Section 2

Direct Methods for Linear Systems

Linear system of equations

In many real-world applications, we need to solve linear system of n equations with n variables $x_1, \dots, x_n$:

$$
\begin{aligned}
E_1 : \qquad & a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\
E_2 : \qquad & a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\
& \vdots \\
E_n : \qquad & a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n
\end{aligned}
$$

We're given a_{ij}, $1 \le i, j \le n$ and b_i, $(1 \le i \le n)$, and want to find $x_1, \dots, x_n$ that satisfy the n equations $E_1, \dots, E_n$.

Linear system of equations

General approach: Gauss elimination.

We use three operations to simplify the linear system:

- Equation E_i can be multiplied by λE_i for any $\lambda \neq 0$: $\lambda E_i \to E_i$
- E_j is multiplied by λ and added to E_i: $\lambda E_j + E_i \to E_i$
- Switch E_i and E_j: $E_i \leftrightarrow E_j$

The goal is to simply the linear system into a triangular form, and apply backward substitution to get $x_1, \ldots, x_n$.

Linear system of equations

Generally, we form the augmented matrix

$$\tilde{A} = [A\ \mathbf{b}], \text{ where } A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

and apply Gaussian elimination to get a triangular form of $\tilde{A}$ then apply backward substitution. Total cost is $O(n^3)$.

Pivoting strategies

Standard Gauss elimination may not work properly in numerical computations.

Example

Apply Gauss elimination to the system

$$\begin{aligned} E_1: \quad 0.003000x_1 + 59.14x_2 &= 59.17 \\ E_2: \quad 5.291x_1 - 6.130x_2 &= 46.78 \end{aligned}$$

with four digits for arithmetic rounding. Compare the result to exact solution $x_1 = 10.00$ *and* $x_2 = 1.000$*.*

Pivoting strategies

Solution: We need to multiply E_1 by $\frac{5.291}{0.003000} = 1763.66\bar{6} \approx 1764$, then subtract it from E_2 and get:

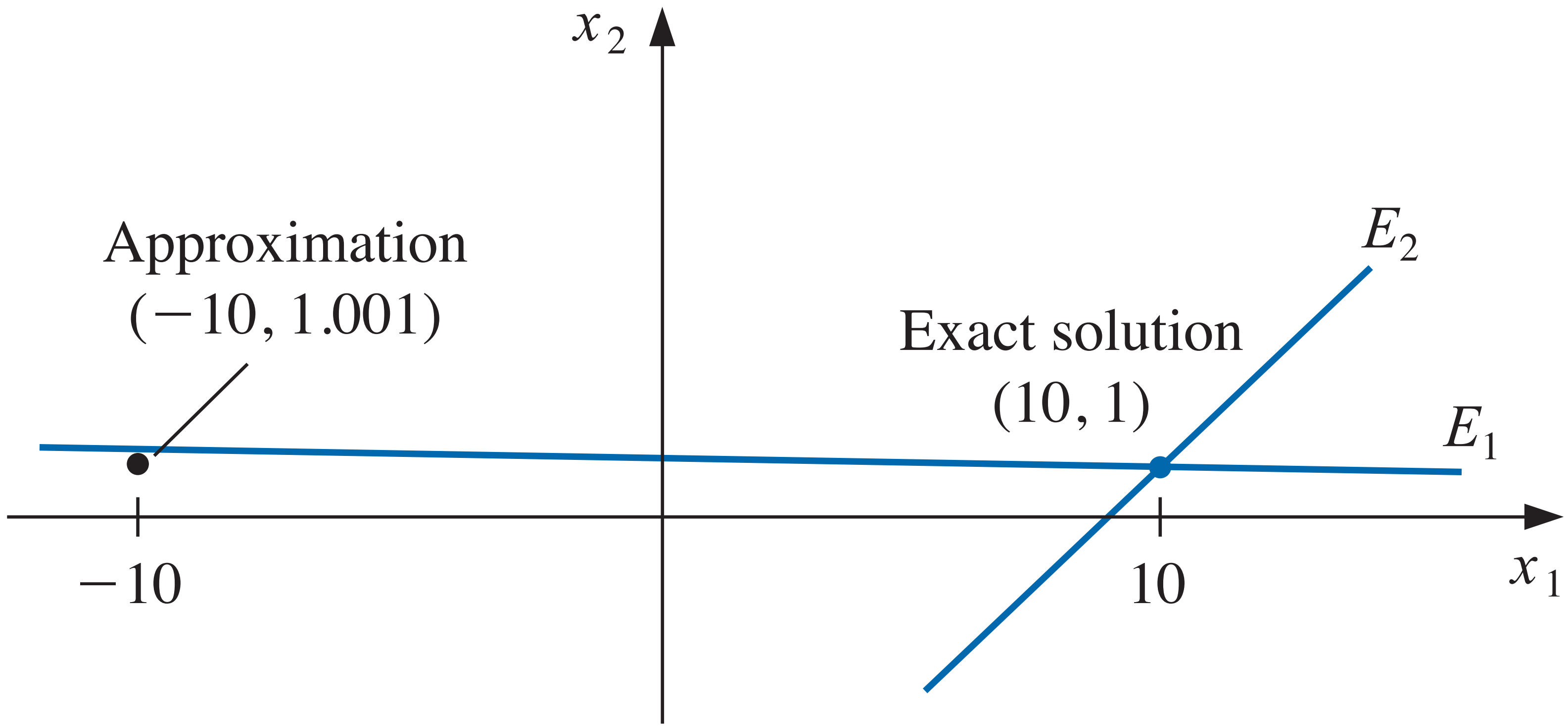
$$\begin{aligned} 0.003000x_1 + 59.14x_2 &\approx 59.17 \\ -104300x_2 &\approx -104400 \end{aligned}$$

