ME 2450 - Numerical Methods

Final Exam Review Notes

- You are allowed 2 sides of an 8 ½ x 11 sheet of paper for notes

- Exam: Friday, April 28, 2006 1:00 – 3:00 pm

Systems of Linear Algebraic Equations

CH. 10 LU Decomposition

- Best when [A] is fixed but {b} changes

$$[A]\{x\} = \{b\}$$

1. LU Decomposition – factor [A] into [L] & [U]

$$[L] = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \qquad [U] = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

$$[A] = [L][U] \qquad [U]\{x\} = \{d\}$$

2. Substitution –

   a. $[L]\{d\} = \{b\} \Rightarrow$ Solve for {d} by forward subs.

   b. $[U]\{x\} = \{d\} \Rightarrow$ Solve for {x} by backward subs.

Note: I have posted a fully worked out example online

CH. 11 Gauss – Seidel: Iterative Methods

Relaxation – Acceleration of the solution assuming we know the direction of the solution.

Relaxation coeff

$$x^{k+1} = (1-\lambda)x^{k} + \lambda x^{*}$$

weighted average solution

old value

new value

Typical Range of λ: 0< λ <2

λ = 1 → No Relaxation

0< λ <1 → Under Relaxation

1< λ <2 → Over Relaxation

- The optimum value of λ is problem specific and usually determined empirically
- For Large numbers of equations that are diagonally dominant GS has less Round-Off error and reduces unnecessary storage of 0's

CH. 11 Gauss – Seidel: Iterative Methods

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \quad \begin{matrix} (1) \\ (2) \\ (3) \end{matrix}$$

1. Solve Equation (1) for x_1, Eq (2) for x_2, Eq (3) for x_3
2. Start iterative procedure by guessing: x^o_1, x^o_2, x^o_3
3. Calculate x^1_1 from x^o_2, x^o_3
4. Calculate x^1_2 from x^1_1, x^o_3
5. Calculate x^1_3 from x^1_1, x^1_2
6. Repeat for new x's

Convergence Check:

$$\left|\varepsilon_{a,i}\right| = \left|\frac{x_i^k - x_i^{k-1}}{x_i^k}\right| \bullet 100\% < \varepsilon_s$$

GS Convergence Criteria:

$$\left|a_{ii}\right| > \sum_{\substack{j=1 \\ j \neq i}}^{n} \left|a_{ij}\right|$$

Sufficient but not necessary

Diagonal Dominance!

CH. 17 Least Squares Regression

Derive expressions (approximating function) that fits the shape of the data (or general trend of the data)

(A) Straight Line Least-Squares fit

$$y = a_0 + a_1 x + e$$

Error or Residual

- Find a fit that minimizes the error

Define: "Sum of the Squares" of the Residual

$$S_r = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} \left(y_i - a_o + a_1 x_i\right)^2 = \sum_{i=1}^{N} \left(y_{i,meas} - y_{i,\mathrm{mod}}\right)^2$$

Minimize S_r and solve for *a's* → *How?*

The "Linear Regression" Method produces the best fit to the data with:

$$a_o = \bar{y} - a_1 \bar{x}$$

$$a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - \left(\sum x_i\right)^2}$$

CH. 17 Least Squares Regression

Goodness of fit Statistics for linear regression

1. Standard Deviation: What does it measure?

$$S_y = \left(\frac{\sum \left(y_i - \bar{y} \right)^2}{n-1} \right)$$

2. Standard Error Estimate: What does it measure?

$$S_{y/x} = \left(\frac{\sum \left(y_i - a_0 - a_1 x_i \right)^2}{n-2} \right)$$

3. Coefficient of determination: represents error reduction due to using straight line regression rather than the average

