linear algebra :

when we solve a system of odes or pdes, very often we run into a situation

$Ax = b$ where A is a general matrix of order $m \times n$ b is usually calculated from pevious time step(s), and x is the solution that we seek.

From fundamental linear algebra, we can use Gaussian Elimination to reduce $Ax=b$ to a triangular system and solve using backward substitution:

For example:

$$\begin{array}{c} \\ m_{21}=\frac{a_{21}}{a_{11}} \\ m_{31}=\frac{a_{31}}{a_{11}} \\ m_{41}=\frac{a_{41}}{a_{11}} \end{array} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

row2 − m_{21} row1
row3 − m_{31} row1
row4 − m_{41} row1

$$\begin{array}{c} \\ \\ m_{32}=\frac{a_{32}^{(2)}}{a_{22}^{(2)}} \\ m_{42}=\frac{a_{42}^{(2)}}{a_{22}^{(2)}} \end{array} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & a_{34}^{(2)} \\ 0 & a_{42}^{(2)} & a_{43}^{(2)} & a_{44}^{(2)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2^{(2)} \\ b_3^{(2)} \\ b_4^{(2)} \end{bmatrix}$$

$$\underset{U}{\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} \\ 0 & 0 & 0 & a_{44}^{(4)} \end{bmatrix}} \cdot \underset{x}{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}} = \underset{b}{\begin{bmatrix} b_1 \\ b_2^{(2)} \\ b_3^{(3)} \\ b_4^{(4)} \end{bmatrix}}$$

use back substitution to solve for $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$

$$x_4 = \frac{b_4^{(4)}}{a_{44}^{(4)}} \qquad x_3 = \frac{b_3^{(3)} - a_{34}^{(3)} x_4}{a_{33}^{(3)}} \quad \ldots$$

More formally: first step of elimination

$$L_1 A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -m_{21} & 1 & 0 & 0 \\ -m_{31} & 0 & 1 & 0 \\ -m_{41} & 0 & 0 & 1 \end{bmatrix} A$$

$$L_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -m_{32} & 1 & 0 \\ 0 & -m_{42} & 0 & 1 \end{bmatrix}$$

$$L_3 L_2 L_1 A = U \quad , \quad A = L_1^{-1} L_2^{-1} L_3^{-1} U$$
$$= LU$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ m_{21} & 1 & 0 & 0 \\ m_{31} & m_{32} & 1 & 0 \\ m_{41} & m_{42} & m_{43} & 1 \end{bmatrix} \rightarrow LU \text{ decomposition}$$

Procedure:

$Ly = b \rightarrow$ Forward sub to solve for y

$Ux = y \rightarrow$ back sub to solve for x

Operation Counts :

1. elimination step : $A \to U$

Add / sub : $(n-1)^2 + (n-2)^2 + \cdots + 1 = \frac{n(n-1)(2n-1)}{6}$

Mult : $(n-1)^2 + (n-2)^2 + \cdots + 1 = \frac{n(n-1)(2n-1)}{6}$

Div : $(n-1) + (n-2) + \cdots + 1 = \frac{n(n-1)}{2}$

2. back substitution :

Add / Sub : $0 + 1 + 2 + \cdots + (n-1) = \frac{n(n-1)}{2}$

Mult / Div : $1 + 2 + 3 + \cdots + n = \frac{n(n+1)}{2}$

Grand Totals :

Add / Sub : $\frac{n(n-1)(2n+5)}{6}$

Mult / Div : $\frac{n(n^2+3n-1)}{3}$

AS , MD $\sim \frac{n^3}{3}$ $\longrightarrow$ faster than multiplying 2 matrices.

Note ① most of the computational expense is in elimination step
back sub. & modifying RHS are order n^2

② much cheaper than other direct solvers, such as Cramer's Rule ($(n+1)!$ operations) or finding inverse matrix A^{-1} ($\frac{8n^3}{3}$)

Vector & Matrix norms :

Definition: Let V be a vector space, and let $N(x)$ be a real valued function defined on V. Then $N(x)$ is a norm if

(N1) $N(x) \geq 0$ for all $x \in V$, $N(x) = 0$ iff $x = 0$

(N2) $N(\alpha x) = |\alpha| N(x)$, for all $x \in V$ and all scalars α.

