# Error in numerical differentiation

Alen Alexanderian*

**Abstract**

We consider approximation errors in numerical differentiation. The discussion focuses mainly on the forward and central difference approximation to the derivative. We also consider complex-step differentiation, and include some numerical experiments to provide further insight.

## 1 Introduction

When using classical numerical differentiation formulas, the error due to truncation decreases as the step size decreases. In the meantime, errors due to inexact function evaluations increase. Beyond a certain point the errors in function evaluation completely dominate the total error. This phenomenon is well-known and discussed in many numerical analysis textbooks; see e.g., [1, Section 3.1.3]. We provide a concise discussion of this behavior in the case of the first order forward difference formula in Section 2. We also provide numerical illustrations, showing the error in numerical differentiation, when using forward and central difference formulas, as well as the complex-step method in Section 3.

## 2 The forward difference formula

Consider a function $f : [a, b] \to \mathbb{R}$, and assume $f \in C^2[a, b]$. For $x \in (a, b)$, and a sufficiently small $h > 0$, we consider the following first order accurate one-sided approximation to $f'(x)$:

$$D_h f(x) := \frac{f(x+h) - f(x)}{h}.$$

By Taylor's theorem,

$$f(x+h) = f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(\xi), \qquad \xi \in (x, x+h).$$

We thus obtain

$$D_h f(x) = f'(x) + \tfrac{1}{2}hf''(\xi).$$

Therefore, the truncation error,

$$E_{\text{trunc}}(h) := f'(x) - D_h f(x),$$

satisfies $E_{\text{trunc}}(h) = -\frac{h}{2} f''(\xi)$. Letting

$$\alpha := \frac{\|f''\|_\infty}{2}, \tag{2.1}$$

where the uniform norm is over $[a, b]$, we obtain $|E_{\text{trunc}}(h)| \le \alpha h$, for $h > 0$ sufficiently small.

Now suppose that the function evaluation is subject to error. Namely, for each $x$, the numerically computed value of $f(x)$ is $\tilde{f}(x)$ with

$$f(x) = \tilde{f}(x) + \varepsilon_x.$$

*North Carolina State University, Raleigh, North Carolina, USA.
E-mail: alexanderian@ncsu.edu
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Let us assume that for each $x \in (a, b)$, $|\varepsilon_x| \le \varepsilon$. Here, $\varepsilon > 0$ is a bound on the error in function evaluation. Subsequently, the computed numerical derivative is given by

$$\tilde{D}_h f(x) := \frac{\tilde{f}(x+h) - \tilde{f}(x)}{h}.$$

Let us consider the total error $E(h) := f'(x) - \tilde{D}_h f(x)$. We have,

$$\begin{aligned} f'(x) - \tilde{D}_h f(x) &= f'(x) - \frac{\tilde{f}(x+h) - \tilde{f}(x)}{h} \\ &= f'(x) - \frac{f(x+h) - \varepsilon_{x+h} - f(x) + \varepsilon_x}{h} \\ &= f'(x) - \frac{f(x+h) - f(x)}{h} + \frac{\varepsilon_{x+h} - \varepsilon_x}{h} \\ &= E_{\text{trunc}}(h) + \frac{\varepsilon_{x+h} - \varepsilon_x}{h} \end{aligned}$$

Therefore, letting $\alpha$ be as in (2.1), the total error can be bounded as follows:

$$|E(h)| \le \alpha h + 2\varepsilon/h.$$

In this error bound, the first term corresponds to the truncation error and the second one is due to error in function evaluation. When $h$ is large, the truncation error dominates. On the other hand, when $h$ is very small, the error due to function evaluation dominates; see Figure 1.

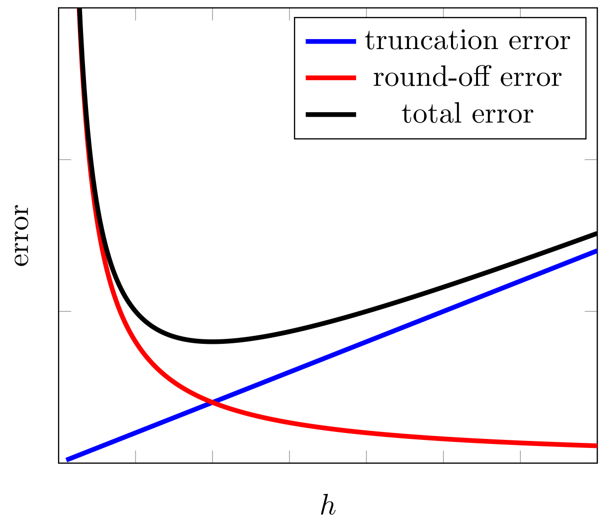


Figure 1: Illustrating the error of the forward difference formula: as $h \to 0$, truncation error decreases while round-off error increases.

