CS182 Introduction to Machine Learning

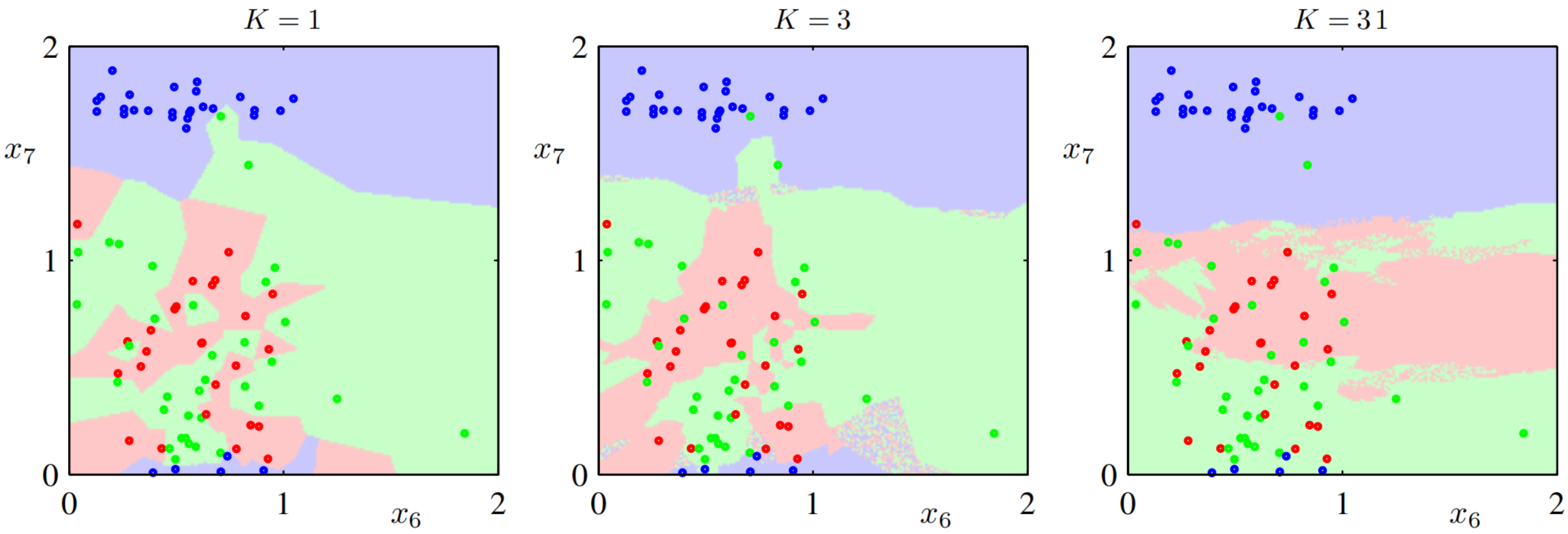
Recitation 2

2025.3.5

Outline

- KNN
- Curse of Dimensionality
- Review(Preview): Linear Algebra

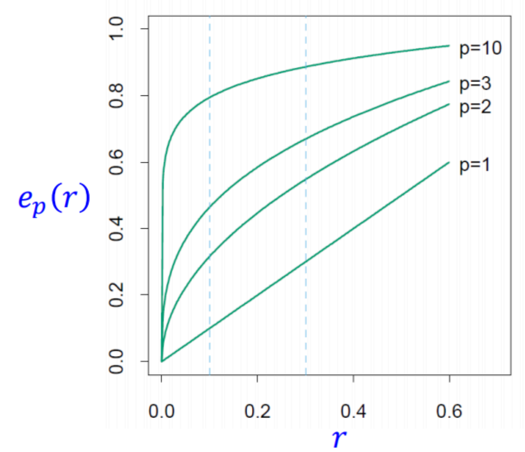
KNN (K-Nearest Neighbors)



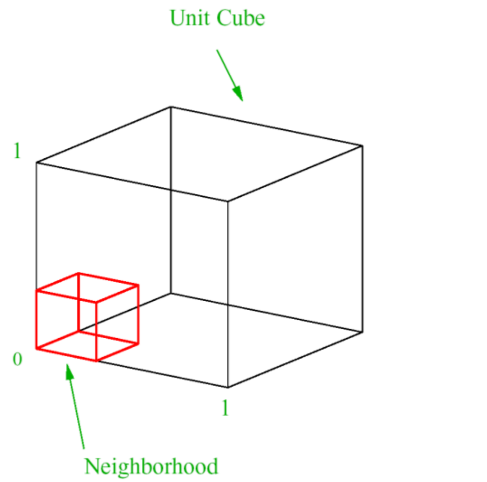
Curse of Dimensionality (维度诅咒)

Local neighborhoods become increasingly global, as the p increases

p: 维度数, e:边长, $r = \frac{e^p}{1}$, $e_p(r) = r^{\frac{1}{p}}$



Reducing r reduces the number of observations and thus the stability.



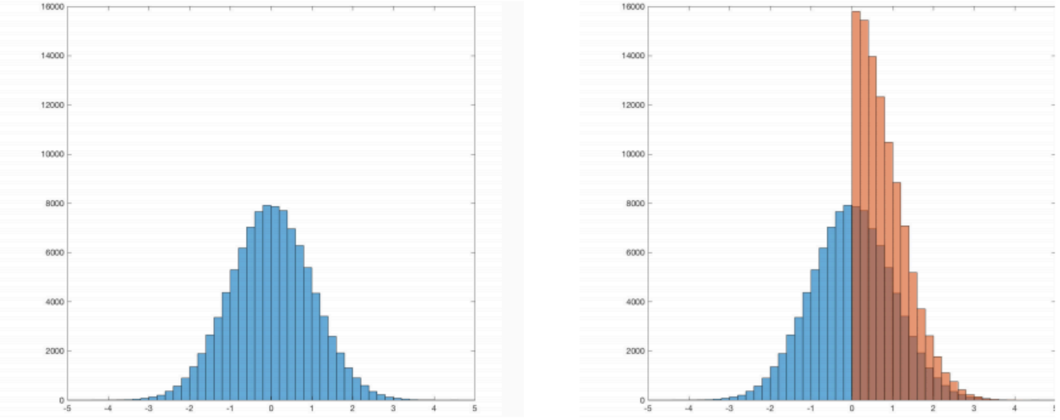
In ten dimensions we need to cover 63% (80%) of the range of each coordinate to capture 1% (10%) of the data.

