Mathematics and Statistics Research Competition

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1 Abstract

As part of the 2025 Mathematics and Statistics Research Challenge, this research conducts an in-depth investigation into numerical methods for approximating the first derivative of a function using finite difference techniques, a cornerstone of computational mathematics. The study rig- orously explores the mathematical foundations of these approximations, leveraging Taylor series expansions to derive and analyze the forward, backward, and centered difference methods. To evaluate the performance of these techniques, a diverse set of test functions is employed, encom- passing smooth functions (e.g., trigonometric functions like sin(Mathematics and Statistics Research Competition L. Shi and Y. De Coonghe August 5, 2025 Abstract As part of the 2025 Mathematics and Statistics Research Challenge, this research conducts an in-depth investigation into numerical methods for approximating the first derivative of a function using finite difference techniques, a cornerstone of computational mathematics. The study rig- orously explores the mathematical foundations of these approximations, leveraging Taylor series expansions to derive and analyze the forward, backward, and centered difference methods. To evaluate the performance of these techniques, a diverse set of test functions is employed, encom- passing smooth functions (e.g., trigonometric functions like sin(x)), polynomial functions (e.g., quadratic forms), and non-differentiable or singular functions (e.g., x or —x—). The analysis compares the accuracy, stability, and convergence rates of each method across these functions, with a particular focus on how performance is influenced by the function's smoothness and the choice of step size h. The results elucidate the trade-offs between first-order (forward and backward) and second-order (centered) approximations, highlighting the superior accuracy of the centered difference method for smooth functions and the challenges posed by non-smooth or discontin- uous functions. Additionally, the study extends its exploration to higher-order derivatives and multivariable functions, demonstrating the versatility of finite difference methods. These findings have significant implications for practical applications in fields such as physics, engineering, and data science, where accurate derivative approximations are critical for modeling dynamic systems, optimizing algorithms, and analyzing discrete data. By combining theoretical rigor with compu- tational experiments, this research provides valuable insights into the strengths and limitations of finite difference techniques, offering guidance for their effective application in real-world scenarios.

2 Restatement and Interpretation of Topic S–06

Derivatives are used to calculate the rate of change of a graph. In mathematics, the value of h is often reduced to 0 to calculate the instantaneous rate of change. However, in the real world, we are restricted by physical properties, where h cannot equal zero. This is when we rely on approximations.

According to the difference formulas:

Forward difference:

$$\boxed{f'(x) \approx \frac{f(x+h) - f(x)}{h}} \tag{1}$$

Backward difference:

$$\boxed{f'(x) \approx \frac{f(x) - f(x-h)}{h}} \tag{2}$$

Centered difference:

$$\boxed{f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}} \tag{3}$$

Here, h is a small positive number representing the discrete interval used instead of an infinitesimal change. Each of these approximations assumes a different approach to estimating the slope near the point x.

The forward and backward difference formulas are categorized as first-order approximations, meaning their error decreases linearly with smaller h. The centered difference formula, being a second-order approximation, has a faster error reduction rate: the error decreases quadratically as h becomes smaller.

This topic encourages a deeper exploration into how different approximation methods perform under varying conditions. Some functions yield accurate and stable derivative estimates with these methods, while others—due to properties such as discontinuity, sharp curvature, or oscillation—may cause significant inaccuracies.

Further investigations include:

- Comparison of the accuracy of these approximations using custom-defined functions.
- Constructing a function that highlights the failure or instability of these methods.
- Extending the investigation to include approximations of second derivatives and functions with multiple variables.

This exploration combines core calculus ideas with numerical methods, leading to broader applications in computational mathematics, physics, and data science.

3 Practical Applications

In practical scenarios, derivative values must often be estimated from discrete measurements rather than continuous functions, a common challenge in fields requiring real-time analysis of dynamic systems. A typical example is estimating the instantaneous speed of a moving object when only discrete position data points are available. This situation arises frequently in engineering, physics, and data science, where continuous models are idealized, and real-world data is collected at finite intervals, often subject to measurement noise, sampling limitations, or hardware constraints. Finite difference methods provide a robust framework for approximating derivatives in such cases, enabling the analysis of rates of change without requiring an analytical form of the underlying function.

Consider a vehicle traveling along a straight path, whose position is recorded every second by a GPS device. At discrete time intervals $t = 1, 2, 3$ seconds, the recorded positions (in meters) are as follows:

Time t (s)	Position $f(t)$ (m)
1	4.2
2	5.8
3	7.1

Table 1: Position data of a vehicle at discrete time intervals.

