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Numerical Differentiation: Approximation and Roundoff Errors

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I. INTRODUCTION

We have already talked about roundoff errors, which are due to the limited precision of the numbers stored in the computer. Here, in addition to roundoff errors, we also discuss the other principle source of error in numerical work, which come from approximations inherent to the numerical method being used. These "approximation errors" would still occur even if we could do the calculations to infinite precision. We will discuss approximation errors for a very simple example, numerical differentiation. There will turn out to be a competition between the requirement of minimizing the approximation error and minimizing the roundoff error. As a result, evaluating the derivative in the simplest way, the final error is always much larger than machine precision. However, with a bit of thought, we shall see that the accuracy can be improved using two techniques that will also be useful later in the course. A discussion is given in Landau, Páez and Bordeianu, Secs. 7.1–7.4.

II. THE BASIC METHOD; FORWARD DIFFERENCE

The basic definition of a derivative is

$$\frac{df}{dx} = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}. \tag{1}$$

Naturally, on the computer we have to choose a finite value for h. However, if one takes h too small then the fractional error in the numerator becomes large because roundoff errors in the values of $f(x+h)$ and $f(x)$ get greatly magnified when these nearly equal numbers are subtracted. On the other hand, if h is too large, the approximation errors (which arise because Eq. (1) is only valid for $h \to 0$) become large.

To investigate the approximation errors consider the Taylor series for $f(x)$, i.e.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) + \cdots , \tag{2}$$

from which we can immediately obtain the *forward difference* algorithm

$$f'(x) = f'_{\rm fd}(x) - \delta_{\rm fd} \tag{3}$$

where

$$f'_{\rm fd}(x) = \frac{f(x+h) - f(x)}{h} \tag{4}$$

and the approximation error, $\delta_{\rm fd}$, is given by the remaining terms in Eq. (2),

$$\delta_{\rm fd} = \frac{h}{2!} f''(x) + \frac{h^2}{3!} f^{(3)}(x) + \frac{h^3}{4!} f^{(4)}(x) + \frac{h^4}{5!} f^{(5)}(x) + \cdots . \tag{5}$$

If h is small $\delta_{\rm fd}$ is dominated by the first term, *i.e.*

$$\delta_{\rm fd} \simeq \frac{h}{2!} f''(x), \tag{6}$$

and so is proportional to h.

Let us next discuss the roundoff error. The fractional error in $f(x)$ and $f(x+h)$ is the machine accuracy, which we call ϵ_m, so actual error in $f(x)$ is $f(x)\,\epsilon_m$. Now $f(x)$ and $f(x+h)$ are almost equal, so the error in the difference is $C f(x)\,\epsilon_m$, where C is a numerical constant of order unity. According to Eq. (4) we divide by h, and hence we find the roundoff error in the derivative to be

$$\delta_{\rm roundoff} = C\,\epsilon_m \frac{f(x)}{h}, \tag{7}$$

Hence the total error, δ, in the forward difference method, roundoff plus approximation, is given by the sum of Eqs. (6) and (7):

$$\delta = C\,\epsilon_m \frac{f(x)}{h} + \frac{h}{2!} f''(x). \tag{8}$$

Hence the optimal choice of h represents a compromise between the conflicting requirements of minimizing the roundoff error, the first term on the RHS of Eq. (8), which requires a large value of h, and minimizing the approximation error, the second term on the RHS of Eq. (8), which requires a small value of h. If we assume that $f''(x)$ and $f(x)$ have similar values, then the optimal choice, obtained by minimizing Eq. (8) with respect to h, is h of order $\sqrt{\epsilon_m}$ which leads to a minimum error also of order $\sqrt{\epsilon_m}$. In other words, we have lost a lot of precision compared with machine precision. For the case of double precision, where $\epsilon_m \simeq 10^{-16}$, the best we accuracy we can achieve with the forward difference algorithm is of order 10^{-8}.

