COURSE 8

4. Numerical methods for solving linear systems

Practical solving of many problems eventually leads to solving linear systems.

Classification of the methods:

- direct methods with low number of unknowns (up to several tens of thousands); they provide the exact solution of the system in a finite number of steps.
- *iterative methods with medium number of unknowns*; it is obtained an approximation of the solution as the limit of a sequence.

- semiiterative methods - with large number of unknowns; it is obtained an approximation of the solution.

4.1. Perturbation of linear systems.

Consider the linear system

$$Ax = b$$
.

Definition 1 The number cond $(A) = ||A|| ||A^{-1}||$ is called **conditioning number** of the matrix A. It measures the sensibility of the solution x of the system Ax = b to the perturbation of A and b.

The system is good conditioned if cond(A) is small (<1000) or it is ill conditioned if cond(A) is great.

Remark 2 1. cond $(A) \ge 1$.

2. cond(A) depends on the norm used.

Consider an example

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix},$$

with the solution $\begin{pmatrix} 1\\1\\1\\1 \end{pmatrix}$.

We perturbate the right hand side:

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} x_1 + \delta x_1 \\ x_2 + \delta x_2 \\ x_3 + \delta x_3 \\ x_4 + \delta x_4 \end{pmatrix} = \begin{pmatrix} 32.1 \\ 22.9 \\ 33.1 \\ 30.9 \end{pmatrix},$$

and obtain the exact solution
$$\begin{pmatrix} 9.2\\ -12.6\\ 4.5\\ -1.1 \end{pmatrix}$$
 .

We have

$$\left| \frac{b_2 - (b_2 + \delta b_2)}{b_2} \right| = \left| \frac{\delta b_2}{b_2} \right| = \frac{1}{229} \approx \frac{1}{200},$$

where δb_i , $i = \overline{1,3}$ denote the perturbations of b, and

$$\left| \frac{x_2 - (x_2 + \delta x_2)}{x_2} \right| = \left| \frac{\delta x_2}{x_2} \right| = 13.6 \approx 10.$$

Thus, a relative error of order $\frac{1}{200}$ on the right hand side (precision of $\frac{1}{200}$ for the data in a linear system) attracts a relative error of order 10 on the solution, 2000 times larger.

Consider the same system, and perturb the matrix A:

$$\begin{pmatrix} 10 & 7 & 8.1 & 7.2 \\ 7.08 & 5.04 & 6 & 5 \\ 8 & 5.98 & 9.89 & 9 \\ 6.99 & 4.99 & 9 & 9.98 \end{pmatrix} \begin{pmatrix} x_1 + \delta x_1 \\ x_2 + \delta x_2 \\ x_3 + \delta x_3 \\ x_4 + \delta x_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix},$$

with exact solution
$$\begin{pmatrix} -81\\137\\-34\\22 \end{pmatrix}$$
.

The matrix A seems to have good properties (symmetric, with deter-

minant 1), and the inverse
$$A^{-1}=\begin{pmatrix} 25 & -41 & 10 & -6 \\ -41 & 68 & -17 & 10 \\ 10 & -17 & 5 & -3 \\ -6 & 10 & -3 & 2 \end{pmatrix}$$
 is also with integer numbers.

This example is very concerning as such orders of the errors in many experimental sciences are considered as satisfactory.

Remark 3 For this example cond (A) = 2984 (in euclidian norm).

Analyze the phenomenon:

lacktriangle In the first case, when b is perturbed, we compare de exact solutions x and $x+\delta x$ of the systems

$$Ax = b$$

and

$$A(x + \delta x) = b + \delta b.$$

Let $\|\cdot\|$ be a norm on \mathbb{R}^n and $\|\cdot\|$ the induced matrix norm.

