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**Date:** October 11, 2025

**Assignment No:** Assignment 3
**Course Code:** DS288/UMC202
**Course Name:** Numerical Methods
**Term:** AUG 2025

## Solution 1

Simpson's rule is an example of a method used for numerical integration. Numerical integration is used when a particular function, i.e. $f(x)$ is too complicated or analytically impossible to integrate.

In such a situation, we can use an interpolating polynomial to obtain a sort of polynomial expression for $f(x)$. Because polynomials can be integrated with ease (and lesser computation), this method is used.

In other words, we will find a $P_n(x)$ such that $f(x) \approx P_n(x)$. Hence, $\int_a^b f(x)dx \approx \int_a^b P_n(x)dx$.

To derive Simpson's $1/3$ rule in this question, we shall be using a set of three points to obtain a quadratic Lagrange interpolating polynomial. Let us call the three points as $(x_0, f(x_0)), (x_1, f(x_1))$ and $(x_2, f(x_2))$.

Because we are asked to calculate the Lagrange interpolating polynomial using three equally spaced points, we can state the following:

$$x_0 = a$$

$$x_1 = x_0 + h = a + h$$

$$x_2 = x_0 + 2h = a + 2h$$

$$\text{where } h = \frac{b-a}{2}$$

Hence, $\int_a^b f(x) \approx \int_{x_0}^{x_2} P_n(x)$.

Let us now find the Lagrange interpolating polynomial:

We know that the formula for Lagrange interpolating polynomial is $f(x) \approx l_0(x) \cdot f(x_0) + l_1(x) \cdot f(x_1) + l_2(x) \cdot f(x_2)$. In this formula:

$$l_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}$$

$$l_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

$$l_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$l_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

Let us now develop an alternative formula for the integration:

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$$f(x) \approx P_n(x)$$

$$\int_a^b f(x)dx \approx \int_a^b P(x)dx$$

$$\int_a^b f(x)dx \approx \int_a^b \left[f\left(x_0\right)l_0(x) + f\left(x_1\right)l_1(x) + f\left(x_2\right)l_2(x)\right]dx$$ Substitute $P_n(x)$.

$$\int_a^b f(x)dx \approx \int_a^b f\left(x_0\right)l_0(x)dx + \int_a^b f\left(x_1\right)l_1(x)dx + \int_a^b f\left(x_2\right)l_2(x)dx$$ Use the summation rule of integration.

$$\int_a^b f(x)dx \approx f\left(x_0\right)\int_a^b l_0(x)dx + f\left(x_1\right)\int_a^b l_1(x)dx + f\left(x_2\right)\int_a^b l_2(x)dx$$ Factor out the constant terms.

By applying the concept of equally spaced points, we can re-write the integration as:

$$\int_a^b f(x)dx \approx f\left(x_0\right)\int_{x_1-h}^{x_1+h} l_0(x)dx + f\left(x_1\right)\int_{x_1-h}^{x_1+h} l_1(x)dx + f\left(x_2\right)\int_{x_1-h}^{x_1+h} l_2(x)dx$$ $a = x_1 - h$ and $b = x_1 + h$

Let us now calculate $l_0(x)$:

$$l_0(x) = \frac{\left(x-x_1\right)\left(x-x_2\right)}{\left(x_0-x_1\right)\left(x_0-x_2\right)}$$

$$l_0(x) = \frac{\left(x-x_1\right)\left(x-\left(x_1+h\right)\right)}{\left(x_0-\left(x_0+h\right)\right)\left(x_0-\left(x_0+2h\right)\right)}$$

$$l_0(x) = \frac{\left(x-x_1\right)\left(x-x_1-h\right)}{(-h)(-2h)}$$

$$l_0(x) = \frac{\left(x-x_1\right)^2 - h\left(x-x_1\right)}{2h^2}$$

Let us integrate $l_0(x)$:

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \int_{x_1-h}^{x_1+h} \frac{\left(x-x_1\right)^2 - h\left(x-x_1\right)}{2h^2}dx$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\int_{x_1-h}^{x_1+h} \left[\left(x-x_1\right)^2 - h\left(x-x_1\right)\right]dx$$

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$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left[\frac{(x-x_1)^3}{3} - \frac{h\,(x-x_1)^2}{2}\right]_{x_1-h}^{x_1+h}$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left\{\left[\frac{(x_1+h-x_1)^3}{3} - \frac{h\,(x_1+h-x_1)^2}{2}\right] - \left[\frac{(x_1-h-x_1)^3}{3} - \frac{h\,(x_1-h-x_1)^2}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left\{\left[\frac{(h)^3}{3} - \frac{h(h)^2}{2}\right] - \left[\frac{(-h)^3}{3} - \frac{h(-h)^2}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left\{\left[\frac{h^3}{3} - \frac{h^3}{2}\right] - \left[\frac{-h^3}{3} - \frac{h\left(h^2\right)}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left\{\left[\frac{h^3}{3} - \frac{h^3}{2}\right] - \left[\frac{-h^3}{3} - \frac{h^3}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left(-\frac{h^3}{6} + \frac{5h^3}{6}\right)$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{1}{2h^2}\left(\frac{2h^3}{3}\right)$$

$$\int_{x_1-h}^{x_1+h} l_0(x)dx = \frac{h}{3}$$

Let us now calculate $l_1(x)$:

$$l_1(x) = \frac{(x-x_0)\,(x-x_2)}{(x_1-x_0)\,(x_1-x_2)}$$

$$l_1(x) = \frac{(x-(x_1-h))\,(x-(x_1+h))}{(x_1-(x_1-h))\,(x_1-(x_1+h))}$$

$$l_1(x) = \frac{(x-x_1+h)\,(x-x_1-h)}{(x_1-(x_1-h))\,(x_1-(x_1+h))}$$

$$l_1(x) = \frac{(x-x_1)^2-h^2}{-h^2}$$

Let us integrate $l_1(x)$:

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \int_{x_1-h}^{x_1+h} \frac{(x-x_1)^2 - h^2}{-h^2} dx$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \int_{x_1-h}^{x_1+h} \left[(x-x_1)^2 - h^2\right] dx$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \left[\frac{(x-x_1)^3}{3} - h^2 x\right]_{x_1-h}^{x_1+h}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \left\{\left[\frac{(x_1+h-x_1)^3}{3} - h^2(x_1+h)\right] - \left[\frac{(x_1-h-x_1)^3}{3} - h^2(x_1-h)\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \left\{\left[\frac{(h)^3}{3} - h^2 x_1 - h^3\right] - \left[\frac{(-h)^3}{3} - h^2 x_1 + h^3\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \left\{\left[-\frac{2h^3}{3} - h^2 x_1\right] - \left[\frac{2h^3}{3} - h^2 x_1\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \left(-\frac{2h^3}{3} - h^2 x_1 - \frac{2h^3}{3} + h^2 x_1\right)$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = -\frac{1}{h^2} \left(-\frac{4h^3}{3}\right)$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \frac{4h}{3}$$

Let us now calculate $l_2(x)$:

$$l_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

$$l_2(x) = \frac{(x-(x_1-h))(x-x_1)}{(x_2-(x_2-2h))(x_2-(x_2-h))}$$

$$l_2(x) = \frac{(x-x_1+h)(x-x_1)}{(2h)(h)}$$

$$l_2(x) = \frac{h(x-x_1) + (x-x_1)^2}{2h^2}$$

Let us integrate $l_2(x)$:

$$\int_{x_1-h}^{x_1+h} l_2(x)dx = \int_{x_1-h}^{x_1+h} \frac{(x-x_1)^2 + h(x-x_1)}{2h^2}dx$$

$$\int_{x_1-h}^{x_1+h} l_2(x)dx = \frac{1}{2h^2}\int_{x_1-h}^{x_1+h} \left[(x-x_1)^2 + h(x-x_1)\right]dx$$

$$\int_{x_1-h}^{x_1+h} l_2(x)dx = \frac{1}{2h^2}\left[\frac{(x-x_1)^3}{3} + \frac{h(x-x_1)^2}{2}\right]_{x_1-h}^{x_1+h}$$

$$\int_{x_1-h}^{x_1+h} l_2(x)dx = \frac{1}{2h^2}\left\{\left[\frac{(x_1+h-x_1)^3}{3} + \frac{h(x_1+h-x_1)^2}{2}\right] - \left[\frac{(x_1-h-x_1)^3}{3} + \frac{h(x_1-h-x_1)^2}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \frac{1}{2h^2}\left\{\left[\frac{(h)^3}{3} + \frac{h(h)^2}{2}\right] - \left[\frac{(-h)^3}{3} + \frac{h(-h)^2}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \frac{1}{2h^2}\left\{\left[\frac{h^3}{3} + \frac{h^3}{2}\right] - \left[\frac{-h^3}{3} + \frac{h(h^2)}{2}\right]\right\}$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \frac{1}{2h^2}\left(\frac{5h^3}{6} - \frac{h^3}{6}\right)$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \frac{1}{2h^2}\left(\frac{2h^3}{3}\right)$$

$$\int_{x_1-h}^{x_1+h} l_1(x)dx = \frac{h}{3}$$

Now that we have the integrations of $l_0(x)$, $l_1(x)$ and $l_2(x)$, we can substitute them back into the original equation:

$$\int_a^b f(x)dx \approx f(x_0)\int_a^b l_0(x)dx + f(x_1)\int_a^b l_1(x)dx + f(x_2)\int_a^b l_2(x)dx$$

$$\int_a^b f(x)dx \approx f(x_0)\left(\frac{h}{3}\right) + f(x_1)\left(\frac{4h}{3}\right) + f(x_2)\left(\frac{h}{3}\right)$$

$$\int_a^b f(x)dx \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

Now, let us find out the reason why Simpson's $1/3$ method gives accurate results for cubic polynomials, despite the fact that the origin is from a quadratic polynomial. The trick for this lies in the error term of the Simpson's $1/3$ rule. The error term for Simpson's $1/3$ rule is as follows:

$$E(f) = -\frac{h^5}{90} f^{(4)}(\xi)$$

If $f(x)$ is a cubic polynomial, i.e $f(x) = a_3x^3 + a_2x^2 + a_1x + a_0$, $f^{(4)}(x) = 0$, for all $x \in \mathbb{R}$. Hence, because the error term is zero, the results of integration shall be accurate until $f(x)$ is a cubic polynomial.

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# Solution 2

## Derivation of formula

In this question, we have been asked to use the composite Simpson's $1/3$ rule to calculate the value of the integration numerically. In the Composite Simpson's $1/3$ rule, we basically split the interval into $n$ intervals, each with a height $h = \frac{b-a}{n}$. We then calculate the integrals of each interval and sum them all up. In mathematical terms, this is what we are doing:

$$\int_b^a f(x)\,dx \approx \int_{x_0}^{x_2} P_1(x)\,dx + \int_{x_2}^{x_4} P_2(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} P_{\frac{n}{2}}(x)\,dx$$

Let us now substitute the formulae for Simpson's $1/3$ formula, as derived in Question 1:

$$\int_b^a f(x)\,dx \approx \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] + \cdots + \frac{h}{3}[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]$$

$$\int_b^a f(x)\,dx \approx \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]$$

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + f(x_n) + 4\sum_{i=1,3,5,\ldots}^{n-1} f(x_i) + 2\sum_{i=2,4,6,\ldots}^{n-2} f(x_i)\right]$$