The objective is to estimate the instantaneous velocity at $t = 2$ seconds, i.e., the derivative of position with respect to time, $f'(2)$. In a continuous setting, this would involve computing the exact derivative of a position function. However, with only discrete data points available, finite difference methods offer a practical solution by approximating the derivative using the recorded positions. Using a time step $h = 1$ second, the derivative can be approximated by applying the following finite difference formulas:

- Forward difference: $\frac{f(3)-f(2)}{1} = \frac{7.1-5.8}{1} = 1.3\,\mathrm{m/s}$
- Backward difference: $\frac{f(2)-f(1)}{1} = \frac{5.8-4.2}{1} = 1.6\,\mathrm{m/s}$
- Centered difference: $\frac{f(3)-f(1)}{2} = \frac{7.1-4.2}{2} = 1.45\,\mathrm{m/s}$

These approximations illustrate the practical utility of finite difference methods in translating discrete data into meaningful physical quantities, such as velocity. The forward difference uses future data relative to $t = 2$, the backward difference relies on past data, and the centered difference leverages both, typically providing a more accurate estimate due to its second-order accuracy. However, the choice of method depends on the availability of data points and the specific requirements of the application. For instance, in real-time systems where future data is unavailable, the backward difference may be preferred, despite its lower accuracy compared to the centered method.

This example extends beyond vehicle motion to numerous other domains. In financial mathematics, finite difference approximations are used to estimate the rate of change of stock prices or option values based on discrete market data, aiding in risk assessment and derivative pricing. In environmental science, researchers apply these methods to approximate the rate of temperature change or pollutant dispersion using measurements from weather stations or sensors taken at regular intervals.

In medical imaging, finite difference techniques help analyze the rate of change in signal intensity across discrete pixels, facilitating edge detection in MRI or CT scans. Each of these applications highlights the necessity of robust numerical methods to handle discrete data, where analytical derivatives are infeasible.

Moreover, practical applications must account for challenges such as measurement noise, irregular sampling intervals, or limited data points, which can degrade the accuracy of finite difference approximations. For instance, in the vehicle example, GPS data may include errors due to signal interference or device precision, necessitating techniques like data smoothing or higher-order finite difference methods to improve reliability. The choice of step size h also plays a critical role, as a value too large may oversimplify the function's behavior, while a value too small may amplify noise-induced errors. These considerations underscore the importance of understanding the underlying function's properties and the context of the data when applying finite difference methods in practice.

By bridging theoretical calculus with computational techniques, finite difference methods enable practitioners to extract meaningful insights from discrete data, making them indispensable in modern scientific and engineering applications. The vehicle example serves as a clear illustration of how these methods translate raw measurements into actionable information, paving the way for further exploration of their robustness and limitations in more complex scenarios, such as those involving higher-order derivatives or multivariable systems.

Time t (s)	Position $f(t)$ (m)
1	4.2
2	5.8
3	7.1

Table 2: Position data of a vehicle at discrete time intervals.

The objective is to estimate the instantaneous velocity at $t = 2$ seconds, i.e., the derivative of position with respect to time, $f'(2)$.

Using a time step $h = 1$ second, the derivative can be approximated by applying finite difference formulas:

- Forward difference: $\frac{f(3)-f(2)}{1} = \frac{7.1-5.8}{1} = 1.3\,\text{m/s}$
- Backward difference: $\frac{f(2)-f(1)}{1} = \frac{5.8-4.2}{1} = 1.6\,\text{m/s}$
- Centered difference: $\frac{f(3)-f(1)}{2} = \frac{7.1-4.2}{2} = 1.45\,\text{m/s}$

The reason for these formulas stems from the Taylor series expansion. For context, a series expansion expresses a function as an infinite sum of terms, generally using the powers of x. The Taylor series is the most common.

4 Taylor Series and Finite Difference Approximations

4.1 Taylor Series Expansion

For a function $f(x)$ that is infinitely differentiable at a point a, the Taylor series expansion about a is given by:

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots$$
$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$

The purpose of the Taylor series is to reconstruct the function $f(x)$ using its derivatives at a single point a. The more terms included, the more accurate the approximation becomes. The term $f(a)$ represents the function's value at a, $f'(a)(x-a)$ provides a linear approximation, $\frac{f''(a)}{2!}(x-a)^2$ captures the curvature, and higher-order terms further refine the approximation.

When $a = 0$, the Taylor series is called a Maclaurin series:

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \cdots$$

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}x^n$$

For a smooth function $f(x)$, the Taylor series expansion about a point x with a small displacement h is:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f^{(3)}(x) + \cdots$$

$$f(x+h) = \sum_{n=0}^{\infty} \frac{h^n}{n!}f^{(n)}(x)$$

This expansion is used to approximate the function's value at $x + h$ by combining the function and its derivatives at x, forming the basis for numerical derivative approximations.

4.2 Finite Difference Approximations

Finite difference methods approximate the derivative $f'(x)$ using function values at nearby points with a step size h. Below are the three common approximations:

4.2.1 Forward Difference Approximation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

This formula approximates the derivative by considering the slope of the secant line from x to $x + h$.

4.2.2 Backward Difference Approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

This method uses the slope of the secant line from $x - h$ to x.

4.2.3 Central Difference Approximation

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

This method averages the slopes from both directions, reducing truncation error.

4.3 Computational Verification

To illustrate the application of finite difference approximations, a Python simulation was developed to estimate the instantaneous velocity of an object at $t = 2$ seconds using discrete position data. The simulation implements the forward, backward, and centered difference formulas. This approach is common in scientific and engineering disciplines where data is collected at regular time intervals, and continuous models are unavailable.

