

1. **Nonlinear Equations** Given scalar equation, $f(x) = 0$,

- (a) Describe I) Newton's Method, II) Secant Method for approximating the solution.
- (b) State sufficient conditions for Newton and Secant to converge. If satisfied, at what rate will each converge?
- (c) Sketch the proof of convergence for Newton's Method.
- (d) Write Newton's Method as a fixed point iteration. State sufficient conditions for a general fixed point iteration to converge.
- (e) Apply the criterion for fixed point iteration to Newton's Method and develop an alternate proof for Newton's Method.

Solution

(a) Newton's method: Given x_0 , let

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \quad n \geq 0.$$

Secant Method: Given x_0, x_1 , let

$$x_{n+1} = x_n - f(x_n) \frac{(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})} \quad n \geq 1.$$

(b) Newton's Method: Let $f(x) = 0$. Assume that there exists an interval $E = [a, b]$ such that $f(x)$, $f'(x)$ and $f''(x)$ are continuous on E , and

$$\frac{\max_{x \in E} |f''(x)|}{2 \min_{x \in E} |f'(x)|} = M,$$

and $M < 1.0$. Then, for any $x_0 \in E$, Newton's method will converge with rate 2.0.

Secant Method: Under the same assumptions, if x_0 and x_1 are in E , the the Secant Method will converge with rate $\frac{1+\sqrt{5}}{2} \approx 1.62$.

(c) See Atkinson, pages 59-60.

(d) Define

$$g(x) = x - \frac{f(x)}{f'(x)}.$$

Newton's method can be cast as: Given x

Numerical quadrature:

2. Assume that a quadrature rule, when discretizing with n nodes, possesses an error expansion of the form

$$I - I_n = \frac{c_1}{n} + \frac{c_2}{n^2} + \frac{c_3}{n^3} + \dots$$

Assume also that we, for a certain value of n , have numerically evaluated I_n , I_{2n} and I_{3n} .

- Derive the best approximation that you can for the true value I of the integral.
- The error in this approximation will be of the form $O(n^{-p})$ for a certain value of p . What is this value for p ?

Solution:

- With three numerically evaluated values, we can solve for three variables. For these we want to choose I , c_1 and c_2 , at which point we only care about the obtained value for I . Abbreviating $\frac{c_1}{n} = d_1$ and $\frac{c_2}{n^2} = d_2$, we thus obtain the relations

$$\begin{aligned} I - I_n &= d_1 + d_2 \\ I - I_{2n} &= \frac{1}{2}d_1 + \frac{1}{4}d_2 \\ I - I_{3n} &= \frac{1}{3}d_1 + \frac{1}{9}d_2 \end{aligned} ,$$

or, written in the usual linear system form (separating 'knowns' from 'unknowns')

$$\begin{bmatrix} 1 & -1 & -1 \\ 1 & -\frac{1}{2} & -\frac{1}{4} \\ 1 & -\frac{1}{3} & -\frac{1}{9} \end{bmatrix} \begin{bmatrix} I \\ d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} I_n \\ I_{2n} \\ I_{3n} \end{bmatrix}$$

from which follows

$$I = \frac{1}{2}(I_n - 8I_{2n} + 9I_{3n}).$$

- With the first two terms in the error expansion eliminated, it will continue from the third term and onwards (with modified coefficients), i.e. the error in the approximation above will be of the form $O(n^{-3})$.

Interpolation / Approximation:

3. The *General Hermite interpolation problem* amounts to finding a polynomial $p(x)$ of degree $n_1 + n_2 + \dots + n_n - 1$ that satisfies

$$\begin{aligned} p^{(i)}(x_1) &= y_1^{(i)}, & i &= 0, 1, \dots, n_1 - 1 \\ &\vdots & & \vdots \\ p^{(i)}(x_n) &= y_n^{(i)}, & i &= 0, 1, \dots, n_n - 1, \end{aligned}$$

where the superscripts denotes derivatives, that is, we specify the first $n_j - 1$ derivatives at the point x_j , for $j = 1, 2, \dots, n$. Show that this problem has a unique solution whenever the x_i are distinct.

