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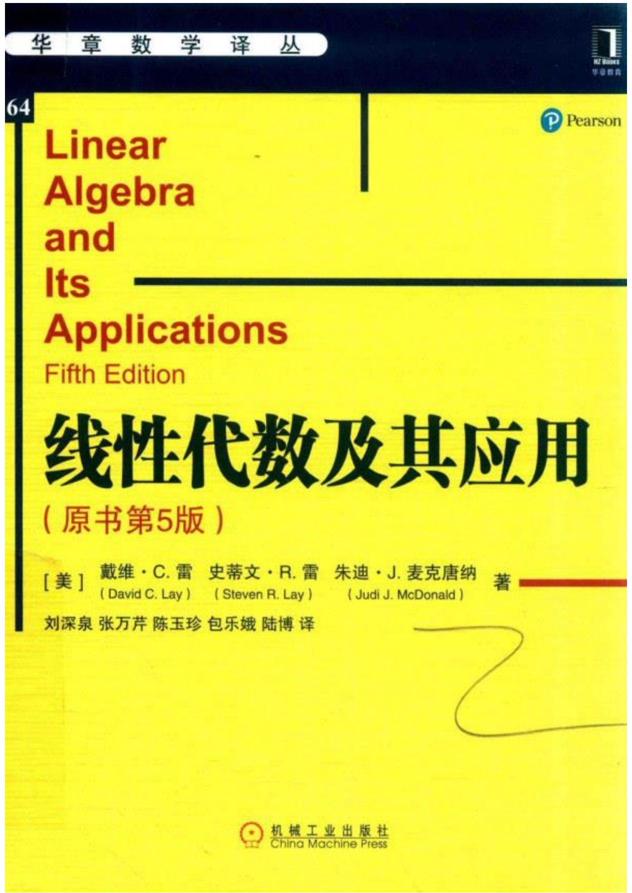
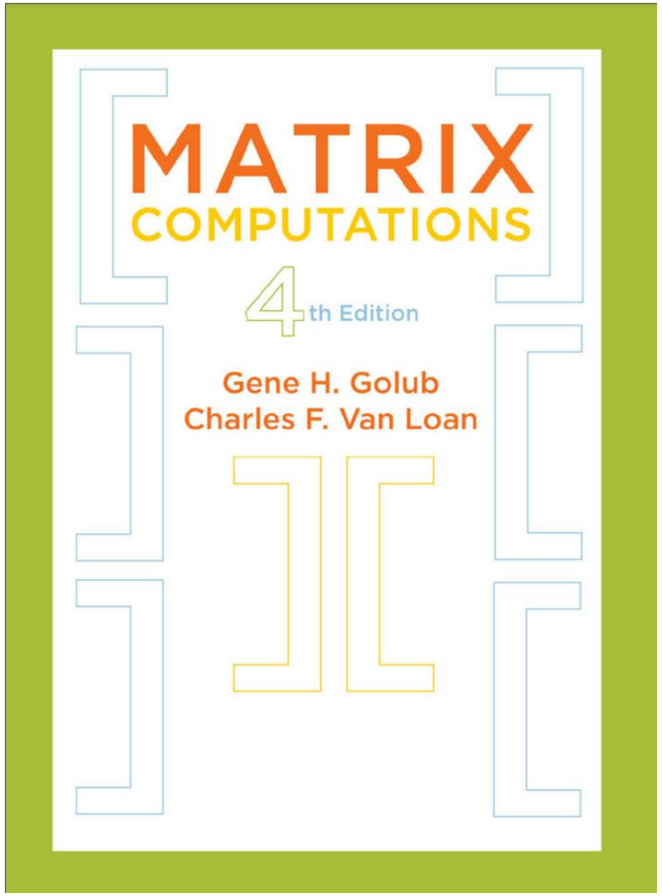
书籍