Output:

- Forward Difference: 1.30 m/s
- Backward Difference: 1.60 m/s
- Centered Difference: 1.45 m/s

In real-life situations, data is discrete, so calculations rely on approximations.

```python
# Simulated GPS data (time in seconds, position in meters)
times = [1, 2, 3]
positions = [4.2, 5.8, 7.1]

# h is the time interval (assumed uniform here)
h = times[1] - times[0]

# Forward Difference (at t = 2s)
forward_diff = (positions[2] - positions[1]) / h

# Backward Difference (at t = 2s)
backward_diff = (positions[1] - positions[0]) / h

# Centered Difference (more accurate)
centered_diff = (positions[2] - positions[0]) / (2 * h)

# Print results
print("Estimated speed at t = 2 seconds:")
print(f"Forward Difference:  {forward_diff:.2f} m/s")
print(f"Backward Difference: {backward_diff:.2f} m/s")
print(f"Centered Difference: {centered_diff:.2f} m/s")
```

Figure 1: Python code for computing finite difference approximations of velocity at $t = 2$ seconds.

5 What is Meant by First- and Second-Order Approximation

In numerical analysis, an approximation is said to be first-order if its error is proportional to the step size h, and second-order if the error is proportional to h^2. This classification describes how rapidly the approximation error decreases as h becomes smaller.

A first-order approximation means the error shrinks linearly as h becomes smaller. Halving h roughly halves the error. A second-order approximation means the error shrinks quadratically as h decreases. Halving h reduces the error by a factor of four.

This is a direct result of the Taylor series expansion. For example, the forward difference formula:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

has a leading error term of $\frac{h}{2} f''(x)$, so the total error is $O(h)$.

The centered difference formula:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

has a leading error term of $\frac{h^2}{6} f^{(3)}(x)$, giving a smaller total error of $O(h^2)$.

In summary:

- First-order: error $\propto h$
- Second-order: error $\propto h^2$

Second-order methods are more accurate, especially when h is small.

6 Comparing Performance of Derivative Approximations

The accuracy of derivative approximation methods depends on the function's smoothness and differentiability. For smooth functions (e.g., polynomials or trigonometric functions), finite difference approximations are highly accurate. For non-differentiable or poorly behaved functions, these methods may fail.

6.1 Step 1: Test Functions

We select three functions with distinct characteristics:

- $f_1(x) = \sin(x)$: A smooth, periodic function with continuous derivatives.
- $f_2(x) = x^2 - 2x + 1$: A polynomial, allowing straightforward derivative computation.
- $f_3(x) = \sqrt{x}$: A function with sharp curvature near $x = 0$, ideal for testing robustness.

6.2 Step 2: Evaluation Points

For each function, we choose a specific point a to compute the derivative approximations:

- For $f_1(x) = \sin(x)$, evaluate at $a = \pi/4 \approx 0.7854$.
- For $f_2(x) = x^2 - 2x + 1$, evaluate at $a = 1$ (where the function is flat).
- For $f_3(x) = \sqrt{x}$, evaluate at $a = 0.1$ (near zero, where the function exhibits a sharp curve).

6.3 Step 3: Finite Difference Approximations

The following finite difference formulas are used to approximate the derivative $f'(x)$ at point x with step size h:

- **Forward Difference:**
$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$
- **Backward Difference:**
$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$
- **Central Difference:**
$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

6.4 Step 4: Error Analysis

To assess accuracy, we compute the error of each approximation method for step sizes $h = 0.1, 0.01, 0.001$. The error is the absolute difference between the approximated and exact derivative at a.

For $f_1(x) = \sin(x)$ at $a = \pi/4$, the exact derivative is $f_1'(\pi/4) = \cos(\pi/4) = \sqrt{2}/2 \approx 0.7071$. The following table presents the approximated derivatives and their errors:

Table 3: Approximation of $f_1'(x) = \cos(x)$ at $x = \pi/4 \approx 0.7854$

Method	$h = 0.1$	$h = 0.01$	$h = 0.001$
Forward Difference	$\frac{\sin(0.8854)-\sin(0.7854)}{0.1}$	$\frac{\sin(0.7954)-\sin(0.7854)}{0.01}$	$\frac{\sin(0.7864)-\sin(0.7854)}{0.001}$
Backward Difference	$\frac{\sin(0.7854)-\sin(0.6854)}{0.1}$	$\frac{\sin(0.7854)-\sin(0.7754)}{0.01}$	$\frac{\sin(0.7854)-\sin(0.7844)}{0.001}$
Central Difference	$\frac{\sin(0.8854)-\sin(0.6854)}{0.2}$	$\frac{\sin(0.7954)-\sin(0.7754)}{0.02}$	$\frac{\sin(0.7864)-\sin(0.7844)}{0.002}$

