Numerical Analysis Problem for Assignment

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1. Take the following steps to determine the rate of convergence of the secant method, given by

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

   (a) Let $e_n = r - x_n$, and subtract both sides of the secant method from r to obtain

$$e_{n+1} = e_n + \frac{(e_{n-1} - e_n)f(r - e_n)}{f(r - e_n) - f(r - e_{n-1})}. \tag{2}$$

   (b) Taylor series expand $f(r - e_n)$ and $f(r - e_{n-1})$ for small e using $f(r) = 0$. Obtain

$$e_{n+1} = e_n + \frac{-e_n f'(r) + \frac{1}{2}e_n^2 f''(r) + \dots}{f'(r) - \frac{1}{2}(e_{n-1} + e_n)f''(r) + \dots}. \tag{3}$$

   (c) For small e, use the Taylor series expansion

$$\frac{1}{1-e} = 1 + e + e^2 + \dots \tag{4}$$

   to obtain

$$|e_{n+1}| = \frac{1}{2}\left|\frac{f''(r)}{f'(r)}\right| |e_n||e_{n-1}|. \tag{5}$$

   (d) Try $|e_{n+1}| = k|e_n|^p$ and $|e_n| = k|e_{n-1}|^p$ to obtain the equation $p^2 = p + 1$. Determine p.

2. Determine the value of m_1 as follows:

   (a) Show that the period-two fixed-point equations, given by

$$x_1 = \mu x_0(1 - x_0), \quad x_0 = \mu x_1(1 - x_1), \tag{6}$$

   with $x_0 = 1/2$ reduces to

$$\mu^3 - 4\mu^2 + 8 = 0. \tag{7}$$

   (b) Using long division, determine the quadratic polynomial obtained from

$$\frac{\mu^3 - 4\mu^2 + 8}{\mu - 2}. \tag{8}$$

   Show that the positive root of this quadratic is $m_1 = 1 + \sqrt{5}$.

3. The area of a rectangle with base h and height $f(h/2)$ is given by $hf(h/2)$. Draw a graph illustrating the midpoint rule. Let $f(x) = a + bx + cx^2$, where a, b, and c are constants. Prove by explicit calculation that

$$\int_0^h f(x)\, dx = hf(h/2) + \frac{h^3}{24} f''(h/2). \tag{9}$$

4. Derive the trapezoidal rule by approximating $f(x)$ by the straight line connecting the points $(0, f(0))$ and $(h, f(h))$:

$$f(x) \approx f(0) + \frac{f(h) - f(0)}{h} x. \tag{10}$$

5. Derive Simpson's rule by approximating $f(x)$ by a quadratic polynomial connecting the points $(0, f(0))$, $(h, f(h))$ and $(2h, f(2h))$.

   (a) Let $g(x) = a + bx + cx^2$. Determine the values of a, b and c such that $g(x)$ passes through the points $(0, f(0))$, $(h, f(h))$ and $(2h, f(2h))$.

   (b) Use $f(x) \approx g(x)$ to derive Simpson's rule.

6. Simpson's 3/8 rule has the elementary formula given by

$$\int_0^{3h} f(x)\, dx = \frac{3h}{8} \left(f(0) + 3f(h) + 3f(2h) + f(3h)\right). \tag{11}$$

   Suppose that $f(x)$ is known at the equally spaced points $a = x_0, x_1, \ldots, x_n = b$, and n is a multiple of three. Let $f_i = f(x_i)$ and $h = x_{i+1} - x_i$. Find the formula for the composite Simpson's 3/8 rule.

7. Determine the weights and nodes of the three-point Legendre-Gauss quadrature rule. You may assume from symmetry that $x_1 = -x_3$, $w_1 = w_3$, and $x_2 = 0$.

8. Consider $I = \displaystyle\int_0^h f(x)\, dx$ with $f(x) = x^3$. Using the trapezoidal rule, compute S_1, S_2, E_1 and E_2, and show that $E_1 = 4E_2$.

9. Consider the Fresnel integrals, defined by

$$C(t) = \int_0^t \cos\left(\frac{1}{2}\pi x^2\right) dx, \quad S(t) = \int_0^t \sin\left(\frac{1}{2}\pi x^2\right) dx. \tag{12}$$

   Write a script using python to plot a Cornu spiral, which is a smooth curve of $C(t)$ versus $S(t)$. Plot your solution over the range $-8 \leq t \leq 8$.

10. Consider the points $(0, 0)$, $(1, 1)$ and $(2, 1)$.

    (a) Find the quadratic polynomial that interpolates these points. What are the interpolated y-values at $x = 1/2$ and $x = 3/2$?

(b) Find the two piecewise linear polynomials that interpolate these points. What are the interpolated y-values at $x = 1/2$ and $x = 3/2$?

