ECE257 Numerical Methods and Scientific Computing

Ordinary Differential Equations
Today’s class:

- Boundary Value Problems
- Eigenvalue Problems
Boundary Value Problems

- Auxiliary conditions
  - $n$-th order equation requires $n$ conditions
  - Initial value conditions
    - All $n$ conditions are specified at the same value of the independent variable
  - Boundary value conditions
    - The $n$ conditions are specified at different values of the independent variable
Initial value conditions

\[
\frac{dy_1}{dt} = f_1(t, y_1, y_2)
\]

\[
\frac{dy_2}{dt} = f_2(t, y_1, y_2)
\]

where at \( t = 0 \), \( y_1 = y_{1,0} \) and \( y_2 = y_{2,0} \)

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Boundary value conditions

\[ \frac{d^2 y}{dx^2} = f(x, y) \]

where at \( x = 0, y = y_0 \) \( x = L, y = y_L \)

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Types of Boundary Conditions

• Simple B.C (Dirichlet B.C): The value of the unknown function is given at the boundary.
  \[ y(a) = y_a \]

• Neumann B.C.: The derivative of the unknown function is given at the boundary.
  \[ \left. \frac{dy}{dx} \right|_{x=a} = \frac{dy(a)}{dx} = \alpha \]

• Mixing B.C.: The combination of the unknown function’s value and derivative is given at the boundary.
  \[ a \cdot \frac{dy(a)}{dx} + b \cdot y(a) = \alpha \]
Boundary Value Problems

• Shooting Method
  – Convert the boundary value problem into an equivalent initial value problem by choosing values for all dependent variables at one boundary

• Relaxation Method
  – Choose values along the range of the integration and gradually adjust values so that they satisfy the integral and boundary values
Shooting Method

- Solve an $N$th order ODE from $x_1$ to $x_2$
- Assume $n_1$ boundary conditions at $x_1$ and $n_2$ boundary conditions at $x_2$
- There are $n_2 = N-n_1$ freely specifiable starting values at $x_1$
- Guess at those $n_2$ values and then solve the resulting initial value ODE at $x_2$
- Check if the boundary conditions are satisfied at $x_2$. If not, adjust the $n_2$ values at $x_1$ and try again.
Shooting Method Example

\[ \frac{d^2y}{dx^2} + 0.01(20 - y) = 0 \quad y(0) = 40, y(10) = 200 \]

• Convert to first-order

\[ \frac{dy}{dx} = z \quad y(0) = 40, y(10) = 200 \]

\[ \frac{dz}{dx} + 0.01(20 - y) = 0 \quad z(0) = 10 \]

• One free unspecified value at x=0 - guess a value for z(0)

• Use RK method or any other method to solve the ODE at x=10
Shooting Method Example

• Using RK method with an initial guess of \( z(0) = 10 \) we get \( y(10) = 168.3797 \)

• The initial condition was \( y(10) = 200 \), so try again

• Using RK method with an initial guess of \( z(0) = 20 \) we get \( y(10) = 285.8980 \)

• With two guesses and a linear ODE, we can interpolate to find the correct value

\[
z(0) = 10 + \frac{20 - 10}{285.8980 - 168.3797} (200 - 168.3797)
= 12.6907
\]
Shooting Method Example
Shooting Method

• If the ODE is non-linear, then you have to recast the problem as solving a series of root problems
• Think of the guessed values as a $n_2$ size vector $V$
• That vector $V$ will generate a $y(x_2)$ vector after solving the ODE
• The $y(x_2)$ vector should equal the boundary value conditions at $x_2$
Shooting Method

\[ \text{discrepancy} = BV_2(x_2, y) - y \]

- Since \( y \) is a function of \( V \), you can create a new discrepancy function \( F \) that is dependent on \( V \)
  \[ \text{discrepancy} = F(V) \]
- The problem then becomes to zero the discrepancy
- We don’t know \( F \) so we can’t use normal root-solving methods
- But we can approach it in a Newton-Raphson manner by iteratively looking at the finite difference derivatives
Shooting Method

