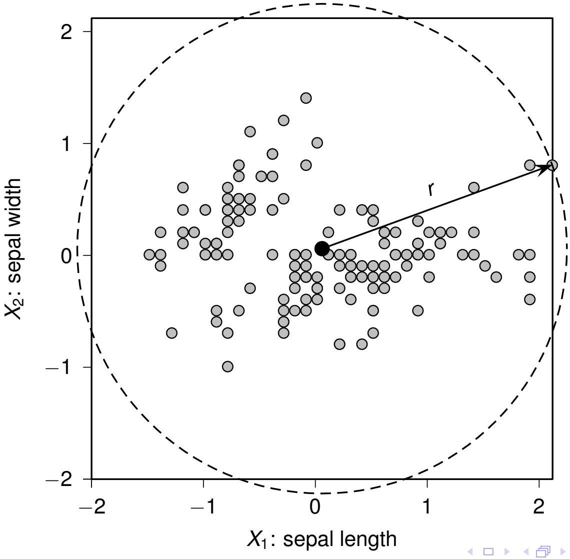
The surface of the hyperball is called a *hypersphere*, and it consists of all the points exactly at distance r from the center of the hyperball

$$S_d(r) = \left\{ \mathbf{x} \mid \; \|\mathbf{x}\| = r \right\}$$

$$\text{or } S_d(r) = \left\{ \mathbf{x} = (x_1, x_2, \dots, x_d) \;\middle|\; \sum_{j=1}^{d} (x_j)^2 = r^2 \right\}$$

Iris Data Hyperspace: Hypercube and Hypersphere

$l = 4.12$ and $r = 2.19$



High-dimensional Volumes

Hypercube: The volume of a hypercube with edge length l is given as

$$\text{vol}(H_d(l)) = l^d$$

HypersphereThe volume of a hyperball and its corresponding hypersphere is identical The volume of a hypersphere is given as

$$\begin{aligned}
\text{In 1 dimension: } & \text{vol}(S_1(r)) = 2r \\
\text{In 2 dimensions: } & \text{vol}(S_2(r)) = \pi r^2 \\
\text{In 3 dimensions: } & \text{vol}(S_3(r)) = \frac{4}{3}\pi r^3 \\
\text{In } d\text{-dimensions: } & \text{vol}(S_d(r)) = K_d r^d = \left(\frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)} \right) r^d
\end{aligned}$$

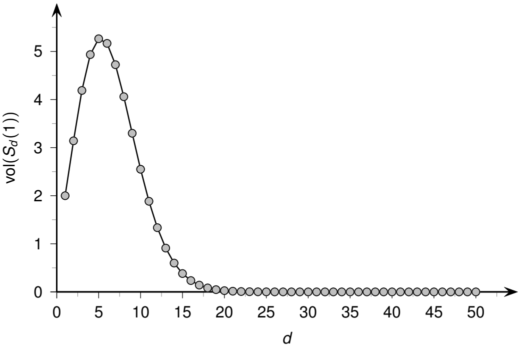
where

$$\Gamma\left(\frac{d}{2}+1\right) = \begin{cases} \left(\frac{d}{2}\right)! & \text{if } d \text{ is even} \\ \sqrt{\pi}\left(\frac{d!!}{2^{(d+1)/2}}\right) & \text{if } d \text{ is odd} \end{cases}$$

Volume of Unit Hypersphere

With increasing dimensionality the hypersphere volume first increases up to a point, and then starts to decrease, and ultimately vanishes. In particular, for the unit hypersphere with $r = 1$,

$$\lim_{d\to\infty} \text{vol}(S_d(1)) = \lim_{d\to\infty} \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2}+1)} \to 0$$



Hypersphere Inscribed within Hypercube

Consider the space enclosed within the largest hypersphere that can be accommodated within a hypercube (which represents the dataspace).

