Remember to write your name! You are allowed to use a calculator. **You are not allowed to use the textbook or your notes or your neighbor**. To receive full credit on a problem you must show **sufficient justification for your conclusion** unless explicitly stated otherwise. You may cite any theorem from Atkinson or from the lectures unless explicitly stated otherwise.

You must do the first problem. You must pick **only** two of the remaining problems. Each problem is 15 points; there are 45 points total.

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1. Quadrature Consider a quadrature of the form

$$\int_{-h}^{h} f(x)\mathrm{d}x \approx h(af(-h) + bf(0) + cf(h)) + dh^2 f'(0).$$

(a) Find coefficients so that the quadrature integrates all cubic polynomials exactly.

Solution: In order to integrate all cubic polynomials exactly we need to integrate all monomials up to x^3 exactly. This leads to the following linear system:

$$h\begin{bmatrix} 1 & 1 & 1 & 0 \\ -h & 0 & h & h \\ h^2 & 0 & h^2 & 0 \\ -h^3 & 0 & h^3 & 0 \end{bmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 2h \\ 0 \\ \frac{2h^3}{3} \\ 0 \end{pmatrix}.$$

The second and fourth equations together imply that $d = 0$, which allows us to reduce the system to

$$h\begin{bmatrix} 1 & 1 & 1 \\ -h & 0 & h \\ h^2 & 0 & h^2 \\ -h^3 & 0 & h^3 \end{bmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 2h \\ 0 \\ \frac{2h^3}{3} \\ 0 \end{pmatrix}.$$

The second and fourth rows are now linearly dependent so we can instead consider (also cancelling factors of h in each row)

$$\begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \\ \frac{2}{3} \end{pmatrix}.$$

Row reducing yields $a = 1/3, b = 4/3, c = 1/3$. This method is just Simpson's rule.

(b) The above quadrature is equivalent to using Hermite interpolation with the available data, and the quadrature error is therefore

$$\int_{-h}^{h} f(x)\mathrm{d}x - h(af(-h) + bf(0) + cf(h)) - dh^2 f'(0) = \int_{-h}^{h} \frac{(x^2 - h^2)x^2}{4!} f^{(4)}(\xi(x))\mathrm{d}x.$$

Use this to find an asymptotic formula for the error in the limit $h \to 0$.

Solution: The function $(x^2 - h^2)x^2$ is negative semi-definite on the interval of integration, so we can use the integral mean value theorem to write

$$\int_{-h}^{h} \frac{(x^2 - h^2)x^2}{4!} f^{(4)}(\xi(x))\mathrm{d}x = f^{(4)}(\eta)\int_{-h}^{h} \frac{(x^2 - h^2)x^2}{4!} f^{(4)}(\xi(x))\mathrm{d}x = -\frac{h^5}{90} f^{(4)}(\eta)$$

for some unknown η in $(-h, h)$. In the limit $h \to 0$ we just have

$$\text{error } \sim -\frac{h^5}{90} f^{(4)}(0).$$

(c) Consider a composite quadrature for integrals on $[a, b]$ based on repeated use of the above formula. Use the asymptotic error estimate derived above to form a 'corrected' composite quadrature similar to the corrected Trapezoid Rule, assuming you know the values of $f^{(3)}(a)$ and $f^{(3)}(b)$.

Solution: The error in the composite rule is

$$\text{Error } = -\frac{h^4}{180}\left[2h\sum_i f^{(4)}(\eta_i)\right]$$

The formula in square brackets is a Riemann sum (actually a midpoint rule) applied to $\int_a^b f^{(4)}(x)\mathrm{d}x$. In the limit $h \to 0$ we have

$$\text{Error } \sim -\frac{h^4}{180}\left[f^{(3)}(b) - f^{(3)}(a)\right].$$

We form a 'corrected' composite rule by adding this back in:

$$\text{Corrected Rule } = \text{ Composite Simpson's Rule } - \frac{h^4}{180}\left[f^{(3)}(b) - f^{(3)}(a)\right].$$

2. Linear Systems Suppose that the LU factorization of $\mathbf{A}$ can be computed without pivoting. Let

$$\mathbf{A} = \begin{bmatrix} \hat{\mathbf{A}} & \boldsymbol{d} \\ \boldsymbol{c}^T & \alpha \end{bmatrix}, \quad \boldsymbol{c}, \boldsymbol{d} \in \mathbb{R}^{n-1}, \quad \alpha \in \mathbb{R}$$

and assume that $\hat{\mathbf{A}} = \hat{\mathbf{L}}\hat{\mathbf{U}}$, the LU-factorization of $\hat{\mathbf{A}}$, has already been computed. Explain how to use this to compute the LU factorization of $\mathbf{A}$. (Note that this can be used to recursively compute an LU factorization by computing LU factorizations of the upper-left $k \times k$ blocks with increasing k.)

