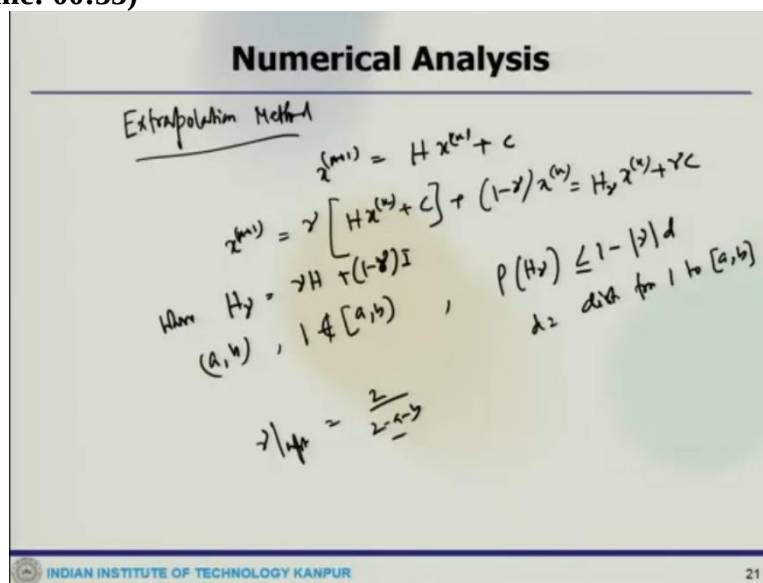


Computational Science in Engineering
Prof. Ashoke De
Department of Aerospace Engineering
Indian Institute of Technology, Kanpur

Lecture - 32
Numeric Analysis

So, we are looking at the different iterative methods for solving the linear system like $Ax = b$ and we have already seen some of these methods like successive over relaxation, Gauss Seidel or Gauss Jacobi kind of method. Now, we will look at some of the other things, like Eigen value kind of things.

(Refer Slide Time: 00:33)



So, before moving there one more quick thing what one can try to look is that this is one of the iterative methods is that extrapolation method. This is quiet, I would say it is some powerful acceleration procedure for iterative method, one of them is this extrapolation method where we can write the iteration formula as

$$x^{(k+1)} = Hx^{(k)} + c$$

where considering one parameter family of extrapolation method is that

$$x^{(k+1)} = \gamma[Hx^{(k)} + c] + (1 - \gamma)x^{(k)} = H_\gamma x^{(k)} + \gamma c$$

Where

$$H_\gamma = \gamma H + (1 - \gamma)I$$

suppose that, we know all the Eigen values of H which lie in the interval of a and b and 1 not belongs to a and b on the real line then,

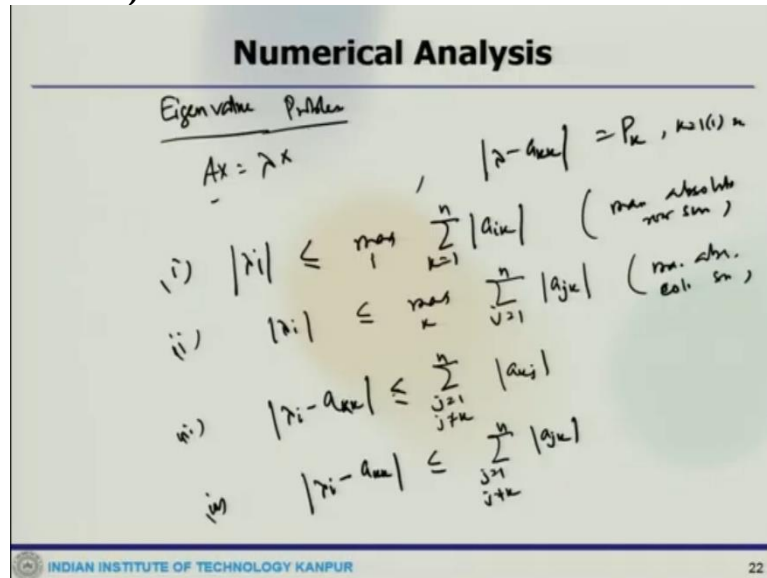
$$\rho(H_\gamma) \leq 1 - |\gamma|d$$

or d is the distance from 1 to a, b, the optimum value of gamma which gives maximum rate of convergence is, so, this is the optimum value which is

$$\gamma_{opt} = \frac{2}{2 - a - b}$$

So, this is what you get.

