Name and section: ____________________

ID number: ____________________

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1. **(10 points)** Use Taylor series to show that the first derivative of a function $f(x)$ at x_0 can be approximated by:

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h} + O(h^2).$$

Solution: Using Taylor series about $x_0 + h$ and $x_0 - h$ we have respectively

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(\xi_1),$$
$$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(\xi_1).$$

By subtracting the above two equations, we obtain the approximation in question:

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6}f'''(\xi),$$

where the truncation term is obtained from $\frac{h^2}{12}\left(f'''(\xi_1) + f'''(\xi_2)\right)$ via the Intermediate Value Theorem in order to find a common ξ between ξ_1 and ξ_2. Note that $x_0 - h \le \xi \le x_0 + h$.

2. **(15 points)** Consider the function:

$$f(x) = \cos(x) + 2x + 1.$$

Find the **second-order Taylor** polynomial P_2 for $f(x)$ about $x_0 = 0$. Then, use the **remainder term** R_2 to find an **upper bound** for

$$\max_{x\in[0,\pi/4]} |f(x) - P_2(x)|.$$

Solution: From the function $f(x)$ and point x_0 given, P_2 reads:

$$P_2(x) = f(0) + f'(0) + \frac{1}{2}f''(0)x^2 \Rightarrow \boxed{P_2(x) = 2 + 2x - \frac{1}{2}x^2}.$$

Next, using the remainder term, we obtain

$$R_2(x) = \frac{f^{(3)}(\xi)}{3!}x^3 \Rightarrow \boxed{R_2(x) = \frac{\sin(\xi)}{6}x^3},$$

with $\xi \in [0, \pi/4]$. Finally, let us find an upper bound for the error by maximizing the remainder term, that is,

$$|R_2(x)| = \left|\frac{\sin(\xi)}{6}x^3\right| \leq \left|\frac{\sin\left(\frac{\pi}{4}\right)}{6}(\pi/4)^3\right| = \frac{\pi^3}{384\sqrt{2}} \approx 0.0570957.$$

3. **(10 points)** Consider the data pairs $\{(x_i, y_i)\}_{i=0}^n$ together with $\rho_j = \prod_{i \neq j} (x_j - x_i)$ and $\psi(x) = \prod_{i=0}^n (x - x_i)$. Note that $j = 0, 1, \ldots, n$. Show that:

$$\rho_j = \psi'(x_j).$$

Then, show that the interpolating polynomial of degree at most n is given by

$$p_n(x) = \psi(x) \sum_{j=0}^{n} \frac{y_j}{(x - x_j)\,\psi'(x_j)}.$$

Solution: Let us calculate ψ' directly:

$$\begin{aligned}
\psi'(x) &= (x - x_1)(x - x_2) + \cdots + (x - x_n) \\
&+ (x - x_0)(x - x_2) + \cdots + (x - x_n) \\
&+ \ldots \\
&+ (x - x_0)(x - x_1) + \cdots + (x - x_{n-2})(x - x_{n-1}) \Rightarrow \\
\psi'(x) &= \prod_{i=1}^{n}(x - x_i) + \prod_{\substack{i=0 \\ i\neq 1}}^{n}(x - x_i) + \cdots + \prod_{i=0}^{n-1}(x - x_i),
\end{aligned}$$

or, in compact form

$$\boxed{\psi'(x) = \sum_{k=0}^{n}\left[\prod_{\substack{i=0 \\ i\neq k}}^{n}(x - x_i)\right]}. \qquad (1)$$

However, at $x = x_j$ with $j = 0, 1, \ldots, n$, only the $k = j$ term survives in Eq. (1). Since, $i \neq k$ and $k = j$, then $i \neq j$ and Eq. (1) yields to

$$\psi'(x_j) = \prod_{\substack{i=0 \\ i\neq j}}^{n}(x_j - x_i) \Rightarrow \boxed{\psi'(x_j) = \rho_j}.$$

Recall that the interpolant can be written using Lagrange basis as

$$\begin{aligned} p_n(x) &= \sum_{j=0}^{n} y_j L_j(x) = \sum_{j=0}^{n} y_j \prod_{\substack{i=0 \\ i\neq j}}^{n} \frac{(x-x_i)}{(x_j-x_i)} = \sum_{j=0}^{n} \frac{y_j}{(x-x_j)} \frac{\prod_{i=0}^{n}(x-x_i)}{\prod_{\substack{i=0 \\ i\neq j}}^{n}(x_j-x_i)} \\ &= \sum_{j=0}^{n} \frac{y_j}{(x-x_j)} \frac{\psi(x)}{\rho_j} = \psi(x) \sum_{j=0}^{n} \frac{y_j}{\psi'(x_j)\,(x-x_j)}. \quad \blacksquare \end{aligned}$$

4. **(20 points)** Let $f(x)$ be written as

$$f(x) = (x-x^*)^m q(x), \quad q(x^*) \neq 0,$$

where x^* is a root of multiplicity m. Write out the **iteration function** $g(x)$ for Newton's method and show that $g'(x^*) = 1 - 1/m \neq 0$. Explain why this implies only **linear** convergence of Newton's method.