We have the systems

$$Ax = b$$

and

$$Ax + A\delta x = b + \delta b \iff A\delta x = \delta b.$$

From $\delta x = A^{-1}\delta b$ we get $\|\delta x\| \le \|A^{-1}\| \|\delta b\|$

and from b = Ax we get $||b|| \le ||A|| \, ||x|| \Leftrightarrow \frac{1}{||x||} \le \frac{||A||}{||b||}$,

so the relative error of the result is bounded by

$$\frac{\|\delta x\|}{\|x\|} \le \left(\|A\| \|A^{-1}\|\right) \frac{\|\delta b\|}{\|b\|} \stackrel{denoted}{=} \text{cond}(A) \frac{\|\delta b\|}{\|b\|}. \tag{1}$$

lacktriangle In the second case, when the matrix A is perturbed , we compare the exact solutions of the linear systems

$$Ax = b$$

and

$$(A + \delta A)(x + \delta x) = b \iff Ax + A\delta x + \delta Ax + \delta A\delta x = b$$
$$\iff A\delta x = -\delta A(x + \delta x).$$

From $\delta x = -A^{-1}\delta A(x+\delta x)$, we get $\|\delta x\| \le \|A^{-1}\| \|\delta A\| \|x+\delta x\|$, or

$$\frac{\|\delta x\|}{\|x + \delta x\|} \le \|A^{-1}\| \|\delta A\| = (\|A\| \|A^{-1}\|) \frac{\|\delta A\|}{\|A\|} = \text{cond}(A) \frac{\|\delta A\|}{\|A\|}.$$
 (2)

4.2. Direct methods for solving linear systems

Why Cramer's method is not suitable for solving linear systems for $n \ge 100$ and it will not be in near future?

For applying Cramer's method for a $n \times n$ system we need in a rough evaluation the following number of operations:

$$\begin{cases} (n+1)! & \text{aditions} \\ (n+2)! & \text{multiplications} \\ n & \text{divisions} \end{cases}$$

Consider, hypothetically, a volume $V=1~\rm km^3$ of cubic processors of each having the side $l=10^{-8}~\rm cm$ (radius of an atom), the time for execution of an operation is equal to the time needed for the light to pass through an atom. (Light speed is 300.000 km/s.)

In this case, the time necessary for solving the $n \times n$ system, $n \ge 100$, will be more than 10^{94} years!

4.2.1. Gauss method for solving linear systems

Consider the linear system Ax = b, i.e.,

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}. \tag{3}$$

The method consists of two stages:

- reducing the system (3) to an equivalent one, Ux = d, with U an upper triangular matrix.
- solving of the upper triangular linear system Ux = d by backward substitution.

At least one of the elements on the first column is nonzero, otherwise A is singular. We choose one of these nonzero elements (using some criterion) and this will be called the first elimination **pivot**.

If the case, we change the line of the pivot with the first line, both in A and in b, and next we successively make zeros under the first pivot:

$$\begin{pmatrix} a_{11}^1 & a_{12}^1 & \dots & a_{1n}^1 \\ 0 & a_{22}^1 & \dots & a_{2n}^1 \\ \vdots & \vdots & & \vdots \\ 0 & a_{n2}^1 & \dots & a_{nn}^1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1^1 \\ b_2^1 \\ \vdots \\ b_n^1 \end{pmatrix}.$$

Analogously, after k steps we obtain the system

$$\begin{pmatrix} a_{11}^1 & a_{12}^1 & \dots & a_{1k}^1 & a_{1,k+1}^1 & \dots & a_{1n}^1 \\ 0 & a_{22}^2 & \dots & a_{2k}^2 & a_{2,k+1}^2 & \dots & a_{2n}^2 \\ \vdots & \vdots & & \vdots & & \vdots & & \vdots \\ 0 & 0 & \dots & a_{kk}^k & a_{k,k+1}^k & \dots & a_{kn}^k \\ 0 & 0 & \dots & 0 & a_{k+1,k+1}^k & \dots & a_{k+1,n}^k \\ \vdots & \vdots & & \vdots & & \vdots & & \vdots \\ 0 & 0 & \dots & 0 & a_{n,k+1}^k & \dots & a_{nn}^k \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \\ x_{k+1} \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1^1 \\ b_2^2 \\ \vdots \\ b_k^k \\ b_{k+1}^k \\ \vdots \\ b_n^k \end{pmatrix} .$$