On the other hand, the exact system without rounding error:

$$\begin{aligned} 0.003000x_1 + 59.14x_2 &\approx 59.17 \\ -104309.37\bar{6}x_2 &\approx -104309.37\bar{6} \end{aligned}$$

Solving the former yields $x_2 = 1.001$ (still close to exact solution 1.000), but $x_1 = \frac{59.17 - 59.14x_2}{0.003000} = -10.00$ (far from exact solution 10.00).

Pivoting strategies



Partial pivoting

- The issue above comes up because the pivot a_{kk} is smaller than the remaining a_{ij} $(i, j > k)$.
- One remedy, called **partial pivoting**, is interchanging rows k and p (where $|a_{ik}| = \max\{|a_{ik}| : i = k, \dots, n\}$).
- Sometimes interchange columns can also be performed.

For example, when we are about to do pivoting for the k-th time (i.e., $a_{kk}x_k$ term), we switch row p and current row k so that

$$p = \operatorname*{argmax}_{k \le i \le n} |a_{ik}|$$

Redo the example above, we will get exact solution.

Scaled partial pivoting

Consider the following example:

$$
\begin{aligned}
E_1: \quad & 30.00x_1 + 591400x_2 = 591700 \\
E_2: \quad & 5.291x_1 - 6.130x_2 = 46.78
\end{aligned}
$$

This is equivalent to example above, except that E_1 is multiplied by 10^4.

If we apply partial pivoting above, we will not exchange E_1 and E_2 since $30.00 > 5.291$, and will end up with the same *incorrect* answer $x_2 = 1.001$ and $x_1 = -10.00$.

To overcome this issue, we can scale the coefficients of each row i by $1/s_i$ where $s_i = \max_{1\le j\le n} |a_{ij}|$. Then apply partial pivoting based on the scaled values.

Scaled partial pivoting

Applying scaled partial pivoting to the example above, we first have

$s_1 = \max\{30.00, 519400\} = 519400, s_2 = \max\{5.291, 6.130\} = 6.130$

Hence we get $\frac{a_{11}}{s_1} = \frac{30.00}{519400} \approx 0.5073 \times 10^{-4}$, and $\frac{a_{21}}{s_2} = \frac{5.291}{6.130} = 0.8631$, the others are ± 1. By comparing $\frac{a_{11}}{s_1}$ and $\frac{a_{21}}{s_2}$, we will exchange E_1 and E_2, and hence obtain

$$
\begin{aligned}
E_1 : &\quad 5.291x_1 - 6.130x_2 = 46.78 \\
E_2 : &\quad 30.00x_1 + 591400x_2 = 591700
\end{aligned}
$$

and apply Gauss elimination to obtain correct answer $x_2 = 1.000$ and $x_1 = 10.00$.