(c) Use Python to plot the three points and the two interpolating functions.

11. Let $y = f(x)$ have known values (x_0, y_0), (x_1, y_1), $\ldots$, (x_n, y_n), and define piecewise cubic polynomials by

$$g_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i, \quad \text{for } i = 0 \text{ to } n-1 \text{ and } x_i \le x \le x_{i+1}.$$

Suppose that the endpoint slopes $f'(x_0) = y_0'$ and $f'(x_n) = y_n'$ are known. From these two extra conditions, determine two extra constraints on the a, b and c coefficients.

12. Consider the points $(0, 0)$, $(1, 1)$, $(2, 1)$ and $(3, 2)$. Using the not-a-knot condition, determine the four-by-four matrix equation for the b coefficients. Solve for the b's as well as the a's, c's and d's, and thus find the cubic spline interpolant. Plot your result. You may use Python to assist in your algebra.

13. The Bessel function of order n, for $n = 0, 1, 2, \ldots$, can be defined by the definite integral

$$J_n(x) = \frac{1}{\pi} \int_0^{\pi} \cos(x \sin\theta - n\theta)\, d\theta. \tag{13}$$

Compute the first five positive roots $j_{n,k}$ $(k = 1, 2, \ldots, 5)$, of the first six Bessel functions $J_n(x)$, $(n = 0, 1, \ldots, 5)$.

14. Consider again the system of equations given by

$$\begin{aligned} \epsilon x_1 + 2x_2 &= 4, \\ x_1 - x_2 &= 1. \end{aligned}$$

The solution of these equations using Gaussian elimination without pivoting was found to be

$$\begin{aligned} x_2 &= \frac{-\frac{4}{\epsilon} + 1}{-\frac{2}{\epsilon} - 1}, \\ x_1 &= \frac{4 - 2x_2}{\epsilon}. \end{aligned}$$

Compute the value of x_2 and x_1 using Python as a calculator. Now, repeat this calculation for the system of equations given by

$$\begin{aligned} 2\epsilon x_1 + 2x_2 &= 4, \\ x_1 - x_2 &= 1. \end{aligned}$$

15. Consider again the system of equations given by

$$\begin{aligned} \epsilon x_1 + 2x_2 &= 4, \\ x_1 - x_2 &= 1. \end{aligned}$$

The solution of these equations using Gaussian elimination with partial pivoting is found to be

$$x_2 = \frac{4-\epsilon}{2+\epsilon}, \quad x_1 = 1 + x_2.$$

Compute the value of x_2 and x_1 using Python as a calculator. Now, repeat this calculation for the system of equations given by

$$\begin{aligned} 2\epsilon x_1 + 2x_2 &= 4, \\ x_1 - x_2 &= 1. \end{aligned}$$

16. Let

$$A = \begin{pmatrix} -3 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{pmatrix}.$$

Using Gaussian elimination with partial pivoting, find the (PL)U decomposition of A, where U is an upper triangular matrix and (PL) is a psychologically lower triangular matrix.

17. A genetic model of recombination is solved using a computational algorithm that scales like $O(3^L)$, where L is the number of loci modeled. If it takes 10 sec to compute recombination when $L = 15$, estimate how long it takes to compute recombination when $L = 16$.

18. Solve the following lower triangular system for x_i in terms of $x_j, j < i$:

$$\begin{pmatrix} a_{11} & 0 & \cdots & 0 & 0 \\ a_{21} & a_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{(n-1)1} & a_{(n-1)2} & \cdots & a_{(n-1)(n-1)} & 0 \\ a_{n1} & a_{n2} & \cdots & a_{n(n-1)} & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{n-1} \\ b_n \end{pmatrix}.$$

Count the total number of multiplication-additions required for a complete solution.

19. The two largest (in absolute value) eigenvalues of an n-by-n matrix with real eigenvalues are $\lambda_1 = 1$ and $\lambda_2 = 1/2$. Give a rough estimate of how many iterations of the power method is required for convergence to an error of less than 10^{-8}.

20. Use the power method (without normalizing the vectors after each iteration) to determine the dominant eigenvalue and corresponding eigenvector of the matrix

$$A = \begin{pmatrix} -5 & 6 \\ 5 & -4 \end{pmatrix}.$$

21. Let

$$A = \begin{pmatrix} -3 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{pmatrix}.$$

Use Python to find the LU decomposition of A, where U is an upper triangular matrix and L is a psychologically lower triangular matrix.

22. Use Python to find the eigenvalues and eigenvectors of the matrix

$$A = \begin{pmatrix} -5 & 6 \\ 5 & -4 \end{pmatrix}.$$

Normalize the eigenvectors so that their second component is one.