The ratio of the volume of the hypersphere of radius r to the hypercube with side length $l = 2r$ is given as

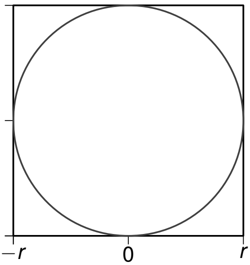
$$\text{In 2 dimensions: } \frac{\text{vol}(S_2(r))}{\text{vol}(H_2(2r))} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4} = 78.5\%$$

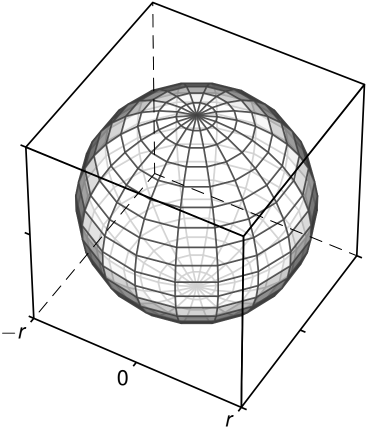
$$\text{In 3 dimensions: } \frac{\text{vol}(S_3(r))}{\text{vol}(H_3(2r))} = \frac{\frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6} = 52.4\%$$

$$\text{In } d \text{ dimensions: } \lim_{d\to\infty} \frac{\text{vol}(S_d(r))}{\text{vol}(H_d(2r))} = \lim_{d\to\infty} \frac{\pi^{d/2}}{2^d\Gamma(\frac{d}{2}+1)} \to 0$$

As the dimensionality increases, most of the volume of the hypercube is in the "corners," whereas the center is essentially empty.

Hypersphere Inscribed inside a Hypercube



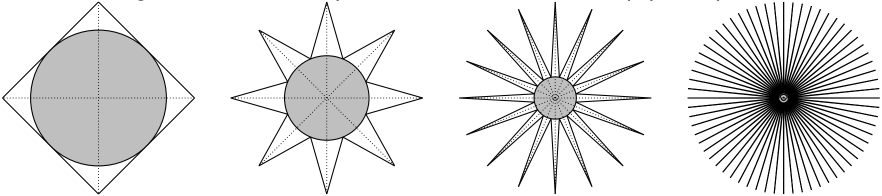


Conceptual View of High-dimensional Space

Two, three, four, and higher dimensions

All the volume of the hyperspace is in the corners, with the center being essentially empty.

High-dimensional space looks like a rolled-up porcupine!



(a) 2D (b) 3D (c) 4D (d) dD

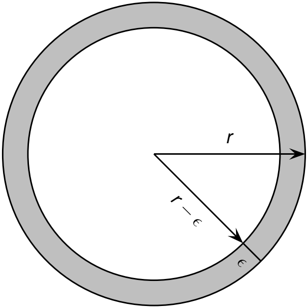
Volume of a Thin Shell

The volume of a thin hypershell of width ϵ is given as

$$\begin{aligned}\text{vol}(S_d(r,\epsilon)) &= \text{vol}(S_d(r)) - \text{vol}(S_d(r-\epsilon)) \\ &= K_d r^d - K_d(r-\epsilon)^d.\end{aligned}$$

The ratio of volume of the thin shell to the volume of the outer sphere:

$$\frac{\text{vol}(S_d(r,\epsilon))}{\text{vol}(S_d(r))} = \frac{K_d r^d - K_d(r-\epsilon)^d}{K_d r^d} = 1 - \left(1 - \frac{\epsilon}{r}\right)^d$$



As d increases, we have

$$\lim_{d\to\infty} \frac{\text{vol}(S_d(r,\epsilon))}{\text{vol}(S_d(r))} = \lim_{d\to\infty} 1 - \left(1 - \frac{\epsilon}{r}\right)^d \to 1$$

Diagonals in Hyperspace

Consider a d-dimensional hypercube, with origin $\mathbf{0}_d = (0_1, 0_2, \ldots, 0_d)$, and bounded in each dimension in the range $[-1, 1]$. Each "corner" of the hyperspace is a d-dimensional vector of the form $(\pm 1_1, \pm 1_2, \ldots, \pm 1_d)^T$.

Let $\mathbf{e}_i = (0_1, \ldots, 1_i, \ldots, 0_d)^T$ denote the d-dimensional canonical unit vector in dimension i, and let $\mathbf{1}$ denote the d-dimensional diagonal vector $(1_1, 1_2, \ldots, 1_d)^T$.

