Centered Difference Formula for the First Derivative

We want to derive a formula that can be used to compute the first derivative of a function at any given point. Our interest here is to obtain the so-called centered difference formula. We start with the Taylor expansion of the function about the point of interest, x,

$$f(x \pm h) \approx f(x) \pm f'(x)h + \frac{f''(x)h^2}{2} \pm \frac{f'''(x)h^3}{3!} + \dots,$$

assuming that h is small. From this expansion we have

$$f(x+h) - f(x-h) \approx 2\left[f'(x)h + \frac{f'''(x)h^3}{3!} + \ldots\right].$$

Solving for $f'(x)$ gives the formula for the centered difference scheme:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} + \frac{f'''(x)h^2}{3!} + \ldots.$$

The centered differencing formula is a second order scheme since the error goes as the second power of h. [Notice that the truncation error depends only on even powers of h. One can actually exploit this fact to obtain even better approximations.] The truncation error is bounded by $Mh^2/3!$ where M is a bound on $|f'''(t)|$ for t near x. Thus the truncation error decreases with decreasing h, yielding more and more accurate results.

However one must also consider the effect of rounding error. Assuming that rounding errors in computing the function values are bounded by the machine ϵ, then the rounding error in evaluating the above formula is $2\epsilon/2h = \epsilon/h$. Thus rounding error increases with decreasing h.

The total computational error, E, is therefore bounded by the sum of these two errors

$$E = \frac{Mh^2}{6} + \frac{\epsilon}{h}.$$

Since the first term coming from truncation decreases with decreasing h and the second term coming from rounding increases with decreasing h, there must be an optimal value for h that represents the best tradeoffs between these two sources of error and gives the smallest total error. To find this optimal value we differentiate E

and set it to zero:

$$\frac{dE}{dh} = \frac{Mh}{3} - \frac{\epsilon}{h^2} = 0.$$

Solving for h gives the optimal value

$$h_{\text{min}} = \left(\frac{3\epsilon}{M}\right)^{1/3}.$$

This optimal value is much larger than the corresponding value obtained for the forward difference formula, which goes like $\sqrt{\epsilon}$.

Inserting this optimal value for h into the expression for

E gives the minimum error that is achieved using this optimal h:

$$
\begin{aligned}
E_{\text{min}} &= \frac{M}{6}\left(\frac{3\epsilon}{M}\right)^{2/3} + \epsilon\left(\frac{M}{3\epsilon}\right)^{1/3} && (1) \\
&= \left(\frac{M^3}{6^3}\frac{3^2\epsilon^2}{M^2}\right)^{1/3} + \left(\epsilon^3\frac{M}{3\epsilon}\right)^{1/3} \\
&= \frac{1}{2}\left(\frac{M\epsilon^2}{3}\right)^{1/3} + \left(\frac{M\epsilon^2}{3}\right)^{1/3} = \frac{3}{2}\left(\frac{M\epsilon^2}{3}\right)^{1/3}.
\end{aligned}
$$