The error term is: $E = \frac{(b-a)h^4}{180} f^{(4)}(\xi)$

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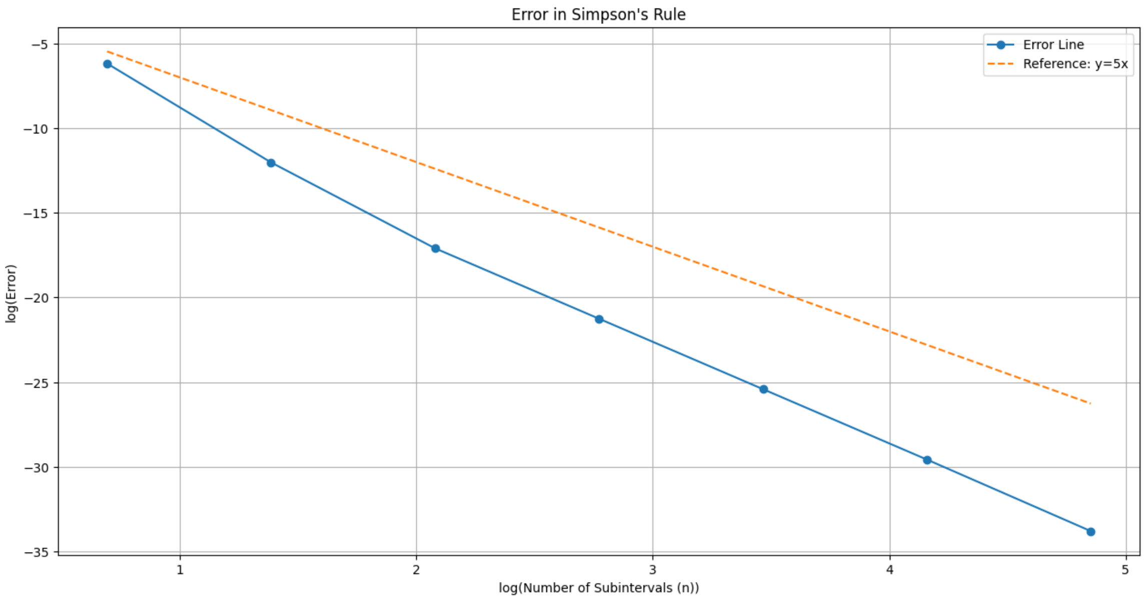
## Results

The convergence graph is as follows:




## Algorithm

The program steps are as follows:

1. The required variables are initialised:
   (a) $a = 0, b = 1$
   (b) components = $[2, 4, 8, 16, 32, 64, 128]$
2. The results of the integrations are calculated using Simpson's composite $1/3$ rule:
   (a) The value of $h$ is calculated.
   (b) The terms of the formula are added, as specified in the above derivation.
   (c) The integration value is multiplied by $\frac{h}{3}$.
3. The error values are calculated. The exact value is $\frac{\pi}{4}$, as specified in the question.
4. The table of results is printed
5. Based on the above calculated error, we plot the graph.

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# Solution 3

## Derivation of formulae

### Derivation of three-point backward difference

The derivation for the three-point backward difference is as follows:

First, let us obtain the Taylor series expansions for $f(x-h)$ and $f(x-2h)$:

$$f(x-h) \approx f(x) - hf'(x) + \frac{h^2}{2}f''(x) + O\left(h^3\right)$$

$$\begin{aligned} f(x-2h) &\approx f(x) - 2hf'(x) + \frac{4h^2}{2}f''(x) + O\left(h^3\right) \\ &\approx f(x) - 2hf'(x) + 2h^2 f''(x) + O\left(h^3\right) \end{aligned}$$

Now, let us solve for $f'(x)$:

$$\begin{aligned} 4f(x-h) - f(x-2h) &\approx 4\left[f(x) - hf'(x) + \frac{h^2}{2}f''(x) + O\left(h^3\right)\right] - \left[f(x) - 2hf'(x) + 2h^2 f''(x) + O\left(h^3\right)\right] \\ 4f(x-h) - f(x-2h) &\approx 4f(x) - 4hf'(x) + 2h^2 f''(x) + 4 \times O\left(h^3\right) - f(x) + 2hf'(x) - 2h^2 f''(x) + O\left(h^3\right) \\ 4f(x-h) - f(x-2h) &\approx 3f(x) - 2hf'(x) + O\left(h^3\right) \\ f'(x) &\approx \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} + O\left(h^2\right) \end{aligned}$$

### Derivation of three-point forward difference

The derivation for the three-point forward difference is as follows:
First, let us obtain the Taylor series expansions for $f(x+h)$ and $f(x+2h)$:

$$f(x+h) \approx f(x) + hf'(x) + \frac{h^2}{2}f''(x) + O\left(h^3\right)$$

$$\begin{aligned} f(x+2h) &\approx f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x) + O\left(h^3\right) \\ f(x+2h) &\approx f(x) + 2hf'(x) + 2h^2 f''(x) + O\left(h^3\right) \end{aligned}$$

Now, let us solve for $f'(x)$:

$$4f(x+h) - f(x+2h) \approx 4\left[f(x) + hf'(x) + \frac{h^2}{2}f''(x) + O\left(h^3\right)\right] - \left[f(x) + 2hf'(x) + 2h^2 f''(x) + O\left(h^3\right)\right]$$

$$4f(x+h) - f(x+2h) \approx 4f(x) + 4hf'(x) + \frac{4h^2}{2}f''(x) + O\left(h^3\right) - f(x) - 2hf'(x) - 2h^2 f''(x) + O\left(h^3\right)$$

$$4f(x+h) - f(x+2h) \approx 3f(x) + 2hf'(x) + O\left(h^3\right)$$

$$f'(x) \approx \frac{4f(x+h) - f(x+2h) - 3f(x)}{2h} + O\left(h^2\right)$$

**Derivation of five-point central difference**

The derivation for the five-point central difference is as follows:
First, let us obtain the Taylor series expansions for $f(x-2h)$, $f(x-h)$, $f(x+h)$ and $f(x+2h)$:

$$f(x+h) \approx f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + O\left(h^5\right)$$

$$f(x-h) \approx f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) - O\left(h^5\right)$$

$$f(x+2h) \approx f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x) + \frac{8h^3}{6}f'''(x) + \frac{16h^4}{24}f^{(4)}(x) + O\left(h^5\right)$$

$$f(x-2h) \approx f(x) - 2hf'(x) + \frac{4h^2}{2}f''(x) - \frac{8h^3}{6}f'''(x) + \frac{16h^4}{24}f^{(4)}(x) - O\left(h^5\right)$$

