MSDM5004
Numerical Methods and Modeling in Science
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Lecture 4

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Properties of SVD

Theorem The nonzero singular values of A are the square roots of the nonzero eigenvalues of A^TA or AA^T.

Proof From $A = U\Sigma V^T$, we have

$$A^TA = V\Sigma^TU^TU\Sigma V^T = V^T\Sigma^T\Sigma V^T,$$

$$AA^T = U\Sigma V^TV\Sigma^TU^T = U\Sigma\Sigma^TU^T.$$

Since U and V are orthogonal matrices, we have that

A^TA is similar to $\Sigma^T\Sigma$ and hence has the same eigenvalues, which are $s_1^2, s_2^2, \cdots, s_n^2$, and

AA^T is similar to $\Sigma\Sigma^T$ and hence has the same eigenvalues, which are $s_1^2, s_2^2, \cdots, s_n^2, 0, \cdots, 0$.

Properties of SVD

Theorem If $A^T = A$, then the singular values of A are the absolute values of the eigenvalues of A.

An example

Determine the singular values of the 5×3 matrix

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix}.$$

Solution We have

$$A^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \end{bmatrix} \text{ and } A^T A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 2 \end{bmatrix}.$$

The eigenvalues of $A^T A$ are $\lambda_1 = s_1^2 = 5$, $\lambda_2 = s_2^2 = 2$, and $\lambda_3 = s_3^2 = 1$.

Thus the singular values of A are $s_1 = \sqrt{5}$, $s_2 = \sqrt{2}$, $s_3 = 1$, Note that for this matrix A

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

the rectangular diagonal matrix Σ is

$$\Sigma = \begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Existence (construction) of SVD

The $A^T A$ is an $n \times n$ symmetric matrix, and it is nonnegative definite:

$$(A^T A)^T = A^T A,$$

$$\mathbf{x}^T (A^T A)\mathbf{x} = (A\mathbf{x})^T A\mathbf{x} = \|A\mathbf{x}\|^2 \geq 0,$$

for any n-vector $\mathbf{x}$.

Thus there exists an orthogonal matrix V, such that

$$A^T A = V D V^T,$$

for some diagonal matrix D. The diagonal entries of D:

$$d_i, \quad i = 1, 2, \cdots, n,$$

are the eigenvalues of $A^T A$ and they are nonnegative.

Choose this V to be the orthogonal matrix $\boxed{V}$ in the SVD of A, and $\boxed{\Sigma}$ in the SVD of A is determined by

$$s_i = \sqrt{d_i}, \quad i = 1, 2, \cdots, n,$$

with these $s_i, i = 1, 2, \cdots, n$ organized in nonincreasing order.

Construction of orthogonal matrix $\boxed{U}$ in the SVD of A.

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

The SVD is equivalent to

$$Av_j = s_j u_j, \qquad j = 1, 2, \cdots, n$$

For the positive singular values s_j, $j = 1, 2, \cdots, k$, we have the first k columns of U:

$$u_j = \frac{1}{s_j} A v_j.$$

The remaining columns of U, which are u_j, $j = k+1, k+2, \cdots, m$, can be chosen such that all the columns of U form an orthogonal basis of $\mathbf{R}^m$.

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \cdots & u_m \end{bmatrix} \begin{bmatrix} s_1 & 0 & \cdots & 0 \\ 0 & s_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & s_n \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix}$$

An example

Determine the singular value decomposition of the 5×3 matrix

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix}.$$

Solution We have

$$A^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \end{bmatrix} \quad \text{so} \quad A^T A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 2 \end{bmatrix}.$$

The eigenvalues of $A^T A$ are $\lambda_1 = s_1^2 = 5$, $\lambda_2 = s_2^2 = 2$, and $\lambda_3 = s_3^2 = 1$.

