Lecture 2 Direct methods for solving linear system

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Outline

Linear system

Necessity

- 1. Computers are good at performing high speed arithmetic operations
- 2. Almost all of the scientific computing problems ends with a solution of a linear system

- Where does the linear system come from?
 - 1. Discretization of ODEs or PDEs
 - 2. Discretization of nonlinear systems
 - 3. Linear programming
 - 4.

Cramer's rule

Cramer's rule

$$\boldsymbol{A} \cdot \boldsymbol{x} = \boldsymbol{b}, \ \ \boldsymbol{A} \in \mathbb{R}^{n \times n}, \ \boldsymbol{x}, \boldsymbol{b} \ \in \mathbb{R}^{n}$$

Case 1. $det(A) \neq 0$, A is nonsingular, then $x_i = \frac{det(A_i)}{det(A)}$, where A_i is the matrix formed by replacing the *i*-th column of A with b.

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Case 2. $det(\mathbf{A}) = 0$, \mathbf{A} is singular, then

- If rank(A, b) = rank(A), infinite solutions;
- If $rank(A, b) \neq rank(A)$, no solution.

Cramer's rule is not suitable for computing (computational efficiency).

Upper triangular system

Upper triangular system

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

where

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

Direct solution by backward substitution

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

Here $\sum_{j=n+1}^{n}$ is defined as 0 when i = n.

Similar strategy holds for other triangular matrices, such as lower, left, right triangular matrices etc.

A simple example

• Order n = 30, Upper triangular matrix

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- ▶ $\boldsymbol{b} = (1, 1, \dots, 1)^T$.
- What is the solution?

Computational efficiency for back substitution

Total number of operations (addition, subtraction, multiplication, division)

$$\sum_{i=n}^{1} \left[2(n - (i+1) + 1) - 1 + 1 + 1 \right] = n^{2}$$

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• Computational efficiency $O(n^2)$.

Outline

Gaussian elimination method

- How to obtain the solution of a general system?
- Idea: Transform the general matrix into upper triangular matrix.
 Step 1: Eliminate the first column.

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Gaussian elimination method

Step 2: Eliminate the second column.

$$\begin{aligned} a_{ij}^{(2)} &\to a_{ij}^{(2)} - \frac{a_{i2}^{(2)}}{a_{22}^{(2)}} a_{2j}^{(2)}, \quad i = 3, \dots, n; \; j = 2, \dots, n \\ & b_i^{(2)} \to b_i^{(2)} - \frac{a_{i2}^{(2)}}{a_{22}^{(2)}} b_2^{(2)}, \quad i = 3, \dots, n \\ \\ a_{11}^{(2)} &= a_{12}^{(2)} & \cdots & a_{1n}^{(2)} & b_1^{(2)} \\ 0 &= a_{22}^{(2)} & \cdots & a_{2n}^{(2)} & b_2^{(2)} \\ 0 &= a_{32}^{(2)} & \cdots & a_{3n}^{(2)} & b_2^{(2)} \\ \vdots &= \vdots & \ddots & \vdots & \vdots \\ 0 &= a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} & b_n^{(2)} \\ \end{aligned} \right) \to \begin{pmatrix} a_{11}^{(3)} &= a_{12}^{(3)} & \cdots & a_{1n}^{(3)} & b_1^{(3)} \\ 0 &= a_{22}^{(3)} & \cdots & a_{3n}^{(3)} & b_2^{(3)} \\ 0 &= 0 & \cdots & a_{3n}^{(3)} & b_3^{(3)} \\ \vdots &= \vdots & \ddots & \vdots & \vdots \\ 0 &= 0 & \cdots & a_{nn}^{(3)} & b_n^{(3)} \\ \end{pmatrix} \end{aligned}$$

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Gaussian elimination method

Step 3: Repeat until the n - 1-th column.

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

$$\begin{pmatrix} a_{11}^{(n-1)} & a_{12}^{(n-1)} & \cdots & a_{1n}^{(n-1)} & b_1^{(n-1)} \\ 0 & a_{22}^{(n-1)} & \cdots & a_{2n}^{(n-1)} & b_1^{(n-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{nn}^{(n-1)} & b_n^{(n-1)} \end{pmatrix} \rightarrow \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} & y_1 \\ 0 & u_{22} & \cdots & u_{2n} & y_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & u_{nn} & y_n \end{pmatrix}$$

Step 4: Backward substitution to obtain x.

$$Ux = y$$

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A simple example

Linear system

Augmented matrix

$$(\boldsymbol{A} \ \boldsymbol{b}) = \left(\begin{array}{rrrr} 1 & 1 & 1 & 6 \\ 2 & 4 & 2 & 16 \\ -1 & 5 & -4 & -3 \end{array}\right)$$

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Gaussian elimination.