- The problem then becomes to zero the discrepancy by solving the following linear system

\[
[\alpha] \cdot \delta V = -F
\]

\[
\alpha_{ij} = \frac{\partial F_i}{\partial V_j}
\]

\[
\frac{\partial F_i}{\partial V_j} \approx \frac{F_i(V_1,\ldots,V_j + \Delta V_j,\ldots,V_{n_2}) - F_i(V_1,\ldots,V_j,\ldots,V_{n_2})}{\Delta V_j}
\]

- The vector \( V \) can be adjusted with the results of the solution

\[
V^{new} = V^{old} + \delta V
\]

- However, you may need multiple cycles to solve for \( V \)
Shooting Method

Guess initial values of \( v_i \) (i=1 to n)
for iter=1 to niters
\[ y_2 = \text{Solve ODE at } x_2 \]
\[ F = BV - y_2 \]
for j=1 to n
\[ v_j = v_j + \Delta v_j \]
\[ y' = \text{Solve ODE at } x_2 \]
\[ F' = BV - y' \]
for i=1 to n
\[ a[i][j] = (F'[i] - F[i]) / \Delta v_j \]
endfor
restore \( v_j \)
endfor
linear solve (a \cdot dv = -F)
\[ v = v + dv \]
check error
endfor
Finite-Difference Method (FDM)

\[ y'' = p(x) y' + q(x) y + r(x) \quad y(a) = \alpha \quad \text{and} \quad y(b) = \beta \]

Approximate the derivatives using numerical difference schemes.

Dividing the range into \( n \) equal segments. \( h = \Delta x = \frac{b - a}{n} \).

\[ y''(x_i) = y_i'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + O(h^2), \]

\[ y'(x_i) = y_i' = \frac{y_{i+1} - y_{i-1}}{2h} + O(h^2) \]
Finite-Difference Method (FDM) (continued)

• Substituting the derivatives by approximations and then we have a set of discretized equations

At \( i = 1, 2, \ldots, n - 1 \)

\[
\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = p_i \frac{y_{i+1} - y_{i-1}}{2h} + q_i y_i + r_i
\]

Multiply both sides by \( h^2 \).

\[
(1 + p_i \frac{h}{2})y_{i-1} - (2 + q_i h^2) y_i + (1 - p_i \frac{h}{2}) y_{i+1} = h^2 r_i
\]
Finite-Difference Method (FDM) (continued)

For \( i = 1 \),

\[-(2 + q_1 h^2) y_1 + (1 - p_1 \frac{h}{2}) y_2 = h^2 r_1 - (1 + p_1 \frac{h}{2}) \alpha\]

For \( i = 2, 3, \ldots, n - 2 \),

\[(1 + p_i \frac{h}{2}) y_{i-1} - (2 + q_i h^2) y_i + (1 - p_i \frac{h}{2}) y_{i+1} = h^2 r_i\]

For \( i = n - 1 \),

\[(1 + p_i \frac{h}{2}) y_{n-2} - (2 + q_i h^2) y_{n-1} = h^2 r_{n-1} - (1 - p_{n-1} \frac{h}{2}) \beta\]
Matrix Form of Equation System

If \( h = \frac{a-b}{7} \) and \( n = 7 \), noticing that \( y(a) = \alpha \) and \( y(b) = \beta \).

\[
\begin{bmatrix}
-(2+q_1h^2) & 1-p_1\frac{h}{2} & 0 & 0 & 0 & 0 \\
1+p_2\frac{h}{2} & -(2+q_2h^2) & 1-p_2\frac{h}{2} & 0 & 0 & 0 \\
0 & 1+p_3\frac{h}{2} & -(2+q_3h^2) & 1-p_3\frac{h}{2} & 0 & 0 \\
0 & 0 & 1+p_4\frac{h}{2} & -(2+q_4h^2) & 1-p_4\frac{h}{2} & 0 \\
0 & 0 & 0 & 1+p_5\frac{h}{2} & -(2+q_5h^2) & 1-p_5\frac{h}{2} \\
0 & 0 & 0 & 0 & 1+p_6\frac{h}{2} & -(2+q_6h^2)
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2 \\
y_3 \\
y_4 \\
y_5 \\
y_6
\end{bmatrix}
= 
\begin{bmatrix}
h^2r_1 - (1+p_1\frac{h}{2})\alpha \\
h^2r_2 \\
h^2r_3 \\
h^2r_4 \\
h^2r_5 \\
h^2r_6 - (1-p_6\frac{h}{2})\beta
\end{bmatrix}
\]
FDM Example