(Refer Slide Time: 02:17)



Now, we move to the Eigen value problems and now, Eigen value problems what we know that, consider an Eigen value problem like, $AX = \lambda X$, now, what we say that let P_k be the sum of the module of elements along the K through excluding diagonal element a_{kk} that every Eigen value of A lies inside of the boundary at least one of the circles. So, which means that,

$$P_k = |\lambda - a_{kk}|$$

where K goes 1 to n.

So, we can have certain properties like

$$i) |\lambda_i| \leq \max_i \sum_{k=1}^n |a_{ik}|$$

So, this is maximum absolute row sum or λ_i

$$ii) |\lambda_i| \leq \max_k \sum_{j=1}^n |a_{jk}|.$$

This is maximum absolute column sum third all the Eigen values lie in the union of a circle,

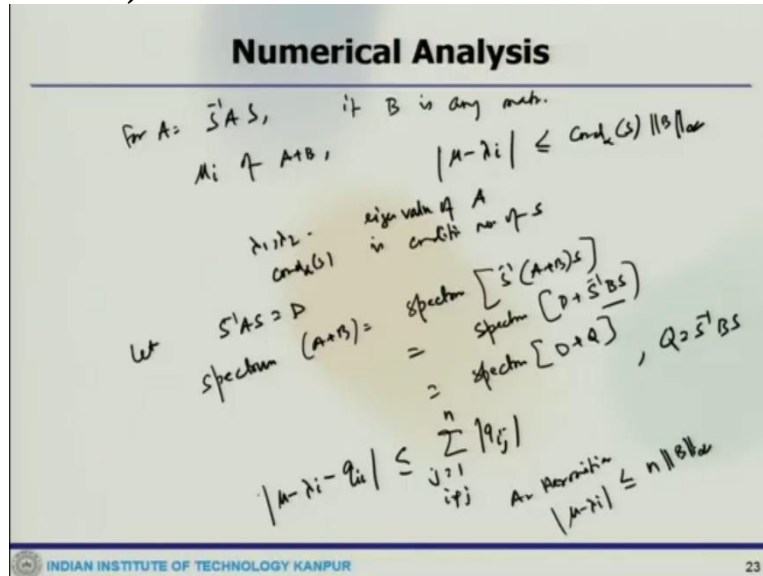
$$iii) |\lambda_i - a_{kk}| \leq \sum_{\substack{j=1 \\ j \neq k}}^n |a_{kj}|$$

And all the Eigen values lie in the union of circles

$$iv) |\lambda_i - a_{kk}| \leq \sum_{\substack{j=1 \\ j \neq k}}^n |a_{jk}|.$$

So, these 4 bounds are independent, hence the required bound is the intersection of these 4 bounds. If A is symmetric then the circle becomes interval on the real line, these bounds are referred as the just scoring circles or just scoring bounds. Now, let us say the matrix A.

(Refer Slide Time: 04:38)



Kind of diagonalized by the similarity transformation like $A = S^{-1}AS$ and if B, this is for A, one can do that and B is any matrix then the Eigen values μ_i of $A + B$ lie in the union of disk like

$$|\mu - \lambda_i| \leq \text{cond}_{\infty}(S) \|B\|_{\infty}$$

Where λ_1, λ_2 these are the Eigen values of A and this is the condition number of S. Usually B is a permutation matrix, so let we have this D then the

$$\text{Spectrum}(A + B) = \text{Spectrum}[S^{-1}(A + B)S]$$

Which, one can write

$$\text{Spectrum}(A + B) = \text{Spectrum}[D + S^{-1}BS] = \text{Spectrum}[D + Q]$$

where Q is written as $S^{-1}BS$ and D is the diagonal matrix. By applying the already discussed theorem, the Eigen values of $A + B$ lie in the unit disk which we can see that

$$|\mu - \lambda_i - q_{ii}| \leq \sum_{\substack{j=1 \\ i \neq j}}^n |a_{ij}|$$

Further if A is Hermitian then the condition simplifies to, like

$$|\mu - \lambda_i| \leq n \|B\|_{\infty}$$

So that is considered method for finding all the Eigen values and Eigen vectors of the given matrix A. So, these are some of the important things that one has to keep in mind.

(Refer Slide Time: 07:04)

Numerical Analysis

Jacobi Method for symmetric Matrices.

