Lecture 15

Last time we studied Pertubations of linear system of equations

Instead of solving $Ax = b$

we are solving $\hat{A}\hat{x} = b$

$$A = \hat{A} + E$$

E matrix that contains error in coefficients

x_0 exact sol^n of $Ax = b$

$\hat{x}_0$ " " " $\hat{A}\hat{x} = b$

$$\| \bar{x}_0 - \hat{x}_0 \| \leq \| A^{-1} \| \| A \| \frac{\| E \|}{\| A \|} \| \hat{x}_0 \|$$

$$\frac{\| \bar{x}_0 - \hat{x}_0 \|}{\| \hat{x}_0 \|} \leq \text{cond}(A) \frac{\| E \|}{\| A \|}$$

Iterative improvement of solution

Solve $Ax = b$ exact $\bar{x}_0$ computed $\hat{x}^{(1)}$

$e = \bar{x}_0 - \hat{x}^{(1)}$ unknown error

Solve $Ae = r = b - A\hat{x}^{(1)}$

$\hat{e}^{(1)}$ approximate sol^n of $Ae = r$

then $\hat{x}^{(2)} = \hat{x}^{(1)} + \hat{e}^{(1)}$ better approx to $\bar{x}_0$ than $\hat{x}^{(1)}$

further ~~compute~~ solve $Ae = \bar{r} = b - A\hat{x}^{(2)}$

to get new correction $\hat{e}^{(2)}$

$$\hat{x}^{(3)} = \hat{x}^{(2)} + \hat{e}^{(2)}$$

One keeps on doing this

stop when $\dfrac{\|\hat{e}^{(k)}\|}{\|\hat{x}^{(k)}\|} \approx 10^{-t}$ if t decimals p/cs accuracy is required

Remark

1) If cond(A) is large then $\hat{e}^{(1)}, \hat{e}^{(2)}, \ldots$ may not decrease in size

2) Solve $A\hat{e} = r$ in DOUBLE PRECESION.

Iterative Methods to solve Linear equations

It is based on fixed point iteration

We want to solve

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

It is equivalent to find zero of

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

We write it in equivalent form

$$\bar{x} = g(\bar{x})$$

A fixed pt ξ of $g(\bar{x})$ will be root of $f(\bar{x})$. i.e. $A\bar{\xi} = \bar{b}$

Iteration initial given $x^{(0)}$

and then we generate the sequence

$$x^{(m+1)} = g(x^{(m)}) \quad m = 0, 1, 2, \ldots$$

For convergence we will need the following theorem

Preliminaries :-

Def^n A set $S \subseteq \mathbb{R}^n$ is closed if any cgt sequence $\{x_n\}$, $x_n \in S$

$\Rightarrow \lim_{n\to\infty} x_n \in S$

Example 1. $\mathbb{R}^n$ is closed

2) $[a,b]$ is closed in $\mathbb{R}$.

3) $[a_1,b_1] \times [a_2,b_2] \times \cdots \times [a_n,b_n]$ is closed in $\mathbb{R}^n$

4) $S=(0,1]$ is Not closed in $\mathbb{R}$

$\{1/n\} \subseteq S$ $\lim_{n\to\infty} \frac{1}{n} = 0 \notin S$

Def^n :- A map $g: S \to S$ is called contractive if $\exists$ ~~k~~ k, $0 < k < 1$ s.t-

$\|g(x) - g(y)\| \leq k\|x-y\|$

$\forall x, y \in S$

Theorem :- Suppose $g: S \to S$, S closed set in $\mathbb{R}^n$. Further assume g is contractive (i.e $\exists K<1$ s.t. $\|g(x)-g(y)\| \leq K\|x-y\|$ $\forall x, y \in S$

Then

1) g has a unique fixed point ξ in S

2) Fixed pt convergence starting with any $x^{(0)}$ in S converges to ξ.

i.e $\lim_{m\to\infty} \|\xi - x^{(m)}\| = 0$

for such a sequence $x^{(m+1)} = g(x^{(m)})$

$m = 0, 1, 2, \ldots$

More explicitly

$$(*) \quad \|\xi - x^{(m)}\| \leq \frac{K}{1-K} \|x^{(m)} - x^{(m-1)}\|$$

~~(K is constant which comes from~~

$$(**) \quad \|\xi - x^{(m)}\| \leq \frac{K^m}{1-K} \|x^{(1)} - x^{(0)}\|$$

This is a non-trivial result.
The difficulty is to show g has a fixed pt ξ

derivation of (*) and (**)