\[ \frac{d^2 y}{dx^2} + 0.01(20 - y) = 0 \quad y(0) = 40, y(10) = 200 \]

\[ p(x) = 0, q(x) = 0.01, r(x) = -0.2 \]
\[ \alpha = 40, \beta = 200 \]

- Set \( n=5, h=2 \)

\[
\begin{bmatrix}
-2.04 & 1 & 0 & 0 \\
1 & -2.04 & 1 & 0 \\
0 & 1 & -2.04 & 1 \\
0 & 0 & 1 & -2.04
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2 \\
y_3 \\
y_4
\end{bmatrix}
= 
\begin{bmatrix}
-40.8 \\
-0.8 \\
-0.8 \\
-200.8
\end{bmatrix}
\]
Eigenvalue problems

- Eigenvalue problems are a special class of boundary-value problem

- Common in engineering systems with oscillating behavior
  - Springs
  - Elasticity
  - RLC circuits
Physics of Eigenvalues & Eigenvectors

A system of two degrees of freedom.

To simplify the problem, we assume that 
\(k_1 = k_2 = k_3 = k\).

\[
m_1 \frac{d^2 x_1}{dt^2} = -kx_1 + k(x_2 - x_1)
\]

\[
m_2 \frac{d^2 x_2}{dt^2} = -kx_2 - k(x_2 - x_1)
\]
Physics of Eigenvalues (continued)

Both masses ($m_1$ & $m_2$) are oscillating w.r.t. their mean positions.

$$x_i = B_i \sin(\omega t) \quad i = 1 \text{ or } 2.$$  
$$\frac{d^2 x_i}{dt^2} = -\omega^2 B_i \sin(\omega t) \quad i = 1 \text{ or } 2.$$

Substituting the above equations into the motion equations and dividing both sides by $\sin(\omega t)$.

$$-\omega^2 m_1 B_1 = -kB_1 + k(B_2 - B_1)$$

$$-\omega^2 m_2 B_2 = -kB_2 - k(B_2 - B_1)$$

$$\begin{bmatrix} \frac{2k}{m_1} - \omega^2 & - \frac{k}{m_1} \\ - \frac{k}{m_2} & \frac{2k}{m_2} - \omega^2 \end{bmatrix} \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} = 0$$
Physics of Eigenvalues (continued)

\[
\begin{bmatrix}
\frac{2k}{m_1} & -\frac{k}{m_1} \\
\frac{k}{m_2} & \frac{2k}{m_2}
\end{bmatrix}
\begin{bmatrix}
B_1 \\
B_2
\end{bmatrix} = \omega^2
\begin{bmatrix}
B_1 \\
B_2
\end{bmatrix}
\quad \leftrightarrow \quad
\begin{bmatrix}
A
\end{bmatrix}\{x\} = \lambda\{x\}
\]

Hence, the \textit{eigenvalues} are related to the \textit{natural frequencies} or periods which are crucial to the design of structures. The \textit{eigenvectors} are related to the \textit{motion} of a structure related to the corresponding natural frequency. For most engineering problems, the \textit{largest} or the \textit{smallest} frequencies are the most important ones to know.
Steps of Solving Eigen-value Problems

• \[ \det[A - \lambda I] = 0 \] leads to an algebraic equation of \( \lambda \).

• Solving the equation for \( \lambda \).
  - Polynomial method (find roots of an equation)
  - Other methods (more efficient): \textbf{Power Method}.

