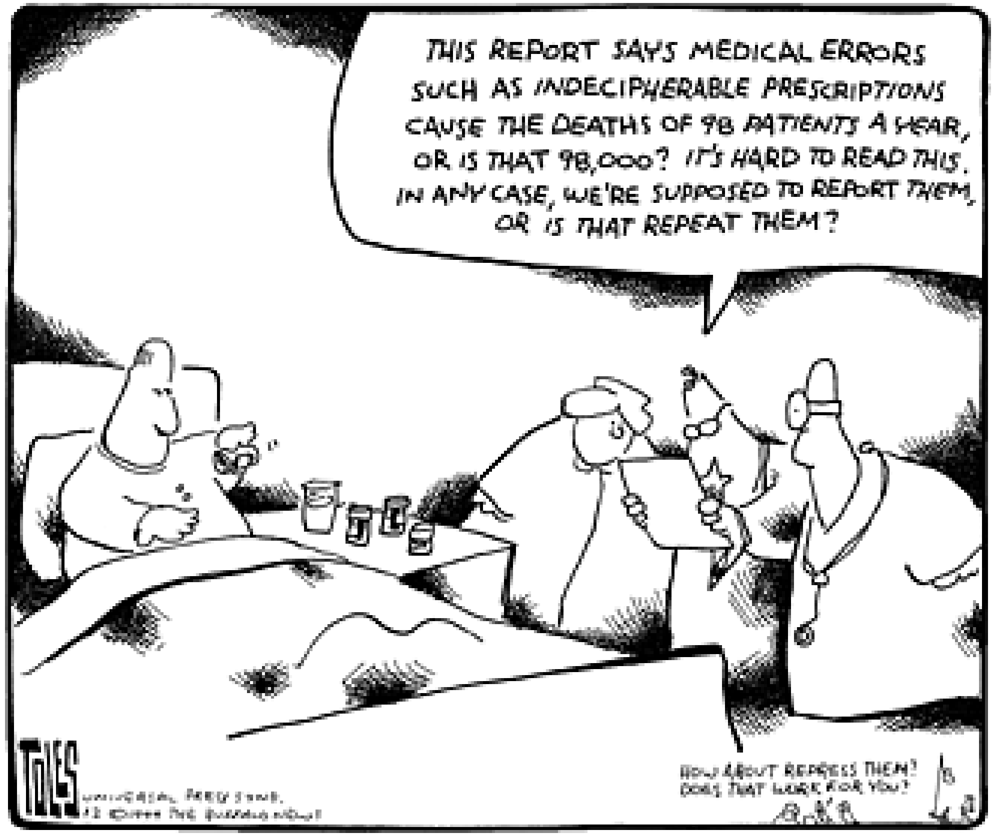
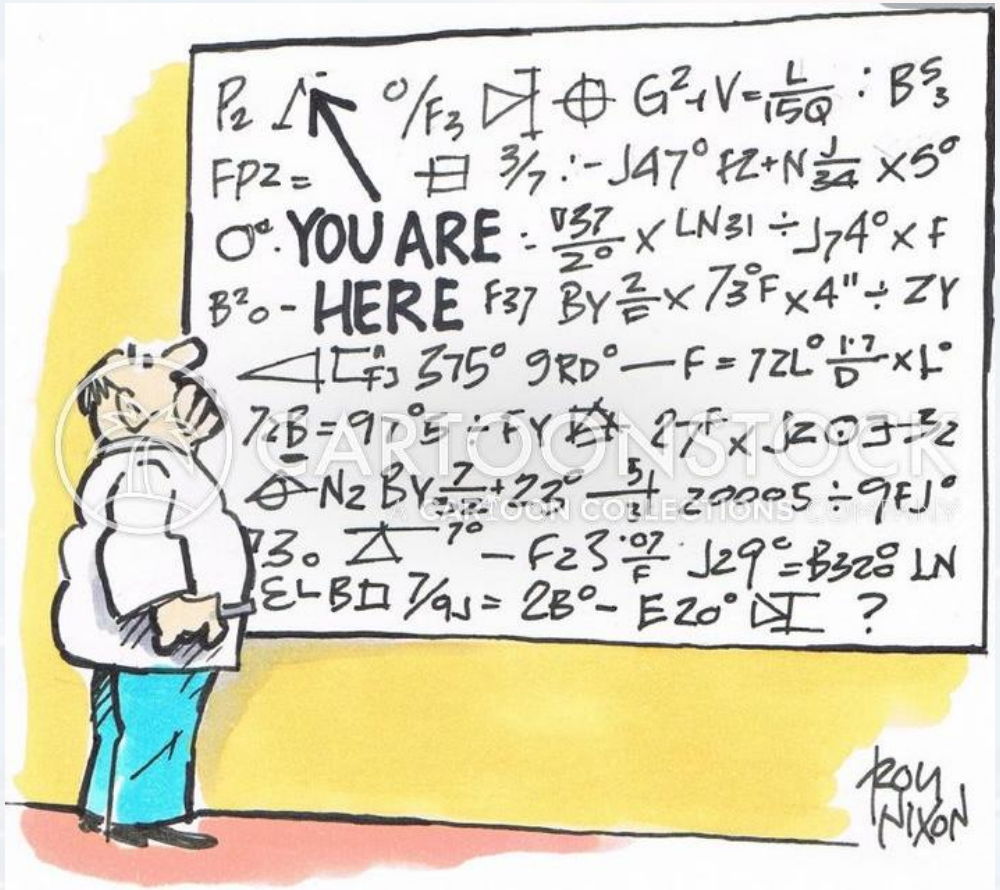
M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