Matrix form of Gaussian elimination method

Gaussian elimination is equivalent to the following LU decomposition

A = LU

and the solution of two triangular systems

$$Ly = b$$
, $Ux = y$

$$\boldsymbol{L} = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & 1 \end{pmatrix}, \quad \boldsymbol{U} = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{pmatrix}$$

The entries l_{ij} in matrix L are the same as those ^{a(k)}_{a(k)} in elimination steps, and the upper triangular matrix U is the same as that in Gaussian elimination.

Gaussian elimination algorithm

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• Gaussian elimination algorithm:

for
$$k = 1, \dots, n - 1$$

for $i = k + 1, \dots, n$
 $l_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}$
for $j = k, \dots, n$
 $a_{ij}^{(k+1)} = a_{ij}^{(k)} - l_{ik}a_{kj}^{(k)}$

Computational efficiency of Gaussian elimination

Total number of triangulation

$$\sum_{k=1}^{n-1} \left[2\left((n+1) - k + 1 \right) + 1 \right] (n - (k+1) + 1) = \frac{2}{3}n^3 + O(n^2)$$

Computational efficiency

$$O\left(\frac{2}{3}n^3\right)$$

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Symmetric positive definite (SPD) system

The matrix form of Gaussian elimination for symmetric positive definite tridiagonal system has the following form

$$A = LU$$

and we have $\boldsymbol{U} = \boldsymbol{D}\boldsymbol{L}^T$, where \boldsymbol{D} is a diagonal matrix with $d_{ii} > 0$.

Cholesky factorization for symmetric positive definite tridiagonal system

$$A = LL^T$$

L can be obtained by the following algorithm

l

$$i_{jj} = \frac{1}{l_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} l_{jk} \right), \quad j = 1, \dots, i-1,$$

 $l_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} l_{ik}^2}$

Computational efficiency of Cholesky factorization

Computational efficiency

$$\sum_{i=1}^{n} \left[\sum_{j=1}^{i-1} (2j-1) + (i-1) + (i-1) + 1 \right] = O\left(\frac{1}{3}n^3\right)$$

 The computational cost is a little less than direct Gaussian elimination by symmetry.

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Tridiagonal system

Tridiagonal system

$$A \cdot x = b$$

where

$$oldsymbol{A} = \left(egin{array}{ccccc} d_1 & c_1 & & & \ a_2 & d_2 & \ddots & & \ a_2 & d_2 & \ddots & & \ & \ddots & \ddots & c_{n-1} \ & & a_n & d_n \end{array}
ight).$$

▶ *LU* decomposition of tridiagonal system

$$\boldsymbol{L} = \begin{pmatrix} 1 & & & \\ \beta_2 & 1 & & \\ & \ddots & & \\ & & \ddots & \ddots \\ & & & \beta_n & 1 \end{pmatrix}, \quad \boldsymbol{U} = \begin{pmatrix} \alpha_1 & c_1 & & \\ & \alpha_2 & \ddots & \\ & & \alpha_2 & \ddots & \\ & & & \ddots & c_{n-1} \\ & & & & \alpha_n \end{pmatrix}$$

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Tridiagonal system

Thomas algorithm

$$\alpha_1 = d_1, \quad \beta_i = \frac{a_i}{\alpha_{i-1}}, \quad \alpha_i = d_i - \beta_i c_i, \quad i = 2, \dots, n$$

Computational efficiency

O(n)

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Numerical solution of a linear system

Numerical solution of a BVP

$$u''(x) = f(x), x \in [0,1], u(0) = u(1) = 0.$$

Numerical discretization

Define $h = \frac{1}{N}$, $x_j = jh, f_j = f(x_j), j = 0, 1, ..., N$, and

$$u''(x_j) \approx \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}$$

then the ODE is reduced to a linear system $A \cdot X = b$, where

$$A = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$
$$X = (u_1, u_2, \dots, u_{N-1})^T, \ b = -h^2(f_1, f_2, \dots, f_{N-1})^T.$$

Numerical solution of a linear system

• Take $f(x) = -\pi^2 \sin \pi x$, we have the exact solution

 $u(x) = \sin \pi x.$

- ▶ Take *N* = 50, we have the linear system and solve it with Thomas algorithm.
- Exact solution v.s. numerical solution



An example

• Linear system Ax = b with

$$\boldsymbol{A} = \left(\begin{array}{rrr} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \end{array} \right), \quad \boldsymbol{b} = \left(\begin{array}{r} 1 \\ 2 \\ 1 \end{array} \right).$$

Gaussian elimination

$$\left(\begin{array}{rrrr} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \end{array}\right) \to \left(\begin{array}{rrrr} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{array}\right)$$

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Even A is nonsingular, Gaussian elimination may NOT be proceeded directly.