A is real sym. matrix.
off-diagonal elements a_{ik}

$$S_1^* = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}, \quad (S_1^*)^T A S_1^* = (S_1^*)^T A S_1^*$$

$$\tan 2\theta = \frac{2a_{ik}}{a_{ii} - a_{kk}}, \quad -\frac{\pi}{4} \leq \theta \leq \frac{\pi}{4}$$

if $a_{ii} = a_{kk}$, then $\theta = \begin{cases} \frac{\pi}{4}, & a_{ik} > 0 \\ -\frac{\pi}{4}, & a_{ik} < 0 \end{cases}$

max. no. of iterations $\sim \frac{n(n-1)}{2}$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

So, let us say, we start with a Jacobi method for symmetric matrices. Let A is a real symmetric matrix then A is reduced to a diagonal matrix by series of orthogonal transformation and which is when the diagonalization is completed the Eigen values are located on the diagonal and the orthogonal matrix of Eigen vectors is obtained as the product of orthogonal function.

So, the off-diagonal elements are a_{ik} , so, these are the magnitude with the largest number. So, what we get that the orthogonal transformation of this, we get

$$S_1^* = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

So, the value of θ is obtained, so that

$$(S_1^*)^{-1} A S_1^* = (S_1^*)^T A S_1^*$$

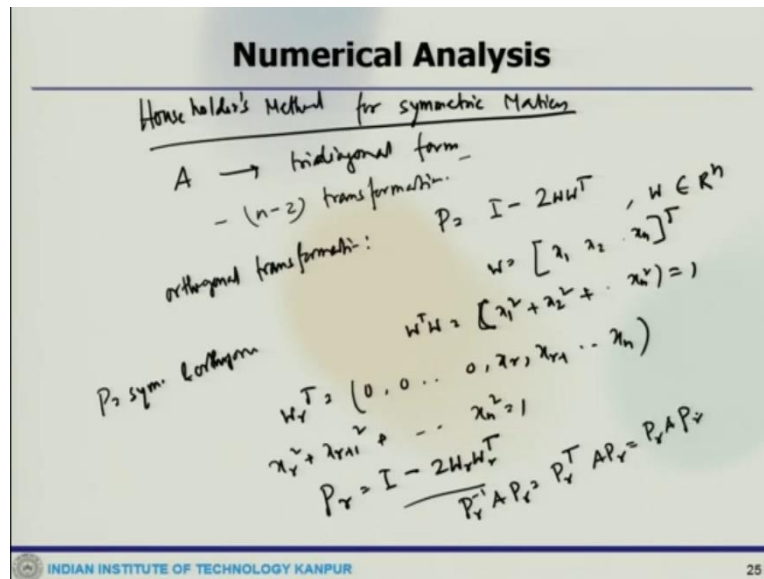
which is diagonalized and we find

$$\tan 2\theta = \frac{2a_{ik}}{a_{ii} - a_{kk}}$$

So, $-\frac{\pi}{4} \leq \theta \leq \frac{\pi}{4}$.

If our $a_{ii} = a_{kk}$ then, one can get down θ is $\frac{\pi}{4}$ and $-\frac{\pi}{4}$ this is for $a_{ik} > 0$, this is for $a_{ik} < 0$. So, the maximum number of rotations required to bring A into a diagonal form, so, this is maximum number of iterations which is record, is roughly $\frac{n(n-1)}{2}$. So, there is a disadvantage of Jacobi method, is that, the elements annihilated by the plane rotation by not necessarily remain 0, during subsequent iteration.

(Refer Slide Time: 09:35)



Now, we will look at some other options or the procedure or the methods like, house holder's method for symmetric matrices, so here in this particular method, A is reduced to tri diagonal form, tri diagonal form by orthogonal transformation. So, let us talk about householder's method for symmetric matrices. So, let us say if householder method is reduced to tri diagonal form by orthogonal transformation, then this reduction is exactly some sort of an $(n - 2)$ transformation.

