

**Computational and Applied Mathematics**

*Solve every problem.*

1. Consider the forward and the centered finite difference formulas

$$D_h^+ f(x_0) = \frac{f(x_0 + h) - f(x_0)}{h}, \quad (1)$$

$$D_h^0 f(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h}, \quad (2)$$

to approximate the derivative of  $f$  at a point  $x_0$ . Assume  $f$  is a smooth function in a neighborhood of  $x_0$  containing the points  $x_0 + h$  and  $x_0 - h$ .

- (a) Prove that  $D_h^+ f(x_0)$  and  $D_h^0 f(x_0)$  approximate  $f'(x_0)$  to  $O(h)$  and  $O(h^2)$ , respectively.
  - (b) Derive an  $O(h^2)$  approximation to  $f'(x_0)$  from  $D_h^+ f(x_0)$  by doing Richardson extrapolation.
  - (c) Take  $f(x) = \sin x$  and  $x_0 = 0$ . Prove that both  $D_h^+ f(x_0)$  and  $D_h^0 f(x_0)$  converge quadratically to  $f'(x_0)$  as  $h \rightarrow 0$  and that in fact they produce the same approximation to  $f'(x_0)$  in this particular case.
2. For functions defined on a closed interval  $[0, 1]$ , we want to compute the following definite integral,

$$I[f] = \int_0^1 f(x) \log(1/x) dx.$$

Here we consider the weight function  $\log(1/x)$ , and denote  $P_n(x)$  as the monic orthogonal polynomials for the corresponding weighted inner product.

- (a) Let  $P_0 = 1$ . Find  $P_1(x)$ , and the corresponding node  $x_1^1$  and weight  $\omega_1^1$  for the 1-point Gaussian quadrature rule.
- (b) Derive a recursive formula for  $P_{n+1}(x)$  using  $P_n(x)$  and  $P_{n-1}(x)$ .
- (c) Consider the normalized orthogonal polynomials  $Q_n(x) = P_n(x)/\|P_n\|$ , where

$$\|P_n\| = \sqrt{\int_0^1 P_n(x)^2 \log(1/x) dx}.$$

Derive a recursive formula for  $Q_{n+1}(x)$  using  $Q_n(x)$  and  $Q_{n-1}(x)$ .

- (d) Use the above recursive formula to show that  $x = \lambda$  is a node of the 4-point Gaussian quadrature if and only if it is an eigenvalue of a symmetric, tridiagonal matrix. Write out the form of the symmetric and tridiagonal matrix explicitly.

3. Let  $A$  be a real  $n \times n$  matrix with distinct eigenvalues such that

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n| \geq 0,$$

with corresponding eigenvectors  $\{v_j\}_{j=1}^n$ .

(a) Show that the power iteration

$$z_m = \frac{A^m z_0}{\|A^m z_0\|_\infty} \longrightarrow \pm \frac{v_1}{\|v_1\|_\infty}, \quad \forall z_0 \in \mathbb{R}^n.$$

(b) Consider the following iteration with initial guess  $x_0 = y_0 = 1$ ,

$$x_{n+1} = x_n + y_n, \quad y_{n+1} = x_{n+1} + x_n.$$

Show that  $y_n/x_n \rightarrow \sqrt{2}$  as  $n \rightarrow \infty$ .

4. Consider the initial value problem

$$y' = f(t, y), \quad 0 < t \leq T. \quad (3)$$

$$y(0) = y_0. \quad (4)$$

Assume  $f$  is continuous and Lipschitz in  $y$  in  $[0, T] \times (-\infty, \infty)$ . Denote  $y_n \approx y(t_n)$ ,  $t_n = nh$ , and  $h = T/N$ , with  $N$  a positive integer, and consider the one-step method

$$y_{n+1} = y_n + \alpha h f(t_n, y_n) + \beta h f(t_n + \gamma h, y_n + \gamma h f(t_n, y_n)),$$

where  $\alpha$ ,  $\beta$  and  $\gamma$  are real parameters.

- (a) Prove that the method is consistent if and only if  $\alpha + \beta = 1$ , and the order of the method can not exceed 2.
- (b) Suppose that a second-order method of the above form is applied to  $f(t, y) = -\lambda y$  with  $\lambda > 0$ , and the initial condition  $y_0 = 1$ . Show that the sequence  $(y_n)_{n \geq 0}$  is bounded if and only if  $h \leq \frac{2}{\lambda}$ . Show further that for such  $h$ ,

$$|y(t_n) - y_n| \leq \frac{1}{6} \lambda^3 h^2 t_n, \quad n \geq 0.$$

5. Let  $u(t, x)$  be the solution of the initial-boundary value problem

$$u_t = Du_{xx}, \quad 0 < x < L, \quad 0 < t \leq T, \quad (5)$$

$$u(0, x) = f(x) \quad (6)$$

$$u(t, 0) = u(t, L) = 0, \quad (7)$$

where  $L > 0$  and  $D > 0$ . Consider the finite difference scheme

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}, \quad j = 1, \dots, M-1, \quad n = 0, 1, \dots, N-1 \quad (8)$$

with  $u_0^n = u_M^n = 0$  for all  $n$  and  $u_j^0 = f(j\Delta x)$ ,  $j = 0, \dots, M$ . Here  $\Delta t = T/N$  and  $\Delta x = L/M$  and  $u_j^n \approx u(n\Delta t, j\Delta x)$ .

- (a) Prove that (8) is consistent with (5).
- (b) Prove that if  $\Delta t \leq \frac{1}{2D}(\Delta x)^2$  the finite difference scheme (8) is stable under the  $l^\infty$  norm.
- (c) Prove that if  $\Delta t \leq \frac{1}{2D}(\Delta x)^2$  the finite difference scheme (8) converges in the  $l^\infty$  norm to the exact solution of (5)-(7).

6. Let  $\psi^\varepsilon(t, x)$  be the solution to the following Schrödinger equation:

$$i\varepsilon \frac{\partial \psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2} \nabla_x^2 \psi^\varepsilon + V(x) \psi^\varepsilon, \quad x = (x_1, \dots, x_n)^T \in \mathbb{R}^n,$$

where  $i = \sqrt{-1}$ ,  $\varepsilon \ll 1$  is a small positive real number (rescaled Planck constant),  $\nabla_x^2 = \sum_{j=1}^n \partial_{x_j}^2$ , and  $V(x) \in C^\infty(\mathbb{R}^n)$  is the potential function.

Consider the WKB expansion

$$\psi^\varepsilon(t, x) = A(t, x) e^{i \frac{S(t, x)}{\varepsilon}},$$

- (a) Derive equations for  $A(t, x)$  and  $S(t, x)$  by asymptotic expansion. (Here both  $A(t, x)$  and  $S(t, x)$  are real-valued functions, and do not depend on  $\varepsilon$ .)
- (b) Define  $u(t, x) = \nabla_x S(t, x) \in \mathbb{R}^n$ . Derive an equation for  $u(t, x)$ . Suppose  $u(0, x) \in C^\infty(\mathbb{R}^n)$ , will  $u(t, x)$  always be in  $C^\infty(\mathbb{R}^n)$  for all  $t > 0$ ? Explain why.