To obtain an *optimal step size*, we can consider minimizing the bound

$$B(h) := \alpha h + 2\varepsilon/h$$

on the total error. This is a simple exercise in calculus. Let us note that

$$B'(h) = \alpha - 2\varepsilon/h^2 \quad \text{and} \quad B''(h) = 4\varepsilon/h^3.$$

Thus, the minimum of $B(h)$ is found by letting $B'(h) = 0$. Letting $C = \sqrt{2/\alpha}$, this yields,

$$h_{\text{opt}} = C\varepsilon^{1/2}.$$

The takeaway message is that when using a forward difference formula for approximating $f'(x)$, given a bound $\varepsilon$ on the error in function evaluations, the optimal step size is in the order of $\varepsilon^{1/2}$. It is worth noting that in the case of a second order central difference formula (cf. Section 3), the optimal step size will be in the order of $\varepsilon^{1/3}$. This can be shown using a similar analysis to the one considered in this section; see [1, Section 3].

# 3 Numerical illustrations

We provide three numerical studies. The first one, presented in Section 3.1, involves an analytic example. The second study, which is presented in Section 3.2, simulates the situation where a function evaluation requires calling a numerical solver. Specifically, in that section we consider a function whose evaluation requires solving an initial value problem (IVP). Subsequently, we examine the impact of the error in numerically computed solution on finite-difference derivative computation. Finally, in Section 3.3, we consider another example involving an IVP, and briefly illustrate complex-step method for numerical differentiation.

## 3.1 Analytic example

Consider the function $f(x) = 1/(x^2 + 1)$. We compute the error in approximating the derivative at $x = 1/5$, when using the following numerical differentiation formulas:

$$D_h^{\text{forward}} f(x) := \frac{f(x+h) - f(x)}{h}, \tag{3.1}$$

$$D_h^{\text{central}} f(x) := \frac{f(x+h) - f(x-h)}{2h}. \tag{3.2}$$

The forward and central difference formulas are, respectively, first and second order accurate. The observed error in computing the derivative using these numerical differentiation formulas is depicted in Figure 2. We note that the optimal step size for the forward difference formula is

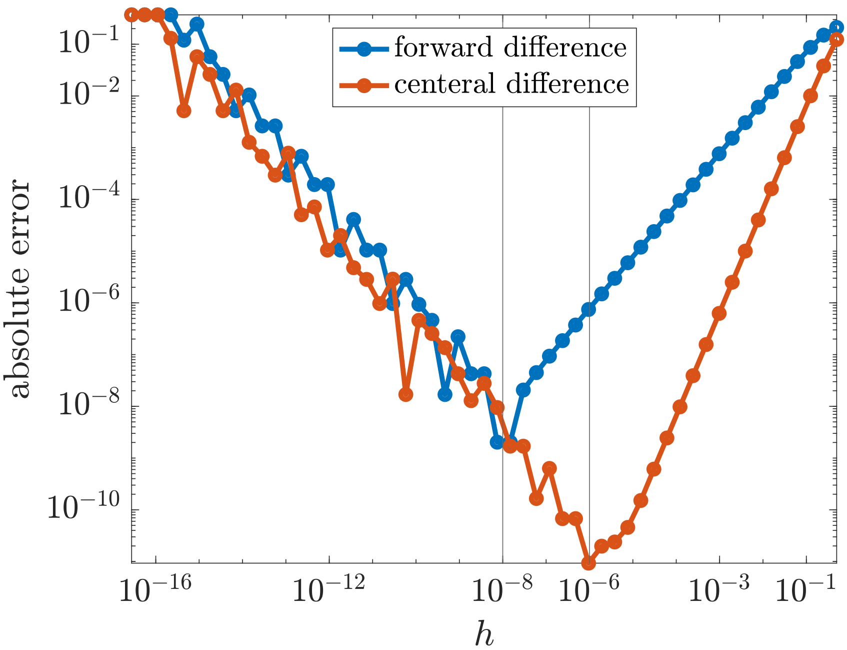


Figure 2: Error in approximating $f'(x)$ at $x = 1/5$ with forward and central difference formulas.

around $10^{-8}$ whereas the optimal step size for the central difference formula is around $10^{-6}$. This is consistent with the analysis in the previous section. Namely, here the error in approximating $f(x)$ is in the order of the machine precision, $\varepsilon \approx 2.2204 \times 10^{-16}$. Note also that $\varepsilon^{1/2} = \mathcal{O}(10^{-8})$ and $\varepsilon^{1/3} = \mathcal{O}(10^{-6})$.