Thus the singular values of A are $s_1 = \sqrt{5}$, $s_2 = \sqrt{2}$, $s_3 = 1$,

$$\Sigma = \begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Using eigenvectors associated with λ_1, λ_2 and λ_3 with norm 1 as the columns of V, we have

$$V = \begin{bmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{6}}{3} & -\frac{\sqrt{3}}{3} & 0 \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{3}}{3} & \frac{\sqrt{2}}{2} \end{bmatrix} \quad \text{and} \quad V^T = \begin{bmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \\ -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

The first 3 columns of U are therefore

$$\mathbf{u}_1 = \frac{1}{\sqrt{5}} \cdot A\left(\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3}, \frac{\sqrt{6}}{6}\right)^T = \left(\frac{\sqrt{30}}{15}, \frac{\sqrt{30}}{15}, \frac{\sqrt{30}}{10}, \frac{\sqrt{30}}{15}, \frac{\sqrt{30}}{10}\right)^T$$

$$\mathbf{u}_2 = \frac{1}{\sqrt{2}} \cdot A\left(\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right)^T = \left(\frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6}, 0, -\frac{\sqrt{6}}{6}, 0\right)^T$$

$$\mathbf{u}_3 = 1 \cdot A\left(-\frac{\sqrt{2}}{2}, 0, \frac{\sqrt{2}}{2}\right)^T = \left(0, 0, \frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2}\right)^T$$

To determine the two remaining columns of U we first need two vectors $\mathbf{x}_4$ and $\mathbf{x}_5$ so that $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{x}_4, \mathbf{x}_5\}$ is a linearly independent set. Then we apply the Gram Schmidt process to obtain $\mathbf{u}_4$ and $\mathbf{u}_5$ so that $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4, \mathbf{u}_5\}$ is an orthogonal set. Two vectors that satisfy are

$$(1, 1, -1, 1, -1)^T \quad \text{and} \quad (0, 1, 0, -1, 0)^T.$$

Normalizing the vectors $\mathbf{u}_i$, for $i = 1, 2, 3, 4$, and 5 produces the matrix U and the singular value decomposition as

$$A = U\Sigma V^T = \begin{bmatrix} \frac{\sqrt{30}}{15} & \frac{\sqrt{6}}{3} & 0 & \frac{\sqrt{5}}{5} & 0 \\ \frac{\sqrt{30}}{15} & -\frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{5}}{5} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{30}}{10} & 0 & \frac{\sqrt{2}}{2} & -\frac{\sqrt{5}}{5} & 0 \\ \frac{\sqrt{30}}{15} & -\frac{\sqrt{6}}{3} & 0 & \frac{\sqrt{5}}{5} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{30}}{10} & 0 & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{5}}{5} & 0 \end{bmatrix} \begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \\ -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

Least squares fitting using SVD

Least-squares fitting problem: To minimize

$$\|A\mathbf{x} - \mathbf{b}\|^2.$$

Using SVD,

$$\|A\mathbf{x} - \mathbf{b}\| = \|U\Sigma V^T\mathbf{x} - \mathbf{b}\| = \|\Sigma V^T\mathbf{x} - U^T\mathbf{b}\|$$

Define $\mathbf{z} = V^T\mathbf{x}$, $\mathbf{c} = U^T\mathbf{b}$. We have

$$\begin{aligned} \|A\mathbf{x} - \mathbf{b}\| &= \|(s_1z_1 - c_1, s_2z_2 - c_2, \ldots, s_kz_k - c_k, -c_{k+1}, \ldots, -c_m)^T\| \\ &= \left\{ \sum_{i=1}^{k} (s_iz_i - c_i)^2 + \sum_{i=k+1}^{m} (c_i)^2 \right\}^{1/2}. \end{aligned}$$

The norm is minimized when the vector $\mathbf{z}$ is chosen with

$$z_i = \begin{cases} \dfrac{c_i}{s_i}, & \text{when } i \le k, \\ \text{arbitrarily}, & \text{when } k < i \le n. \end{cases}$$

Because $\mathbf{c} = U^t\mathbf{b}$ and $\mathbf{x} = V\mathbf{z}$ are both easy to compute, the least squares solution is also easily found.