Solution: From Newton's method written as $x_{k+1} = g(x_k)$ with $k = 0, 1, \ldots,$ we know that

$$g(x) = x - \frac{f(x)}{f'(x)} \Rightarrow g(x) = x - \frac{(x-x^*)^m q(x)}{m(x-x^*)^{m-1}q(x) + (x-x^*)^m q'(x)},$$

or, by simplifying the fraction therein, we arrive at

$$\boxed{g(x) = x - \frac{(x-x^*)q(x)}{mq(x) + (x-x^*)q'(x)}}. \tag{2}$$

Next, we take the derivative of Eq. (2) with respect to x and obtain (after some algebra)

$$g'(x) = 1 - \frac{mq^2(x) + (x-x^*)^2 q'^2(x) - (x-x^*)^2 q(x) q''(x)}{\left[mq(x) + (x-x^*)q'(x)\right]^2}. \tag{3}$$

Thus, the evaluation of Eq. (3) at $x = x^*$ yields to

$$g'(x^*) = 1 - \frac{1}{m} \neq 0, \tag{4}$$

since $m > 1$. Note also, that $q(x^*) \neq 0$.

Finally, and based on Eq. (4), we conclude that Newton's method converges linearly. To show that, recall the Taylor expansion of $g(x)$ about x^*

$$\begin{aligned} g(x) &= g(x^*) + g'(x^*)(x-x^*) + \frac{g''(\xi)}{2}(x-x^*)^2 \xrightarrow{(x=x_k)} \\ x_{k+1} &= x^* + g'(x^*)(x_k - x^*) + \frac{g''(\xi)}{2}(x_k-x^*)^2 \Rightarrow \\ \frac{x_{k+1}-x^*}{x_k - x^*} &= g'(x^*) + \frac{g''(\xi)}{2}(x_k - x^*) \Rightarrow \\ \lim_{k\to\infty} \frac{|x_{k+1}-x^*|}{|x_k-x^*|} &= |g'(x^*)|, \end{aligned}$$

or, via Eq. (4)

$$\boxed{\lim_{k\to\infty} \frac{|x_{k+1} - x^*|}{|x_k - x^*|} = \left|1 - \frac{1}{m}\right|}. \tag{5}$$

The latter equation reveals that the covergence factor is given by $\rho = |1-\frac{1}{m}|$ which is **less** than 1, $\forall m > 1$, thus, convergence of Newton's method is guaranteed. Furthermore, the rate of convergence is $\alpha = 1$ which signals that Newton's method will converge **linearly** in this case.

5. **(20 points)** Given a function $f(x)$ and the interval $[a, b]$, **derive** the Trapezoidal rule denoted by I_{trap}. Subsequently, consider Simpson's rule:

$$I_{\text{Simp}} = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right], \tag{6}$$

and the definite integral $\int_0^1 f(x)\,dx$. Suppose the Trapezoidal and Simpson's rules applied to this integral give the values 4 and 2, respectively, i.e., $I_{\text{trap}} = 4$ and $I_{\text{Simp}} = 2$. What is $f(1/2)$?

Solution: To derive the Trapezoidal rule, we interpolate the function $f(x)$ at the endpoints of the interval, that is, we have the abscissae $x_0 = a$ and $x_1 = b$. This way, the Lagrange polynomials of degree 1 are given by

$$\begin{aligned} L_0(x) &= \frac{x-b}{a-b}, \\ L_1(x) &= \frac{x-a}{b-a}, \end{aligned}$$

where the corresponding weights $a_j = \int_a^b L_j(x)\,dx$ with $j = 1, 2$ read

$$\begin{aligned} a_0 &= \frac{b-a}{2}, \\ a_1 &= a_0. \end{aligned}$$

Thus, the Trapezoidal method can be obtained via

$$I_{\text{trap}} = \sum_{j=0}^{1} a_j f(x_j) \Rightarrow \boxed{I_{\text{trap}} = \frac{b-a}{2}\left[f(a) + f(b)\right]}. \tag{7}$$

Finally, let us utilize Eq. (7) with $a = 0$ and $b = 1$ while $I_{\text{trap}} = 4$:

$$\frac{1}{2}\left[f(0) + f(1)\right] = 4 \Rightarrow \boxed{f(0) + f(1) = 8}. \tag{8}$$

However, from Eq. (6), we have

$$I_{\text{Simp}} = 2 \Rightarrow \frac{1}{6}\left[f(0) + 4f\left(\frac{1}{2}\right) + f(1)\right] = 2 \Rightarrow f(0) + f(1) + 4f\left(\frac{1}{2}\right) = 12, \quad (9)$$

which results in $\boxed{f\,(1/2) = 1}$.