Let us now cancel out the even-ordered derivatives, i.e. $f''(x)$, $f^{(4)}(x)$, etc.:

$$\begin{aligned} &f(x+h) - f(x-h) \\ &\quad = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + O(h^5) - f(x) + hf'(x) - \frac{h^2}{2}f''(x) \\ &\qquad + \frac{h^3}{6}f'''(x) - \frac{h^4}{24}f^{(4)}(x) + O(h^5) \end{aligned}$$

$$\therefore f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + O(h^5)$$

$$
\begin{aligned}
&f(x+2h) - f(x-2h) \\
&\quad = f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x) + \frac{8h^3}{6}f'''(x) + \frac{16h^4}{24}f^{(4)}(x) + O(h^5) - f(x) + 2hf'(x) \\
&\qquad - \frac{4h^2}{2}f''(x) + \frac{8h^3}{6}f'''(x) - \frac{16h^4}{24}f^{(4)}(x) + O(h^5)
\end{aligned}
$$

$$\therefore f(x+2h) - f(x-2h) = 4hf'(x) + \frac{8h^3}{3}f'''(x) + O(h^5)$$

Now, let us cancel out the $f'''(x)$ term:

$$8\left[f(x+h) - f(x-h)\right] - \left[f(x+2h) - f(x-2h)\right] = 8\left(2hf'(x) + \frac{h^3}{3}f'''(x) + O(h^5)\right) - \left(4hf'(x) + \frac{8h^3}{3}f'''(x) + O(h^5)\right)$$

$$8\left[f(x+h) - f(x-h)\right] - \left[f(x+2h) - f(x-2h)\right] = 16hf'(x) + \frac{8h^3}{3}f'''(x) + 80(h^5) - 4hf'(x) - \frac{8h^3}{3}f'''(x) - O(h^5)$$

Finally, let us solve for $f'(x)$:

$$f'(x) = \frac{8\left[f(x+h) - f(x-h)\right] - \left[f(x+2h) - f(x-2h)\right]}{12h} + O(h^4)$$

$$f'(x) = \frac{8f(x+h) + f(x-2h) - 8f(x-h) - f(x+2h)}{12h} + O(h^4)$$

## Summary

The summary of the derivations is as follows:

| Formula Name | Formula | Error |
|---|---|---|
| 3-Point Backward Difference | $\dfrac{3f(x) - 4f(x-h) + f(x-2h)}{2h}$ | $O(h^2)$ |
| 3-Point Forward Difference | $\dfrac{4f(x+h) - f(x+2h) - 3f(x)}{2h}$ | $O(h^2)$ |
| 5-Point Central Difference | $\dfrac{8f(x+h) + f(x-2h) - 8f(x-h) - f(x+2h)}{12h}$ | $O(h^4)$ |

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## Analytical derivation

For obtaining the error of the numerically calculated, derivative, we shall require an analytical (true) derivative. This can be calculated as follows:

$$f'(x) = \frac{d}{dx}(e^x \sin x)$$

$$f'(x) = e^x \left(\frac{d}{dx}(\sin x)\right) + (\sin x)\left(\frac{d}{dx}(e^x)\right)$$

$$f'(x) = e^x(\cos x) + e^x(\sin x)$$

$$f'(x) = e^x(\sin x + \cos x)$$

The analytical value of $f'(x)$ at $x = \frac{\pi}{4}$ is as follows:

$$f'\left(\frac{\pi}{4}\right) = e^{\frac{\pi}{4}}\left(\sin\frac{\pi}{4} + \cos\frac{\pi}{4}\right)$$

$$f'\left(\frac{\pi}{4}\right) = e^{\frac{\pi}{4}}\left(\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2}\right)$$