And the orthogonal transformations can be of the form, so the orthogonal transformation which will be the form of like

$$P = I - 2WW^T$$

where, W belongs to $\mathbb{R}^n$ and W consist of

$$W = [x_1 \ x_2 \ x_3 \ \dots \ x_n]^T$$

and

$$W^T W = [x_1^2 + x_2^2 + x_3^2 + \dots + x_n^2] = 1$$

So, P here is symmetric and orthogonal, the vector W_r constructed with the first $(r - 1)$ components as 0s. So that is,

$$W_r^T = (0, 0, \dots, 0, x_r, x_{r+1}, x_n)$$

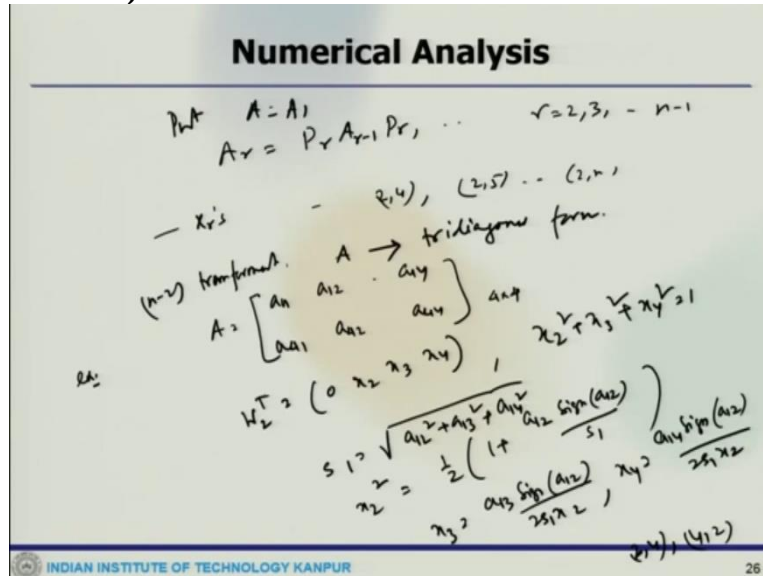
With $[x_1^2 + x_2^2 + x_3^2 + \dots + x_n^2] = 1$. So, this choice W_r of the matrices one can write like,

$$P_r = I - 2W_r W_r^T$$

So, the similarity transformation which one can write as,

$$P_r^{-1} A P_r = P_r^T A P_r = P_r A P_r$$

(Refer Slide Time: 12:24)



Now, here, if we put $A = A_1$ and formed successively then what we can get?

$$A_r = P_r A_{r-1} P_r$$

So, which is r goes from 2, 3 to $(n-1)$. At the first transformation we first find x_r , so that we get zones in the position (1,3), (1,4), (1,n) and the corresponding position, so, in the first column. In the second transformation, we find essentially x_r , such that we get zones in the position like (2,4), (2,5), .. (2,n), something like that and in the corresponding position in the second column.

So, similarly, in $(n-1)$ transformations A essentially reduced to a tri diagonal form. So, the remaining procedure is same as like other. Now, we can just take an example, like consider an example like this and see

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{14} \\ \vdots & \vdots & \ddots & \vdots \\ a_{41} & a_{42} & \vdots & a_{44} \end{bmatrix}$$

which is a 4×4 system. So, this is 4×4 system. For the first transformation the choice of

$$W_2^T = (0 \quad x_2 \quad x_3 \quad x_4)$$

Where $x_2^2 + x_3^2 + x_4^2 = 1$ and we find

$$s_1 = \sqrt{a_{12}^2 + a_{13}^2 + a_{14}^2}$$

And

$$x_2^2 = \frac{1}{2} \left(1 + \frac{a_{12} \text{sign}(a_{12})}{s_1} \right)$$

And

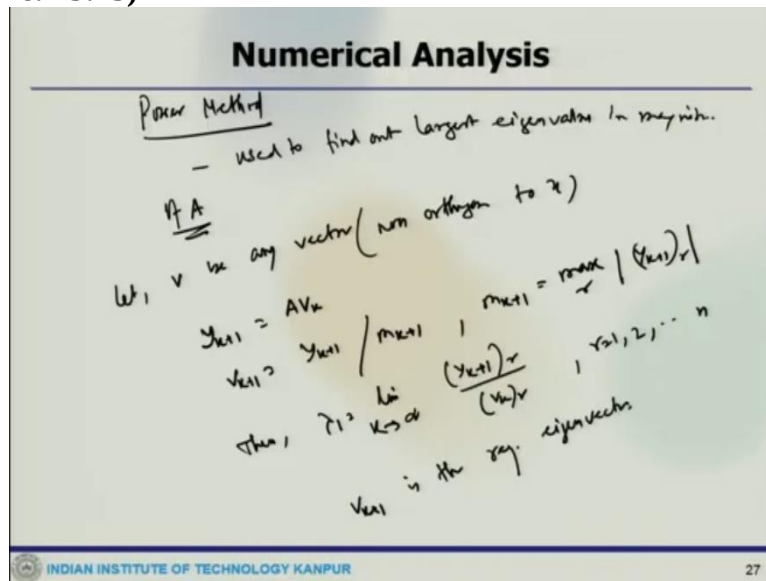
$$x_3 = \frac{a_{13} \text{sign}(a_{12})}{2S_1 x_2}$$

