Books:

1. Trefethen, L and Bau D., Numerical Linear Algebra, SIAM

2. Gene Golub and Van Loan, Matrix Computation

3. J. W. Demmel, Applied numerical linear Algebra

- Linear Systems

  - Gauss-elimination
  - LU decomposition

$Ax = b$, with $A = (a_{ij})_{n\times n}$, $b = (b_i)_{n\times 1}$

Exm. Find the parabola $y = A + Bx + Cx^2$ that passes through $(1,1)$, $(2,-1)$ and $(3,1)$.

Soln: We obtain

$$A + B + C = 1$$
$$A + 2B + 4C = -1$$
$$A + 3B + 9C = 1$$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$$

Let, $A = [\bar{a}_1\ \bar{a}_2\ \bar{a}_3 \dots \bar{a}_n]$ where $\bar{a}_i$'s are column vectors.

Cramer's Rule :- For $\det(A) \neq 0$, the linear system $Ax = b$ has the unique solution,

$$x_i = \frac{\det(A_i)}{\det(A)}, \quad i = 1(1)n$$

where A_i is the matrix obtained from A, replacing $\bar{a}_i$ by b.

$\Rightarrow \quad A = \frac{14}{2} = 7, \quad B = \frac{-16}{2} = -8, \quad C = \frac{4}{2} = 2$

Cramer's Rule is simple and elegant, but computationally a disaster.

<u>Computational Cost</u> :-

Let, R_n be the no of operations (Multiplication and addition) to calculate an $n \times n$ determinant.

\# Determinant is expanded as a sum of $(n-1)$ order minors, multiplied by element.

Then, $R_n = nR_{n-1} + n + (n-1)$

$= nR_{n-1} + 2n - 1$

Let, M_n be the no of operations in Cramer's Rule

$M_n = (n+1)R_n + n$ [Computing $(n+1)$ $n \times n$ determinants and n divisions]

We have $R_2 = 3$

$M_2 = 11$

So, $R_n \sim O(n!)$ & $M_n \sim O((n+1)!)$. This is too large for large n.

$\Rightarrow$ For 8 eqns, we need to do 25,40,160 operations in 700 hrs if one can perform one operation per sec.

$\Rightarrow$ No information if $\det(A) = 0$.

Exm.

$$\left.\begin{aligned} x + 2y + z &= 1 \\ 2x + 4y + 2z &= 2 \\ x + 2y &= 1 \end{aligned}\right\} \det(A) = 0$$

But infinite soln

$x + 2y = 1, \; z = 0$. whole line.

Gauss Elimination :-

$$2x + 3y + 5z = 1$$
$$4y + z = 5$$
$$3z = 15$$

$$\Rightarrow \left.\begin{aligned} z &= 15/3 = 5 \\ y &= \frac{5-5}{4} = 0 \\ x &= \frac{1-25}{2} = -12 \end{aligned}\right\} \text{Back - substitution}$$

$$A = \begin{pmatrix} 2 & 3 & 5 \\ 0 & 4 & 1 \\ 0 & 0 & 3 \end{pmatrix} \quad \text{upper - triangular.}$$

Aim: Gauss elimination converts any matrix A into an equivalent upper triangular form.

$$Ax = b \Rightarrow Ux = b_1$$
$$\downarrow$$
Back - subs.

Exm.

$$2x + 3y = 5 \quad \cdots (\text{i})$$
$$x + y = 3 \quad \cdots (\text{ii})$$

$$\begin{pmatrix} 2 & 3 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 5 \\ 3 \end{pmatrix}$$

$(\text{ii}) - \frac{1}{2} \times (\text{i})$:

$$2x + 3y = 5$$
$$-\frac{y}{2} = \frac{1}{2}$$

$$\begin{pmatrix} 2 & 3 \\ 0 & -1/2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Use back-substitution to get

$$y = -1$$
$$x = 4$$

In matrix form,

$$[A \mid b] = \left(\begin{array}{cc|c} 2 & 3 & 5 \\ 1 & 1 & 3 \end{array}\right) \xrightarrow{R_2 - \frac{1}{2}R_1} \left(\begin{array}{cc|c} 2 & 3 & 5 \\ 0 & -1/2 & 1/2 \end{array}\right)$$

Augmented matrix.

Theorem : For any square matrix A, $\exists$ one non-singular matrix M such that $U = MA$ is upper triangular.

How are we getting $\begin{pmatrix} 2 & 3 \\ 0 & -\frac{1}{2} \end{pmatrix}$ from $\begin{pmatrix} 2 & 3 \\ 1 & 1 \end{pmatrix}$?