$$f'\left(\frac{\pi}{4}\right) = \sqrt{2}e^{\frac{\pi}{4}}$$

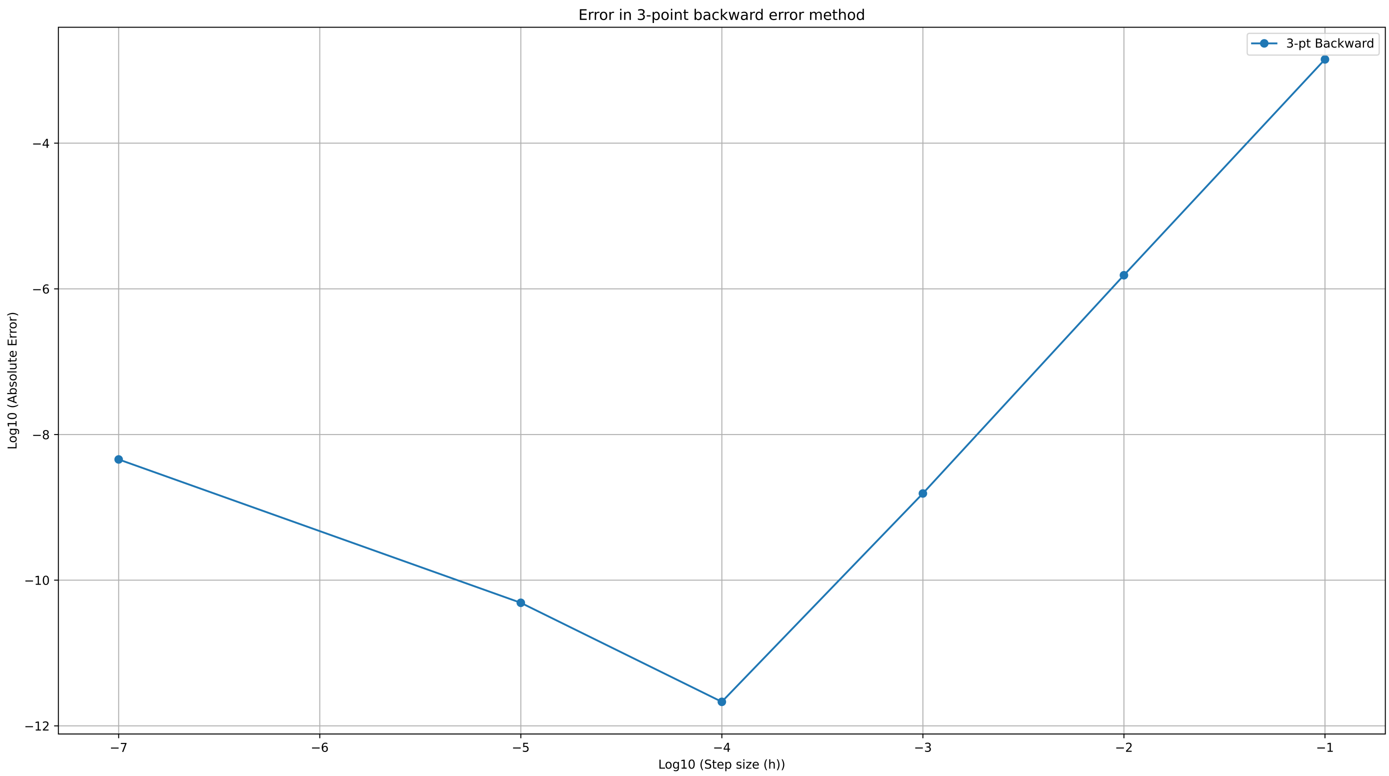
## Results

The comparison table is as follows:

| h | 3-pt Backward | 3-pt Forward | 5-pt Central |
|---|---|---|---|
| $10^{-1}$ | 3.1003558975 | 3.1034671876 | 3.1018077506 |
| $10^{-2}$ | 3.1017648574 | 3.1017679592 | 3.1017663980 |
| $10^{-3}$ | 3.1017663923 | 3.1017663954 | 3.1017663938 |
| $10^{-4}$ | 3.1017663938 | 3.1017663938 | 3.1017663938 |
| $10^{-5}$ | 3.1017663938 | 3.1017663938 | 3.1017663938 |
| $10^{-7}$ | 3.1017663893 | 3.1017663860 | 3.1017663898 |

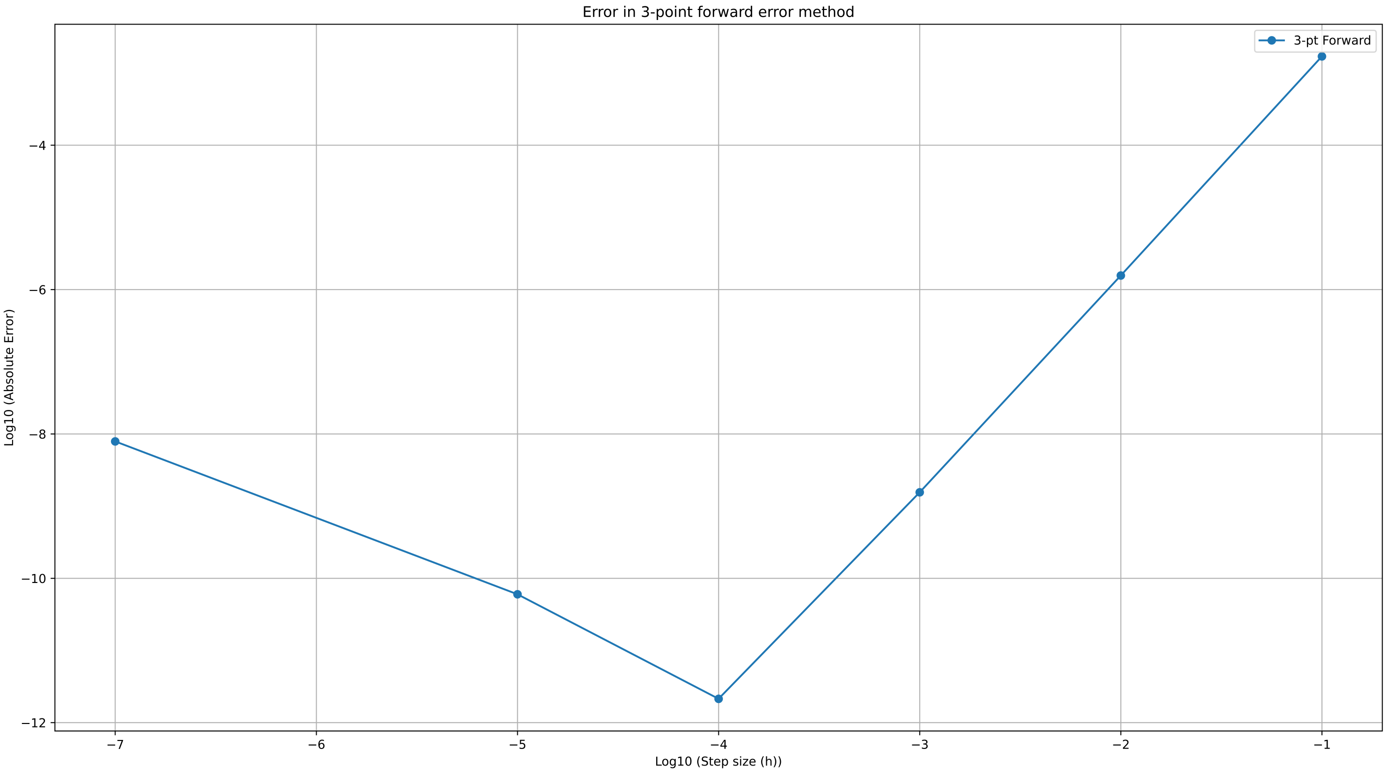
The exact value, as calculated above, is 3.1017663938.