高维情况下, 距离, cosine similarity等度量方式失效.

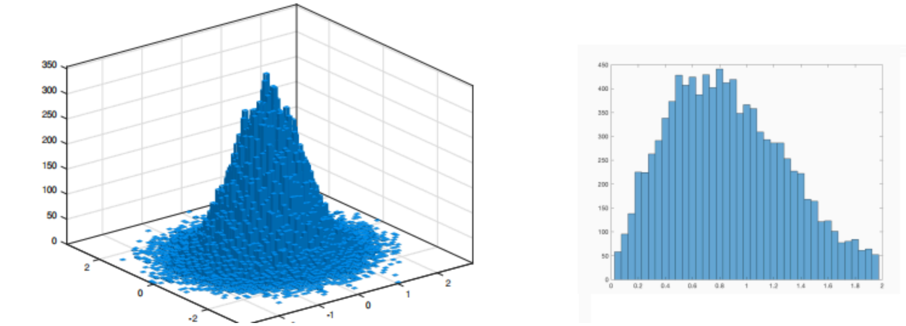
e.g. 1维, 2维 Gaussian distribution PDF集中在均值附近, 但是在高维空间中, 大部分数据点都位于边界附近

Curse of Dimensionality (维度诅咒)

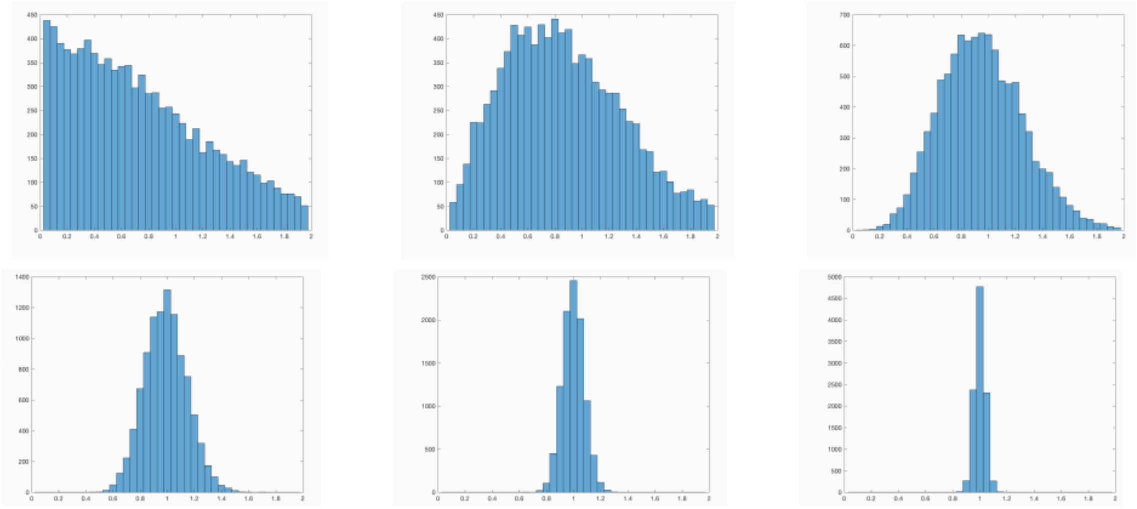
distribution of a one-dimensional Gaussian vector $x \in \mathbb{R}^1$ and of its length $\|x\| \in \mathbb{R}$, with 100.000 samples



distribution of a two-dimensional Gaussian vector $x \in \mathbb{R}^2$ and of its length $\|x\| \in \mathbb{R}$, with 100.000 samples



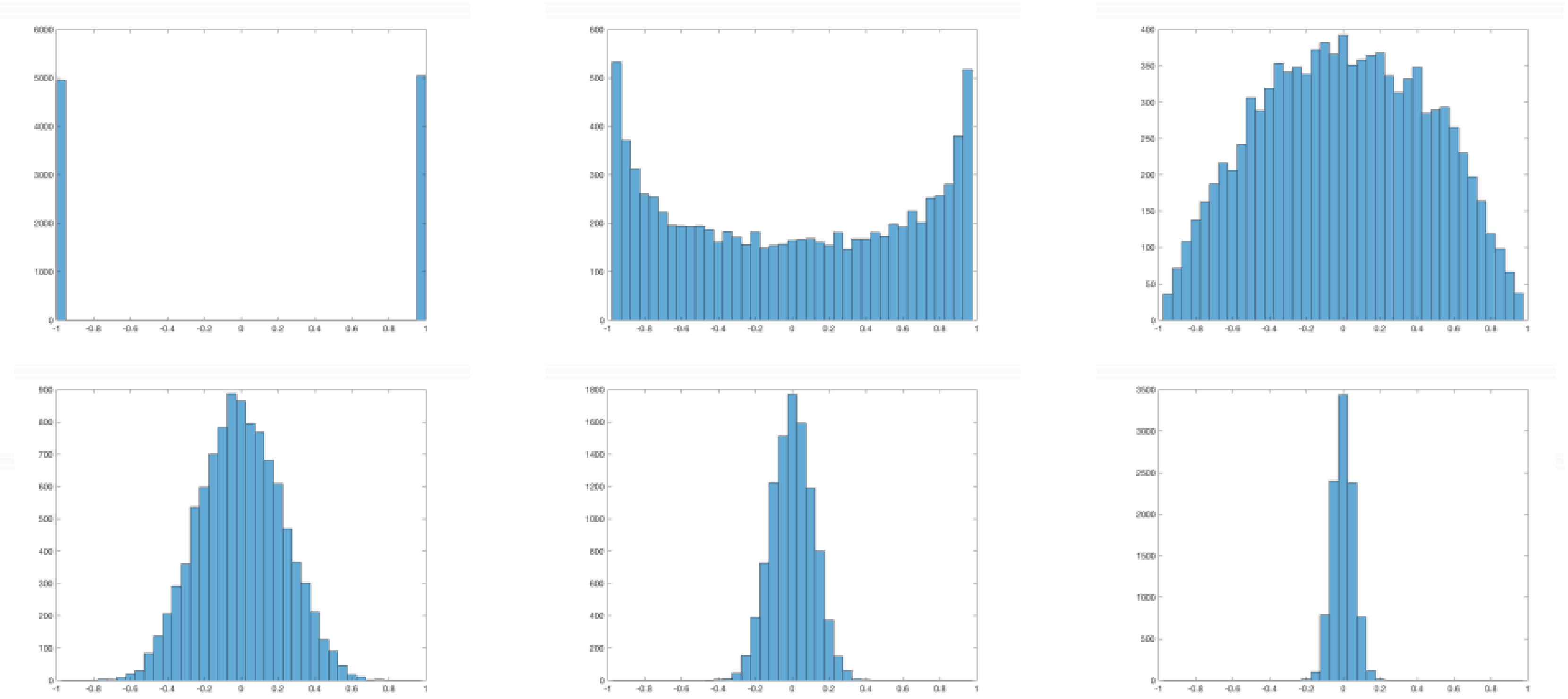
the length $\|x\| \in \mathbb{R}$ of a Gaussian vector $x \in \mathbb{R}^p$, for $p = 1, 2, 5, 20, 80, 320$; with 10.000 samples in each case



Curse of Dimensionality (维度诅咒)

Two Gaussian random vectors are nearly orthogonal in high dimensions

For 10.000 samples of pairs (x_1, x_2) of independent Gaussian vectors $x_1, x_2 \in \mathbb{R}^p$, the histogram of the normalized inner product $\frac{\langle x_1, x_2 \rangle}{\|x_1\| \cdot \|x_2\|}$ is shown for $p = 1, 2, 5, 20, 80, 320$. This shows that two such vectors are close to orthogonal in high dimensions. Note that 0 is, also in small dimensions, the expectation of the normalized inner product.



外差(Extrapolation), 内插(Interpolation).

外差是指在已知数据范围之外做预测的过程。在高维情况下，由于数据点之间的距离普遍较大，模型往往需要在大量空白或未探索的空间中进行预测，这通常会导致预测不准确。

内插是指在已知数据点之间进行预测的过程。在低维空间，数据点比较密集，内插通常可以较好地进行。然而在高维空间，即使是最近的邻居也可能相距甚远，这使得内插的效果大打折扣。

Review(Preview): Linear Algebra

- 为什么用到线性代数：
  - 线性代数是描述空间和变换的工具，让描述问题变得简单
  - 大量学习算法通过建模输入空间到输出空间的变换来解决问题
  - 线性代数的矩阵分解理论提供了寻找主成分的理论基础
- 用哪些线性代数：
  - 矩阵的基本运算和性质(回忆一下特殊矩阵：对称矩阵、对角矩阵、单位矩阵、正交矩阵、上三角矩阵)
  - 常用的两种矩阵分解: 特征值分解、SVD分解
  - 最小二乘法
  - 矩阵求导*(由于将向量记作行向量还是列向量有分歧，因此有两套矩阵求导公式，请注意如果没有特殊说明，我们均默认列向量)

linear algebra in CS

> 你们觉得你们现在学的东西没有用，并不是因为它真的没有用，只是你们还没有遇到要用到那门课的时候

linear algebra in CS

- 一个CS的学生, 在大学期间其实会多次重新学习线性代数
- 学习过的内容不需要你牢牢记住, 但是需要你知道它的存在, 以及它的用途, 以及清楚的知道你需要的时候去哪里找

linear algebra in CS

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「大学招生简直诡计多端...某个uc数学系的博士生说，现在愿意修线性代数的美国本科生越来越少了，后来他们改了个名字大概叫Math Foundationsof MachineLearning，爆满，学生给教授写邮件要去上这门课，其实还是线性代数。」

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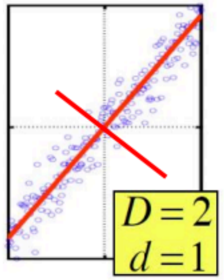
linear algebra in IML

Principal Component Analysis (PCA)

$(X X^T)v = \lambda v$, so v (the first PC) is the eigenvector of sample correlation/covariance matrix $X X^T$



Sample variance of projection $v^T X X^T v = \lambda v^T v = \lambda$

Thus, the eigenvalue λ denotes the amount of variability captured along that dimension (aka amount of energy along that dimension).

Eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots$

- The 1st PC v_1 is the the eigenvector of the sample covariance matrix $X X^T$ associated with the largest eigenvalue
- The 2nd PC v_2 is the the eigenvector of the sample covariance matrix $X X^T$ associated with the second largest eigenvalue
- And so on …

linear algebra in IML

- for optimizations

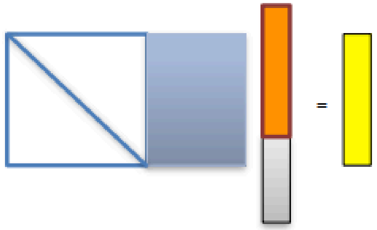
将 $\boldsymbol{Ax}=\boldsymbol{b}$ 的任一解 $\boldsymbol{x}$ 用非基变量表示为

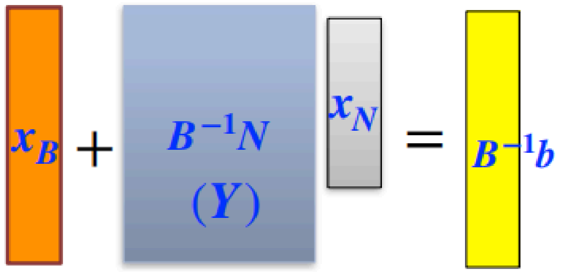
$$x_1 = \bar{b}_1 - \sum_{j=m+1}^{n} y_{1j}x_j$$

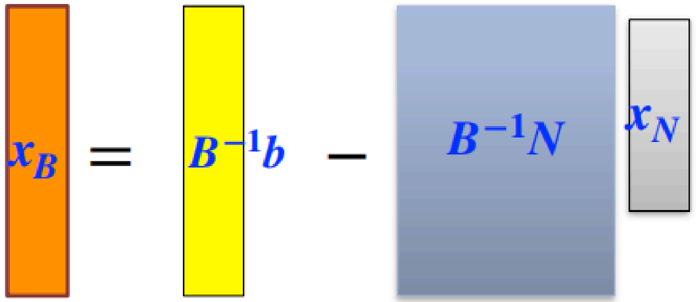
$$x_2 = \bar{b}_2 - \sum_{j=m+1}^{n} y_{2j}x_j$$

$$\vdots$$

$$x_m = \bar{b}_m - \sum_{j=m+1}^{n} y_{mj}x_j$$







Review(Preview) Outline

- Trace, Transpose, Inverse, Symmetric, Determinant, Rank
- Quadratic Form
- Positive (Semi) Definite Matrix
- Orthogonal Matrix
- Eigenvalues Decomposition
- Singular Value Decomposition

Trace 迹

> only for square matrix

$$\mathrm{Tr}(A) = \sum_{i=1}^{n} a_{ii}$$

- $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$
- matrix inner product
  $< A, B >= \mathrm{Tr}(A^\top B) = \mathrm{Tr}(B^\top A)$

> $<\mathbf{x}, \mathbf{y}>=\mathbf{x}^\top \mathbf{y} = \mathbf{y}^\top \mathbf{x}$

- $\mathrm{Tr}(aA + bB) = a\,\mathrm{Tr}(A) + b\,\mathrm{Tr}(B)$

> Trace is a linear operator

Transpose 转置

$(A^\top)_{ij} = (A)_{ji}$

- $(AB)^\top = B^\top A^\top$
- $AA^\top$ must be a symmetric matrix

Inverse 逆

- nonsingular matrix $\leftrightarrow$ invertible matrix
  $AB = BA = I_n$
  $B = A^{-1}$
  otherwise, A is singular and has no inverse
  $(|A| = 0)$

> singular: 奇异的. 所以一个所有元素都随机的矩阵大概率是可逆的
> i.e. 奇异矩阵是不可逆矩阵
> e.g. $A \in \mathbb{R}^{1\times 1}$, A is singular if and only if $a_{11} = 0$

Properties of Inverse

- inverse matrix of A is unique
  B, C are A's inverse matrices
  $B = BI_n = B(AC) = (BA)C = I_nC = C$
- $(A^{-1})^{-1} = A$
- $(AB)^{-1} = B^{-1}A^{-1}$

> proof: $(AB)(B^{-1}A^{-1}) = A(BB^{-1})A^{-1} = AA^{-1} = I_n$

- $(A^\top)^{-1} = (A^{-1})^\top \to A^{-T}$

> proof: $A^\top(A^{-1})^\top = (A^{-1}A)^\top = I_n$

Symmetric matrix 对称矩阵

- $A^\top = A$

all properties of symmetric matrix are based on this definition(this time)
(more propertires later such as similarity and diagonalizable)

- $\forall A_{m\times n}, AA^\top$ or $A^\top A$ are symmetric matrix
- 全体对称矩阵的集合: $\mathbb{S}^n$

Determinant 行列式

- a function mapping a matrix A into a scalar $\det(A)$ or $|A|$
- $A^{-1} = \frac{1}{|A|} A^*$
- $A^* = [C_{ij}]^\top$, C_{ij} is the cofactor of a_{ij}
- $C_{ij} = (-1)^{i+j} M_{ij}$, M_{ij} is the minor of a_{ij}
- the most simple usage: invertibility

Determinant Properties

> compare with the elementary row(column) operations

1. B is obtained from A by interchanging two rows(columns)
   $|B| = -|A|$
2. B is obtained from A by multiplying one row(column) by a nonzero scalar k
   $|B| = k|A|$
3. B is obtained from A by adding a multiple of one row(column) to another row(column)
   $|B| = |A|$

Determinant Properties

$$|A^\top| = |A|$$
$$|\lambda A| = \lambda^n |A|$$
$$|AB| = |A||B|$$
$$|A^{-1}| = \frac{1}{|A|}$$

Triangular Matrix 上/下三角矩阵

- upper triangular matrix

  the elements **below** the diagonal are all zero

  (the elements on the diagonal can be zero or not)

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix},$$

then elements on the diagonal of A^k are $a_{11}^k, a_{22}^k, \cdots, a_{nn}^k$

- similar to the lower triangular matrix

Triangular Matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}$$

- $\det(A) = \prod_{i=1}^{n} a_{ii}$
- and the lower triangular matrix is the same

Diagonal Matrix 对角矩阵

- for diagonal matrix Λ, $\Lambda_{ij} = 0$ for $i \neq j$
  so it can be written as $\Lambda = \mathrm{diag}(d_1, d_2, \cdots, d_n)$
- the power of diagonal matrix is easy to compute
  $\Lambda^k = \mathrm{diag}(d_1^k, d_2^k, \cdots, d_n^k)$
  $\rightarrow$ similarity and diagonalizable
- the diagonal matrix Λ is invertible if and only if $\forall i, d_i \neq 0$

> $$|\Lambda| = \prod_{i=1}^{n} d_i$$

Row space, Column space and Null space

A is a $m \times n$ matrix

- row space 行空间
  $row(A) = span\{\mathbf{r}_1, \cdots, \mathbf{r}_m\}$
- column space 列空间
  $col(A) = span\{\mathbf{c}_1, \cdots, \mathbf{c}_n\}$
- null space 零空间
  $null(A) = \{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \mathbf{0}\}$
- left null space 左零空间
  $null(A^\top) = \{\mathbf{x} \in \mathbb{R}^m : A^\top\mathbf{x} = \mathbf{0}\}$

Fundamental Matrix Spaces

Definition 4.31. 对$m \times n$-矩阵A，以下六个向量空间被称为A的基本空间(*the fundamental spaces of A*):

- A的行空间$Row(A)$,
- A的列空间$Col(A)$,
- $A^\top$的行空间$Row(A^\top)$,
- $A^\top$的列空间$Col(A^\top)$,
- A的零空间$Null(A)$,
- $A^\top$的零空间$Null(A^\top)$。

- 行空间和零空间互为正交补
- 列空间和左零空间互为正交补

正交补(Orthogonal Complements)

> 正交: $col(A) \perp null(A)$, 补: $col(A) + null(A) = \mathbb{R}^n$

Row space, Column space and Null space

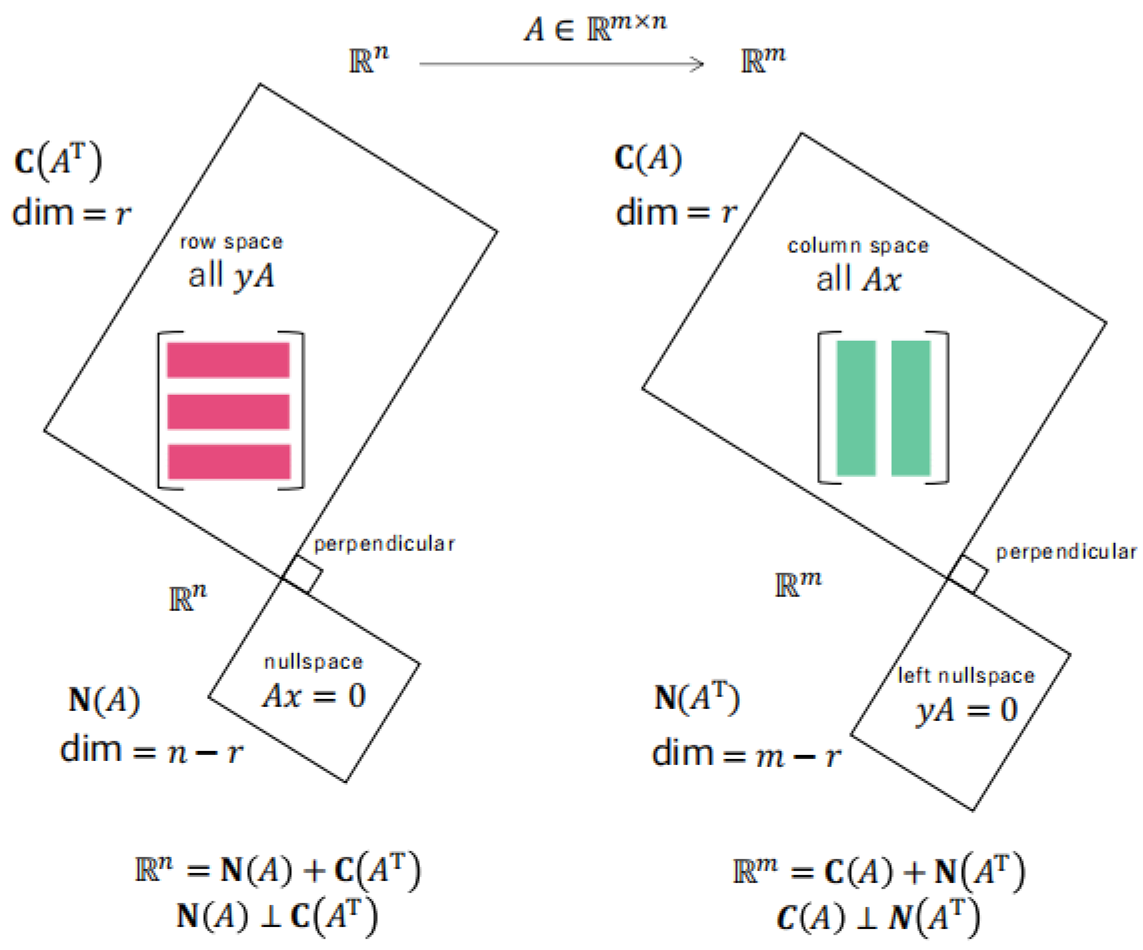


Figure 5: 四个子空间

Rank, Nullity 秩, 零化度

- $rank(A) = \dim(row(A)) = \dim(col(A))$
  A 的秩 = A 的行阶梯矩阵的首一个数
  最本质: 非0奇异值的个数

  $\Rightarrow rank(A) \leq \min(n, m)$

- $rank(A)$ 可看作行阶梯矩阵的首一(非零行/主元) 个数
  $nullity(A) = \dim(Null(A))$ 可看作自由元的个数
  $\Rightarrow rank(A) + nullity(A) = n$

rank property

- $A \in \mathbb{R}^{m \times n}$
  $rank(A) \leq \min(m, n)$
- $rank(AB) \leq \min(rank(A), rank(B))$
- $rank(A^\top A) = rank(A)$

Equivalent expression

$A \in M_{n\times n}$

- A可逆；
- $A\boldsymbol{x}=\boldsymbol{0}$只有平凡解；
- A的简化阶梯型为单位矩阵；
- A是一组初等矩阵的乘积；
- $A\boldsymbol{x}=\boldsymbol{b}$对任何$n\times 1$的列向量$\boldsymbol{b}$都有解；
- $A\boldsymbol{x}=\boldsymbol{b}$对任何$n\times 1$的列向量$\boldsymbol{b}$都有且只有一个解；
- $\det(A)\neq 0$；
- A的所有n个行向量线性无关；
- A的所有n个列向量线性无关；
- $span(Row(A))=\mathbb{R}^n$；
- $span(Col(A))=\mathbb{R}^n$；
- A的所有n个行向量构成$\mathbb{R}^n$的一组基底；
- A的所有n个列向量构成$\mathbb{R}^n$的一组基底；
- $rank(A)=n$；
- $Null(A)=0$。

Norm 范数

满足:

- triangle inequality
  $\|\mathbf{x}+\mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$
  when $p=2$: triangle inequality
- $\|\mathbf{x}\| \geq 0, \|\mathbf{x}\| = 0 \Leftrightarrow \mathbf{x} = \mathbf{0}$
- $\forall a, \|a\mathbf{x}\| = |a| \|\mathbf{x}\|$

则$\|\cdot\|$是一个范数

> all norm $f: \mathbb{R}^n \to \mathbb{R}$ are convex.

Norm

- p-norm of a vector $\mathbf{v} = (v_1, \cdots, v_n)$

  $|| \mathbf{v} ||_p = \sqrt[p]{|v_1|^p + |v_2|^p + \cdots + |v_n|^p}$

- 0-norm: the number of nonzero entries in $\mathbf{v}$

  $0 - norm$不是范数$(non - convex)$!

- 1-norm / L1-norm:

  $|| \mathbf{v} ||_1 = |v_1| + |v_2| + \cdots + |v_n|$

- 2-norm(Euclidean norm, L2-norm):

  $|| \mathbf{v} ||_2 = \sqrt{v_1^2 + v_2^2 + \cdots + v_n^2}$

- ∞-norm:

  $|| \mathbf{v} ||_\infty = \max\{|v_1|, |v_2|, \cdots, |v_n|\}$

Norm

p-norm : $\| \mathbf{v} \|_p = \sqrt[p]{|v_1|^p + |v_2|^p + \cdots + |v_n|^p}$, $p \geq 1$

- 0 norm is actually not a norm, but metric(度量)
- Hölder's inequality (赫尔德不等式)

  $$p, q \geq 1, \frac{1}{p} + \frac{1}{q} = 1$$

  $$\sum_{i=1}^{n} |a_i b_i| \leq \| x \|_p \|y\|_q$$

  $$\sum_{i=1}^{n} |a_i b_i| \leq \| x \|_1 \|y\|_\infty$$

- Cauchy inequality ($p = q = 2$)

  $$\sum_{i=1}^{n} |a_i b_i| \leq \sqrt{\sum_{i=1}^{n} a_i^2} \sqrt{\sum_{i=1}^{n} b_i^2}$$

Norms for matrices

- p-norm: $\|A\|_p = \max_{\|\mathbf{x}\|_p \neq 0} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p}$
- 1-norm(列范数): $\|A\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^{m} |a_{ij}|$
- 2-norm(spectral norm, 谱范数): $\|A\|_2 = \sqrt{\lambda_{\max}(A^\top A)}$
- ∞-norm(行范数): $\|A\|_\infty = \max_{1 \leq i \leq m} \sum_{j=1}^{n} |a_{ij}|$
- Frobenius norm: $\|A\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2} = \sqrt{\mathrm{Tr}(A^\top A)}$
- Nuclear norm(核范数): $\|A\|_* = \sum_{i=1}^{\min(m,n)} \sigma_i(A)$

Dual Norm 对偶范数

范数$\|\cdot\|$的对偶范数$\|\cdot\|_*$定义为

$$\|\mathbf{x}\|_* = \sup_{\|\mathbf{z}\|\leq 1} < \mathbf{x}, \mathbf{z} >$$

e.g.

- $\|\mathbf{x}\|_1$ & $\|\mathbf{x}\|_\infty$
- $\|\mathbf{x}\|_2$ & $\|\mathbf{x}\|_2$
- $\|X\|_2$ & $\|X\|_*$

性质:

$$\mathbf{x}^\top \mathbf{z} \leq \|\mathbf{x}\|_* \|\mathbf{z}\|$$

> proof: $\|\mathbf{x}\|_* = \sup_{\|\mathbf{z}\|\leq 1} \mathbf{x}^\top \mathbf{z} \geq \mathbf{x}^\top \frac{\mathbf{z}}{\|\mathbf{z}\|} \Rightarrow \mathbf{x}^\top \mathbf{z} \leq \|\mathbf{x}\|_* \|\mathbf{z}\|$

点到点的距离

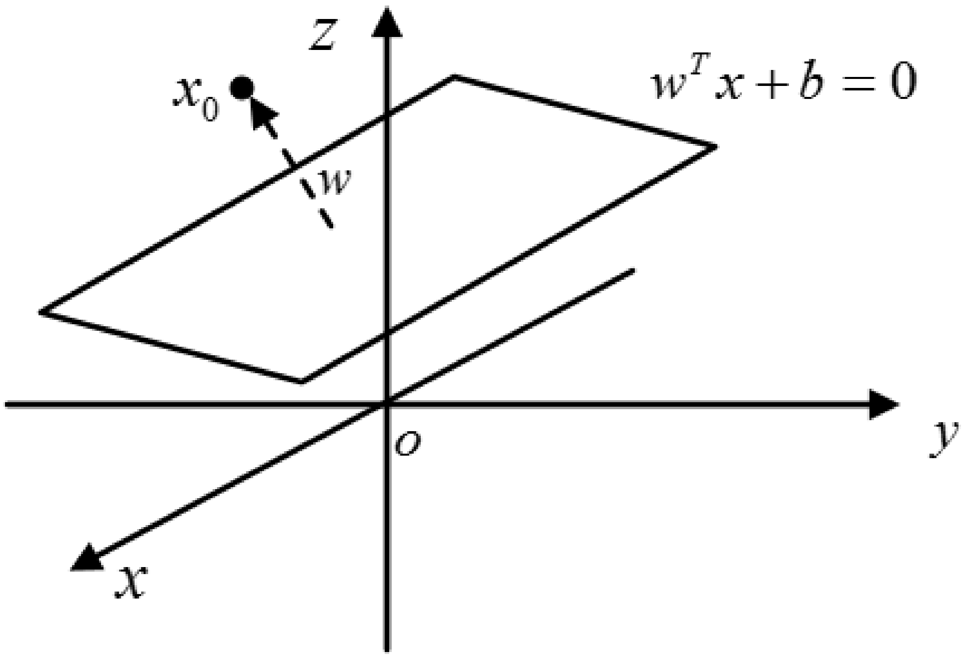
the Euclidean distance between $\mathbf{u}$ and $\mathbf{v}$

$$d(u,v) = d(u,v) = \|\mathbf{u}-\mathbf{v}\| = \sqrt{(u_1-v_1)^2+(u_2-v_2)^2+\cdots+(u_n-v_n)^2}$$

