REVIEW Lecture 6:

- **Direct Methods for solving linear algebraic equations**
  - LU decomposition/factorization
    - Separates time-consuming elimination for $A$ from that for $b$ / $B$
      
      $$ A = L \cdot U \quad \Rightarrow \quad L \vec{y} = \vec{b} \quad \U \vec{x} = \vec{y} $$
    - Derivation, assuming no pivoting needed:
      $$ a_{ij} = \sum_{k=1}^{\min(i,j)} m_{ik} a_{kj}^{(k)} $$
    - Number of Ops: Same as for Gauss Elimination
    - Pivoting: Use pivot element “pointer vector”
    - Variations: Doolittle and Crout decompositions, Matrix Inverse

- **Error Analysis for Linear Systems**
  - Matrix norms
  - Condition Number for Perturbed RHS and LHS:
    $$ K(A) = \| A^{-1} \| \| A \| $$

- **Special Matrices**: Intro
TODAY (Lecture 7): Systems of Linear Equations III

• **Direct Methods**
  - Gauss Elimination
  - LU decomposition/factorization
  - Error Analysis for Linear Systems
  - Special Matrices: LU Decompositions
    - Tri-diagonal systems: Thomas Algorithm
    - General Banded Matrices
      - Algorithm, Pivoting and Modes of storage
      - Sparse and Banded Matrices
  - Symmetric, positive-definite Matrices
    - Definitions and Properties, Choleski Decomposition

• **Iterative Methods**
  - Jacobi’s method
  - Gauss-Seidel iteration
  - Convergence
Reading Assignment

  
Special Matrices

- Certain Matrices have particular structures that can be exploited, i.e.
  - Reduce number of ops and memory needs

- Banded Matrices:
  - Square banded matrix that has all elements equal to zero, excepted for a band around the main diagonal.
  - Frequent in engineering and differential equations:
    - Tri-diagonal Matrices
    - Wider bands for higher-order schemes
  - Gauss Elimination or LU decomposition inefficient because, if pivoting is not necessary, all elements outside of the band remain zero (but direct GE/LU would manipulate these zero elements anyway)

- Symmetric Matrices

- Iterative Methods:
  - Employ initial guesses, than iterate to refine solution
  - Can be subject to round-off errors
Forced Vibration of a String

Consider the case of a Harmonic excitation

\[ f(x,t) = -f(x) \cos(\omega t) \]

Applying Newton’s law leads to the wave equation:

With separation of variables, one obtains the equation for modal amplitudes, see eq. (1) below:

Differential Equation for the amplitude:

\[ \frac{d^2y}{dx^2} + k^2y = f(x) \quad (1) \]

Boundary Conditions:

\[ y(0) = 0 \ , \ y(L) = 0 \]
Special Matrices: Tri-diagonal Systems

Forced Vibration of a String

\[ f(x,t) \]

\[ x_i \quad \rightarrow \quad Y(x,t) \]

Harmonic excitation

\[ f(x,t) = f(x) \cos(\omega t) \]

Differential Equation:

\[ \frac{d^2y}{dx^2} + k^2y = f(x) \quad (1) \]

Boundary Conditions:

\[ y(0) = 0 , \quad y(L) = 0 \]

Finite Difference

\[ \frac{d^2y}{dx^2} \bigg|_{x_i} \approx \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} + O(h^2) \]

Discrete Difference Equations

\[ y_{i-1} + ( (kh)^2 - 2 ) y_i + y_{i+1} = f(x_i)h^2 \]

Matrix Form:

\[
\begin{bmatrix}
(kh)^2 - 2 & 1 & \cdots & \cdots & 0 \\
1 & (kh)^2 - 2 & 1 & \cdots & \\
\vdots & \vdots & \ddots & \ddots & \\
\vdots & \vdots & \ddots & \ddots & \\
0 & \cdots & \cdots & 1 & (kh)^2 - 2 \\
\end{bmatrix}
\]

\[ \bar{y} = \begin{bmatrix}
f(x_1)h^2 \\
\cdots \\
f(x_i)h^2 \\
\cdots \\
f(x_n)h^2 \\
\end{bmatrix} \]

Tridiagonal Matrix

If \( kh < 1 \) or \( kh > \sqrt{3} \) symmetric, negative or positive definite: No pivoting needed

