Numerical Differentiation

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1 Motivation

Calculating the exact (= analytical) **numerical value of a derivative** can be complicated and time consuming. When computation time is valuable, we might prefer a **quick approximation** to a slow, exact calculation. Numerical differentiation is a set of techniques to obtain numerical values of derivatives by **using function values**. Generally, numerical differentiation delivers approximations of the numerical value of the derivative that **converge to the true value**.

2 What is a Derivative?

Instantaneous rate of change of a function with respect to one of its variables

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

3 Finite Difference Methods

We can approximate a derivative by lying a secant through two function points and computing the slope of this secant. The most simple case is the **two-point formula**

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

which has an approximation error of $O(h)$. This means the approximation error will converge to zero as fast as h will converge to zero. You can derive the approximation error by writing the Taylor series of $f(x+h)$ around x.
We can get an even better estimate with the **three-point formula**:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h},$$

where the error is $O(h^2)$, i.e. converges to zero faster.

4 Problems of Finite Difference Methods

With large values of h the approximation is quite inaccurate (**truncation error)**. However, if h converges to zero, the difference between function values might become so small, that a computer rounds the number to zero (**subtraction cancellation error**). This means the approximation from the finite difference methods only converge to the true value of the derivative in a certain range of h values, then it deteriorates.
The larger the power of h in the big O $(O(h), O(h^2)O(h^3)...)$, the faster the approximation will converge to the true value of the derivative. But this is no guarantee that convergence will occur before the subtractive cancellation error sets in.

5 Richardson Extrapolation

The Richardson Extrapolation combines several approximations with slower convergence to obtain an approximation with faster convergence. For example, we can arrive at the **five-point formula** with an $O(h^4)$ error

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}.$$

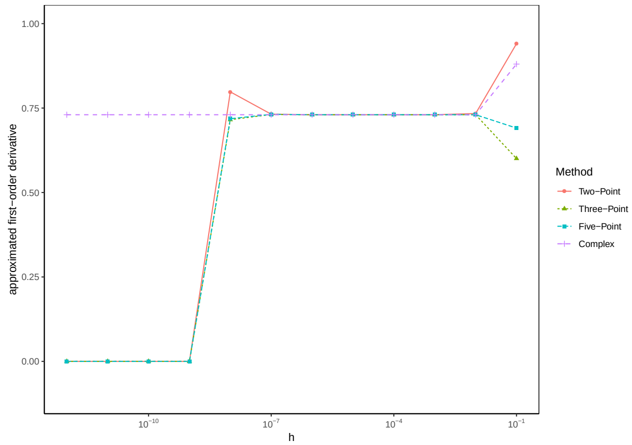

Figure 1: Convergence and deterioration graphically of the first derivative of $f(x) = x^2 sin(1/x)$ at $x = 0.1$ and $h = 0.01$. Find it on Github here.

$h^{(\dots)}$	two-point	three-point	five-point	complex
0.01^1	0.94	0.60	0.69	0.88
0.01^2	0.73	0.73	0.73	0.73
0.01^3	0.73	0.73	0.73	0.73
0.01^4	0.73	0.73	0.73	0.73
0.01^5	0.73	0.73	0.73	0.73
0.01^6	0.73	0.73	0.73	0.73
0.01^7	0.73	0.73	0.73	0.73
0.01^8	0.80	0.72	0.72	0.73
0.01^9	0.00	0.00	0.00	0.73
0.01^{10}	0.00	0.00	0.00	0.73
0.01^{11}	0.00	0.00	0.00	0.73
0.01^{12}	0.00	0.00	0.00	0.73

Table 1: Convergence and deterioration of the same function numerically

6 Higher-Order Derivatives

We can compute higher-order derivatives by applying our formulas from above. The second-order derivative can be estimated by plugging in the approximations for the first-order derivatives

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

When estimating higher-order derivative, convergence will become slower.

7 Applications

A policeman who measures the speed of passing cars with a radar gun uses numerical differentiation. The first-order derivative of the position is the velocity and the second-order derivative is the acceleration. Numerical differentiation is also used to find optima of profit functions in economics or in gradient-based optimizers in machine learning.

8 Some Dos and Don'ts

Do use numerical differentiation if an analytic solution would take long and an approximation of the derivative is acceptable. Then numerical differentiation can save computation time.
Don't use numerical differentiation if an exact value is needed. A small error can compile to large errors if the approximated derivative is used in many follow-up computations. Numerical differentiation also might not work well if the function cannot be evaluated at arbitrary points.

References

Jaan Kiusalaas. *Numerical Methods in Engineering with MATLAB.* Cambridge University Press, p. 182 - 195, 2005.
C. Woodford, C. Phillips. *Numerical Methods with Worked Examples: Matlab Edition.* Springer, p. 119-128, 2012.