The absolute error plot for the 3-point backward difference is as follows:



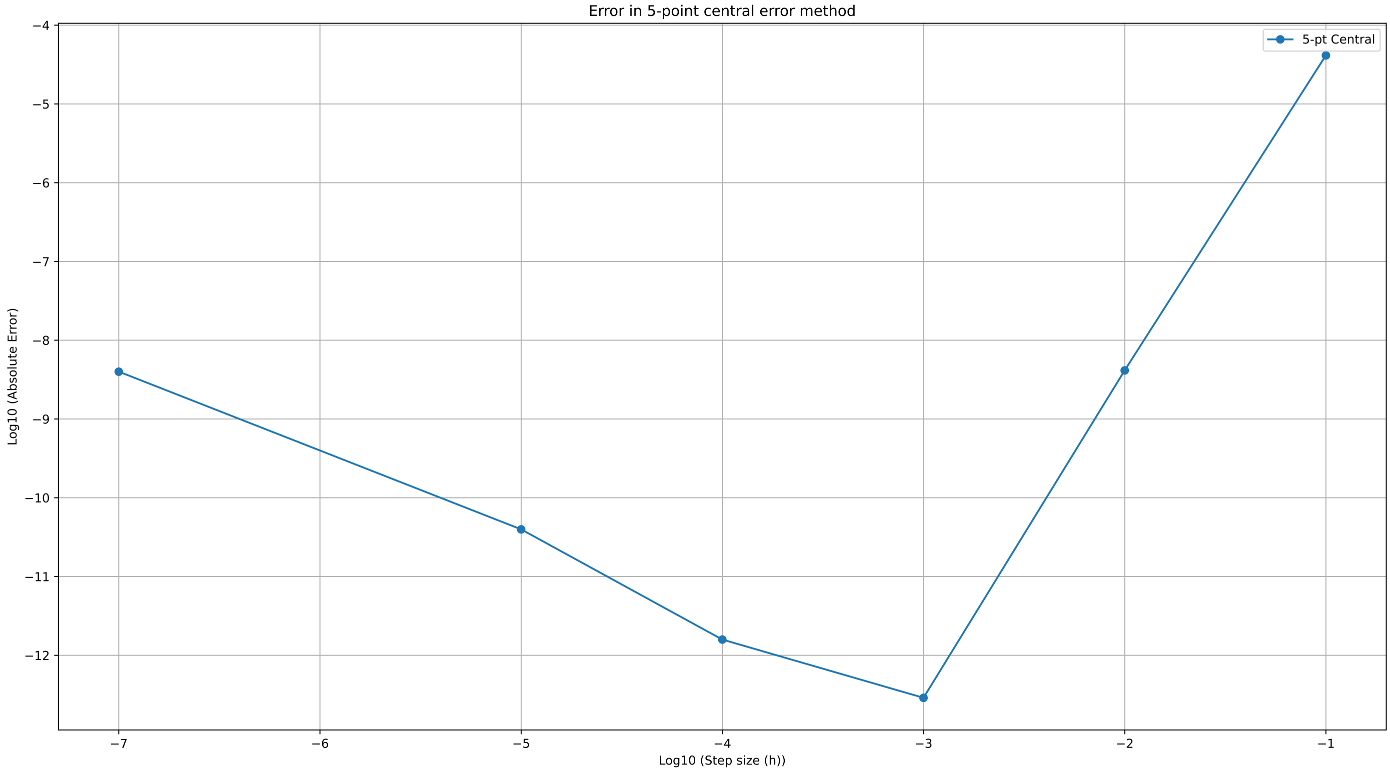

As can be seen in the plot, the optimal step size is $10^{-4}$.

The absolute error plot for the 3-point forward difference is as follows:




As can be seen in the plot, the optimal step size is $10^{-4}$.

The absolute error plot for the 5-point central difference is as follows:




As can be seen in the plot, the optimal step size is $10^{-3}$.

## Algorithm

The program steps are as follows:

1. The required variables are initialised:
   (a) $x = \frac{\pi}{4}$
   (b) step_sizes = $[10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-7}]$
2. The three point backward, three point forward and five point central derivatives are calculated using the formulae derived above.
3. The exact value of the derivative is calculated using the analytical method given above.
4. The table of results is printed
5. The errors are calculated for each method and step size.
6. Based on the above calculated error, we plot (and save) the graphs.

# Solution 4

## Theory

We are trying to find a polynomial $P(x)$ that minimises the sum of squares of errors between the values evaluated by the polynomial and the actual values. In other words, we want to minimise the error term, $E$:

$$E = \sum_{i=1}^{n} (y_i - P(x_i))^2$$

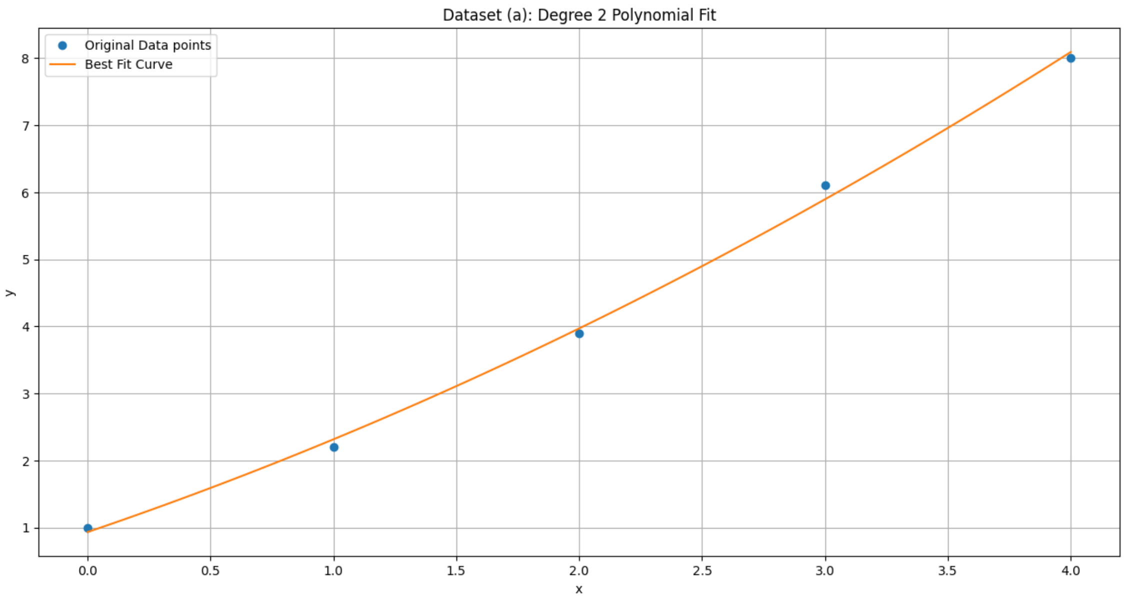
## Part (a)