Consider the angle θ_d between the diagonal vector $\mathbf{1}$ and the first axis $\mathbf{e}_1$, in d dimensions:

$$\cos\theta_d = \frac{\mathbf{e}_1^T\mathbf{1}}{\|\mathbf{e}_1\|\;\|\mathbf{1}\|} = \frac{\mathbf{e}_1^T\mathbf{1}}{\sqrt{\mathbf{e}_1^T\mathbf{e}_1}\sqrt{\mathbf{1}^T\mathbf{1}}} = \frac{1}{\sqrt{1}\sqrt{d}} = \frac{1}{\sqrt{d}}$$

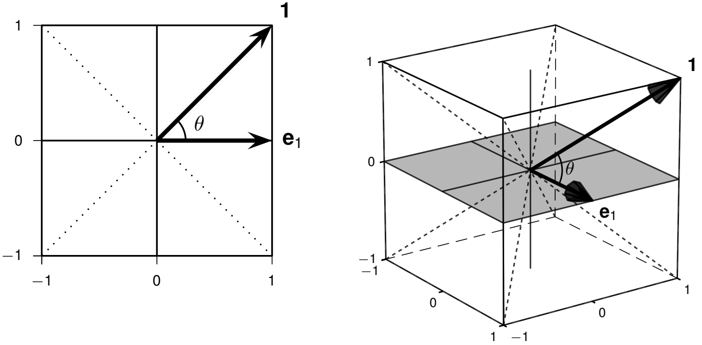
As d increases, we have

$$\lim_{d\to\infty}\cos\theta_d = \lim_{d\to\infty}\frac{1}{\sqrt{d}} \to 0$$

which implies that

$$\lim_{d\to\infty}\theta_d \to \frac{\pi}{2} = 90^\circ$$

Angle between Diagonal Vector $\mathbf{1}$ and $\mathbf{e}_1$



(a) In 2D (b) In 3D

In high dimensions all of the diagonal vectors are perpendicular (or orthogonal) to all the coordinates axes! Each of the 2^{d-1} new axes connecting pairs of 2^d corners are essentially orthogonal to all of the d principal coordinate axes! Thus, in effect, high-dimensional space has an exponential number of orthogonal "axes."

Density of the Multivariate Normal

Consider the standard multivariate normal distribution with $\boldsymbol{\mu} = \mathbf{0}$, and $\boldsymbol{\Sigma} = \mathbf{I}$

$$f(\mathbf{x}) = \frac{1}{(\sqrt{2\pi})^d} \exp\left\{-\frac{\mathbf{x}^T\mathbf{x}}{2}\right\}$$

The peak of the density is at the mean. Consider the set of points $\mathbf{x}$ with density at least α fraction of the density at the mean

$$\frac{f(\mathbf{x})}{f(\mathbf{0})} \geq \alpha$$

$$\exp\left\{-\frac{\mathbf{x}^T\mathbf{x}}{2}\right\} \geq \alpha$$

$$\mathbf{x}^T\mathbf{x} \leq -2\ln(\alpha)$$

$$\sum_{i=1}^{d}(x_i)^2 \leq -2\ln(\alpha)$$

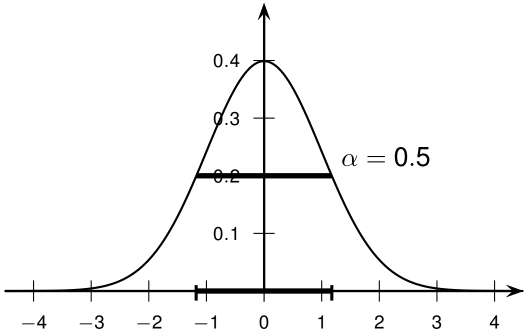
The sum of squared IID random variables follows a chi-squared distribution χ^2_d. Thus,

$$P\left(\frac{f(\mathbf{x})}{f(\mathbf{0})} \geq \alpha\right) = F_{\chi^2_d}(-2\ln(\alpha))$$

where $F_{\chi^2_q}$ is the CDF.