And

$$x_4 = \frac{a_{14} \text{sign}(a_{12})}{2S_1 x_2}$$

So, the transformation reduces to zeros in the first row and first column and one more transformation produces zeros in the like (2, 4) position and (4, 2) position. So, this is how one has to carry out these systems for the solution.

(Refer Slide Time: 15:13)



Now, we can look at another method like called power method. So, this method is kind of, is normally used to determine the largest Eigen value in magnitude. And so, this used to find out largest Eigen value in magnitude and the corresponding Eigen vector of A. Fastest convergence is obtained when λ_i are distinct and far separated. So, let us say, let V be any vector which is obviously non orthogonal to x in the space spanned by the Eigen vectors.

Then we can have this algorithm like

$$y_{k+1} = AV_k$$

Where

$$V_{k+1} = \frac{y_{k+1}}{m_{k+1}}$$

where m_{k+1} is estimated as

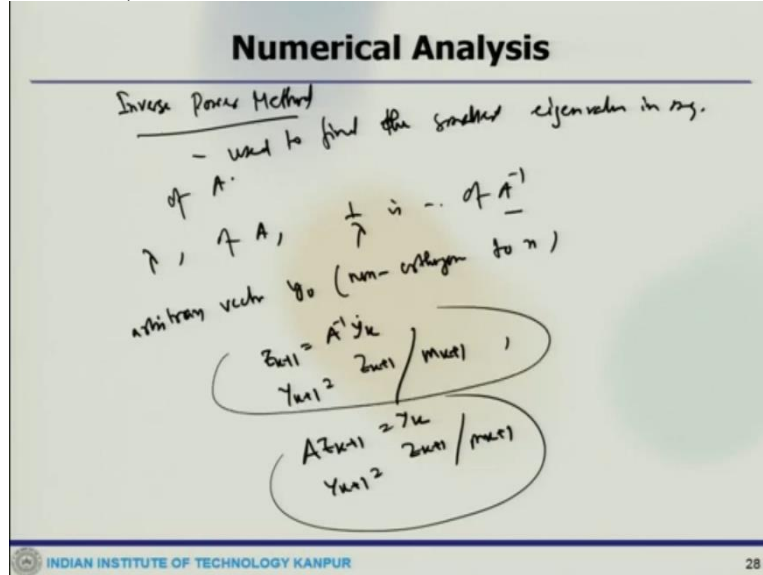
$$m_{k+1} = \max_r |(y_{k+1})_r|$$

Then, what we have,

$$\lambda_1 = \lim_{k \rightarrow \infty} \frac{(y_{k+1})_r}{(V_k)_r}$$

where r goes from 1, 2 like n and V_{k+1} is the required Eigen vector.

(Refer Slide Time: 17:12)



So, similarly, you can have inverse power method, so, what happens there? Like in this particular method can give approximation to any Eigen value. However, this is used to find the smallest Eigen value in magnitude and the corresponding Eigen vector of matrix A . The Eigen vectors are computed very accurately by this method. Further, the method is powerful to calculate accurately the Eigen vectors when the Eigen values are not well separated.

So, in this case power method converges very slowly. So, let us say if λ is an Eigen value of A then $\frac{1}{\lambda}$ is an Eigen value of A inverse, so, corresponding to the same Eigen vector. The smallest Eigen value in magnitude of A is the largest Eigen value in magnitude of A^{-1} which is correct. So, let us choose an arbitrary vector, y_0 which is again non orthogonal to x , so, we can apply the power method on A^{-1} .

What we can write

$$Z_{k+1} = A^{-1} y_k$$

and

$$y_{k+1} = \frac{Z_{k+1}}{m_{k+1}}$$

and m_{k+1} has the same meaning in the power method. And so, what we write that

$$A Z_{k+1} = y_k$$

and

$$y_{k+1} = \frac{Z_{k+1}}{m_{k+1}}$$

So, we find Z_{k+1} by solving this set of equations.

