MA 3021: Numerical Analysis I Direct and Iterative Methods for Solving Linear Systems



Suh-Yuh Yang (楊肅煜)

Department of Mathematics, National Central University Jhongli District, Taoyuan City 32001, Taiwan

syyang@math.ncu.edu.tw http://www.math.ncu.edu.tw/~syyang/

A system of linear equations

We are interested in solving systems of linear equations having the form:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n = b_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \dots + a_{3n}x_n = b_3$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n = b_n$$

This is a system of *n* equations in the *n* unknowns, x_1, x_2, \dots, x_n . The elements a_{ij} and b_i are assumed to be prescribed real numbers.

Ax = b

We can rewrite this system of linear equations in a matrix form:

<i>a</i> ₁₁	<i>a</i> ₁₂	<i>a</i> ₁₃	•••	a_{1n}		<i>x</i> ₁		b_1	
<i>a</i> ₂₁	a ₂₂	a ₂₃	• • •	a_{2n}		<i>x</i> ₂		b_2	
<i>a</i> ₃₁	<i>a</i> ₃₂	a ₃₃	• • •	a _{3n}		<i>x</i> ₃	=	b_3	
÷	÷	÷	γ_{i_1}	÷		÷		÷	
<i>a</i> _{n1}	a_{n2}	a_{n3}	•••	a _{nn}		<i>x</i> _{<i>n</i>}		b_n	

We can denote these matrices by *A*, *x*, and *b*, giving the simpler equation:

Ax = b.

Matrix

A matrix is a rectangular array of numbers such as

 $\begin{bmatrix} 3.0 & 1.1 & -0.12 \\ 6.2 & 0.0 & 0.15 \\ 0.6 & -4.0 & 1.3 \\ 9.3 & 2.1 & 8.2 \end{bmatrix}, \begin{bmatrix} 3 & 6 & \frac{11}{7} & -17 \end{bmatrix}, \begin{bmatrix} 3.2 \\ -4.7 \\ 0.11 \end{bmatrix}.$ $4 \times 3 \text{ matrix} \qquad 1 \times 4 \text{ matrix} \qquad 3 \times 1 \text{ matrix} \\ a \text{ row vector} \qquad a \text{ column vector}$

Matrix properties

- If A is a matrix, the notation a_{ij}, (A)_{ij}, or A(i, j) is used to denote the element at the intersection of the *i*th row and the *j*th column. For example, let A be the first matrix on the previous slide. Then a₃₂ = A₃₂ = A(3, 2) = −4.0.
- ② The transpose of a matrix is denoted by A^{\top} and is the matrix defined by $(A^{\top})_{ij} = a_{ji}$. If a matrix *A* has the property $A = A^{\top}$, we say that *A* is symmetric.
- The $n \times n$ matrix

$$I := I_n := I_{n \times n} := \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

is called an identity matrix. Note that IA = A = AI for any $n \times n$ matrix A.

Algebraic operations

- Scalar * Matrix: If A is a matrix and λ is a scalar, then λA is defined by $(\lambda A)_{ij} = \lambda a_{ij}$.
- 2 *Matrix* + *Matrix:* If $A = (a_{ij})$ and $B = (b_{ij})$ are $m \times n$ matrices, then A + B is defined by $(A + B)_{ij} = a_{ij} + b_{ij}$.
- So *Matrix* * *Matrix:* If *A* is an $m \times p$ matrix and *B* is a $p \times n$ matrix, then *AB* is an $m \times n$ matrix defined by:

$$(AB)_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj}, \qquad 1 \le i \le m, \ 1 \le j \le n.$$

What is the cost of *AB*?

Answer: *mnp* multiplications and mn(p-1) additions.

Right inverse and left inverse

If *A* and *B* are two matrices such that AB = I, then we say that *B* is a right inverse of *A* and that *A* is a left inverse of *B*. For example,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ \alpha & \beta \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I_{2\times 2}, \quad \forall \alpha, \beta \in \mathbb{R}.$$
$$\begin{bmatrix} 1 & 0 \\ 0 & 1 & \beta \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I_{2\times 2}, \quad \forall \alpha, \beta \in \mathbb{R}.$$

Notice that right inverse and left inverse may not unique.

Theorem: A square matrix can possess at most one right inverse. *Proof:* Let AB = I. Then $\sum_{j=1}^{n} b_{jk}A^{(j)} = I^{(k)}$, $1 \le k \le n$. So, the columns of A form a

basis for \mathbb{R}^n . Therefore, the coefficients b_{jk} above are uniquely determined.

2 Theorem: If *A* and *B* are square matrices such that AB = I, then BA = I.

Proof: Let C = BA - I + B. Then AC = ABA - AI + AB = A - A + I = I. Since right inverse for square matrix is at most one, B = C. Hence, C = BA - I + B = BA - I + C, i.e., BA = I.

Inverse

• If a square matrix *A* has a right inverse *B*, then *B* is unique and BA = AB = I. We then call *B* the inverse of *A* and say that *A* is invertible or nonsingular. We denote $B = A^{-1}$.

2 Example:

$$\begin{bmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I_{2 \times 2}.$$

- If A is invertible, then the system of equations Ax = b has the solution x = A⁻¹b. If A⁻¹ is not available, then in general, A⁻¹ should not be computed solely for the purpose of obtaining x.
- How do we get this A^{-1} ?