## 3.2 An example involving an initial value problem

We consider the IVP,

$$\begin{aligned} Y'(x) &= \frac{1}{4} Y(x)\Big(1 - \frac{Y(x)}{20}\Big), \quad x > 0, \\ Y(0) &= 1. \end{aligned} \tag{3.3}$$

The exact solution to this IVP is given by

$$Y(x) = \frac{20}{1 + 19e^{-x/4}}. \quad (3.4)$$

We let $y(x)$ be the numerical solution of the IVP at a given $x$; i.e., $y(x) \approx Y(x)$. In the present study, we use a second order Runge–Kutta (RK2) method for solving the IVP. Subsequently, the numerical solution is used for approximating the derivative $Y'(x)$:

$$Y'(x) \approx \tilde{D}_h Y(x) := \frac{y(x+h) - y(x)}{h}. \quad (3.5)$$

The present study is substantially different from the one in the previous section. There, we had used the analytic formula for evaluating the function. In that case, there error in function evaluation was in the order of the machine precision. Here, the error in evaluating $Y(x)$ is dominated by the error of the RK2 solver. The latter is controlled by the grid resolution within the solver.

In Figure 3, we show the error $E(h) := |Y'(x) - \tilde{D}_h Y(x)|$ at $x = 1$ with two different grid resolutions used for the RK2 solver. The low-resolution grid results in (relative and absolute) error of the order $\mathcal{O}(10^{-6})$. On the other hand, the higher resolution grid yields an error of $\mathcal{O}(10^{-9})$. This suggests that the optimal step size for these two cases would be on the order of $10^{-3}$ and $10^{-5}$, respectively. This is consistent with the results in Figure 3.

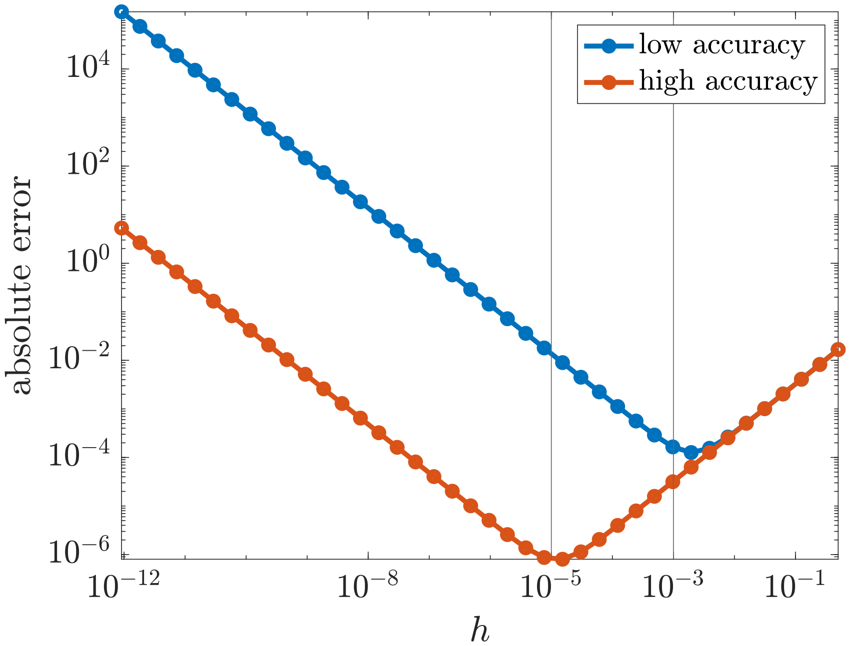


Figure 3: Error $|Y'(x) - \tilde{D}_h Y(x)|$ in approximating $Y'(x)$ at $x = 1$ using (3.5), for low- and high-resolution numerical grids used in the RK2 solver. Note that we have access to the analytic expression for the derivative from the description of the IVP.

### 3.3 A brief detour: complex-step differentiation

Consider the following IVP, which describes Newton's law of heating/cooling:

$$\frac{dT}{dt} = -\alpha\big(T(t) - T_{\text{amb}}\big), \quad t \in [0, t_f],$$
$$T(0) = T_0.$$

Here, $T(t)$ is temperature of an object at time $t$, $T_{\text{amb}}$ is the ambient temperature, $\alpha$ is a heat transfer coefficient, and $t_f$ is the final time. We consider $\alpha$ as an uncertain model parameter. Therefore, we may consider the state variable $T$ as a function, $\alpha \mapsto T(\cdot; \alpha)$. For the present example, we use

$T_0 = 5$, $T_{\text{amb}} = 15$, and $t_f = 8$. This final time is chosen so that the system has not yet reached steady state. We assume a nominal value of $\alpha_0 = 0.35$ for $\alpha$.

We focus on the following function:

$$f(\alpha) := T(t_f; \alpha).$$

That is, we consider the temperature at the final time as a function of the parameter $\alpha$. Suppose we wish to compute $f'(\alpha)$ at $\alpha = \alpha_0$. This is a simple example of a common problem in scientific computing: computing the sensitivity of a model with respect to uncertain model parameters. As before, we consider the case where the IVP is solved using a numerical method. In the present experiment, we rely on a fourth order Runge Kutta method. Note also that the present IVP can be easily solved analytically. Therefore, we can compute the error in the numerically computed derivative by comparing the results with the analytical expression for the derivative. The latter is straightforward to derive and is thus omitted for brevity.

Here, we consider a different perspective on numerical differentiation: the complex-step method [2, 3]. Assuming that $f$ admits a suitable extension to the complex plane and is sufficiently regular, it can be shown that the complex-step method provides a second order accurate approximation to the derivative. We will not delve into the technical aspects of the complex-step method. See [4, Section 8.4] for a detailed discussion and references on complex-step differentiation. Here, we only provide a couple of numerical experiments.

The complex-step approximation to $f'(\alpha_0)$ is given by

$$f'(\alpha_0) \approx \frac{\operatorname{Im}\big(f(\alpha_0 + \mathrm{i}h)\big)}{h}.$$

Here, $\mathrm{i}$ denotes the imaginary unit.

In Figure 4 (left), we compare the error in computing $f'(\alpha)\big|_{\alpha=\alpha_0}$ when using the complex-step method and the classical central difference formula (3.2). As before, we note that the error in computing the derivative is limited by the accuracy of function evaluations. We also observe the second order accuracy of both numerical differentiation formulas. However, unlike the central difference formula, the complex-step method does not suffer from subtractive cancellation errors. Namely, when using the complex-step method, the errors due to function evaluation are not amplified as successively smaller step sizes are used. In Figure 4 (right), we consider the error of complex-step differentiation, when using two different accuracy levels for the RK4 solver. The results reiterate the earlier conclusions that the complex step method does not suffer from error due to subtractive cancellation, but its accuracy is limited by the accuracy of the function evaluation.

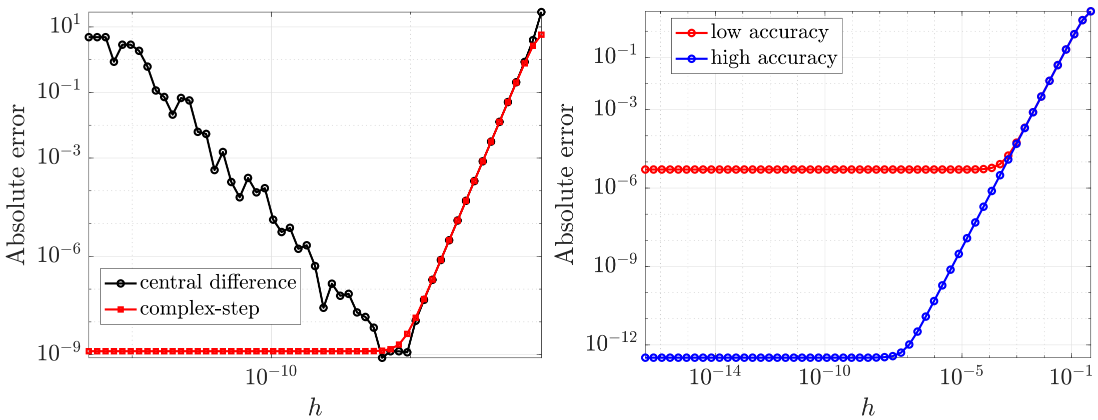


Figure 4: Left: the error of the central and complex-step differentiation formulas for computing $f'(\alpha_0)$. Right: the error of the complex-step method with low- and high-fidelity function evaluation.

## 4 Conclusion

While the study in this brief note is of academic nature, the takeaway message is important for practical computations: in numerical differentiation, the expected accuracy is limited by the accuracy of the function evaluations. This puts a limit on how small of a step size one may choose, when using classical numerical differentiation formulas based on finite-differences. Beyond a certain point, the errors in function evaluation dominate the total error and corrupt the results.

The studies in Sections 3.2 and 3.3 are particularly relevant to real applications, where one often has access to only approximate function evaluations through numerical solvers. In such cases, choosing a step size for computing derivatives numerically via finite-differences requires care. On the other hand, as noted in Section 3.3, when applicable, the complex-step method can be used to great effect. It avoids subtractive cancellation errors, allowing one to safely use a very small step size, e.g., $h = 10^{-12}$, to achieve maximal accuracy.

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