(N3) $N(x+y) \leq N(x) + N(y)$, for all $x, y \in V$

$\Rightarrow$ triangular inequality

$$\| x - z \| \leq \| x - y \| + \| y - z \|$$

$\Rightarrow$ reverse triangle inequality

$$\big| \| x \| - \| y \| \big| \leq \| x - y \|$$

Note: the p-norm for $1 \leq p < \infty$ is defined as

$$\| x \|_p = \left[\sum_{1}^{n} |x_j|^p \right]^{1/p}, \quad x \in C^n$$

Note: the maximum norm

$$\| x \|_\infty = \max_{1 \leq j \leq n} |x_j|, \quad x \in C^n$$

Matrix Norms: N1, N2 and N3

(N4) $\|AB\| \leq \|A\|\|B\|$

(N5) matrix & vector norms be compatible

$$\|Ax\|_v \leq \|A\| \, \|x\|_v \qquad x \in V$$

$$\|Ax\|_2 = \left[\sum_{i=1}^{n} \left|\sum_{j=1}^{n} a_{ij} x_j\right|^2\right]^{1/2}$$

$$\leq \left[\sum_{i=1}^{n} \left\{\sum_{j=1}^{n} |a_{ij}|^2\right\} \left\{\sum_{j=1}^{n} |x_j|^2\right\}\right]^{1/2}$$

C-S inequality $|(x,y)^2| \leq (x,x)(y,y)$

$$\therefore \quad \|Ax\|_2 \leq F(A) \|x\|_2 \, , \quad F(A) = \left[\sum_{i,j=1}^{n} |a_{ij}|^2\right]^{1/2}$$ the Frobenius norm

$$F(AB) = \left[\sum_{i,j=1}^{n} \left|\sum_{k=1}^{n} a_{ik} b_{kj}\right|^2\right]^{1/2}$$

$$\leq \left[\sum_{i,j=1}^{n} \left\{\sum_{k=1}^{n} |a_{ik}|^2\right\} \left\{\sum_{k=1}^{n} |b_{kj}|^2\right\}\right]^{1/2} = F(A)F(B),$$

$\therefore$ (N4) is satisfied $\Longrightarrow$ $F(A)$ is a matrix norm.

Given a vector norm $\|\cdot\|_v$,
the associated matrix norm $\|A\| = \text{Supremum} \dfrac{\|Ax\|_v}{\|x\|_v}$

$$\|Ax\|_1 = \sum_{i=1}^{n}\left|\sum_{j=1}^{n} a_{ij} x_j\right| \leq \sum_{i=1}^{n}\sum_{j=1}^{n} |a_{ij}|\,|x_j|$$

$$\leq \sum_{j=1}^{n} |x_j| \sum_{i=1}^{n} |a_{ij}|$$

define $c \equiv \underset{1\leq j\leq n}{\text{Max}} \sum_{i=1}^{n} |a_{ij}|$

$$\|Ax\|_1 \leq c\,\|x\|_1$$

$$\therefore \quad \frac{\|Ax\|_1}{\|x\|_1} \leq c$$

$$\|A\|_1 \leq c$$

if $x = e^{(k)}$, the k th unit vector $\|x_k\|_1 = 1$

$$\|Ax\|_1 = \sum_{i=1}^{n}\left|\sum_{j=1}^{n} a_{ij} x_j\right| = \sum_{i=1}^{n} |a_{ik}| = c$$

$$\Rightarrow \|A\|_1 = \underset{1\leq j\leq n}{\text{Max}} \sum_{i=1}^{n} |a_{ij}| \longrightarrow \text{column norm}$$

similarly, we can derive $\|A\|_\infty$ from the operator norm

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

$$\|A\|_2 = \sqrt{r_\sigma(A^*A)} \qquad r_\sigma(A) = \max_{\lambda\in\sigma(A)} |\lambda| \quad \text{spectral radius}$$

