Note Title 3/23/2011

Numerical Differentiation

$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} - \frac{h^2}{6} f'''(\xi)$$

$$f'_{comp} = \frac{f(a+h) + E_1 - \{ f(a-h) + E_2 \}}{2h}$$

E_1, E_2 : round-off errors

$$f'(a) = f'_{comp} + \underbrace{\frac{E_2 - E_1}{2h}}_{\text{does not decrease}} - \frac{h^2}{6} f'''(\xi)$$

Numerical Integration

$$\int_a^b f(x)\,dx \simeq \frac{h}{2}\left(f(a)+f(b)\right) + h\sum_{i=1}^{n-1} f(t_i) \doteq T_n \,.$$

$$T_n^{\text{comp.}} = T_n + \frac{h}{2}\left(E_0 + E_n\right) + h\sum_{i=1}^{n-1} E_i$$

Round-off error

Note Title 2/7/2011

System of linear equations

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$

$$\vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n$$

$Ax = b$, $A = [a_{ij}]$: coefficient matrix

$b = [b_1 \; b_2 \cdots b_n]^T$: Right Hand Side

$x = [x_1 \; x_2 \cdots x_n]^T$: unknown vector

$[A \;\; b]$: $n \times (n+1)$: augmented matrix.

$Ax = b$. If A is invertible, then the system has a unique solution: $x = A^{-1}b$.

Cramer's Rule

$$x_j = \frac{\begin{vmatrix} a_{11} & \cdots & b_1 & a_{1n} \\ a_{21} & & b_2 & a_{2n} \\ \vdots & & \vdots & \vdots \\ a_{n1} & & b_n & a_{nn} \end{vmatrix}}{\det A}, \quad j = 1, \cdots, n.$$

too expensive

Upper triangular system.

$$u_{11} x_1 + u_{12} x_2 + \cdots + u_{1n} x_n = y_1$$

$$u_{22} x_2 + \cdots + u_{2n} x_n = y_2$$

$$u_{n-1,n-1} x_{n-1} + u_{n-1,n} x_n = y_{n-1}$$

$$u_{nn} x_n = y_n$$

$\det(U) = u_{11} u_{22} \cdots u_{nn} \neq 0$

$\Rightarrow u_{ii} \neq 0$

$$x_n = \frac{y_n}{u_{nn}}, \quad x_{n-1} = \frac{y_{n-1} - u_{n-1,n} x_n}{u_{n-1,n-1}}, \quad \ldots$$

Aim: To replace $Ax = b$ by an <u>equivalent</u> upper triangular system $Ux = y$ using elementary row transformations of the type

$$R_i \longrightarrow R_i - \alpha R_j ,$$

where $\alpha \in \mathbb{R}$, R_i : ith row of the augmented matrix.

Additional Assumption

$$
\left[\begin{array}{cccc|cc}
a_{11} & a_{12} & \cdots & a_{1k} & \cdots & a_{1n} \\
a_{21} & a_{22} & \cdots & a_{2k} & \cdots & a_{2n} \\
\vdots & & & & & \\
a_{k1} & a_{k2} & \cdots & a_{kk} & \cdots & a_{kn} \\
\hline
\vdots & & & & & \\
a_{n1} & a_{n2} & \cdots & a_{nk} & \cdots & a_{nn}
\end{array}\right]
\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \\ \vdots \\ x_n \end{bmatrix}
=
\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \\ \vdots \\ b_n \end{bmatrix}.
$$

A_k : principal leading submatrix.

Assumption : $\det(A_k) \neq 0, \quad k = 1, 2, \cdots, n$

Gauss elimination method

1 flop (floating point operation)

= 1 addition / subtraction + 1 multiplication / division.