Introduction to Computational Techniques in Physics: syllabus

Week	Date	Topic
1	June 12th	Programming Environment & UIs for Python, Programming Fundamentals
2	*June 19th*	Basic Types in Python
3	June 26th	Parsing, Data Processing and File I/O, Visualization
4	July 3rd	Functions, Map & Lambda
5	July 10th	Random Numbers & Probability Distributions, Interpreting Measurements
6	**July 17th**	**Numerical Integration and Differentiation**
7	July 24th	Root finding, Interpolation
8	July 31st	Systems of Linear Equations, Ordinary Differential Equations (ODEs)
9	Aug 7th	Stability of ODEs, Examples
10	Aug 14th	Final Project Presentations



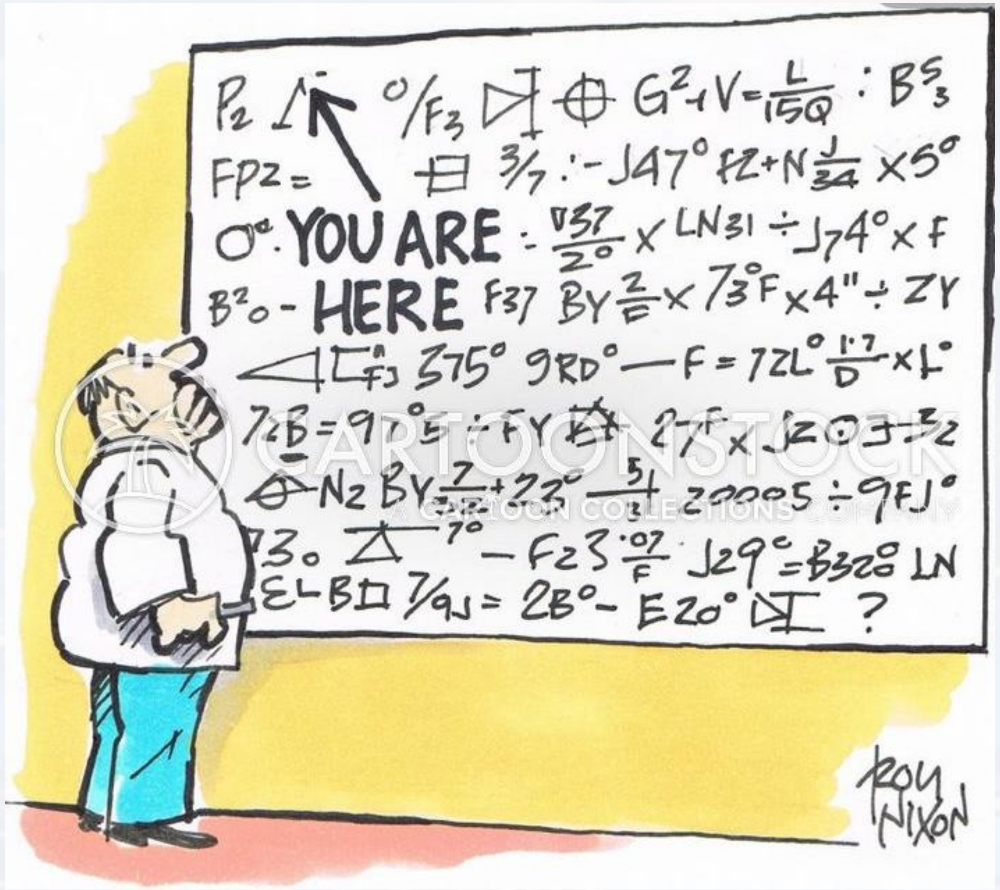
Outline:

