Scientific Computing Homework #4

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Problem 1. (a) *What is the degree of Simpson's rule for numerical quadrature?*

(b) *What is the degree of an n-point Gaussian quadrature rule?*

Solution. (a) 3.

(b) $2n - 1$.

□

Problem 2. *What is the degree of each of the following types of numerical quadrature rules?*

(a) *An n-point Newton-Cotes rule, where n is odd*

(b) *An n-point Newton-Cotes rule, where n is even*

(c) *An n-point Gaussian rule*

(d) *What accounts for the difference between the answers to parts a and b?*

(e) *What accounts for the difference between the answers to parts b and c?*

Solution. (a) n.

(b) $n - 1$.

(c) $2n - 1$.

(d) The difference is due to cancellation of positive and negative errors, as illustrated for the midpoint and Simpson's rules in the following figure, which, on the left, shows a linear polynomial and the constant function interpolating it at the midpoint and, on the right, a cubic and the quadratic interpolaing it at the midpoints and endpoints. Integration of the linear polynomial by the midpoint rule yields two congruent triangles of equal area. The inclusion of one of the triangles compensates exactly for the omission of the other. A simiar phenomenon occurs for the cubic polynomial, where the two shaded regions also have equal areas, so that the addition of one compensates for the subtraction of the other. Such cancellation does not occur, however, for an n-point Newton-Cotes rule if n is even.

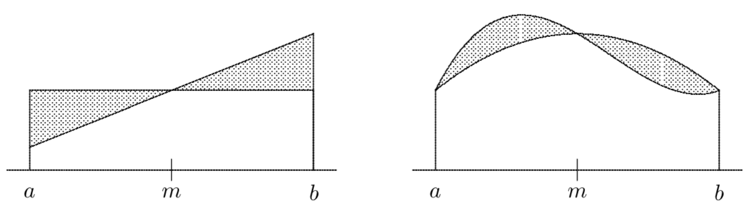

Figure 1: Cancellation of errors in midpoint (left) and Simpson (right) rules.

(e)
- In Newton-Cotes rules, the n nodes are prespecified and the n corresponding weights are then optimally chosen to maximize the degree of the resulting quadrature rules. With only n parameters free to be chosen, the resulting degree is generally $n - 1$.
- In Gaussian rule, the locations of the nodes are also freely chosen, then there are $2n$ free parameters, so that a degree of $2n - 1$ is achievable.

□

Problem 3. *Rank the following types of quadrature rules in order of their degree for the same number of nodes (1 for highest degree, etc.):*

(a) Newton-Cotes

(b) Gaussian

(c) Kronrod

Solution. 1. Gaussian; 2. Kronrod; 3. Newton-Cotes. □

Problem 4. *Why is Monte Carlo* not *a practical method for computing one-dimensional integrals?*

Solution. The error goes to zero as $1/\sqrt{n}$, which means, for example, that to gain an additional decimal digit of accuracy the number of sample points must be increased by a factor of 100. Therefore, for computing one-dimensional integrals, Monte Carlo method is so inefficient, which may require millions of evaluations of the integrand. □

Problem 5. *Explain how a quadrature rule can be used to solve an integral equation numerically. What type of computational problem results?*

Solution. We approximate the integral equation

$$\int_a^b K(s,t)u(t)\,\mathrm{d}t = f(s),$$

by

$$\sum_{j=1}^{n} w_j K(s_i,t_j)u(t_j) = f(s_i), \quad i = 1,\ldots,n,$$

where t_j and w_j $(j = 1,\ldots,n)$ are the nodes and weights of a quadrature rule.
Now we can solve the above *system of linear algebratic equations* $A\mathbf{x} = \mathbf{b}$, where $a_{ij} = w_j K(s_i,t_j), b_i = f(s_i)$, and $x_j = u(t_j)$, which can be solved for $\mathbf{x}$ to obtain a discrete sample of approximate values of the solution function u.
As we have seen, the result is solving a system of linear algebraic equations. □

Problem 6. *With an initial value of $y_0 = 1$ at $t_0 = 0$ and a time step of $h = 1$, compute the approximate solution value y_1 at time t_1 for the ODE $y' = -y$ using each of the following two numerical methods. (Your answers should be numbers, not formulas.)*

(a) Euler's method

(b) Backward Euler method

Solution. (a)

$$y_1 = y_0 + hf(t_0,y_0) = y_0 - hy_0 = 1 - 1 = 0.$$

(b)

$$y_1 = y_0 + hf(t_1,y_1) = y_0 - hy_1 \Rightarrow y_1 = \frac{y_0}{1+h} = \frac{1}{1+1} = 0.5.$$

□

Problem 7. *Consider the IVP*

$$y'' = y$$

for $t \geq 0$, with initial values $y(0) = 1$ and $y'(0) = 2$.