$$S_t = \sum \left(y_i - \bar{y} \right)^2$$

$$S_r = \sum \left(y_i - a_0 + a_1 x_i \right)^2$$

$$r^2 = \frac{S_t - S_r}{S_t}$$

$$r = \sqrt{\frac{S_t - S_r}{S_t}} \longrightarrow$$ Correlation coefficient

CH. 17 Least Squares Regression

(B) Non-Linear Relationships: convert to linear

1. Exponential $y = a_1 e^{b_1 x}$

2. Power Model $y = a_2 x^{b_2}$

3. Saturation Growth Rate $y = a_3 \dfrac{x}{b_2 + x}$

(C) Polynomial Regression

$$y = a_0 + a_1 x + a_1 x^2 + \ldots + a_m x^m + e$$

- Follow minimization procedure from linear regression

- Solve a system of m+1 equations with standard error:

$$S_{y/x} = \left(\frac{S_r}{n-(m+1)} \right)$$

(D) Multiple Linear Regression: y is a function of 2 or more independent variables

$$y = a_0 + a_1 x + a_2 x_2 + \ldots + a_m x_m + e$$

- Follow minimization procedure from linear regression

- Solve a system of m dimension with standard error:

$$S_{y/x} = \left(\frac{S_r}{n-(m+1)} \right)$$

CH. 21 Numerical Integration

Integrate data & functions

(A) Newton-Cotes Integration Formula:

$$I = \int_a^b f(x)dx \approx \int_a^b f_n(x)dx$$

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_{n-1}x^{n-1} + a_n x^n$$

Open & Closed Form Methods:

1. Trapazoidal Rule & Error → Multiple Application
2. Simpson's Rule & Error
    1. 1/3 Rule for even number of segments
    2. 3/8 rule for odd number of segments

CH. 22 Numerical Integration

(B) Gauss Quadrature → Wise positioning of points for integration to reduce error

Two Point Guass Legendre formulation

$$I = \int_{-1}^{1} f(x_d)dx_d \approx c_0 f(x_0) + c_1 f(x_1)$$

c_o, c_1 are constants (and unknown)
x_o, x_1 are unknown Gauss points

We need 4 Eqns. For our 4 unknowns, we choose the following polynomials: $y=1$, $y=x$, $y=x^2$, $y=x^3$

$$\int_{-1}^{1} f(x_d)dx_d = c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} 1 dx_d = 1$$

$$\int_{-1}^{1} f(x_d)dx_d = c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x_d dx_d = 0$$

$$\int_{-1}^{1} f(x_d)dx_d = c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x_d^2 dx_d = 2/3$$

$$\int_{-1}^{1} f(x_d)dx_d = c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x_d^3 dx_d = 0$$

Solving we obtain:

$$\left.\begin{aligned} c_o &= c_1 = 1 \\ x_o &= -x_1 \\ x_o &= \frac{-1}{\sqrt{3}} \end{aligned}\right\} \quad \boxed{I \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

2pt Gauss-Legendre Forumula

CH. 22 Numerical Integration

(B) Gauss Quadrature → Apply 2pt formula to an integral of the form:

$$I = \int_a^b f(x)dx \approx \frac{b-a}{2}\left[c_0 f(x_o^{trans}) + c_1 f(x_1^{trans})\right]$$

To transform the x-locations we use:

$$x = \frac{b+a}{2} + \frac{b-a}{2} x_d$$

$$dx = \frac{b-a}{2} dx_d$$

Substituting the Gauss points for the 2pt formula we obtain:

$$x_o^{trans} = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{-1}{\sqrt{3}}\right)$$

$$x_1^{trans} = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right)$$

CH. 25 Runge-Kutta Methods

- Classification of Differential Equations
- Solution of ODE's
- Initial Value Problems
- Boundary Value Problems

Note: I have posted handout online for classification

Solve ODE's of the form:

$$\frac{dy}{dx} = f(x, y)$$

Numerical Solution form:

$$y_{i+1} = y_i + \phi h$$

Step size

New estimate

Current value

slope

1. Euler's Method

$$y_{i+1} = y_i + f(x_i, y_i)h$$

- Local truncation error – $O(h^2)$
- Global truncation error – $O(h)$

CH. 25 Runge-Kutta Methods

2. Huen's Method – Predictor/Corrector
   - Predictor Equation

$$y_{i+1}^{0} = y_i + f(x_i, y_i)h$$

   - Corrector Equation

$$y_{i+1} = y_i + \underbrace{\frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^{0})}{2}}_{\text{Average slope}} h$$

