Numerical Differentiation

- In calculus, it is easier to differentiate than to integrate. But in numerical calculation, the opposite is true.
- Some basic formulas:
  - ◇ Forward-difference,
  $$f^{'}(c) = \frac{f(c+h) - f(c)}{h} + O(h).$$
  - ◇ Central-difference,
  $$f^{'}(c) = \frac{f(c+h) - f(c-h)}{2h} + 0(h^2).$$
  - ◇ Central-difference for the second derivative,
  $$f^{''}(c) = \frac{f(c-h) - 2f(c) + f(c+h)}{h^2} + 0(h^2)$$
  - ◇ There are many more systematic way of deriving other formulas to approximate derivatives. But the above three are workhorses that are put to service in many applications.
- Limitations on numerical differentiation.
  - ◇ In exact arithmetic, it is true that as h goes to zero, the approximation get more accurate. In practice, there is a lower bound on h beyond which no improvement on accuracy should be expected.
    - ▷ Due to roundoff errors, suppose
    $$\begin{aligned} f(c+h) &= \hat{f}(c+h) + E^{+}, \\ f(c-h) &= \hat{f}(c-h) + E^{-} \end{aligned}$$
    where $\hat{f}$ represents the floating point value of f.

- ▷ Using the central-difference formula, we would calculate $\hat{f}'(c) = \frac{\hat{f}(c+h)-\hat{f}(c-h)}{2h}$. Thus the error is given by

$$f'(c) - \hat{f}'(c) = \frac{E^+ - E^-}{2h} + 0(h^2). \tag{1}$$

- ▷ The second term in the above is stable and converges to zero as $h \to 0$.
- ▷ The first term becomes unbounded as $h \to 0$, since the numerator $E^+ - E^-$ is approximately equal to the machine accuracy and is bounded away from zero.
- ▷ Using double precision in calculation can help to delay but not prevent this from happening too soon.

◇ A rule of thumb is that *if the formula is of order r, then the step should not be smaller than $\epsilon^{1/(r+1)}$ where ϵ is the machine accuracy.* For example, we cannot expect more than half machine precision if a forward difference scheme is used.