6. **(25 points)** Let A be the following 2×2 matrix:

$$A = \begin{bmatrix} a & -b \\ -a & a \end{bmatrix},$$

where a and b are real numbers satisfying $a > 0$, $b > 0$ and $a > b$. Show that both the Jacobi and Gauss-Seidel methods **converge** for this type of matrices for **any** initial guess.

Solution: At first, we have to construct the respective *iteration matrices* T. In principle, the latter are given by:

$$T = \mathbb{I} - M^{-1}A,$$

with $A = M - N$, where $M = D$ and $M = E$ (lower triangular matrix) for the Jacobi and Gauss-Seidel methods, respectively. Equivalently, the iteration matrices for Jacobi and Gauss-Seidel methods based on the following splitting $A = L + D + U$ can be written as:

$$\begin{aligned} R_J &= -D^{-1}(U + L), \\ R_{GS} &= -(L + D)^{-1} U, \end{aligned}$$

respectively, where L is strictly lower triangular matrix, U is strictly upper triangular matrix and D is a diagonal matrix, **all** extracted from A.

Let us calculate the matrix T for the respective cases. In particular we have

$$\begin{aligned} T_J &= \mathbb{I} - D^{-1}A \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} a & 0 \\ 0 & a \end{bmatrix}^{-1} \begin{bmatrix} a & -b \\ -a & a \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{1}{a}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} a & -b \\ -a & a \end{bmatrix} \\ &= \begin{bmatrix} 0 & \frac{b}{a} \\ 1 & 0 \end{bmatrix}, \end{aligned}$$

and similarly

$$\begin{aligned} T_{GS} &= \mathbb{I} - E^{-1}A \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} a & 0 \\ -a & a \end{bmatrix}^{-1} \begin{bmatrix} a & -b \\ -a & a \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{1}{a}\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} a & -b \\ -a & a \end{bmatrix} \\ &= \begin{bmatrix} 0 & \frac{b}{a} \\ 0 & \frac{b}{a} \end{bmatrix}, \end{aligned}$$

where T_J and T_{GS} are the iteration matrices for the Jacobi and Gauss-Seidel methods, respectively.

Next, we have to calculate the spectral radii of these matrices. To do so, we have to find the spectrum of the respective matrices. Specifically, and as far as Jacobi's method is concerned, we have that

$$|T_J - \lambda \mathbb{I}| = 0 \Rightarrow \boxed{\lambda = \pm\sqrt{\frac{b}{a}}}.$$

On equally footing and for the Gauss-Seidel method we obtain

$$|T_{GS} - \lambda \mathbb{I}| = 0 \Rightarrow \boxed{\lambda = 0 \quad \text{or} \quad \lambda = \frac{b}{a}}.$$

Since the by definition the spectral radii are given by

$$\rho(T) = \max\{|\lambda|, / \, \lambda \text{ the eigenvalues of } T\},$$

we conclude that

$$\begin{aligned} \rho(T_J) &= \sqrt{\frac{b}{a}}, \\ \rho(T_{GS}) &= \frac{b}{a}. \end{aligned}$$

It is straightforward to see that both radii are < 1 since $a > b \Rightarrow 1 > b/a$ with $a > 0$ and $b > 0$. Based on the theorem about stationary method convergence, if $\rho(T) < 1$, then the method will converge, which **is** the case here. In other words, both Jacobi and Gauss-Seidel methods **will** converge for **any** initial guess.

Duration: 2hrs
Good luck and happy summer!

Formula sheet

- Lagrange polynomial of degree n:

$$L_j(x) = \prod_{\substack{i=0 \\ i\neq j}}^{n} \frac{(x - x_i)}{(x_j - x_i)}.$$

- The inverse of a 2×2 matrix A:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad A^{-1} = \frac{1}{ad - bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

- Trapezoidal rule:

$$I_{\text{trap}} = \frac{b-a}{2}\left[f(a) + f(b)\right].$$