Complete pivoting

For each of the n steps, find the largest magnitude among all coefficients a_{ij} for $k \leq i, j \leq n$. Then switch rows and/or columns so that the one with largest magnitude is in the pivot position.

This requires $O(n^3)$ comparisons. Only worth it if the accuracy improvement justifies the cost.

Linear algebra: quick review

We call A an $m \times n$ (m-by-n) **matrix** if A is an array of mn numbers with m rows and n columns

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

We may simply denote it by $A = [a_{ij}]$, when its size is clear in the context.

Linear algebra: quick review

- We call two matrices equal, i.e., $A = B$, if $a_{ij} = b_{ij}$ for all i, j.
- The sum of two matrices of same size is: $A \pm B = [a_{ij} \pm b_{ij}]$.
- Scalar multiplication of A by $\lambda \in \mathbb{R}$ is $\lambda A = [\lambda a_{ij}]$.
- We denote the matrix of all zeros by 0, and $-A = [-a_{ij}]$.

Linear algebra: quick review

The set of all $m \times n$ matrices forms a **vector space**:

- $A + B = B + A$
- $(A + B) + C = A + (B + C)$
- $A + 0 = 0 + A$
- $A + (-A) = 0$
- $\lambda(A + B) = \lambda A + \lambda B$
- $(\lambda + \mu)A = \lambda A + \mu A$
- $\lambda(\mu A) = (\lambda\mu)A$
- $1A = A$

Linear algebra: quick review

For matrix A of size $m \times n$ and (column) vector b of dimension n, we define the matrix-vector multiplication (product) by

$$Ab = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{n} a_{1j} b_j \\ \sum_{j=1}^{n} a_{2j} b_j \\ \vdots \\ \sum_{j=1}^{n} a_{mj} b_j \end{bmatrix}$$

Linear algebra: quick review

For matrix A of size $m \times n$ and matrix B of size $n \times k$, we define the matrix-matrix multiplication (product) by

$$AB = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1k} \\ b_{21} & b_{22} & \cdots & b_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nk} \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{j=1}^n a_{1j} b_{j1} & \sum_{j=1}^n a_{1j} b_{j1} & \cdots & \sum_{j=1}^n a_{1j} b_{jk} \\ \sum_{j=1}^n a_{2j} b_{j1} & \sum_{j=1}^n a_{2j} b_{j1} & \cdots & \sum_{j=1}^n a_{2j} b_{jk} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{j=1}^n a_{mj} b_{j1} & \sum_{j=1}^n a_{mj} b_{j1} & \cdots & \sum_{j=1}^n a_{mj} b_{jk} \end{bmatrix} \in \mathbb{R}^{m \times k}$$

That is, if $C = AB$, then $[c_{ij}] = [\sum_r a_{ir} b_{rj}]$ for all i, j.

Linear algebra: quick review

Some properties of matrix product

- $A(BC) = (AB)C$
- $A(B + D) = AB + AD$
- $\lambda(AB) = (\lambda A)B = A(\lambda B)$

Remark

Note that $AB \neq BA$ in general, even if both exists.

Linear algebra: quick review

Some special matrices

- Square matrix: A is of size $n \times n$
- Diagonal matrix: $a_{ij} = 0$ if $i \neq j$.
- Identity matrix of order n: $I = [\delta_{ij}]$ where $\delta_{ij} = 1$ if $i = j$ and $= 0$ otherwise.
- Upper triangle matrix: $a_{ij} = 0$ if $i > j$.
- Lower triangle matrix: $a_{ij} = 0$ if $i < j$.

Linear algebra: quick review

Definition (Inverse of matrix)

An $n \times n$ matrix A is said to be **nonsingular** *(or* **invertible***) if there exists an $n \times n$ matrix, denoted by A^{-1}, such that $A(A^{-1}) = (A^{-1})A = I$. Here A^{-1} is called the* **inverse** *of matrix A.*

Definition

An $n \times n$ matrix A without an inverse is called **singular** *(or* **noninvertible***)*

Linear algebra: quick review

Several properties of inverse matrix:

- A^{-1} is unique.
- $(A^{-1})^{-1} = A$.
- If B is also nonsingular, then $(AB)^{-1} = B^{-1}A^{-1}$.

