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

   (a) Describe I) Newtons 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

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

Secant Method: Given x_0, x_1, let

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

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

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

and $\eta M < 1.0$. 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 $\frac{1+\sqrt{5}}{2} \simeq 1.62$.

(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_0, let

$$x_{n+1} = g(x_n), \qquad n \geq 1.$$

Fixed point convergence: Let $D \subset \Re$ be a closed, bounded interval such that, for $x \in D$,

(I) $g(D) \subset D$.

(II) $\lambda = \max_{x \in D} |g'(x)| < 1.0$.

(e) We want to find an interval, $D = [\alpha - \eta, \alpha + \eta]$ for which

(I) $g(D) \subset D$.

(II) $g'(x) = 1 - \frac{f'(x)^2 - f(x)f''(x)}{f'(x)^2} = \frac{f(x)f''(x)}{f'(x)^2} \in (-1, 1)$.

Toward that end, assume $f(x)$, $f'(x)$ and $f''(x)$ are continuous in a neighborhood of α and $f'(\alpha) \neq 0$. Then, there exists an interval, E, containing α in which

$$\frac{\max_{x \in E} |f(x)f''(x)|}{\min_{x \in E} |f'(x)^2|} \leq \lambda < 1.0,$$

Chose $D \subseteq E$. Then, for some $\xi \in [\alpha, x]$,

$$|g(x) - \alpha| = |g(\alpha) - \alpha + g'(\xi)(x - \alpha)| \leq \lambda |x - \alpha|,$$

which establishes $g(D) \subset D$.

Numerical quadrature:

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

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

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

a. Derive the best approximation that you can for the true value I of the integral.

b. 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:

a. 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

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

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

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

b. 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 $a_1 + a_2 + \ldots + a_n - 1$ that satisfies

$$
\begin{aligned}
p^{(i)}(x_1) &= y_1^{(i)}\,, \quad i = 0, 1, \ldots, a_1 - 1 \\
&\;\vdots \qquad\qquad\qquad\quad \vdots \\
p^{(i)}(x_n) &= y_n^{(i)}\,, \quad i = 0, 1, \ldots, a_n - 1\,,
\end{aligned}
$$

where the superscripts denotes derivatives, that is, we specify the first $a_j - 1$ derivatives at the point x_j, for $j = 1, 2, \ldots, n$. 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 $a_1 + a_2 + \ldots + a_n = N$ conditions. Let the interpolation polynomial of degree $N-1$ be $p(x) = \beta_0 + \beta_1 x + \ldots + \beta_{N-1}x^{N-1}$. Each of the given conditions form one line in a linear system for the coefficients:

$$
\begin{bmatrix}
1 & x_1 & \cdots & \cdots & x_1^{N-1} \\
0 & 1 & \cdots & \cdots & (N-1)x_1^{N-2} \\
 & & \ddots & \cdots & \cdots \\
1 & x_2 & \cdots & \cdots & x_2^{N-1} \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{bmatrix}
\begin{bmatrix}
\beta_0 \\ \beta_1 \\ \vdots \\ \vdots \\ \beta_{N-1}
\end{bmatrix}
=
\begin{bmatrix}
y_1^{(0)} \\ y_1^{(1)} \\ \vdots \\ \vdots \\ \vdots
\end{bmatrix}
$$

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 a_1 at x_1, i.e. a factor $(x - x_1)^{a_1}$; then likewise a factor of $(x - x_2)^{a_2}$, 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

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

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

(b) What is the Frobenius norm of this special ∂A?

(c) Prove that it is the smallest such perturbation.

(d) Extra Credit: Is it unique?

Solution

(a) Start with the singular value decomposition of A,

$$A = U\Sigma V^*,$$

where U and V are unitary, and

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix},$$

where $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_n > 0$. The last inequality stems from that assumption that A is nonsingular.

Consider the perturbation

$$\partial A = U\Gamma V^*$$

where

$$\Gamma = \begin{bmatrix} 0 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & \sigma_n \end{bmatrix},$$

Clearly,

$$A - \partial A = U(\Sigma - \Gamma)V^*$$

is singular.