III. THE MIDPOINT METHOD (CENTRAL DIFFERENCE)

We shall now see that we can do much better than the forward difference algorithm with essentially no extra computing. Let us subtract Eq. (2) with h replaced by $h/2$, from the same equation with h replaced by $-h/2$. Clearly all the even powers of h vanish and we get

$$f(x+h/2) - f(x-h/2) = hf'(x) + \frac{2}{3!}\left(\frac{h}{2}\right)^3 f^{(3)}(x) + \frac{2}{5!}\left(\frac{h}{2}\right)^5 f^{(5)}(x) + \cdots , \tag{9}$$

This gives us the *midpoint method* (called the *central difference* method by Landau and Páez) $f'(x) = f'_{\mathrm{m}p}(x) - \delta_{\mathrm{m}p}$ where

$$f'_{\mathrm{m}p}(x) = \frac{f(x+h/2) - f(x-h/2)}{h} \tag{10}$$

and the approximation error is given by the remaining terms in Eq. (9),

$$\delta_{\mathrm{m}p} = \frac{h^2}{24} f^{(3)}(x) + \frac{h^4}{1920} f^{(5)}(x) + \cdots . \tag{11}$$

The error is now of order h^2, and so is much smaller for small h than that of the forward difference approximation which is order h. Intuitively, the reason is that the slope of a chord between two points on a curve is a much better approximation to the slope of the curve at the midpoint that at either end, see Fig. 1.

The roundoff error will similar to that of the forward difference method, *i.e.* proportional to $1/h$.

IV. MIDPOINT + ERROR EXTRAPOLATION

With a bit of extra work we can do even better than the midpoint method. Suppose we take Eq. (9) with h replaced by $2h$, *i.e.*

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2}{3!}h^3 f^{(3)}(x) + \frac{2}{5!}h^5 f^{(5)}(x) + \cdots . \tag{12}$$

We see that the leading contribution to the error in the derivative, the h^3 term, is eight times larger in Eq. (12) than in Eq. (9). Hence if subtract Eq. (12) from eight times Eq. (9) the leading contribution to the error will cancel and we will get a higher order approximation. This technique is called *error extrapolation* and is often associated with the name of Richardson. The result is

$$8\left[f(x+h/2) - f(x-h/2)\right] - \left[f(x+h) - f(x-h)\right] = 6hf'(x) - \frac{h^5}{80} f^{(5)}(x) + \cdots . \tag{13}$$

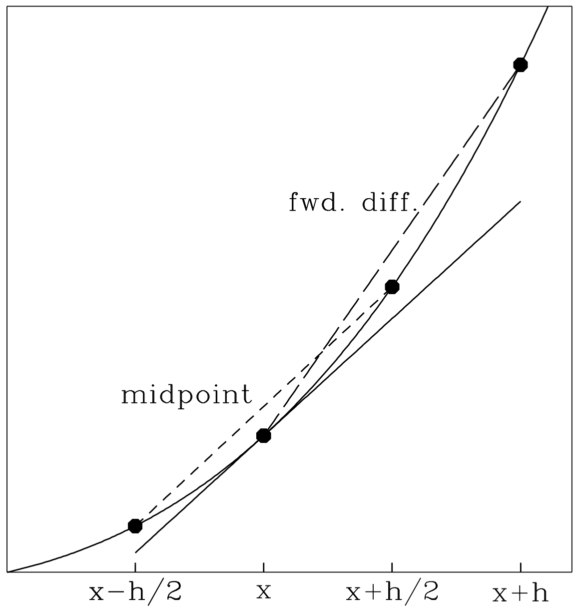

FIG. 1: The solid curve is the function and the solid straight line is the tangent to the curve at x whose slope is $f'(x)$. The long dashed line is the chord from x to $x+h$, whose slope is the forward difference approximation to the derivative. The short dashed line is the chord from $x-h/2$ to $x+h/2$, whose slope is the midpoint (central difference) approximation to the derivative. Clearly the latter is a better approximation to $f'(x)$ than the forward difference approximation since the slope of the chord is a much better approximation to the slope of the curve at the midpoint than at either end.

Hence our approximation for $f'(x)$, obtained by combining the midpoint and error extrapolation techniques, is $f'(x) = f'_{\rm errext}(x) - \delta_{\rm errext}$ where

$$f'_{\rm errext}(x) = \frac{1}{6h}\left\{8\left[f(x+h/2) - f(x-h/2)\right] - \left[f(x+h) - f(x-h)\right]\right\} \tag{14}$$

and

$$\delta_{\rm errext} = -\frac{h^4}{480} f^{(5)}(x) + \cdots , \tag{15}$$

so the leading error is of order h^4.

