Numerical Analysis : [MA214]
Lecture 12

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September 5, 2017

Last time we did Gauss Elimination (GE). We have a system of equations.

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

We can write it as $Ax = b$ where $A = (a_{ij})$,

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

After doing Row transformation we convert it into an equivalent system

$$Ux = \overline{b} \quad \text{where } U \text{ is upper tringular.}$$

Then x can be solved by back substitution.

If GE can be done without row interchange then A can be factored as $A = LU$ where L is lower triangular and U is upper triangular.

To solve $Ax = b$. Then $LUx = b$

Set $Ux = y$. Solve $Ly = b$ by forward substitution.

Then solve $Ux = y$ by back substitution.

Advantage of LU factorization:- Advantage of LU factorization is when we have to solve $Ax = b$ for many different values of b.

Question:- Which classes of matrices admit LU decomposition?

We have to find classes of matrices for which Gauss Elimination can be performed effectively without row interchanges.

The classes of matrices are

1. Strictly diagonally dominant matrices.
2. positive definite matrices.

Recall:- An $n \times n$ matrices $A = (a_{ij})$ is said to be strictly diagonally dominated if

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

Example:-

$$A = \begin{bmatrix} 7 & 2 & 0 \\ 3 & 5 & -1 \\ 0 & 5 & -6 \end{bmatrix}$$

A is strictly diagonally dominant. Note

$$A^t = \begin{bmatrix} 7 & 3 & 0 \\ 2 & 5 & 5 \\ 0 & -1 & -6 \end{bmatrix}$$

is not strictly diagonally dominant.

Theorem

A strictly diagonally dominant matrix A is non-singular.

Proof:-

We prove by contradiction. Suppose A is singular.

$$\implies \quad \text{there exists} \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \neq 0 \quad \text{such that} \quad Ax = 0.$$

Let k be index for which $0 < |x_k| = max_{1 \leq j \leq n} \ |x_j|$

Since $Ax = 0$, we have $\sum_{j=0}^{n} a_{ij} x_j = 0$ for each $i = 1, 2, \cdots, n$

When $i = k$, $\sum_{j=0}^{n} a_{kj} x_j = 0 \implies a_{kk} x_k = -\sum_{j \neq k} a_{kj} x_j$.

$$\implies |a_{kk}||x_k| \leq \sum_{j \neq k} |a_{kj}||x_j| \implies |a_{kk}| \leq \sum_{j \neq k} |a_{kj}| \frac{|x_j|}{x_k} \leq \sum_{j \neq k} |a_{kj}|$$

This inequality contradicts the strict diagonal dominance of A.

Positive definte matrices

A matrix A is positive definite if

1. it is symmetric $i.e$, $A^t = A$.
2. $x^t A x > 0$ for every n-dimensional vector $x \neq 0$.

Remark : A positive definite matrix is non-singular.

Proof.

$$
\begin{aligned}
\text{If} \quad Ax &= 0 \\
\Longrightarrow x^t A x = 0 & \\
\Longrightarrow x &= 0
\end{aligned}
$$

$\square$

Cholesky's Algorithm

Given a positive definite $n \times n$ matrix A. It factors into LL^t where L is lower triangular.

Example

$$A = \begin{bmatrix} 4 & 2 & 14 \\ 2 & 17 & -5 \\ 14 & -5 & 83 \end{bmatrix}$$

.

$$A = LL^t$$

$$A = \begin{bmatrix} 4 & 2 & 14 \\ 2 & 17 & -5 \\ 14 & -5 & 83 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{12} & l_{13} \\ 0 & l_{22} & l_{23} \\ 0 & 0 & l_{33} \end{bmatrix}$$

$$
\begin{aligned}
l_{11}^2 &= 4 &\implies\quad l_{11} &= 2\\
l_{21} l_{11} &= 2 &\implies\quad l_{21} &= 1\\
l_{31} l_{11} &= 14 &\implies\quad l_{31} &= 7
\end{aligned}
$$

$$
\begin{aligned}
l_{21}^2 + l_{22}^2 &= 17 &\implies\quad & l_{22}^2 = 16 \implies l_{22} = 4\\
l_{21} l_{31} + l_{32} l_{22} &= -5 &\implies\quad & 7 + 4 l_{32} = -5 \implies l_{32} = -3\\
l_{31}^2 + l_{32}^2 + l_{33}^2 &= 83 &\implies\quad & 49 + 9 + l_{33}^2 = 83 \implies l_{33} = 5
\end{aligned}
$$

$$
\text{So} \quad L = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 4 & 0 \\ 7 & -3 & 5 \end{bmatrix}
$$

Cholesky's Algorithm

To factor A into LL^t where L is lower triangular (here A is positive definite). Let $L = (l_{ij})$.

