降维

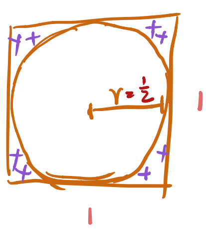
解决：

- 过拟合
  - 增加 data
  - 正则化
  - 降维 →
    - 直接降维 → 特征选择
    - 线性降维 →
      - PCA
      - MDS
    - 非线性降维 → 流形
      - Isomap
      - LLE

如果一直增加特征维数，由于样本分布越来越稀疏，如果要避免过拟合的出现，就不得不持续增加样本数量。

- 维度灾难

$\boxed{\text{几何角度}}$



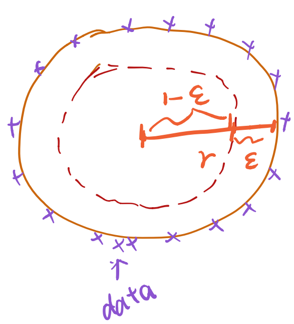
D：维度

$V_{超立方体} = 1$

$V_{超球体} = k \cdot R^D = k \cdot (0.5)^D \quad D \to \infty$

$\to 0$ 说明里面为空

即 D↑，数据稀疏化



$V_{外} = k \cdot 1^D = k$

$V_{环形带} = V_{外} - V_{内}$

$= k - k \cdot (1-\varepsilon)^D$

$$\frac{V_{环形带}}{V_{外}} = \frac{k - k \cdot (1-\varepsilon)^D}{k} = 1 - (1-\varepsilon)^D$$

$$\forall\ 0<\varepsilon<1 \qquad \lim_{D\to\infty}(1-\varepsilon)^D=0 \qquad \Rightarrow \lim_{D\to\infty}\frac{V_{环}}{V_{外}}=1$$ 一个空壳

维度太高，距离都很大，样本间距离就没有实际意义了

[样本均值，样本方差的矩阵表示]：

Data： $X=(x_1, x_2 \cdots x_N)^T_{N\times p} = \begin{pmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Np} \end{pmatrix}_{N\times p}$

p维

$x_i \in R^p \quad i=1,2,3\cdots N \qquad 1_N=\begin{pmatrix}1\\ \vdots \\ 1\end{pmatrix}_{N\times 1} \qquad H_N=I_N-\frac{1}{N}1_N1_N^T$

[p维]

Sample mean： $\underline{\bar{X}_{p\times 1}}=\frac{1}{N}\sum_{i=1}^{N}x_i=\frac{1}{N}X^T1_N$

Sample covariance： $\underline{S_{p\times p}}=\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})(x_i-\bar{x})^T=\frac{1}{N}X^THX$

① $\bar{x}=\frac{1}{N}\sum_{i=1}^{N}x_i=\frac{1}{N}\underbrace{(x_1\ x_2 \cdots x_N)}_{X^T}\underline{\begin{pmatrix}1\\ \vdots \\ 1\end{pmatrix}_{N\times 1}}=\frac{1}{N}X^T1_N$

② $S=\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})(x_i-\bar{x})^T$

$=\frac{1}{N}\underbrace{(x_1-\bar{x}\quad x_2-\bar{x}\quad x_3-\bar{x}\ \cdots\ x_N-\bar{x})}\begin{pmatrix}(x_1-\bar{x})^T\\ (x_2-\bar{x})^T \\ \vdots \\ (x_N-\bar{x})^T\end{pmatrix}$

$$(x_1\ \ x_2 \cdots x_N) - (\bar{x}\ \ \bar{x} \cdots \bar{x})$$

$$X^T - \bar{x}\underbrace{(1\ \ 1\ \ 1 \cdots 1)}_{1_N^T}$$

$$X^T - \frac{1}{N}X^T 1_N \bar{X} 1_N^T$$

$$X^T\left(1_N - \frac{1}{N}1_N 1_N^T\right)$$

$$= \frac{1}{N}X^T\underbrace{\left(1_N - \frac{1}{N}1_N 1_N^T\right)}_{H_{N\times N}\text{中心矩阵}} \cdot \left(1_N - \frac{1}{N}1_N 1_N^T\right)^T X$$

