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JTMS-MAT-13: Numerical Methods

Sample Exam Solutions

Question 1:

Consider the linear system of equations Ax = b with

$$5x_1 + 2x_2 - 2x_3 = 10$$
$$x_1 + 6x_2 - 2x_3 = -6$$
$$x_2 + 4x_3 = 8$$

(a) Given the starting point $\vec{x}_0 = \vec{0}$, compute the next iterate \vec{x}_1 of the Jacobi iteration.

 $\begin{pmatrix} 5 & 2 \\ 1 & 6 \end{pmatrix}$

- (b) Write down a sufficient condition on a linear system to yield convergence of the Jacobi iteration.
- (c) Given the two equations $2x_1 + 5x_2 = 16$ and $3x_1 + x_2 = 11$, formulate this as a system of equations Ax = b in such an order that convergence is guaranteed and, using the starting point $\vec{x}_0 = \vec{0}$, compute the next iterate \vec{x}_1 of the Gauss-Seidel iteration.
- (a) The system of equations is:

 \mathbf{So}

$$D = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \quad D^{-1} = \begin{pmatrix} 1/5 & 0 & 0 \\ 0 & 1/6 & 0 \\ 0 & 0 & 1/4 \end{pmatrix}, \quad D^{-1}A = \begin{pmatrix} 1/5 & 0 & 0 \\ 0 & 1/6 & 0 \\ 0 & 0 & 1/4 \end{pmatrix} \begin{pmatrix} 5 & 2 & -2 \\ 1 & 6 & -2 \\ 0 & 1 & 4 \end{pmatrix},$$

Hence

$$x_{n+1} = (I - D^{-1}A)x_n + D^{-1}b = \begin{pmatrix} 0 & -2/5 & 2/5 \\ -1/6 & 0 & 1/3 \\ 0 & 1/4 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} 1/5 & 0 & 0 \\ 0 & 1/6 & 0 \\ 0 & 0 & 1/4 \end{pmatrix} \begin{pmatrix} 10 \\ -6 \\ 8 \end{pmatrix}.$$

Thus, with initial guess $\vec{x}_0 = (0, 0, 0)^T$, then $\vec{x}_1 = (2, 1, 2)^T$.

- (b) The Jacobi method converges if the matrix is diagonally dominant.
- (c) The diagonally dominant linear system is

$$\left(\begin{array}{cc} 3 & 1 \\ 2 & 5 \end{array}\right) \left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) = \left(\begin{array}{c} 11 \\ 16 \end{array}\right).$$

From A, then

$$D+L = \left(\begin{array}{cc} 3 & 0\\ 2 & 5 \end{array}\right), \quad U = \left(\begin{array}{cc} 0 & 1\\ 0 & 0 \end{array}\right).$$

Furthermore,

$$(D+L)^{-1} = \frac{1}{15} \begin{pmatrix} 5 & 0 \\ -2 & 3 \end{pmatrix} \implies (D+L)^{-1} b = \frac{1}{15} \begin{pmatrix} 5 & 0 \\ -2 & 3 \end{pmatrix} \begin{pmatrix} 11 \\ 16 \end{pmatrix} = \begin{pmatrix} 11/3 \\ 26/15 \end{pmatrix}$$

Hence when $\vec{x}_0 = \vec{0}$, then $\vec{x}_1 = (11/3, 26/15)$.

Question 2:

Take the function

$$f(x) = x^2 - 4x + 1$$

We want to find root of this function.

- (a) Taking the starting point $x_0 = 2$. Why can we not apply the Newton method?
- (**b**) Derive the secant method from the Newton method.
- (c) Using the points $x_0 = 2$ and $x_1 = 3$ carry out one step of the secant method.
- (d) Show that we can formally apply the Newton method with the starting point $x_0 = 3$ and do one iteration.
- (e) By calculating the actual root(s) of the function, which of the two schemes of (c) and (d) has the lower error with respect to the closest root? Briefly describe if you would expect that from their convergence behaviour.
- (a) The Newton method may be problematic to apply when f'(x) = 0 in the search interval, which is the case with f' = 2(x 2).
- (**b**) Newton's method is

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

The Secant method approximates the derivative $f'(x_n)$ by using a finite difference of the function at two successive points, x_n and x_{n-1} , instead of using the actual derivative

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Substituting this approximation into the Newton-Raphson formula gives:

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

(c) With $x_0 = 2$ and $x_1 = 3$, then f(2) = -3, f(3) = -2, so then

$$x_2 = x_1 - f(x_1) \frac{x_1 - x_0}{f(x_1) - f(x_0)} = 3 - (-2) \frac{3 - 2}{(-2) - (-3)} = 3 + 2\frac{1}{1} = 5.$$

(d) Given $x_0 = 3$, we calculate $f(x_0)$ and $f'(x_0)$:

$$f(x_0) = f(3) = 3^2 - 4 \cdot 3 + 1 = 9 - 12 + 1 = -2$$

$$f'(x_0) = f'(3) = 2 \cdot 3 - 4 = 6 - 4 = 2$$

Now apply the Newton-Raphson formula to find x_1 :

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 3 - \frac{-2}{2} = 4$$

(e) The function has roots $2 \pm \sqrt{3}$, so the relevant root is $2 + \sqrt{3} \approx 3.732$. The error from Newton method is $|\sqrt{3}-2| \approx 0.2679$, whereas the for the secant method the error is $|\sqrt{3}-3| \approx 1.2679$. So the newton method gives a better approximation after one iterate, which given the quadratic convergence, rather than linear, is to be expected.

Question 3: Consider the interpolation problem

We try to fit the function $p(x) = a \sin(x/2) + b \cos(2x)$.

- (a) Solve the resulting overdetermined system to find the free coefficients a and b by either using the 3×2 collocation matrix and its transpose or by writing down the system of normal equations. Both methods are based on the minimization of the sum of squared errors.
- (b) Briefly describe the terms over-determined and under-determined in the context of linear systems of equations.
- (a) The function is $f(x) = a \sin(x/2) + b \cos(2x)$. We need to minimize the sum of the squared errors:

$$E = \sum_{i=1}^{n} \left(y_i - \left(a \sin(x_i/2) + b \cos(2x_i) \right) \right)^2$$

Given points: (0,1) gives $\sin(0) = 0$, $\cos(0) = 1$ and $(\pi, -1)$ gives $\sin(\pi/2) = 1$, $\cos(2\pi) = 1$ and finally $(3\pi, 2)$ gives $\sin(3\pi/2) = -1$, $\cos(6\pi) = 1$. Thus, formulate the matrix equation $A\vec{x} = \vec{y}$ where:

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \vec{x} = \begin{pmatrix} a \\ b \end{pmatrix}, \quad \vec{y} = \begin{pmatrix} 1 \\ -1 \\ 2 \end{pmatrix}$$

The least squares solution is found by solving:

$$A^T A \vec{x} = A^T \vec{y}$$

Calculate
$$A^T A$$
 and $A^T \vec{y}$:

$$A^T A = \begin{pmatrix} 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$$

$$A^T \vec{y} = \begin{pmatrix} 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 2 \end{pmatrix} = \begin{pmatrix} -3 \\ 2 \end{pmatrix}$$
Solving:

$$\begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -3 \\ 2 \end{pmatrix}$$
This leads to:

$$a = -\frac{3}{2}, \text{ and } b = \frac{2}{3}.$$

(b) An over-determined linear system is a system of linear equations in which there are more equations than unknowns. An over-determined linear system can be written as Ax = b, where A is an $m \times n$ matrix with m > n, i.e. more rows than columns. An under-determined linear system is a system of linear equations in which there are fewer equations than unknowns, so the matrix A has more columns than rows.

Question 4:

For the ordinary differential equation

$$y'(t) = -y(t) + t^2, \quad y(0) = 1.$$

- (a) Perform one step each with the forward Euler and backward Euler schemes, with the step h = 1/2 starting at y(0).
- (b) Perform one step of the so called Heun's third-order method which follows the Butcher array



with the step h = 1/2 starting at y(0).

- (c) Show that $y(t) = t^2 2t e^{-t} + 2$ is a solution to the ODE with the initial condition y(0) = 1 and compute the errors for (a) and (b).
- (d) Briefly explain the terms explicit and implicit in this context. Which of the above methods are implicit, which are explicit? What is the advantage of implicit methods compared to explicit methods, what is their disadvantage?
- (a) The formula for the forward Euler method is:

$$y_{n+1} = y_n + hf(t_n, y_n)$$
 where $f(t, y) = -y + t^2$.