• Given the eigenvalues \( \lambda \), obtain the corresponding eigenvectors \( \{x\} \).
Eigenvalue Example

\[ m_1 = m_2 = 40, k = 200 \]

\[
\begin{bmatrix}
10 - \omega^2 & -5 \\
-5 & 10 - \omega^2
\end{bmatrix}
\begin{bmatrix}
B_1 \\
B_2
\end{bmatrix}
= 0
\]

\[
\det[A - \lambda I] = (10 - \omega^2)(10 - \omega^2) - (-5)(-5)
\]

\[
= (\omega^2)^2 - 20\omega^2 + 75 = 0
\]

\[ \omega^2 = 15 \text{ or 5} \]

At \ \omega^2 = 15, \ B_1 = -B_2 \text{ and at } \omega^2 = 5, \ B_1 = B_2 \]
Eigenvalue Example

(a) First mode

(b) Second mode

$T_F = 1.625$

$T_F = 2.815$
Boundary value eigenvalue problems

- Polynomial Method
  - Similar to Finite-Difference Method

- Power Method
  - Hotelling’s Method
Power Method

The **Power Method** is an *iterative* procedure for determining the *dominant (largest) eigenvalue* of the matrix $A$ and the *corresponding eigenvector*.

Example

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
= \lambda
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
\]

1. Guess a solution for the eigenvector, $x_1 = 1$, $x_2 = 1$, $x_3 = 1$. 
Example of Power Method (Continued)

substituting the eigenvector into the left-hand-side of Eq.

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix}
\begin{bmatrix}
1 \\
1 \\
1
\end{bmatrix}
= 
\begin{bmatrix}
1.778 \\
0 \\
1.778
\end{bmatrix}
\]

2. Normalize the approximate eigenvector (the right-hand-side), so that the element of the largest absolute value becomes either 1 or -1.

\[
\begin{bmatrix}
1.778 \\
0 \\
1.778
\end{bmatrix}
= 1.778
\begin{bmatrix}
1 \\
0 \\
1
\end{bmatrix}
\]

3. Using the current normalized eigenvector \( \{x\}^T = \begin{bmatrix} 1 & 0 & 1 \end{bmatrix} \) as the guess and repeat steps 1 and 2.
Example of Power Method (Continued)

substituting the eigenvector into the left-hand-side of Eq.

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix}
\begin{bmatrix}
1 \\
0 \\
1
\end{bmatrix}
= 
\begin{bmatrix}
3.556 \\
-3.556 \\
3.556
\end{bmatrix}
= 3.556 \begin{bmatrix}
1 \\
-1 \\
1
\end{bmatrix}
\]

4. Examine the relative error of \( \lambda \),

\[
\varepsilon_a = \left| \frac{\lambda_{i+1} - \lambda_i}{\lambda_{i+1}} \right| = \left| \frac{3.556 - 1.778}{3.556} \right| = 50\%.
\]

if \( \varepsilon_a \) is greater than the tolerance error, the iteration continues.

Otherwise, the eigenvalue \( \lambda \), and the eigenvector \( \{x\} \) are obtained.
Example of Power Method (Continued)

Third Iteration

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 5.333 \\ -7.111 \\ 5.333 \end{bmatrix} = \begin{bmatrix} -0.75 \\ -7.111 \\ 1 \end{bmatrix}
\]

\[\varepsilon_a = \left| \frac{-7.111 - 3.556}{-7.111} \right| = 150\%\]

Fourth Iteration

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix} \begin{bmatrix} -0.75 \\ 1 \\ -0.75 \end{bmatrix} = \begin{bmatrix} -4.444 \\ 6.222 \\ -4.444 \end{bmatrix} = \begin{bmatrix} -0.714 \\ 6.222 \\ -0.714 \end{bmatrix}
\]

\[\varepsilon_a = \left| \frac{6.222 - (-7.111)}{6.222} \right| = 214\%\]
Example of Power Method (Continued)

Fifth Iteration

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix} \begin{bmatrix}
-0.714 \\
1 \\
-0.714
\end{bmatrix} = \begin{bmatrix}
-4.317 \\
6.095 \\
-4.317
\end{bmatrix} = \begin{bmatrix}
-0.708 \\
1 \\
-0.708
\end{bmatrix}
\]

\[\varepsilon_a = \left| \frac{6.095 - 6.222}{6.095} \right| = -2.08\%
\]