$$\|\xi - x^{(m)}\| = \|g(\xi) - g(x^{m-1})\|$$
$$\leq K\|\xi - x^{(m-1)}\|$$

By Δ triangle inequality
$$\|\xi - x^{(m-1)}\| \leq \|\xi - x^{(m)}\| + \|x^{(m)} - x^{(m-1)}\|$$
$$\leq K\|\xi - x^{(m-1)}\| + \|x^{(m)} - x^{(m-1)}\|$$

$$(1-K)\|\xi - x^{(m-1)}\| \leq \|x^{(m)} - x^{(m-1)}\|$$

so $$\|\xi - x^{(m)}\| \leq \frac{K}{1-K}\|x^{(m)} - x^{(m-1)}\|$$

This proves (*)
$$\|x^{(m)} - x^{(m-1)}\| = \|g(x^{(m-1)}) - g(x^{(m-2)})\|$$
$$\leq K\|x^{(m-1)} - x^{(m-2)}\|$$

$$\|\xi - x^{(m)}\| \leq \frac{K^2}{1-K}\|x^{(m-1)} - x^{(m-2)}\|$$

$$\vdots$$

$$\leq \frac{K^m}{1-K}\|x^{(1)} - x^{(0)}\|$$

All iteration schemes to solve $Ax = b$ is based on the notion of approximate inverse, by this we mean any matrix C for which

$$\| I - CA \| < 1$$

in some matrix norm

Lemma If C is an approximate inverse for the matrix A, i.e., if $\| I - CA \| < 1$ in some matrix norm, then both C and A are invertible.

Proof Suppose if possible C or A is NOT invertible

$\Rightarrow \det(CA) = \det C \cdot \det A = 0$

so CA is not invertible

$\Rightarrow \exists\ \bar{x} \neq 0$ such that $CA\bar{x} = 0$

But then

$$0 \neq \|\bar{x}\| = \|(I - CA)x\|$$

$$\leq \|I - CA\| \, \|\bar{x}\|$$

$$< \|\bar{x}\|$$

this is a contradiction.

So A, C are invertible.

Iteration function

Let C be an approximate inverse to A

$$g(\bar{x}) = C\bar{b} + (I - CA)\bar{x}$$

$$= \bar{x} + C(\bar{b} - A\bar{x})$$

If $A\bar{\xi} = \bar{b}$ i.e $\bar{\xi}$ is a solution of $A\bar{x} = \bar{b}$

then $g(\xi) = \xi$.

conversely if $g(\xi) = \xi$

$$\bar{\xi} = \bar{\xi} + C(\bar{b} - A\bar{\xi})$$

$$0 = C(\bar{b} - A\bar{\xi})$$

C is invertible. So $\bar{b} - A\bar{\xi} = 0$

so $A\bar{\xi} = \bar{b}$ i.e ξ is a solution of $A\bar{x} = \bar{b}$.

Check

$$g(x) - g(y) = (I - CA)(\bar{x} - \bar{y})$$

$$\|g(x) - g(y)\| = \|(I - CA)(\bar{x} - \bar{y})\|$$

$$\leq \|I - CA\| \, \|x - y\|$$

So g is contractive with $K = \|I - CA\| < 1$

$S = \mathbb{R}^n$ is closed

Thus the fixed pt iteration

$$x^{(m+1)} = x^{(m)} + C(b - Ax^{(m)}) \quad m \geq 0$$

~~starting with any x_0 will converge to unique soln of $Ax = b$~~

starting with any $x^{(0)}$ will converge to the unique solution ξ of $A\bar{x} = \bar{b}$

Two most common choices of C

$$A = (a_{ij}) = \hat{L} + \hat{D} + \hat{U}$$

$\hat{L} = (l_{ij})$ $\quad l_{ij} = \begin{cases} a_{ij} & i > j \\ 0 & i \le j \end{cases}$

$\hat{D} = (d_{ij})$ $\quad d_{ij} = \begin{cases} a_{ii} & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$

$\hat{U} = (u_{ij})$ $\quad u_{ij} = \begin{cases} 0 & \text{if } i \ge j \\ a_{ij} & \text{if } i < j \end{cases}$

Example

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 3 & 0 & 0 \\ 6 & 7 & 0 \end{pmatrix}}_{\hat{L}} + \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 8 \end{pmatrix}}_{\hat{D}} + \underbrace{\begin{pmatrix} 0 & 2 & 3 \\ 0 & 0 & 5 \\ 0 & 0 & 0 \end{pmatrix}}_{\hat{U}}.$$

We assume all diagonal entries of A are non-zero

(if this is not so at the outset, we can do row changes to ensure this condition is satisfied. We can always do this since A is invertible)