23. The algorithm for solving the system of two equations and two unknowns,

$$f(x, y) = 0, \quad g(x, y) = 0,$$

is given by the following two-step process.

(a) Solve the linear system for Δx_n and Δy_n given by

$$\begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix} \begin{pmatrix} \Delta x_n \\ \Delta y_n \end{pmatrix} = \begin{pmatrix} -f \\ -g \end{pmatrix}.$$

(b) Advance the iterative solution, using

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

Write down the corresponding algorithm for three equations and three unknowns.

24. The fixed-point solutions of the Lorenz equations satisfy

$$\sigma(y - x) = 0, \quad rx - y - xz = 0, \quad xy - \beta z = 0.$$

Find analytically three fixed-point solutions for (x, y, z) as a function of the parameters σ, β, and r. What are the numerical values for the fixed points when $r = 28$, $\sigma = 10$, and $\beta = 8/3$?

25. Complete a Python code that uses Newton's method to determine the fixed-point solutions of the Lorenz equations. Solve using the parameters $r = 28$, $\sigma = 10$, and $\beta = 8/3$. Use as your three initial guesses $x = y = z = 1$, $x = y = z = 10$, and $x = y = z = -10$.

26. Determine a fractal that arises from using Newton's method to compute the fixed-point solutions of the Lorenz equations. Use the parameter values $r = 28$, $\sigma = 10$, and $\beta = 8/3$. Initial values (x_0, z_0) are taken on a grid in the x-z plane with always $y_0 = 3\sqrt{2}$. For assessment purposes, the computational grid and the graphics code will be given in the Learner Template. To pass the assessment, every pixel in your figure needs to be colored correctly.

(Hint: Some grid points may require as many as 33 Newton iterations to converge while others may require as few as three. Unfortunately, if you uniformly use 33 Newton iterations at every grid point. You can accelerate your code by using a `while` loop instead of a `for` loop.)

27. Let $\dot{x} = b$, with initial condition $x(0) = x_0$ and b a constant. With $t = n\Delta t$, show that the Euler method results in the exact solution

$$x(t) = x_0 + bt. \tag{14}$$

28. Let $\dot{x} = bt$, with initial condition $x(0) = x_0$ and b a constant. With $t = n\Delta t$, show that the Modified Euler method results in the exact solution

$$x(t) = x_0 + \frac{1}{2}bt^2. \tag{15}$$

29. Construct Ralston's method, which is a second-order Runge-Kutta method corresponding to $\alpha = \beta = 3/4$, $a = 1/3$ and $b = 2/3$.

30. Consider the ODE given by

$$\frac{dy}{dx} = f(x), \tag{16}$$

with $y(0)$ as the initial value. Use the second-order Runge-Kutta methods given by the midpoint rule and the modified Euler method to derive two elementary quadrature formulas.

31. Consider the ODE given by

$$\frac{dy}{dx} = f(x), \tag{17}$$

with $y(0)$ as the initial value. Use the standard fourth-order Runge-Kutta method to derive Simpson's rule.

32. Write down the modified Euler method for the system of equations given by

$$\dot{x} = f(t, x, y, z), \quad \dot{y} = g(t, x, y, z), \quad \dot{z} = h(t, x, y, z). \tag{18}$$

33. Using the Dormand-Prince method, suppose that a user requests an error tolerance of $\varepsilon = 10^{-6}$, and suppose the time step attempted was $\Delta t = 0.01$ and that $e = |x_{n+1} - X_{n+1}| = 1.1 \times 10^{-6}$. Is the current time step accepted? What time step will be used next? Assume a safety factor of 0.9.

34. The Lorenz equations are a system of nonlinear ODEs that pioneered the study of chaos. The Lorenz equations are given by

$$\dot{x} = \sigma(y - x), \quad \dot{y} = x(r - z) - y, \quad \dot{z} = xy - \beta z, \tag{19}$$

where σ, β and r are constants. Edward Lorenz studied the solution for $\sigma = 10$, $\beta = 8/3$ and $r = 28$, and the result is now known as the Lorenz attractor, an example of what is now more generally known as a strange attractor. Compute the Lorenz attractor and plot z versus x and y, using the python. Remove the transient before plotting.

35. The dimensionless, unforced pendulum equation is given by

$$\ddot{\theta} + \alpha\dot{\theta} + \sin\theta = 0, \tag{20}$$

where α is the only free parameter.

Consider initial conditions with the mass at the bottom, $\theta(0) = 0$. Using the shooting method, determine the smallest positive value of $\dot{\theta}(0)$ such that the mass becomes exactly balanced at the top ($\theta = \pi$). Plot this value of $\dot{\theta}(0)$ versus α for $0 \le \alpha \le 2$.