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

Example:

$$A = \begin{bmatrix} 1 & -2 \\ -3 & 4 \end{bmatrix}$$

$$\|A\|_1 = 2+4 = 6$$

$$\|A\|_\infty = 3+4 = 7$$

$$\|A\|_2 \Rightarrow \quad A^*A = \begin{bmatrix} 10 & -14 \\ -14 & 20 \end{bmatrix} \quad \lambda = 15 \pm \sqrt{221}$$

$$\therefore \|A\|_2 = \sqrt{15+\sqrt{221}} \approx 5.46$$

Theorem: Let A be a square matrix. If $r_\sigma(A) < 1$, then $(I-A)^{-1}$ exists and it can be expressed as a convergent series

$$(I-A)^{-1} = I + A + A^2 + \cdots + A^m + \cdots$$

$\Rightarrow$ First existence:

Assume $(I-A)\cdot x = 0$ if $x \neq 0$. A has an eigenvalue $= 1$

but $r_\sigma(A) < 1$ $\therefore$ $x = 0$ is the only solution

$\Rightarrow$ $(I-A)^{-1}$ exists

$$\Rightarrow (I-A)(I + A + A^2 + \cdots + A^m) = I - A^{m+1}$$

$$\therefore I + A + A^2 + \cdots + A^m = \frac{I - A^{m+1}}{I - A}$$

Since $r_\sigma(A) < 1$ $A^{m+1} \to 0$ as $m \to \infty$

$$\therefore (I-A)^{-1} = I + A + A^2 + \cdots + A^m + \cdots$$

$\Rightarrow$ Let A be a square matrix, if for some operator matrix norm $\|A\| < 1$, then $(I-A)^{-1}$ exists and has the geometric series expression $(I-A)^{-1} = I + A + A^2 + \cdots + A^m + \cdots$

$$\|(I-A)^{-1}\| \leq \frac{1}{I - \|A\|}$$

Example:

$$\begin{aligned} 6x_1 + 2x_2 + 2x_3 &= -2 \\ 2x_1 + \tfrac{2}{3}x_2 + \tfrac{1}{3}x_3 &= 1 \\ x_1 + 2x_2 - x_3 &= 0 \end{aligned} \qquad \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.6 \\ -3.8 \\ -5.0 \end{bmatrix}$$

Gaussian Elmination:

$$\left[\begin{array}{ccc|c} 6 & 2 & 2 & -2 \\ 2 & \frac{2}{3} & \frac{1}{3} & 1 \\ 1 & 2 & -1 & 0 \end{array}\right]$$

$$\left[\begin{array}{ccc|c} 6 & 2 & 2 & -2 \\ 0 & 0 & -\frac{1}{3} & \frac{5}{3} \\ 0 & \frac{5}{3} & -\frac{4}{3} & \frac{1}{3} \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 6.000 & 2.000 & 2.000 & -2.000 \\ 0.0 & 0.0001 & -0.3333 & 1.667 \\ 0.0 & 1.667 & -1.333 & 0.3334 \end{array}\right]$$

$$\left[\begin{array}{ccc|c} 6 & 2 & 2 & -2 \\ 0 & 5/3 & -4/3 & 1/3 \\ 0 & 0 & -1/3 & 5/3 \end{array}\right]$$

$x_3 = -5$

$x_2 = -3.8$

$x_1 = 2.6$.

Computationally

$$\left[\begin{array}{ccc|c} 6.000 & 2.000 & 2.000 & -2.000 \\ 0.0 & 0.0001 & -0.3333 & 1.6667 \\ 0.000 & 0.000 & 5555 & -27790 \end{array}\right]$$

$x_1 = 1.335$

$x_2 = 0.0$

$x_3 = -5.003$

needs to conduct partial pivoting : $C = \max\limits_{k \le j \le n} |a_{jk}^{(k)}|$

if $|a_{kk}^{(k)}| < c$, interchange rows to avoid zero pivots.