Jacobi iteration

$$C = \hat{D}^{-1}$$

This converges if $\| I - \hat{D}^{-1} A \| < 1$ for some norm

$$x^{(m+1)} = x^{(m)} + \hat{D}^{-1} (b - A x^{(m)})$$

$$x_i^{(m+1)} = \frac{b_i - \sum_{j \neq i} a_{ij} x_i^{(m)}}{a_{ii}}$$

$i = 1, 2, \ldots, n$

Example

$$10x_1 - x_2 = 9$$

$$-x_1 + 10x_2 - 2x_3 = 7$$

$$-2x_2 + 10x_3 = 6$$

$$x_1 = 0.1x_2 + 0.9$$

$$x_2 = 0.1x_1 + 0.2x_3 + 0.7$$

$$x_3 = 0.2x_2 + 0.6$$

Jacobi iteration

initial $x_1^{(0)} = 0$

$x_2^{(0)} = 0$

$x_3^{(0)} = 0$

iteration scheme

$$x_1^{(m+1)} = 0.1x_2^{(m)} + 0.9$$

$$x_2^{(m+1)} = 0.1x_1^{(m)} + 0.2x_3^{(m)} + 0.7$$

$$x_3^{(m+1)} = 0.2x_2^{(m)} + 0.6.$$

Iterations

m	0	1	2	3	4
$x_1^{(m)}$	0	0.9	0.97	0.991	0.9941
$x_2^{(m)}$	0	0.7	0.91	0.941	0.9555
$x_3^{(m)}$	0	0.6	0.72	0.782	0.7564

m	5	6	7	8	9
$x_1^{(m)}$	0.99555	0.995069	0.995778	0.995115	0.9957189
$x_2^{(m)}$	0.95069	0.957775	0.951151	0.957889	0.951174
$x_3^{(m)}$	0.7911	0.758220	0.791558	0.758311	0.791578

Converging nicely to exact soln (in 6 sig digits)

$$x_1 = 0.995789$$

$$x_2 = 0.957895$$

$$x_3 = 0.791579$$

$$A = \hat{L} + \hat{D} + \hat{U}$$

for Jacobi Method

$$C = \hat{D}^{-1}$$

For Gauss-Seidel iteration

$$C = (\hat{L} + \hat{D})^{-1}$$

$$x^{(m+1)} = x^{(m)} + (\hat{L} + \hat{D})^{-1}(b - Ax^{(m)})$$

$$(\hat{L} + \hat{D})(x^{(m+1)}) = (\hat{L} + \hat{D} - A)x^{(m)} + b$$

$$\hat{D}\, x^{(m+1)} = -L\, x^{(m+1)} - \hat{U}\, x^{(m)} + b$$

This gives the formula

$$x_i^{(m+1)} = \frac{-\sum_{j<i} a_{ij}\, x_j^{(m+1)} - \sum_{j>i} a_{ij}\, x_j^{(m)} + b_i}{a_{ii}}$$

$$i = 1, 2, \ldots, n$$

This converges if for some matrix norm

$$\| I - CA \| < 1$$

$$I - CA = I - (\hat{L}+\hat{D})^{-1}(\hat{L}+\hat{D}+\hat{U})$$

$$= (\hat{L}+\hat{D})^{-1}\hat{U}$$

i.e if $\| C\hat{U} \| < 1$ then Gauss-Seidel method converges

Example Same example as before

$$10x_1 - x_2 = 9$$

$$-x_1 + 10x_2 - 2x_3 = 7$$

$$-2x_2 + 10x_3 = 6$$

$$x_1 = 0.1x_2 + 0.9$$

$$x_2 = 0.1x_1 + 0.2x_3 + 0.7$$

$$x_3 = 0.2x_2 + 0.6$$

Iteration Scheme

$$x_1^{(m+1)} = 0.1\, x_2^{(m)} + 0.9$$

$$x_2^{(m+1)} = 0.1\, x_1^{(m+1)} + 0.2\, x_3^{(m)} + 0.7$$

$$x_3^{(m+1)} = 0.2\, x_2^{(m+1)} + 0.6$$

(note the difference from Jacobi-Method)
in Gaus-Siedel while computing $x_i^{(m+1)}$ we can use $x_j^{(m+1)}$ for $j < i$

initial approximation $= (\bar{0}, \bar{0}, \bar{0})$

m	0	1	2	3	4
$x_1^{(m)}$	0	0.9	0.979	0.98495	0.995748
$x_2^{(m)}$	0	0.79	0.9495	0.957475	0.957874
$x_3^{(m)}$	0	0.758	0.7899	0.791495	0.791575

m	5	6
$x_1^{(m)}$	0.995787	0.995789
$x_2^{(m)}$	0.957894	0.957895
$x_3^{(m)}$	0.791571	0.791579

Gauss-Seidel iteration is usually faster than Jacobi iteration (not always but!)