Ans:

Elementary matrix differs from the identity matrix by one single elementary operation.

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \xrightarrow{R_2 - \frac{1}{2}R_1} \begin{pmatrix} 1 & 0 \\ -\frac{1}{2} & 1 \end{pmatrix} = L_1$$

$$L_1 A = \begin{pmatrix} 1 & 0 \\ -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 2 & 3 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 3 \\ 0 & -\frac{1}{2} \end{pmatrix} = U$$

$$\therefore \quad A = L_1^{-1} U = \begin{pmatrix} 1 & 0 \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 2 & 3 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

$$= \underline{LU}.$$

This is called LU decomposition.

Exm.

$$A = \begin{pmatrix} -3 & +2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{pmatrix} \qquad b = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}$$

$$[A|b] \xrightarrow[R_3 + R_1]{R_2 + 2R_1} \left(\begin{array}{ccc|c} -3 & 2 & -1 & 1 \\ 0 & -2 & 5 & 4 \\ 0 & -2 & 3 & 2 \end{array}\right) \xrightarrow{R_3 - R_2} \left(\begin{array}{ccc|c} -3 & 2 & -1 & 1 \\ 0 & -2 & 5 & 4 \\ 0 & 0 & -2 & -2 \end{array}\right)$$

With back. subs, the soln is:

$z = 1$
$y = \frac{1}{2}$
$x = -\frac{1}{3}$

$$L_2 L_1 A = U$$

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

$$\therefore \quad A = L_1^{-1} L_2^{-1} U$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} U.$$

LU decomposition

$$A = LU$$

$$Ax = b \Rightarrow LUx = b$$

Let, $Ux = y$ then $Ly = b$

Forward subs: $Ly = b$

Backward subs: $Ux = y$

Difficulty :- (I) $A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$: Gauss-elimination fails

(II)

$$\begin{pmatrix} 10^{-4} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Original Soln : $x_1 = \frac{1}{1-10^{-4}}$, $x_2 = 2 - \frac{1}{1-10^{-4}}$

$$\left(\begin{array}{cc|c} 10^{-4} & 1 & 1 \\ 1 & 1 & 2 \end{array}\right) \xrightarrow{R_2 - 10^4 R_1} \left(\begin{array}{cc|c} 10^{-4} & 1 & 1 \\ 0 & -9999 & -9998 \end{array}\right)$$

So, $x_2 = 0.9999 \simeq 1$

$x_1 = 0$

Remedy:

$$\frac{1.2567}{10^{-4}} = 12567$$

$$\frac{1.26}{10^{-4}} = 12600$$

Error margin: 33

To avoid these round-off error from small pivots/ Zero pivots, row interchanges are made (Partial pivoting) or both rows and columns are interchanged (Complete pivoting)

Exm

$$A = \begin{pmatrix} -2 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -8 & 4 \end{pmatrix}$$

We interchange rows to place the largest element of 1st column in the pivot

$$A \xrightarrow{P_{12}} \begin{pmatrix} 6 & -6 & 7 \\ -2 & 2 & -1 \\ 3 & -8 & 4 \end{pmatrix} \xrightarrow[R_3 - \frac{1}{2}R_1]{R_2 + \frac{1}{3}R_1} \begin{pmatrix} 6 & -6 & 7 \\ 0 & 0 & 4/3 \\ 0 & -5 & 1/2 \end{pmatrix}$$

$$\xrightarrow{P_{23}} \begin{pmatrix} 6 & -6 & 7 \\ 0 & -5 & 1/2 \\ 0 & 0 & 4/3 \end{pmatrix} = U$$

P_{12} & P_{23} are permutation matrices.

$\Rightarrow$ A permutation matrix P is an identity matrix with permuted rows.

Property:

1. (I) PX is same as X with rows permuted
   XP is same as X with columns permuted
2. (II) $P^{-1} = P^T$
3. (III) $\det(P) = \pm 1$
4. (IV) $P_1 P_2$ is also a permutation matrix.

