Lecture 14

Last time we did Numerical differentiation.

We derived 3 formula

$$f'(a) \approx \frac{f(a+h) - f(a)}{h} \qquad O(h) \text{ approx}$$

$$f'(a) \approx \frac{f(a+h) - f(a-h)}{2h} \qquad O(h^2) \text{ approx}$$

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h}$$

$O(h^2)$ approx

---x---x---

Then we discussed on how Numerical differentiation is a "bad" process.

i.e if we reduce h (to decrease truncation error) we end up increasing round-off error

So Numerical diff has to be done with care

One way to increase accuracy is to use Richardson extrapolation

$$f'(a) = \frac{f(a+h)-f(a-h)}{2h} + c_2 h^2 + c_4 h^4 + c_6 h^6 + \cdots$$

c_2, c_4, c_6 are constants.

Today we do

Numerical methods to solve

Linear system of equations

Suppose we have a system of equation

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

We want to find a solution.

In applications n is large (at least 1000). So doing it by hand is out of question. We have to use computers.

It is convenient to use matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

$$\bar{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \bar{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Thus we have to solve

$$A\bar{x} = \bar{b}$$

This system either has

1) a unique solution
2) no solution
3) infinitely many solutions

Example

1) $$x_1 + x_2 = 1$$
$$x_1 - x_2 = 0$$
has unique solution $x_1 = x_2 = \frac{1}{2}$.

2) $$\left.\begin{aligned} x_1 + x_2 &= 1 \\ 2x_1 + 2x_2 &= 3 \end{aligned}\right\}$$ has no solution

3) $$2x_1 - x_2 = 3$$
$$4x_1 - 2x_2 = 6$$
has infinitely many solⁿˢ
$$\{ (x_1, x_2) \mid 2x_1 - x_2 = 3 \}$$

For most application the system $A\bar{x} = \bar{b}$ has a unique solution

Theory

$A\bar{x} = \bar{b}$ has unique solution

iff A is an invertible matrix

i.e. there exists a matrix B s/t

$$BA = AB = I_n$$

$I_n = n \times n$ identity matrix

$$= \begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & \ddots \; 1 \end{bmatrix}$$

B is usually denoted by A^{-1}

$$A^{-1}(A\bar{x}) = A^{-1}\bar{b}$$

$\bar{x} = A^{-1}\bar{b}$. is the

unique solution

In practice

Computation of A^{-1} takes too many computations.

Usually we don't need it.

In practice there is a two step procedure to find sol^n of $\underline{A\bar{x}=\bar{b}}$.

<u>Step 1</u> (Gaussian Elimination)

$A\bar{x}=\bar{b}$ is transformed to an equivalent system $U\bar{x}=\tilde{b}$

where $U=(u_{ij})$ is an upper triangular matrix

i.e $u_{ij}=0$ for $i>j$

i.e

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdot & \cdot & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ & & & & \\ 0 & 0 & \cdots & 0 & u_{nn} \end{pmatrix}$$

$A\bar{x} = b$ equivalent to $Ux = \tilde{b}$ means that $\bar{x}_0$ is a solution of $Ax = b$ iff $\bar{x}_0$ is a solution of $Ux = \tilde{b}$

<u>Step 2</u> Solving

$$U\bar{x} = \tilde{b}$$

We do step 2 first.

<u>note</u> that by equivalence $Ax = b$ has a <u>unique</u> solution x_0 iff $Ux = \tilde{b}$ has a unique solution

Thus U is invertible matrix

Exercise

Show that an upper triangular matrix $U = (u_{ij})$ is invertible iff all diagonal entries (i.e u_{ii}) is non-zero

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Step 2 sol^n of $U\bar{x} = \tilde{b}$

$$u_{11}x_1 + u_{12}x_2 + \cdots + u_{1n}x_n = \tilde{b}_1$$
$$u_{22}x_2 + \cdots + u_{2n}x_n = \tilde{b}_2$$
$$\vdots$$
$$u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n = \tilde{b}_{n-1}$$
$$u_{n,n}x_n = \tilde{b}_n$$

$$x_n = \frac{\tilde{b}_n}{u_{nn}}.$$

$$x_{n-1} = \frac{\tilde{b}_{n-1} - u_{n-1,n}x_n}{u_{n-1,n-1}}$$

$$\vdots$$

$$x_i = \frac{\tilde{b}_i - \sum_{j>i} u_{ij} x_j}{u_{ii}}$$

for $i = n-1, n-2, \dots, 2, 1$

This process is called back-substitution

Example

$$3x_1 + x_2 + 2x_3 = 6$$
$$4x_2 + 2x_3 = 7$$
$$3x_3 = 9$$

- $x_3 = 3$
- $4x_2 + 6 = 7$

$$x_2 = \frac{1}{4}$$

$$3x_1 + \frac{1}{4} + 6 = 6$$

$$x_1 = -\frac{1}{12}.$$

Gaussian Elimination

Recall two linear systems $Ax = b$ and $\tilde{A}x = \tilde{b}$ are equivalent if any solution of one is a solution of the other

