L28: Numerical Differentiation

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E7 Spring 2017, University of California at Berkeley

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Version: release

Welcome Back!
I hope you had a great Spring Break!

Image by Anita Martinz, retrieved from https://en.wikipedia.org/wiki/File:Colorful_spring_garden.jpg on April 2nd 2017

Announcements

Lab 10 is due on April 7 at 12 pm (noon)

Question 2, test case 1: it is okay if `coefficients(4,5)` is `0`

`coefficients(4,5)` is correct if `abs(coefficients(4,5)) < 1e-15`

Today:

- Numerical Differentiation (Chapter 17)

Wednesday (April 5):

- Numerical Integration (Chapter 18)

Friday (April 7):

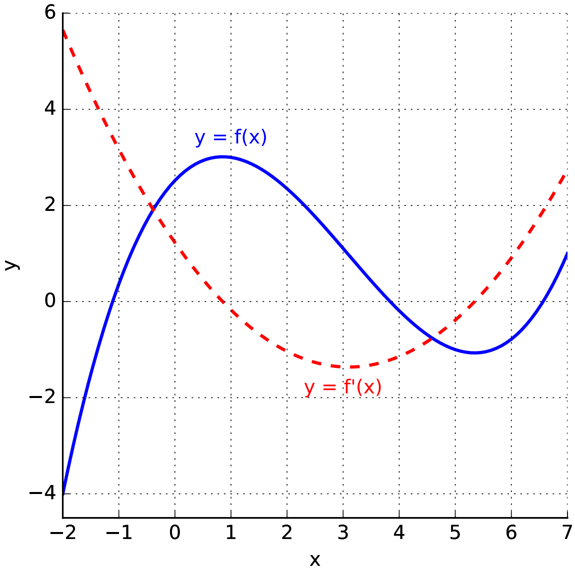
- Project discussion, tips, and recommendation
- Other discussion

Programming project:

- **Due on April 28 at 11:59 pm**
- Instructions are available on bCourses
- "Random" components were removed from the project

Warm-up: draw derivatives by hand

Can you draw the derivative of this function?



Warm-up: draw derivatives by hand

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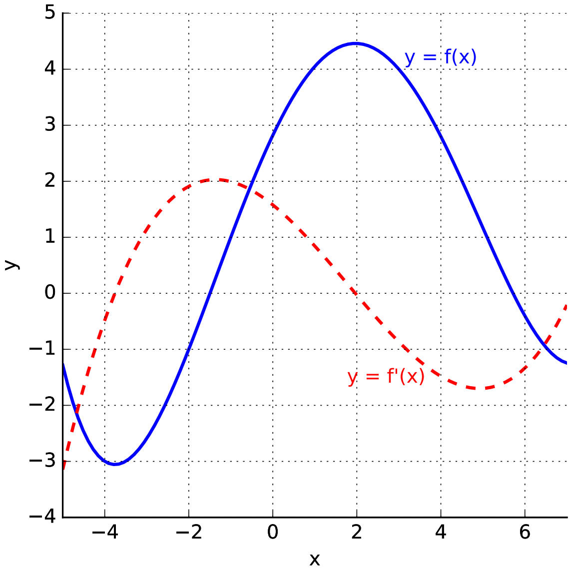
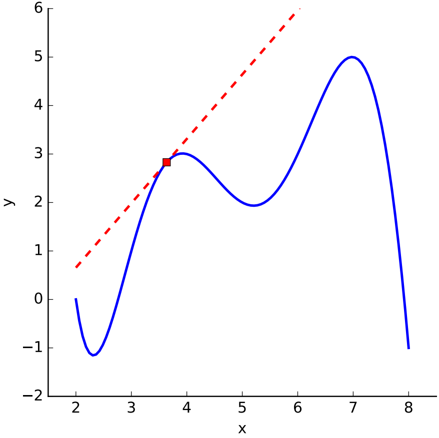


Definition of the derivative

Consider a function f that is differentiable at x

The derivative $f'(x)$ of f at x measures the **local rate of change of f**

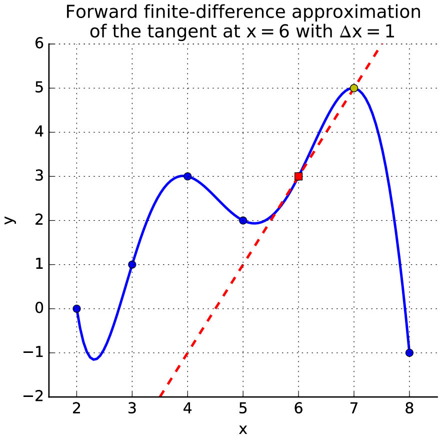
$$
\begin{aligned}
f'(x) &= \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \\
&= \lim_{\text{run} \to 0} \frac{\text{rise}}{\text{run}} \\
&= \text{slope of the tangent at } x
\end{aligned}
$$



Examples:

- Velocity measures the rate of change of the location
- Acceleration measures the rate of change of the velocity

Task: estimate the derivative of this function at $x = 6$



Choice 1:

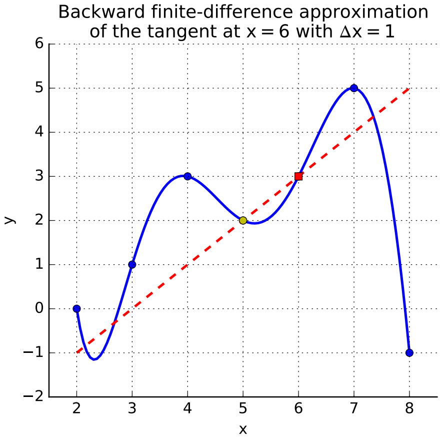
Use values at $x = 6$ and $x = 7$

$$\text{slope} = \frac{\text{rise}}{\text{run}}$$

$$\text{slope} \approx \frac{f(7) - f(6)}{7 - 6}$$
$$= \frac{5 - 3}{7 - 6} = 2$$

We just used a forward finite-difference approximation!

Task: estimate the derivative of this function at $x = 6$



Choice 2:

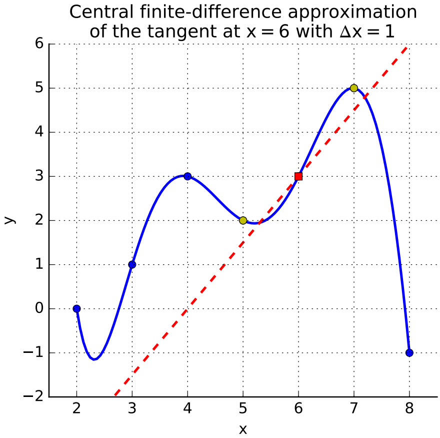
Use values at $x = 6$ and $x = 5$

$$\text{slope} = \frac{\text{rise}}{\text{run}}$$

$$\text{slope} \approx \frac{f(6) - f(5)}{6 - 5}$$
$$= \frac{3 - 2}{6 - 5} = 1$$

We just used a backward finite-difference approximation!

Task: estimate the derivative of this function at $x = 6$



Choice 3:

Use values at $x = 5$ and $x = 7$

$$\text{slope} = \frac{\text{rise}}{\text{run}}$$

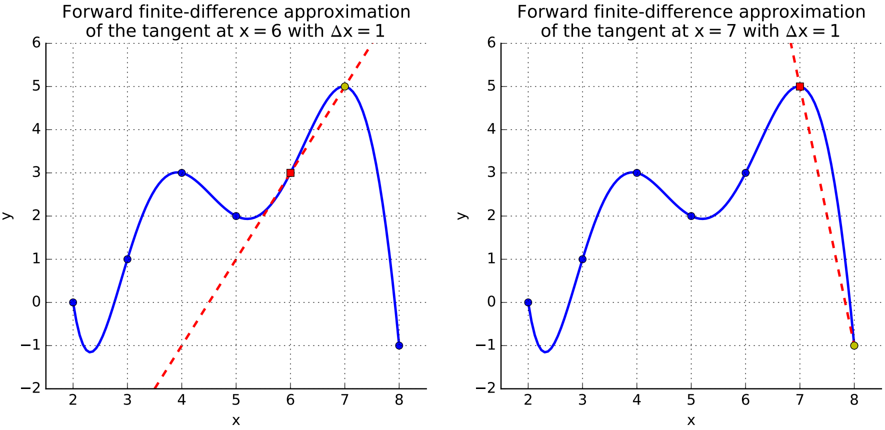
$$\text{slope} \approx \frac{f(7) - f(5)}{7 - 5}$$
$$= \frac{5 - 2}{7 - 5} = 1.5$$

We just used a central finite-difference approximation!

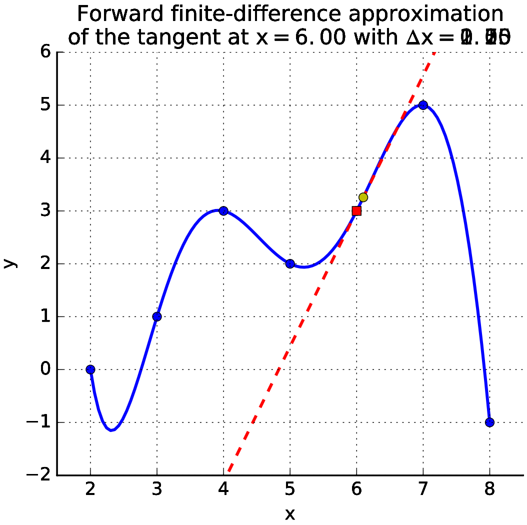
Introduction to finite-difference methods

The accuracy of finite-difference approximations depends on:

- The finite-difference method used
- The function whose derivative we are approximating
- The location at which we are estimating the derivative
- The spacing of the points used



In general, finite-difference approximations become more accurate as the spacing between the points used to calculate the derivative is reduced



Introduction to finite-difference methods

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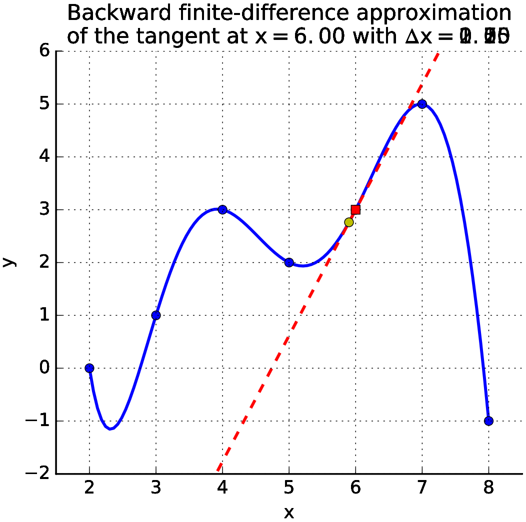

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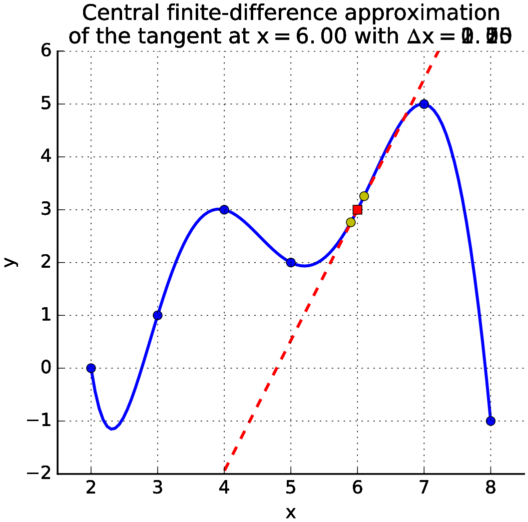


Finite-difference approximations: the math

Finite-difference approximations are derived by "combining" different Taylor series expansions of the function of interest

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \dots$$

Consider a set of m equally-spaced data points of coordinates (x_i, y_i), $i \in \{1, 2, \dots, m\}$. Call Δx the spacing between consecutive points

$$f(x_{i+1}) = f(x_i) + \frac{f'(x_i)}{1!}\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \dots$$

$$f(x_{i-1}) = f(x_i) + \frac{f'(x_i)}{1!}(-\Delta x) + \frac{f''(x_i)}{2!}(-\Delta x)^2 + \frac{f'''(x_i)}{3!}(-\Delta x)^3 + \dots$$

Finite-difference approximations: the math

$$f(x_{i+1}) = f(x_i) + \frac{f'(x_i)}{1!}\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \ldots \quad (1)$$

$$f(x_{i-1}) = f(x_i) - \frac{f'(x_i)}{1!}\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \ldots \quad (2)$$

From (1), obtain the first-order forward finite-difference approximation:

$$\begin{aligned} f'(x_i) &= \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{f''(x_i)}{2!}\Delta x - \frac{f'''(x_i)}{3!}(\Delta x)^2 - \ldots \\ &= \frac{f(x_{i+1}) - f(x_i)}{\Delta x} + \mathcal{O}(\Delta x) \\ &\approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x} \end{aligned}$$

Finite-difference approximations: the math

From (2), obtain the first-order backward finite-difference approximation:

$$
\begin{aligned}
f'(x_i) &= \frac{f(x_i) - f(x_{i-1})}{\Delta x} + \frac{f''(x_i)}{2!}\Delta x - \frac{f'''(x_i)}{3!}(\Delta x)^2 - \dots \\
&= \frac{f(x_i) - f(x_{i-1})}{\Delta x} + \mathcal{O}(\Delta x) \\
&\approx \frac{f(x_i) - f(x_{i-1})}{\Delta x}
\end{aligned}
$$

From (1) and (2), obtain the second-order central finite-difference approximation:

$$
\begin{aligned}
f'(x_i) &= \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} - \frac{f'''(x_i)}{3!}(\Delta x)^2 - \frac{f'''''(x_i)}{5!}(\Delta x)^4 - \dots \\
&= \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + \mathcal{O}((\Delta x)^2) \\
&\approx \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}
\end{aligned}
$$

Error term and order of the approximation

Forward approximation:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} + \mathcal{O}(\Delta x)$$
$$\approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x}$$

Central approximation:

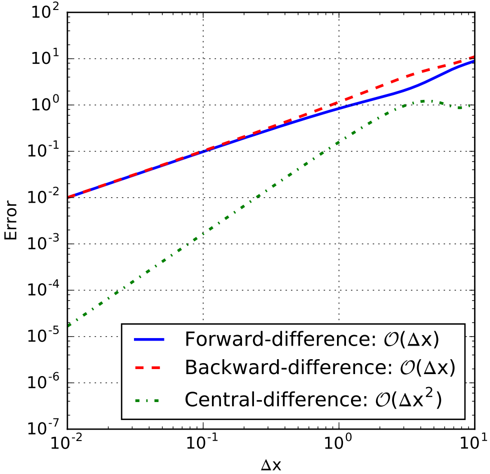
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + \mathcal{O}((\Delta x)^2)$$
$$\approx \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}$$

The error term ($\mathcal{O}(\Delta x)$, $\mathcal{O}((\Delta x)^2)$, $\mathcal{O}((\Delta x)^n)$, etc.):

- Is made up of the remaining terms resulting from combining the Taylor series (n: exponent of Δx in the lowest-order term)
- **Describes how the error varies with the size of Δx**
  - **$\mathcal{O}((\Delta x)^n)$: the error is roughly proportional to $(\Delta x)^n$ (We say that the method is of order n)**

Error term and order of the approximation

Error versus Δx for different finite-difference approximations, when calculating the derivative of $x \mapsto \sin(x) + x^2$ at $x = 0$



The slope of the line in a log-log plot indicates the order of the method

IMPORTANT practice question

We use a 2^{nd}- and a 4^{th}-order finite-difference formula to estimate the derivative of a function, using equally-spaced points (spacing is Δx).

Which of the following statements are true?

(A) The error made when using the 4^{th}-order formula is always smaller than the error made when using the 2^{nd}-order formula

(B) On average, if we reduce Δx by a factor of 2, the error made when using the 2^{nd}-order formula is divided by 4

(C) On average, if we reduce Δx by a factor of 2, the error made when using the 4^{th}-order formula is divided by 4

(D) On average, if we reduce Δx by a factor of 2, the error made when using the 4^{th}-order formula is divided by 16

(E) The error made when using the 4^{th}-order formula is always twice as small as the error made when using the 2^{nd}-order formula

Higher-order formulae and higher-order derivatives

One can obtain **higher-order formulae** by using more data points and/or by combining more Taylor series expansions. For example (see textbook for derivations):

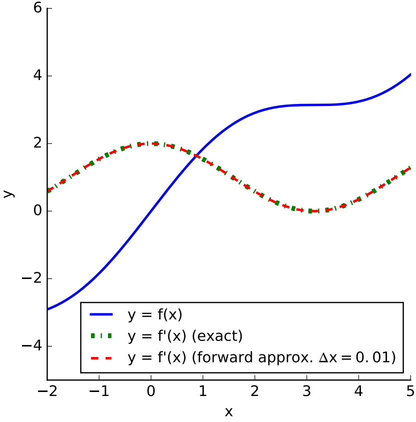
$$f'(x_i) = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12\Delta x} + \mathcal{O}((\Delta x)^4)$$

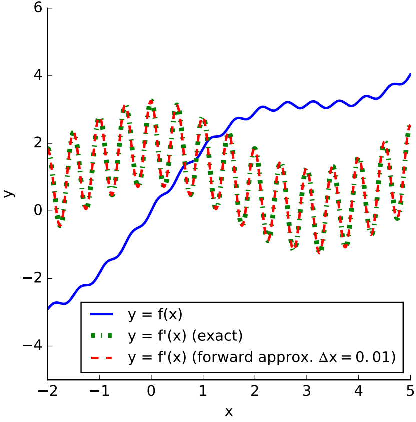
One can obtain **formulae for higher-order derivatives** by using more data points and/or by combining more Taylor series expansions. For example (see textbook for derivations):

$$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{(\Delta x)^2} + \mathcal{O}((\Delta x)^2)$$

Differentiation is very sensitive to noise in the original function

For example:





Consider using linear regression before calculating the derivative?