Calculating y_1 using $y_0 = 1$, $t_0 = 0$ and $h = \frac{1}{2}$. As $f(t_0, y_0) = -y_0 + t_0^2 = -1$, then $y_1 = y_0 + hf(t_0, y_0) = 1 - \frac{1}{2} = \frac{1}{2}$. Thus, the forward Euler estimate after one step is $y_1 = \frac{1}{2}$.

The formula for the backward Euler method is:

$$u_{n+1} = u_n + hf(t_{n+1}, u_{n+1})$$

Calculate u_1 using u_0 and $h = \frac{1}{2}$, solving the implicit equation:

$$u_1 = u_0 + h(-u_1 + t_1^2)$$

where $t_1 = t_0 + h = \frac{1}{2}$ and $t_1^2 = (\frac{1}{2})^2 = \frac{1}{4}$. Hence,

$$u_1 = 1 + \frac{1}{2}(-u_1 + \frac{1}{4}) \Rightarrow u_1 = \frac{3}{4}$$

Thus, the backward Euler estimate after one step is $u_1 = \frac{3}{4}$.

(b) The Butcher array yields:

$$u_{n+1} = u_n + \frac{h}{4} \left(K_1 + 3K_3 \right)$$

where

$$K_{1} = f(u_{n}, t_{n})$$

$$K_{2} = f(u_{n} + hK_{1}/3, t_{n} + h/3)$$

$$K_{3} = f(u_{n} + 2hK_{2}/3, t_{n} + 2h/3)$$

Thus, $K_1 = \frac{1}{2}$, so that $K_2 = f(1 + \frac{1}{6}, \frac{1}{6}) = -\frac{41}{36}$ and $K_3 = f(1 - \frac{41}{54}, \frac{1}{3}) = -\frac{13}{54} + \frac{1}{9} = -\frac{7}{54}$. Thus, the approximation according to the scheme is:

$$u_1 = 1 + \frac{h}{4} \left(K_1 + 3K_3 \right) = 1 + \frac{1}{8} + \frac{-21}{216} = \frac{(216 + 27 - 21)}{216} = \frac{222}{216} = \frac{111}{108}$$

(c) Differentiating yields $y' = 2t - 2 + e^{-t}$, which is the righthand side of the ordinary differential equation. The value of the function at $t_1 = 1/2$ is $y_1 = 5/4 - e^{-1/2}$. Thus, the error for the forward Euler method is given by $|1 - e^{-1/2}|$, and for the backwards Euler is $|1/2 - e^{-1/2}|$.

For the Runge-Kutta scheme $|5/4 - 111/108 - e^{-1/2}| = |2/9 - e^{-1/2}|$.

(d) An explicit scheme computes the next step entirely in terms of previous solutions, whereas an implicit does not. The forward Euler scheme is explicit, as is Heun's third order scheme. The Backwards Euler scheme is implicit. Implicit schemes, can be more accurate but requires manipulation, or the solution of additional equations in order to compute each iterate.

Question 5: Given the following integral

$$\int_{0}^{2\pi/\sqrt{3}} \sin(t) f(t) \,\mathrm{d}t$$

with some function f(t).

- (a) Derive the Legendre polynomial with n = 1 and its two Gaussian nodes.
- (b) Evaluate the integral with $f(t) = \cos(t)$, using Gaussian quadrature based on the Gaussian nodes found in (a).
- (c) Show that $\sin^2(t)/2$ is the indefinite integral. Using this, compute the exact solution. How large is the error of Gaussian quadrature?
- (d) What specific integration rule does this kind of Gaussian quadrature correspond to (neglecting the exact choice of nodes)?
- (a) The Legendre polynomial for n = 1 takes the form $q = a + bx + cx^2$, with a normalization condition q(1) = 1 and two orthogonality conditions

$$\int_{-1}^{1} (a + bx + cx^{2}) dx = 0$$
$$\int_{-1}^{1} x (a + bx + cx^{2}) dx = 0$$

These yield a + b + c = 1, and

$$\left[ax + \frac{b}{2}x^2 + \frac{c}{3}x^3\right]_{-1}^{1} = 0 \Rightarrow 2a + \frac{2}{3}c = 0$$
$$\left[\frac{a}{2}x^2 + \frac{b}{3}x^3 + \frac{c}{4}x^4\right]_{-1}^{1} = 0 \Rightarrow b = 0$$
$$-\frac{1}{2} \text{ and } c = -\frac{3}{2}. \text{ Hence } q = \frac{1}{2}\left(3x^2 - 1\right). \text{ This has roots } \pm \sqrt{\frac{1}{3}}.$$

