

Journal of Engineering Science and Technology Management

| ISSN (Online) 2828 -7886 |



Article

Round-Off and Truncation Error Trade-Off in Finite-Difference Numerical Differentiation: Optimal Step-Size Determination

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DOI: 10.31004/jestm.v6i3.449

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ARTICLE INFORMATION

Volume 6 Issue 3

Received: 01 June 2026

Accepted: 22 Oktober 2026

Publish Online: 26 October 2026

Online: at <https://JESTM.org>

Keywords

numerical differentiation,
finite difference,
round-off error,
truncation error,
optimal step size

ABSTRACT

Numerical differentiation by finite differences is an inherently ill-conditioned operation in which two antagonistic error sources, truncation and round-off, govern the attainable accuracy. The objective of this study is to quantify this trade-off and to determine the step size that minimises the total error of the centred finite-difference operator. Using the smooth test function $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$ evaluated at $x_0 = 0.5$, the first derivative was approximated for step sizes from 100 to 10^{-10} in IEEE-754 double precision, and the true, truncation, round-off, and total errors were measured and compared with a Taylor-series error model. The results reproduce the characteristic U-shaped error curve: truncation dominates for large h with second-order slope, round-off dominates for small h with slope minus one, and the minimum true error of 5.42×10^{-12} occurs at $h = 10^{-6}$, in close agreement with the analytical optimum $h_{opt} = (3\epsilon|f|/M_3)^{1/3}$. The centred scheme is shown to be markedly more accurate than the forward scheme. The study concludes that an a-priori optimal step size can be reliably predicted, providing practical guidance for derivative-based engineering computation.

1. Introduction

The evaluation of derivatives lies at the heart of computational engineering: it underpins sensitivity analysis, the solution of differential equations, optimisation, root-finding, and the calibration of physical models. When the underlying function is known only through discrete samples or through a black-box simulator, its analytical derivative is unavailable and one must resort to numerical differentiation. The finite-difference family of approximations, derived from truncated Taylor expansions, is the most widely used tool for this purpose because of its simplicity and generality (Chapra & Canale, 2021; Fornberg, 1988), and such derivative computations arise routinely in the mathematical modelling and MATLAB/Simulink simulation of dynamic engineering systems (Nugraha, 2024).

Unlike numerical integration, which is a smoothing and therefore well-conditioned operation, numerical differentiation amplifies perturbations and is intrinsically ill-conditioned (Higham, 2002). Two error mechanisms act in opposition. The truncation (or discretisation) error arises from neglecting higher-order terms of the Taylor series and decreases as the step size h is reduced. The round-off error arises from the finite precision of floating-point arithmetic and from the subtractive cancellation of nearly equal function values; it grows without bound as h tends to zero. Consequently there exists an intermediate, optimal step size that balances the two contributions and minimises the total error (Burden, Faires & Burden, 2016).

Despite being a textbook result, the practical determination of this optimal step size is frequently overlooked by practitioners, who often select h heuristically and thereby waste several digits of accuracy. The research gap addressed here is the absence, in much applied work, of a quantitative, reproducible demonstration that links the observed error behaviour to a closed-form predictor of the optimum. The objectives of this paper are therefore threefold: (i) to characterise empirically the truncation–round-off trade-off for a representative smooth function in double precision; (ii) to validate a Taylor-series error model and a closed-form expression for the optimal step size; and (iii) to compare the accuracy and order of the forward and centred difference operators. The significance of the work is that it converts a qualitative “rule of thumb” into a verified, ready-to-use guideline for

derivative-based numerical computation.

2. Literature Review

Finite-difference approximations of derivatives have a long and well-documented history in numerical analysis. Classical treatments derive forward, backward, and centred formulae from Taylor series and establish their orders of accuracy (Stoer & Bulirsch, 2002; Süli & Mayers, 2003). General procedures for generating finite-difference weights on arbitrary grids were systematised by Fornberg (1988), while LeVeque (2007) provides a modern account of their use in the discretisation of differential equations. The interaction between discretisation and floating-point error is analysed in depth by Higham (2002), who formalises the notions of conditioning, backward stability, and subtractive cancellation that explain why differentiation degrades for very small step sizes.