(a) Express this second-order ODE as an equivalent system of two first-order ODEs.

(b) What are the corresponding initial conditions for the system of ODEs in part a?

(c) Are solutions of this system stable?

(d) Perform one step of Euler's method for this ODE system using a step size of $h = 0.5$.

(e) Is Euler's method stable for this problem using this step size?

(f) Is the backward Euler method stable for this problem using this step size?

Solution. (a) Define the new unknowns $u_1(t) = y(t)$ and $u_2(t) = y'(t)$, then we have

$$\begin{bmatrix} u_1' \\ u_2' \end{bmatrix} = \begin{bmatrix} u_2 \\ u_1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}.$$

(b)

$$\begin{bmatrix} u_1(0) \\ u_2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

(c) The eigenvalues of the matrix

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

are $1(> 0)$ and -1, thus solutions of this system are unstable.

(d)

$$\mathbf{u}_1 = \mathbf{u}_0 + hA\mathbf{u}_0 = \begin{bmatrix} 1 & 2 \end{bmatrix}^T + 0.5 \begin{bmatrix} 2 & 1 \end{bmatrix}^T = \begin{bmatrix} 2 & 2.5 \end{bmatrix}^T.$$

(e) The eigenvalues of the matrix $I + hA$ are $1.5(> 1)$ and 0.5, therefore, Euler's method is unstable for this problem using this step size.

(f) The formula for the backward Euler method is

$$\mathbf{u}_{n+1} = \mathbf{u}_n + hA\mathbf{u}_{n+1} \Rightarrow \mathbf{u}_{n+1} = (I - hA)^{-1}\mathbf{u}_n,$$

the eigenvalues of the matrix $(I - hA)^{-1}$ are $2(> 1)$ and $2/3$, therefore, backward Euler's method is unstable for this problem using this step size.

□

Problem 8. *Applying the midpoint quadrature rule on the interval $[t_k, t_{k+1}]$ leads to the implicit* midpoint method

$$y_{k+1} = y_k + h_k f(t_k + h_k/2, (y_k + y_{k+1})/2)$$

for solving the ODE $y' = f(t, y)$. Determine the order of accuracy and the stability region of this method.

Solution. Applying Taylor's theorem yields

$$\begin{aligned} y(t_{k+1}) &= y(t_k) + h_k y'(t_k) + \frac{h_k^2}{2} y''(t_k) + \mathcal{O}(h_k^3); \\ f\left(t_k + \frac{h_k}{2}, \frac{y(t_k) + y(t_{k+1})}{2}\right) &= f(t_k, y(t_k)) + \frac{h_k}{2} f_t(t_k, y(t_k)) + \frac{y(t_{k+1}) - y(t_k)}{2} f_y(t_k, y(t_k)) + \mathcal{O}(h_k^2) \\ &= y'(t_k) + \frac{h_k}{2}\left(f_t(t_k, y(t_k)) + f_y(t_k, y(t_k)) y'(t_k)\right) + \mathcal{O}(h_k^2) \\ &= y'(t_k) + \frac{h_k}{2} y''(t_k) + \mathcal{O}(h_k^2). \end{aligned}$$

Therefore

$$\begin{aligned} y(t_{k+1}) - \left[y(t_k) + h_k f\left(t_k + \frac{h_k}{2}, \frac{y(t_k) + y(t_{k+1})}{2}\right)\right] &= y(t_k) + h_k y'(t_k) + \frac{h_k^2}{2} y''(t_k) + \mathcal{O}(h_k^3) \\ &\quad - \left\{y(t_k) + h_k\left[y'(t_k) + \frac{h_k}{2} y''(t_k) + \mathcal{O}(h_k^2)\right]\right\} \\ &= \mathcal{O}(h_k^3), \end{aligned}$$

which shows that the implicit midpoint method is of order 2.
To determine the stability of the implicit midpoint method, we apply it to the scalar test ODE $y' = \lambda y$, obtaining

$$y_{k+1} = y_k + \frac{\lambda h_k}{2}(y_k + y_{k+1}),$$

which implies that

$$y_k = \left(\frac{1 + h_k\lambda/2}{1 - h_k\lambda/2}\right)^k y_0.$$

Thus, the stability region of the implicit midpoint method is

$$\mathcal{D} = \left\{ z \in \mathbb{C} : \left|\frac{1+z}{1-z}\right| < 1 \right\}.$$