An example

Use the singular value decomposition technique to determine the least squares polynomial of degree two for the data given in the table:

i	x_i	y_i
1	0	1.0000
2	0.25	1.2840
3	0.50	1.6487
4	0.75	2.1170
5	1.00	2.7183

Solution We need to find the least squares polynomial

$$P_2(x) = a_0 + a_1 x + a_2 x^2.$$

In order to express this in matrix form, we let

$$\mathbf{x} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 1.0000 \\ 1.2840 \\ 1.6487 \\ 2.1170 \\ 2.7183 \end{bmatrix}, \quad \text{and}$$

$$A = \begin{bmatrix} 1 & x_0 & x_0^2 \\ 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0.25 & 0.0625 \\ 1 & 0.5 & 0.25 \\ 1 & 0.75 & 0.5625 \\ 1 & 1 & 1 \end{bmatrix}.$$

The singular value decomposition of A has the form $A = U\Sigma V^T$, where

$$U = \begin{bmatrix} -0.2945 & -0.6327 & 0.6314 & -0.0143 & -0.3378 \\ -0.3466 & -0.4550 & -0.2104 & 0.2555 & 0.7505 \\ -0.4159 & -0.1942 & -0.5244 & -0.6809 & -0.2250 \\ -0.5025 & 0.1497 & -0.3107 & 0.6524 & -0.4505 \\ -0.6063 & 0.5767 & 0.4308 & -0.2127 & 0.2628 \end{bmatrix},$$

$$\Sigma = \begin{bmatrix} 2.7117 & 0 & 0 \\ 0 & 0.9371 & 0 \\ 0 & 0 & 0.1627 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \text{and} \quad V^T = \begin{bmatrix} -0.7987 & -0.4712 & -0.3742 \\ -0.5929 & 0.5102 & 0.6231 \\ 0.1027 & -0.7195 & 0.6869 \end{bmatrix}.$$

$$\mathbf{c} = U^T \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} -0.2945 & -0.6327 & 0.6314 & -0.0143 & -0.3378 \\ -0.3466 & -0.4550 & -0.2104 & 0.2555 & 0.7505 \\ -0.4159 & -0.1942 & -0.5244 & -0.6809 & -0.2250 \\ -0.5025 & 0.1497 & -0.3107 & 0.6524 & -0.4505 \\ -0.6063 & 0.5767 & 0.4308 & -0.2127 & 0.2628 \end{bmatrix}^T \begin{bmatrix} 1 \\ 1.284 \\ 1.6487 \\ 2.117 \\ 2.7183 \end{bmatrix}$$

$$= \begin{bmatrix} -4.1372 \\ 0.3473 \\ 0.0099 \\ -0.0059 \\ 0.0155 \end{bmatrix},$$

and the components of $\mathbf{z}$ are

$$z_1 = \frac{c_1}{s_1} = \frac{-4.1372}{2.7117} = -1.526, \quad z_2 = \frac{c_2}{s_2} = \frac{0.3473}{0.9371} = 0.3706, \quad \text{and}$$

$$z_3 = \frac{c_3}{s_3} = \frac{0.0099}{0.1627} = 0.0609.$$

This gives the least squares coefficients in $P_2(x)$ as

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \mathbf{x} = V\,\mathbf{z} = \begin{bmatrix} -0.7987 & -0.5929 & 0.1027 \\ -0.4712 & 0.5102 & -0.7195 \\ -0.3742 & 0.6231 & 0.6869 \end{bmatrix} \begin{bmatrix} -1.526 \\ 0.3706 \\ 0.0609 \end{bmatrix} = \begin{bmatrix} 1.005 \\ 0.8642 \\ 0.8437 \end{bmatrix},$$

Note that the least square error of the solution is

$$||A\mathbf{x} - \mathbf{b}||_2 = \sqrt{c_4^2 + c_5^2} = \sqrt{(-0.0059)^2 + (0.0155)^2} = 0.0165.$$