V. NUMERICAL RESULTS

We have seen that the approximation errors in the forward difference, midpoint and combined midpoint-error extrapolation approximations, are of order h, h^2 and h^4 respectively. The power of h in the leading contribution to the error is called the *order* of the method. In all three cases the roundoff error, which dominates for very small h, varies as h^{-1}.

For many problems, higher order methods give better results. This is the case here provided we are differentiating a smooth function. The figure below shows numerical results for these three approximations for the derivative of $\ln(1+x)$ at $x = 1$, with double precision. The calculations were done with the g77 compiler under linux. Some compilers do internal computations in higher precision than the precision specified, so results on your computer *may* look somewhat different.

One sees that even for a not-very-small value of h, such as 0.1, the combined midpoint-error extrapolation approximation gives a very small error, about 10^{-7}. With an optimal choice of h, the minimum error is about 10^{-13}, which is not very far short of machine precision, $\simeq 10^{-16}$.

However, we should emphasize that higher order is not *always* better. You see that the error in the higher order approximations involves higher order derivatives. If the function is being evaluated at or near a singularity, these can become very large. In this case a lower order method is to be preferred. In addition, *very* high order methods are rarely worthwhile because the gain in accuracy is not enough to compensate for the extra complexity of the calculation. It is better to use a somewhat lower order method with a smaller value of h. For the present problem, the midpoint method is a good choice, because it improves the accuracy a lot relative to the forward difference approximation with almost no increase in computing.

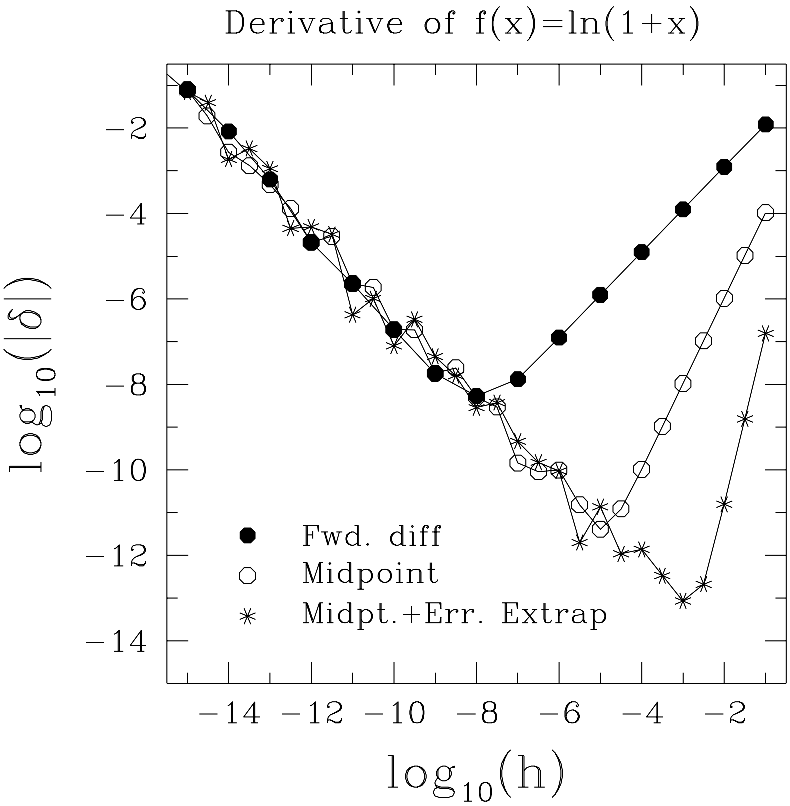

FIG. 2: A log-log plot of the absolute value of the error as a function of h for the approximations discussed in the text. Note that for small h the roundoff error dominates, it is the same for all three methods, and varies as h^{-1}. For larger h, in the regions where the curves have positive slope, the approximation error dominates and it varies as h, h^2 and h^4 for the forward difference, midpoint, and midpoint plus error extrapolation methods, respectively.