(Refer Slide Time: 19:09)

Numerical Analysis

Shift of origin
 Shift Power Method
 Shifted inverse Power Method
 $Z^{(k+1)} = (A - qI)Z^{(k)}$
 $Z^{(k+1)} = (A - qI)^{-1}Z^{(k)}$
 $(A - qI)Z^{(k+1)} = Z^{(k)}$

Tridiagonal system
 $Ax = b$
 $A = \begin{bmatrix} a_1 & -r_1 & & 0 \\ -p_2 & a_2 & -r_2 & \\ & -p_3 & a_3 & -r_3 \\ 0 & & -p_n & a_n \end{bmatrix}$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR 29

Now, there could be like shift of origin that means power and inverse power methods can be used to the shift of origin. So, either it can have like, shift power method. In that case, one can write that

$$Z^{(k+1)} = (A - qI)Z^{(k)}$$

we can use the Eigen value for this from the Eigen given number q or other case it could be shifted inverse power method. So, in this case one can write

$$Z^{(k+1)} = (A - qI)^{-1}Z^{(k)}$$

Or

$$(A - qI)Z^{(k+1)} = Z^{(k)}$$

This can be used to find an Eigen value which is closest to a given number q . In both the cases normalization is done as given here. So, this is how the normalization is done. Now, we talk about some special system like, one is the solution of that tri diagonal system. So, let us say, we consider a system which is $Ax = b$ and it has a special case of tri diagonal system of equation arisen in the numerical solution of differential equation.

(Refer Slide Time: 21:10)

Numerical Analysis

$$-p_j x_{j-1} + q_j x_j - r_j x_{j+1} = b_j \quad 1 \leq j \leq n$$

p_1, r_n are given, q_0, r_{n+1} are unknown

assume that $p_j > 0, q_j > 0, r_j > 0, q_j \geq p_j + r_j$
 $1 \leq j \leq n$

$$x_j = \alpha_j x_{j+1} + \beta_j \quad 1 \leq j \leq n$$

$$x_{j-1} = \alpha_{j-1} x_j + \beta_{j-1}$$

$$x_j = \frac{r_j}{q_j - p_j \alpha_{j-1}} x_{j+1} + \frac{b_j + p_j \beta_{j-1}}{q_j - p_j \alpha_{j-1}}$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

30

So, this if you look at particularly, this is written as that form

$$-p_j x_{j-1} + q_j x_j - r_j x_{j+1} = b_j$$

where j lies between 1, 2. So, essentially every row of this matrix has only 3, so, it is a like, one is the main diagonal then you have one up diagonal, the 2 up diagonal terms which in this case. So, where p_1, r_n are given and x_0, x_{n+1} are known from the boundary condition of the given problem.

Let us say, assume that we have $p_j > 0, q_j > 0, r_j > 0$ and $q_j \geq p_j + r_j$. So, for $1 \leq j \leq n$ that is A is diagonally dominant, however, the requirement is a sufficient condition. Now, to get the solution of this particular equation, we write the difference relations like

$$x_j = \alpha_j x_{j+1} + \beta_j$$

where, $1 \leq j \leq n$.

So, this guy we can have

$$x_{j-1} = \alpha_{j-1} x_j + \beta_{j-1}$$

Now, from this if we eliminate x_{j-1} , what do we get,

$$x_j = \frac{r_j}{q_j - p_j \alpha_{j-1}} x_{j+1} + \frac{b_j + p_j \beta_{j-1}}{q_j - p_j \alpha_{j-1}}$$

So, when you compare this guy, like this with this, what we get?