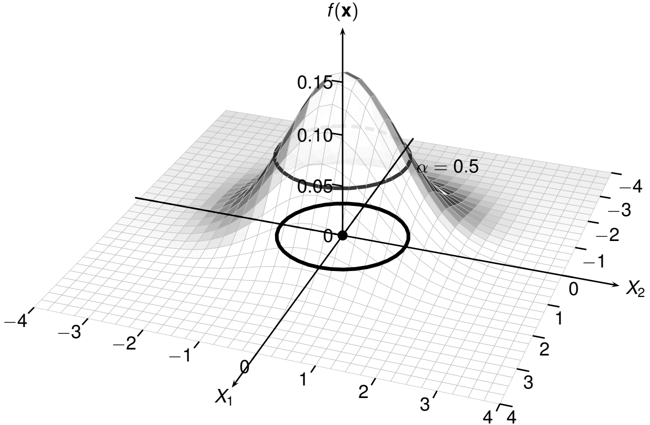
Density Contour for α Fraction of the Density at the Mean: One Dimension

Let $\alpha = 0.5$, then $-2\ln(0.5) = 1.386$ and $F_{\chi^2_1}(1.386) = 0.76$. Thus, 24% of the density is in the tail regions.



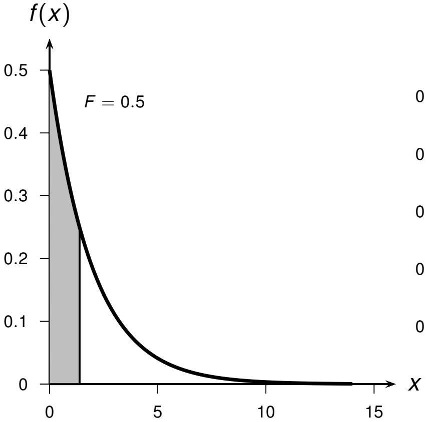
Density Contour for α Fraction of the Density at the Mean: Two Dimensions

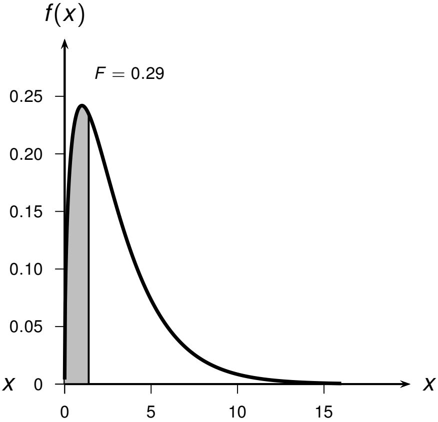
Let $\alpha = 0.5$, then $-2\ln(0.5) = 1.386$ and $F_{\chi^2_2}(1.386) = 0.50$. Thus, 50% of the density is in the tail regions.



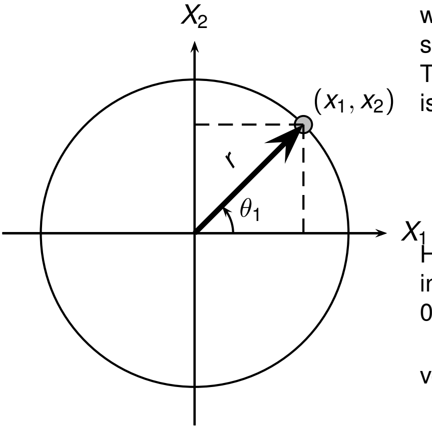
Chi-Squared Distribution: $P(f(\mathbf{x})/f(\mathbf{0}) \geq \alpha)$

This probability decreases rapidly with dimensionality. For 2D, it is 0.5. For 3D it is 0.29, ie., 71% of the density is in the tails. By $d = 10$, it decreases to 0.075%, that is, 99.925% of the points lie in the extreme or tail regions.





Hypersphere Volume: Polar Coordinates in 2D



The point $\mathbf{x} = (x_1, x_2)$ in polar coordinates

$$x_1 = r\cos\theta_1 = rc_1$$
$$x_2 = r\sin\theta_1 = rs_1$$

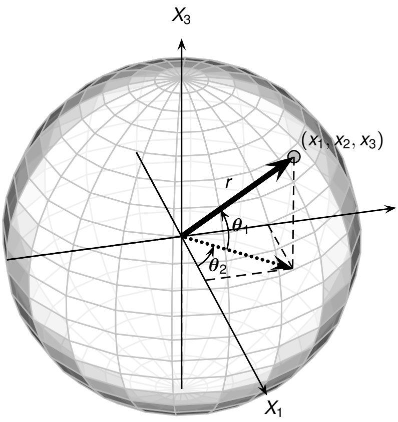
where $r = \|\mathbf{x}\|$, and $\cos\theta_1 = c_1$ and $\sin\theta_1 = s_1$.
The *Jacobian matrix* for this transformation is given as