Solution: The LU factorization of $\mathbf{A}$ has the form

$$\mathbf{A} = \begin{bmatrix} \hat{\mathbf{A}} & \boldsymbol{d} \\ \boldsymbol{c}^T & \alpha \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{L}} & \mathbf{0} \\ \boldsymbol{l}^T & 1 \end{bmatrix}\begin{bmatrix} \hat{\mathbf{U}} & \boldsymbol{u} \\ \mathbf{0}^T & u \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{L}}\hat{\mathbf{U}} & \hat{\mathbf{L}}\boldsymbol{u} \\ \boldsymbol{l}^T\hat{\mathbf{U}} & \boldsymbol{l}^T\boldsymbol{u} + u \end{bmatrix}$$

Matching blocks yields the following systems:

$$\hat{\mathbf{L}}\boldsymbol{u} = \boldsymbol{d} \Rightarrow \boldsymbol{u} = \mathbf{L}^{-1}\boldsymbol{d}$$

$$\hat{\mathbf{U}}^T\boldsymbol{l} = \boldsymbol{c} \Rightarrow \boldsymbol{l} = \mathbf{U}^{-T}\boldsymbol{c}$$

$$\boldsymbol{l}^T\boldsymbol{u} + u = \alpha, \Rightarrow u = \alpha - \boldsymbol{l}^T\boldsymbol{u}$$

To compute the missing components of the LU factorization of $\mathbf{A}$, first compute $\boldsymbol{l}$ and $\boldsymbol{u}$ by solving the appropriate lower-triangular systems, then find $u = \alpha - \boldsymbol{l}^T\boldsymbol{u}$.

3. Rootfinding/Nonlinear Equations Consider the fixed-point iteration $x_{k+1} = 2^{x_k - 1}$. (Recall $2^x = e^{x\ln(2)}$.)

(a) What are the fixed points?
Solution: The fixed points of $2x = 2^x$ are $x = 1, 2$.

(b) Which fixed points are stable, i.e. locally convergent?
Solution: $g(x) = 2^{x-1}$, $g'(x) = \ln(2)2^{x-1}$. Plugging in the fixed points $g'(1) = \ln(2)$ and $g'(2) = 2\ln(2)$. The first is stable since $|\ln(2)| < 1$ while the second is unstable since $|2\ln(2)| > 1$.

(c) For each fixed point, what is the order of convergence (i.e. linear, quadratic, etc)?
Solution: Convergence is linear for $x = 1$ since $g' \neq 0$. There is no convergence at $x = 2$.

(d) Formulate Newton's method for $f(x) = x - 2^{x-1}$. What is the order of convergence for each root?
Solution: Newton's method is

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$

Here $f'(x) = 1 - \ln(2)2^{x-1}$, so

$$x_{k+1} = x_k - \frac{x_k - 2^{x_k-1}}{1 - \ln(2)2^{x_k-1}} = \frac{2^{x_k-1}(1 - x_k\ln(2))}{1 - \ln(2)2^{x_k-1}}.$$

The function is smooth and both the roots are simple ($f'(1) \neq 0$ and $f'(2) \neq 0$) so Newton's method will converge quadratically for both roots.

4. Interpolation

(a) Let $x_1, \ldots, x_n$ be n distinct points, and suppose that $p_{n-1}(x)$ interpolates $f(x)$ at $x_1, \ldots, x_{n-1}$ while $q_{n-1}(x)$ interpolates $f(x)$ at $x_2, \ldots, x_n$ (p and q are polynomials of degree $\leq n-1$). Show that

$$p_n(x) = \frac{(x - x_1)q_{n-1}(x) - (x - x_n)p_{n-1}(x)}{x_n - x_1}$$

is a polynomial of degree $\leq n$ that interpolates $f(x)$ at $x_1, \ldots, x_n$.

Solution: First note that p_n is a sum of polynomials of degree at most n, so it is a polynomial of degree at most n. Second note:

$$p_n(x_1) = \frac{-(x_1 - x_n)p_{n-1}(x_1)}{x_n - x_1} = f(x_1)$$

$$p_n(x_n) = \frac{(x_n - x_1)q_{n-1}(x_n)}{x_n - x_1} = f(x_n)$$

$$p_n(x_j) = \frac{(x_j - x_1)q_{n-1}(x_j) - (x_j - x_n)p_{n-1}(x_j)}{x_n - x_1} = \frac{(x_j - x_1) - (x_j - x_n)}{x_n - x_1} f(x_j) = f(x_j)$$

(b) The above fact can be used to develop a recursive algorithm for finding an interpolating polynomial. Consider the following table

$$\begin{array}{cc|cc} x_1 & f_1 & & \\ x_2 & f_2 & P_{1,2}(x) & \\ x_3 & f_3 & P_{2,3}(x) & P_{1,2,3}(x) \end{array}$$

where $P_{1,2}(x)$ interpolates $f(x)$ at points x_1 and x_2, $P_{2,3}(x)$ interpolates at x_2 and x_3, and $P_{1,2,3}(x)$ interpolates at all the points. Assume that the nodes are $-1, 0, 1$ and values are $f(-1) = -1$, $f(0) = 0$, $f(1) = 1$, and give explicit expressions for all 3 P polynomials in the table above using the recursion from (a).