Theorem Let $A\bar{x} = \bar{b}$ be a linear system and suppose we subject this system to a seq of operations of the following kind

(i) Multiplication of one equation by a non-zero constant

(ii) Addition of a multiple of one equation to another equation

(iii) Interchange of two equations

If this system of operations produces a

new system $\tilde{A}x = \tilde{b}$, then the systems $Ax = b$ and $\tilde{A}x = \tilde{b}$ are equivalent.

In particular A is invertible iff $\tilde{A}$ is invertible.

Gaussian Elimination

It is possible to convert $Ax = b$ to equivalent system $Ux = \tilde{b}$ by using the above 3 operation

Example

$$
\begin{aligned}
x_1 - x_2 + 2x_3 &= -6 \\
2x_1 - 2x_2 + 3x_3 &= -14 \\
x_1 + x_2 + x_3 &= -2
\end{aligned}
$$

$$\left[\begin{array}{ccc|c} 1 & -1 & 2 & -6 \\ 2 & -2 & 3 & -14 \\ 1 & 1 & 1 & -2 \end{array}\right]$$

augmented matrix

$R_2 - 2R_1$

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

$R_3 - R_1$

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

$R_2 \leftrightarrow R_3$

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

$-x_3 = -2$ so $x_3 = 2$

$2x_2 - x_3 = 4$ $\quad x_2 = 3$

$x_1 - x_2 + 2x_3 = -6$

$x_1 - 3 + 4 = -6$

$x_1 = -7$

Algorithim for Gaussian Elimination

- To solve $Ax = b$
- $W = [A \,\vdots\, b]$ "augumented matrix"

Step 1 for $i = 1, \ldots, n-1$ do Steps 2, 3, 4

Step 2 Let p be the smallest integer with $i \le p \le n$ and $a_{pi} \neq 0$

If no integer p can be found then output "no unique sol^n exists" & stop

$$\left[\begin{array}{c} \vdots \end{array} \right]$$

Step 3 If $p \neq i$ then interchange Row $R_i \leftrightarrow$ Row R_j

Step 4 for $j = i+1, \ldots, n$ do steps 5 & 6

Step 5 Set $m_{ji} = \dfrac{a_{ji}}{a_{ii}}$

Step 6 perform $R_j - m_{ji} R_i$

Step 7 If $a_{nn} = 0$ then "no unique sol^n exist". & stop

Step 8 U = first n columns of W

$\tilde{b}$ = last column of W

Then $Ax = b$ is equivalent to $Ux = \tilde{b}$ where U is upper triangular matrix.

Operation Count

We count the number of multiplication / division & addition / substraction to do GE.

In general, the amount of time required to perform a multiplication or division on a computer is approximately the same and is considerably greater than that required to perform an addition or substraction

No arithmetic operation is performed until Step 5 in the algorithm

Step 5 requires that $n-i$ division be performed

In Step 6 we replace row R_j by

$R_j - m_{ji} R_i$

This requires m_{ji} be multiplied to each term in R_i.

This requires $(n-i)(n-i+1)$ multiplications

Afterwards each term of the resulting equation is subtracted from the corresponding term in R_j. This requires $(n-i)(n-i+1)$ substractions

Thus for each $i = 1, 2, \ldots, n-1$ the operations required are

[Multiplication / division]

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

[Addition / substractions]

$$(n-i)(n-i+1)$$

Total multiplication / division

$$\sum_{i=1}^{n-1}(n-i)(n-i+2) = \frac{2n^3+3n^2-5n}{6}$$

Total addition / substraction

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

For backsubstition (i.e step 2)

One can show one require

$\frac{n^2+n}{2}$ multiplication / division

$\frac{n^2-n}{2}$ addition / subtraction

Note that for large n

n^3 is considerably larger than n^2

for example when $n = 100$

100^2 is 1% of 100^3

Thus GE is $O(n^3/3)$ operation

Tridiagonal matrix

$$\begin{bmatrix} a_1 & b_1 & & & & \\ c_1 & a_2 & b_2 & & 0 & \\ & c_2 & a_3 & & & \\ & & & & & \\ & 0 & & & & b_{n-1} \\ & & & & c_{n-1} & a_n \end{bmatrix}$$

$A = [a_{ij}]$ is said to be tridiagonal if $a_{ij} = 0$ for $|i-j| > 1$

$Ax = b$ for tridiagonal systems can be solved in $O(n)$ steps.