If $a_{kk}^k\neq 0$, denote $m_{ik}=\frac{a_{ik}^k}{a_{kk}^k}$ and we get $a_{ij}^{k+1}=a_{ij}^k-m_{ik}a_{kj}^k,\quad j=k,...,n$

$$a_{ij}^{k+1} = a_{ij}^k - m_{ik} a_{kj}^k, \quad j = k, ..., n$$

 $b_i^{k+1} = b_i^k - m_{ik} b_k^k, \quad i = k+1, ..., n.$

After n-1 steps we obtain the system

$$\begin{pmatrix} a_{11}^{1} & a_{12}^{1} & \dots & a_{1n}^{1} \\ 0 & a_{22}^{2} & \dots & a_{2n}^{2} \\ 0 & 0 & \dots & a_{3n}^{3} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & a_{nn}^{n-1} \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \\ \vdots \\ x_{n} \end{pmatrix} = \begin{pmatrix} b_{1}^{1} \\ b_{2}^{2} \\ b_{3}^{3} \\ \vdots \\ b_{n}^{n-1} \end{pmatrix}.$$

Remark 4 The total number of elementary operations is of order $\frac{2}{3}n^3$.

Example 5 Consider the system

$$\left(\begin{array}{cc} 0.0001 & 1 \\ 1 & 1 \end{array}\right) \left(\begin{array}{c} x \\ y \end{array}\right) = \left(\begin{array}{c} 1 \\ 2 \end{array}\right).$$

Gauss algorithm yields: $m_{11} = \frac{a_{21}}{a_{11}} = \frac{1}{0.0001}$

$$\begin{pmatrix} 0.0001 & 1 \\ 1 - 0.0001 * m_{11} = 0 & 1 - 1 * m_{11} = -9999 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$
$$= \begin{pmatrix} 1 \\ 2 - 1 * m_{11} = -9998 \end{pmatrix}$$
$$\Rightarrow y = \frac{9998}{9999} = 0.(9998) \approx 1.$$

Replacing in the first equation we get

$$x = 1.000(1000) \approx 1.$$

By division with a pivot of small absolute value there could be induced errors. For avoiding this there are two ways:

A) Partial pivoting: finding an index $p \in \{k, ..., n\}$ such that:

$$\left|a_{p,k}^{k}\right| = \max_{i=\overline{k},n} \left|a_{i,k}^{k}\right|.$$

B) Total pivoting: finding $p, q \in \{k, ..., n\}$ such that:

$$\left| a_{p,q}^k \right| = \max_{i,j = \overline{k}, n} \left| a_{ij}^k \right|,$$

Example 6 Solve the following system of equations using partial pivoting:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 3 & 1 & 5 \\ -1 & 1 & -5 & 3 \\ 3 & 1 & 7 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 10 \\ 31 \\ -2 \\ 18 \end{bmatrix}.$$

The pivot is a_{41} . We interchange the 1-st line and the 4-th line. We have

$$\begin{bmatrix} 3 & 1 & 7 & -2 \\ 2 & 3 & 1 & 5 \\ -1 & 1 & -5 & 3 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 18 \\ 31 \\ -2 \\ 10 \end{bmatrix},$$

then

Subtracting multiplies of the first equation from the three others gives

$$\begin{array}{c} \textit{pivot element} \rightarrow \\ m_{32} = \frac{1.33}{2.33} \\ m_{42} = \frac{0.66}{2.33} \end{array} \left[\begin{array}{cccccc} 3 & 1 & 7 & -2 & | & 18 \\ 0 & 2.33 & -3.66 & 6.33 & | & 19 \\ 0 & 1.33 & -2.66 & 2.33 & | & 4 \\ 0 & 0.66 & -1.33 & 1.66 & | & 4 \end{array} \right].$$

Subtracting multiplies, of the second equation from the last two equations, gives

$$pivot \ element \rightarrow \left[\begin{array}{ccc|ccc|c} 3 & 1 & 7 & -2 & | & 18 \\ 0 & 2.33 & -3.66 & 6.33 & | & 19 \\ 0 & 0 & -0.57 & -1.28 & | & -6.85 \\ m_{43} = \frac{0.28}{0.57} & 0 & 0 & -0.28 & -0.14 & | & -1.42 \end{array} \right].$$