Solution: Putting values into the table:

$$\begin{array}{cc|cc} -1 & -1 & & \\ 0 & 0 & x & \\ 1 & 1 & x & \frac{(x+1)x-(x-1)x}{2} = x \end{array}$$

(c) The above table can also be used to compute *values* of the interpolating polynomial. Add another point $x_4 = 2$ with value $f_4 = f(2) = 8$. Without computing the new interpolating polynomial, use the table to compute the *value* of the interpolating polynomial at $x = 1/2$.
Solution: We will need to plug in for $x = 1/2$ in the third column, so we need to figure out the polynomial in the third column, fourth row:

$$\begin{array}{cc|ccc} -1 & -1 & & & \\ 0 & 0 & x & & \\ 1 & 1 & x & P_{1,2,3}(x) & \\ 2 & 8 & -6+7x & P_{2,3,4}(x) & P_{1,2,3,4}(x) \end{array}$$

Next we plug in $x = 1/2$:

$$\begin{array}{cc|ccc} -1 & -1 & & & \\ 0 & 0 & \frac{1}{2} & & \\ 1 & 1 & \frac{1}{2} & P_{1,2,3}(\frac{1}{2}) & \\ 2 & 8 & -\frac{5}{2} & P_{2,3,4}(\frac{1}{2}) & P_{1,2,3,4}(\frac{1}{2}) \end{array}$$

Now compute

$$P_{1,2,3}(1/2) = \frac{(1/2+1)(1/2) - (1/2-1)(1/2)}{2} = \frac{1}{2}$$

and similarly for

$$P_{2,3,4}(1/2) = \frac{(1/2-0)(-5/2) - (1/2-2)(1/2)}{2} = -\frac{1}{4}$$

Finally

$$P_{1,2,3,4}(1/2) = \frac{(1/2+1)(-1/4) - (1/2-2)(1/2)}{3} = \frac{1}{8}$$

5. Approximation

(a) Find the coefficients a_j and b_j to minimize

$$\int_{-\pi}^{\pi} \left(\cos((n+1)x) - \left[a_0 + \sum_{i=1}^{n} a_j \cos(jx) + b_j \sin(jx) \right] \right)^2 \mathrm{d}x.$$

Solution: The coefficients are

$$a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos((n+1)x)\mathrm{d}x = 0, \;\; a_j = \frac{1}{\pi} \int_{-\pi}^{\pi} \cos((n+1)x)\cos(jx)\mathrm{d}x = 0$$

$$b_j = \frac{1}{\pi} \int_{-\pi}^{\pi} \cos((n+1)x)\sin(jx)\mathrm{d}x = 0$$

(b) Let $p(x)$ be the trig polynomial of degree at most n that minimizes $\int_{-\pi}^{\pi}(f(x)-p(x))^2\mathrm{d}x$ for some periodic, continuously-differentiable f. Show that $q(x)=p'(x)$ is the trig polynomial of degree at most n that minimizes $\int_{-\pi}^{\pi}(f'(x)-q(x))^2\mathrm{d}x$.

Solution: Denote the optimal approximations to f and f' by

$$p(x) = a_0 + \sum_{j=1}^{n} a_j \cos(jx) + b_j \sin(jx)$$

$$q(x) = c_0 + \sum_{j=1}^{n} c_j \cos(jx) + d_j \sin(jx).$$

The coefficients are, by definition

$$c_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} f'(x)\mathrm{d}x = \frac{1}{2\pi}(f(\pi)-f(-\pi)) = 0.$$

$$c_j = \frac{1}{\pi}\int_{-\pi}^{\pi} f'(x)\cos(jx)\mathrm{d}x = \frac{j}{\pi}\int_{-\pi}^{\pi} f(x)\sin(jx)\mathrm{d}x = jb_j$$

$$d_j = \frac{1}{\pi}\int_{-\pi}^{\pi} f'(x) sin(jx)\mathrm{d}x = -\frac{j}{\pi}\int_{-\pi}^{\pi} f(x)\cos(jx)\mathrm{d}x = -ja_j$$

It is now trivial to note that $p'(x)$ is exactly equal to $q(x)$.

(c) Let $p(x)$ be the polynomial of degree at most $n \geq 1$ that minimizes $\int_{-1}^{1}(f(x)-p(x))^2\mathrm{d}x$ for some continuously-differentiable f. Show by example that the polynomial $q(x)$ of degree at most $n-1$ that minimizes $\int_{-1}^{1}(f'(x)-q(x))^2\mathrm{d}x$ is not necessarily $p'(x)$.

Solution: Let $n=1$ and $f(x)=x^2$. The optimal linear $n=1$ least-squares approximation to $f(x)$ is

$$p(x) = \frac{1}{3}.$$

The optimal constant $n=0$ approximation is just

$$q(x) = p(x) = \frac{1}{3} \neq p'(x) = 0.$$