Numerical Modeling

Unit 4: Solution for System of Equations

Numerical Solution for a System of Equations

- Linear System of Equations
  - Representation using Matrices
  - Gaussian Elimination, backward substitution
  - Pivoting and Scaling
  - LU Decomposition
- Nonlinear System of Equations
  - Newton Method

Linear System of Equations: Representation using Matrices

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = & b_1 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = & b_2 \\ \dots\dots\dots & \dots\dots \\ a_{n1}x_1 + a_{n2}x_2 + \dots\dots + a_{nn}x_n = & b_n \end{cases}$$

Matrice format: Ax=b,

Where:

$$A = (a_{ij}) = \begin{bmatrix} a_{11} & a_{12} & \dots\dots & a_{1n} \\ a_{21} & a_{22} & \dots\dots & a_{2n} \\ \dots & \dots & \dots. & \dots. \\ a_{n1} & a_{n2} & \dots\dots & a_{nn} \end{bmatrix} \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_n \end{bmatrix}$$

Linear System of Equations: Gaussian Elimination

1. Iterative transformations applied to A to get to an upper triangular form

2. Use "backward substitution" to find the solution

$$\overline{A} = [A, b] = \left[\begin{array}{ccccc} a_{11} & a_{12} & \ldots & a_{1n} & : & a_{1,n+1} \\ a_{21} & a_{22} & \ldots & a_{2n} & : & a_{2,n+1} \\ \ldots & \ldots & \ldots & \ldots & : & \ldots. \\ a_{n1} & a_{n2} & \ldots & a_{nn} & : & a_{n,n+1} \end{array} \right]$$

$$\hat{A} = \left[\begin{array}{ccccc} a_{11} & a_{12} & \ldots & a_{1n} & : & a_{1,n+1} \\ 0 & a_{22} & \ldots & a_{2n} & : & a_{2,n+1} \\ \ldots & \ldots & \ldots & \ldots & : & \ldots \\ 0 & \ldots.. & 0 & a_{nn} & : & a_{n,n+1} \end{array} \right]$$

Linear System of Equations: Gaussian Elimination

1. Iterative transformations applied to A to get to an upper triangular form

2. Use "backward substitution" to find the solution

$$M^{(1)} = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ -m_{21} & 1 & & & \vdots \\ \vdots & 0 & & & \vdots \\ \vdots & \vdots & & & 0 \\ -m_{n1} & 0 & \cdots & 0 & 1 \end{bmatrix}$$

$$m_{j,1} = \frac{a_{j1}}{a_{11}}$$

$$A^{(2)}x = M^{(1)}Ax = M^{(1)}b = b^{(2)}$$

Linear System of Equations: Gaussian Elimination

```
>> A=[1 1 0 1; 2 1 -1 1; -1 2 3 -1;3 -1 -1 2]
A =

   1   1   0   1
   2   1  -1   1
  -1   2   3  -1
   3  -1  -1   2

>> P=[0 0 0 1; 0 1 0 0; 0 0 1 0; 1 0 0 0]
P =

   0   0   0   1
   0   1   0   0
   0   0   1   0
   1   0   0   0

>> P*A
ans =

   3  -1  -1   2
   2   1  -1   1
  -1   2   3  -1
   1   1   0   1

>> A*P
ans =

   1   1   0   1
   1   1  -1   2
  -1   2   3  -1
   2  -1  -1   3
```

Switching rows (permutation) in the matrix A

Use a square permutation matrix
 - obtained by switching rows/columns in the identity matrix

PA=A'
Where A' is the matrix A where the same 2 rows are switched

AP=A"
Where A' is the matrix A where the same 2 columns are switched

Linear System of Equations: Pivoting Strategies

- Avoid small numbers for the pivot value
- Switch rows so that the pivot is equal to max value
- Normalize the coefficients (scale factor)

$$PivotRowJ = max\left|a_{kj}\right|, k \geqslant j$$

$$ScaleRowJ = s_j = max\left|a_{ji}\right|, n \geqslant i > 0$$

$$PivotRowJ = max\frac{\left|a_{kj}\right|}{s_j}, k \geqslant j$$

Linear System of Equations: LU Decomposition

- Write matrix A as a product of 2 matrices (one lower triangular form and one upper triangular form)
- We use the Gausian elimination to create the upper triangular matrix
- Each elimination can be represented as a product with one of these matrices

$$M^{(1)} = \begin{bmatrix} 1 & 0 & \dots. & \dots. & 0 \\ -m_{21} & 1 & & & : \\ : & 0 & & & : \\ : & : & & & 0 \\ -m_{n1} & 0 & \dots. & 0 & 1 \end{bmatrix}$$

$$M^{(k)} = \begin{bmatrix} 1 & 0 & \dots & \dots & \dots & \dots & 0 \\ 0 & 1 & & & & & : \\ : & 0 & 1 & & & & : \\ : & & 0 & 1 & & & : \\ : & & & -m_{k+1,k} & & & : \\ : & & & & & & : \\ : & & & & 0 & 1 & 0 \\ 0 & \dots & 0 & -m_{n,k} & 0 & 0 & 1 \end{bmatrix}$$

$$m_{j,2} = \frac{a_{j2}^{(2)}}{a_{22}^{(2)}}$$

2-nd column

Linear System of Equations: LU Decomposition

Ax=b,

- Decomposition
  - A=LU
  - LUx=b
- Forward substitution
  - Ly=b
- Backward substitution
  - Ux=y

$$A^{(2)}x = M^{(1)}Ax = M^{(1)}b = b^{(2)}$$

$$A^{(n)} = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \cdots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & \vdots \\ \vdots & & & a_{n-1,n}^{(n-1)} \\ 0 & \dots & 0 & a_{nn}^{(n)} \end{bmatrix}$$