Low-rank approximation based on SVD

SVD of A $\quad A = U\Sigma V^T$

$$\begin{bmatrix} \\ & A & \\ \\ \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \cdots & u_m \end{bmatrix} \begin{bmatrix} s_1 & 0 & \cdots & 0 \\ 0 & s_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & s_n \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} v_1^T \\ \hline v_2^T \\ \hline \vdots \\ \hline v_n^T \end{bmatrix}$$

$$A = \sum_{j=1}^{n} s_j u_j v_j^T = \sum_{j=1}^{k} s_j u_j v_j^T,$$

where s_j, $j = 1, 2, \cdots, k$, are the positive singular values.

Each $s_j u_j v_j^T$ is an $m \times n$ rank-1 matrix

If the singular values s_j, $j = r+1, r+2, \cdots$, are small, we approximate them by 0 to have the low-rank apprxomation

$$A = \sum_{j=1}^{k} s_j u_j v_j^T \approx \sum_{j=1}^{r} s_j u_j v_j^T.$$

Here the approximate matrix has rank $r < k$, where k is the rank of A.

Relationship with PCA

The approximation with SVD in statistics or machine learning is often called *Principal Component Analysis* (PCA).

MATLAB function for SVD

MATLAB has a built-in function for SVD.

```
>> help svd
 svd   Singular value decomposition.
   [U,S,V] = svd(X) produces a diagonal matrix S, of the same
   dimension as X and with nonnegative diagonal elements in
   decreasing order, and unitary matrices U and V so that
   X = U*S*V'.

   S = svd(X) returns a vector containing the singular values.

   [U,S,V] = svd(X,0) produces the "economy size"
   decomposition. If X is m-by-n with m > n, then only the
   first n columns of U are computed and S is n-by-n.
   For m <= n, svd(X,0) is equivalent to svd(X).

   [U,S,V] = svd(X,'econ') also produces the "economy size"
   decomposition. If X is m-by-n with m >= n, then it is
   equivalent to svd(X,0). For m < n, only the first m columns
   of V are computed and S is m-by-m.
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Chapter 6

Direct methods for solving linear systems

1. Gaussian elimination

Review

$$\begin{cases} x_1 - 2x_2 + x_3 = 0 & (1) \\ \quad\;\; 2x_2 - 8x_3 = 8 & (2) \\ -4x_1 + 5x_2 + 9x_3 = -9 & (3) \end{cases}$$

$$\left[\begin{array}{ccc|c} 1 & -2 & 1 & 0 \\ 0 & 2 & -8 & 8 \\ -4 & 5 & 9 & -9 \end{array}\right]\begin{array}{c}(1)\\(2)\\(3)\end{array} \rightarrow \left[\begin{array}{ccc|c} 1 & -2 & 1 & 0 \\ 0 & 2 & -8 & 8 \\ 0 & -3 & 13 & -9 \end{array}\right]\begin{array}{c}(1)\\(2)\\(3)\end{array} \rightarrow \left[\begin{array}{ccc|c} 1 & -2 & 1 & 0 \\ 0 & 1 & -4 & 4 \\ 0 & -3 & 13 & -9 \end{array}\right]\begin{array}{c}(1)\\(2)\\(3)\end{array} \rightarrow$$

replace (3) by (3) + (1) $*$ 4

(2) $* \frac{1}{2}$

replace (3) by (3) + (2) $*$ 3

/ Backward substitution

$$\left[\begin{array}{ccc|c} 1 & -2 & 1 & 0 \\ 0 & 1 & -4 & 4 \\ 0 & 0 & 1 & 3 \end{array}\right]\begin{array}{c}(1)\\(2)\\(3)\end{array} \rightarrow \left[\begin{array}{ccc|c} 1 & -2 & 1 & 0 \\ 0 & 1 & 0 & 16 \\ 0 & 0 & 1 & 3 \end{array}\right]\begin{array}{c}(1)\\(2)\\(3)\end{array} \rightarrow$$