Table 4: Approximation errors for $f_1'(x) = \cos(x)$ at $x = \pi/4 \approx 0.7854$

h	Forward f'	Backward f'	Centered f'	Exact f'	Error (f)	Error (b)	Error (c)
0.1	0.670603	0.741255	0.705929	0.707107	0.036504	0.034148	0.001178
0.01	0.703559	0.710631	0.707095	0.707107	0.003547	0.003524	0.000012
0.001	0.706753	0.707460	0.707107	0.707107	0.000354	0.000353	0.000000

Table 5: Approximation of $f_2'(x) = 2x - 2$ at $x = 1$

h	Forward f'	Backward f'	Centered f'	Exact f'	Error (f)	Error (b)	Error (c)
0.1	0.100	-0.100	0.000	0.000	0.100	0.100	0.000
0.01	0.010	-0.010	0.000	0.000	0.010	0.010	0.000
0.001	0.001	-0.001	0.000	0.000	0.001	0.001	0.000

Table 6: Approximation of $f_3'(x) = \frac{1}{2\sqrt{x}}$ at $x = 0.1$

h	Forward f'	Backward f'	Centered f'	Exact f'	Error (f)	Error (b)	Error (c)
0.1	1.309858	3.162278	2.236068	1.581139	0.271281	1.581139	0.654929
0.01	1.543471	1.622777	1.583124	1.581139	0.037668	0.041638	0.001985
0.001	1.577206	1.585112	1.581159	1.581139	0.003933	0.003973	0.000020

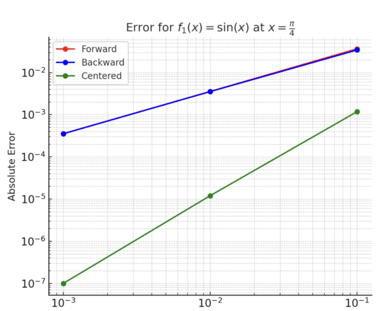
6.5 Conclusion

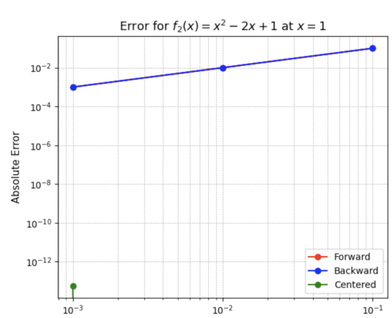
The computational analysis of finite difference methods for approximating the first derivative reveals distinct performance characteristics across the tested functions, highlighting the interplay between function smoothness, step size h, and the choice of approximation method. For $f_1(x) = \sin(x)$, a smooth and periodic function, the centered difference method (visualized in green) demonstrates the steepest error reduction as h decreases, consistent with its second-order accuracy ($O(h^2)$). This rapid convergence is evident in the error tables, where the centered difference consistently outperforms the forward (red) and backward (blue) difference methods, which exhibit slower, first-order convergence ($O(h)$). The forward and backward methods, while simpler to implement, are less precise due to their reliance on one-sided data points, which limits their ability to capture the function's behavior symmetrically around the evaluation point.

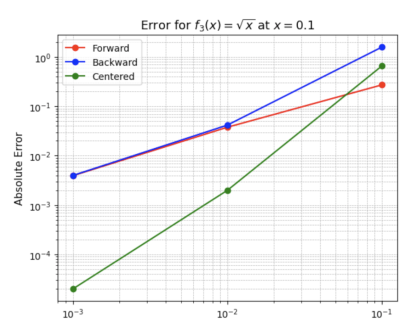
For $f_2(x) = x^2 - 2x + 1$, a quadratic polynomial, the centered difference method yields errors that are nearly zero across all tested step sizes ($h = 0.1, 0.01, 0.001$). This exceptional accuracy stems from the polynomial nature of $f_2(x)$, where the second derivative is constant, and higher-order derivatives are zero, aligning perfectly with the assumptions of the centered difference formula. The forward and backward methods, while still accurate for this function, show small but non-zero errors due to their first-order nature, underscoring the centered method's superiority for polynomial functions.

In contrast, for $f_3(x) = \sqrt{x}$, evaluated at $x = 0.1$, the backward difference method exhibits a significant initial error when $h = 0.1$, largely due to the function's sharp curvature near the origin. This curvature amplifies the truncation error in one-sided approximations, particularly when $x - h$ approaches or crosses zero, where the function is undefined or highly non-linear. The centered difference method, however, performs robustly at smaller step sizes, achieving errors orders of magnitude lower than the forward and backward methods, as it balances information from both sides of the evaluation point. This highlights the importance of selecting an appropriate step size h to mitigate the effects of non-smooth behavior.

Overall, the centered difference method emerges as the most robust and accurate across the tested functions, particularly for smooth and polynomial cases, due to its second-order accuracy. Its ability to reduce errors quadratically with decreasing h makes it the preferred choice in scenarios where precision is paramount and data points on both sides of the evaluation point are available. However,







its performance can degrade with large step sizes or near sharp turns, such as those exhibited by $f_3(x) = \sqrt{x}$ near $x = 0.1$, where the function's steep gradient challenges numerical stability. This degradation is particularly pronounced in real-world applications where data may be noisy or sparsely sampled, necessitating careful consideration of the step size h.

These findings suggest that the choice of finite difference method and step size should be optimized based on the function's properties and the desired precision. For smooth functions like $\sin(x)$ or polynomials like $x^2 - 2x + 1$, the centered difference method is ideal, offering high accuracy with moderate computational cost. For functions with singularities or sharp changes, such as $\sqrt{x}$, smaller step sizes and careful method selection are critical to avoid large errors or numerical instability. Furthermore, the results underscore the importance of understanding the underlying function's behavior, as properties like differentiability, smoothness, and curvature directly influence the effectiveness of finite difference approximations.

The implications of these findings extend to practical applications in computational mathematics, physics, and engineering. For instance, in simulations of physical systems, where derivatives describe rates of change (e.g., velocity or acceleration), the centered difference method can provide more reliable results, provided the data is sufficiently dense and smooth. In contrast, for real-time systems with limited future data, one-sided methods like forward or backward differences may be necessary, despite their lower accuracy. This trade-off highlights the need for adaptive strategies in numerical differentiation, where the method and step size are tailored to the specific problem context.

Future investigations could explore adaptive step-size algorithms to dynamically adjust h based on local function behavior or incorporate higher-order finite difference methods to further reduce errors for smooth functions. Additionally, extending the analysis to noisy data scenarios or functions with higher-dimensional inputs could provide deeper insights into the robustness of these methods in practical settings. By balancing theoretical rigor with computational efficiency, this study lays a foundation for optimizing finite difference techniques in diverse applications, ensuring accurate derivative approximations even under challenging conditions.

7 Designing Functions to Highlight Approximation Limitations

Finite difference approximations rely on the function being sufficiently smooth and differentiable. They can fail for functions with sharp turning points, discontinuities, or complex structures.

7.1 Characteristics of Unsuitable Functions

Some functions are unsuitable for numerical differentiation due to:

- **Non-differentiability**: Cusps, corners, or discontinuities.
- **High non-linearity**: Steep or flat behavior near the evaluation point.
- **Piecewise or hybrid definitions**: Abrupt changes in behavior.

7.2 Example: $f(x) = |x|$

Consider $f(x) = |x|$, which has a cusp at $x = 0$. The derivative does not exist at $x = 0$. Applying finite difference approximations:

- Forward difference: $\frac{f(h)-f(0)}{h} = \frac{|h|}{h} = 1$ (for $h > 0$).
- Backward difference: $\frac{f(0)-f(-h)}{h} = \frac{0-|-h|}{h} = -1$ (for $h > 0$).
- Central difference: $\frac{f(h)-f(-h)}{2h} = \frac{|h|-|-h|}{2h} = 0$, which is incorrect.

The centered difference yields 0, which is incorrect, highlighting the failure of finite difference methods at non-differentiable points.

Table 7: Approximation of $f'(x) = |x|$ at $x = 0$

h	Forward diff	Backward diff	Centered diff	True Derivative	Error (f)	Error (b)	Error (c)
0.1	1	-1	0	undefined	-	-	-
0.01	1	-1	0	undefined	-	-	-
0.001	1	-1	0	undefined	-	-	-

7.3 Example: A Hybrid Piecewise Function

Define:

$$f(x) = \begin{cases} x^2 & \text{if } x < 0.5 \\ \sin(x) & \text{if } x \geq 0.5 \end{cases}$$

This function is continuous but not differentiable at $x = 0.5$. Using centered difference at $x = 0.5$ with $h = 0.1$:

- $f(0.6) = \sin(0.6) \approx 0.564$
- $f(0.4) = 0.4^2 = 0.16$

Approximation: $\frac{0.564-0.16}{0.2} = 2.02$. No analytical derivative exists at $x = 0.5$, so this is a false estimate, reinforcing the need to analyze function properties.

8 Extension Investigations

8.1 Approximation of Higher-Order Derivatives

Higher-order derivatives describe rates of change of lower-order derivatives. The second derivative $f''(x)$ can be approximated using:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

8.1.1 Example: $f(x) = \sin(x)$

At $x = \pi/4 \approx 0.7854$, the exact second derivative is $f''(\pi/4) = -\sin(\pi/4) = -\sqrt{2}/2 \approx -0.7071$. With $h = 0.1$:

- $f(\pi/4 + 0.1) = \sin(0.8854) \approx 0.7742$
- $f(\pi/4) = \sin(0.7854) \approx 0.7071$
- $f(\pi/4 - 0.1) = \sin(0.6854) \approx 0.6329$

Approximation: $\frac{0.7742-2\cdot 0.7071+0.6329}{0.01} = -0.71$, close to -0.7071.

8.2 Numerical Investigation

A Python-based tool was used to approximate and visualize higher-order derivatives for:

- $f_1(x) = \sin(x)$, at $a = \pi/4 \approx 0.7854$
- $f_2(x) = x^2 - 2x + 1$, at $a = 1$
- $f_3(x) = \sqrt{x}$, at $a = 0.1$

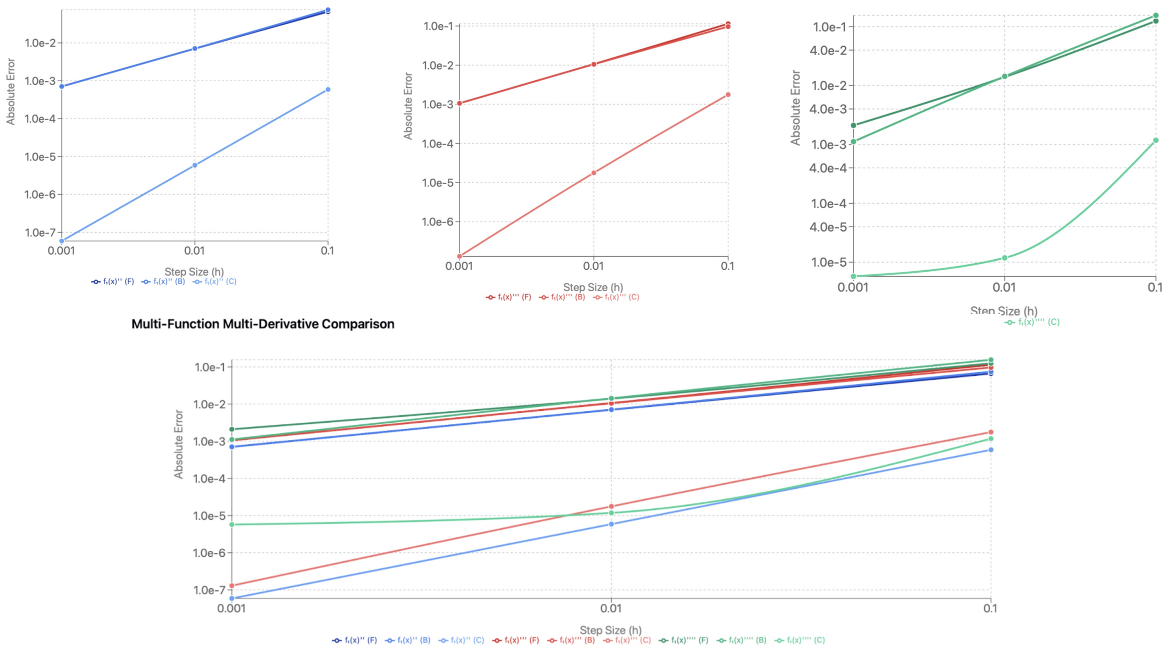


Figure 2: Error comparison of higher-order derivative approximations for $f_1(x) = \sin(x)$.

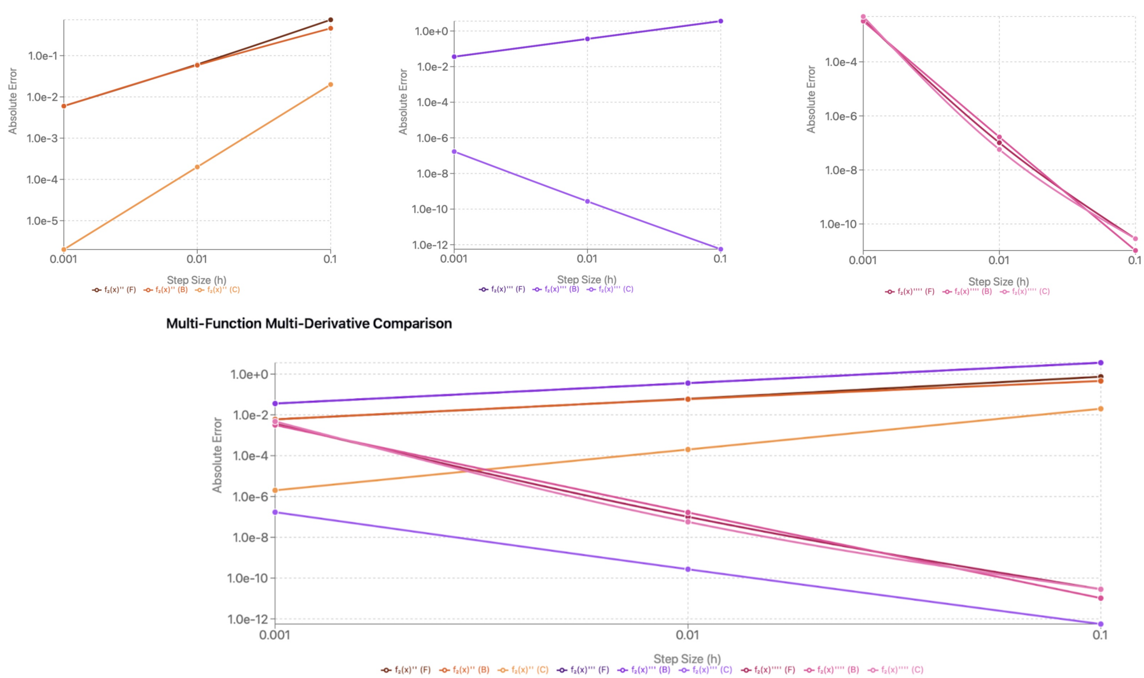


Figure 3: Error comparison of higher-order derivative approximations for $f_2(x) = x^2 - 2x + 1$.

