# ME360 Lecture 20.

## Ch.5. Numerical Differentiation and Integration.

We will cover a few methods in this chapter in preparation of Ch.6. solving ordinary differential equations numerically.

1. Numerical Differentiation - Finite difference
   (a). two-point forward-difference
   (b). three-point centered-difference
   (c). extrapolation
2. Numerical Integration - Newton-Cotes
   (a). Trapezoid Rule
   (b). Simpson's Rule

### 5.1.1 Finite difference formulas

By definition:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \quad \text{(if limit exists)}$$

Taylor's theorem (if $f$ is twice continuously differentiable)

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(c)$$

where $c$ is between $x$ and $x+h$.

Combining the two equations above, we get:

**Two-point forward-difference formula**

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(c)$$

where $c$ is between $x$ and $x+h$.

To get the numerical formula based on the formula above, we compute the approximation.

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{(if } h \text{ is small)}$$

With this approximation, we treat the term $\frac{h}{2}f''(c)$ as error.

We can reduce the error by making $h$ smaller. The two-point forward-difference formula is a first-order method for approximating the first derivative.

In general, if the error is $O(h^n)$, we call the formula an order $n$ approximation.

(Note: see Sauer P.254-255 on the discussion of this method being first order and the concept of convergence).

Example: Use two-point forward-difference formula with $h=0.1$ to approximate the derivatives of $f(x)=1/x$ at $x=2$.

$$f'(x) \approx \frac{f(x+h)-f(x)}{h} = \frac{1/2.1 - 1/2}{0.1} \approx \boxed{-0.2381}$$

Error analysis for this approximation:
We can compute the analytical form of $f(x)$.

$$f'(x) = \left(\frac{1}{x}\right)' = -\frac{1}{x^2} \Rightarrow f'(2) = -0.25$$

The error is $-0.2381-(-0.25)=0.0119$
We now compare this error to the formula, where the error should be $hf''(c)/2$, where $c$ is between $x$ & $x+h$.
(Here $x=2.0$, $x+h=2.1$)

$$f''(x) = \left(-\frac{1}{x^2}\right)' = \frac{2}{x^3}$$

So the error should be between

$$0.1 \times \frac{2}{2^3} \times \frac{1}{2} \approx 0.0125 \text{ and } 0.1 \times \frac{2}{2.1^3} \times \frac{1}{2} \approx 0.0108$$

Our error 0.0119 is consistent with the result.

We can have a more accurate way to estimate the derivative by using a second-order formula.

According to Taylor's Theorem, if f is three times continuously differentriable, then

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(c_1)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(c_2)$$

where $x-h < c_2 < x < c_1 < x+h$.

Subtracting the two equations gives the following three-point formula

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12}f'''(c_1) - \frac{h^2}{12}f'''(c_2)$$

By using the generalized Intermediate Value theorem (see details on Sauer P.255-256), we can rewrite the error term to get the Three-point centered-difference formula:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6}f'''(c)$$

where $x-h < c < x+h$

**Example:** Use the three-point centered-difference formula with $h=0.1$ to approximate the derivative of $f(x) = 1/x$ at $x=2$.

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} = \frac{1/2.1 - 1/1.9}{0.2} \approx -0.2506$$

The error is 0.0006, an improvement from the two-point forward-difference formula.

**Notes on float point computing**

Since we are trying to subtract two nearly equal numbers, it breaks the cardinal rule of floating point computing. There is no way to improve it as finding derivatives is an inherently unstable process.

## Equations for higher derivatives.

Using the Taylor Expansions.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(iv)}(c_1)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(iv)}(c_2)$$

where $x-h < c_2 < x < c_1 < x+h$

Adding the two equations together, we can single out the second derivative.

$$f(x+h) + f(x-h) - 2f(x) = h^2 f''(x) + \frac{h^4}{24}f^{(iv)}(c_1) + \frac{h^4}{24}f^{(iv)}(c_2)$$

Using generalized Intermediate Value Theorem to combine the error, we have Three-Point centered-difference formula for second derivative:

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \frac{h^2}{12}f^{(iv)}(c)$$

for some $c$ between $x-h$ and $x+h$.