华章数学译丛
64
Pearson
Linear Algebra and Its Applications
Fifth Edition
线性代数及其应用
（原书第5版）
[美] 戴维·C. 雷 史蒂文·R. 雷 朱迪·J. 麦克唐纳 著
(David C. Lay) (Steven R. Lay) (Judi J. McDonald)
刘深泉 张万芹 陈玉珍 包乐娥 陆博 译
机械工业出版社
China Machine Press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4th Edition
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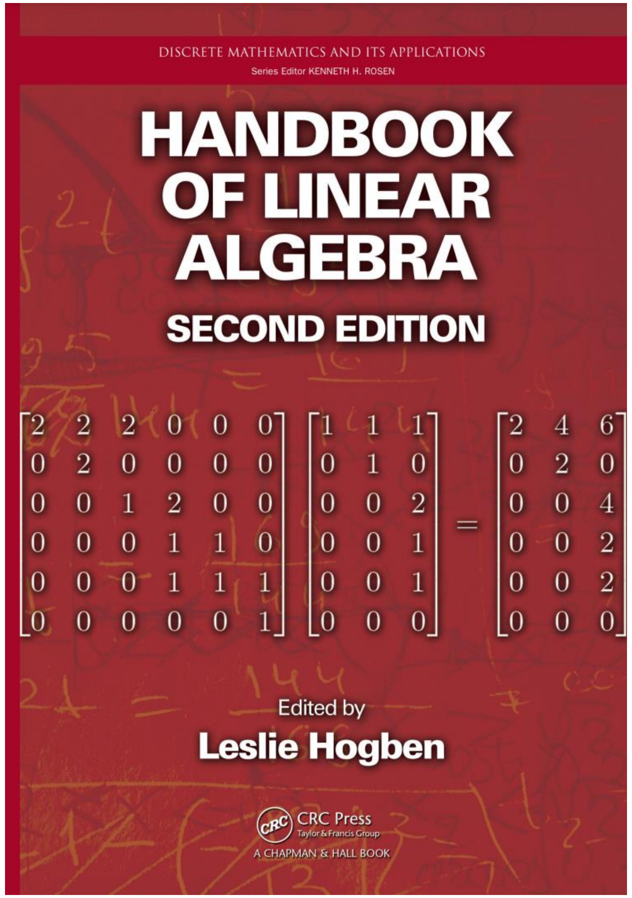
Charles F. Van Loan


DISCRETE MATHEMATICS AND ITS APPLICATIONS
Series Editor KENNETH H. ROSEN
HANDBOOK OF LINEAR ALGEBRA
SECOND EDITION
Edited by
Leslie Hogben
CRC Press
Taylor & Francis Group
A CHAPMAN & HALL BOOK

软件

- BLAS / LAPACK (接口规范)
  https://netlib.org/
- Intel MKL (商业) / OpenBLAS (开源)
  https://www.intel.cn/content/www/cn/zh/developer/tools/oneapi/onemkl.html
  https://www.openblas.net/
- Eigen / Armadillo
  https://eigen.tuxfamily.org/
  https://arma.sourceforge.net/
- MATLAB / Mathematica

矩阵乘法

Algorithm 1.1.5 (*ijk* Matrix Multiplication) If $A \in \mathbb{R}^{m\times r}$, $B \in \mathbb{R}^{r\times n}$, and $C \in \mathbb{R}^{m\times n}$ are given, then this algorithm overwrites C with $C + AB$.

for $i = 1{:}m$
  for $j = 1{:}n$
    for $k = 1{:}r$
      $C(i,j) = C(i,j) + A(i,k)\cdot B(k,j)$
    end
  end
end

Loop Order	Inner Loop	Inner Two Loops	Inner Loop Data Access
ijk	dot	vector $\times$ matrix	A by row, B by column
jik	dot	matrix $\times$ vector	A by row, B by column
ikj	saxpy	row gaxpy	B by row, C by row
jki	saxpy	column gaxpy	A by column, C by column
kij	saxpy	row outer product	B by row, C by row
kji	saxpy	column outer product	A by column, C by column

线性方程组

$$\begin{bmatrix} 1 & 3 & 2 \\ 1 & 8 & 5 \\ 1 & 2 & 7 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 10 \\ 5 \\ 8 \end{bmatrix}$$

1. 平面“$x + 3y + z = 10$”, “$x + 8y + 5z = 5$”, “$x + 2y + 7z = 8$”的交集.

2. 三个列向量$\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$, $\begin{bmatrix} 3 \\ 8 \\ 2 \end{bmatrix}$, $\begin{bmatrix} 2 \\ 5 \\ 7 \end{bmatrix}$的线性组合能否得到$\begin{bmatrix} 10 \\ 5 \\ 8 \end{bmatrix}$? 如果能, 是否唯一?

高斯消元

解方程组$\begin{cases}3x_1+5x_2=9\\6x_1+7x_2=4\end{cases}$'

将第一行乘2然后从第二行减去, 得到$\begin{cases}3x_1+5x_2=9\\ \ -3x_2=-14\end{cases}$, 这是一个三角形方程组.

$$\begin{bmatrix}1 & 0\\-2 & 1\end{bmatrix}\begin{bmatrix}3 & 5\\6 & 7\end{bmatrix}=\begin{bmatrix}3 & 5\\0 & -3\end{bmatrix}$$

找到单位下三角阵L和上三角阵U使得$A=LU$.

那么解方程组$Ax=b$可以化为两步$Ly=b, Ux=y \ \Rightarrow \ Ax=LUx=Ly=b$.