点到平面的距离

点$\mathbf{x}_0 \in \mathbb{R}^n$到高维超平面 (hyperplane) $H = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{w}^\top \mathbf{x} + b = 0\}$的距离为

$$d = \frac{|\mathbf{w}^\top \mathbf{x}_0 + b|}{\|\mathbf{w}\|}$$



Projection Theorem

- orthogonal projection of $\mathbf{u}$ on $\mathbf{v}$

  $$\mathbf{w}_1 = proj_{\mathbf{v}}(\mathbf{u}) = \frac{\mathbf{u} \cdot \mathbf{v}}{||\,\mathbf{v}\,||^{\,2}}\mathbf{v}$$

- the vector component of $\mathbf{u}$ orthogonal to $\mathbf{v}$

  $$\mathbf{w}_2 = \mathbf{u} - \mathbf{w}_1 = \mathbf{u} - proj_{\mathbf{v}}(\mathbf{u}) = \mathbf{u} - \frac{\mathbf{u} \cdot \mathbf{v}}{||\,\mathbf{v}\,||^{\,2}}\mathbf{v}$$

Quadratic Form 二次型

- $Q(\mathbf{x}) = \mathbf{x}^\top A\mathbf{x}$
- $Q(\mathbf{x}) = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_i x_j$

e.g.

$$Q(\mathbf{x}) = x_1^2 + 2x_1x_2 + 3x_2^2$$

$$Q(\mathbf{x}) = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Positive (Semi) Definite Matrix (半)正定矩阵

- $A \in \mathbb{S}^n$: symmetric matrix
  $A^\top = A$
- $A \in \mathbb{S}^n_+$: symmetric positive semi-definite matrix
  $A^\top = A, A \succeq 0 : \forall \mathbf{x} \in \mathbb{R}^n, \mathbf{x}^\top A\mathbf{x} \geq 0$
- $A \in \mathbb{S}^n_{++}$: symmetric positive definite matrix
  $A^\top = A, A \succ 0 : \forall \mathbf{x} \in \mathbb{R}^n \backslash \{\mathbf{0}\}, \mathbf{x}^\top A\mathbf{x} > 0$

> $\forall A \in \mathbb{S}^n_+$, A can be decomposed as $A = BB^\top$

正定矩阵的判定方法

- 所有的特征值均> 0
- 二次型 $Q(\mathbf{x}) = \mathbf{x}^\top A\mathbf{x} > 0, \forall \mathbf{x} \neq \mathbf{0}$
- 顺序主子式均> 0

e.g. $A^\top A$是正定矩阵

> $\forall x, x^\top A^\top Ax = \|Ax\|^2 \geq 0 \Leftrightarrow A^\top A \succeq 0 \Leftrightarrow A^\top A$的特征值都是非负的

同理, $AA^\top$的特征值一定都是非负的

Orthogonal 正交

- $\mathbf{u}, \mathbf{v}$ are orthogonal **iff** $\mathbf{u} \cdot \mathbf{v} = 0$
- orthogonal set

  $\mathbf{v}_1, \cdots, \mathbf{v}_n$ are orthogonal

  $\|\mathbf{v}_1 + \cdots + \mathbf{v}_n\| = \|\mathbf{v}_1\| + \cdots + \|\mathbf{v}_n\|$

Orthogonal Matrix 正交矩阵

- $A^\top A = AA^\top = I_n$
  $A^{-1} = A^\top$

e.g. rotation matrix $R = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$

正交矩阵性质

- A 是正交矩阵 $\Leftrightarrow$ A 的行/列向量组成的集合是正交规范集合
- 正交矩阵的行/列向量是**标准正交基底**
- A是正交矩阵 $\Leftrightarrow A^\top$是正交矩阵
- A是正交矩阵 $\Leftrightarrow \|A\mathbf{x}\| = \|\mathbf{x}\|$
- A是正交矩阵 $\Leftrightarrow A\mathbf{x} \cdot A\mathbf{y} = \mathbf{x} \cdot \mathbf{y}$
- A是正交矩阵 $\Leftrightarrow A^{-1}$也是正交矩阵
- A, B是正交矩阵 $\Rightarrow AB$也是正交矩阵
- A是正交矩阵 $\Rightarrow |A| = 1$ or $|A| = -1$

eigenvalue 特征值

$A\mathbf{x} = \lambda\mathbf{x}$
$(\lambda I - A)\mathbf{x} = \mathbf{0}$

$\mathbf{x} \neq \mathbf{0}$
$\left|\lambda I - A\right| = 0$

- $p(\lambda) = \left|\lambda I - A\right|$: eigen polynomial 特征多项式
- $p(\lambda) = 0$: characteristic equation 特征方程

eigenvector 特征向量

$A\mathbf{x} = \lambda\mathbf{x}$
$(A - \lambda I)\mathbf{x} = \mathbf{0}$
$\mathbf{x} \neq \mathbf{0}$

- the nontrivial solutions of $(A - \lambda I)\mathbf{x} = \mathbf{0}$
- $\mathbf{x} \in null(A - \lambda I)$
- $\mathbf{x}$: the eigenvectors(特征向量) of A corresponding to λ
- $null(A - \lambda I)$: the eigenspace(特征空间) of A corresponding to λ