The existence of an optimal step size that minimises the sum of truncation and round-off errors is discussed in standard texts (Chapra & Canale, 2021; Heath, 2018; Press, Teukolsky, Vetterling & Flannery, 2007), where the centred-difference optimum is shown to scale with the cube root of machine epsilon. To circumvent the cancellation problem altogether, alternative differentiation strategies have been proposed, most notably the complex-step derivative approximation, which attains near-analytical accuracy for the first derivative by avoiding the subtraction of nearly equal real numbers (Martins, Sturdza & Alonso, 2003). Higher-order and weighted schemes that improve efficiency for related numerical problems continue to be developed (Jayaraman, 2019). Building on this body of work, and on the present authors’ related studies on the mathematical modelling and dynamic simulation of engineering systems, in which numerical differentiation and integration are intrinsic (Nugraha, 2024; Pratama, Nugraha & Jami’in, 2025), the contribution of this paper is a compact, fully reproducible verification of the error model on a controlled test problem, together with a side-by-side comparison of operator orders.

3. Research Methodology

3.1 Test function and reference derivative

A fourth-degree polynomial was adopted as the test function because it is smooth, has bounded higher derivatives, and admits an exact

analytical derivative that serves as the error reference:

$$f(x_0 \pm h) = f(x_0) \pm h f'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{6} f'''(x_0) + \mathcal{O}(h^4) \quad (1)$$

The test function and the slope to be approximated are $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$, with analytical derivative $f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25$. At the evaluation point $x_0 = 0.5$ the exact values are $f(x_0) = 0.925$ and $f'(x_0) = -0.9125$, while the third derivative $f'''(x_0)$

= -2.1 controls the leading truncation term (Figure 1).

3.2 Finite-difference operators

Two operators were considered. The forward difference, obtained from a single forward Taylor expansion, is first-order accurate:

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi), \quad \xi \in (x_0, x_0 + h) \quad (2)$$

Subtracting the backward expansion from the forward expansion cancels the even-order terms

and yields the centred difference, which is second-order accurate:

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{h^2}{6} f'''(\xi) + \mathcal{O}(h^4) \quad (3)$$

Here ξ denotes an unknown point in the relevant interval. Equation (3) shows that halving h reduces the centred truncation error by a factor of four, whereas Eq. (2) reduces it only by a factor of two.

3.3 Error model

The truncation error of the centred operator is bounded by the magnitude of the leading neglected term,

$$E_t(h) = \frac{h^2}{6} |f'''(\xi)| \leq \frac{h^2}{6} M_3, \quad M_3 = \max_x |f'''(x)| \quad (4)$$

where M_3 is a bound on the third derivative. The round-off error originates from representing and subtracting the function values in finite precision; if each evaluation carries a relative error of order ε (the machine epsilon, $\varepsilon \approx 2.22 \times 10^{-16}$ in double precision), the propagated error in the quotient behaves as

$$E_r(h) \approx \frac{\varepsilon |f(x_0)|}{h} \quad (5)$$

Adding the two contributions gives the total-error model

$$E(h) \approx \frac{M_3}{6} h^2 + \frac{\varepsilon |f(x_0)|}{h} \quad (6)$$

Minimising Eq. (6) by setting its derivative with respect to h to zero,

$$\frac{dE}{dh} = \frac{M_3}{3} h - \frac{\varepsilon |f(x_0)|}{h^2} = 0 \quad (7)$$

yields the closed-form optimal step size

$$h_{\text{opt}} = \left(\frac{3\varepsilon |f(x_0)|}{M_3} \right)^{1/3} \sim \varepsilon^{1/3} \quad (8)$$

which, for functions whose magnitude and third derivative are of order unity, simplifies to the familiar estimate $h_{\text{opt}} \approx (3\varepsilon)^{1/3} \approx 9 \times 10^{-6}$ (Heath, 2018).