Step 1 Set $l_{ii} = \sqrt{a_{11}}$.

Step 2 For $j = 2, 3, \cdots, n$, Set $l_{j1} = \frac{a_{j1}}{l_{11}}$.

Step 3 For $i = 2, 3, \cdots, n-1$, do steps 4 and 5.

Step 4 Set $l_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} l_{ik}^2}$

Step 5 $j = i+1, \cdots, n$, set $l_{ji} = \frac{a_{ji} - \sum_{k=1}^{i-1} l_{jk} l_{ik}}{l_{ii}}$.

Step 6 set $l_{nn} = \sqrt{a_{nn} - \sum_{k=1}^{n-1} l_{nk}^2}$.

Why do Cholesky's factorization?

LU factorization requires $\theta(n^3/3)$ multiplication and division and $\theta(n^3/3)$ addition and subtraction.

The LL^t Cholesky's factorization requires $\theta(n^3/6)$ multiplication and division and $\theta(n^3/6)$ addition and subtraction.

Thus it requires only 50% of calculations.

Disadvantage of Cholesky's algorithm: It is valid only for positive definite matrices.

Note that LU decomposition is possible if GE can be done without row changes.

What to do when GE has row changes?

A $n \times n$ permutation matrix $P = (p_{ij})$ is obtained by rearranging the rows of identity matrix I.

Example : $I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$R_2 \leftrightarrow R_3 \quad P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ is 3×3 permutation matrix .

$A = (a_{ij})_{3\times 3}$

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

Two Useful properties of permutation matrices

Suppose $k_1, k_2, \cdots, k_n$ is a permutation of $1, 2, \cdots, n$ and the permutation matrix $P = (p_{ij})$ is defined by

$$p_{ij} = \begin{cases} 1 & \text{if } \ j = k, \\ 0 & otherwise. \end{cases}$$

Then

1. PA permutes the rows of A.
2. P^{-1} exists and $P^{-1} = P^t$.

PLU factorization of a matrix

Let A be a matrix. Suppose if possible we have done some row change while doing Gauss Elimination on A.

This implies that there exists a permutation matrix P such that GE can be done on PA without any row changes.

$$Thus, \quad PA = LU$$

$$Solving \quad Ax = b$$

$$PAx = Pb = b'$$

$$LUx = b'$$

$$y = Ux$$

$$\text{first solve} \quad Ly = b'$$

$$\text{Then solve} \quad Ux = y$$

Example

$$A = \begin{bmatrix} 0 & 1 & -1 & 1 \\ 1 & 1 & -1 & 2 \\ -1 & -1 & 1 & 0 \\ 1 & 2 & 0 & 2 \end{bmatrix}, \ then\ R_1 \leftrightarrow R_2\ gives\ \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ -1 & -1 & 1 & 0 \\ 1 & 2 & 0 & 2 \end{bmatrix},$$

$$R_3 + R_1 \quad and \quad R_4 - R_1\ give \ \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & 0 & 2 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$

$$R_3 \leftrightarrow R_4\ gives\ \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \ R_3 - R_2\ gives\ \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & 2 \end{bmatrix} = U$$

$$P = R_1 \leftrightarrow R_2 \ \textit{and} \ R_3 \leftrightarrow R_4 \text{ done on identity matrix}$$

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

$$PA = \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ 1 & 2 & 0 & 2 \\ -1 & -1 & 1 & 0 \end{bmatrix}, \ R_3 - R_1 \ \textit{and} \ R_4 + R_1 \ \textit{give} \ \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

$$R_3 - R_2 \ \textit{gives} \ \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & 2 \end{bmatrix} = U \ \textit{and} \ L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$

Errors associated with Gauss Elimination

Example :

$$\begin{aligned} 0.0003x_1 + 1.566x_2 &= 1.569 \\ 0.3454x_1 - 2.436x_2 &= 1.018 \\ \text{Exact answer } x_1 = 10, & \quad x_2 = 1 \end{aligned}$$

corresponding in 4 sig digits

$$\begin{bmatrix} 0.0003 & 1.566 & : & 1.569 \\ 0.3454 & -2.436 & : & 1.018 \end{bmatrix}$$

$$m_{21} = \frac{0.3454}{0.0003} = 1,151$$

$$a_{22}^{(2)} = -2.436 - (1151)(1.566) = -1804$$

$$\begin{aligned} b_{22}^{(2)} &= 1.018 - (1151)(1.566) \\ &= -1805 \end{aligned}$$

$$\left[\begin{array}{cccc} 0.0003 & 1.566 & : & 1.569 \\ 0 & -1804 & : & -1805 \end{array} \right]$$

$$x_2 = \frac{-1805}{-1804} = 1.001$$

Hence from the first equation

$$\begin{aligned} x_1 &= \frac{1.569 - (1.566)(1.001)}{0.0003} \\ &= 3.333 \end{aligned}$$

Exact is 10

So x_1 has lot of error.