replace (2) by (2) + (3) $*$ 4

replace (1) by (1) − (3)

$$\left[\begin{array}{ccc|c} 1 & -2 & 0 & -3 \\ 0 & 1 & 0 & 16 \\ 0 & 0 & 1 & 3 \end{array}\right]\begin{array}{c}(1)\\(2)\\(3)\end{array} \rightarrow \left[\begin{array}{ccc|c} 1 & 0 & 0 & 29 \\ 0 & 1 & 0 & 16 \\ 0 & 0 & 1 & 3 \end{array}\right]$$

replace (1) by (1) + (2) $*$ 2

Algorithm

Elimination

Step 1: Eliminate the first column.

$$a_{ij} \rightarrow a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}, \quad i = 2, \ldots, n; \; j = 1, \ldots, n$$

$$b_i \rightarrow b_i - \frac{a_{i1}}{a_{11}} b_1, \quad i = 2, \ldots, n$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{pmatrix} \rightarrow \begin{pmatrix} a_{11}^{(2)} & a_{12}^{(2)} & \cdots & a_{1n}^{(2)} & b_1^{(2)} \\ 0 & a_{22}^{(2)} & \cdots & a_{2n}^{(2)} & b_2^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} & b_n^{(2)} \end{pmatrix}$$

Step 2: Eliminate the second column.

$$a_{ij}^{(2)} \rightarrow a_{ij}^{(2)} - \frac{a_{i2}^{(2)}}{a_{22}^{(2)}} a_{2j}^{(2)}, \quad i = 3, \ldots, n; \; j = 2, \ldots, n$$

$$b_i^{(2)} \rightarrow b_i^{(2)} - \frac{a_{i2}^{(2)}}{a_{22}^{(2)}} b_2^{(2)}, \quad i = 3, \ldots, n$$

$$\begin{pmatrix} a_{11}^{(2)} & a_{12}^{(2)} & \cdots & a_{1n}^{(2)} & b_1^{(2)} \\ 0 & a_{22}^{(2)} & \cdots & a_{2n}^{(2)} & b_2^{(2)} \\ 0 & a_{32}^{(2)} & \cdots & a_{3n}^{(2)} & b_3^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} & b_n^{(2)} \end{pmatrix} \rightarrow \begin{pmatrix} a_{11}^{(3)} & a_{12}^{(3)} & \cdots & a_{1n}^{(3)} & b_1^{(3)} \\ 0 & a_{22}^{(3)} & \cdots & a_{2n}^{(3)} & b_2^{(3)} \\ 0 & 0 & \cdots & a_{3n}^{(3)} & b_3^{(3)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{nn}^{(3)} & b_n^{(3)} \end{pmatrix}$$

$\ldots$

Step $n-1$: Eliminate the $(n-1)$-th column.

$$a_{ij}^{(n-1)} \to a_{ij}^{(n-1)} - \frac{a_{n-1,j}^{(n-1)}}{a_{n-1,n-1}^{(n-1)}} a_{i,n-1}^{(n-1)}, \quad i = n;\ j = n-1, n$$

$$\begin{pmatrix} a_{11}^{(n-1)} & a_{12}^{(n-1)} & \cdots & a_{1n}^{(n-1)} & b_1^{(n-1)} \\ 0 & a_{22}^{(n-1)} & \cdots & a_{2n}^{(n-1)} & b_1^{(n-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{nn}^{(n-1)} & b_n^{(n-1)} \end{pmatrix}$$

Backward substitution

$$\boldsymbol{U} \cdot \boldsymbol{x} = \boldsymbol{b}$$

where

$$\boldsymbol{U} = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \ddots & \vdots \\ & & \ddots & \ddots \\ & & & u_{nn} \end{pmatrix}$$

and $u_{ii} \neq 0, i = 1, \ldots, n.$

$$x_i = (b_i - \sum_{j=i+1}^{n} u_{ij} x_j)/u_{ii}, \quad i = n, n-1, \ldots, 1$$

For a matrix of size n, the computational cost (total number of operations) of Gaussian elimination is *$O(n^3)$.*

Elimination: $O(n^3)$

Backward substitution: $O(n^2)$

