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,
    \[ f'(c) = \frac{f(c + h) - f(c - h)}{2h} + O(h^2). \]
  ◦ Central-difference for the second derivative,
    \[ f''(c) = \frac{f(c - h) - 2f(c) + f(c + h)}{h^2} + O(h^2). \]
  ◦ 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
      \[
      f(c + h) = \hat{f}(c + h) + E^+, \\
      f(c - h) = \hat{f}(c - h) + E^-
      \]
    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
\[
f'(c) - \hat{f}'(c) = \frac{E^+ - E^-}{2h} + O(h^2). \tag{1}
\]
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 \( \epsilon \) is the machine accuracy. For example, we cannot expect more than half machine precision if a forward difference scheme is used.