Plausible explanation

$a_{11} = 0.0003$ is very small. So the algorithm performs badly for a_{11} is "near zero".

However consider the system in example but with first equation multiplied by 10^m where m is some integer.

$$\begin{aligned} (0.0003)10^m x_1 + (1.566)10^m x_2 &= (1.569)10^m \\ 0.3454x_1 - 2.436x_2 &= 1.018 \end{aligned}$$

$$m_{21} = \frac{0.3454}{(0.0003)10^m} = (1,151)10^{-m}$$

$$a_{22}^{(2)} = -2.436 - (1151)10^{-m}(1.566)10^m = -1804$$

$$\textit{Similarly} \quad b_{22}^{(2)} = -1805$$

So we get $x_2 = 1.001$ and finally $x_1 = 3.333$.

Explanation of the error

$|a_{11}|$ is small compared with $|a_{12}|$. Thus a small error in computed value of x_2 leads to a large error in x_1.

$$\left|\frac{a_{12}}{a_{11}}\right| \equiv 5220$$

$$\left|\frac{a_{22}}{a_{21}}\right| \equiv 6$$

So we do $R_1 \longleftrightarrow R_2$

We get

$$m_{11} = \frac{0.0003}{0.3454} = 0.0008681$$

So now new second equation becomes

$$1.568x_2 = 1.568 \implies x_2 = 1$$

and from "new" first equation we get $x_1 = 10$.

Scaled partial pivoting

$$\text{Let} \quad s_i = max_{1 \le j \le n} |a_{ij}|$$

scale factor for row i, $s_i \neq 0$, since otherwise all entries in row i is zero. It implies that A is singular.

$$\frac{|a_{p1}|}{s_p} = max_{1 \le k \le n} \frac{|a_{k1}|}{s_k}$$

$$\text{perform} \quad R_1 \longleftrightarrow R_p \quad \text{if } p \neq 1$$

In a similar manner before eliminating variable x_i from rows $i+1, i+2, \cdots, n$.

We select the smallest integer $p \geq i$ with

$$\frac{|a_{pi}|}{s_p} = max_{i \le k \le n} \frac{|a_{ki}|}{s_k}$$

$$\text{perform} \quad R_i \longleftrightarrow R_p \quad \text{if } p \neq i$$

Example

$$\begin{aligned} 2.11x_1 - 4.21x_2 + 0.921x_3 &= -2.01 \\ 4.01x_1 + 10.2x_2 - 1.12x_3 &= -3.09 \\ 1.09x_1 + 0.987x_2 + 0.832x_3 &= 4.21 \end{aligned}$$

$$s_1 = 4.21 \quad s_2 = 10.2 \quad s_3 = 1.09$$

$$\begin{aligned} \frac{|a_{11}|}{s_1} &= \tfrac{2.11}{4.21} = 0.501 \\ \frac{|a_{21}|}{s_2} &= \tfrac{4.01}{10.2} = 0.393 \\ \frac{|a_{31}|}{s_3} &= \tfrac{1.09}{1.09} = 1 \end{aligned}$$

So we do $R_1 \longleftrightarrow R_3$.

$$\begin{bmatrix} 1.09 & 0.987 & 0.832 & : & 4.21 \\ 4.01 & 10.2 & -1.12 & : & -3.09 \\ 2.11 & -4.21 & 0.921 & : & 2.01 \end{bmatrix}$$

$$R_2 - \frac{4.01}{1.09} R_1 \text{ and } R_3 - \frac{2.11}{1.09} R_1 \text{ give } \begin{bmatrix} 1.09 & 0.987 & 0.832 & : & 4.21 \\ 0 & 6.57 & -4.18 & : & -18.6 \\ 0 & -6.12 & -0.689 & : & -6.16 \end{bmatrix}$$

Note $s_2 = 10.2$ and $s_3 = 4.21$, since we did $R_1 \leftrightarrow R_3$

$$\begin{aligned} \frac{|a_{22}|}{s_2} &= \tfrac{6.57}{10.2} &= 0.644 \\ \frac{|a_{32}|}{s_3} &= \tfrac{6.12}{4.21} &= 1.45 \end{aligned}$$

So we do $R_3 \leftrightarrow R_2$ and do further computation.