Notice that the minimum computational error scales as

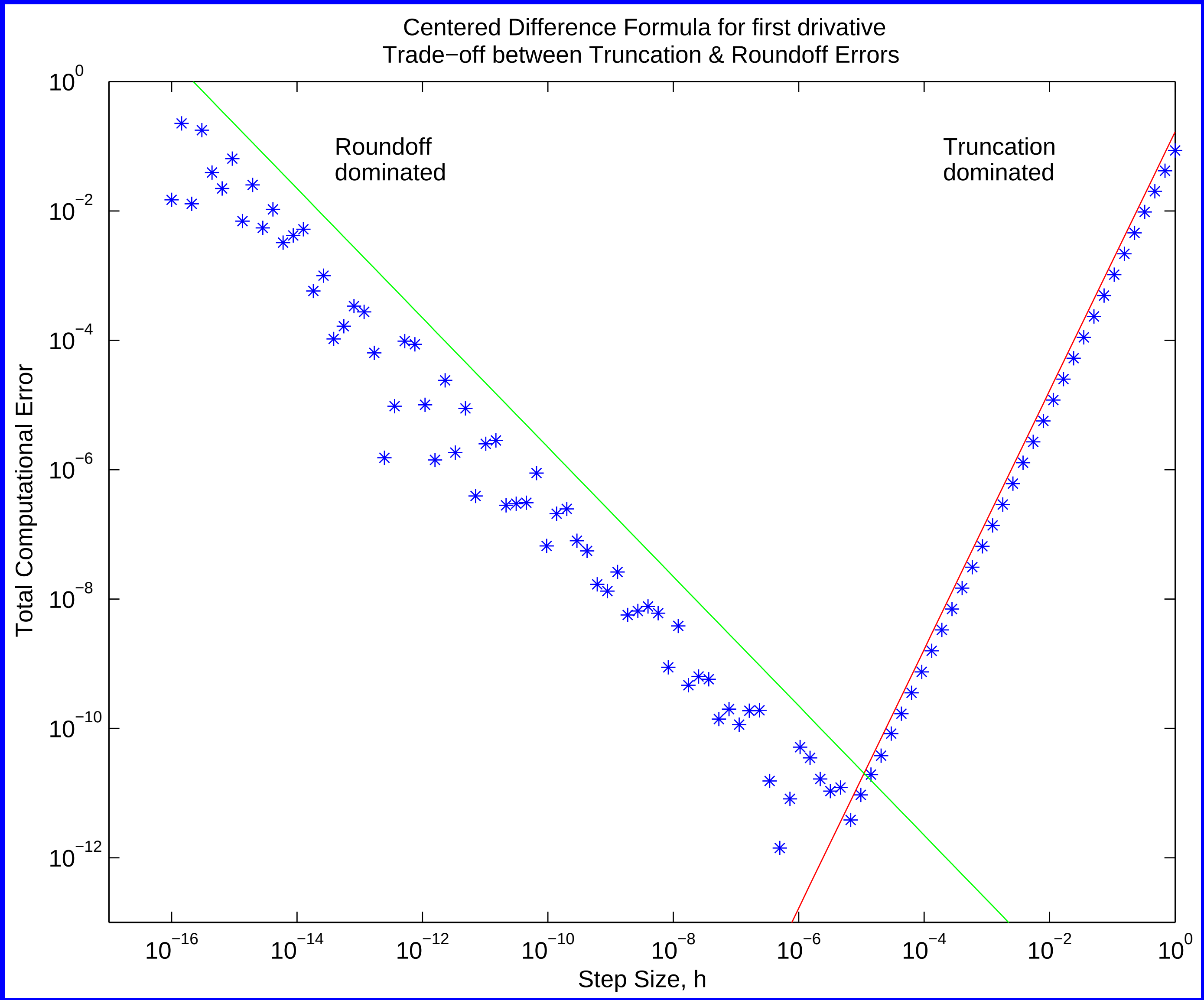
$\epsilon^{2/3}$ and is therefore much smaller than the corresponding value for the case of the forward differencing scheme whose minimum computational error goes as $\sqrt{\epsilon}$. Also notice that two-thirds of that error is due to rounding. Recall that for the first order forward differencing scheme, both truncation and round contribute equally to the minimal total computational error.

One can derive even high-order schemes to approximate the first derivative of a function. The following important general remarks can be made.

The higher the order of the scheme is,

1. the more accurate is the result,
2. the larger is the optimal step size h to achieve the minimum error,
3. the larger is the proportion of the error due to rounding,
4. the more complicated the formula is and the more time-consuming it is to compute the derivative.

It is not always obvious which order of scheme to use. At any rate, it is very seldom that one has to use higher than fourth order schemes.


Centered Difference Formula for first drivative
Trade−off between Truncation & Roundoff Errors
Roundoff dominated
Truncation dominated
Total Computational Error
Step Size, h
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−16
10^−14
10^−12
10^−10
10^−8
10^−6
10^−4
10^−2
10^0