Derivatives

Taylor Series

Integrals

Diffusion Example



Outline:

Derivatives

Taylor Series

Integrals

Diffusion Example

motivation:

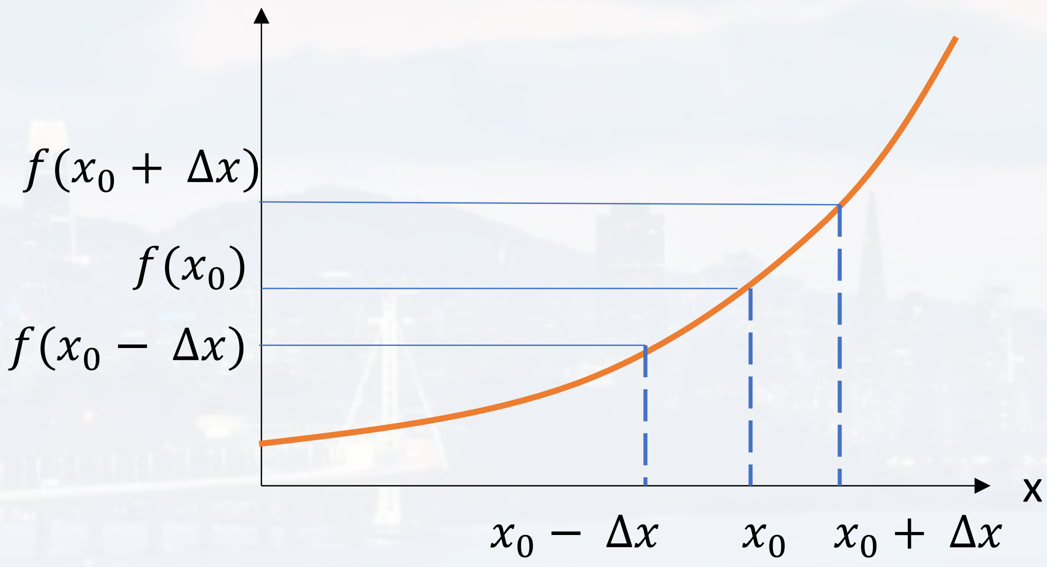
- optimization algorithms (gradient descent and related)
- ANNs learn via **backpropagation** → chain rule
- approximation methods (Taylor series)
- maximum entropy distributions (data analysis, data modelling)
- error estimation and error propagation
- and more…

slope of a function at $x = x_0$

$$\left.\frac{df^+}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

$$\left.\frac{df^-}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x}$$

finite differences Δx & Δy



$$\boxed{\left.\frac{df}{dx}\right|_{x=x_0} = \frac{1}{2}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} + \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}}$$