□

Problem 9. *Consider the two-point BVP for the second-order scalar ODE*

$$u'' = u, \quad 0 < t < b,$$

with boundary conditions

$$u(0) = \alpha, \quad u(b) = \beta.$$

(a) *Rewrite the problem as a first-order system of ODEs with separated boundary conditions.*

(b) *Show that the fundamental solution matrix for the resulting linear system of ODEs is given by*

$$Y(t) = \begin{bmatrix} \cosh(t) & \sinh(t) \\ \sinh(t) & \cosh(t) \end{bmatrix}.$$

(c) *Are the solutions to this ODE stable?*

(d) *Determine the matrix $Q \equiv B_0 Y(0) + B_b Y(b)$ for this problem.*

(e) *Determine the rescaled solution matrix $\Phi(t) = Y(t)Q^{-1}$.*

(f) *What can you say about the conditioning of Q, the norm of $\Phi(t)$, and the stability of solutions to this BVP as the right endpoint b grows?*

Solution. (a) Define the new unknowns $y_1(t) = u(t)$ and $y_2(t) = u'(t)$, then we have

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} y_2 \\ y_1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix},$$

with separated linear boundary conditions

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_1(b) \\ y_2(b) \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

(b) Solving $\mathbf{y}' = A\mathbf{y}$ with initial condition $\mathbf{y}(0) = \mathbf{e}_1 = \begin{bmatrix} 1 & 0 \end{bmatrix}^T$, we obtain $\mathbf{y}(t) = \begin{bmatrix} \cosh(t) & \sinh(t) \end{bmatrix}^T$, with $\mathbf{y}(0) = \mathbf{e}_2 = \begin{bmatrix} 0 & 1 \end{bmatrix}^T$, $\mathbf{y}(t) = \begin{bmatrix} \sinh(t) & \cosh(t) \end{bmatrix}^T$. Therefore the fundamental solution matrix is

$$Y(t) = \begin{bmatrix} \cosh(t) & \sinh(t) \\ \sinh(t) & \cosh(t) \end{bmatrix}.$$

(c) The solutions to this ODE are stable, since growth in the solution is limited by the boundary conditions.

(d)

$$Q = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cosh(b) & \sinh(b) \\ -\sinh(b) & \cosh(b) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \cosh(b) & \sinh(b) \end{bmatrix}.$$

(e)

$$\begin{aligned} \Phi(t) = Y(t)Q^{-1} &= \begin{bmatrix} \cosh(t) & \sinh(t) \\ \sinh(t) & \cosh(t) \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -\frac{\cosh(b)}{\sinh(b)} & \frac{1}{\sinh(b)} \end{bmatrix} \\ &= \frac{1}{\sinh(b)} \begin{bmatrix} \sinh(b-t) & \sinh(t) \\ -\cosh(b-t) & \cosh(t) \end{bmatrix} \end{aligned}$$

(f) As b grows, the condition number of Q and the norm of $\Phi(t)$ grow as well, and the stability of solutions to this BVP decreases.

□

Problem 10. *Consider the two-point BVP*

$$u'' = u^3 + t, \quad a < t < b,$$

with boundary conditions

$$u(a) = \alpha, \quad u(b) = \beta.$$

To use the shooting method to solve this problem, one needs a starting guess for the initial slope $u'(a)$. One way to obtain such a starting guess for the initial slope is, in effect, to do a "preliminary shooting" in which we take a single step of Euler's method with $h = b - a$.

(a) Using this approach, write out the resulting algebraic equation for the initial slope.

(b) What starting value for the inital slope results from this approach?

Solution. (a)

$$u(b) = u(a) + hu'(a) \Rightarrow hu'(a) = u(b) - u(a).$$

(b)

$$u'(a) = \frac{u(b) - u(a)}{h} = \frac{\beta - \alpha}{b - a}.$$

□