(b) Evaluating

Thus, a =

$$\int_{0}^{2\pi/\sqrt{3}} \sin\left(t\right) \cos\left(t\right) \mathrm{d}t = \sum_{i=0}^{1} \tilde{A}_i f(\tilde{x}_i)$$

where \tilde{A}_i and \tilde{x}_i are transformed from the domain [-1,1] to $[0,2\pi/\sqrt{3}]$. But, firstly, to find the correct values of A_0 , A_1 on [-1,1], exploit the fact that the approximation is exact for polynomials, i.e.

$$\int_{-1}^{1} 1 dx = 2 = A_0 f(x_0) + A_1 f(x_1) = A_0 + A_1 \quad \text{when} \quad f(x) = 1$$

and

$$\int_{-1}^{1} x dx = 0 = A_0 f(x_0) + A_1 f(x_1) = \frac{1}{\sqrt{3}} (A_1 - A_0) \quad \text{when} \quad f(x) = x.$$

Hence $A_0 = A_1 = 1$. Thus, $\tilde{A}_0 = \frac{b-a}{2}A_0 = \frac{\pi}{\sqrt{3}}$ and similarly, $\tilde{A}_1 = \frac{b-a}{2}A_1 = \frac{\pi}{\sqrt{3}}$. The Gauss points scale via

$$\tilde{x}_0 = \frac{b+a}{2} + \frac{b-a}{2}x_0 = \frac{\pi}{\sqrt{3}} - \frac{\pi}{3}$$
$$\tilde{x}_1 = \frac{b+a}{2} + \frac{b-a}{2}x_1 = \frac{\pi}{\sqrt{3}} + \frac{\pi}{3}$$

Thus,

$$\sum_{i=0}^{1} \tilde{A}_i f(\tilde{x}_i) = \frac{\pi}{\sqrt{3}} \sin\left(\frac{\pi}{\sqrt{3}} - \frac{\pi}{3}\right) \cos\left(\frac{\pi}{\sqrt{3}} - \frac{\pi}{3}\right) + \frac{\pi}{\sqrt{3}} \sin\left(\frac{\pi}{\sqrt{3}} + \frac{\pi}{3}\right) \cos\left(\frac{\pi}{\sqrt{3}} + \frac{\pi}{3}\right) \approx 0.4236$$

(c) If $F = \frac{1}{2}\sin^2(x)$, then the derivative $F' = \sin(x)\cos(x)$, so it is the indefinite integral of f. Thus, the integral can be evaluated as

$$\left[F(x)\right]_{0}^{2\pi/\sqrt{3}} = \frac{1}{2}\sin^{2}\left(\frac{2\pi}{\sqrt{3}}\right) - \frac{1}{2}\sin^{2}\left(0\right) \approx 0.1091$$

Thus, the error is given by |0.1091 - 0.4236| = 0.3145.

(d) This corresponds to the Trapezium rule, as we use linear interpolation between the two data points.

Question 6: Given the following interpolation problem with points p_i at nodes u_i

Consider the Newton polynomials

$$p_i(u) = \prod_{j=0}^{i-1} (u - u_i)$$
 with $p_0(u) = 1$.

- (a) Derive the collocation matrix for the given interpolation problem.
- (b) Write down the collocation matrix for the case of Lagrange interpolation.
- (c) Use the collocation matrix from (a) to compute the interpolating polynomial $p_2(u)$ for the first two points only (i.e. i = 0 and i = 1).

(a) The collocation matrix is given by:

$$\Phi = \begin{pmatrix} 1 & 0 & 0 \\ 1 & u_1 - u_0 & 0 \\ 1 & u_2 - u_0 & (u_2 - u_1)(u_2 - u_0) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 3 & 0 \\ 1 & 2 & 10 \end{pmatrix}.$$

- (b) The collocation matrix is the identity matrix.
- (c) The linear system to solve $\Phi \alpha = p$, where p is the vector given by $p(x_i)$, which yields $(\alpha_1, \alpha_2)^T = (1, -1)^T$, so that the interpolating polynomial is p = 1 x, as the first Newton polynomial is given by $x x_0$.