**Name and section:** ____________________

**ID number:** ____________________

**E-mail:** ____________________

1. (5 points) Use Taylor series to show that the second derivative of a function $f(x) \in C^4$ at a point $x_0$ can be approximated by:

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

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

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f''''(\xi_1),$$
$$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f''''(\xi_2).$$

By adding the above two equations, we obtain:

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

where the truncation term is obtained from $\frac{h^2}{48}\left(f''''(\xi_1) + f''''(\xi_2)\right)$ via the Intermediate Value Theorem in order to find a common $\xi$ between $\xi_1$ and $\xi_2$. Note that $x_0 - h \leq \xi \leq x_0 + h$.

2. (15 points) Let $f(x)$ be a continuous function in $[a,b]$ and differentiable in $(a,b)$. Show that the error in the Trapezoidal rule is

$$E(f) = -\frac{f''(\eta)}{12}(b-a)^3,$$

for some $\eta \in [a,b]$.

**Solution:** Recall that

$$f(x) - p_n(x) = f[x_0, x_1, \ldots, x_n, x]\prod_{i=0}^{n}(x - x_i)$$

and

$$E(f) = \int_a^b f[x_0, x_1, \ldots, x_n, x] \prod_{i=0}^{n} (x - x_i)\ dx. \tag{1}$$

In the Trapezoidal rule, we consider $n = 1$ with abscissae: $x_0 = a$ and $x_1 = b$. Then Eq. (1) becomes

$$E(f) = \int_a^b f[a, b, x]\,(x - a)\,(x - b)\ dx.$$

Note that the function $(x-a)(x-b)$ is a non-positive function, or equivalently, it does not change sign over $[a, b]$. Then, the Integral Mean Value Theorem applies here and we obtain:

$$\begin{aligned} E(f) &= f[a, b, \xi] \int_a^b (x - a)\,(x - b)\ dx \\ &= -\frac{f[a, b, \xi]}{6}\,(b - a)^3\,, \end{aligned} \tag{2}$$

for some $\xi \in [a, b]$. Upon using the formula in the appendix (connecting the divided differences with ordinary derivatives) Eq. (2) becomes

$$\boxed{E(f) = -\frac{f''(\eta)}{12}\,(b - a)^3},$$

for some $\eta \in [a, b]$. ■

3. (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

$$\boxed{g(x) = x - \frac{(x - x^*)q(x)}{mq(x) + (x - x^*)q'(x)}}. \tag{3}$$

Next, we take the derivative of Eq. (3) with respect to $x$ and obtain (after some algebra)

$$g'(x) = 1 - \frac{mq^2(x) + (x - x^*)^2 q'^2(x) - (x - x^*)^2 q(x) q''(x)}{[mq(x) + (x - x^*)q'(x)]^2}. \tag{4}$$

Thus, the evaluation of Eq. (4) at $x = x^*$ yields to

$$g'(x^*) = 1 - \frac{1}{m} \neq 0, \tag{5}$$

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

Finally, and based on Eq. (5), 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. (5)

$$\boxed{\lim_{k\to\infty} \frac{|x_{k+1} - x^*|}{|x_k - x^*|} = \left|1 - \frac{1}{m}\right|}. \tag{6}$$

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.

4. (15 points) Let the data pairs $(-1, 5)$, $(0, 1)$ and $(1, 1)$. Find the **Lagrange form** and **Newton form** of the interpolating polynomial $p_2(x)$. Please, state which is which. Then, expand out the Lagrange and Newton forms to verify that they agree with each other. Explain why.

**Solution:** At first, we have the following table:

| | | | |
|---|---|---|---|
| $x$ | $-1$ | 0 | 1 |
| $y$ | 5 | 1 | 1 |

Then, using Lagrange interpolation $p_2(x)$ is given by:

$$\begin{aligned} p_2(x) &= \sum_{j=0}^{2} y_j L_j(x) \\ &= y_0 \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} + y_1 \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} + y_2 \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}, \end{aligned}$$

or

$$\boxed{p_2(x) = \frac{5}{2}x(x-1) - (x-1)(x+1) + \frac{1}{2}x(x+1)},$$

which corresponds to the **Lagrange form**. Note that expanding $p_2(x)$ out, we obtain

$$p_2(x) = 1 - 2x + 2x^2, \tag{7}$$

which is the **standard form**. Furthermore, a quick check reveals that $p_2(x_i) = y_i$ holds for $i = 0, 1, 2$.

Next, by utilizing the formulas for the divided differences in the appendix, we end up with the corresponding divided difference table:

| $i$ | $x_i$ | $f[\cdot]$ | $f[\cdot,\cdot]$ | $f[\cdot,\cdot,\cdot]$ |
|---|---|---|---|---|
| 0 | $-1$ | 5 | – | – |
| 1 | 0 | 1 | $-4$ | – |
| 2 | 1 | 1 | 0 | 2 |

Thus, extracting its diagonal entries yields the coefficients for the Newton interpolation polynomial. This way, the **Newton form** is given by

$$\boxed{p_2(x) = 5 - 4\,(x+1) + 2x\,(x+1)},$$

which is precisely (after some algebra) the same polynomial as the one in Eq. (7).

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

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

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

**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 $a_j = \displaystyle\int_a^b L_j(x)\,dx$ with $j = 1, 2$ read

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

Thus, the Trapezoidal method is obtained via

$$I_{\text{trap}} = \sum_{j=0}^{1} a_j f(x_j) \Rightarrow \boxed{I_{\text{trap}} = \frac{b-a}{2}\left[f(a) + f(b)\right]}. \tag{8}$$

Finally, let us utilize Eq. (8) with $a = 0$ and $b = 2$ while $I_{\text{trap}} = 1$:

$$\boxed{f(0) + f(2) = 1}. \tag{9}$$

However, from Eq. (8), we have

$$I_{\text{Simp}} = 1/2 \Rightarrow \frac{1}{3}\left[f(0) + 4f\,(1) + f(2)\right] = 1/2 \Rightarrow f(0)+f(2)+4f\,(1) = 3/2, \tag{10}$$

which results in $\boxed{f\,(1) = 1/8}$.

6. (25 points) Let $A$ be the following $2 \times 2$ 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:

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

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 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.

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**Duration: 2hrs**

Good luck and happy Christmas Holidays!

# Formula sheet

- Relationship between divided differences and ordinary derivatives:

$$f[x_0, x_1, \dots, x_n] = \frac{f^{(n)}(\eta)}{n!},$$

for some $\eta \in [a, b]$ and $x_i$ for $i = 0, \dots, n$ are **distinct** points in $[a, b]$.

- Lagrange polynomial of degree $n$:

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

- Divided differences:
  Given points $x_0, x_1, \dots, x_n$ for arbitrary indices $0 \leq i < j \leq n$, then

$$\begin{aligned} f[x_i] &= f(x_i), \\ f[x_i, \dots, x_j] &= \frac{f[x_{i+1}, \dots, x_j] - f[x_i, \dots, x_{j-1}]}{x_j - x_i}. \end{aligned}$$

- Trapezoidal rule:

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

- The inverse of a $2 \times 2$ matrix $A$:

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