Step 1:

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{bmatrix} \to \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} & b_2^{(1)} \\ \vdots & & & & \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} & b_n^{(1)} \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{bmatrix} \longrightarrow \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} & b_2^{(1)} \\ \vdots & & & & \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} & b_n^{(1)} \end{bmatrix}$$

$a_{11} \neq 0$ (why?), Define $m_{i1} = \dfrac{a_{i1}}{a_{11}}, \; i = 2, \cdots, n$

$$R_i \longrightarrow R_i - m_{i1} R_1, \quad i = 2, \cdots, n$$

$$a_{ij}^{(1)} = a_{ij} - m_{i1} a_{1j}, \quad b_i^{(1)} = b_i - m_{i1} b_1, \quad \begin{matrix} i = 2, \cdots, n \\ j = 2, \cdots, n. \end{matrix}$$

$(n-1)n$ mult. $+$ $(n-1)n$ subtractions $+$ $n-1$ divisions

$$A_2 = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \longrightarrow \begin{bmatrix} a_{11} & a_{12} \\ 0 & a_{22}^{(1)} \end{bmatrix}$$

$$\det(A_2) = a_{11}\, a_{22}^{(1)} \implies a_{22}^{(1)} \neq 0$$

$\neq 0$ by assumption

Perform similar operations on $(n-1) \times n$ matrix.

$$[A : b] \longrightarrow [A^{(1)} : b^{(1)}] \longrightarrow [A^{(2)} : b^{(2)}]$$

$[A : b] \longrightarrow [A^{(1)} : b^{(1)}]$

$(n-1)n$ multi. + $(n-1)n$ subtractions + $n-1$ divisions

$[A^{(1)} : b^{(1)}] \longrightarrow [A^{(2)} : b^{(2)}]$

$(n-2)(n-1)$ mult. + $(n-2)(n-1)$ sub. + $n-2$ divisions.

Total number of operations : $[A : b] \longrightarrow [U : y]$

$\left[(n-1)^2 + (n-2)^2 + \cdots + 1\right] + \left[(n-1) + (n-2) + \cdots + 1\right]$ flops

$+ \left[(n-1) + (n-2) + \cdots + 1\right]$ divisions

$= \dfrac{(n-1)n(2n-1)}{6} + \dfrac{(n-1)n}{2}$ flops $+ \dfrac{(n-1)n}{2}$ divisions

$O\left(\frac{n^3}{3}\right)$

Back Substitution

$Ax = b \longrightarrow Ux = y$. $U = [u_{ij}]$

$u_{ii} \neq 0$, $i = 1, \cdots, n$, $u_{ij} = 0$ if $i > j$.

$u_{ii} x_i + u_{i,i+1} x_{i+1} + \cdots + u_{in} x_n = y_i$: ith eq^n

$$x_i = \frac{y_i - \sum_{j=i+1}^{n} u_{ij} x_j}{u_{ii}}, \quad i = n, n-1, \cdots, 1.$$

Number of operations $= \sum_{i=1}^{n-1} (n-i)$ flops + n divisions

$= \frac{(n-1)n}{2}$ flops + n divisions $\qquad O\left(\frac{n^2}{2}\right)$

Definition : A is said to be positive - definite

if i) $A^T = A$ ii) $x^T A x > 0$ if $x \neq \bar{0}$

$Au = \lambda u$, $u \neq \bar{0}$ $\Rightarrow$ $\lambda = \dfrac{u^T A u}{u^T u} > 0$

eigenvalues of A are > 0.

$\det(A) =$ product of eigenvalues > 0

A_k : principal leading submatrix of A of order k.

Claim: A_k is positive definite

Proof: $A^T = A \implies a_{ij} = a_{ji}$, $i, j = 1, \cdots, n$

$\implies a_{ij} = a_{ji}$, $i, j = 1, \cdots, k \implies A_k^T = A_k$

Claim: If $y \neq \overline{0}$, then $y^T A_k y > 0$

Proof:

Let $y = [y_1\ y_2 \cdots y_k]^T$ be such that at least one $y_p \neq 0$. Define $x = [y, \underbrace{0, 0, \cdots, 0}_{n-k}]^T$.

Then $$y^T A_k y = \sum_{i=1}^{k} \sum_{j=1}^{k} a_{ij}\, y_i\, y_j$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}\, x_i\, x_j = x^T A x > 0$$

Thus A_k is positive definite and hence $\det(A_k) > 0$.

$A = M^T M$, M : invertible.

$A^T = A$. $x^T A x = x^T M^T M x$

$= y^T y = \sum_{i=1}^{n} y_i^2$

$x \neq \bar{0} \implies Mx \neq \bar{0} \implies y^T y > 0$.

A : positive definite.

Converse is true : Cholesky decomposition