$$J(\theta_1) = \begin{pmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_1}{\partial \theta_1} \\ \frac{\partial x_2}{\partial r} & \frac{\partial x_2}{\partial \theta_1} \end{pmatrix} = \begin{pmatrix} c_1 & -rs_1 \\ s_1 & rc_1 \end{pmatrix}$$

Hypersphere volume is obtained by integration over r and θ_1 (with $r > 0$, and $0 \leq \theta_1 \leq 2\pi$):

$$\text{vol}(S_2(r)) = \int_r \int_{\theta_1} \left|\det(J(\theta_1))\right| \, dr \, d\theta_1$$
$$= \int_0^r \int_0^{2\pi} r \, dr \, d\theta_1 = \int_0^r r \, dr \int_0^{2\pi} d\theta_1$$

Hypersphere Volume: Polar Coordinates in 3D



$\mathbf{x} = (x_1, x_2, x_2)$ in polar coordinates

$$\begin{aligned} x_1 &= r\cos\theta_1\cos\theta_2 = rc_1c_2 \\ x_2 &= r\cos\theta_1\sin\theta_2 = rc_1s_2 \\ x_3 &= r\sin\theta_1 = rs_1 \end{aligned}$$

The Jacobian matrix is given as

$$X_2 J(\theta_1, \theta_2) = \begin{pmatrix} c_1c_2 & -rs_1c_2 & -rc_1s_2 \\ c_1s_2 & -rs_1s_2 & rc_1c_2 \\ s_1 & rc_1 & 0 \end{pmatrix}$$

The volume of the hypersphere for $d = 3$ is obtained via a triple integral with $r > 0$, $-\pi/2 \le \theta_1 \le \pi/2$, and $0 \le \theta_2 \le 2\pi$

$$\begin{aligned} \text{vol}(S_3(r)) &= \int_r \int_{\theta_1} \int_{\theta_2} \left|\det(J(\theta_1, \theta_2))\right| \, dr \, d\theta_1 \, d\theta_2 \\ &= \frac{4}{3}\pi r^3 \end{aligned}$$

Hypersphere Volume in d Dimensions

The determinant of the d-dimensional Jacobian matrix is

$$\det(J(\theta_1, \theta_2, \ldots, \theta_{d-1})) = (-1)^d r^{d-1} c_1^{d-2} c_2^{d-3} \ldots c_{d-2}$$

The volume of the hypersphere is given by the d-dimensional integral with $r > 0$, $-\pi/2 \leq \theta_i \leq \pi/2$ for all $i = 1, \ldots, d-2$, and $0 \leq \theta_{d-1} \leq 2\pi$:

$$\begin{aligned}
\mathrm{vol}(S_d(r)) &= \int_r \int_{\theta_1} \int_{\theta_2} \ldots \int_{\theta_{d-1}} \Big| \det(J(\theta_1, \theta_2, \ldots, \theta_{d-1})) \Big| \; dr \; d\theta_1 \; d\theta_2 \ldots d\theta_{d-1} \\
&= \int_0^r r^{d-1} dr \int_{-\pi/2}^{\pi/2} c_1^{d-2} d\theta_1 \; \ldots \int_{-\pi/2}^{\pi/2} c_{d-2} d\theta_{d-2} \int_0^{2\pi} d\theta_{d-1} \\
&= \frac{r^d}{d} \frac{\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} \frac{\Gamma\left(\frac{d-2}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{d-1}{2}\right)} \ldots \frac{\Gamma(1)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{3}{2}\right)} 2\pi \\
&= \frac{\pi \Gamma\left(\frac{1}{2}\right)^{d/2-1} r^d}{\frac{d}{2}\Gamma\left(\frac{d}{2}\right)} \\
&= \left(\frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)}\right) r^d
\end{aligned}$$