36. Consider the two-body problem where the solution for the relative coordinates is a circular orbit of unit radius, that is,

$$\mathbf{r} = \cos(\omega t)\mathbf{i} + \sin(\omega t)\mathbf{j}. \tag{21}$$

Sketch the orbits of m_1 and m_2 for (a) $m_1 = m_2$ and (b) $m_1 = 3m_2$.

37. By solving a system of differential equations, determine the orbit of two masses using Newton's law and the universal law of gravitation. Display an animation of the orbit.

38. Using Taylor series approximations for $y(x+2h)$, $y(x+h)$, $y(x-h)$ and $y(x-2h)$, derive a central difference approximation for the first derivative $y'(x)$ that is accurate to $O(h^4)$.

39. Show that the solution of the discrete Laplace equation at grid point (i, j) on a uniform grid is just the average value of the solution at the neighboring four grid points.

40. What are the k coordinates for the four corners of a rectangular box with n_x and n_y grid points in the x- and y-directions, respectively?

41. Construct the matrix equation for the discrete Laplace equation on a four-by-four grid. When k indexes a boundary point, assume that $\Phi_k = b_k$ is known.

42. On a rectangular grid with n_x and n_y grid points, how many interior points are there and how many boundary points? What percentage of grid points are boundary points when $n_x = n_y = 100$, and what percentage when $n_x = n_y = 1000$?

43. Using the direct method, solve the Laplace equation inside a unit square. Set the boundary conditions to be zero on the left and bottom sides, and to go from zero to one across the top, and from one to zero down the right side. Model these boundary conditions as

$$\Phi = x(2-x) \quad \text{for} \quad y = 1; \quad \Phi = y(2-y) \quad \text{for} \quad x = 1. \tag{22}$$

44. The Jacobi, Gauss-Seidel and SOR methods can also be used to solve a system of linear equations. Consider the system of equations given by

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1, \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= b_2, \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3. \end{aligned}$$

By solving the ith equation for x_i, write down the Jacobi iteration method for this system.

45. Using the Jacobi method, solve the Laplace equation inside a unit square. Set the boundary conditions to be zero on the left and bottom sides, and to go from zero to one across the top, and from one to zero down the right side. Model these boundary conditions as

$$\Phi = x(2-x) \quad \text{for} \quad y = 1; \quad \Phi = y(2-y) \quad \text{for} \quad x = 1. \tag{23}$$

46. Use the second-order Runge-Kutta method known as the modified Euler method to write a two-step process for solving the one-dimensional diffusion equation.

47. Consider the one-dimensional advection equation given by

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}. \tag{24}$$

Using the second-order central difference approximation for the spatial derivative and the first-order Euler method for the time integration, derive the FTCS scheme for the advection equation.

48. Analyze the stability of the FTCS scheme for the advection equation, given by

$$u_j^{l+1} = u_j^l - \frac{c\Delta t}{2\Delta x}\left(u_{j+1}^l - u_{j-1}^l\right). \tag{25}$$

49. Consider the one-dimensional advection equation given by

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}. \tag{26}$$

(a) By computing the spatial derivative at the advanced time step t_{l+1}, derive the implicit discrete advection equation.

(b) Analyze its stability.

50. Consider the one-dimensional advection equation given by

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}. \tag{27}$$

The explicit Lax scheme for the advection equation is given by

$$u_j^{l+1} = \frac{1}{2}\left(u_{j+1}^l + u_{j-1}^l\right) - \frac{c\Delta t}{2\Delta x}\left(u_{j+1}^l - u_{j-1}^l\right). \tag{28}$$

Analyze its stability and derive the Courant-Friedrichs-Lewy (CFL) stability criterion, which is widely used in fluid turbulence simulations.

51. (a) Derive a second-order method for the x-derivative at boundary points. When x is a boundary point on the left, use the Taylor series

$$\begin{aligned} y(x+h) &= y(x) + hy'(x) + \frac{1}{2}h^2y''(x) + O(h^3), \\ y(x+2h) &= y(x) + 2hy'(x) + 2h^2y''(x) + O(h^3). \end{aligned}$$

When x is a boundary point on the right, use the Taylor series

$$\begin{aligned} y(x-h) &= y(x) - hy'(x) + \frac{1}{2}h^2y''(x) + O(h^3), \\ y(x-2h) &= y(x) - 2hy'(x) + 2h^2y''(x) + O(h^3). \end{aligned}$$

(b) No-flux boundary conditions set $\partial u/\partial x$ equal to zero on the boundaries. Using the results of Part (a), determine two homogeneous equations that need to be satisfied for no-flux boundary conditions.

52. Solve the one-dimensional diffusion equation for $|x| \leq L$ using the Crank-Nicolson method. Assume no-flux boundary conditions. Use the results of 1(b).

53. Solve the two-dimensional diffusion equation on a square with u equal to zero on the boundaries.