Linear algebra: quick review

Definition (Transpose)

The **transpose** *of an* $m \times n$ *matrix* $A = [a_{ij}]$ *is the* $n \times m$ *matrix* $A^\top = [a_{ji}]$.

Sometimes $A^\top$ is also written as A^t, A', A^T.

- $(A^\top)^\top = A$
- $(AB)^\top = B^\top A^\top$
- $(A + B)^\top = A^\top + B^\top$
- If A is nonsingular, then $(A^{-1})^\top = (A^\top)^{-1}$.

Linear algebra: quick review

Definition (Determinant)

- *If $A = [a]$ is a 1×1 matrix, then* $\det(A) = a$.
- *If A is $n \times n$ where $n > 1$, then the* **minor** M_{ij} *is the determinant of the $(n-1) \times (n-1)$ submatrix of A by deleting its ith row and jth column.*
- *The* **cofactor** A_{ij} *associated with the minor M_{ij} is defined by $A_{ij} = (-1)^{i+j} M_{ij}$.*
- *The* **determinant** *of the $n \times n$ matrix A, denoted by* $\det(A)$ *(or $|A|$), is given by either of the followings:*

$$\det(A) = \sum_{j=1}^{n} a_{ij} A_{ij} = \sum_{j=1}^{n} (-1)^{i+j} a_{ij} M_{ij}, \quad \textit{for any } i = 1, \dots, n$$

$$\det(A) = \sum_{i=1}^{n} a_{ij} A_{ij} = \sum_{j=1}^{n} (-1)^{i+j} a_{ij} M_{ij}, \quad \textit{for any } j = 1, \dots, n$$

Linear algebra: quick review

Some properties of determinant

- If A has any zero row or column, then $\det(A) = 0$.
- If two rows (or columns) of A are the same, or one is a multiple of the other, then $\det(A) = 0$.
- Switching two rows (or columns) of A results in a matrix with determinant $-\det(A)$.
- Multiplying a row (or column) of A by λ results in a matrix with determinant $\lambda \det(A)$.
- $(E_i + \lambda E_j) \to E_i$ results in a matrix of the same determinant.

Linear algebra: quick review

Some properties of determinant

- $\det(AB) = \det(A)\det(B)$ if A and B are square matrices of same size.
- $\det(A^\top) = \det(A)$
- A is singular if any only if $\det(A) = 0$.
- If A is nonsingular, then $\det(A) \neq 0$ and $\det(A^{-1}) = \det(A)^{-1}$.
- If A is an upper or lower triangular matrix, then $\det(A) = \prod_{i=1}^{n} a_{ii}$.

Linear algebra: quick review

The following statements are equivalent:

- $Ax = 0$ has unique solution $x = 0$.
- $Ax = b$ has a unique solution for every b.
- A is nonsingular, i.e., A^{-1} exists.
- $\det(A) \neq 0$.

Matrix factorization

Gauss elimination can be used to compute **LU factorization** of a square matrix A:

$$A = LU$$

where L is a lower triangular matrix, and U is an upper triangular matrix.

Matrix factorization

If we have **LU factorization** of A, then

$$Ax = LUx = L(Ux) = b$$

so we solve x easily:

1. Solve y from $Ly = b$ by forward substitution;
2. Solve x from $Ux = y$ by backward substitution.

Total cost is $O(2n^2)$.

Matrix factorization

The cost reduction from $O(n^3/3)$ to $O(2n^2)$ is huge, especially for large n:

n	$n^3/3$	$2n^2$	% Reduction
10	$3.\bar{3} \times 10^2$	2×10^2	40
100	$3.\bar{3} \times 10^5$	2×10^4	94
1000	$3.\bar{3} \times 10^8$	2×10^6	99.4

Unfortunately, LU factorization itself requires $O(n^3)$ in general.

LU factorization

Now let's see how to obtain LU factorization by Gauss elimination.

Suppose we can perform Gauss elimination without any row exchange. In first round, we use a_{11} as the pivot and cancel each of $a_{21}, \dots, a_{n1}$ by

$$(E_j - m_{j1}E_1) \to E_j \quad \text{where } m_{j1} = \frac{a_{j1}}{a_{11}}, \quad j = 2, \dots, 4$$

This is equivalent to multiplying $M^{(1)}$ to A and get $A^{(2)} := M^{(1)}A$ where

$$M^{(1)} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ -m_{21} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -m_{n1} & 0 & \cdots & 1 \end{bmatrix} \text{ and } A^{(2)} = \begin{bmatrix} a_{11} & * & \cdots & * \\ 0 & * & \cdots & * \\ \vdots & \vdots & \ddots & \vdots \\ 0 & * & \cdots & * \end{bmatrix}$$

LU factorization

In second round, we use <u>current</u> a_{22} as the pivot and cancel each of $a_{32}, \dots, a_{n2}$ by

$$(E_j - m_{j2}E_2) \to E_j \quad \text{where } m_{j2} = \frac{a_{j2}}{a_{22}}, \quad j = 3, \dots, 4$$

This is equivalent to multiplying $M^{(2)}$ to $A^{(2)}$ and get $A^{(3)} := M^{(2)}A^{(2)}$ where

$$M^{(2)} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & -m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -m_{n2} & 0 & \cdots & 1 \end{bmatrix} \text{ and } A^{(3)} = \begin{bmatrix} a_{11} & * & * & \cdots & * \\ 0 & * & * & \cdots & * \\ 0 & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & * & \cdots & * \end{bmatrix}$$

LU factorization

When Gauss elimination finishes (total $n-1$ rounds), we will get an upper triangular matrix U:

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

Define matrix L

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

Note that L is lower triangular (because each M is lower triangular, and inverse and product of lower triangular matrices are still lower triangular). So we get the LU factorization of A:

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

LU factorization

It is easy to check that:

$$M^{(1)} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ -m_{21} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -m_{n1} & 0 & \cdots & 1 \end{bmatrix} \text{ and } (M^{(1)})^{-1} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ m_{n1} & 0 & \cdots & 1 \end{bmatrix}$$

$$M^{(2)} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & -m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -m_{n2} & 0 & \cdots & 1 \end{bmatrix} \text{ and } (M^{(2)})^{-1} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & m_{n2} & 0 & \cdots & 1 \end{bmatrix}$$

LU factorization

and finally there is

$$L = (M^{(1)})^{-1} \cdots (M^{(n-2)})^{-1} (M^{(n-1)})^{-1} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ m_{21} & 1 & 0 & \cdots & 0 \\ m_{31} & m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ m_{n1} & m_{n2} & m_{n3} & \cdots & 1 \end{bmatrix}$$

To summarize, the LU factorization of A gives L as above, and U as the result of Gauss elimination of A.

Gauss elimination row exchange

If Gauss elimination is done with row exchanges, then we will get LU factorization of PA where P is some row permutation matrix.

For example, to switch rows 2 and 4 of a 4×4 matrix A, the permutation matrix P is

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

Some properties of permutation matrices:

- If P_1, P_2 are permutations, then $P_2 P_1$ is still permutation.
- $P^{-1} = P^\top$.

Diagonally dominate matrices

Now we consider two types of matrices for which Gauss elimination can be used effectively without row interchanges.

Definition (Diagonally dominate matrices)

An $n \times n$ matrix A is called **diagonally dominate** *if*

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|, \quad \forall i = 1, 2, \dots, n$$

An $n \times n$ matrix A is called **strictly diagonally dominate** *if*

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|, \quad \forall i = 1, 2, \dots, n$$

Diagonally dominate matrices

Example

Consider the following matrices:

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

$$B = \begin{bmatrix} 7 & 2 & 0 \\ 3 & 5 & -1 \\ 0 & 5 & -6 \end{bmatrix} \quad C = \begin{bmatrix} 6 & 4 & -3 \\ 4 & -2 & 0 \\ -3 & 0 & 1 \end{bmatrix}$$

A (and $A^\top$) is diagonally dominate, B is strictly diagonally dominate, $B^\top, C, C^\top$ are not diagonally dominate.

Diagonally dominate matrices

Theorem

If A is strictly diagonally dominant, then A is nonsingular. Moreover, Gauss elimination can be performed without row interchange to obtain the unique solution of $Ax = b$.

Diagonally dominate matrices

Proof.

If A is singular, then $Ax = 0$ has nonzero solution x. Suppose x_k is the component of x with largest magnitude:

$$|x_k| > 0 \quad \text{and} \quad |x_k| \geq |x_j|, \ \forall j \neq k$$

Then the product of x and the k-th row of A gives

$$a_{kk}x_k + \sum_{j \neq k} a_{kj}x_j = 0$$

From this we obtain

$$|a_{kk}| = \left| -\sum_{j \neq k} \frac{a_{kj}x_j}{x_k} \right| \leq \sum_{j \neq k} \frac{|x_j|}{|x_k|}|a_{kj}| \leq \sum_{j \neq k} |a_{kj}|$$

Contradiction. So A is nonsingular. □

Diagonally dominate matrices

Proof (cont.) Now let's see how Gauss elimination works when A is strictly diagonally dominant. Consider 1st and ith ($i \geq 2$) rows of A:

$$|a_{11}| > \sum_{j \neq 1} |a_{1j}|, \quad |a_{ii}| > \sum_{j \neq i} |a_{ij}|$$

If we perform $E_i - \frac{a_{i1}}{a_{11}} E_1 \to E_i$, the new values in row i are $a_{i1}^{(2)} = 0$ and $a_{ij}^{(2)} = a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}$ for $j \geq 2$. Therefore

$$\begin{aligned}\sum_{\substack{j=2\\ j\neq i}}^{n} |a_{ij}^{(2)}| &\leq \sum_{\substack{j=2\\ j\neq i}}^{n} |a_{ij}| + \sum_{\substack{j=2\\ j\neq i}}^{n} \left|\frac{a_{1j}}{a_{11}}\right| |a_{i1}| < |a_{ii}| - |a_{i1}| + \frac{|a_{11}| - |a_{1i}|}{|a_{11}|} |a_{i1}| \\ &= |a_{ii}| - \frac{|a_{1i}|}{|a_{11}|} |a_{i1}| \leq \left| |a_{ii}| - \frac{|a_{1i}|}{|a_{11}|} |a_{i1}| \right| = |a_{ii}^{(2)}|\end{aligned}$$

As i is arbitrary, we know A remains strictly diagonally dominant after first round. By induction we know A stays as strictly diagonally dominant and Gauss elimination can be performed without row interexchange.

Positive definite matrices

Definition (Positive definite matrix)

A matrix A is called **positive definite** *(PD) if it is symmetric and $x^\top Ax > 0$ for any $x \neq 0$*

Remark

In some texts, A is called positive definite as long as $x^\top Ax > 0$ for any $x \neq 0$, so A is not necessarily symmetric. In these texts, the matrix in our definition above is called **symmetric positive definite** *(SPD).*

Positive definite matrices

We first have the following formula: if $x = (x_1, \dots, x_n)^\top$ and $A = [a_{ij}]$, then

$$x^\top A x = \sum_{i,j} a_{ij} x_i x_j$$

Positive definite matrices

Example

Show that the matrix A below is PD:

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

Solution: First A is symmetric. For any $x \in \mathbb{R}^3$, we have

$$\begin{aligned} x^\top Ax &= 2x_1^2 - 2x_1x_2 + 2x_2^2 - 2x_2x_3 + 2x_3^2 \\ &= x_1^2 + (x_1^2 - 2x_1x_2 + x_2^2) + (x_2^2 - 2x_2x_3 + x_3^2) + x_3^2 \\ &= x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 \end{aligned}$$

Therefore $x^\top Ax = 0$ if and only if $x_1 = x_2 = x_3 = 0$. So A is PD.

Positive definite matrices

Theorem

If A is an $n \times n$ positive definite matrix, then

- *A is nonsingular;*
- *$a_{ii} > 0$ for all i;*
- *$\max_{i \neq j} |a_{ij}| \leq \max_i |a_{ii}|$;*
- *$(a_{ij})^2 < a_{ii}a_{jj}$ for any $i \neq j$.*

Positive definite matrices

Proof.