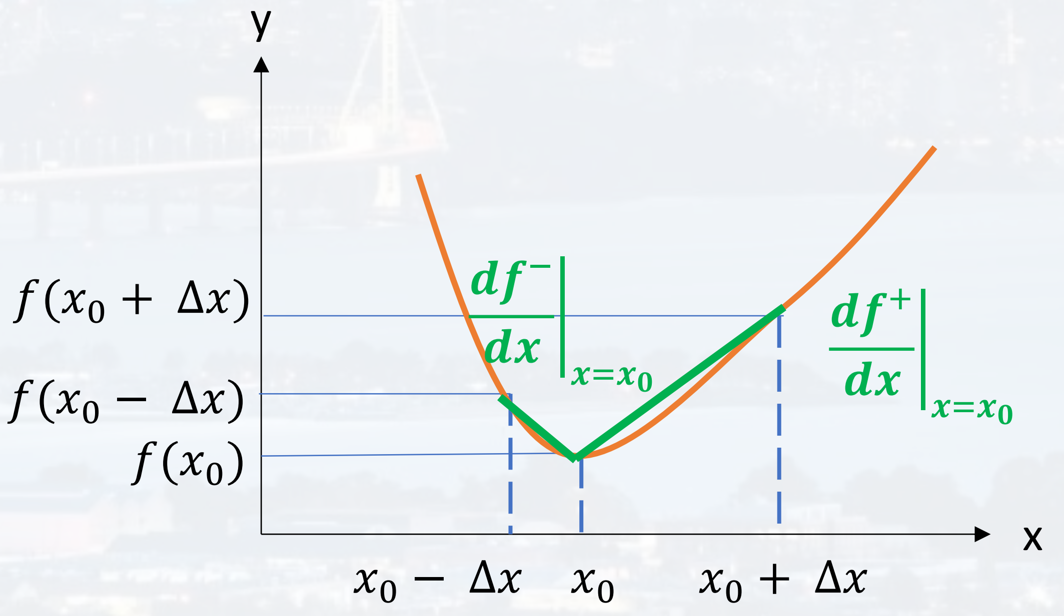
1st derivative at $x = x_0$

$$\left.\frac{df}{dx}\right|_{x=x_0} = \frac{1}{2}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} + \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x\to 0}\frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x}$$

1st derivative at x $= x_0$

change* of the slope of a function at $x = x_0$, aka *curvature

$$\left.\frac{d^2f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x\to 0}\frac{1}{\Delta x}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} - \left.\frac{df^-}{dx}\right|_{x=x_0}\right)$$



$$\boxed{\left.\frac{df}{dx}\right|_{x=x_0} = \frac{1}{2}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} + \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}}$$

1st derivative at x $= x_0$

change of the slope of a function at $x = x_0$, aka *curvature*

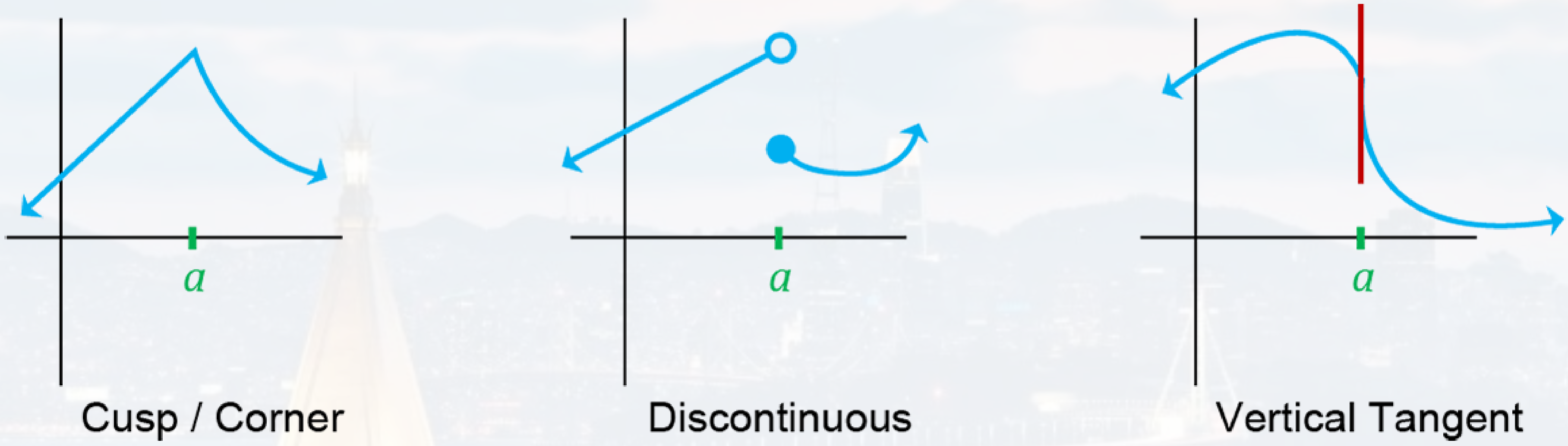
$$\left.\frac{d^2f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{1}{\Delta x}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} - \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2}$$

$$\boxed{\left.\frac{d^2f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2}}$$