- Can be solved iteratively
- Local truncation error – $O(h^3)$
- Global truncation error – $O(h^2)$
- 2^{nd} order accurate

CH. 25 Runge-Kutta Methods

3. 4th order Runge-Kutta
   - Can achieve Taylor Series accuracy without evaluating higher order derivatives.

$$y_{i+1} = y_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

$$y_{i+1} = y_i + \phi h$$

Slope Estimates:

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + 0.5h, y_i + .5k_1 h)$$

$$k_3 = f(x_i + 0.5h, y_i + .5k_2 h)$$

$$k_4 = f(x_i + h, y_i + k_3 h)$$

- Note the recursive nature of the k's
- Recall where coefficients come from
- Global truncation error – $O(h^4)$
- 4th order accurate

CH. 25 Runge-Kutta Methods

4. Systems of ODEs
   - Higher order ODEs can be broken down into a system of first order ODEs that can be solved using Runge-Kutta Methods
   - Example:

$$y'' + ay' + c\sin y = 0$$

$$y(0) = 1$$
$$y'(0) = -1$$

$$\downarrow$$

$$\frac{dy}{dx} = z$$
$$\frac{dz}{dx} = -az - c\sin y$$

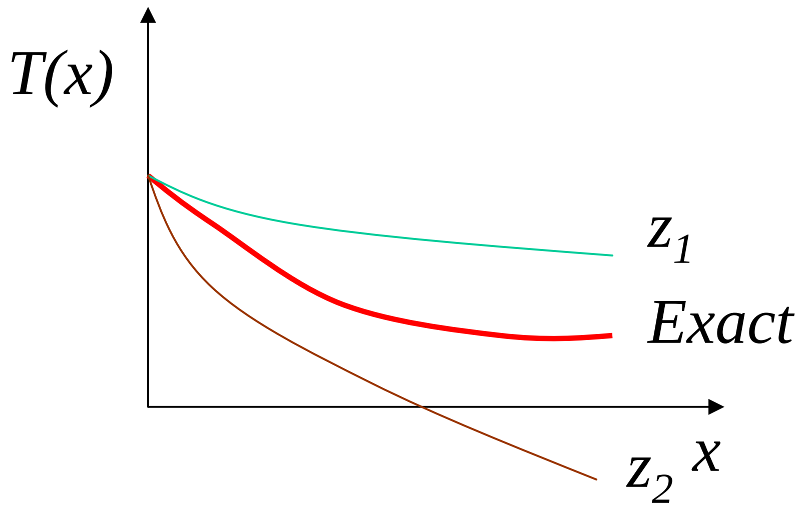
$$\longrightarrow$$

$$y_{i+1} = y_i + \varphi_1 h$$
$$z_{i+1} = z_i + \varphi_2 h$$

$$y(0) = 1$$
$$z(0) = -1$$

CH. 27 Boundary Value Problems

1. Shooting Method
   - Convert a boundary value problem into an initial value problem.
   - Solve the problem iteratively



   - Linear ODE Approach
   - Non-Linear ODE Approach

CH. 27 Boundary Value Problems

2. Finite Difference Equations

- Alternative to the shooting method
- Substitute finite difference equations for derivatives in the original ODE.
- This will give us a set of simultaneous algebraic equations that are solved a *nodes* using techniques like Gauss-Seidel, LU Decomposition, etc.

- Advantage over shooting method:
    - Shooting method can become difficult for higher order equations where we have to assume two or more conditions

CH. 29 Partial Differential Equations: Finite Difference: Elliptical Equations

Poisson's equation:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = R(x, y)$$

Can be written using central differencing as:

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} - 2T_{j} + T_{j-1}}{\Delta y^2} = R_{i,j}$$

The resulting system of algebraic equations can be solved using standard techniques developed in Chapters 9-11