Hint: Set up the linear system for a small problem, recognize the pattern, and prove the general result.

Solution:

In all, there are $n_1 + n_2 + \dots + n_n = N$ conditions. Let the interpolation polynomial of degree $N - 1$ be $p(x) = a_0 + a_1x + \dots + a_{N-1}x^{N-1}$. Each of the given conditions form one line in a linear system for the coefficients:

$$\begin{bmatrix} 1 & x_1 & \text{\textcircled{£}} & \text{\textcircled{£}} & \dots & x_1^{N-1} \\ 0 & 1 & \text{\textcircled{£}} & \text{\textcircled{£}} & \dots & (N-1)x_1^{N-2} \\ & & \bullet & \text{\textcircled{£}} & \dots & \text{\textcircled{£}} \\ 1 & x_2 & \text{\textcircled{£}} & \text{\textcircled{£}} & \dots & x_2^{N-1} \\ \text{\textcircled{£}} & \text{\textcircled{£}} & \text{\textcircled{£}} & \text{\textcircled{£}} & \dots & \text{\textcircled{£}} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ \text{\textcircled{£}} \\ \text{\textcircled{£}} \\ \dots \\ \text{\textcircled{£}} \end{bmatrix} = \begin{bmatrix} y_1^{(0)} \\ y_1^{(1)} \\ \text{\textcircled{£}} \\ \text{\textcircled{£}} \\ \dots \\ \text{\textcircled{£}} \end{bmatrix}$$

The task is to show that this $N \times N$ coefficient matrix is nonsingular, as this will imply both existence and uniqueness. One way to do this is to let the right hand side (RHS) be zero, and show that the problem then has only the zero solution.

With the RHS zero, the conditions that are imposed require $p(x)$ to have a zero of degree n_1 at x_1 , i.e. a factor $(x - x_1)^{n_1}$; then likewise a factor of $(x - x_2)^{n_2}$, etc. These required factors will imply that the polynomial $p(x)$ will have a total of N zeros (counting multiplicities). This is one above the actual degree of $p(x)$, implying that all the coefficients of $p(x)$ must be zero.

4. Linear Algebra

Consider the $n \times n$, nonsingular matrix, A . The Frobenius norm of A is given by

$$\|A\|_F = \left(\sum_{i,j} a_{ij}^2 \right)^{1/2}$$

- (a) Construct the perturbation, δA , with smallest Frobenius norm such that $A + \delta A$ is singular. (Hint: use one of the primary decompositions of A .)

Clearly,

$$A - A = U(\quad)V$$

is singular.

- (b) Denote the columns of $U = [\underline{u}_1, \underline{u}_2, \dots, \underline{u}_n]$ and $V = [\underline{v}_1, \underline{v}_2, \dots, \underline{v}_n]$. The fact that U and V are unitary implies that $\underline{u}_j^T \underline{u}_j = \underline{v}_j^T \underline{v}_j = 1$, for $j = 1, \dots, n$. We can write

$$A = \sum_{j=1}^n \underline{u}_j \underline{v}_j^T$$

and the Frobenius norm is

$$\|A\|_F^2 = \sum_{j=1}^n \sum_{k=1}^n (\underline{u}_j^T \underline{u}_k)^2 (\underline{v}_j^T \underline{v}_k)^2 = \sum_{j=1}^n 1 = n,$$

or

$$\|A\|_F = \sqrt{n}.$$

- (c) Suppose A is any perturbation such that $A - A$ is singular. Then, there exists a vector of unit length, denoted by \underline{w} , such that

$$A\underline{w} = A\underline{w}.$$

Now,

$$\min_{\|\underline{z}\|=1} \frac{A\underline{z}}{\|\underline{z}\|} = \min_{\|\underline{w}\|=1} A\underline{w} = \sqrt{n}.$$