Another example

• Linear system Ax = b with

$$\boldsymbol{A} = \left(\begin{array}{rrr} 1 & 1 & 1 \\ 1 & 1.0001 & 2 \\ 1 & 2 & 2 \end{array} \right), \quad \boldsymbol{b} = \left(\begin{array}{r} 1 \\ 2 \\ 1 \end{array} \right).$$

Gaussian elimination

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1.0001 & 2 & 2 \\ 1 & 2 & 2 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 0.0001 & 1 & 1 \\ 0 & 0 & 9999 & 10000 \end{pmatrix}$$

- ▶ If the precision t = 3, we will have x̄ = (0,0,1.000). But the roundoff exact solution is x = (1.000, -1.0001, 1.0001). It is totally different!
- Even direct Gaussian elimination could be applied, the result may be very bad!
- We need pivoting technique.

Outline

Pivoting

- What is pivoting?
- Complete pivoting is to let the largest element of the submatrix lie on the diagonal by interchanging rows or columns. A partial pivoting (or column pivoting) is to let the largest element in one column lie on the diagonal by interchanging two rows.

The partial pivoting is more used.

Pivoting

 Example 1: Complete pivoting (move 3 — the largest one among the matrix — to a₁₁)

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 2 & 2 & 3 \end{pmatrix} \rightarrow \begin{pmatrix} 2 & 2 & 3 \\ 1 & 1 & 2 \\ 1 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 3 & 2 & 2 \\ 2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

Example 2: partial pivoting (move 2 — the largest one among the first column — to a₁₁)

$$\left(\begin{array}{rrrr} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 2 & 2 & 3 \end{array}\right) \rightarrow \left(\begin{array}{rrrr} 2 & 2 & 3 \\ 1 & 1 & 2 \\ 1 & 1 & 1 \end{array}\right)$$

Pivoting

Pivoting

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

Pivoting

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1.0001 & 2 & 2 \\ 1 & 2 & 2 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 0.0001 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0.9999 & 1 \end{pmatrix}$$

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The numerical solution will be x = (1, -1, 1).

Matrix form for pivoting

Matrix form for pivoting by row

$$PA = LU$$

where \boldsymbol{P} is a permutation matrix.

Pivoting by row makes the computation more robust and stable.

Outline

Vector norms

Define $oldsymbol{x} = (x_1, x_2, \dots, x_n)$,

Vector norms (definition of length)

$$\begin{array}{ll} 2-\operatorname{norm} & \|\boldsymbol{x}\|_2 = (\sum_{i=1}^n x_i^2)^{\frac{1}{2}} & \operatorname{Euclidean \ norm} \\ \infty - \operatorname{norm} & \|\boldsymbol{x}\|_{\infty} = \max_i |x_i| \\ 1 - \operatorname{norm} & \|\boldsymbol{x}\|_1 = \sum_{i=1}^n |x_i| \\ p - \operatorname{norm} & \|\boldsymbol{x}\|_p = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}} \end{array}$$

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Properties of vector norms

1.
$$\|x\| \ge 0$$
 and $\|x\| = 0$ iff $x = 0$,
2. $\|kx\| = |k| \cdot \|x\|$,

3. $\|x+y\| \le \|x\| + \|y\|$ (Triangle inequality).

Matrix norms

Define $A = (a_{ij})_{n \times n}$

Matrix norm

Induced norm (subordinate norm)

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

From the definition of vector norms, we have

$$2 - \operatorname{norm} \qquad \|\boldsymbol{A}\|_{2} = \sqrt{\lambda_{\max}(\boldsymbol{A}^{T}\boldsymbol{A})} \ (= \sigma_{\max})$$
$$\infty - \operatorname{norm} \qquad \|\boldsymbol{A}\|_{\infty} = \max_{i} \sum_{j=1}^{n} |a_{ij}|$$
$$1 - \operatorname{norm} \qquad \|\boldsymbol{A}\|_{1} = \max_{j} \sum_{i=1}^{n} |a_{ij}|$$