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

$$\partial A = \sigma_n \underline{u}_n \underline{v}_n^*$$

and the Frobenius norm is

$$\|\partial A\|_F^2 = \sigma_n^2 \sum_i \sum_j |(\underline{u}_n)_i|^2 |(\underline{v}_n)_j|^2 = \sigma_n^2,$$

or

$$\|\partial A\|_F = \sigma_n$$

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

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

Now,

$$\min_{\underline{z} \neq 0} \frac{\|A\underline{z}\|}{\|\underline{z}\|} = \min_{\|\underline{w}\|=1} \|Aw\| = \sigma_n$$

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

$$\|A\|_F = (\sum_i \sigma_i^2)^{1/2}.$$

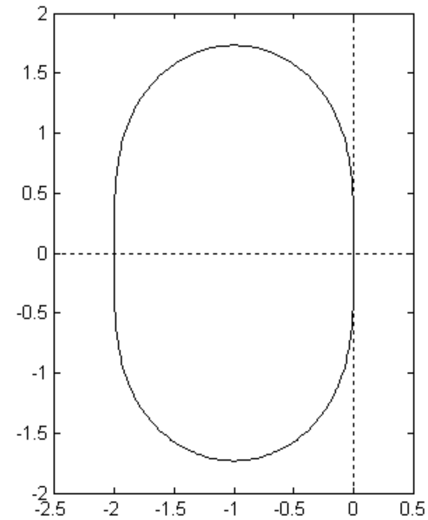
Thus,

$$\|\partial A\| \geq \sigma_n.$$

(d) The answer depends on A. If the smallest singular value of A is unique, then the smallest perturbation is unique. Any other perturbation, $\partial \widehat{A}$ for which $A - \partial \widehat{A}$ is singular will, itself, have a second nonzero singular value, and thus, a larger Frobenius norm. If there are multiplies of the smallest singular values of A, then there are multiple choices of ∂A with Frobenius norm equal to σ_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 in the domain, and that its vertical extremes are taken at $(-1 \pm \sqrt{3}\, i)$.

Note: If your solution utilizes that the stability domain is symmetric around the line $\operatorname{Re} \xi = -1$, that symmetry has also to be proved.

Solution:

a. Let the intermediate value at time t_{n+1} be denoted y^*_{n+1}. The two steps are then

$$\begin{cases} y^*_{n+1} &= y_n + k f(t_n, y_n) \\ y_{n+1} &= y_n + \frac{k}{2}(f(t_{n+1}, y^*_{n+1}) + f(t_n, y_n)) \end{cases}$$

b. There is a general theorem to the effect that, with a predictor of order p and a corrector of order q, the order of the combined predictor-corrector scheme will be $\min(p+1, q)$. In the present case, $p = 1$ and $q = 2$, resulting in second order. One (of many possible) direct verifications will be noted in the solution to part c below.

c. We obtain a scheme's stability domain by applying it to the special ODE $y' = \lambda y$. In the present case, eliminating the intermediate y^*_{n+1}, leads then to

$$y_{n+1} = y_n + \tfrac{k}{2}(\lambda(y_n + k\lambda y_n) + \lambda y_n),$$

which, following the standard variable change $k\lambda = \xi$, simplifies to

$$y_{n+1} = (1 + \xi + \tfrac{1}{2}\xi^2) y_n.$$

At this point, we can find the order of the scheme by inspecting how far the expansion in ξ, here $h(\xi) = 1 + \xi + \frac{1}{2}\xi^2$, agrees with the Taylor expansion for e^{ξ}. Thus, the scheme is of order 2.

The outer edge of the stability domain, displayed in the figure above, is the contour line in the complex ξ-plane for where $|h(\xi)| = 1$. Writing $h(\xi) = \frac{1}{2}(1 + (\xi+1)^2)$, this implies that $(\xi+1)^2$ should fall on the periphery of a circle with radius 2, centered at $\xi = -1$. This circle extends between -3 and +1 along the real axis. After taking the square root and subtracting one, we obtain the stability domain, which thus has as its extreme points $\pm\sqrt{-3} - 1$ and $\pm\sqrt{1} - 1$.

6. **Partial Differential Equations**

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

$$-\partial_x(a(x)\partial_x u(x)) + b(x)\partial_x u = f, \qquad x \in [0,1]$$

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

(a) 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_c^h and A_u^h, that the FD method yields.

(b) 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_c^h, and II) Upwind Differences, A_u^h.