LU分解

用分块矩阵的观点:

$$A = \begin{bmatrix} \alpha & w^T \\ v & B \end{bmatrix}$$
$$LU = \begin{bmatrix} 1 & 0 \\ ?_3 & ?_4 \end{bmatrix}\begin{bmatrix} ?_1 & ?_2 \\ 0 & ?_5 \end{bmatrix}$$

$$1 \times ?_1 + 0 \times 0 = \alpha \Rightarrow ?_1 = \alpha$$
$$1 \times ?_2 + 0 \times ?_5 = w^T \Rightarrow ?_2 = w^T$$
$$?_3 \times ?_1 + ?_4 \times 0 = v \Rightarrow ?_3 = \frac{1}{\alpha} v$$
$$?_3 \times ?_2 + ?_4 \times ?_5 = B \Rightarrow ?_4\, ?_5 = \mathrm{B} - \frac{1}{\alpha} v w^T$$

而$?_4$ 是单位下三角阵, $?_5$是上三角阵, 因此再对$\mathrm{B} - \frac{1}{\alpha} v w^T$进行LU分解.

LU分解

实际中常用部分主元的LU分解, 即每次迭代时, 选取第一列中绝对值最大的作为α, 行交换到第一行, 得到

$$PA = LU.$$

如果$\alpha = 0$则LU分解无法继续, 此时矩阵A秩亏.

因为只有L的对角线以下, U的对角线及以上需要存储, 所以通常存储在同一个跟A一样大的数组上.即

$$\begin{bmatrix} \alpha & w^T \\ v & B \end{bmatrix} \to \begin{bmatrix} \alpha & w^T \\ v/\alpha & B - vw^T/\alpha \end{bmatrix}$$

ZW3D:

VxMatFullPvtLuD: 求PLU分解

VxMatFullPvtFBS: 已知PLU分解, 求解线性方程组

VxMatGetInv: 用PLU分解求逆

Eigen::PartialPivLU
xgesv

四个基本子空间

行空间 $C(A^T)$ (row space)

行的线性组合, $N(A)$的正交补, dim = rank

零空间 $N(A)$ (null space, kernel)

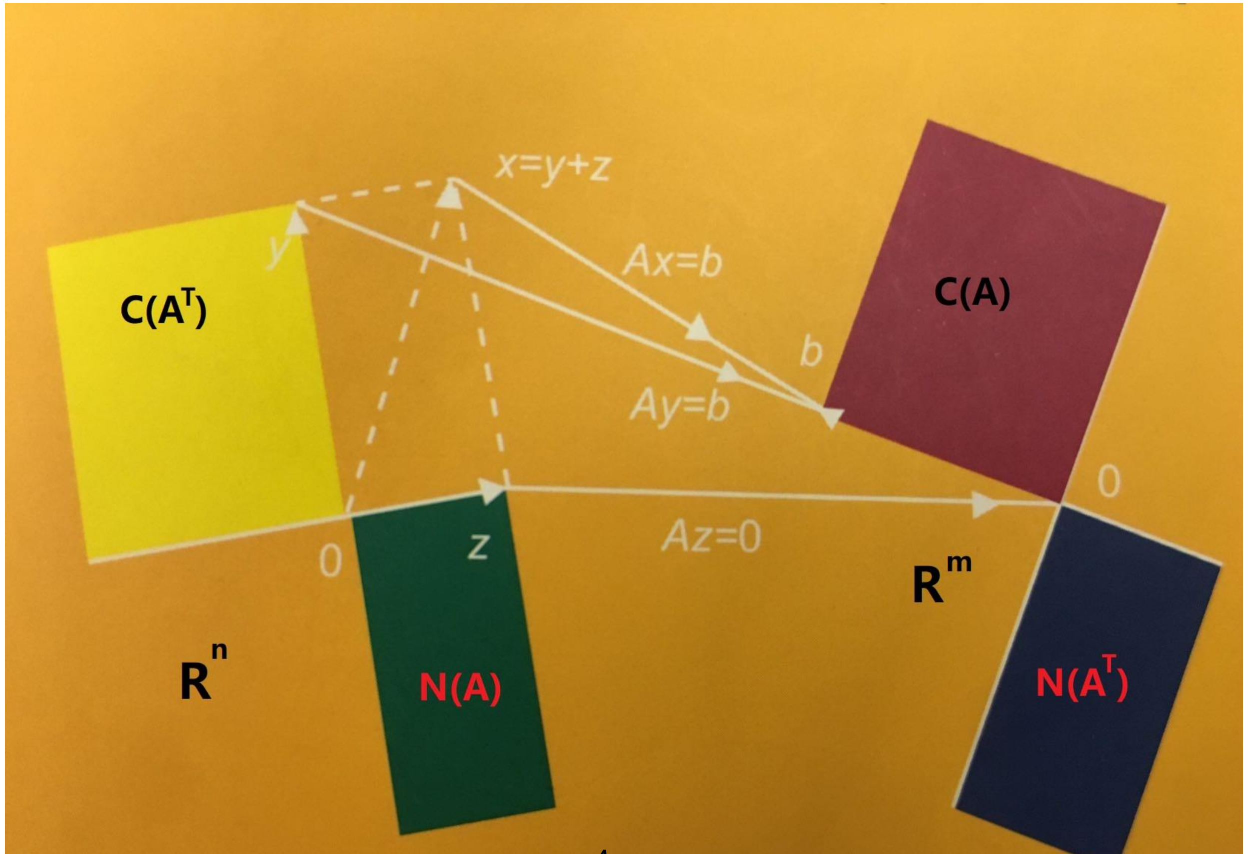
$Ax = 0$的解空间, $C(A^T)$的正交补, dim = n - rank