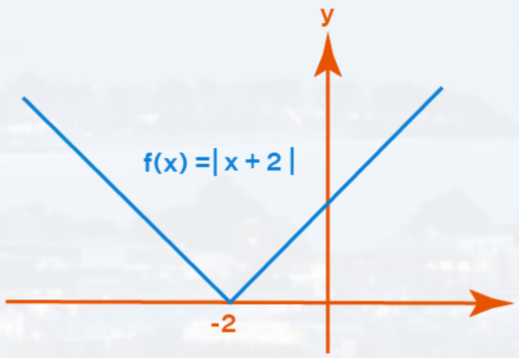
2nd derivative at x $= x_0$

…and so on

derivatives are not always defined:



function needs to be **continuous *and* differentiable**



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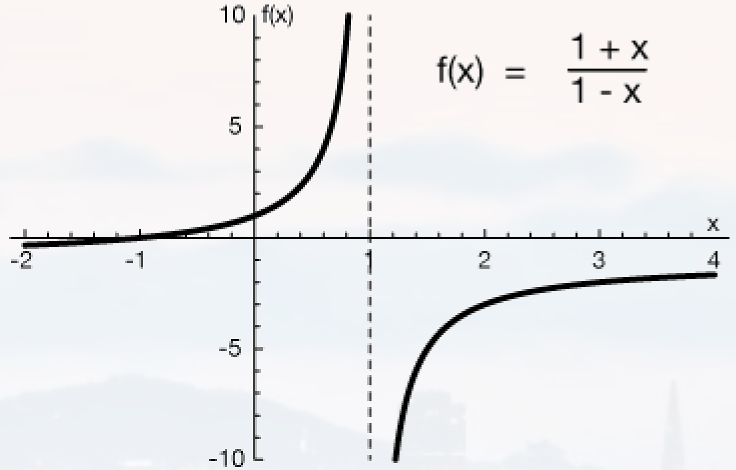
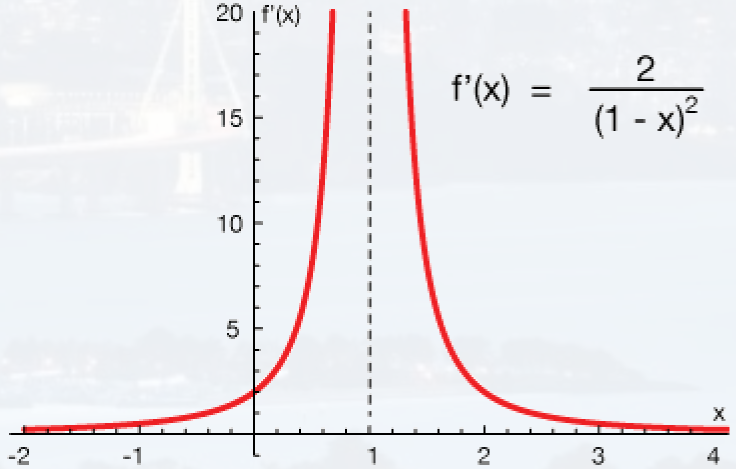




function needs to be **continuous *and* differentiable** example: $f(x) = \sqrt{x}$

$$\left.\frac{df}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{\sqrt{x_0 + \Delta x} - \sqrt{x_0 - \Delta x}}{2\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{\left(\sqrt{x_0 + \Delta x} - \sqrt{x_0 - \Delta x}\right)\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)}{2\,\Delta x\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)}$$

$$= \lim_{\Delta x \to 0} \frac{x_0 + \Delta x - x_0 + \Delta x}{2\,\Delta x\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)}$$

$$= \lim_{\Delta x \to 0} \frac{2\Delta x}{2\,\Delta x\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)} = \frac{1}{2\sqrt{x_0}}$$

$a \in \mathbb{C}$
$n \in \mathbb{R}$

rules: $$\frac{d}{dx}\, a x^n = a\, n x^{n-1}$$

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx} f(x) + \frac{d}{dx} g(x)$$

sum rule: derivatives are linear

$$\frac{d}{dx}[f(x) g(x)] = g(x) \frac{d}{dx} f(x) + f(x) \frac{d}{dx} g(x)$$

product rule

$$\frac{d}{dx} \boldsymbol{f}[\boldsymbol{g}(\boldsymbol{x})] = \frac{df(x)}{dg(x)} \frac{d}{dx} g(x)$$