(c) For constant $a > 0$, $b > 0$, use Gershgorin bounds to establish bounds on the eigenvalues of A_u^h, the **upwind** difference matrix.

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

$$\partial_t u = a\partial_{xx}u(x) - b\partial_x u, \qquad x \in [0,1]$$

(d) Write the **Forward** Euler scheme for this equation using I) Centered Differences II) Upwind Differences for the advection term.

(e) Write a simple relationship, in terms of a, b, h and δt that guarantees the stability of **Forward** Euler and **Upwind** Differences.

Solution

(a) Start by defining a mesh of points: Let $h = 1/n$ and define $x_j = jh$ for $j = 0, \ldots, n$. The Centered Difference stencil for the first term is

$$\frac{-a(x_i - h/2)u_{i-1} + (a(x_i - h/2) + a(x_i + h/2))u_i - a(x_i + h/2)u_{i+1}}{h^2}$$
$$= -(a(x_i)u'(x_i))' + \frac{h^2}{24}\left((a(\xi_i)u^{(3)}(\xi_i))' + (a(\eta_i)u'(\eta_i))^{(3)}\right),$$

where $\xi_i, \eta_i \in [x_{i-1}, x_{i+1}]$.
The Centered Difference stencil for the second term is

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

where $\eta_i \in [x_{i-1}, x_{i+1}]$.
The Upwind Difference stencil for the second term is, for $b(x_i) > 0$,

$$b(x_i)\frac{-u(x_{i-1}) + u(x_i)}{h} = b(x_i)u'(x_i) - \frac{h}{2}b(x_i)u''(\eta_i),$$

where $\eta_i \in [x_{i-1}, x_i]$ and, for $b(x_i) < 0$,

$$b(x_i)\frac{-u(x_i) + u(x_{i+1})}{h} = b(x_i)u'(x_i) + \frac{h}{2}b(x_i)u''(\eta_i),$$

where $\eta_i \in [x_i, x_{i+1}]$.

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

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

With upwind differences, the system is, for $b(x_i) > 0$,

$$A^h_c = \frac{1}{h^2}tri\left[-(a(x_i - h/2) + hb(x_i));\quad (a(x_i - h/2) + a(x_i + h/2) + hb(x_i));\quad - a(x_i + h/2)\right]$$

and, for $b(x_i) < 0$,

$$A^h_u = \frac{1}{h^2}tri\left[-a(x_i - h/2);\quad (a(x_i - h/2) + a(x_i + h/2) - hb(x_i));\quad -(a(x_i + h/2) - hb(x_i))\right].$$

(b) Let $a > 0$ and $b > 0$ be constants. If the product of the off diagonal terms is positive, that is, if

$$a^2 - (bh)^2/4 \geq 0, \quad \text{or} \quad \frac{bh}{2a} \leq 1.0,$$

then the centered difference matrix will be an M-matrix with real eigenvalues. The upwind matrix has real eigenvalues for every a, b, and h.

(c) For upwind differences and constant coefficients, $a > 0$, $b > 0$, we have the matrix

$$A_u^h = \frac{1}{h^2} tri\,[-(a+bh);\ (2a+bh);\ \ -a]\,.$$

Gershgorin bounds imply that spectrum of A_u^h is contained in the interval $[0, \frac{4a+2bh}{h^2}]$.

(d) The Forward Euler stencil for Centered Differences is

$$u_i^{\ell+1} = u_i^\ell + \frac{\delta t}{h^2}[(a+bh/2)u_{i-1}^\ell - (2a)u_i^\ell + (a-bh/2)u_{i+1}^\ell]$$

and for Upwind Differences is

$$u_i^{\ell+1} = u_i^\ell + \frac{\delta t}{h^2}[(a+bh)u_{i-1}^\ell - (2a+bh)u_i^\ell + au_{i+1}^\ell].$$

(e) The stability condition is that the eigenvalues of the operator on the right-hand side of the equation above are inside (or on) the unit circle. Using the fact that all eigenvalues A_u^h are real, and the Gershgorin bounds from above, this is guaranteed if

$$1 - \delta t \frac{4a+2bh}{h^2} \geq -1,$$

or

$$\delta t \frac{4a+2bh}{h^2} \leq 2.$$

Notice that for $a = 1$ and $b = 0$ this is the familiar bound $\delta t/h^2 \leq 1/2$.