列空间 $C(A)$ (column space, range space)

列的线性组合, $N(A^T)$的正交补, dim = rank

左零空间 $N(A^T)$ (left null space)

$A^T x = 0$的解空间, $C(A)$的正交补, dim = m - rank



行空间 ⊕ 零空间 $\xrightarrow{A}$ 列空间 ⊕ 左零空间

行空间 $\xrightarrow{A}$ 列空间

奇异值分解 (SVD)

任意$A \in \mathbb{R}^{m\times n}$有

$$A = U\Sigma V^T$$

其中

$$U = [\boldsymbol{u}_1 \quad \cdots \quad \boldsymbol{u}_m] \in \mathbb{R}^{m\times m}$$
$$V = [\boldsymbol{v}_1 \quad \cdots \quad \boldsymbol{v}_n] \in \mathbb{R}^{n\times n}$$

是正交矩阵,

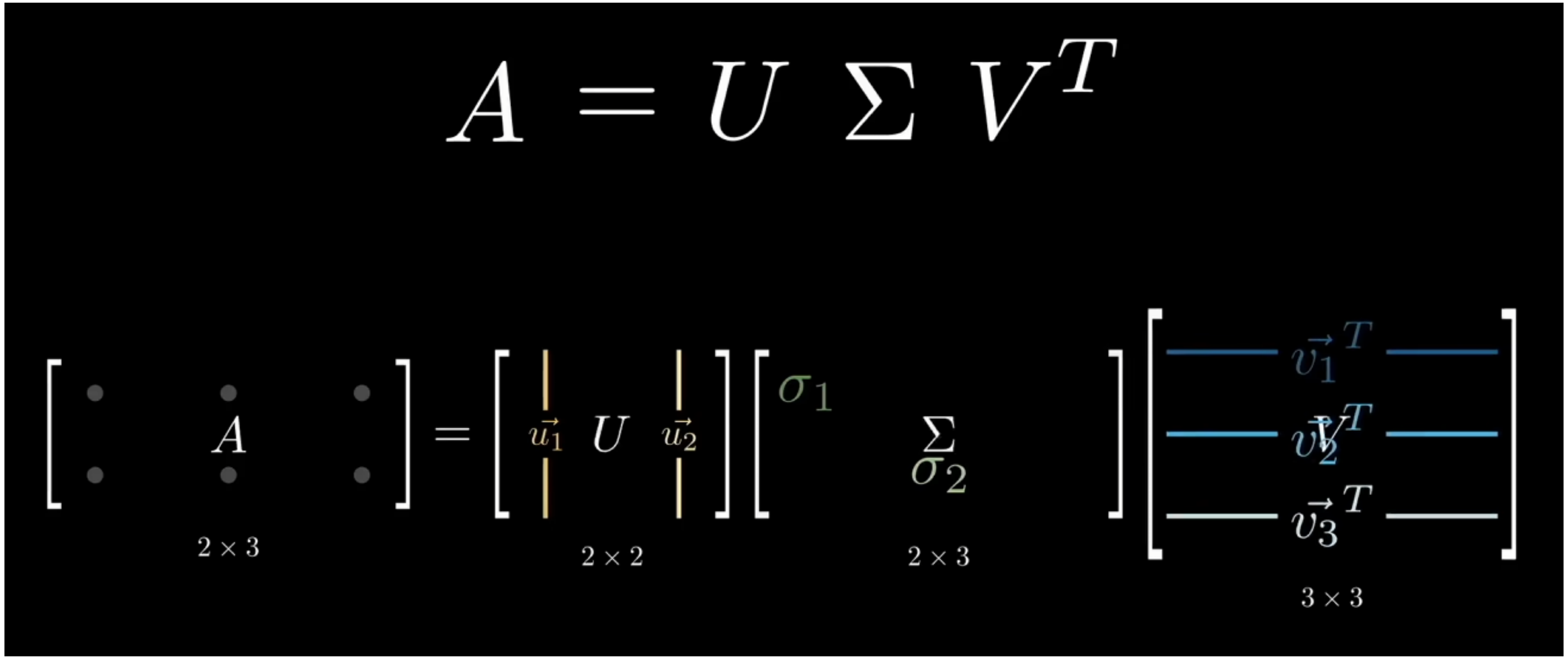
$$\Sigma = diag(\sigma_1, \cdots, \sigma_r) \in \mathbb{R}^{m\times n}$$

是对角矩阵.

换句话说，秩r矩阵表示为r个秩1矩阵的和

$$A = \sum_{i=1}^{r} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$$

奇异值分解 (SVD)



奇异值分解 (SVD)

$$V = [\underbrace{v_1 \quad v_2}_{r} \quad \cdots \quad \underbrace{v_n}_{n-r}]$$

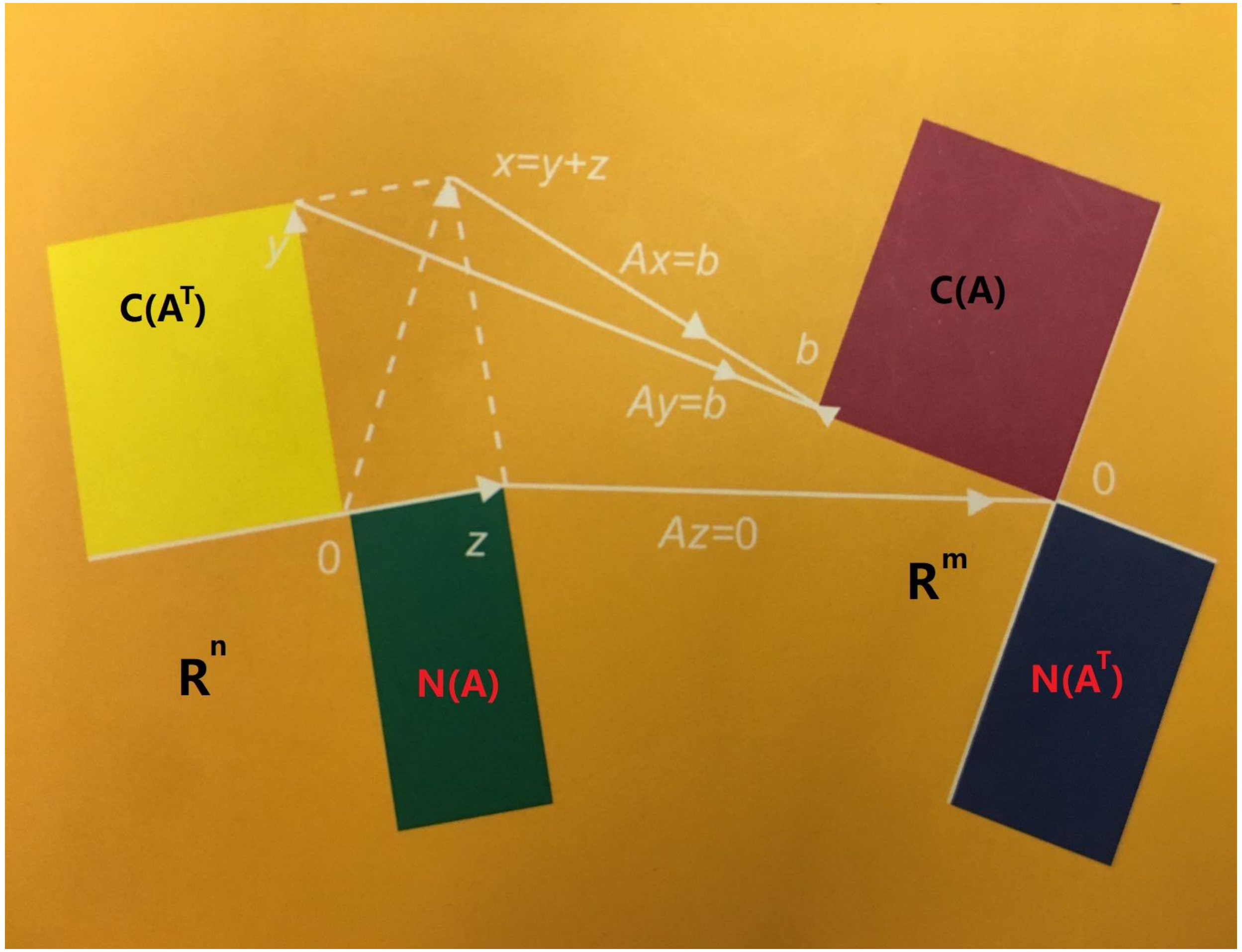
$$U = [\underbrace{u_1 \quad u_2}_{r} \quad \cdots \quad \underbrace{u_m}_{m-r}]$$

ZW3D:

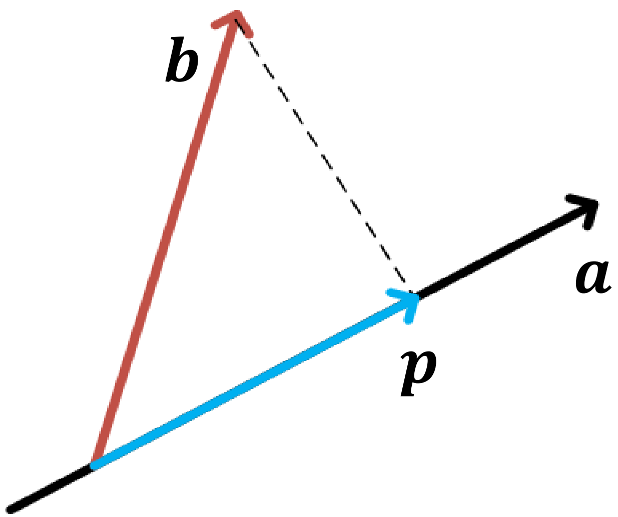
VxMatSvd: 求奇异值分解

VxMatSvdFBS: 用奇异值分解解线性方程组

Eigen::BDCSVD
Eigen::JacobiSVD
xgesvd



投影到向量上



$\boldsymbol{a}$上的单位向量: $\frac{\boldsymbol{a}}{\|\boldsymbol{a}\|_2}$.

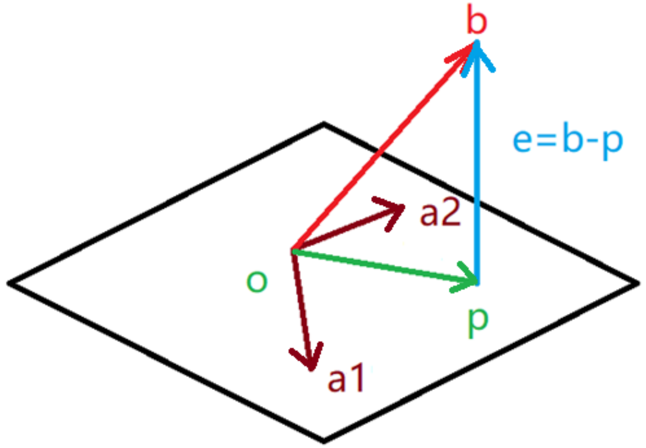
$\boldsymbol{b}$在$\boldsymbol{a}$上的投影长度: $\frac{1}{\|\boldsymbol{a}\|_2}\boldsymbol{a}^T\boldsymbol{b}$.

向量$\boldsymbol{b}$往向量$\boldsymbol{a}$上投影:

$$\boldsymbol{p} = \left(\frac{1}{\|\boldsymbol{a}\|_2}\boldsymbol{a}^T\boldsymbol{b}\right)\frac{\boldsymbol{a}}{\|\boldsymbol{a}\|_2} = \frac{\boldsymbol{a}\boldsymbol{a}^T}{\boldsymbol{a}^T\boldsymbol{a}}\boldsymbol{b}.$$

投影矩阵: $\frac{\boldsymbol{a}\boldsymbol{a}^T}{\boldsymbol{a}^T\boldsymbol{a}}$.

投影到列空间



设$A=[\boldsymbol{a}_1 \quad \boldsymbol{a}_2]$线性无关, 要求$\boldsymbol{b}$到$C(A)$的投影$\boldsymbol{p}$.

已知$\boldsymbol{e}=\boldsymbol{b}-\boldsymbol{p}$且$\boldsymbol{a}_1^T\boldsymbol{e}=\boldsymbol{a}_2^T\boldsymbol{e}=0$, 有

$$A^T(\boldsymbol{b}-\boldsymbol{p})=\boldsymbol{0}.$$

$\boldsymbol{p}$在$C(A)$上所以有$A\boldsymbol{x}=\boldsymbol{p}$, 那么

$$A^TA\boldsymbol{x}=A^T\boldsymbol{b}.$$

所以$\boldsymbol{p}=A(A^TA)^{-1}A^T\boldsymbol{b}$.

矩阵$(A^TA)^{-1}A^T$称为矩阵A的左逆.

最小二乘解

线性方程组$A\boldsymbol{x}=\boldsymbol{b}$如果$\boldsymbol{b}\notin C(A)$则无解. 我们可以把$\boldsymbol{b}$投影到$C(A)$上再求解, 即

$$A^TA\hat{\boldsymbol{x}}=A^T\boldsymbol{b}.$$

此时$\hat{\boldsymbol{x}}=(A^TA)^{-1}A^T\boldsymbol{b}$, 即用左逆替代矩阵的逆.

因为$\frac{d}{d\boldsymbol{x}}(A\boldsymbol{x}-\boldsymbol{b})^T(A\boldsymbol{x}-\boldsymbol{b})=2A^T(A\boldsymbol{x}-\boldsymbol{b})$, 所以$\hat{\boldsymbol{x}}$处$\|A\boldsymbol{x}-\boldsymbol{b}\|_2$取得极值.

类似的有右逆$\mathrm{A}^{\mathrm{T}}(AA^T)^{-1}$, 对应$Ax=b$的最小范数解.