Gaussian elimination is essential an LU factorization

$$\mathbf{A}\mathbf{x} = \mathbf{b} \qquad A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix}$$

$$A = LU \qquad \mathbf{A}\mathbf{x} = \mathbf{b} \Longleftrightarrow L\mathbf{y} = \mathbf{b} \quad U\mathbf{x} = \mathbf{y}$$

$$L = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ m_{n1} & \cdots & m_{n,n-1} & 1 \end{bmatrix} \qquad U = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \cdots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_{n-1,n}^{(n-1)} \\ 0 & \cdots & 0 & a_{nn}^{(n)} \end{bmatrix}$$

lower-triangular matrix   upper-triangular matrix

Once the LU factorization of a matrix is determined, it can be used repeatedly.

In MATLAB: [L U]=lu(A)

Step k in the elimination is equivalent to $M^{(k)}A^{(k)}$

$$M^{(k)} = \begin{bmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & 0 & & \ddots & \ddots & & \vdots \\ \vdots & \vdots & -m_{k+1,k} & & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & 0 & & \ddots & 0 \\ 0 \cdots & 0 & -m_{n,k} & 0 & \cdots & 0 & 1 \end{bmatrix}$$

$$m_{j,k} = \frac{a_{jk}^{(k)}}{a_{kk}^{(k)}}$$

$$M^{(n-1)} \cdots M^{(2)} M^{(1)} A = U$$

$$L^{(k)} = [M^{(k)}]^{-1} = \begin{bmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & & & \vdots \\ \vdots & \ddots & 0 & \ddots & & & \vdots \\ \vdots & & \vdots & m_{k+1,k} & \ddots & & \vdots \\ \vdots & & \vdots & \vdots & 0 & \ddots & \vdots \\ \vdots & & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & m_{n,k} & 0 & \cdots\ 0 & 1 \end{bmatrix}$$

$$L = L^{(1)} L^{(2)} \cdots L^{(n-1)} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ m_{n1} & \cdots & m_{n,n-1} & 1 \end{bmatrix},$$

$$A = LU$$

2. Pivoting

In the k-th step in the elimination, we determine the smallest $p \geq k$ such that

$$|a_{pk}^{(k)}| = \max_{k \leq i \leq n} |a_{ik}^{(k)}|$$

and interchange the k-th and p-th rows.

e.g.

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \end{pmatrix} \to \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

LU factorization

$$PA = LU$$

where P is a permutation matrix (obtained by rearranging rows from the identity matrix).

e.g.

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

3. Tridiagonal linear system: Thomas algorithm

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & \cdots & 0 \\ a_{21} & a_{22} & a_{23} & \ddots & & \vdots \\ 0 & a_{32} & a_{33} & a_{34} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & a_{n-1,n} \\ 0 & \cdots & \cdots & 0 & a_{n,n-1} & a_{nn} \end{bmatrix}$$

$$A\mathbf{x} = \mathbf{b} \iff L\mathbf{y} = \mathbf{b} \qquad U\mathbf{x} = \mathbf{y}$$

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & \cdots & 0 \\ l_{21} & l_{22} & \ddots & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & l_{n,n-1} & l_{nn} \end{bmatrix} \qquad U = \begin{bmatrix} 1 & u_{12} & 0 & \cdots & 0 \\ 0 & 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & u_{n-1,n} \\ 0 & \cdots & \cdots & 0 & 1 \end{bmatrix}.$$