The number of the eigenvectors of A corresponding to λ_i is same as the multiplicity of roots of λ_i of $p(\lambda)$

eigenvalue and eigenvector

$$A = \begin{bmatrix} 0 & 0 & -2 \\ 1 & 2 & 1 \\ 1 & 0 & 3 \end{bmatrix}$$

find the eigenvalues and eigenvectors of A

相似对角化 Diagonalization

若一个矩阵A可写作$\Lambda = P^{-1}AP$,即$A = P\Lambda P^{-1}$, 则称A可对角化(diagonalizable)

usage:
$A^n = P\Lambda P^{-1}P\Lambda P^{-1} \cdots P\Lambda P^{-1} = P\Lambda^n P^{-1}$

特征值分解 / 谱分解 Eigenvalues Decomposition

将A对角化为 $A = P\Lambda P^{-1}$:

1. 求A的特征值和特征向量
2. 将特征向量组成P
   原因: $A = P\Lambda P^{-1} \Leftrightarrow AP = P\Lambda$

Λ: 特征值
P: 特征空间的基拼成(对应特征值)

若某个特征值的几何重数(特征空间的维度)小于代数重数(特征值的重数), 则A不可对角化

Orthogonal Diagonalization 正交对角化

- **实对称矩阵**不同特征值对应的特征向量彼此正交

  proof:

  设$\lambda_1 \neq \lambda_2$, 其对应的特征向量为$\mathbf{x}_1, \mathbf{x}_2$

  $A\mathbf{x}_1 = \lambda_1\mathbf{x}_1, A\mathbf{x}_2 = \lambda_2\mathbf{x}_2$

  $\mathbf{x}_1^\top A\mathbf{x}_2 = \mathbf{x}_1^\top \lambda_2\mathbf{x}_2 = \lambda_2\mathbf{x}_1^\top\mathbf{x}_2$

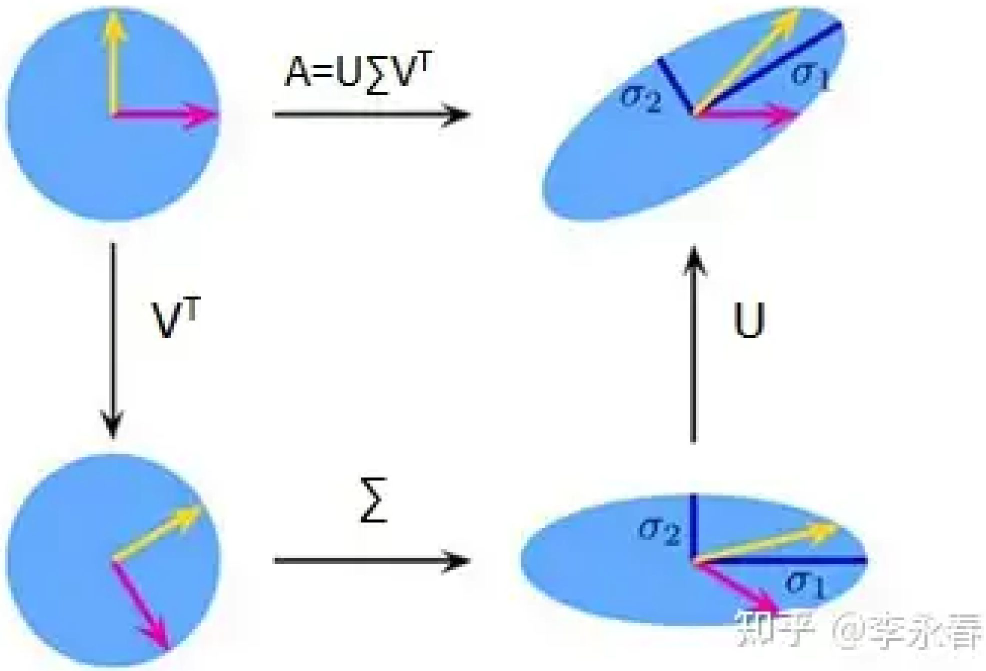
  $(A\mathbf{x}_1)^\top\mathbf{x}_2 = (\lambda_1\mathbf{x}_1)^\top\mathbf{x}_2$

  $(\lambda_2 - \lambda_1)\mathbf{x}_1^\top\mathbf{x}_2 = x_1^\top A\mathbf{x}_2 - x_1^\top A^\top\mathbf{x}_2 = 0$

Orthogonal Diagonalization 正交对角化

- 若将**实对称矩阵**的每个特征值对应的特征向量的基**施密特正交化**得到P,则P是正交矩阵, i.e. $P^\top P = I$
- 实对称矩阵一定可以相似对角化 $\Rightarrow$ 一定可以正交对角化 $A = P\Lambda P^{-1} \Rightarrow A = P\Lambda P^\top$

Singular Value Decomposition(SVD) 奇异值分解



整个 SVD 分解过程可以视为: 首先通过 $V^\top$ 把数据旋转到一个新的坐标系，在这个坐标系中通过 Σ 对数据进行不同程度的拉伸(或压缩), 最后通过 U 可以将这些变化映射回原始或另一个适当的空间.

SVD

记录 A 的奇异值分解为 $A = U\Sigma V^\top$, 其中 U 和 V 是正交矩阵，Σ 是对角矩阵.

- V & Σ
  $A^\top A = V\Sigma^\top U^\top U\Sigma V^\top = V\Sigma^\top\Sigma V^\top$
  $AA^\top V = V\Sigma^2$
  对于V的每个列向量v_i, $A^\top Av_i = \sigma_i^2 v_i$
  所以Σ为$A^\top A$的特征值的平方根, V为正交规范化的特征向量拼成的矩阵
- U: 同理可得$AA^\top u_i = \sigma^2 u_i$
  设奇异值σ_i的左奇异向量为u_i, 右奇异向量为v_i, 则
  $Av_i = U\Sigma V^\top v_i = U\Sigma e_i = \sigma_i u_i$
  同理: $A^\top u_i = \sigma_i v_i$
  由于U是正交矩阵, 所以求解方程组 $\mathbf{x} \cdot \mathbf{u}_i = 0$的解即可得到$U$

SVD

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} \sqrt{3} & 0 \\ 0 & \sqrt{2} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$