最小二乘解

条件数: $\kappa_2(A) = \frac{\sigma_{max}(A)}{\sigma_{min}(A)}$.

设误差矩阵E, $\|E\|_2 \approx u\|A^TA\|_2$, 解方程

$$(A^TA + E)\tilde{x} = A^Tb$$

代替解

$$A^TA\hat{x} = A^Tb$$

则有

$$\frac{\|\tilde{x} - \hat{x}\|_2}{\|\hat{x}\|_2} \approx u\kappa_2(A^TA) = u\kappa_2(A)^2$$

即计算误差被平方了。

正交矩阵

向量$\boldsymbol{a}$与$\boldsymbol{b}$正交: $\boldsymbol{a}^T\boldsymbol{b} = 0$.

一组n个n维单位向量两两正交: $[\boldsymbol{q}_1 \quad \boldsymbol{q}_2 \quad \cdots]$ 满足

$$\boldsymbol{q}_i^T\boldsymbol{q}_j = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

构成$\mathbb{R}^{n\times n}$的正交矩阵.

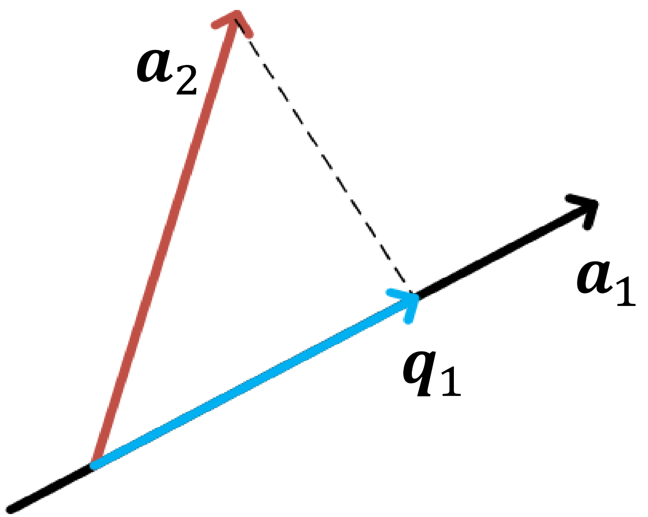
正交矩阵Q有:

$$Q^TQ = QQ^T = I$$
$$\det(Q) = \pm 1$$
$$Q^TQ\boldsymbol{y} = Q^T\boldsymbol{b} \Leftrightarrow \boldsymbol{y} = Q^T\boldsymbol{b}$$

Gram-Schmidt

给定各列线性无关的矩阵$A = [\boldsymbol{a}_1 \quad \boldsymbol{a}_2 \quad \cdots]$

如何正交化得到Q?



1. $\boldsymbol{x}_1 = \boldsymbol{a}_1$, $\boldsymbol{q}_1 = \boldsymbol{x}_1/\lambda_1$.
2. $\boldsymbol{x}_2 = (I - \boldsymbol{q}_1\boldsymbol{q}_1^T)\boldsymbol{a}_2$, $\boldsymbol{q}_2 = \boldsymbol{x}_2/\lambda_2$.
3. $\boldsymbol{x}_3 = (I - \boldsymbol{q}_1\boldsymbol{q}_1^T - \boldsymbol{q}_2\boldsymbol{q}_2^T)\boldsymbol{a}_3$, $\boldsymbol{q}_3 = \boldsymbol{x}_3/\lambda_3$.

…

QR分解

A的各列线性无关, 将A分解为一个正交矩阵Q和一个上三角矩阵R的乘积.

$$\lambda_1 \boldsymbol{q}_1 = \boldsymbol{x}_1 = \boldsymbol{a}_{\boldsymbol{1}}$$
$$\lambda_2 \boldsymbol{q}_2 = \boldsymbol{x}_2 = \boldsymbol{a}_{\boldsymbol{2}} - \boldsymbol{q}_1 \boldsymbol{q}_1^T \boldsymbol{a}_2$$
$$\lambda_3 \boldsymbol{q}_3 = \boldsymbol{x}_3 = \boldsymbol{a}_{\boldsymbol{3}} - \boldsymbol{q}_1 \boldsymbol{q}_1^T \boldsymbol{a}_3 - \boldsymbol{q}_2 \boldsymbol{q}_2^T \boldsymbol{a}_3$$

$$A = QR = [\mathrm{q}_1 \ \ \mathrm{q}_2 \ \ \mathrm{q}_3] \begin{bmatrix} \lambda_1 & \boldsymbol{q}_1^T \boldsymbol{a}_2 & \boldsymbol{q}_1^T \boldsymbol{a}_3 \\ 0 & \lambda_2 & \boldsymbol{q}_2^T \boldsymbol{a}_3 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$

如果A是一个长方形矩阵, $R = \begin{bmatrix} \lambda_1 & * & * \\ 0 & \lambda_2 & * \\ 0 & 0 & \lambda_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

QR分解

最小二乘方程组$A^TA\boldsymbol{x} = A^T\boldsymbol{b}$可以化为

$$R^TR\boldsymbol{x} = A^T\boldsymbol{b},$$

然后$R^T\boldsymbol{y} = A^T\boldsymbol{b}, R\boldsymbol{x} = \boldsymbol{y}$两步三角形方程组求解.