chain rule

outer derivative **inner derivative**

$a \in \mathbb{C}$
$n \in \mathbb{R}$

special derivatives

$$\frac{d}{dx}\, e^x = e^x$$

the actual definition of e

$$\frac{d}{dx}\, b^x = \ln(b)\, b^x$$

$b > 0$

$$\frac{d}{dx}\, log_b(x) = \frac{1}{x \ln(b)}$$

$$\frac{d}{dx}\, sin(x) = \cos(x)$$

$$\frac{d}{dx}\, cos(x) = -\sin(x)$$

$a \in \mathbb{C}$
$n \in \mathbb{R}$

$$\frac{d}{dx} ax^n = a\, nx^{n-1}$$

$$\frac{d}{dx} 3x^5 = 15x^4$$

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx} f(x) + \frac{d}{dx} g(x)$$

$$\frac{d}{dx}[3x^5 - 2x] = 15x^4 - 2$$

$$\frac{d}{dx}[f(x)g(x)] = g(x)\frac{d}{dx} f(x) + f(x)\frac{d}{dx} g(x)$$

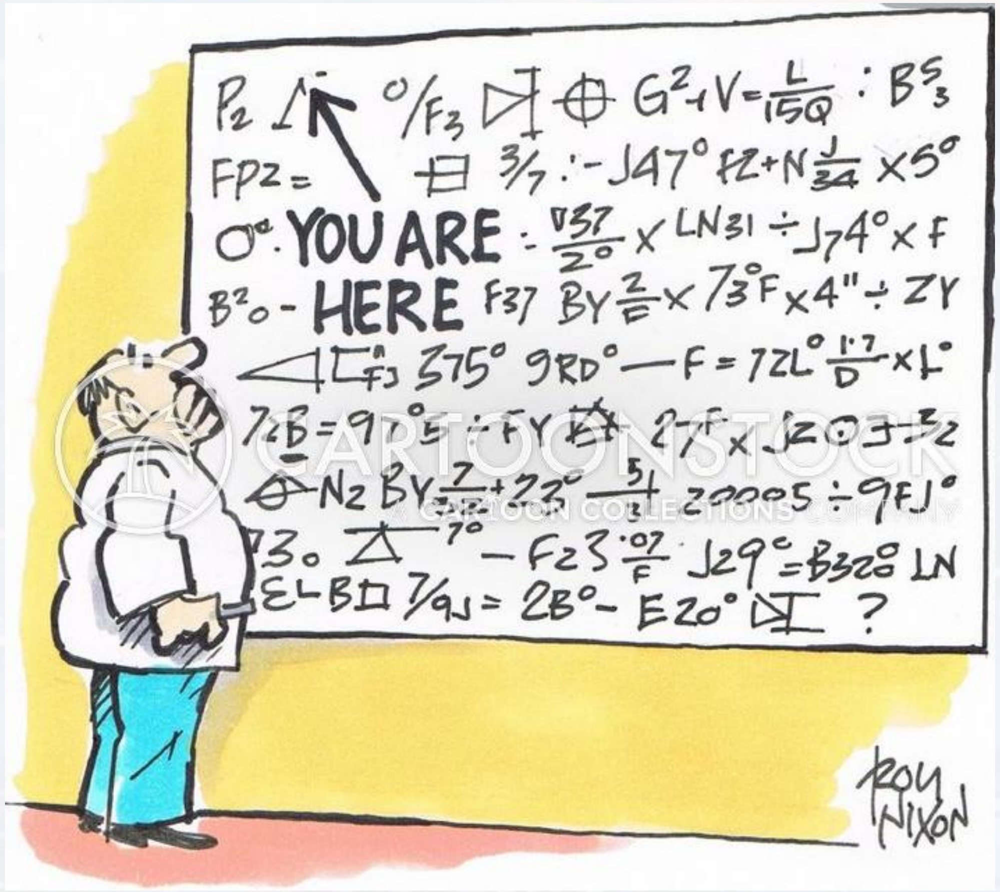
$$\frac{d}{dx}[3x^5 \sin(x)] = 15x^4 \sin(x) + 3x^5 \cos(x)$$

$$\frac{d}{dx} f[g(x)] = \frac{df(x)}{dg(x)} \frac{d}{dx} g(x)$$

outer derivative inner derivative

$$\frac{d}{dx} \sin(3x^5) = \cos(3x^5)\, 15x^4$$

outer derivative inner derivative



Outline:

- Derivatives
- **Taylor Series**
- Integrals
- Diffusion Example

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=x_0} (x - x_0)^n$$

n = 0: $f(x) \approx f(x_0)$

n = 1: $f(x) \approx f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} (x - x_0)$ tangent on f at $x = x_0$

$$\frac{f(x) - f(x_0)}{x - x_0} \approx \left.\frac{df}{dx}\right|_{x=x_0}$$

$$\left.\frac{df^+}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

definition of the 1st derivative!