It is easier to compute since in Jacobi iteration two iterates must be kept in memory while in Gauss-Seidel only one vector is required to be kept in memory

Gauss-Seidel iteration can be shown to be convergent if the coefficient matrix A is strictly row diagonally-dominant.

It also converges if A is true definite (i.e A is symmetric and for all $x \neq 0$ $x^t A x > 0$)

Proposition

Suppose A is strictly diagonally dominant. Then the Jacobi-iteration converge

Proof $A = (a_{ij})$ is strictly row diagonally dominant.

$$\text{So} \quad |a_{ii}| > \sum_{j \neq i} |a_{ij}| \qquad i = 1, 2, \ldots, n$$

$\hat{D} = \text{diag}(a_{11}, a_{22}, \ldots, a_{nn})$ be the diagonal of A

Recall $\|x\|_\infty = \max_i |x|$

$$\|B\|_\infty = \max_{1 \le i \le n} \sum_{1 \le j \le n} |b_{ij}|$$

$$\|I - \hat{D}^{-1}A\|_\infty = \max_i \left\{ 1 - \sum_{j=1}^{n} \frac{|a_{ij}|}{|a_{ii}|} \right\}$$

$$= \max_i \left\{ \sum_{j \neq i} \frac{|a_{ij}|}{|a_{ii}|} \right\}$$

$$< 1$$

Thus $\hat{D}^{-1}$ is an approximate inverse to A

Therefore the Jacobi-Method converges

Remark

Recall that C is an approximate inverse to A if in some matrix norm

$$\|I - CA\| < 1$$

Note that in some other matrix norm it is possible that

$$\|I - CA\|' > 1$$

Example

$$B = \begin{bmatrix} 0.9 & 0.9 \\ 0 & 0 \end{bmatrix}$$

$$\|B\|_\infty = 1.8 > 1$$

$$\|B\|_1 = 0.9 < 1$$

This makes it important to find ways of telling whether $\|B\| < 1$ in some matrix norm (without having to try out all possible matrix norms)

Def^n

$\rho(B)$ = spectral radius of B

$= \max \{ |\lambda| \mid \lambda \text{ is an eigenvalue of } B \}$

Theorem There exists for any $\varepsilon > 0$, a vector norm on $\mathbb{R}^n$ for ~~which~~ which the associated matrix norm of B satisfies

$$\|B\| \leq \rho(B) + \varepsilon$$

Corollary C is an approximate inverse for A

$$\Leftrightarrow \quad \rho(I - CA) < 1$$

Remark :- Iterative methods are usually applied to large linear systems with sparse coefficient matrix.

Numerical Methods To solve initial value differential equations

$$\frac{dy}{dx} = f(x,y) \qquad x_0 \le x \le x_n$$

$$y(x_0) = y_0$$

We assume that all partial derivatives to f exist.

By theory there exists a unique solution to the above initial value problem (in a neighbhaurhood of (x_0, y_0))

However we cannot hope for exact solutions

Example $\frac{dy}{dx} = \sin(x^2 + y^2) \qquad 0 \le x \le 1$

$$y(0) = 1$$

We cannot find exact answer to above equation

Numerical integration by Taylor Series

$$(*) \quad \frac{dy}{dx} = f(x,y) \qquad y(x_0) = y_0$$

If $y(x)$ is exact solution of $(*)$ then we can expand $y(x)$ into a Taylor series about the point x_0

$$(**) \quad y(x) = y_0 + (x-x_0)\,y'(x_0) + \frac{(x-x_0)^2}{2!}\,y''(x_0) + \cdots$$

The derivatives in this expression are not known explicitly since the solution is unknown. However if f is sufficiently differentiable they can be obtained by taking the total derivative of $(*)$ with respect to x, keeping in mind that y itself is a function of x

$$y' = f(x,y)$$

$$y'' = f' = f_x + f_y f$$

$$y''' = f'' = f_{xx} + f_{xy} f + f_{yx} f + f_{yy} f^2 + f_y f_x + f_y^2 f$$

Continuing in this manna we can express any derivative of y in terms of f and its partial derivatives. It is already clear however, that unless f is a very simple function the higher total derivatives become increasingly complex.

