NUMERICAL DIFFERENTIATION

James T. Smith
San Francisco State University

In calculus classes, you compute derivatives algebraically: for example,

$$f(x) = x^2 + \frac{1}{x} \qquad\qquad f'(x) = 2x - \frac{1}{x^2} \,.$$

This technique requires your knowing the formula for f and the appropriate differentiation rule. What if you don't know a rule? One way is to refer to the definition of the derivative as the limit of the differential quotient

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \,.$$

and evaluate the quotient for smaller and smaller h until successive values don't change significantly. You can accept the last value as an adequate approximation to the derivative. The function $f(x) = \arctan x$ is a good example. You don't learn its derivative very early in calculus classes, so you might want to use this method. On the other hand, there *is* a formula,

$$\frac{d}{dx} \arctan x = \frac{1}{1 + x^2} \,,$$

so you can check the accuracy of the differential quotient approximation. Figure 1 gives the results for a typical argument x, with a succession of smaller and smaller h values.

The error seems closely tied to the size of h, until that gets too small. The method works well here, but there seems to be a limit to the accuracy. Consider a less successful case:

$$f(x) = \sin \frac{1.1\pi}{x} \qquad\qquad x = 0.1 \quad h = 0.01$$

$$f'(x) = -\frac{1.1\pi}{x^2} \cos \frac{1.1\pi}{x} = -\frac{1.1\pi}{0.01} \cos 11\pi = 110\pi \approx 346$$

$$\frac{f(x+h) - f(x)}{h} = \frac{\sin \dfrac{1.1\pi}{0.11} - \sin \dfrac{1.1\pi}{0.1}}{0.01} = \frac{\sin 10\pi - \sin 11\pi}{0.01} = 0 \,.$$

Clearly, you must take care when you approximate a derivative this way! In these notes, you'll see how to predict this method's behavior, so you can avoid taking h too small, and avoid catastrophes like the second example.

6 December 2002

$f(x) = \arctan x \qquad x = 1.2345678 \qquad f'(x) = 0.3961718$

Approximating $f'(x)$ by $\dfrac{f(x+h)-f(x)}{h}$

Error = Approximation – $f'(x)$

h	*Approximation*	*Error*
1.0E+0	0.2600244	–1.4E–1
1.0E–1	0.3775191	–1.9E–2
1.0E–2	0.3942415	–1.9E–3
1.0E–3	0.3959781	–1.9E–4
1.0E–4	0.3961524	–1.9E–5
1.0E–5	0.3961698	–1.9E–6
1.0E–6	0.3961710	–7.2E–7
1.0E–7	0.3961682	–3.6E–6
1.0E–8	0.3961375	–3.4E–5

Figure 1 Approximating a derivative by a differential quotient

A major tool for analyzing approximation errors is the mean-value theorem, considered in your first calculus course. The theorem relates a difference in function arguments to the resulting difference in function values, as follows.

> Suppose function f is defined and continuous at each point x in a closed interval $a \le x \le b$, and differentiable at each interior point. Then for some interior point ξ,
>
> $$\frac{f(b)-f(a)}{b-a} = f'(\xi).$$

The geometric interpretation is striking: the theorem says that at some point $<\xi, f(\xi)>$ the graph of f has the same slope as the secant through points $<a, f(a)>$ and $<b, f(b)>$. Since the derivative isn't based on geometry, the proof of the theorem, found in calculus texts, requires detailed analysis. In some cases you can actually calculate ξ: for example, if $f(x) = x^2$, then $\xi = \frac{1}{2}(a+b)$. In general, however, the theorem just asserts existence of ξ, and gives no information about its exact value.

To use the mean-value theorem to analyze the error

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

resulting from approximating $f'(x)$ by the differential quotient, first let $a, b = x, x + h$ so that $b - a = h$. The theorem yields ξ between a and b such that

$$\varepsilon = f'(\xi) - f'(x).$$

Now apply it again with f replaced by f', and $a, b = x, \xi$. You get η between x and ξ such that

$$|\varepsilon| = |f'(\xi) - f'(x)| = |(\xi - x) f''(\eta)| \le hM_2,$$

provided M_2 is an upper bound for *all* values $|f''(\eta)|$ with η between x and $x + h$. Thus, the approximation error doesn't exceed hM_2. From Taylor's theorem, considered in later calculus classes, you can derive a smaller error bound $\frac{1}{2}hM_2$. The following paragraphs use this version to analyze the behavior of the differential quotients in the earlier examples.