(Refer Slide Time: 23:24)

Numerical Analysis

$$\alpha_j = \frac{r_j}{q_j - p_j \alpha_{j-1}}, \quad \beta_j = \frac{b_j + p_j \beta_{j-1}}{q_j - p_j \alpha_{j-1}}$$

if $x_0 = A, \alpha_0 = 0, \beta_0 = A$, for all x ,
 $x_0 = \alpha_0 x_1 + \beta_0$

$\alpha_j, \beta_j, 1 \leq j \leq n$
 $\alpha_1 = \frac{r_1}{q_1}, \quad \beta_1 = \frac{b_1 + p_1 A}{q_1}$
 $\alpha_n = \frac{r_n}{q_n - p_n \alpha_{n-1}}, \quad \beta_n = \frac{b_n + p_n \beta_{n-1}}{q_n - p_n \alpha_{n-1}}$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR
31

That,

$$\alpha_j = \frac{r_j}{q_j - p_j \alpha_{j-1}}$$

and

$$\beta_j = \frac{b_j + p_j \beta_{j-1}}{q_j - p_j \alpha_{j-1}}$$

If $x_0 = A$ and $\alpha_0 = 0, \beta_0 = A$, then the relation

$$x_0 = \alpha_0 x_1 + \beta_0$$

holds for all x_1 . The remaining α_j, β_j , for $1 \leq j \leq n$, which can be calculated as

$$\alpha_1 = \frac{r_1}{q_1}$$

$$\beta_1 = \frac{b_1 + p_1 A}{q_1}$$

Similarly,

$$\alpha_n = \frac{r_n}{q_n - p_n \alpha_{n-1}}$$

$$\beta_n = \frac{b_n + p_n \beta_{n-1}}{q_n - p_n \alpha_{n-1}}$$

(Refer Slide Time: 24:44)

Numerical Analysis

if $x_{n+1} = B$ is prescribed,

$$\begin{aligned}
 x_n &= \alpha_n B + \beta_n \\
 x_{n-1} &= \alpha_{n-1} x_n + \beta_{n-1} \\
 &\vdots \\
 x_1 &= \alpha_1 x_2 + \beta_1, \quad |\alpha_j| \leq 1
 \end{aligned}$$

Pentagonal system (Five diagonal)

Matrix A is:

$$\begin{bmatrix}
 x_1 & s_1 & t_1 & & \\
 t_2 & x_2 & s_2 & t_2 & \\
 t_3 & s_3 & -x_3 & s_3 & t_3 \\
 & & & & \\
 & & & & x_n & s_n & t_n
 \end{bmatrix}$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR 32

Now, if $x_{n+1} = B$ is prescribed then the solution of the tri diagonal system would become like

$$\begin{aligned}
 x_n &= \alpha_n B + \beta_n \\
 x_{n-1} &= \alpha_{n-1} x_n + \beta_{n-1} \\
 &\vdots \\
 x_1 &= \alpha_1 x_2 + \beta_1
 \end{aligned}$$

the procedure convergence for $|\alpha_j| \leq 1$, this method is equivalent to the Gauss elimination and minimizes the storage in the machine computation, as only 3 diagonals are to be stored.

So, if the problem to be solved by the tri diagonal system. Now, this is a special system there is another special system, one is called a pentagonal system or 5 diagonal system. So, in this case also the $Ax = b$. So, this is the, r is the diagonal term and the last but one will have 4 digit.

(Refer Slide Time: 26:28)

Numerical Analysis

Equation for $2 \leq j \leq n-2$:

$$p_j x_{j-2} + q_j x_{j-1} + r_j x_j + s_j x_{j+1} + t_j x_{j+2} = b_j$$

Derivation of x_j :

$$\begin{aligned}
 x_j &= \frac{1}{r_j} [b_j - p_j x_{j-2} - q_j x_{j-1} - s_j x_{j+1} - t_j x_{j+2}] \\
 &= \frac{1}{r_j} [b_j - p_j x_{j-2} - q_j x_{j-1} - s_j x_{j+1} - t_j x_{j+2}]
 \end{aligned}$$

Intermediate terms:

$$\begin{aligned}
 p^* &= q_j - p_j \beta_{j-2} \\
 q^* &= b_j - p_j \beta_{j-2} - q_j \beta_{j-1} \\
 r^* &= r_j - p_j \beta_{j-2} - q_j \beta_{j-1} - s_j \beta_j - t_j \beta_{j+1}
 \end{aligned}$$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR 33