Subtracting multiplies, of the third equation form the last one, gives the upper triangular system

$$\begin{bmatrix} 3 & 1 & 7 & -2 & | & 18 \\ 0 & 2.33 & -3.66 & 6.33 & | & 19 \\ 0 & 0 & -0.57 & -1.28 & | & -6.85 \\ 0 & 0 & 0 & 0.5 & | & 2 \end{bmatrix}.$$

The process of the back substitution algorithm applied to the triangular system produces the solution

$$x_4 = \frac{2}{0.5} = 4$$

$$x_3 = \frac{-6.85 + 1.28x_4}{-0.57} = 3$$

$$x_2 = \frac{19 + 3.66x_3 - 6.33x_4}{2.33} = 2$$

$$x_1 = \frac{18 - x_2 - 7x_3 + 2x_4}{3} = 1$$

Example 7 Solve the system:

$$\begin{cases} 2x + y = 3\\ 3x - 2y = 1 \end{cases}$$

Sol.

$$\begin{cases} 2x + y = 3\\ 3x - 2y = 1 \end{cases}$$

The extended matrix is

$$\begin{bmatrix}
 2 & 1 & | & 3 \\
 3 & -2 & | & 1
 \end{bmatrix}$$

and the pivot is 3. We interchange the lines:

$$\left[\begin{array}{ccc|c}
3 & -2 & | & 1 \\
2 & 1 & | & 3
\end{array}\right]$$

We have $L_2 - \frac{2}{3}L_1 \rightarrow L_2$ and obtain

$$\begin{bmatrix}
3 & -2 & | & 1 \\
0 & \frac{7}{3} & | & \frac{7}{3}
\end{bmatrix}$$

so the system becames

$$\begin{cases} 3x - 2y = 1 \\ \frac{7}{3}y = \frac{7}{3} \end{cases}.$$

Solution is

$$\begin{cases} x = 1 \\ y = 1 \end{cases}.$$

Example 8 Solve the system:

$$\begin{cases} x_1 + x_2 + x_3 = 4 \\ 2x_1 - 2x_2 + 3x_3 = 5 \\ x_1 - x_2 + 4x_3 = 5. \end{cases}$$

4.2.2. Gauss-Jordan method ("total elimination" method)

Consider the linear system Ax = b, i.e.,

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}. \tag{4}$$

We make transformations, like in Gauss elimination method, to make zeroes in the lines i+1, i+2,...,n and then, also in the lines 1, 2, ..., i-1 such that the system to be reducing to:

$$\begin{pmatrix} a_{11}^{1} & 0 & \dots & 0 \\ 0 & a_{22}^{2} & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & a_{nn}^{n} \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \\ \vdots \\ x_{n} \end{pmatrix} = \begin{pmatrix} b_{1}^{1} \\ b_{2}^{2} \\ b_{3}^{3} \\ \vdots \\ b_{n}^{n} \end{pmatrix}.$$

The solution is obtained by

$$x_i = \frac{b_i^i}{a_{ii}^i}, \quad i = 1, ..., n.$$

4.2.3. Factorization methods - LU methods

Definition 9 A $n \times n$ matrix A is strictly diagonally dominant if

$$|a_{ii}| > \sum_{j=1, j \neq i}^{n} |a_{ij}|, \text{ for } i = 1, 2, ..., n.$$

Theorem 10 If A is a strictly diagonally dominant matrix, then A is nonsingular and moreover, Gaussian elimination can be performed on any linear system Ax = b without row or column interchanges, and the computations are stable with respect to the growth of rounding errors.

Theorem 11 If A is strictly diagonally dominat then it can be factored into the product of a lower triangular matrix L and an upper triangular matrix U, namely A = LU.