$P_{23} M_1 P_{12} A = U$ where

$$P_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad P_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix}$$

$$(P_{23} M_1 P_{23}) P_{23} P_{12} A = U$$

$$\Rightarrow \quad PA = (P_{23} M_1^{-1} P_{23}) U = P_{23} \begin{pmatrix} 1 & 0 & 0 \\ -1/3 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix} P_{23} \; U$$

$$PA = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ -\frac{1}{3} & 0 & 1 \end{pmatrix} U = LU.$$

$$P = P_{23} P_{12} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Operation Count :-

GE :

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \xrightarrow[R_3 - \frac{a_{31}}{a_{11}} R_1]{R_2 - \frac{a_{21}}{a_{11}} R_1} \begin{pmatrix} \text{---} & \text{---} & \text{---} \\ 0 & \boxed{} & \\ 0 & & \end{pmatrix}$$

In step i, we eliminate x_i from $(n-i)$ equations or $(n-i)$ rows. This needs $n-i$ divisions in computing the multiplier $m_{ji} \left(= \frac{a_{ji}}{a_{ii}}\right)$ and $(n-i)^2$ multiplications and as many subtractions. Since we do a total $(n-1)$ steps, the total ~~no~~ no of operations is

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

$$= \sum_{k=1}^{n-1} (k + 2k^2) = \frac{n(n-1)}{2} + \frac{n(n-1)(2n-1)}{3}$$

$$= \frac{2}{3} n^3 - \frac{n^2}{2} - \frac{n}{6}$$

$$= O(n^3)$$

Back Substitutions :

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

The solution x_i is given by,

$$x_i = \frac{1}{a_{ii}} \left(b_i - \sum_{J=i+1}^{n} a_{iJ} x_J \right)$$

For x_i, we make $(n-i)$ multiplications and as many subtractions and 1 division. So, total no of operations

$$= 2 \sum_{i=1}^{n} (n-i) + n = 2 \sum_{K=1}^{n-1} K + n$$

$$= n(n-1) + n = n^2$$

Therefore, forward and backward substitution cost $O(n^2)$ operations

$A = LU$. How does the eigenvalues of A & L, U connects?

$$LU = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = A$$

$eig(L) = 1, 1$ $\qquad$ $eig(A) = 0, 2$.

$eig(U) = 1, 0$

Is $\det(A) \neq 0$ enough for LU decomposition?

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 1 & 3 & 4 \end{pmatrix} \xrightarrow[R_3 - R_1]{R_2 - 2R_1} \begin{pmatrix} 1 & 2 & 3 \\ 0 & 0 & -1 \\ 0 & 1 & 1 \end{pmatrix}$$

But $\det(A) = 1 \neq 0$.

Theorem :-

a) Any square matrix A, singular or non-singular, has a factorization $PA = LU$, with P permutation matrix, L unit lower triangular matrix and U upper-triangular.

b) A non-singular matrix A is LU diagonalizable iff all leading principal submatrices of A are non-singular.

c) If A is a singular matrix of rank k, then it admits an LU factorization if the first k leading minors are non-zero. [Converse not true] $A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

Proof

(b) $A = LU \Rightarrow$ leading minors are non-zero

In terms of block matrices:

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{pmatrix}$$

$$= \begin{pmatrix} L_{11}U_{11} & L_{12}U_{12} \\ L_{21}U_{11} & L_{21}U_{12} + L_{22}U_{22} \end{pmatrix}$$

where A_{11} is a leading principal submatrix of order $1 \le J \le n$, as are L_{11} and U_{11}.

So, $\det(A_{11}) = \det(L_{11}) \det(U_{11})$
$= \det(U_{11}) \neq 0$

L is unit triangular & U is non-singular.

leading minors are non-zero $\Rightarrow A = LU$.

The proof is by induction on the size of the matrix A.

$n = 1$. $\quad a_{11} = l_{11} u_{11} = 1 . a_{11}$.

Assume that the result is true for $n = K-1$. Let, $\tilde{A}$ is a square matrix of order K.

We need to find unique triangular matrices L & U of order $(K-1)$, unique $(K-1)\times 1$ vectors l and u, and a unique non-zero number α such that the following decomposition holds:

$$\tilde{A} = \begin{pmatrix} A & b \\ c^T & \delta \end{pmatrix} = \begin{pmatrix} L & 0 \\ l^T & 1 \end{pmatrix} \begin{pmatrix} U & u \\ 0 & \alpha \end{pmatrix} = \begin{pmatrix} LU & Lu \\ l^T U & l^T u + \alpha \end{pmatrix}$$

By the induction hypothesis, $\exists$ unique matrices L and U of order $(k-1)$ such that $A = LU$. We get

$$u = L^{-1} b, \quad l^T = c^T U^{-1}, \quad \alpha = \delta - l^T u.$$

So, u, l and α are unique. Also, U is non-singular

Therefore,
$$0 \neq \det(\tilde{A}) = \det \begin{pmatrix} L & 0 \\ l^T & 1 \end{pmatrix} \det \begin{pmatrix} U & u \\ 0 & \alpha \end{pmatrix}$$
$$= \alpha \det(U)$$

$\therefore \quad \underline{\alpha \neq 0}.$

Result: If A is positive definite, i.e. $x^T A x > 0 \quad \forall x \neq 0$, then all leading principal minors of A are non-zero.