- If $Ax = 0$, then $x^\top Ax = 0$ and hence $x = 0$ since A is PD. So A is nonsingular.
- Set $x = e_i$, where $e_i \in \mathbb{R}^n$ has 1 as the i-th component and zeros elsewhere. Then $x^\top Ax = e_i^\top Ae_i = a_{ii} > 0$.
- For any k, j, define $x, z \in \mathbb{R}^n$ such that $x_j = z_k = z_j = 1$ and $x_k = -1$, and $x_i = z_i = 0$ if $i \neq k, j$. Then we can show

$$0 < x^\top Ax = a_{jj} + a_{kk} - a_{kj} - a_{jk}$$
$$0 < z^\top Az = a_{jj} + a_{kk} + a_{kj} + a_{jk}$$

  Note that $a_{kj} = a_{jk}$, so we get $|a_{kj}| < \frac{a_{jj}+a_{kk}}{2} \leq \max_i a_{ii}$.
- For any $i \neq j$, set $x \in \mathbb{R}^n$ such that $x_i = \alpha$ and $x_j = 1$, and 0 elsewhere. Therefore $0 < x^\top Ax = a_{ii}\alpha^2 + 2a_{ij}\alpha + a_{jj}^2$ for any α. This implies that $4a_{ij}^2 - 4a_{ii}a_{jj} < 0$.

Positive definite matrices

Definition (Leading principal submatrix)

A **leading principal submatrix** *of A is the $k \times k$ upper left submatrix*

$$A_k = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix}$$

Positive definite matrices

Theorem

A symmetric matrix A is PD if and only if every leading principal submatrix has a positive determinant.

Example

Use the Theorem above to check A is PD:

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

Positive definite matrices

Theorem

A matrix A is PD if and only either of the followings is true:

- *There exist a lower triangular matrix L with all 1 on its diagonal and a diagonal matrix D with all diagonal entries positive, such that $A = LDL^\top$.*
- *There exists a lower triangular matrix L with all diagonal entries positive such that $A = LL^\top$ (Cholesky factorization).*
- *Gauss elimination of A without row interchanges can be performed and all pivot elements are positive.*

Band matrices

Definition (Band matrix)

An $n \times n$ matrix A is called **band matrix** *if there exist p, q such that a_{ij} can be nonzero only if $i - q \leq j \leq i + p$. The band width is defined by $w = p + q + 1$.*

Definition (Tridiagonal matrix)

A band matrix with $p = q = 1$ is called **tridiagonal** *matrix.*

Crout factorization

The **Crout factorization** of a tridiagonal matrix is $A = LU$ where L is lower triangle, U is upper triangle, and both L, U are tridiagonal:

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

Note that a tridiagonal matrix A has $3n-2$ unknowns, and the L and U together also have $3n-2$ unknowns.

Crout factorization

Theorem

A tridiagonal matrix A has a Crout factorization if either of the following statements is true:

- *A is positive definite;*
- *A is strictly diagonally dominant;*
- *A is diagonally dominant,* $|a_{11}| > |a_{12}|$, $|a_{nn}| > |a_{n,n-1}|$, *and* $a_{i,i-1}, a_{i,i+1} \neq 0$ *for all* $i = 2, \ldots, n-1$.

Crout factorization

With the special form of A, L and U, we can obtain the Crout factorization $A = LU$ by solving l_{ij} ($i = 1, \dots, n$ and $j = i-1, i$) and $u_{i,i+1}$ ($i = 1, \dots, n-1$) from

$$
\begin{aligned}
a_{11} &= l_{11} \\
a_{i,i-1} &= l_{i,i-1}, && \text{for } i = 2, \dots, n \\
a_{i,i} &= l_{i,i-1} u_{i-1,i} + l_{ii}, && \text{for } i = 2, \dots, n \\
a_{i,i+1} &= l_{ii} u_{i,i+1}, && \text{for } i = 1, \dots, n-1
\end{aligned}
$$

When we use Crout factorization to solve $Ax = b$, the cost is only $5n-4$ multiplications/divisions and $3n-3$ additions/subtractions.