Thus, the largest singular value of A must be greater than or equal to \sqrt{n} . Since multiplication by a unitary matrix does not change the Frobenius norm, the Frobenius norm of a general matrix is

$$\|A\|_F = \left(\sum_{i=1}^n \sigma_i^2 \right)^{1/2}.$$

Thus,

$$\|A\|_F \geq \sqrt{n}.$$

- (d) The answer depends on A . If the smallest singular value of A is unique, then the smallest perturbation is unique. Any other perturbation, \hat{A} for which $A - \hat{A}$ is singular will, itself, have a second nonzero singular value, and thus, a larger Frobenius norm. If there are multiples of the smallest singular values of A , then there are multiple choices of A with Frobenius norm equal to \sqrt{n} .

Numerical ODE:

5. Consider using forward Euler (same as AB1; Adams-Bashforth of first order) as a predictor, and the trapezoidal rule (same as AM2; Adams Moulton of second order) as a corrector for solving the ODE $y' = f(t, y)$.
 - a. Write down the explicit steps that need to be taken in order to advance the numerical solution from time t_n to time $t_{n+1} = t_n + k$.
 - b. Determine the order of the combined scheme. In case you know a theorem that gives the order directly, you may quote this *in its general form*, i.e. do not just state the answer in the present special case.
 - c. The figure to the right illustrates the stability domain of the scheme. Prove that $(-2, 0)$ is the leftmost point

6. Partial Differential Equations

Consider the steady-state, advection-diffusion equation in one space dimension:

$$-\frac{d}{dx}(a(x)\frac{du}{dx}) + b(x)u = f, \quad x \in [0, 1]$$

with boundary conditions $u(0) = u(1) = 0$ and the assumption that $a(x)$ is continuous and $a(x) > 0$ for $x \in [0, 1]$

- Describe the finite difference (FD) method for approximating the solution using I) Centered Differences, II) Upwind Differences on the advection term. Let h represent the mesh spacing and assume a uniform mesh. In each case above, describe the linear systems, A and \tilde{A} , that the FD method yields.
- Assume $a > 0$ and $b > 0$ are constant. State a relationship between a , b , and h that assures the eigenvalues of the linear system are real for I) Centered Differences, A , and II) Upwind Differences, \tilde{A} .
- For constant $a > 0$, $b > 0$, use Gershgorin bounds to establish bounds on the eigenvalues of A , the **upwind** difference matrix.

Now consider the parabolic equation (assume $a > 0$ and $b > 0$ are constant)

$$u_t = a \frac{\partial^2 u}{\partial x^2} - b \frac{\partial u}{\partial x}, \quad x \in [0, 1]$$

- Write the **Forward** Euler scheme for this equation using I) Centered Differences II) Upwind Differences for the advection term.
- Write a simple centered difference scheme for the diffusion term.

where $\xi \in [x_{-1}, x_{+1}]$.

The Centered Difference stencil for the second term is

$$b(x) \frac{-u(x_{-1}) + u(x_{+1})}{2h} = b(x)u'(x) + \frac{h^2}{12}b(x)u^{(3)}(\xi),$$

where $\xi \in [x_{-1}, x_{+1}]$.

The Upwind Difference stencil for the second term is, for $b(x) > 0$,

$$b(x) \frac{-u(x_{-1}) + u(x)}{h} = b(x)u'(x) - \frac{h}{2}b(x)u''(\xi),$$

where $\xi \in [x_{-1}, x]$ and, for $b(x) < 0$,

$$b(x) \frac{-u(x) + u(x_{+1})}{h} = b(x)u'(x) + \frac{h}{2}b(x)u''(\xi),$$

where $\xi \in [x, x_{+1}]$.

With centered differences, the linear system is tridiagonal, denoted by

$$A = \frac{1}{h^2} \text{tri} \left[-\left(a(x-h/2) + \frac{1}{2}b(x)\right); \left(a(x-h/2) + a(x+h/2)\right); -\left(a(x+h/2) - \frac{1}{2}b(x)\right) \right]$$

(c) For upwind differences and constant coefficients, $a >$