Note: for \( 0 < kh < 1 \) Negative definite => Write: \( A' = -A \) and \( \bar{y}' = -\bar{y}' \) to render matrix positive definite

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Numerical Fluid Mechanics
Special Matrices: Tri-diagonal Systems

General Tri-diagonal Systems: Bandwidth of 3

\[
\begin{bmatrix}
  a_1 & c_1 & \cdots & & 0 \\
  b_2 & a_2 & c_2 & & \\
  & \ddots & \ddots & \ddots & \\
  b_i & a_i & c_i & \ddots & \\
  0 & \cdots & b_n & a_n & \\
\end{bmatrix}
\begin{bmatrix}
  f_1 \\
  . \\
  . \\
  . \\
  \end{bmatrix}
= \begin{bmatrix}
  x_1 \\
  . \\
  . \\
  . \\
\end{bmatrix}
\]

LU Decomposition

\[
\bar{A} = \bar{L}\bar{U}
\]

\[
\begin{align*}
\bar{L}\bar{y} &= \bar{f} \\
\bar{U}\bar{x} &= \bar{y}
\end{align*}
\]

Three steps for LU scheme:

1. Decomposition (GE): 
   \[ a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik}a_{kj}^{(k)}, \quad m_{ik} = a_{ik}^{(k)}/a_{kk}^{(k)} \]
2. Forward substitution 
   \[ \bar{L}\bar{y} = \bar{f} \]
3. Backward substitution 
   \[ \bar{U}\bar{x} = \bar{y} \]
Special Matrices: Tri-diagonal Systems

Thomas Algorithm

By identification with the general LU decomposition, one obtains,

\[ a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik}a_{kj}^{(k)}, \quad m_{ik} = a_{ik}^{(k)}/a_{kk}^{(k)} \]

1. Factorization/Decomposition

\[ \alpha_1 = a_1 \]
\[ \beta_k = \frac{b_k}{\alpha_{k-1}}, \quad \alpha_k = a_k - \beta_k c_{k-1}, \quad k = 2, 3, \ldots n \]

2. Forward Substitution

\[ y_1 = f_1, \quad y_i = f_i - \beta_i y_{i-1}, \quad i = 2, 3, \ldots n \]

3. Back Substitution

\[ x_n = \frac{y_n}{\alpha_n}, \quad x_i = \frac{y_i - c_i x_{i+1}}{\alpha_i}, \quad i = n - 1, \ldots 1 \]

Number of Operations: Thomas Algorithm

- LU Factorization: \(3(n-1)\) operations
- Forward substitution: \(2(n-1)\) operations
- Back substitution: \(3(n-1)+1\) operations
- Total: \(8(n-1) \sim O(n)\) operations
Special Matrices: 
General, Banded Matrix

General Banded Matrix \((p \neq q)\)
\[
\begin{align*}
j > i + p & \quad a_{ij} = 0 \\
i > j + q &
\end{align*}
\]

Banded Symmetric Matrix \((p = q = b)\)
\[
\begin{align*}
a_{ij} &= a_{ji} , \quad |i - j| \leq b \\
a_{ij} &= a_{ji} = 0 , \quad |i - j| > b
\end{align*}
\]

\(w = 2b + 1\) is called the bandwidth
\(b\) is the half-bandwidth

\(p\) super-diagonals
\(q\) sub-diagonals
\(w = p + q + 1\) bandwidth
Special Matrices:
General, Banded Matrix

LU Decomposition via Gaussian Elimination
If No Pivoting: the zeros are preserved

\[
L = \begin{bmatrix}
0 & \cdots & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & 0 \\
\end{bmatrix}
\]

\[
U = \begin{bmatrix}
0 & \cdots & \cdots & \cdots \\
0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
\end{bmatrix}
\]

\[
m_{ij} = \frac{a_{ij}^{(j)}}{a_{jj}^{(j)}} = 0 \quad \text{if } j > i \text{ or } i > j + q
\]

(General case) (Banded)

\[
u_{ij} = a_{ij}^{(i)} = a_{ij}^{(i-1)} - m_{i,i-1} a_{i-1,j}^{(i-1)}
\]

(General case) (Banded)
Consider pivoting the 2 rows as below:

Then, the bandwidth of $L$ remains unchanged,

$$m_{ij} = 0 \quad \text{if} \quad j > i \quad \text{or} \quad i > j + q$$

but the bandwidth of $U$ becomes as that of $A$

$$u_{ij} = 0 \quad \text{if} \quad i > j \quad \text{or} \quad j > i + p + q$$

$$w = p + 2q + 1 \text{ bandwidth}$$
Special Matrices: General, Banded Matrix

Compact Storage

Matrix size: $n^2$

Matrix size: $n(p+2q+1)$

Needed for Pivoting only

Diagonal (length n)
Skyline storage applicable when no pivoting is needed, e.g. for banded, symmetric, and positive definite matrices: FEM and FD methods. Skyline solvers are usually based on Cholesky factorization (which preserves the skyline).
Special Matrices: Symmetric (Positive-Definite) Matrix

Symmetric Coefficient Matrices:

- If no pivoting, the matrix remains symmetric after Gauss Elimination/LU decompositions

Proof: Show that if \( a_{ij}^{(k)} = a_{ji}^{(k)} \) then \( a_{ij}^{(k+1)} = a_{ji}^{(k+1)} \) using:

\[
a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik}a_{kj}^{(k)}, \quad m_{ik} = a_{ik}^{(k)}/a_{kk}^{(k)}
\]

- Gauss Elimination symmetric (use only the upper triangular portion of \( A \)):

\[
a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik}a_{kj}^{(k)}
\]

\[
m_{ik} = \frac{a_{ki}^{(k)}}{a_{kk}^{(k)}}, \quad i = k + 1, k + 2, \ldots, n \quad j = i, i + 1, \ldots, n
\]

- About half the total number of ops than full GE
Special Matrices: Symmetric, Positive Definite Matrix

1. Sylvester Criterion:
A symmetric matrix is Positive Definite if and only if:
\[ \det(A_k) > 0 \quad \text{for} \quad k=1,2,\ldots,n, \quad \text{where} \quad A_k \text{ is matrix of } k \text{ first lines/columns} \]

Symmetric Positive Definite matrices frequent in engineering

2. For a symmetric positive definite \( A \), one thus has the following properties

a) The maximum elements of \( A \) are on the main diagonal

b) For a Symmetric, Positive Definite \( A \): No pivoting needed

c) The elimination is stable: \( |a_{ii}^{(k+1)}| \leq 2 |a_{ii}^{(k)}| \). To show this, use \( a_{kj}^2 \leq a_{kk} a_{jj} \) in

\[
a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)} \\
m_{ik} = \frac{a_{ki}^{(k)}}{a_{kk}^{(k)}}, \quad i = k + 1, k + 2, \ldots, n \quad j = i, i + 1, \ldots, n
\]
Special Matrices: Symmetric, Positive Definite Matrix

The general GE

\[
\begin{align*}
    a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)} \\
    m_{ik} &= \frac{a_{ki}^{(k)}}{a_{kk}^{(k)}}, \quad i = k + 1, k + 2, \ldots, n \quad j = i, i + 1, \ldots, n
\end{align*}
\]

becomes:

\[
\overline{A} = \overline{L}\overline{U} = \overline{U}^\dagger \overline{U}
\]

Choleski Factorization

\[
\overline{U}^\dagger = [m_{ij}]
\]

where

\[
\begin{align*}
    m_{kk} &= \left( a_{kk} - \sum_{\ell=1}^{k-1} m_{k\ell} \overline{m}_{k\ell} \right)^{1/2} \\
    m_{ik} &= \frac{a_{ik} - \sum_{\ell=1}^{k-1} m_{i\ell} \overline{m}_{k\ell}}{m_{kk}}, \quad i = k + 1, \ldots, n
\end{align*}
\]

No pivoting needed

† Complex Conjugate and Transpose
Linear Systems of Equations: **Iterative Methods**

Sparse (large) Full-bandwidth Systems (frequent in practice)

Iterative Methods are then efficient

Analogous to iterative methods obtained for roots of equations, i.e. Open Methods: Fixed-point, Newton-Raphson, Secant

Example of Iteration equation

\[
\begin{align*}
A x &= b &\Rightarrow & A x - b = 0 \\
x &= x + A x - b &\Rightarrow & x^{k+1} = x^k + A x^k - b = (A + I) x^k - b
\end{align*}
\]

General Stationary Iteration Formula

\[
x^{k+1} = B x^k + c & \quad k = 0, 1, 2, \ldots
\]