QR分解的软件实现一般基于Householder变换或MGS.

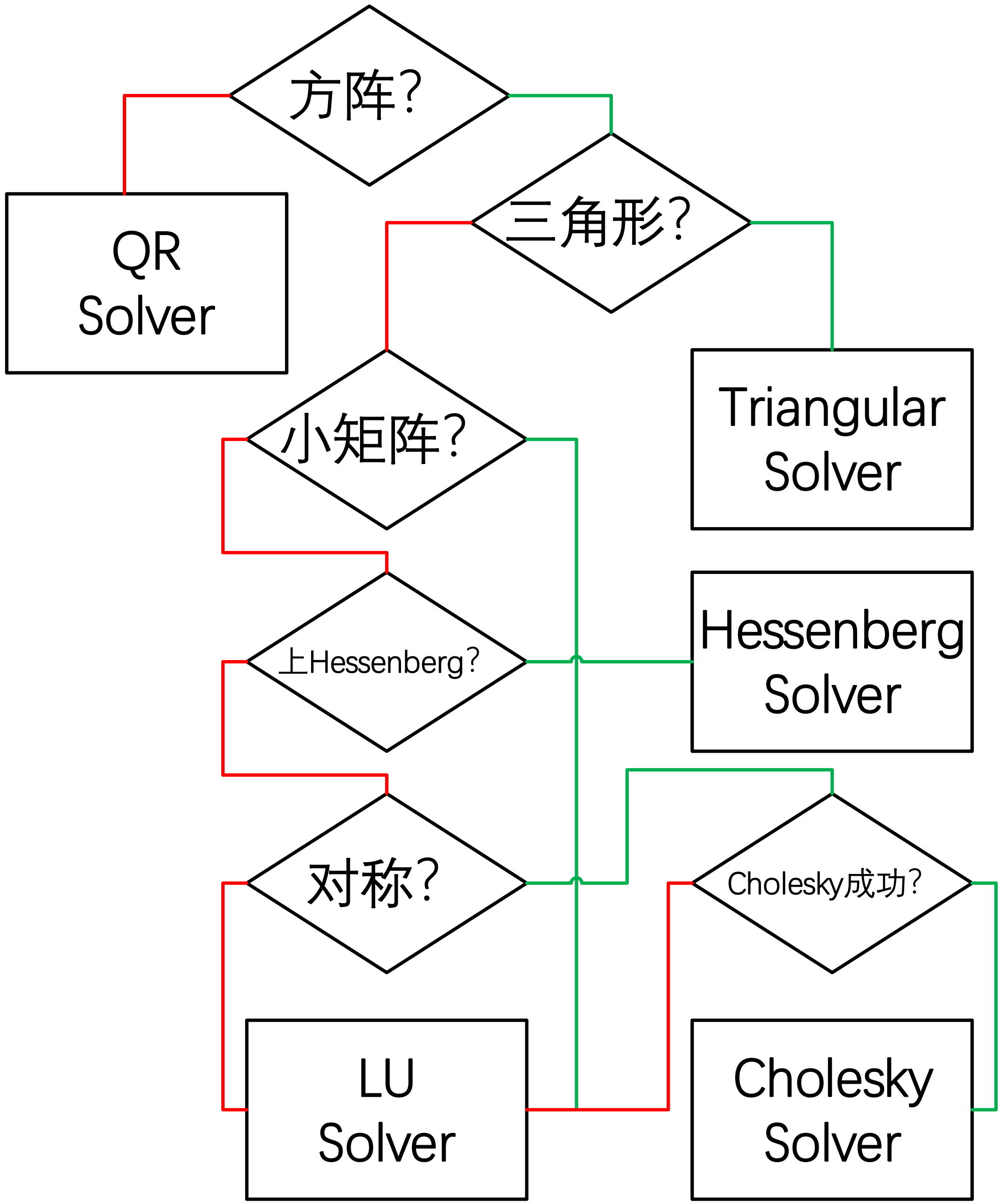
如果矩阵列不满秩, 可以用带主元的QR分解, 此时称为RRQR(Rank Revealing QR Factorization).

ZW3D:

VxHouseholderQR

Eigen::HouseholderQR

xgeqr


方阵?
QR Solver
三角形?
小矩阵?
Triangular Solver
上Hessenberg?
Hessenberg Solver
对称?
Cholesky成功?
LU Solver
Cholesky Solver