$$= \frac{1}{N}X^T H \cdot H^T X$$

$$\boxed{= \frac{1}{N}X^T H X}$$

$$\begin{cases} H = 1_N - \frac{1}{N}1_N 1_N^T \\ H^T = \left(1_N - \frac{1}{N}1_N 1_N^T\right) = 1_N - \frac{1}{N}1_N 1_N^T = H \end{cases}$$

$$H^2 = H \cdot H = \left(1_N - \frac{1}{N}1_N 1_N^T\right)\left(1_N - \frac{1}{N}1_N 1_N^T\right)$$

$$= 1_N - \frac{2}{N}1_N 1_N^T + \underbrace{\frac{1}{N^2}1_N \underbrace{1_N^T 1_N}_{N} 1_N^T}_{\frac{1}{N}\begin{pmatrix} 1 & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}_{N\times N}}$$

$$= 1_N - \frac{1}{N}1_N 1_N^T = H$$

$$\Rightarrow H^n = H$$

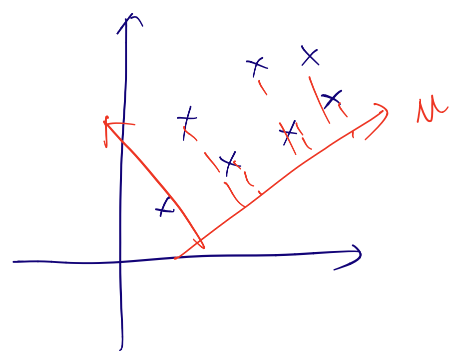
[主成分分析(PCA) - 最大投影方差角度]:

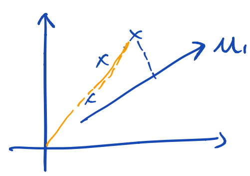
data, Mean, Covariance ... 同上

一个中心：原始特征空间的重构

使相关 → 无关 (正交基)

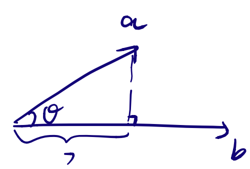
两个基本点：
- 最大投影方差 $\Longrightarrow$
- 最小重构距离





首先：中心化 $\Rightarrow$ $x_i - \bar{x}$

$x_i - \bar{x}$ $\quad u_1 \quad \|u_1\| = 1$



$|\vec{b}| = 1$

$$? = |\vec{a}| \cdot \cos\theta$$

$$\because \ \vec{a} \cdot \vec{b} = |\vec{a}||\vec{b}|\cos\theta = |\vec{a}| \cdot \cos\theta$$

$$\Rightarrow \ ? = \vec{a} \cdot \vec{b} = a^T b$$

[方差] $J = \frac{1}{N} \sum_{i=1}^{N} \left((x_i - \bar{x})^T u_1 \right)^2$ 中心化后均值为0 $\quad s.t.\ u_1^T u_1 = 1$

$$= \frac{1}{N} \sum_{i=1}^{N} u_1^T (x_i - \bar{x}) (x_i - \bar{x})^T u_1$$

$$= u_1^T \left(\sum_{i=1}^{N} \frac{1}{N} (x_i - \bar{x})(x_i - \bar{x})^T \right) u_1$$

$$= u_1^T \cdot S \cdot u_1$$

$$\begin{cases} \hat{u}_1 = \arg\max \, u_1^T \cdot S \cdot u_1 \\ \text{s.t.} \quad u_1^T u = 1 \end{cases}$$

$$\mathcal{L}(u_1, \lambda) = u_1^T \cdot S \cdot u_1 + \lambda(1 - u_1^T u_1)$$

$$\frac{\partial \mathcal{L}}{\partial u_1} = 2Su_1 - \lambda \cdot 2u_1 = 0$$

$$Su_1 = \lambda u_1$$

方差矩阵

特征向量

特征值