For
$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & \cdots & \cdots & a_{nn} \end{pmatrix},$$
we assume
$$A_k = \begin{pmatrix} a_{11} & \cdots & a_{1k} \\ \vdots & & \\ a_{k1} & \cdots & a_{kk} \end{pmatrix}$$
as the kth principal leading submatrix.

Assume, if possible A_k is singular. Then, $\exists$ a vector

$$\begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} \neq 0 \quad \text{such that} \quad A_k \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} = 0$$

let,
$$\bar{x}_0 = \begin{pmatrix} x_1 \\ \vdots \\ x_k \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$
Then, $\bar{x}_0^T A \bar{x}_0 = 0$ and $\bar{x}_0 \neq 0$

This contradicts that A is positive definite. So, A_k is non-singular.

Converse is not true.
$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
$\det(A_1) \neq 0$
$\det(A_2) \neq 0$
but A is not p.d.

Symmetric Positive Definite Matrix :

If $A^T = A$ and $x^T A x > 0 \quad \forall x \neq 0$, then A is called s.p.d.

Theorem:

i) If X is non-singular, then A is s.p.d iff $X^T A X$ is spd.

ii) If A is spd, then any principal submatrix A_K is spd

iii) A is spd iff $A = A^T$ and all eigenvalues are +ve

iv) If A is spd, then $a_{ii} > 0$ and $\max |a_{ij}| = \max_i a_{ii} > 0$

v) A is spd iff $\exists$ a unique lower triangular non-singular matrix L, with +ve diagonal entries such that $A = LL^T$. This is called the cholesky factorization of A.

Proof:

i) If X is non-singular, then $Xx \neq 0 \quad \forall x \neq 0$, and thus
$$x^T(X^T A X)x > 0 \quad \forall x \neq 0 \text{ if } A \text{ is spd.}$$

~~Since A is spd, this implies that $X^T A X$ is spd~~

The opposite implication is true as X is invertible.

ii) Do yourself

iii) Let, X be the real, orthogonal eigenvecter matrix of A so that $X^T A X = D$, diagonal matrix of real eigenvalues λ_i. $\cancel{x^T A x = x^T \lambda}$

$$x^T D x = \sum \lambda_i x_i^2$$

D is spd iff $\lambda_i > 0 \ \forall i$ Now apply (i).

(iv) Let, A is spd.

Let, e_k be the kth column of the identity matrix.

Then $e_k^T A e_k = a_{kk} > 0 \quad \forall k$.

If $|a_{mn}| = \max_{ij} |a_{ij}|$, but $m \neq n$, choose

$\bar{x}_0 = e_m - \text{sign}(a_{mn}) e_n$.

Then $\bar{x}_0^T A \bar{x}_0 = a_{mm} + a_{nn} - 2|a_{mn}| \leq 0$, contradicts that A is spd. So, $\max_{ij} |a_{ij}| = \max_i a_{ii}$.

v) Let, $A = LL^T$ with L non-singular.

Then,
$$x^T A x = x^T L L^T x$$
$$= (L^T x)^T L^T x$$
$$= \|L^T x\|_2^2 > 0 \quad \text{for } x \neq 0$$

So, A is spd.

Now let A is spd. Therefore $A = LU$ with diagonal elements of L being all 1.

Since A is invertible, we write $U = D\bar{U}$ with D diagonal matrix and diagonal elements of $\bar{U}$ all 1.

So, $A = LD\bar{U}$

Hence, $A^T = \bar{U}^T D L^T = A = LU$

By the uniqueness of LU decomposition, $L = \bar{U}^T$. $\Rightarrow \bar{U} = L^T$.

So, $A = LDL^T$.

Now, A being ~~β~~ spd

$$d_{ii} = e_i^T D e_i = e_i^T L^{-1} A (L^T)^{-1} e_i$$

$$= (L^{-T} e_i)^T A (L^{-T} e_i) > 0$$

Set $D^{1/2} = \text{diag}\left(\sqrt{d_{11}}, \sqrt{d_{22}}, \ldots \sqrt{d_{nn}}\right)$

then $A = (LD^{1/2})(LD^{1/2})^T = \bar{L}\bar{L}^T$

This completes the result.

<u>H.W</u>. 1. If A is strictly diagonally dominant, i.e

$$|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \quad \forall i$$

then A is LU decomposible

Hint: Use Gauss-- elimination.

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2. Let, A is spd. Show that $|a_{ij}| < \sqrt{a_{ii} a_{jj}}$