LU factorization for tridiagonal linear system (The Thomas algorithm)

1. Find L and U, such that $A = LU$

$$a_{11} = l_{11};$$

$$a_{i,i-1} = l_{i,i-1}, \quad \text{for each } i = 2, 3, \ldots, n;$$

$$a_{ii} = l_{i,i-1}u_{i-1,i} + l_{ii}, \quad \text{for each } i = 2, 3, \ldots, n;$$

$$a_{i,i+1} = l_{ii}u_{i,i+1}, \quad \text{for each } i = 1, 2, \ldots, n-1.$$

2. Solve $L\mathbf{y} = \mathbf{b}$

3. Solve $U\mathbf{x} = \mathbf{y}$

Computational cost (total number of operations) is *O(n).*

4. Matrix norm and condition number

Norm of a vector

The l_2 and l_∞ norms for the vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ are defined by

$$\|\mathbf{x}\|_2 = \left\{\sum_{i=1}^{n} x_i^2\right\}^{1/2} \quad \text{and} \quad \|\mathbf{x}\|_\infty = \max_{1\le i\le n} |x_i|.$$

Example

Determine the l_2 norm and the l_∞ norm of the vector $\mathbf{x} = (-1, 1, -2)^t$.

Solution The vector $\mathbf{x} = (-1, 1, -2)^t$ in $\mathbb{R}^3$ has norms

$$\|\mathbf{x}\|_2 = \sqrt{(-1)^2 + (1)^2 + (-2)^2} = \sqrt{6}$$

and

$$\|\mathbf{x}\|_\infty = \max\{|-1|, |1|, |-2|\} = 2.$$

Norm of a matrix

$$A = (a_{ij})_{n\times n}$$ vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$

$$\|\boldsymbol{A}\| = \max_{\boldsymbol{x}\neq 0} \frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|}$$

$2-$ norm $\qquad \|\boldsymbol{A}\|_2 = \sqrt{\lambda_{\max}(\boldsymbol{A}^T\boldsymbol{A})}$

(maximum eigenvalue)

$\infty-$ norm $\qquad \|\boldsymbol{A}\|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$

Properties

1. $\|\boldsymbol{A}\| \geq 0$ and $\|\boldsymbol{A}\| = 0$ iff $\boldsymbol{A} = 0$,
2. $\|k\boldsymbol{A}\| = |k| \cdot \|\boldsymbol{A}\|$,
3. $\|\boldsymbol{A} + \boldsymbol{B}\| \leq \|\boldsymbol{A}\| + \|\boldsymbol{B}\|$
4. $\|\boldsymbol{A}\boldsymbol{B}\| \leq \|\boldsymbol{A}\| \cdot \|\boldsymbol{B}\|$,
5. $\|\boldsymbol{A}\boldsymbol{x}\| \leq \|\boldsymbol{A}\| \cdot \|\boldsymbol{x}\|$.

Stability of the solution

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

$$\boldsymbol{A}(\boldsymbol{x} + \delta\boldsymbol{x}) = \boldsymbol{b} + \delta\boldsymbol{b}$$

$$\delta\boldsymbol{x} = \boldsymbol{A}^{-1}\delta\boldsymbol{b}$$

$$||\delta\boldsymbol{x}|| \leq ||\boldsymbol{A}^{-1}||\,||\delta\boldsymbol{b}|| = ||\boldsymbol{A}^{-1}||\,||\boldsymbol{A}\boldsymbol{x}||\frac{||\delta\boldsymbol{b}||}{||\boldsymbol{b}||} \leq ||\boldsymbol{A}^{-1}||\,||\boldsymbol{A}||\,||\boldsymbol{x}||\frac{||\delta\boldsymbol{b}||}{||\boldsymbol{b}||}.$$

$$\frac{||\delta\boldsymbol{x}||}{||\boldsymbol{x}||} \leq Cond(A)\frac{||\delta\boldsymbol{b}||}{||\boldsymbol{b}||}$$

$$Cond(A) = ||\boldsymbol{A}|| \cdot ||\boldsymbol{A}^{-1}||$$

Condition number