If conditions of Theorem 10 are fulfilled then

$$Ax = b \iff LUx = b$$

where

$$L = \begin{pmatrix} l_{11} & 0 & \dots & 0 \\ l_{21} & l_{22} & \dots & 0 \\ \vdots & & & & \\ l_{n1} & l_{n2} & \dots & l_{nn} \end{pmatrix} \qquad U = \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & & & & \\ 0 & 0 & \dots & u_{nn} \end{pmatrix}.$$

We solve the systems in two stages:

First stage: Solve Lz = b,

Second stage: Solve Ux = z.

Methods for computing matrices L and U: **Doolittle method** where all diagonal elements of L have to be 1; **Crout method** where all diagonal elements of U have to be 1 and **Choleski method** where $l_{ii} = u_{ii}$ for i = 1, ..., n.

Remark 12 LU factorizations are modified forms of Gauss elimination method.

Doolittle method

We consider that the hypotesis of Theorem 10 is fulfilled, so $a_{kk} \neq 0$, $k = \overline{1, n-1}$. Denote

$$l_{i,k} := \frac{a_{i,k}^{(k-1)}}{a_{k,k}^{(k-1)}}, \quad i = \overline{k+1, n}$$

$$t^{(k)} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ l_{k+1,k} \\ \vdots \\ l_{n,k} \end{bmatrix},$$

having zeros for the first k-th lines, and

$$M_k = I_n - t^{(k)} e_k \in \mathcal{M}_{n \times n}(\mathbb{R})$$
 (5)

$$I_n = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & & & & \\ 0 & 0 & \dots & 1 \end{pmatrix}$$
 is the identity matrix of order n .

 $a_{i,k}^{(0)}$ are elements of A; $a_{i,k}^{(1)}$ are elements of $M_1 \cdot A$; ...; $a_{i,k}^{(k-1)}$ are elements of $M_{k-1} \dots \cdot M_1 \cdot A$.

Definition 13 The matrix M_k is called **Gauss matrix**, the components $l_{i,k}$ are called **Gauss multiplies** and the vector $t^{(k)}$ is **Gauss vector**.

Remark 14 If $A \in \mathcal{M}_{n \times n}(\mathbb{R})$, then the Gauss matrices M_1, \ldots, M_{n-1} can be determined such that

$$U = M_{n-1} \cdot M_{n-2} \dots M_2 \cdot M_1 \cdot A$$

is an upper triangular matrix. Moreover, if we choose

$$L = M_1^{-1} \cdot M_2^{-1} \dots M_{n-1}^{-1}$$

then

$$A = L \cdot U$$
.

Example 15 Find LU factorization for the matrix

$$A = \left(\begin{array}{cc} 2 & 1 \\ 6 & 8 \end{array}\right).$$

Solve the system $\begin{cases} 2x_1 + x_2 = 3 \\ 6x_1 + 8x_2 = 9 \end{cases}.$

Sol.

$$M_{1} = I_{2} - t^{(1)}e_{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 \\ \frac{6}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 3 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -3 & 1 \end{pmatrix}.$$

We have

$$U = M_1 A = \begin{pmatrix} 1 & 0 \\ -3 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 \\ 6 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 0 & 5 \end{pmatrix}$$

$$L = M_1^{-1} = \left(\begin{array}{cc} 1 & 0 \\ 3 & 1 \end{array}\right).$$

So

$$A = \begin{pmatrix} 2 & 1 \\ 6 & 8 \end{pmatrix} = L \cdot U = \begin{pmatrix} 1 & 0 \\ 3 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 \\ 0 & 5 \end{pmatrix}.$$

We have

$$L \cdot U \cdot x = \begin{pmatrix} 3 \\ 9 \end{pmatrix}$$
$$Ux = z$$

and

$$\begin{pmatrix} 1 & 0 \\ 3 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 9 \end{pmatrix} \Rightarrow z = \begin{pmatrix} 3 \\ 0 \end{pmatrix}$$
$$\begin{pmatrix} 2 & 1 \\ 0 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 0 \end{pmatrix} \Rightarrow x = \begin{pmatrix} 1.5 \\ 0 \end{pmatrix}.$$