Equivalent systems

Let two linear systems be given, each consisting of *n* equations with *n* unknowns:

Ax = b and Bx = d.

If the two systems have precisely the same solutions, we call them equivalent systems.

- 2 Note that *A* and *B* can be very different.
- Thus, to solve a linear system of equations, we can instead solve any equivalent system. This simple idea is at the heart of our numerical procedures.

Elementary operations

- Let *E_i* denote the *i*-th equation in the system *Ax* = *b*. The following are the elementary operations which can be performed:
 - Interchanging two equations in the system: $\mathcal{E}_i \leftrightarrow \mathcal{E}_j$;
 - Multiplying an equation by a nonzero number: $\lambda \mathcal{E}_i \rightarrow \mathcal{E}_i$;
 - Adding to an equation a multiple of some other equation:
 E_i + λ*E_j* → *E_i*.
- Theorem on equivalent systems: If one system of equations is obtained from another by a finite sequence of elementary operations, then the two systems are equivalent.

Elementary operations (cont'd)

- An elementary matrix is defined to be an n × n matrix that arises when an elementary operation is applied to the n × n identity matrix.
- 2 Let A_i be the *i*-th row of matrix A. The elementary operations expressed in terms of the rows of matrix A are:
 - The interchange of two rows in $A: A_i \leftrightarrow A_j$;
 - Multiplying one row by a nonzero constant: $\lambda A_i \rightarrow A_i$;
 - Adding to one row a multiple of another: $A_i + \lambda A_j \rightarrow A_i$.
- So Each elementary row operation on *A* can be accomplished by multiplying *A* on the left by an elementary matrix.

Examples

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \\ a_{21} & a_{22} & a_{23} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ \lambda a_{21} & \lambda a_{22} & \lambda a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ \lambda a_{21} & \lambda a_{22} & \lambda a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{21} & a_{22} & a_{23} \\ \lambda a_{21} + a_{31} & \lambda a_{22} + a_{32} & \lambda a_{23} + a_{33} \end{bmatrix}$$

Invertible matrix

If matrix A is invertible, then there exists a sequence of elementary row operations can be applied to A, reducing it to I,

 $E_m E_{m-1} \cdots E_2 E_1 A = I.$

② This gives us an equation for computing the inverse of a matrix:

 $A^{-1} = E_m E_{m-1} \cdots E_2 E_1 = E_m E_{m-1} \cdots E_2 E_1 I.$

Remark: This is not a practical method to compute A^{-1} .

Eigenvalue and eigenvector

Let $A \in \mathbb{C}^{n \times n}$ be a square matrix. If there exists a nonzero vector $x \in \mathbb{C}^n$ and a scalar $\lambda \in \mathbb{C}$ such that

 $Ax = \lambda x$,

then λ is called an eigenvalue of A and x is called the corresponding eigenvector of A.

Remark: Computing λ and x is a major task in numerical linear algebra.

Theorem on nonsingular matrix properties

For an $n \times n$ real matrix A, the following properties are equivalent:

- The inverse of A exists; that is, A is nonsingular
- 2 The determinant of A is nonzero
- The rows of *A* form a basis for \mathbb{R}^n
- The columns of *A* form a basis for \mathbb{R}^n
- Solution As a map from \mathbb{R}^n to \mathbb{R}^n , *A* is injective (one to one)
- As a map from \mathbb{R}^n to \mathbb{R}^n , *A* is surjective (onto)
- O The equation Ax = 0 implies x = 0
- So For each $b \in \mathbb{R}^n$, there is exactly one $x \in \mathbb{R}^n$ such that Ax = b
- A is a product of elementary matrices
- 0 is not an eigenvalue of *A*

Some easy-to-solve systems:

1. Diagonal Structure

$$\begin{bmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ 0 & a_{22} & 0 & \cdots & 0 \\ 0 & 0 & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

The solution is: (provided $a_{ii} \neq 0$ for all $i = 1, 2, \cdots, n$)

$$x = \left(\frac{b_1}{a_{11}}, \frac{b_2}{a_{22}}, \frac{b_3}{a_{33}}, \cdots, \frac{b_n}{a_{nn}}\right)^\top.$$

- If $a_{ii} = 0$ for some index *i*, and if $b_i = 0$ also, then x_i can be any real number. The number of solutions is infinity.
- If $a_{ii} = 0$ and $b_i \neq 0$, no solution of the system exists.
- What is the complexity of the method? *n* divisions.

2. Lower Triangular Systems

$$\begin{bmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & 0 & \cdots & 0 \\ a_{31} & a_{32} & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}.$$

Some simple observations:

• If $a_{11} \neq 0$, then we have $x_1 = b_1/a_{11}$.

 Once we have x₁, we can simplify the second equation, x₂ = (b₂ − a₂₁x₁)/a₂₂, provided that a₂₂ ≠ 0.
 Similarly, x₃ = (b₃ − a₃₁x₁ − a₃₂x₂)/a₃₃, provided that a₃₃ ≠ 0.
 In general, to find the solution to this system, we use forward substitution (assume that a_{ii} ≠ 0 for all *i*).

2. Lower Triangular Systems (cont'd)

• Algorithm of forward substitution:

input
$$n$$
, (a_{ij}) , $b = (b_1, b_2, \cdots, b_n)^{\top}$
for $i = 1$ to n do
 $x_i \leftarrow \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j\right) / a_{ii}$

end do

output
$$x = (x_1, x_2, \cdots, x_n)^\top$$

- Complexity of forward substitution:
 - *n* divisions.
 - the number of multiplications: 0 for x_1 , 1 for x_2 , 2 for x_3 , \cdots total = 0 + 1 + 2 + \cdots + $(n 1) \approx (n + 1)n/2 = O(n^2)$.
 - the number of subtractions: same as the number of multiplications = $O(n^2)$.

Forward substitution is an $O(n^2)$ algorithm.

• **Remark:** forward substitution is a sequential algorithm (not parallel at all).

3. Upper Triangular Systems

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ 0 & 0 & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}.$$

The formal algorithm to solve for *x* is called backward substitution. It is also an $O(n^2)$ algorithm. Assume that $a_{ii} \neq 0$ for all *i*:

Т

input
$$n$$
, (a_{ij}) , $b = (b_1, b_2, \cdots, b_n)$
for $i = n : -1 : 1$ do
 $x_i \leftarrow (b_i - \sum_{j=i+1}^n a_{ij} x_j) / a_{ii}$

end do output $x = (x_1, x_2, \cdots, x_n)^\top$

LU decomposition (factorization)

Suppose that *A* can be factored into the product of a lower triangular matrix *L* and an upper triangular matrix *U*:

A = LU.

Then, Ax = LUx = L(Ux). Thus, to solve the system of equations Ax = b, it is enough to solve this problem in two stages:

Lz = b solve for z, Ux = z solve for x.

Basic Gaussian elimination

Let $A^{(1)} = (a_{ij}^{(1)}) = A = (a_{ij})$ and $b^{(1)} = b$. Consider the following linear system Ax = b:

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 34 \\ 27 \\ -38 \end{bmatrix}$$

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.

pivot row = row1.
pivot element:
$$a_{11}^{(1)} = 6$$
.
row2 - $(12/6)$ *row1 \rightarrow row2.
row3 - $(3/6)$ *row1 \rightarrow row3.
row4 - $(-6/6)$ *row1 \rightarrow row4.

$$\implies \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & -12 & 8 & 1 \\ 0 & 2 & 3 & -14 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ 21 \\ -26 \end{bmatrix}$$

multipliers: 12/6, 3/6, (-6)/6

Basic Gaussian elimination (cont'd)

We have the following equivalent system $A^{(2)}x = b^{(2)}$:

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & -12 & 8 & 1 \\ 0 & 2 & 3 & -14 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ 21 \\ -26 \end{bmatrix}$$

.

pivot row = row2.

pivot element
$$a_{22}^{(2)} = -4$$
.
row3 - (-12/-4)*row2 → row3.
row4 - (2/-4)*row2 → row4.

$$\implies \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 4 & -13 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ -9 \\ -21 \end{bmatrix}.$$

Itiplier: $(-12)/(-4), 2/(-4)$

multip

Basic Gaussian elimination (cont'd)

We have the following equivalent system $A^{(3)}x = b^{(3)}$:

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 4 & -13 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ -9 \\ -21 \end{bmatrix}$$

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pivot row = row3.

pivot element
$$a_{33}^{(3)} = 2$$
.
row4 - (4/2)*row3 \rightarrow row4

$$\implies \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ -9 \\ -3 \end{bmatrix}$$

multiplier: 4/2

Basic Gaussian elimination (cont'd)

Finally, we have the following equivalent upper triangular system $A^{(4)}x = b^{(4)}$:

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ -9 \\ -3 \end{bmatrix}$$

Using the backward substitution, we have

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ -3 \\ -2 \\ 1 \end{bmatrix}$$

The LU decomposition

Display the multipliers in an unit lower triangular matrix $L = (\ell_{ij})$:

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

Let $U = (u_{ij})$ be the final upper triangular matrix $A^{(4)}$. Then we have

$$U = \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix}$$

and one can check that A = LU (the Doolittle Decomposition).

Some remarks

- The entire elimination process will break down if any of the pivot elements are 0.
- **2** The total number of arithmetic operations:

$$M/D = \frac{n^3}{3} + n^2 - \frac{n}{3}$$
$$A/S = \frac{n^3}{3} + \frac{n^2}{2} - \frac{5n}{6}$$

 \therefore The GE is an $O(n^3)$ algorithm.

Vector norm

A vector norm on \mathbb{R}^n is a real-valued function $\|\cdot\| : \mathbb{R}^n \to \mathbb{R}$ with the properties:

() $||x|| \ge 0$, $\forall x \in \mathbb{R}^n$, and ||x|| = 0 if and only if x = 0;

2
$$||\alpha x|| = |\alpha|||x||, \forall x \in \mathbb{R}^n \text{ and } \alpha \in \mathbb{R};$$

◎ $||x + y|| \le ||x|| + ||y||, \forall x, y \in \mathbb{R}^n$ (the triangle inequality).

Note: ||x|| is called the norm of *x*, the length or magnitude of *x*.

Some vector norms on \mathbb{R}^n and distance

• Let
$$x = (x_1, x_2, \cdots, x_n)^\top \in \mathbb{R}^n$$
:

- The 2-norm (Euclidean norm, or ℓ^2 norm): $||x||_2 = \sqrt{\sum_{i=1}^n x_i^2}$
- The infinity norm (ℓ^{∞} -norm): $||x||_{\infty} = \max_{1 \le i \le n} |x_i|$
- The 1-norm $(\ell^1$ -norm): $||x||_1 = \sum_{i=1}^n |x_i|$

2 Let
$$x = (x_1, x_2, \cdots, x_n)^\top$$
, $y = (y_1, y_2, \cdots, y_n)^\top \in \mathbb{R}^n$. Then
• $||x - y||_2 = \sqrt{\sum_{i=1}^n (x_i - y_i)^2}$
• $||x - y||_{\infty} = \max_{1 \le i \le n} |x_i - y_i|$
• $||x - y||_1 = \sum_{i=1}^n |x_i - y_i|$

The difference between the above norms

- What is the unit ball $\{x \in \mathbb{R}^2 : ||x|| \le 1\}$ for the three norms above?
 - 2-norm: a circle
 - ∞-norm: a square
 - 1-norm: a diamond

Example: Let *x* = (−1, 1, −2)^T ∈ ℝ³. Then
$$\|x\|_{2} = \sqrt{(-1)^{2} + 1^{2} + (-2)^{2}} = \sqrt{6},$$

$$\|x\|_{\infty} = \max_{1 \le i \le 3} |x_{i}| = \max\{|-1|, |1|, |-2|\} = 2,$$

$$\|x\|_{1} = \sum_{i=1}^{3} |x_{i}| = |-1| + |1| + |-2| = 4.$$

Solution Cauchy-Buniakowsky-Schwarz inequality: For $x = (x_1, x_2, \cdots, x_n)^\top, y = (y_1, y_2, \cdots, y_n)^\top \in \mathbb{R}^n$, we have $\sum_{i=1}^n |x_i y_i| \le \left(\sum_{i=1}^n x_i^2\right)^{1/2} \left(\sum_{i=1}^n y_i^2\right)^{1/2} = ||x||_2 ||y||_2.$

Convergence of sequences in \mathbb{R}^n

- **Definition:** Let $x, x^{(k)} \in \mathbb{R}^n$ for $k = 1, 2, \cdots$. Then $\lim_{k \to \infty} x^{(k)} = x$ with respect to the norm $\|\cdot\| \iff$ $\forall \varepsilon > 0, \exists$ an integer $N(\varepsilon) > 0$ such that if $k \ge N(\varepsilon)$ then $\|x^{(k)} - x\| < \varepsilon$.
- $\lim_{k \to \infty} x^{(k)} = x \text{ with respect to } \| \cdot \|_{\infty} \iff \lim_{k \to \infty} x_i^{(k)} = x_i \text{ for } i = 1, 2, \cdots, n.$
- **Solution Example:** $x^{(k)} = (x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, x_4^{(k)})^\top = (1, 2 + \frac{1}{k}, \frac{3}{k^2}, e^{-k} \sin(k))^\top.$ $\therefore \lim_{k \to \infty} 1 = 1, \lim_{k \to \infty} (2 + \frac{1}{k}) = 2, \lim_{k \to \infty} \frac{3}{k^2} = 0, \lim_{k \to \infty} e^{-k} \sin(k) = 0.$ $\therefore \lim_{k \to \infty} x^{(k)} = x = (1, 2, 0, 0)^\top \text{ with respect to } \|\cdot\|_{\infty} \text{ norm.}$

All vector norms on \mathbb{R}^n are equivalent

• For each $x \in \mathbb{R}^n$, $||x||_{\infty} \le ||x||_2 \le \sqrt{n} ||x||_{\infty}$.

Proof: Let $|x_j| = ||x||_{\infty}$. Then

$$||x||_{\infty}^{2} = |x_{j}|^{2} = x_{j}^{2} \le \sum_{i=1}^{n} x_{i}^{2} = ||x||_{2}^{2} \le \sum_{i=1}^{n} x_{j}^{2} = nx_{j}^{2} = n||x||_{\infty}^{2}.$$

2 In fact, all vector norms on \mathbb{R}^n are equivalent!

Matrix norm

Let *A* be an $n \times n$ real matrix. If $\|\cdot\|$ is any vector norm on \mathbb{R}^n , then

$$||A|| := \max\{||Ax|| : x \in \mathbb{R}^n, ||x|| = 1\}$$

$$\iff ||A|| := \max\{\frac{||Ax||}{||x||} : x \in \mathbb{R}^n, x \neq 0\}$$

defines a norm on the vector space of all $n \times n$ real matrices. (This is called the matrix norm associated with the given vector norm)

Proof:

$$\|A + B\| = \max\{\|(A + B)x\| : \|x\| = 1\} \le \max\{\|Ax\| + \|Bx\| : \|x\| = 1\} \\ \le \max\{\|Ax\| : \|x\| = 1\} + \max\{\|Bx\| : \|x\| = 1\} = \|A\| + \|B\|.$$

Some additional properties

Some matrix norms

Let $A_{n \times n} = (a_{ij})$ be an $n \times n$ real matrix. Then The ∞ -matrix norm:

$$||A||_{\infty} = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$$

2 The 1-matrix norm:

$$||A||_1 = \max_{1 \le j \le n} \sum_{i=1}^n |a_{ij}|$$

• The 2-matrix norm (ℓ^2 -matrix norm):

 $||A||_2 = \max_{||x||_2 = 1} ||Ax||_2$

Example

We consider the matrix

$$A = \left[\begin{array}{rrrr} 1 & 0 & 2 \\ 0 & 1 & -1 \\ -1 & 1 & 1 \end{array} \right]$$

• The characteristic polynomial $p(\lambda)$ of A is given by

$$p(\lambda) = \det(A - \lambda I)$$

= $(1 - \lambda)\{(1 - \lambda)^2 + 1\} + (-1)\{-2(1 - \lambda)\}$
= $(1 - \lambda)\{\lambda^2 - 2\lambda + 4\}.$

The eigenvalues of *A* are $\lambda_1 = 1$, $\lambda_2 = 1 + \sqrt{3}i$ and $\lambda_3 = 1 - \sqrt{3}i$.

• The spectral radius $\rho(A)$ of matrix *A* is defined by

 $\rho(A) = \max\{|\lambda|: \lambda \text{ is an eigenvalue of } A\}.$

For matrix *A*, we have $\rho(A) = \max\{|1|, |1 + \sqrt{3}i|, |1 - \sqrt{3}i|\} = 2$.

The 2-matrix norm

- $||A||_2$ is not easy to compute.
- Since $A^{\top}A$ is symmetric, $A^{\top}A$ has *n* real eigenvalues, $\lambda_1, \lambda_2, \dots, \lambda_n \in \mathbb{R}$. Moreover, one can prove that they are all nonnegative. Then

$$\rho(A^{\top}A) := \max_{1 \le i \le n} \{\lambda_i\} \ge 0.$$

is called the spectral radius of $A^{\top}A$.

③ Then the ℓ^2 -matrix norm of *A* is given by

$$\|A\|_2 = \sqrt{\rho(A^\top A)}.$$

The ℓ^2 -matrix norm is also called the spectral norm.

Properties of matrix norm

Let *A* be an $n \times n$ real matrix. Then

- Then the ℓ^2 -matrix norm of *A* is given by $||A||_2 = \sqrt{\rho(A^{\top}A)}$. The ℓ^2 -matrix norm is also called the spectral norm.
- 2 $\rho(A) \leq ||A||$ for any matrix norm $|| \cdot ||$.

Proof: Suppose that λ is an eigenvalue of A with eigenvector x and ||x|| = 1.

$$\implies |\lambda| = |\lambda| ||x|| = ||\lambda x|| = ||Ax|| \le ||A|| ||x|| = ||A||$$
$$\implies \rho(A) = \max |\lambda| \le ||A||$$

■ For any *n* × *n* matrix *A* and any ε > 0, ∃ a matrix norm $\|\cdot\|$ such that $ρ(A) \le \|A\| \le ρ(A) + ε$.

Example

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

$$A^{\top}A = \begin{bmatrix} 1 & 1 & -1 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ -1 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 2 & -1 \\ 2 & 6 & 4 \\ -1 & 4 & 5 \end{bmatrix}$$

$$\det(A^{\top}A - \lambda I) = \det\begin{bmatrix} 3 - \lambda & 2 & -1 \\ 2 & 6 - \lambda & 4 \\ -1 & 4 & 5 - \lambda \end{bmatrix} = -\lambda(\lambda^2 - 14\lambda + 42)$$

$$\Longrightarrow \lambda = 0, 7 + \sqrt{7}, 7 - \sqrt{7}$$

$$\Longrightarrow ||A||_2 = \sqrt{\rho(A^{\top}A)} = \sqrt{7 + \sqrt{7}} \approx 3.106$$

Convergence

Definition: An $n \times n$ matrix A is said to be convergent (to zero matrix) if $\lim_{k \to \infty} (A^k)_{ij} = 0$ for $i, j = 1, 2, \dots, n$.

2 Example:

$$A = \begin{bmatrix} \frac{1}{2} & 0\\ \frac{1}{4} & \frac{1}{2} \end{bmatrix} \Longrightarrow A^2 = \begin{bmatrix} \frac{1}{4} & 0\\ \frac{1}{4} & \frac{1}{4} \end{bmatrix} \Longrightarrow A^3 = \begin{bmatrix} \frac{1}{8} & 0\\ \frac{3}{16} & \frac{1}{8} \end{bmatrix} \Longrightarrow \cdots$$
$$A^k = \begin{bmatrix} (\frac{1}{2})^k & 0\\ \frac{k}{2^{k+1}} & (\frac{1}{2})^k \end{bmatrix}, \quad \lim_{k \to \infty} (\frac{1}{2})^k = 0, \quad \lim_{k \to \infty} \frac{k}{2^{k+1}} = 0.$$

 $\therefore A$ is a convergent matrix

Equivalent statements

The following statements are equivalent:

- A is a convergent matrix
- ② $\lim_{n \to \infty} ||A^n|| = 0$ for some natural matrix norm
- ◎ $\lim_{n\to\infty} ||A^n|| = 0$ for all natural matrix norms
- $\textcircled{0} \rho(A) < 1$
- $\lim_{n \to \infty} A^n x = 0 \text{ for all } x$

Iterative methods

- Basic idea: $Ax = b \implies x = Tx + c$ for some fixed matrix *T* and vector *c*
- 2 Given $x^{(0)}, x^{(k)} := Tx^{(k-1)} + c$ for $k = 1, 2, \cdots$
- Onsider a linear system:

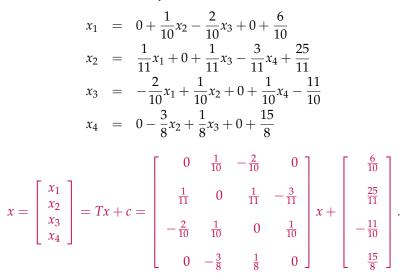
$$10x_1 - x_2 + 2x_3 + 0 = 6$$

-x₁ + 11x₂ - x₃ + 3x₄ = 25
2x₁ - x₂ + 10x₃ - x₄ = -11
0 + 3x₂ - x₃ + 8x₄ = 15

Exact unique solution: $x = (1, 2, -1, 1)^{\top}$

The Jacobi iterative method

We first rewrite the linear system as



The Jacobi iterative method (cont'd)

If $x^{(0)} = (0, 0, 0, 0)^{\top}$, then $x^{(1)} = Tx^{(0)} + c = \begin{bmatrix} \frac{6}{10} \\ \frac{25}{11} \\ -\frac{11}{10} \\ \frac{15}{8} \end{bmatrix} = \begin{bmatrix} 0.6000 \\ 2.2727 \\ -1.1000 \\ 1.8750 \end{bmatrix}.$

$$\implies x^{(2)} = Tx^{(1)} + c \implies \cdots$$
$$\implies \frac{\|x^{(10)} - x^{(9)}\|_{\infty}}{\|x^{(10)}\|_{\infty}} = \frac{8.0 \times 10^{-4}}{1.9998} < 10^{-3} \text{ stop!} \quad x \approx x^{(10)}.$$

The Jacobi iterative method (cont'd)

$$Ax = b, a_{ii} \neq 0 \text{ for all } i = 1, 2, \cdots, n.$$

Given $x^{(k-1)}, k \ge 1.$
For $i = 1, 2, \cdots, n,$
 $x_i^{(k)} = \frac{-\sum_{j=1, j \neq i}^n a_{ij} x_j^{(k-1)} + b_i}{a_{ii}}.$

Theoretical setting

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} a_{11} & & & \\ & a_{22} & & \\ & & \ddots & & \\ & & & a_{nn} \end{bmatrix}$$
$$-\begin{bmatrix} 0 & & & \\ -a_{21} & 0 & & \\ \vdots & \ddots & \ddots & \\ -a_{n1} & \cdots & -a_{nn-1} & 0 \end{bmatrix} - \begin{bmatrix} 0 & -a_{12} & \cdots & -a_{1n} \\ & \ddots & \ddots & \vdots \\ & & & -a_{n-1n} \\ & & & 0 \end{bmatrix}$$

 $\Longrightarrow A = D - L - U$

D: diagonal matrix L: lower triangular matrix U: upper triangular matrix

Theoretical setting (cont'd)

$$Ax = b$$

$$\implies Dx = (L + U)x + b$$

$$\implies x = D^{-1}(L + U)x + D^{-1}b$$

The Jacobi iterative method:

$$x^{(k)} = D^{-1}(L+U)x^{(k-1)} + D^{-1}b, \quad k = 1, 2, \cdots$$

Notation:
$$x^{(k)} = T_J x^{(k-1)} + c_J$$
, where $T_J := D^{-1}(L+U)$, $c_J := D^{-1}b$

The Gauss-Seidel iterative method

$$Ax = b, a_{ii} \neq 0 \text{ for all } i = 1, 2, \cdots, n.$$

Given $x^{(k-1)}, k \ge 1.$
For $i = 1, 2, \cdots, n,$
$$x_i^{(k)} = \frac{-\sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^n a_{ij} x_j^{(k-1)} + b_i}{a_{ii}}.$$

Example

Letting
$$x^{(0)} = (0, 0, 0, 0)^{\top}$$
, for $k = 1, 2, \cdots$
 $x_1^{(k)} = 0 + \frac{1}{10}x_2^{(k-1)} - \frac{2}{10}x_3^{(k-1)} + 0 + \frac{6}{10}$
 $x_2^{(k)} = \frac{1}{11}x_1^{(k)} + 0 + \frac{1}{11}x_3^{(k-1)} - \frac{3}{11}x_4^{(k-1)} + \frac{25}{11}$
 $x_3^{(k)} = -\frac{2}{10}x_1^{(k)} + \frac{1}{10}x_2^{(k)} + 0 + \frac{1}{10}x_4^{(k-1)} - \frac{11}{10}$
 $x_4^{(k)} = 0 - \frac{3}{8}x_2^{(k)} + \frac{1}{8}x_3^{(k)} + 0 + \frac{15}{8}$
 $\implies \frac{\|x^{(5)} - x^{(4)}\|_{\infty}}{\|x^{(5)}\|_{\infty}} = 4.0 \times 10^{-4} < 10^{-3} \text{ stop! } x \approx x^{(5)}.$

Theoretical setting

$$Ax = b, A = D - L - U \Longrightarrow (D - L)x^{(k)} = Ux^{(k-1)} + b$$
. That is,

 $a_{11}x_1^{(k)} = -a_{12}x_2^{(k-1)} - \cdots - a_{1n}x_n^{(k-1)} + b_1$ $a_{21}x_1^{(k)} + a_{22}x_2^{(k)} = -a_{23}x_2^{(k-1)} - \dots - a_{2n}x_n^{(k-1)} + b_2$ $\begin{array}{rcl}
\vdots & = & \vdots \\
a_{n1}x_1^{(k)} + a_{n2}x_2^{(k)} + \dots + a_{nn}x_n^{(k)} & = & b_n
\end{array}$ $\implies x^{(k)} = (D-L)^{-1}Ux^{(k-1)} + (D-L)^{-1}b$ for $k = 1, 2, \cdots$ The Gauss-Seidel iterative method: $x^{(k)} = T_S x^{(k-1)} + c_S$, where $T_{s} := (D - L)^{-1}U$ and $c_{s} := (D - L)^{-1}b$. **Note:** $a_{ii} \neq 0$, $i = 1, 2, \cdots, n \iff D - L$ is nonsingular!

Theorem on convergence

• For any $x^{(0)} \in \mathbb{R}^n$, the sequence $\{x^{(k)}\}$ defined by $x^{(k)} := Tx^{(k-1)} + c, \quad k \ge 1,$

converges to the unique solution of $x = Tx + c \iff \rho(T) < 1$.

2 A lemma: If $\rho(T) < 1$, then $(I - T)^{-1}$ exists and

$$(I-T)^{-1} = I + T + T^2 + \dots (:= \sum_{n=0}^{\infty} T^n).$$

Corollaries

• $x^{(0)} \in \mathbb{R}^n$, $x^{(k)} := Tx^{(k-1)} + c$, $k \ge 1$. If ||T|| < 1 for any natural matrix norm then $\{x^{(k)}\}$ converges to the unique solution of x = Tx + c and

•
$$||x - x^{(k)}|| \le ||T||^k ||x - x^{(0)}||.$$

• $||x - x^{(k)}|| \le \frac{||T||^k}{1 - ||T||} ||x^{(1)} - x^{(0)}||.$

② If *A* is strictly diagonally dominant, then for any $x^{(0)} \in \mathbb{R}^n$, both the Jacobi and Gauss-Seidel methods give sequences { $x^{(k)}$ } that converge to the unique solution of Ax = b (x = Tx + c).

Successive Over-Relaxation (SOR)

1 The Gauss-Seidel method:

$$x_i^{(k)} = \frac{1}{a_{ii}} \left\{ -\sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^n a_{ij} x_j^{(k-1)} + b_i \right\}$$

2 Successive over-relaxation:

$$x_i^{(k)} = (1-\omega)x_i^{(k-1)} + \frac{\omega}{a_{ii}} \left\{ -\sum_{j=1}^{i-1} a_{ij}x_j^{(k)} - \sum_{j=i+1}^n a_{ij}x_j^{(k-1)} + b_i \right\}, \ \omega > 0$$

In general,

- $\omega = 1$: the Gauss-Seidel method
- $0 < \omega < 1$: when G-S diverges
- $\omega > 1$: when G-S converges

SOR (cont'd)

$$\begin{aligned} a_{ii}x_{i}^{(k)} + \omega \sum_{j=1}^{i-1} a_{ij}x_{j}^{(k)} &= (1-\omega)a_{ii}x_{i}^{(k-1)} - \omega \sum_{j=i+1}^{n} a_{ij}x_{j}^{(k-1)} + \omega b_{i} \\ \implies (D-\omega L)x^{(k)} &= \left((1-\omega)D + \omega U\right)x^{(k-1)} + \omega b \\ \implies x^{(k)} &= (D-\omega L)^{-1}\left((1-\omega)D + \omega U\right)x^{(k-1)} + \omega(D-\omega L)^{-1}b \\ \implies x^{(k)} &= T_{\omega}x^{(k-1)} + c_{\omega} \end{aligned}$$

Example

Onsider a linear system:

Exact unique solution: $x = (3, 4, -5)^{\top}$.

2 Let $x^{(0)} = (1, 1, 1)^{\top}$. The G-S method:

$$\begin{cases} x_1^{(k)} &= -0.75x_2^{(k-1)} + 6\\ x_2^{(k)} &= -0.75x_1^{(k)} + 0.25x_3^{(k-1)} + 7.5\\ x_3^{(k)} &= 0.25x_2^{(k)} - 6 \end{cases}$$

• Let $x^{(0)} = (1, 1, 1)^{\top}$. The SOR with $\omega = 1.25$: $\begin{cases}
x_1^{(k)} = -0.25x_1^{(k-1)} - 0.9375x_2^{(k-1)} + 7.5 \\
x_2^{(k)} = -0.9375x_1^{(k)} - 0.25x_2^{(k-1)} + 0.3125x_3^{(k-1)} + 9.375 \\
x_3^{(k)} = 0.3125x_2^{(k)} - 0.25x_3^{(k-1)} - 7.5
\end{cases}$

Theorems on convergence

- If $a_{ii} \neq 0$, $i = 1, 2, \dots, n$, then $\rho(T_{\omega}) \ge |\omega 1|$. This implies the SOR method can converge only if $0 < \omega < 2$.
- 2 If *A* is SPD, $0 < \omega < 2$, then the SOR method converges for any $x^{(0)}$.

Some error analysis

- Suppose that we want to solve the linear system Ax = b, but b is somehow perturbed to b (this may happen when we convert a real b to a floating-point b).
- Then actual solution would satisfy a slightly different linear system

$$A\widetilde{x} = \widetilde{b}.$$

- **Question**: Is \tilde{x} very different from the desired solution *x* of the original system?
- Of course, the answer should depend on how good the matrix A is.
- **(**) Let $\|\cdot\|$ be a vector norm, we consider two types of errors:
 - absolute error: $||x \tilde{x}||$
 - relative error: $||x \tilde{x}|| / ||x||$

The absolute error

For the absolute error, we have

$$||x - \widetilde{x}|| = ||A^{-1}b - A^{-1}\widetilde{b}|| = ||A^{-1}(b - \widetilde{b})|| \le ||A^{-1}|| ||b - \widetilde{b}||.$$

Therefore, the absolute error of *x* depends on two factors: the absolute error of *b* and the matrix norm of A^{-1} .

The relative error

For the relative error, we have

$$\begin{aligned} \|x - \widetilde{x}\| &= \|A^{-1}b - A^{-1}\widetilde{b}\| = \|A^{-1}(b - \widetilde{b})\| \\ &\leq \|A^{-1}\| \|b - \widetilde{b}\| = \|A^{-1}\| \|Ax\| \frac{\|b - \widetilde{b}\|}{\|b\|} \\ &\leq \|A^{-1}\| \|A\| \|x\| \frac{\|b - \widetilde{b}\|}{\|b\|}. \end{aligned}$$

That is

$$\frac{\|x - \tilde{x}\|}{\|x\|} \le \|A^{-1}\| \|A\| \frac{\|b - \tilde{b}\|}{\|b\|}.$$

Therefore, the relative error of *x* depends on two factors: the relative error of *b* and $||A|| ||A^{-1}||$.

Condition number

• Therefore, we define a condition number of the matrix *A* as $\kappa(A) := \|A\| \|A^{-1}\|.$

 $\kappa(A)$ measures how good the matrix *A* is.

2 Example: Let $\varepsilon > 0$ and

$$A = \begin{bmatrix} 1 & 1+\varepsilon \\ 1-\varepsilon & 1 \end{bmatrix} \Longrightarrow A^{-1} = \varepsilon^{-2} \begin{bmatrix} 1 & -1-\varepsilon \\ -1+\varepsilon & 1 \end{bmatrix}$$

Then $||A||_{\infty} = 2+\varepsilon$, $||A^{-1}||_{\infty} = \varepsilon^{-2}(2+\varepsilon)$, and
 $\kappa(A) = \left(\frac{2+\varepsilon}{\varepsilon}\right)^2 \ge \frac{4}{\varepsilon^2}.$

.

Condition number (cont'd)

- For example, if $\varepsilon = 0.01$, then $\kappa(A) \ge 40000$.
- 2 What does this mean?

It means that the relative error in *x* can be 40000 times greater than the relative error in *b*.

- So If $\kappa(A)$ is large, we say that A is ill-conditioned, otherwise A is well-conditioned.
- In the ill-conditioned case, the solution is very sensitive to the small changes in the right-hand vector *b* (higher precision in *b* may be needed).

Another way to measure the error

Consider the linear system Ax = b. Let \tilde{x} be a computed solution (an approximation to *x*).

Residual vector:

$$r = b - A\tilde{x}$$

2 Error vector:

$$e = x - \tilde{x}$$

O They satisfy

$$Ae = r$$

(Proof:
$$Ae = Ax - A\tilde{x} = b - A\tilde{x} = r$$
)

Moreover, we have

$$\frac{1}{\kappa(A)} \frac{\|r\|}{\|b\|} \le \frac{\|e\|}{\|x\|} \le \kappa(A) \frac{\|r\|}{\|b\|}.$$

(Theorem on bounds involving condition number)

Proof of the Theorem

$$\therefore Ae = r$$

$$\therefore e = A^{-1}r$$

$$\therefore \|e\|\|b\| = \|A^{-1}r\|\|Ax\| \le \|A^{-1}\|\|r\|\|A\|\|x\|$$

$$\therefore \frac{\|e\|}{\|x\|} \le \kappa(A) \frac{\|r\|}{\|b\|}$$

On the other hand, we have $\|r\| \|x\| = \|Ae\| \|A^{-1}b\| \le \|A\| \|e\| \|A^{-1}\| \|b\|.$ $\therefore \frac{1}{\kappa(A)} \frac{\|r\|}{\|b\|} \le \frac{\|e\|}{\|x\|}$