Compatibility condition for \(Ax=b\) to be the solution:

Write \(c = C b\)

\[
A^{-1} b = B A^{-1} b + C b
\]

\[
(I - B) A^{-1} = C \quad \text{or} \quad B = I - CA
\]

\(ps: \) \(B\) and \(c\) could be function of \(k\) (non-stationary)
Convergence

\[ \left| \overline{x}^{(k+1)} - \overline{x} \right| \to 0 \quad \text{for} \quad k \to \infty \]

Iteration – Matrix form

\[ \overline{x}^{(k+1)} = \overline{B} \overline{x}^{(k)} + \overline{c} \quad , \quad k = 0, \ldots \]

Convergence Analysis

\[
\begin{align*}
\overline{x}^{(k+1)} &= \overline{B} \overline{x}^{(k)} + \overline{c} \\
\overline{x} &= \overline{B} \overline{x} + \overline{c} \\
\Rightarrow \quad \overline{x}^{(k+1)} - \overline{x} &= \overline{B} (\overline{x}^{(k)} - \overline{x}) \\
&= \overline{B} \cdot \overline{B} (\overline{x}^{(k-1)} - \overline{x}) \\
&= \overline{B}^{k+1} (\overline{x}^{(0)} - \overline{x})
\end{align*}
\]

\[
\left| \overline{x}^{(k+1)} - \overline{x} \right| \leq \left| \overline{B}^{k+1} \right| \left| \overline{x}^{(0)} - \overline{x} \right| \leq \left| \overline{B} \right|^{k+1} \left| \overline{x}^{(0)} - \overline{x} \right|
\]

Sufficient Condition for Convergence:

\[ \left| \overline{B} \right| < 1 \]
\[ \|B\| < 1 \text{ for a chosen matrix norm} \]

Infinite norm often used in practice

\[ \|A\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^{m} |a_{i,j}| \]

“Maximum Column Sum”

\[ \|A\|_\infty = \max_{1 \leq i \leq m} \sum_{j=1}^{n} |a_{i,j}| \]

“Maximum Row Sum”

\[ \|A\|_F = \left( \sum_{i=1}^{m} \sum_{j=1}^{n} |a_{i,j}|^2 \right)^{1/2} \]

“The Frobenius norm” (also called Euclidean norm)

\[ \|A\|_2 = \sqrt{\lambda_{\text{max}}(A^*A)} \]

“The l-2 norm” (also called spectral norm)
Convergence

\[ \| \mathbf{x}^{(k+1)} - \mathbf{x} \| \to 0 \quad \text{for} \quad k \to \infty \]

Iteration – Matrix form

\[ \mathbf{x}^{(k+1)} = \mathbf{B} \mathbf{x}^{(k)} + \mathbf{c} , \quad k = 0, \ldots \]

Convergence Analysis

\[ \mathbf{x}^{(k+1)} = \mathbf{B} \mathbf{x}^{(k)} + \mathbf{c} \]

\[ \mathbf{x} = \mathbf{B} \mathbf{x} + \mathbf{c} \]

\[ \Rightarrow \mathbf{x}^{(k+1)} - \mathbf{x} = \mathbf{B} (\mathbf{x}^{(k)} - \mathbf{x}) \]

\[ = \mathbf{B} \cdot \mathbf{B} (\mathbf{x}^{(k-1)} - \mathbf{x}) \]

\[ = \mathbf{B}^{k+1} (\mathbf{x}^{(0)} - \mathbf{x}) \]

\[ \Rightarrow \quad \| \mathbf{x}^{(k+1)} - \mathbf{x} \| \leq \| \mathbf{B}^{k+1} \| \| \mathbf{x}^{(0)} - \mathbf{x} \| \leq \| \mathbf{B} \|^{k+1} \| \mathbf{x}^{(0)} - \mathbf{x} \| \]

Necessary and Sufficient Condition for Convergence:

Spectral radius of \( \mathbf{B} \) is smaller than one:

\[ \rho(\mathbf{B}) = \max_{i=1 \ldots n} | \lambda_i | < 1, \quad \text{where} \quad \lambda_i = \text{eigenvalue}(\mathbf{B}_{n \times n}) \]

(proof: use eigendecomposition of \( \mathbf{B} \))

(This ensures \( \| \mathbf{B} \| < 1 \)
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