If $f(x) = \arctan x$, then

$$f''(x) = \frac{-2x}{\left(1 + x^2\right)^2} \ ,$$

and you can verify that $|f''(\eta)| \le 1$ for all η between $x = 1.2345678$ and $x + 1$. Thus you can take $M_2 = 1$, and the approximation error shouldn't exceed $\frac{1}{2}h$. That's true in figure 1 for $h > 10^{-6}$, but it fails afterward. There's no contradiction in the mathematics—this analysis neglected something that happened in producing figure 1. Before turning to that, however, consider the second example $f(x) = \sin(1.1\pi/x)$:

$$f''(x) = \frac{2.2\pi}{x^3}\cos\frac{1.1\pi}{x} + \frac{(1.1\pi)^2}{x^4}\sin\frac{1.1\pi}{x} \ .$$

From the graph of f'' you can see that the largest value $M_2 \approx 101000$ of $|f''(x)|$ on the interval $0.10 \le x \le 0.11$ occurs at $x \approx 0.104$. With $h = 0.01$ you get the error bound $\frac{1}{2}hM_2 > 500$, which agrees with the example and suggests that the approximation may be very inaccurate.

Why did the error ε in figure 1 stop decreasing with h in spite of the bound $\varepsilon \le \frac{1}{2}hM_2$? The analysis that led to this inequality assumed that the difference quotient was computed exactly. But that's not true. In particular, calculating f with any computer involves roundoff error. The two f values in the quotient are almost equal, so when you subtract them, roundoff errors may form a more significant part of the result. Consider a simpler situation with a different function f:

$$2.00000005003 - 2.00000004001 = 1.002\cdot 10^{-8}$$

$f(x+h)$ $f(x)$

Roundoff errors are in the 12th digit of the f values.

Resulting error is in the 4th digit of the difference.

This effect, *subtractive cancellation error*, is bad by itself. But in the difference quotient, it's multiplied by a large factor, because h is tiny. Thus you can expect that something will go wrong with this approximation. Can you predict when?

It's not difficult to use elementary calculus to determine when the error stops decreasing. Suppose the function values actually computed are

$$f^*(x+h) = f(x+h) + e_1 \qquad f^*(x) = f(x) + e_2,$$

where $f(x+h), f(x)$ are exact values and e_1, e_2 are roundoff errors. Then the total error in the approximation is

$$\left|\frac{f^*(x+h) - f^*(x)}{h} - f'(x)\right| = \left|\frac{f(x+h) - f(x)}{h} - f'(x) + \frac{e_1 - e_2}{h}\right|$$
$$\leq \left|\frac{f(x+h) - f(x)}{h} - f'(x)\right| - \left|\frac{e_1 - e_2}{h}\right|.$$

With *Turbo Pascal* **`Real`** arithmetic, used to compute Figure 1, $|e_1|, |e_2| \leq 10^{-12}$. Thus the total error is bounded by

$$E(h) = \frac{hM_2}{2} + \frac{2\times 10^{-12}}{h} = \frac{h}{2} + \frac{2\times 10^{-12}}{h}.$$

$E(h)$ is smooth and approaches ∞ as h approaches $0+$ or ∞, hence it has a minimum value at some $h > 0$ where

$$0 = E'(h) = \frac{1}{2} - \frac{2\times 10^{-12}}{h^2},$$

i.e. $h^2 = 4\times 10^{-12}$, $h = 2\times 10^{-6}$. That the total approximation error is bounded by a function $E(h)$ with a minimum value at $h = 2\times 10^{-6}$ suggests that the error will stop decreasing between $h = 10^{-5}$ and 10^{-6}. Figure 1 confirms that.

The previous discussion was devoted to computing a derivative in a situation where you could calculate the function at will, but had no rule for differentiating it. What if you only have a table of function values? If you need an approximation to $f'(x)$ for a tabulated argument x, and $x + h$ is the next one, then you can use the differential quotient

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

and from the formula $\frac{1}{2}hM_2$ predict the size of the approximation error (as long as h is not so small as to cause subtractive cancellation roundoff error buildup). Of course, you'd have to know M_2. If you don't, you shouldn't trust approximate derivatives calculated this way. After all, you could construct another function g agreeing with f at arguments x and $x + h$. By making g'' large enough (increasing M_2) you could make g' differ wildly from f'. The differential quotient formula would still yield an approximation to $f'(x)$, not $g'(x)$.

If you're designing a table of values $f(x)$ to facilitate calculating $f'(x)$ by differential quotient approximation, and you know M_2, then you can ensure that the approximation error will not exceed a specified tolerance T by selecting h so that $\frac{1}{2}hM_2 < T$. You shouldn't select h small enough, though, to cause subtractive cancellation roundoff error buildup.

Many derivative approximation formulas more accurate than the differential quotient are studied in numerical analysis. These two are used in the commercial software package *MathCAD* :

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h} \qquad \tfrac{1}{6}M_3h^2$$

$$f'(x) \approx \frac{f(x-2h)-8f(x-h)+8f(x+h)-f(x+2h)}{12h} \qquad \tfrac{1}{30}M_5h^4.$$

The expressions at right are error bounds, disregarding roundoff error. In general, M_k stands for an upper bound of the values $|f^{(k)}(x)|$ with x in the region of interest. You should be able to construct corresponding examples and error analyses analogous to the ones in these notes. That would test your understanding and show you how much more accurate these formulas are.

Reference

Richard L. BURDEN and J. Douglas FAIRES, *Numerical analysis*, 6th ed., Brooks/Cole, 1997. §4.1.