Frobenius norm (why is it NOT an induced norm?)

$$\|\mathbf{A}\|_F = (\sum_{i,j=1}^n a_{ij}^2)^{\frac{1}{2}}$$

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Properties of induced matrix norms

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Properties of induced matrix norms:

1.
$$\|\boldsymbol{A}\| \ge 0$$
 and $\|\boldsymbol{A}\| = 0$ iff $\boldsymbol{A} = 0$

2.
$$||kA|| = |k| \cdot ||A||$$
,

- 3. $\|A + B\| \le \|A\| + \|B\|$ (Triangle inequality),
- 4. $||AB|| \le ||A|| \cdot ||B||$,
- 5. $||Ax|| \leq ||A|| \cdot ||x||.$

Stability for the solution of linear system

Example

$$\boldsymbol{A} = \left(\begin{array}{cc} 2.0002 & 1.9998\\ 1.9998 & 2.0002 \end{array}\right), \quad \boldsymbol{b} = \left(\begin{array}{c} 4\\ 4 \end{array}\right)$$

The exact solution

$$x = (1, 1)^T$$

• Add perturbation $\delta \boldsymbol{b} = (0.0002, -0.0002)^T$ to \boldsymbol{b} , i.e. we have

$$\tilde{\boldsymbol{b}} = (4.0002, 3.9998)^T$$

The perturbed solution

$$\tilde{\boldsymbol{x}} = (1.5, 0.5)^T$$

 \blacktriangleright Relative error for solution and perturbation in $\infty\text{-norm}$

$$\frac{\|\tilde{\boldsymbol{x}} - \boldsymbol{x}\|_{\infty}}{\|\boldsymbol{x}\|_{\infty}} = \frac{1}{2}, \quad \frac{\|\tilde{\boldsymbol{b}} - \boldsymbol{b}\|_{\infty}}{\|\boldsymbol{b}\|_{\infty}} = \frac{1}{20000}$$

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The relative error is amplified 10000 times!!!

Condition number

Condition number

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

For l^2 -norm we have

$$Cond_2(\mathbf{A}) = \|\mathbf{A}\|_2 \cdot \|\mathbf{A}^{-1}\|_2$$

If A is symmetric, we have

$$Cond_2(\boldsymbol{A}) = rac{\lambda_{\max}(\boldsymbol{A})}{\lambda_{\min}(\boldsymbol{A})}.$$

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Remark 1: $Cond(\mathbf{A}) \ge 1$. Remark 2: If $det(\mathbf{A}) \approx 0$, $Cond(\mathbf{A}) \gg 1$.

High condition number matrix — Hilbert Matrix

• Hilbert matrix $H_n = (h_{ij})_{i,j=1}^n$ is defined as

$$h_{ij} = \frac{1}{i+j-1}$$

- Hilbert matrix is a Symmetric Positive Definite (SPD) matrix
- Determinant of H_n
- $n \quad \det(H_n)$ 1 1
 2 8.33333 × 10⁻²
 3 4.62963 × 10⁻⁴
 4 1.65344 × 10⁻⁷
 5 3.74930 × 10⁻¹²
 6 5.36730 × 10⁻¹⁸

• $Cond_2(H_5) \sim O(10^5).$

Explanation of condition number

Original problem Ax = b;
 Perturbed problem A(x + δx) = b + δb;
 Subtracting two equations we have

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

Take norm we have

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

With condition

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

we have

Condition number

- Condition number characterize the stability If Cond(A) ≫ 1, stability is very bad; If Cond(A) ~ 1, stability is good.
- Lesson we should learn:

We should avoid handle the bad condition number problem in applications!

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Stability

Loosely speaking, stability is to indicate how sensitive the solution of a problem may be to small relative changes in the input data. It is often quantized by condition number of a problem or an algorithm.

- Stability of the original problem ("Well-posedness") This means the well-posedness of the original problem. The linear system with high condition number is a typical ill-posed example, which is called the unstable problem.
- Stability of numerical algorithm

This means the condition of the algorithm. The Gaussian elimination without pivoting for some linear system will be unstable.

Homework assignment 2

- 1. Using Thomas algorithm to solve the second order ODEs with one language (except matlab) (n=30, 50, 100). Compare the numerical solution with exact solution.
- 2. Compute 2-, 1- and ∞ -condition number of n by n symmetric tridiagonal matrix

$$A_n = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix}$$

versus n with matlab and plot it as a figure.