## 5.1.2 Rounding Error

The equations we proposed so far all break the advise from Ch.0, and this is the bottle neck of numerical differentiation.

To understand the problem better, we consider the following example.

**Example**: Approximate the derivative of $f(x) = e^x$ at $x = 0$.

Two point: $$f'(x) \approx \frac{e^{x+h} - e^x}{h}$$

Three point: $$f'(x) \approx \frac{e^{x+h} - e^{x-h}}{2h}$$

We know the correct value is $f'(x) = e^x \Rightarrow f'(0) = e^0 = 1$.

(see table on Sauer P. 257)

At the beginning, error decreases as $h$ decreases, but then error starts to increase, and this is caused by losing significance in floating point computation. In addition, it is being magnified by dividing by a small number.

Let's study the effect of rounding errors more generally by analyze the three-point formula.

- Denote floating point version of the input $f(x+h)$ as $\hat{f}(x+h)$. These two values differ by a number on the order of machine precision.
- We also assume $f(x-h)$ & $f(x+h)$ are around 1 so relative & absolute errors are roughly the same.

$$\hat{f}(x+h) = f(x+h) + \epsilon_1 \quad \& \quad \hat{f}(x-h) = f(x-h) + \epsilon_2$$

$$|\epsilon_1|, |\epsilon_2| \approx \epsilon_{mach}$$

Plug these numbers in the three-point formula.

$$f'(x)_{correct} - f'(x)_{machine} = f'(x) - \frac{\hat{f}(x+h) - \hat{f}(x-h)}{2h}$$

$$= f'(x) - \frac{f(x+h) + \epsilon_1 - (f(x-h) + \epsilon_2)}{2h}$$

$$= \left(f'(x) - \frac{f(x+h) - f(x-h)}{2h}\right) + \frac{\epsilon_2 - \epsilon_1}{2h}$$

$$= \left(f'(x)_{correct} - f'(x)_{formula}\right) + \text{error}_{rounding}$$

Three sources of error

1. truncation error (from floating point representation)
2. difference between correct derivative and correct approximating formula.
3. rounding error (loss of significance of the computer-implemented formula).

The rounding error has absolute value.

$$\left|\frac{\epsilon_2-\epsilon_1}{2h}\right| \leq \frac{2\epsilon_{mach}}{2h} = \frac{\epsilon_{mach}}{h}$$

$\epsilon_{mach}$ : Machine precision

Therefore, the absolute value of the error of the machine approximation of $f'(x)$ is bounded above by

$$E(h) \equiv \underbrace{\frac{h^2}{6} f'''(c)}_{\text{error from formula approximation}} + \underbrace{\frac{\epsilon_{mach}}{h}}_{\text{rounding error}} \qquad x-h < c < x+h$$

We can find the minimum value of $E(h)$ by solving $E'(h)=0$.

$$E'(h) = \frac{M}{3}h - \frac{\epsilon_{mach}}{h^2} = 0 \qquad |f'''(c)| \approx |f'''(x)| = M$$

Solve $h$ for the above equation, we get

$$h = (3\epsilon_{mach}/M)^{1/3}$$

What does this value mean?

When $h > (3\epsilon_{mach}/M)^{1/3}$ (or, we can assume $M$ is order one here, so $h > (3\epsilon_{mach})^{1/3} \approx 10^{-5}$ in double precision), decreasing $h$ will increase the accuracy of the algorithm.

When $h < (3\epsilon_{mach}/M)^{1/3}$, decreasing $h$ may increase the error of the algorithm.

### 5.1.3 Extrapolation

If you are interested, read Sauer P. 259-260.

### In class exercise: