Chapter 4: Numerical Differentiation and Integration

Lecture 1:

Numerical Differentiation

Motivation

Example: Money flow into a branch of a bank in different days is given in Table

Question: Estimate money flow rate in 2^{nd} and in 3^{rd} days

Time (working days)	Money (million $)
1	3.2
2	4.8
4	9.5
7	18.8

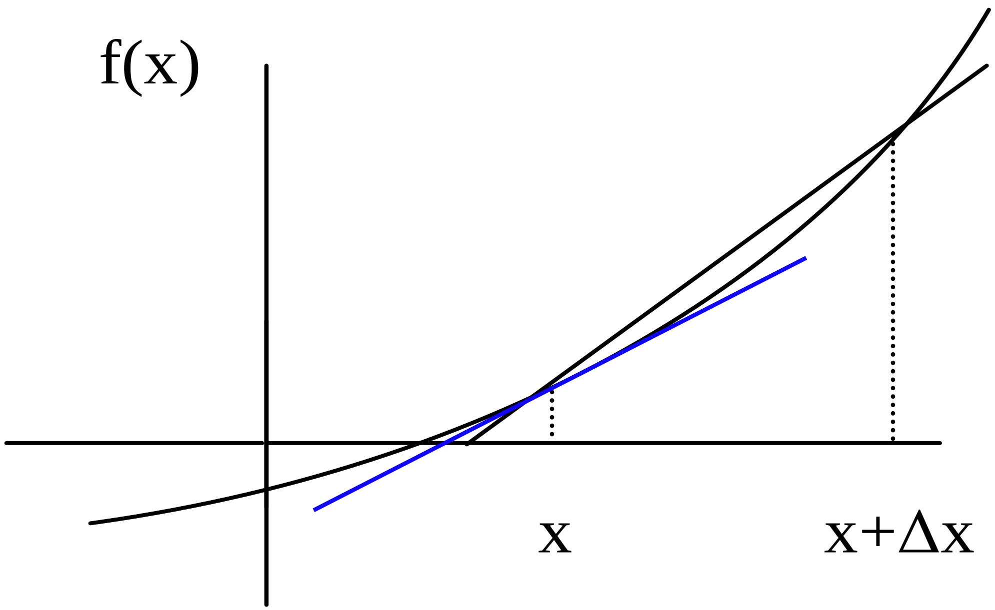
Aim: Approximate derivatives of tabulated or "complicated" functions

Forward Difference Approximation

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For small $\Delta x > 0$:

$$\boxed{f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}}$$

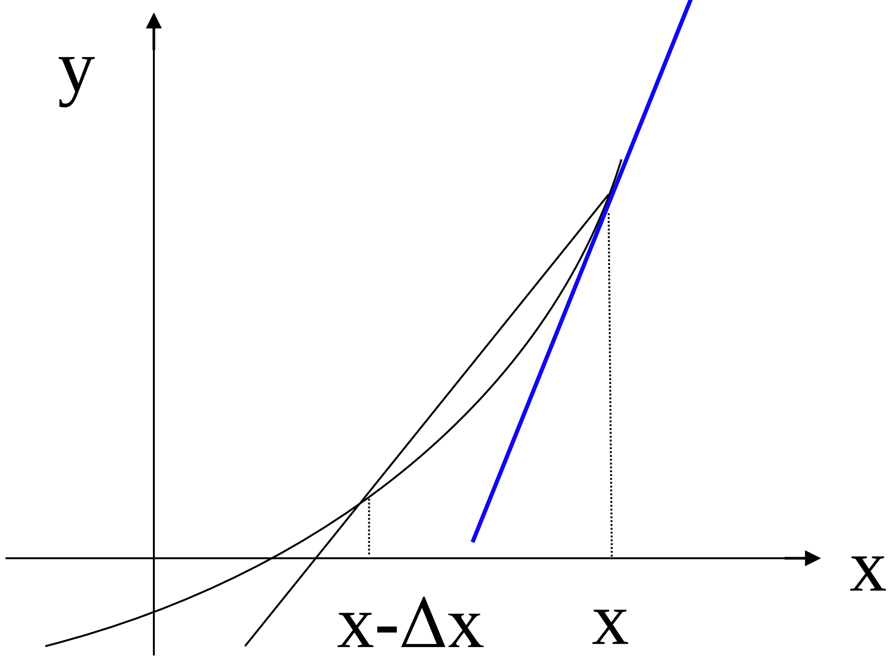


Backward Difference Approximation

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For small $\Delta x > 0$:

$$\boxed{f'(x) \approx \frac{f(x) - f(x-\Delta x)}{\Delta x}}$$



Derive the forward difference approximation from Taylor series

Taylor series expansion of a function for x near x_0:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \ldots = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

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

Substituting for convenience $\Delta x = x_{i+1} - x_i$

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

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

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

$$\boxed{\begin{gathered} f(x) = g(x) + O(x) \Leftrightarrow \\ |\, f(x) - g(x) \,| \leq K\,|\,x\,| \text{ as } x \to 0 \end{gathered}}$$

Derive the central difference approximation from Taylor series

$$x_{i-1} = x_i - \Delta x, \quad x_{i+1} = x_i + \Delta x, \quad x_{i+k} = x_i + k\Delta x$$

From Taylor series

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

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

Subtracting equation (2) from equation (1)

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

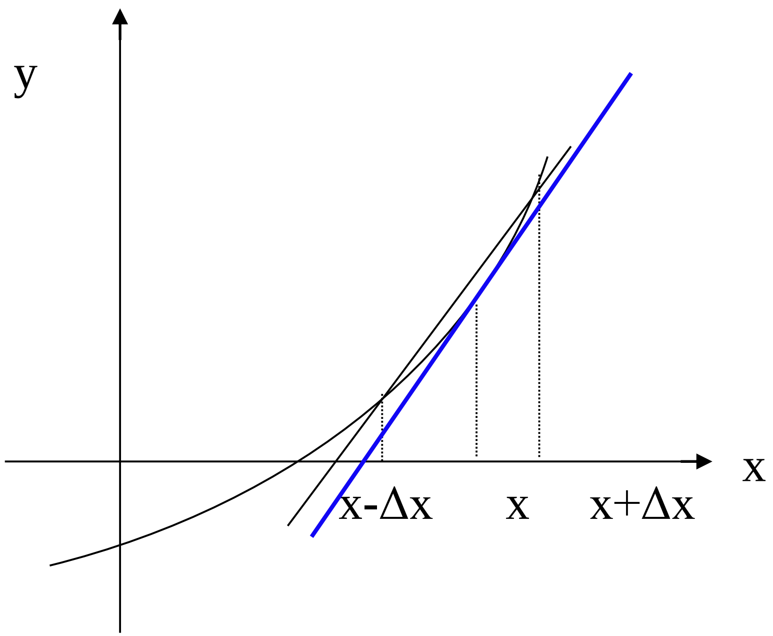
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} - \frac{f'''(x_i)}{3!}(\Delta x)^2 + \ldots = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + O(\Delta x)^2$$

Central Difference Approximation:

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

Central Difference Approximation

$$\boxed{f'(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}}$$



Example

Use FDA, BDA, and CDA to estimate the derivative and calculate the corresponding error

$$f(x) = x^3 + 2x^2 - 3x + 4$$

at $x_0 = 1$, use $\Delta x = 0.1$

Solution: Exact value

$$f(x) = x^3 + 2x^2 - 3x + 4$$

$$f'(x) = 3x^2 + 4x - 3$$

$$f'(1) = 3 + 4 - 3 = 4$$

Approximations of the derivative

$$\boxed{\begin{array}{l} f(x) = x^3 + 2x^2 - 3x + 4 \\ \text{at } x_0 = 1, \text{ use } \Delta x = 0.1 \end{array}}$$

$$\text{FDA: } f'(1) \approx \frac{f(1+\Delta x) - f(1)}{\Delta x} = \frac{f(1.1) - f(1)}{0.1} = \frac{4.4510 - 4}{0.1} = 4.51$$

$$E_1 = 4 - 4.51 = \text{-}0.51, \quad |\varepsilon_1| = \frac{0.51}{4} = 0.1275 = 12.75\%$$

$$\text{BDA: } f'(1) \approx \frac{f(1) - f(1-\Delta x)}{\Delta x} = \frac{f(1) - f(0.9)}{0.1} = \frac{4 - \ 3.6490}{0.1} = 3.51$$

$$\mathrm{E}_2 = 4 - 3.51 = 0.49 \quad |\varepsilon_2| = \frac{0.49}{4} = 0.1225 = 12.25\%$$

$$\text{CDA: } f'(1) \approx \frac{f(1+\Delta x) - f(1-\Delta x)}{2\Delta x} = \frac{f(1.1) - f(0.9)}{0.2} = \frac{4.451 - 3.649}{0.2} = 4.01$$

$$\mathrm{E}_3 = 4 - 4.01 = -0.01 \quad |\varepsilon_3| = \frac{0.01}{4} = 0.0025 = 0.25\%$$

Approximations of Higher Derivatives

One can use Taylor series to approximate higher order derivatives

For example $\quad x_{i+k} = x_i + k\Delta x,\ k = 1,2$

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

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

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

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

Formula of forward and backward difference approximation of 2nd derivative

So we get the **forward difference approximation** of 2nd derivative:

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

Similarly, we get the formula of **backward difference approximation** of 2nd derivative:

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

Central difference approximation of 2nd derivative

$$f\left(x_{i+1}\right)=f\left(x_i\right)+f'\left(x_i\right)\Delta x+\frac{f''\left(x_i\right)}{2!}\left(\Delta x\right)^2+\frac{f'''\left(x_i\right)}{3!}\left(\Delta x\right)^3+\frac{f''''\left(x_i\right)}{4!}\left(\Delta x\right)^4\dots$$

$$f\left(x_{i-1}\right)=f\left(x_i\right)-f'\left(x_i\right)\Delta x+\frac{f''\left(x_i\right)}{2!}\left(\Delta x\right)^2-\frac{f'''\left(x_i\right)}{3!}\left(\Delta x\right)^3+\frac{f''''\left(x_i\right)}{4!}\left(\Delta x\right)^4\dots$$

$$x_{i+1}=x_i+\Delta x,\quad x_{i-1}=x_i-\Delta x$$

Adding these equations gives

$$f\left(x_{i+1}\right)+f\left(x_{i-1}\right)=2f\left(x_i\right)+f''\left(x_i\right)\left(\Delta x\right)^2+f'''\left(x_i\right)\frac{\left(\Delta x\right)^4}{12}+\dots$$

$$f''\left(x_i\right)=\frac{f\left(x_{i+1}\right)-2f\left(x_i\right)+f\left(x_{i-1}\right)}{\left(\Delta x\right)^2}-\frac{f''''\left(x_i\right)\left(\Delta x\right)^2}{12}+\dots=\frac{f\left(x_{i+1}\right)-2f\left(x_i\right)+f\left(x_{i-1}\right)}{\left(\Delta x\right)^2}+O(\left(\Delta x\right)^2)$$

$$\boxed{f''\left(x_i\right)\approx\frac{f\left(x_{i+1}\right)-2f\left(x_i\right)+f\left(x_{i-1}\right)}{\left(\Delta x\right)^2}}$$

HIGH-ACCURACY DIFFERENTIATION FORMULAS

Substitute

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

into

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

we get FDA:

$$\boxed{f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)}$$

CDA:

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

HIGH-ACCURACY DIFFERENTIATION FORMULAS…

Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives (see Textbook)

FDA:

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} + O(h^2)$$

CDA:

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} + O(h^4)$$

Unequally spaced data

We can use 2nd-order Lagrange interpolating polynomial passing though 3 data points

$$(x_{i-1}, f(x_{i-1})),\ (x_i, f(x_i)),\ (x_{i+1}, f(x_{i+1}))$$

Then the derivative is given by:

$$f'(x) = f(x_{i-1})\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})}$$
$$+ f(x_{i+1})\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \quad \text{for } x_{i-1} \le x \le x_{i+1}$$

It is as good as CDA

Partial Derivatives

Partial derivatives along a single dimension are computed in the same fashion as ordinary derivatives

For example, we can use CDA for a function $z = f(x, y)$

$$\frac{\partial f}{\partial x}(x, y) \approx \frac{f(x+\Delta x, y) - f(x-\Delta x, y)}{2\Delta x}$$

$$\frac{\partial f}{\partial y}(x, y) \approx \frac{f(x, y+\Delta y) - f(x, y-\Delta y)}{2\Delta y}$$

Forward difference approximation of partial derivatives:

$$\frac{\partial f}{\partial x}(x,y) \approx \frac{f\left(x+\Delta x, y\right) - f\left(x,y\right)}{\Delta x}$$

$$\frac{\partial f}{\partial y}(x,y) \approx \frac{f\left(x, y+\Delta y\right) - f\left(x,y\right)}{\Delta y}$$

Central difference approximation of second partial derivatives:

$$\frac{\partial^2 f}{\partial x^2}(x,y) \approx \frac{f\left(x+\Delta x, y\right) - 2f\left(x,y\right) + f(x-\Delta x, y)}{(\Delta x)^2}$$

$$\frac{\partial^2 f}{\partial y^2}(x,y) \approx \frac{f\left(x, y+\Delta y\right) - 2f\left(x,y\right) + f(x, y-\Delta y)}{(\Delta y)^2}$$

$$\frac{\partial^2 f}{\partial x \partial y} \approx \frac{f\left(x+\Delta x, y+\Delta y\right) - f(x+\Delta x, y-\Delta y) - f(x-\Delta x, y+\Delta y) + f(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}$$

Example

Use FDA, BDA, and CDA to estimate the second derivative and calculate the corresponding error

$$f(x) = x^3 + 2x^2 - 3x + 4$$

$$\text{at } x_0 = 1, \text{ use } \Delta x = 0.1$$

Solution: Exact value

$$f(x) = x^3 + 2x^2 - 3x + 4$$

$$f'(x) = 3x^2 + 4x - 3$$

$$f''(x) = 6x + 4$$

$$f''(1) = 6 + 4 = 10$$

Approximations of the second derivative

$$\text{FDA: } f''(1) \approx \frac{f(1+2\Delta x) - 2f(1+\Delta x) + f(1)}{(\Delta x)^2} = \frac{f(1.2) - 2f(1.1) + f(1)}{0.01} = 10.6$$

$$E_1 = 10 - 10.6 = -0.6, \qquad |\varepsilon_1| = \frac{0.6}{10} = 0.06 = 6\%$$

$$\text{BDA: } f''(1) \approx \frac{f(1-2\Delta x) - 2f(1-\Delta x) + f(1)}{(\Delta x)^2} = \frac{f(0.8) - 2f(0.9) + f(1)}{0.01} = 9.4$$

$$E_2 = 10 - 9.4 = 0.6, \qquad |\varepsilon_2| = \frac{0.6}{10} = 0.06 = 6\%$$

$$\text{CDA: } f''(1) \approx \frac{f(1+\Delta x) - 2f(1) + f(1-\Delta x)}{(\Delta x)^2} = \frac{f(1.1) - 2f(1) + f(0.9)}{0.01} = 10$$

$$E_3 = 10 - 10 = 0.0$$

Exercise 1

Use FDA, BDA, and CDA to approximate
a) the derivative and
b) second derivative
and *calculate* the error and relative error

$$f(x) = e^{x}(x+1)$$

$$\text{at } x_0 = 1, \text{ use } \Delta x = 0.1$$

Exercise 2

Use FDA, BDA, and CDA to approximate the indicated partial derivatives and calculate the error

$$\frac{\partial f}{\partial x}(x, y), \quad \text{and} \quad \frac{\partial f}{\partial y}(x, y)$$

where $f(x, y) = \ln(\sqrt{x+1} + y^2 + 2)$

at $(x, y) = (0, 0)$, use $\Delta x = \Delta y = 0.1$

Homework Chapter 4: Deadline 3 weeks

$\overline{(m-2)(n-2)}$ is the two last digits of your student ID number

Problem 1: Use FDA, BDA, and CDA to estimate a) the derivative and b) second derivative and *calculate* the corresponding error

$$f(x) = mx^2 e^{nx} \text{ at } x_0 = 1, \text{ use } \Delta x = 0.1$$

Problem 2: Use FDA, BDA, CDA, or an interpolating polynomial if needed, to estimate 1st and 2nd derivatives

x	1	1.2	1.5
y	6+1/n	2/m	8

Homework Chapter 4

Problems 3-5: Problems 23.24, 23.25 in Textbook (page 672)

Problem 23.26

Problem 6: Use FDA, BDA, and CDA to estimate the indicated partial derivatives and and *calculate* the corresponding error

$$f(x,y) = xe^{nx+my}$$

Estimate f_x, f_y, f_{xx}, f_{yy} at $x_0 = m, y_0 = -n,$ use $\Delta x = \Delta y = 0.1$

Homework Chapter 4

Problem 7: Given the integral

$$I = \int_{-2}^{2} e^{-mx^2/n} dx$$

a) Evaluate I using trapezoidal rule with n=6. Estimate the error. How large do we need to choose n such in trapezoidal rule such that $|error| \leq 10^{-8}$?

b) Evaluate I using Simpson's rule with n=6. Estimate the error. How large do we need to choose n such in trapezoidal rule such that $|error| \leq 10^{-8}$?