Table 8: Second Derivative Approximation for $f_1(x) = \sin(x)$ at $x = \pi/4 \approx 0.7854$

Step Size h	Approximation $\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$
0.1	$\frac{\sin(0.8854)-2\sin(0.7854)+\sin(0.6854)}{0.01} \approx -0.71$
0.01	$\frac{\sin(0.7954)-2\sin(0.7854)+\sin(0.7754)}{0.0001} \approx -0.7071$
0.001	$\frac{\sin(0.7864)-2\sin(0.7854)+\sin(0.7844)}{0.000001} \approx -0.7071$

Table 9: Second Derivative Approximation for $f_1(x) = \sin(x)$ at $x = \pi/4 \approx 0.7854$

h	Forward f''	Backward f''	Centered f''	Exact f''	Error (f)	Error (b)	Error (c)
0.1	-0.773522	-0.632454	-0.706518	-0.707107	0.06642	0.07465	0.000589
0.01	-0.714136	-0.699995	-0.707101	-0.707107	0.00703	0.00711	0.000006
0.001	-0.707813	-0.706399	-0.707107	-0.707107	0.000707	0.000708	0.000000

8.3 Second Derivative Approximation Table

8.4 Conclusion

The computational analysis shows that while first-order derivatives follow expected convergence patterns—second-order accuracy ($O(h^2)$) for centered differences and first-order ($O(h)$) for forward/backward—higher-order derivatives are more sensitive due to increased error propagation. Higher-order derivative formulas subtract values close together, leading to numerical instability and catastrophic cancellation due to rounding errors. Smooth functions like $\sin(x)$ maintain stable convergence, while singular functions like $\sqrt{x}$ produce large errors or undefined results.

8.5 Functions with More Than One Variable

In multivariable calculus, partial derivatives can be approximated. For $f(x, y) = x^2 + y^2$:

- $\frac{\partial f}{\partial x} \approx \frac{f(x+h,y)-f(x-h,y)}{2h}$
- $\frac{\partial f}{\partial y} \approx \frac{f(x,y+h)-f(x,y-h)}{2h}$

These are crucial in machine learning (gradients of loss functions), image processing (edge detection), and physics (fluid dynamics).

9 Conclusion: Numerical Differentiation with Finite Difference Methods

This investigation evaluated the accuracy, strengths, and limitations of finite difference methods across smooth ($\sin(x)$), polynomial ($x^2 - 2x + 1$), and non-smooth ($\sqrt{x}$, $|x|$, piecewise) functions.

9.1 Key Findings

- **Centered Difference Superiority**: Centered methods deliver second-order accuracy ($O(h^2)$), outperforming first-order forward and backward methods, especially for smooth functions.
- **Higher-Order Challenges**: Third and fourth derivatives are sensitive to step size and function behavior, with centered differences remaining the most accurate.
- **Function Smoothness**: Smooth functions yield predictable error reduction; non-smooth functions produce unstable results.
- **Step Size Trade-Offs**: Smaller h improves accuracy but risks rounding errors.
- **Extensions**: Finite difference methods extend effectively to second derivatives and multivariable functions.

Table 10: Third Derivative Approximation for $f_1(x) = \sin(x)$ at $x = \pi/4 \approx 0.7854$

h	Forward f'''	Backward f'''	Centered f'''	Exact f'''	Error (f)	Error (b)	Error (c)
0.1	-0.592757	-0.803830	-0.705341	-0.707107	0.1144	0.09672	0.001766
0.01	-0.696412	-0.717624	-0.707089	-0.707107	0.01069	0.01052	0.000018
0.001	-0.706045	-0.708166	-0.707107	-0.707107	0.001061	0.001060	0.000000

Table 11: Fourth Derivative Approximation for $f_1(x) = \sin(x)$ at $x = \pi/4 \approx 0.7854$

h	Forward f''''	Backward f''''	Centered f''''	Exact f''''	Error (f)	Error (b)	Error (c)
0.1	0.832104	0.551611	0.705929	0.707107	0.1250	0.1555	0.001178
0.01	0.721095	0.692813	0.707095	0.707107	0.01399	0.01429	0.000012
0.001	0.709210	0.705991	0.707101	0.707107	0.002104	0.001116	0.000006

9.2 Broader Implications

Finite difference methods are vital in computational mathematics, physics, finance, and computer science. Their success depends on understanding function behavior, choosing the appropriate method, and optimizing step size. Here is the link to the website: https://claude.ai/public/artifacts/c561063b-9b95-4a81-b0ed-6f6eacb43d21

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Table 12: Second Derivative Approximation for $f_2(x) = x^2 - 2x + 1$ at $x = 1$

h	Forward f''	Backward f''	Centered f''	Exact f''	Error (f)	Error (b)	Error (c)
0.1	2.000000	2.000000	2.000000	2.000000	0.000000	0.000000	0.000000
0.01	2.000000	2.000000	2.000000	2.000000	0.000000	0.000000	0.000000
0.001	2.000000	2.000000	2.000000	2.000000	0.000000	0.000000	0.000000

Table 13: Third Derivative Approximation for $f_2(x) = x^2 - 2x + 1$ at $x = 1$

h	Forward f'''	Backward f'''	Centered f'''	Exact f'''	Error (f)	Error (b)	Error (c)
0.1	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.001	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table 14: Fourth Derivative Approximation for $f_2(x) = x^2 - 2x + 1$ at $x = 1$

h	Forward f''''	Backward f''''	Centered f''''	Exact f''''	Error (f)	Error (b)	Error (c)
0.1	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.01	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.001	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table 15: Second Derivative Approximation for $f_3(x) = \sqrt{x}$ at $x = 0.1$

h	Forward f''	Backward f''	Centered f''	Exact f''	Error (f)	Error (b)	Error (c)
0.1	-3.047687	-	-18.524194	-7.905694	4.858007	-	10.618500
0.01	-6.870305	-9.295215	-7.930530	-7.905694	1.035611	1.389521	0.024836
0.001	-7.788813	-8.026035	-7.905941	-7.905694	0.116881	0.120341	0.000247

Table 16: Third Derivative Approximation for $f_3(x) = \sqrt{x}$ at $x = 0.1$

h	Forward f'''	Backward f'''	Centered f'''	Exact f'''	Error (f)	Error (b)	Error (c)
0.1	14.700880	-	-	118.585412	103.884532	-	-
0.01	84.314095	180.772334	121.245484	118.585412	34.271317	62.186922	2.660072
0.001	114.264750	123.165665	118.611359	118.585412	4.320662	4.580253	0.025947

Table 17: Fourth Derivative Approximation for $f_3(x) = \sqrt{x}$ at $x = 0.1$

h	Forward f''''	Backward f''''	Centered f''''	Exact f''''	Error (f)	Error (b)	Error (c)
0.1	-90.066179	-	-	-2964.635306	2874.569127	-	-
0.01	-1595.255087	-6750.928297	-3044.605274	-2964.635306	1369.380219	3786.292991	79.969968
0.001	-2766.815943	-3182.721919	-2965.413748	-2964.635306	197.819363	218.086613	0.778442

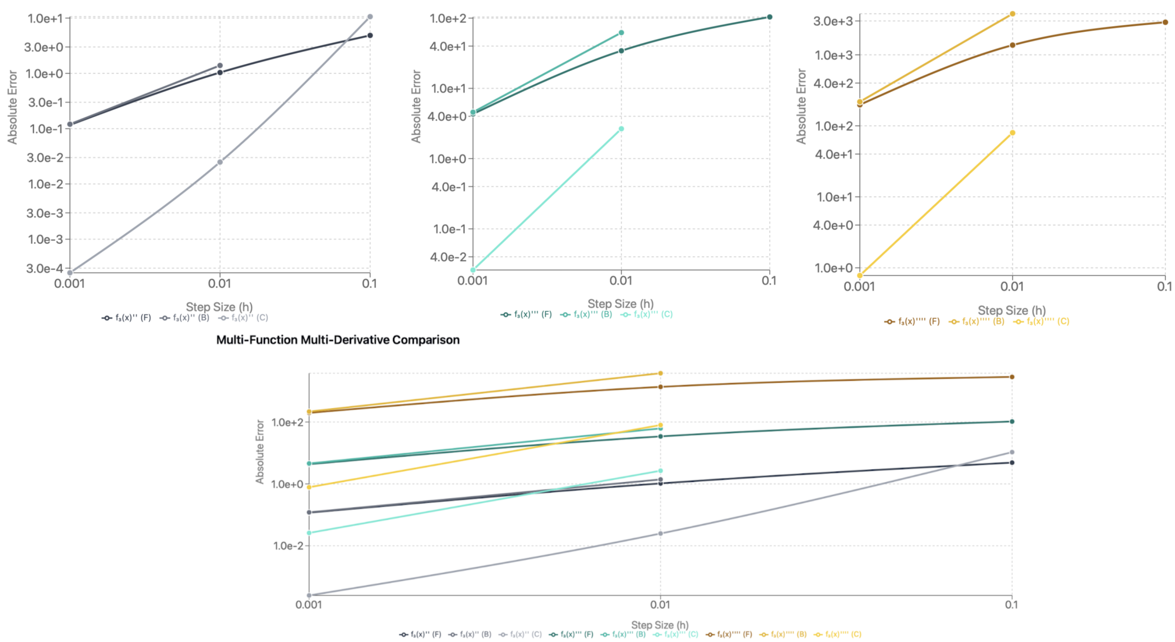

Figure 4: Error comparison of higher-order derivative approximations for $f_3(x) = \sqrt{x}$.