For practical reasons then one must limit the number of terms in the expression (**) to a reasonable number.

If we assume that the truncated series (**) is a good approximation for a step of length h (i.e., for $x - x_0 = h$ we can then evaluate y at $x_0 + h$, re-evaluate the derivatives y', y'' etc and then use (**) to proceed to the next step.

Thus we obtain a discrete set of values y_n which are approximation to the true solution at the points $x_n = x_0 + nh$ $(n = 0, 1, 2, \ldots)$

(Q3)

Remark:- We will always denote the value of the exact solution $*$ at a point x_n by $y(x_n)$ and of an approximate solution by y_n

define

$$T_k(x,y) = f(x,y) + \frac{h}{2} f'(x,y) + \frac{h^2}{3!} f''(x,y) + \cdots + \frac{h^{k-1}}{k!} f^{(k-1)}(x,y)$$

Algorithm 1 (Taylor algorithm of order k)

To find an approximate solution of the diff equation

$$y' = f(x,y)$$
$$y(a) = y_0$$

over an interval $[a,b]$

1. choose a step size $h = \frac{b-a}{N}$

   Set $x_n = a + nh$ $\quad n = 0, 1, 2, \ldots, N$

2. Generate approximation y_n to $y(x_n)$ from the recursion

$$y_{n+1} = y_n + h\, T_k(x_n, y_n) \qquad n = 0, 1, 2 \ldots, N-1$$

Taylor's theorem with remainder shows that the local error of Taylor's algorithm of order k is

$$E = \frac{h^{k+1} f^{(k)}(\xi, y(\xi))}{(k+1)!} \qquad x_n < \xi < x_n + h$$

$$= \frac{h^{(k+1)}}{(k+1)!} y^{(k+1)}(\xi).$$

Example Use Taylor's method of order 2 to solve

$$\frac{dy}{dx} = y - x^2 + 1 \qquad 0 \le x \le 2$$

$$y(0) = 0.5$$

$$f' = \frac{d}{dx}(y - x^2 + 1)$$

$$= \frac{dy}{dx} - 2x$$

$$= y - x^2 + 1 - 2x$$

$$T_2(x_i, y_i) = f(x_i, y_i) + \frac{h}{2} f'(x_i, y_i)$$

$$= y_i - x_i^2 + 1 + \frac{h}{2}(y_i - x_i^2 - 2x_i + 1)$$

$$= \left(1 + \frac{h}{2}\right)(y_i - x_i^2 + 1) - hx_i$$

Taylors method of order 2

$$y_0 = 0.5$$

$$y_{i+1} = y_i + h\left[\left(1 + \frac{h}{2}\right)(y_i - x_i^2 + 1) - hx_i\right]$$

Exact solution to above d.e is

$$y(x) = (x+1)^2 - 0.5e^x$$

x_i	Exact $y(x_i)$	Taylor order 2 y_i	Error
0.0	0.5	0.5	0
0.2	0.8292986	0.8300	0.0007014
0.4	1.2140877	1.2158	0.0017123
0.6	1.6489406	1.6520760	0.0031354
0.8	2.1272295	2.1323327	0.0051032
1.0	2.6408591	2.6486459	0.0077812
1.2			
1.4			
1.6			
1.8			0.0422123
2.0	5.3054720	5.3476843	

On setting $k=1$ in our Algorithm we obtain Euler's Method

$$y_{n+1} = y_n + h f(x_n, y_n)$$

local error $E = \frac{h^2}{2} y''(\xi)$

$$x_n \le \xi \le x_{n+1}$$

Example :- $\frac{dy}{dx} = y - x^2 + 1 \qquad 0 \le x \le 2$

$y(0) = 0.5$

$h = 0.2 \qquad x_n = 0.2\,n$

$$y_{n+1} = y_n + 0.2\,(y_n - 0.04\,n^2 + 1)$$

Exact solution

$$y(x) = (x+1)^2 - 0.5\,e^x$$

x_i	Euler method y_i	Exact $y(x_i)$	Error $\lvert y_i - y(x_i) \rvert$
0	0.5	0.5	0
0.2	0.8	0.8292986	0.0292981
0.4	1.152	1.2140877	0.0620877
0.6	1.5504	1.6489406	0.0985406
0.8	1.9884800	2.1272295	0.1387495
1.0	2.4581760	2.6408591	0.1826831
1.2			
1.4			
1.6			
1.8			
2.0	4.8657845	5.3054720	0.4396854

Notice error grows slightly as the value of x increases.

This controlled error growth is a consequence of the stability of Eulers method which implies that the error is expected to grow in no worse than a linear manner.