So, here the equation would lead to like

$$p_j x_{j-2} + q_j x_j + r_j x_j + s_j x_{j+1} + t_j x_{j+2} = b_j$$

So, this is what the Penta diagonal system and $2 \leq j \leq n-2$. For the solution assume the recurrence relation like,

$$x_j = \alpha_j - \beta_j x_{j+1} - \gamma_j x_{j+2}$$

Where $0 \leq j \leq n$ and we can say that

$$x_{j-1} = \alpha_{j-1} - \beta_{j-1} x_j - \gamma_{j-1} x_{j+1}$$

$$x_{j-2} = \alpha_{j-2} - \beta_{j-2} x_{j-1} - \gamma_{j-2} x_j$$

So, all these if we substitute these are the things, if we substitute back in here then, finally, we get the

$$x_j = \frac{1}{r^*} [(b_j - p^*) - (s_j - \gamma_{j-1} + q^*) x_{j+1} - t_j x_{j+2}]$$

Where

$$q^* = q_j - p_j \beta_{j-2}$$

$$p^* = p_j \alpha_{j-2} + \alpha_{j-1} q^*$$

And

$$r^* = r_j - p_j \gamma_{j-2} - \beta_{j-1} q^*$$

(Refer Slide Time: 28:30)

Numerical Analysis

$$\alpha_j = \frac{(b_j - p^*)}{r^*}$$

$$\beta_j = \frac{(s_j - \gamma_{j-1} + q^*)}{r^*}$$

$$\gamma_j = \frac{t_j}{r^*}$$

Let, $j=0$, $x_0 = \alpha_0 - \beta_0 x_1 - \gamma_0 x_2$
if $x_0 = \alpha_0$, $\beta_0 = \gamma_0 = 0$

$j=1$, $x_1 = \alpha_1 - \beta_1 x_2 - \gamma_1 x_3$

$j=2$, $x_2 = \alpha_2 - \beta_2 x_3 - \gamma_2 x_4$

INDIAN INSTITUTE OF TECHNOLOGY KANPUR 34

So, when we compare this, we get,

$$\alpha_j = \frac{(b_j - p^*)}{r^*}$$

$$\beta_j = \frac{(s_j - \gamma_{j-1} + q^*)}{r^*}$$

$$\gamma_j = \frac{t_j}{r^*}$$

So, now, we can set $j = 0$ then we get

$$x_0 = \alpha_0 - \beta_0 x_1 - \gamma_0 x_2$$

So, this equation is satisfied for all x_1 and x_2 , only if

$$x_0 = \alpha_0, \quad \beta_0 = 0 = \gamma_0$$

So, if x_0 is prescribed then α_0 is known, if only given system to solve then we can have $\alpha_0 = x_0 = 0$.

For $j = 1$ we get

$$x_1 = \alpha_1 - \beta_1 x_2 - \gamma_1 x_3$$

So, the equation should be identical with the first equation, so which is,

$$x_1 = \frac{1}{r_1} (b_1 - s_1 x_2 - t_1 x_3)$$

So, comparing this it gets us

$$\alpha_1 = \frac{b_1}{r_1}$$

$$\beta_1 = \frac{s_1}{r_1}$$

and

$$\gamma_1 = \frac{t_1}{r_1}$$

(Refer Slide Time: 29:52)

Numerical Analysis

$d_i, \beta_i, \gamma_i \quad i=2, \dots, n$

$x_n = d_n - \beta_n x_{n+1} - \gamma_n x_{n+2}$

Let, $\gamma_n = 0, \quad x_{n+1} = g_{n+1}$

Also, $\beta_n = 0, \quad x_n = d_n - \beta_n x_{n+1}$

or $x_n = d_n$

x_{n+1}, x_{n+2}

INDIAN INSTITUTE OF TECHNOLOGY KANPUR 35

So, the remaining values $\alpha_i, \beta_i, \gamma_i$, for $i = 2$ to n which are obtained using these particular expressions, here given and then we can get

$$x_n = \alpha_n - \beta_n x_{n+1} - \gamma_n x_{n+2}$$

So, if we set $\gamma_n = 0$ then if the problem is derived from the boundary value problem in which the values or the inputs are prescribed, so, $x_{n+1} = g_{n+1}$ which is given otherwise we set $\beta_n = 0$. So that we get $x_n = \alpha_n - \beta_n x_{n+1}$ or $x_n = \alpha_n$.

So, the values of $x_{n-1}, x_{n-2}, \dots, x_1$ are obtained from the back substitution of these equations here, what is given here? So, you see, why do you have this special system or tri diagonal, penta diagonal system, this is how you can kind of calculate the different elements and these are the special systems and which would be the outcome of your governing equations and you end up in the linear system. So that pretty much what we wanted to discuss on the system of linear equations. And we will stop it here and continue the things in the next session.