Linear System of Equations: LU Decomposition

Ax=b

$$A^{(n)} = M^{(n-1)} \ldots M^{(1)} A = U$$

$$LU = A$$

$$[M^{(1)}]^{-1} \ldots [M^{(n-1)}]^{-1} M^{(n-1)} \ldots M^{(1)} A = A$$

$$L = [M^{(1)}]^{-1} \ldots [M^{(n-1)}]^{-1}$$

$$M^{(k)} = \begin{bmatrix} 1 & 0 & \ldots & \ldots & \ldots & \ldots & 0 \\ 0 & 1 & & & & & \vdots \\ \vdots & 0 & 1 & & & & \vdots \\ \vdots & & 0 & 1 & & & \vdots \\ \vdots & & & -m_{k+1,k} & & & \vdots \\ \vdots & & & & & & \vdots \\ \vdots & & & & 0 & 1 & 0 \\ 0 & \ldots & 0 & -m_{n,k} & 0 & 0 & 1 \end{bmatrix}$$

$$[M^{(k)}]^{-1} = \begin{bmatrix} 1 & 0 & \ldots & \ldots & \ldots & \ldots & 0 \\ 0 & 1 & & & & & \vdots \\ \vdots & 0 & 1 & & & & \vdots \\ \vdots & & 0 & 1 & & & \vdots \\ \vdots & & & m_{k+1,k} & & & \vdots \\ \vdots & & & & & & \vdots \\ \vdots & & & & 0 & 1 & 0 \\ 0 & \ldots & 0 & m_{n,k} & 0 & 0 & 1 \end{bmatrix}$$

Nonlinear System of Equations

- Nonlinear Equation: $f(x_1 + .. + x_n) \neq f(x_1) + .. + f(x_2)$

- System of Nonlinear Equations:

$$\begin{cases} f_1(x_1, .., x_n) = & 0 \\ f_2(x_1, .., x_n) = & 0 \\ \ldots\ldots\ldots & \ldots \\ f_n(x_1, .., x_n) = & 0 \end{cases}$$

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Solution of Equations in One Variable

Newton Method: find x so that f(x) = 0

Taylor's Theorem: if

- $x_0 \in [a, b]$; $f \in C^n[a, b]$ and $f^{(n+1)}$
- For every $x \in [a, b]$ we can find a value $g(x) \in [a, b]$ so that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n+1)}(g(x))}{(n+1)!}(x - x_0)^{n+1}$$

For $n = 1$ we get: $f(x) = f(x_0)+(x-x_0)f'(x_0)+(1/2)(x-x_0)^2 f''(g(x))$

Simplification 1: We try to find a root so $f(x) = 0$

Simplification 2: The Newton method works for small $(x-x_0)$. In this case $(x-x_0)^2$ is very small and can be ignored

With these simplifications we get $f(x_0)+(x-x_0)f'(x_0) =\sim 0$

or: $x =\sim x_0 - f(x_0)/ f'(x_0)$

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Nonlinear System of Equations: Newton Method

- Nonlinear Equation: $f(x_1 + .. + x_n) \neq f(x_1) + .. + f(x_2)$

- System of Nonlinear Equations:
$$\begin{cases} f_1(x_1, .., x_n) = & 0 \\ f_2(x_1, .., x_n) = & 0 \\ \cdots\cdots\cdots & \cdots \\ f_n(x_1, .., x_n) = & 0 \end{cases}$$

- Jacobian Matrix:
$$J = \begin{bmatrix} j_{11} & j_{12} & \cdots\cdot & j_{1n} \\ j_{21} & j_{22} & \cdots\cdot & j_{2n} \\ \cdots & \cdots & \cdots\cdot & \cdots\cdot \\ j_{n1} & j_{n2} & \cdots\cdots & j_{nn} \end{bmatrix} \qquad j_{ab}(x) = \frac{\delta f_a}{\delta x_b}(x)$$

$$\frac{\delta f}{\delta x_k}(x_1, .., x_n) = \lim_{h->0} \frac{f(x_1,..,x_k+h,..x_n) - f(x_1,..,x_n)}{h}$$
$$\frac{\delta f}{\delta x_k}(x_1, .., x_n) = \lim_{h->0} \frac{f(x_1,..,x_k+h,..x_n) - f(x_1,..,x_k-h,..x_n)}{2h}$$

Nonlinear System of Equations: Newton Method

- Start from the expression: $x_{k+1} = x_k - f(x_k)/f'(x_k)$

- Vector form:

$$X_{k+1} = X_k - F(X_k)/J(X_k)$$
$$X_{k+1} - X_k = -F(X_k)/J(X_k)$$
$$X_{k+1} - X_k = -J^{-1}(X_k)F(X_k)$$

- Linear form:

$$J(X_k) * (X_{k+1} - X_k) = -F(X_k)$$

!

$$J(X_k) * Y = \boxed{-F(X_k)} \qquad A \cdot Y = \boxed{B}$$
$$Y = X_{k+1} - X_k$$

$$-\begin{pmatrix} f_1(1,1,1) \\ f_2(1,1,1) \\ f_3(1,1,1) \end{pmatrix}$$

- Apply Gaussian Elimination to the linear form