The coefficients are: $0.1357$, $1.2471$, $0.9314$.

The polynomial produced using these coefficients is: $P(x) = 0.1357x^2 + 1.2471x + 0.9314$.

The mean square error is: $0.014629$.

The graph showing the best fit is as follows:




As can be seen in the graph, the best fit curve is very close to the actual data points.

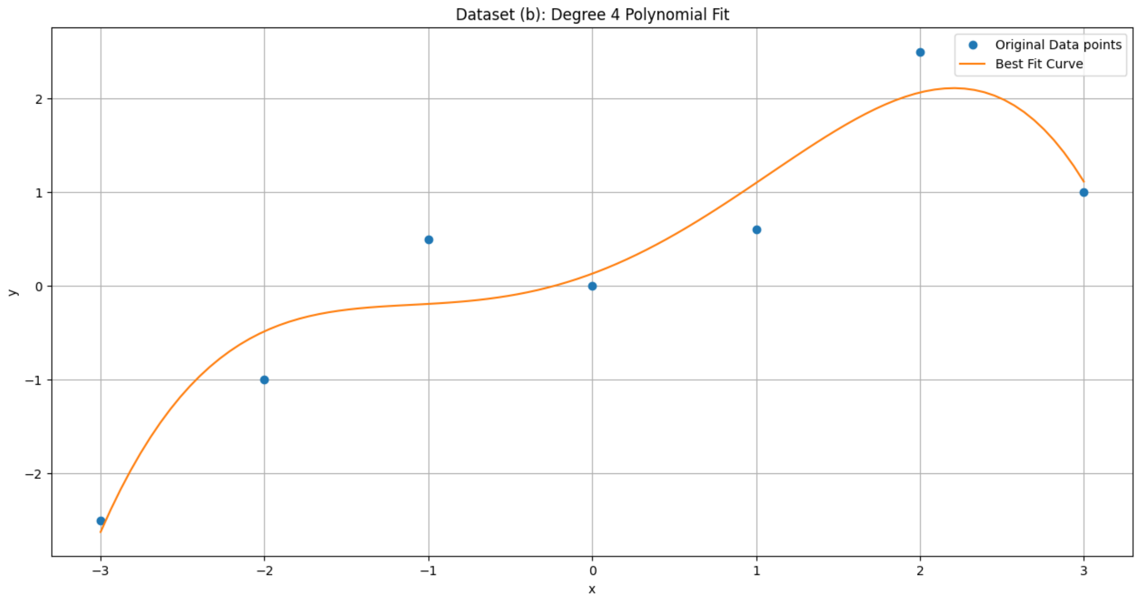
## Part (b)

The coefficients are: $-0.0527$, $-0.0028$, $0.3754$, $0.6480$, $0.1299$.

The polynomial produced using these coefficients is: $P(x) = -0.0527x^4 + -0.0028x^3 + 0.3754x^2 + 0.6480x + 0.1299$.

The mean square error is: $0.175634$.

The graph showing the best fit is as follows:




As can be seen in the graph, the best fit curve is very close to the actual data points.

## Algorithm

The program steps are as follows:

1. We first solve the question 4 (a). We initialise the points and requrired degree for best fit polynomial for this question.
2. We calculate the coefficients of the best fit polynomial using the following method:
   (a) We construct the Vandermonde matrix.
   (b) We convert the Vandermonde matrix into a system of normal equations by multiplying the transpose of the matrix.
   (c) We do the same thing on the other side of the equation for consistency.
   (d) We solve the system of normal equations using `np.linalg.solve()`.
   (e) This calculates the coefficients of the best fit line, but in ascending order. Hence, we reverse the list of coeffients before returning it.

3. We output the coefficients in descending order and the corresponding best-fit polynomial.
4. We calculated the mean square error (MSE) and output it.
5. We plot the best fit line and the original points on the same plot, for comparison.
6. We repeat steps 1-5 for question 4 (b).

| | | | |
|---|---|---|---|
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# Solution 5

## Part (a) - Derivation of Composite Trapezoidal Rule

The original trapezoidal rule is as follows:

$$\int_a^b f(x)dx \approx \frac{1}{2}(\text{width})(\text{sum of sides}) = \frac{1}{2}(b-a)(f(a)+f(b))$$

We also know that the absolute error in this method is: $\frac{h^3}{12}f''(\xi)$, where $h = b-a$.
Just like for composite Simpson's rule, we can split the Trapezoidal rule into multiple intervals. Let $h = \frac{b-a}{n}$, $x_i = a + (i \times h)$, and $x_n = a + (nh) = b$.

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx$$

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n-1} \frac{1}{2}(x_{i+1}-x_i)(f(x_i)+f(x_{i+1}))$$

$$\approx \sum_{i=0}^{n-1} \frac{h}{2}(f(x_i)+f(x_{i+1}))$$

$$\approx \frac{h}{2}\sum_{i=0}^{n-1}(f(x_i)+f(x_{i+1}))$$

$$\approx \frac{h}{2}[(f(x_0)+f(x_1)) + (f(x_1)+f(x_2)) + \cdots + (f(x_{n-1})+f(x_n))]$$

$$\approx \frac{h}{2}[f(x_0)+2f(x_1)+2f(x_2)+\cdots+2f(x_{n-1})+f(x_n)]$$

$$\approx \frac{h}{2}[f(x_0)+f(x_n)+2(f(x_1)+f(x_2)+\cdots+f(x_{n-1}))]$$

$$\approx \frac{h}{2}\left[f(x_0)+f(x_n)+2\sum_{i=1}^{n-1}f(x_i)\right]$$

| | | | |
|---|---|---|---|
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## Part (b)

The integral values are as follows:

| a \n | 10 | 50 | 500 | 3000 |
|---|---|---|---|---|
| **0.5** | 0.9213 | 0.9225 | 0.9226 | 0.9226 |
| **1.0** | 1.4887 | 1.4935 | 1.4936 | 1.4936 |
| **2.0** | 1.7623 | 1.7641 | 1.7642 | 1.7642 |
| **5.0** | 1.7726 | 1.7725 | 1.7725 | 1.7725 |

## Part (c)

The error values are as follows:

| a \n | 10 | 50 | 500 | 3000 |
|---|---|---|---|---|
| **0.5** | 0.851191 | 0.849944 | 0.849892 | 0.849892 |
| **1.0** | 0.283717 | 0.279002 | 0.278808 | 0.278806 |
| **2.0** | 0.010193 | 0.008369 | 0.008292 | 0.008291 |
| **5.0** | 0.000183 | 0.000000 | 0.000000 | 0.000000 |

## Part (d)

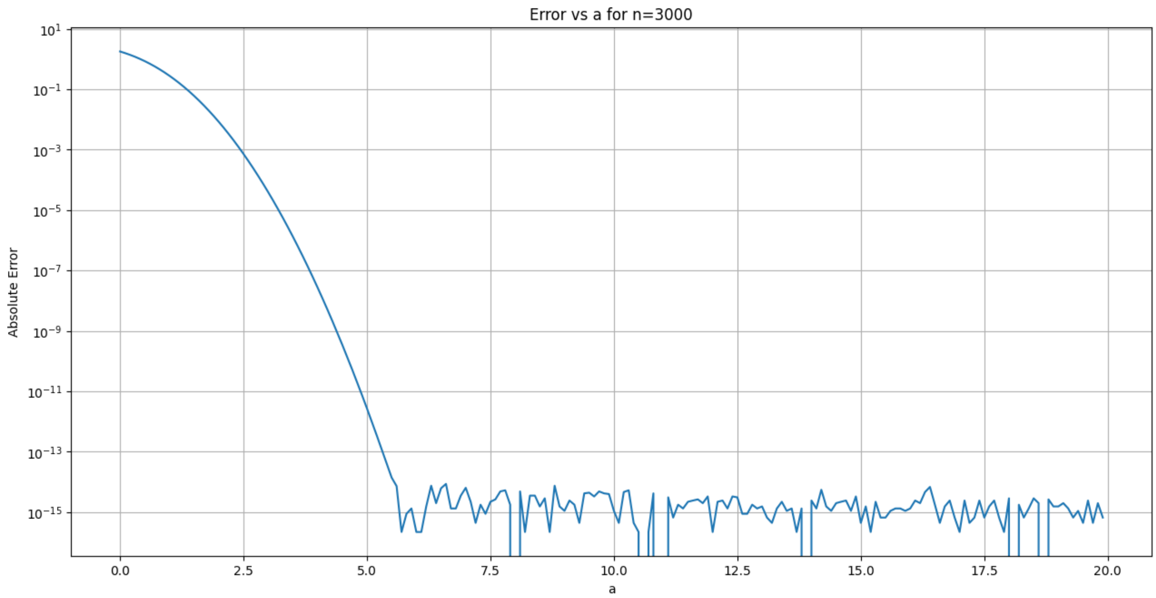
The table is as follows:

Table 1: Numerical Integration Results and Errors

| a | n | Approximate Value | Absolute Error |
|---|---|---|---|
| 0.5 | 10 | 0.9213 | 0.851191 |
| 0.5 | 50 | 0.9225 | 0.849944 |
| 0.5 | 500 | 0.9226 | 0.849892 |
| 0.5 | 3000 | 0.9226 | 0.849892 |
| 1.0 | 10 | 1.4887 | 0.283717 |
| 1.0 | 50 | 1.4935 | 0.279002 |
| 1.0 | 500 | 1.4936 | 0.278808 |
| 1.0 | 3000 | 1.4936 | 0.278806 |
| 2.0 | 10 | 1.7623 | 0.010193 |
| 2.0 | 50 | 1.7641 | 0.008369 |
| 2.0 | 500 | 1.7642 | 0.008292 |
| 2.0 | 3000 | 1.7642 | 0.008291 |
| 5.0 | 10 | 1.7726 | 0.000183 |
| 5.0 | 50 | 1.7725 | 0.000000 |
| 5.0 | 500 | 1.7725 | 0.000000 |
| 5.0 | 3000 | 1.7725 | 0.000000 |

## Part (e)

The graph is as follows:




We can see from the graph that the absolute error decreases from $a = 0.0$ to $a \approx 5.5$ After this, the value of the error is fluctuating, albeit always in the order of $10^{-14}$. This is due to the floating point calculation errors.

Hence, to obtain an accurate value of the integration, it is best to use a relatively small value of $a$. This ensures that the floating point errors are kept in control.

## Algorithm

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**Course Code:** DS288/UMC202
**Course Name:** Numerical Methods
**Term:** AUG 2025

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[2] Lecture Notes

[3] Strang, G. (2006). Linear Algebra and Its Applications. Thomson, Brooks/Cole.