3.4 Computational procedure

All computations were performed in IEEE-754 double precision. The derivative was approximated for the eleven step sizes $h = 10^0, 10^{-1}, \dots, 10^{-10}$. For each h the centred and forward estimates were formed, the true error was

computed as the absolute difference from the analytical derivative, and the truncation and round-off components were evaluated from Eqs. (4) and (5). The optimal step size was located both empirically, as the minimiser of the measured true error, and analytically, from Eq. (8); the two were then compared. The procedure is deterministic and fully reproducible.

4. Results and Discussion

4.1 Step-size dependence of the error

Table 1. Centred-difference estimate of $f'(0.5)$ and the true error of the centred and forward operators versus step size (exact value $f'(0.5) = -0.9125$).

Step size h	Centred $f'(0.5)$	True error (centred)	True error (forward)
1×10^0	-1.262500000000	3.50×10^{-1}	1.33×10^0
1×10^{-1}	-0.916000000000	3.50×10^{-3}	9.11×10^{-2}
1×10^{-2}	-0.912535000000	3.50×10^{-5}	8.79×10^{-3}
1×10^{-3}	-0.912500350000	3.50×10^{-7}	8.75×10^{-4}
1×10^{-4}	-0.912500003500	3.50×10^{-9}	8.75×10^{-5}
1×10^{-5}	-0.912500000033	3.32×10^{-11}	8.75×10^{-6}
1×10^{-6}	-0.912500000005	5.42×10^{-12}	8.75×10^{-7}
1×10^{-7}	-0.912499999450	5.50×10^{-10}	8.66×10^{-8}
1×10^{-8}	-0.912500003336	3.34×10^{-9}	8.89×10^{-9}
1×10^{-9}	-0.912500019989	2.00×10^{-8}	3.55×10^{-8}
1×10^{-10}	-0.912500075501	7.55×10^{-8}	7.55×10^{-8}

Table 2 decomposes the centred error into its modelled truncation and round-off components and compares their sum with the measured true error. The agreement is excellent in both asymptotic regimes: for $h \geq 10^{-3}$ the true error coincides with the truncation estimate ($0.35h^2$) to

Table 1 lists the centred-difference estimate of $f'(0.5)$ together with the true error of both operators. As h decreases from 10^0 to 10^{-6} , the centred true error falls monotonically from 3.50×10^{-1} to 5.42×10^{-12} , a reduction of more than eleven orders of magnitude. Below $h = 10^{-6}$ the error reverses and grows again, signalling the onset of round-off dominance. The forward operator is consistently less accurate, by roughly two orders of magnitude in the truncation-dominated region, confirming its lower order.

three significant figures, whereas for $h \leq 10^{-8}$ it follows the round-off estimate ($\epsilon|f|/h$). Near the optimum the two components are comparable, which is precisely the balance condition that defines h_{opt} .

Table 2. Modelled truncation and round-off error components, their sum, and the measured true error of the centred operator.

Step size h	Truncation E_t	Round-off E_r	Total (model)	True error
1×10^0	3.50×10^{-1}	2.05×10^{-16}	3.50×10^{-1}	3.50×10^{-1}
1×10^{-2}	3.50×10^{-5}	2.05×10^{-14}	3.50×10^{-5}	3.50×10^{-5}
1×10^{-4}	3.50×10^{-9}	2.05×10^{-12}	3.50×10^{-9}	3.50×10^{-9}
1×10^{-5}	3.50×10^{-11}	2.05×10^{-11}	5.55×10^{-11}	3.32×10^{-11}
1×10^{-6}	3.50×10^{-13}	2.05×10^{-10}	2.06×10^{-10}	5.42×10^{-12}
1×10^{-8}	3.50×10^{-17}	2.05×10^{-8}	2.05×10^{-8}	3.34×10^{-9}
1×10^{-10}	3.50×10^{-21}	2.05×10^{-6}	2.05×10^{-6}	7.55×10^{-8}

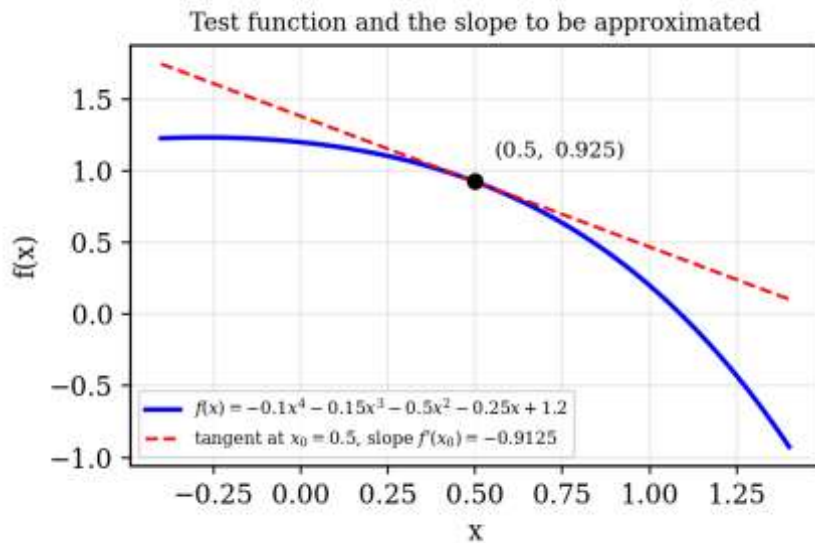


Figure 1. The fourth-degree test function and the tangent line of slope $f'(x_0) = -0.9125$ at $x_0 = 0.5$ that the finite-difference operators approximate.

4.2 The U-shaped error curve

Figure 2 presents the four error curves on logarithmic axes. The truncation curve is a straight line of slope +2 and the round-off curve a straight line of slope -1, so that the modelled total error forms the classic V (or U) shape whose vertex marks the optimum. The measured true

error tracks the model closely and reaches its minimum at $h = 10^{-6}$. The right-hand branch rises with unit slope because the round-off contribution scales as $1/h$: a tenfold reduction in h multiplies the round-off error tenfold, the signature of catastrophic cancellation between the nearly equal values $f(x_0+h)$ and $f(x_0-h)$.

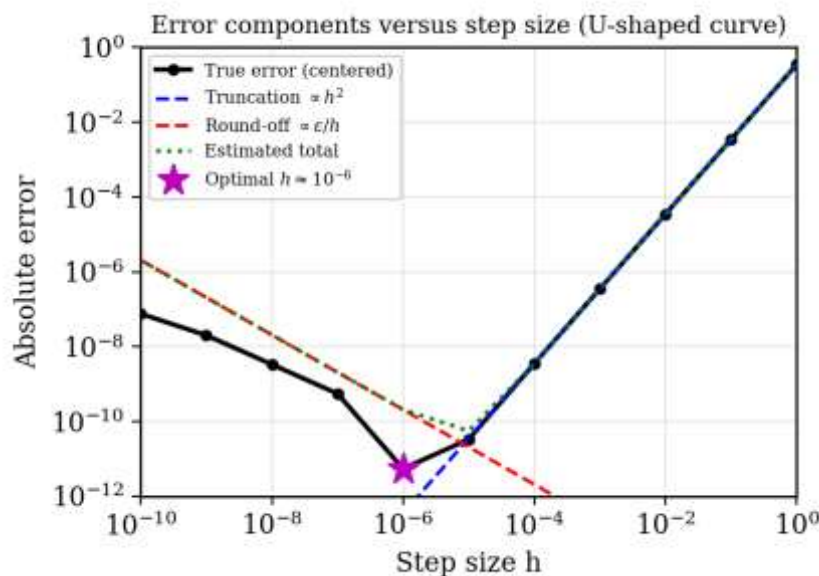


Figure 2. Error components of the centred operator versus step size. Truncation (slope +2) and round-off (slope -1) intersect at the optimal step size $h \approx 10^{-6}$ (magenta star).

4.3 Optimal step size

The empirically observed optimum, $h = 10^{-6}$ with true error 5.42×10^{-12} , agrees with the analytical prediction of Eq.

(8). Substituting $\varepsilon = 2.22 \times 10^{-16}$, $|f(x_0)| = 0.925$, and $M_3 = 2.1$ gives $h_{\text{opt}} = 6.6 \times 10^{-6}$, of the same order of magnitude as the observed value; the simplified estimate $(3\varepsilon)^{1/3} = 8.7 \times 10^{-6}$ is equally

consistent. The residual factor-of-a-few discrepancy is expected, because Eq. (8) predicts the minimiser of the modelled total error rather than of the actual error, and because the constant in the round-off bound is only an order-of-magnitude estimate. The practical conclusion is unaffected: a step size near 10^{-6} , rather than the smallest representable number, secures the best accuracy for this class of problem.

4.4 Operator order

Figure 3 contrasts the true errors of the two operators against reference slopes. In the truncation-dominated region the centred error decreases as h^2 while the forward error decreases only as h , so the accuracy gap widens by one order of magnitude for every order-of-magnitude reduction in h . This quantitative confirmation of the theoretical orders motivates the routine preference for centred (or higher-order) operators whenever function evaluations on both sides of x_0 are available (Süli & Mayers, 2003).

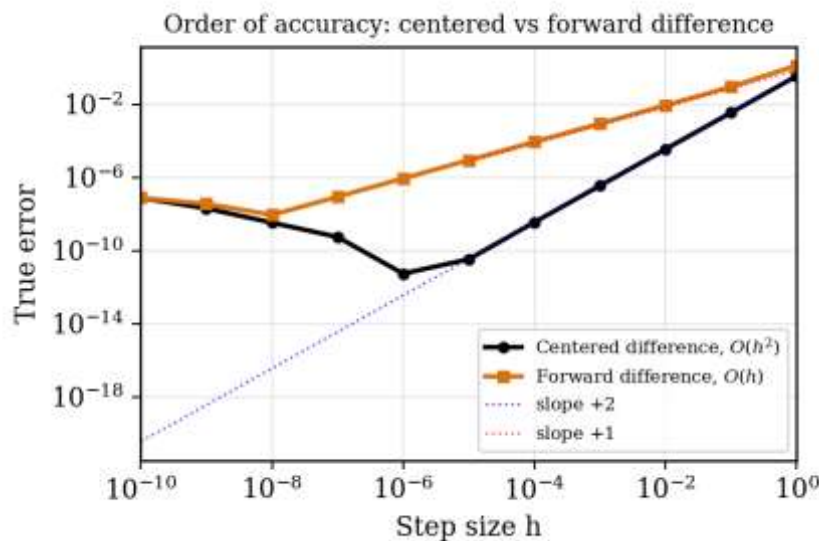


Figure 3. True error of the centred (slope +2) and forward (slope +1) operators, demonstrating their respective second- and first-order accuracy.

Taken together, the results validate the truncation–round-off error model quantitatively and confirm that the optimal step size is predictable a priori. The findings are consistent with the classical theory (Higham, 2002; Chapra & Canale, 2021) and provide a clean, reproducible reference case that can be embedded in teaching and in the verification of derivative-based engineering codes.

5. Conclusion

This study quantified the competition between truncation and round-off error in finite-difference numerical differentiation and demonstrated how to choose the step size that minimises the total error. For the smooth fourth-degree test function evaluated at $x_0 = 0.5$ in double precision, the centred operator attained a minimum true error of 5.42×10^{-12} at $h = 10^{-6}$, in agreement with the closed-form optimum $h_{\text{opt}} = (3\epsilon|f|/M_3)^{1/3}$. The measured errors reproduced

the U-shaped curve predicted by the Taylor-series model, with truncation governing the large- h branch at second order and round-off governing the small- h branch at order minus one. The centred operator was shown to be one to two orders of magnitude more accurate than the forward operator across the truncation-dominated range, in accordance with their respective orders of accuracy.

The principal contribution is a fully reproducible verification that the optimal step size can be predicted analytically rather than chosen by trial and error, yielding immediate practical guidance for sensitivity analysis, optimisation, and the discretisation of differential equations. Future work will extend the analysis to second derivatives, to non-smooth and noisy data, to Richardson-extrapolated and complex-step schemes that mitigate cancellation, and to adaptive step-size selection driven by run-time error estimates.

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