The sixth iteration

\[
\begin{bmatrix}
3.556 & -1.778 & 0 \\
-1.778 & 3.556 & -1.778 \\
0 & -1.778 & 3.556
\end{bmatrix} \begin{bmatrix}
-0.708 \\
1 \\
-0.708
\end{bmatrix} = \begin{bmatrix}
-4.296 \\
6.074 \\
-4.296
\end{bmatrix} = \begin{bmatrix}
-0.707 \\
1 \\
-0.707
\end{bmatrix}
\]

\[\varepsilon_a = \left| \frac{6.074 - 6.095}{6.074} \right| = 0.35\%\]
Inverse Power Method

- The **Power Method** can be modified to provide the *smallest (lowest) (magnitude) eigenvalue* and its *eigenvector*. The modified method is known as the **inverse power method**.

- The smallest eigenvalue $\lambda$ in the matrix $A$ corresponds to $1/\lambda$ the largest eigenvalue in the inverse matrix $A^{-1}$.
General I-P Method

The combination of Shifted Power Method and I-P method can be used to determine all the eigenvalues and their related eigenvectors.

• Deflation  **Hotelling’s Method** for symmetric matrices
  • First, normalize the largest eigenvector found by the sum of the squares of the elements in the eigenvector

\[
\{X\} = \frac{\{X\}}{\sqrt{\sum_{k=1}^{n} x_k^2}}
\]
General I-P Method

• Then create new $A_2$ matrix

\[
[A]_2 = [A]_1 - \lambda_1 \{X\}_1 \{X\}_1^T
\]

\[
[A]_2 \{X\}_j = [A]_1 \{X\}_j - \lambda_1 \{X\}_1 \{X\}_1^T \{X\}_j
\]

\[
\begin{cases}
[A]_2 \{X\}_j = \lambda_j \{X\}_j & j \neq 1 \\
[A]_2 \{X\}_1 = [A]_2 \{X\}_1 - \lambda_1 \{X\}_1 & j = 1
\end{cases}
\]

• The new $A_2$ matrix has the same eigenvalues as before except that the largest eigenvalue has been replaced with 0.
Hotelling’s Method

\[ A = \begin{bmatrix} 3.556 & -1.778 & 0 \\ -1.778 & 3.556 & -1.778 \\ 0 & -1.778 & 3.556 \end{bmatrix}, \lambda_1 = 6.074, x_1 = \begin{bmatrix} -0.707 \\ 1 \\ -0.707 \end{bmatrix} \]

Modified \( A_2 \)

\[ A_2 = \begin{bmatrix} 3.556 & -1.778 & 0 \\ -1.778 & 3.556 & -1.778 \\ 0 & -1.778 & 3.556 \end{bmatrix} - 6.074 \begin{bmatrix} -0.707 \\ 1 \\ -0.707 \end{bmatrix} \begin{bmatrix} -0.707 \\ 1 \\ -0.707 \end{bmatrix} \]
Hotelling’s Method

\[
A_2 = \begin{bmatrix} 3.556 & -1.778 & 0 \\ -1.778 & 3.556 & -1.778 \\ 0 & -1.778 & 3.556 \end{bmatrix} - 6.074 \begin{bmatrix} 0.5 & -0.707 & 0.5 \\ -0.707 & 1 & -0.707 \\ 0.5 & -0.707 & 0.5 \end{bmatrix}
\]

\[
A_2 = \begin{bmatrix} 0.519 & 2.516 & -3.037 \\ 2.516 & -2.518 & 2.516 \\ -3.037 & 2.516 & 0.519 \end{bmatrix}
\]
Exam 2

• Parts 4, 6, and 7 of book
• Optimization
• Numerical Integration and Differentiation
• Ordinary Differential Equations
Next Lecture

- Partial Differential Equations
- Read Chapter PT8, 29
- HW6 due 11/16
- Exam 2 11/9