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=x_0} (x - x_0)^n$$

n = 0: $f(x) \approx f(x_0)$

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n = 2: $f(x) \approx f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} (x - x_0) + \frac{1}{2} \left.\frac{d^2 f}{dx^2}\right|_{x=x_0} (x - x_0)^2$

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=x_0} (x - x_0)^n$$

n = 0: $f(x) \approx f(x_0)$

n = 1: $f(x) \approx f(x_0) + \frac{df}{dx}\Big|_{x=x_0} (x - x_0)$ tangent on f at $x = x_0$

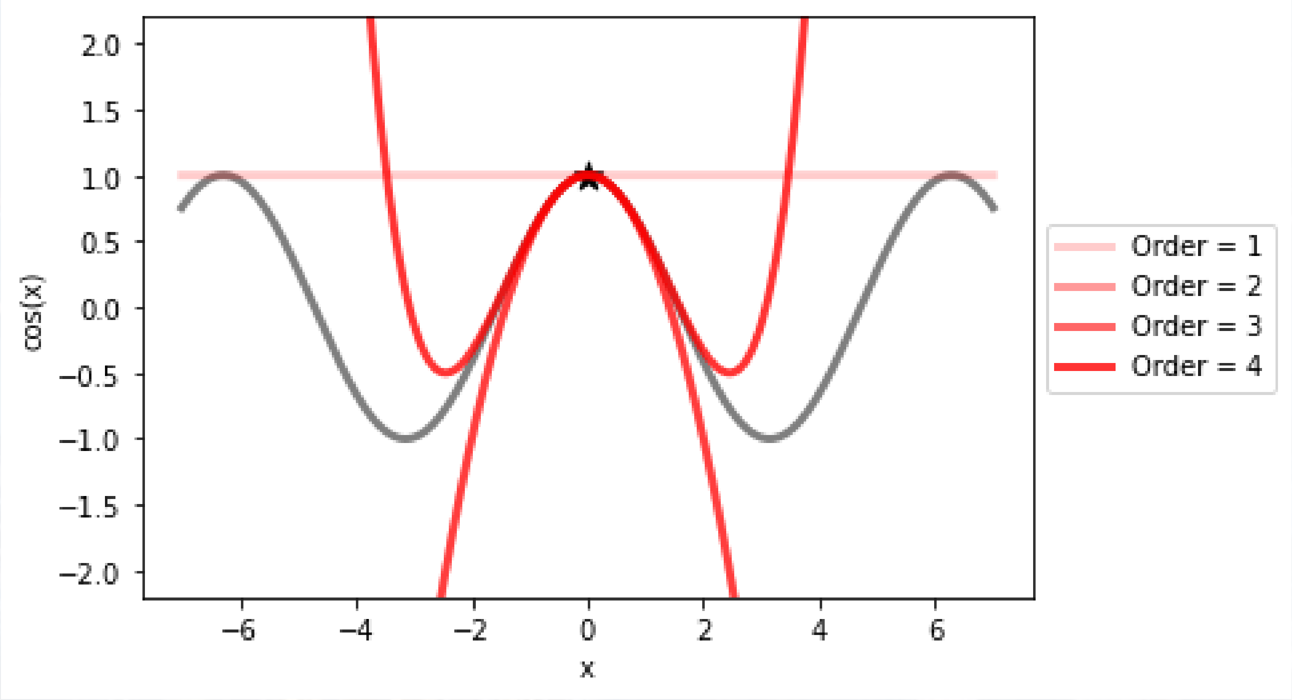
n = 2: $f(x) \approx f(x_0) + \frac{df}{dx}\Big|_{x=x_0} (x - x_0) + \frac{1}{2} \frac{d^2 f}{dx^2}\Big|_{x=x_0} (x - x_0)^2$

<u>exercise:</u>

- write down the Taylor Series of *sin(x)*, *cos(x)* and e^x at $x_0 = 0$
- express all three series as an infinite sum
- try to combine all three equations by introducing a new mathematical object $\boldsymbol{i}$ which only property is $\boldsymbol{i^2 = -1}$

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=x_0} (x - x_0)^n$$

run the function `PlotTaylorSeries.py`



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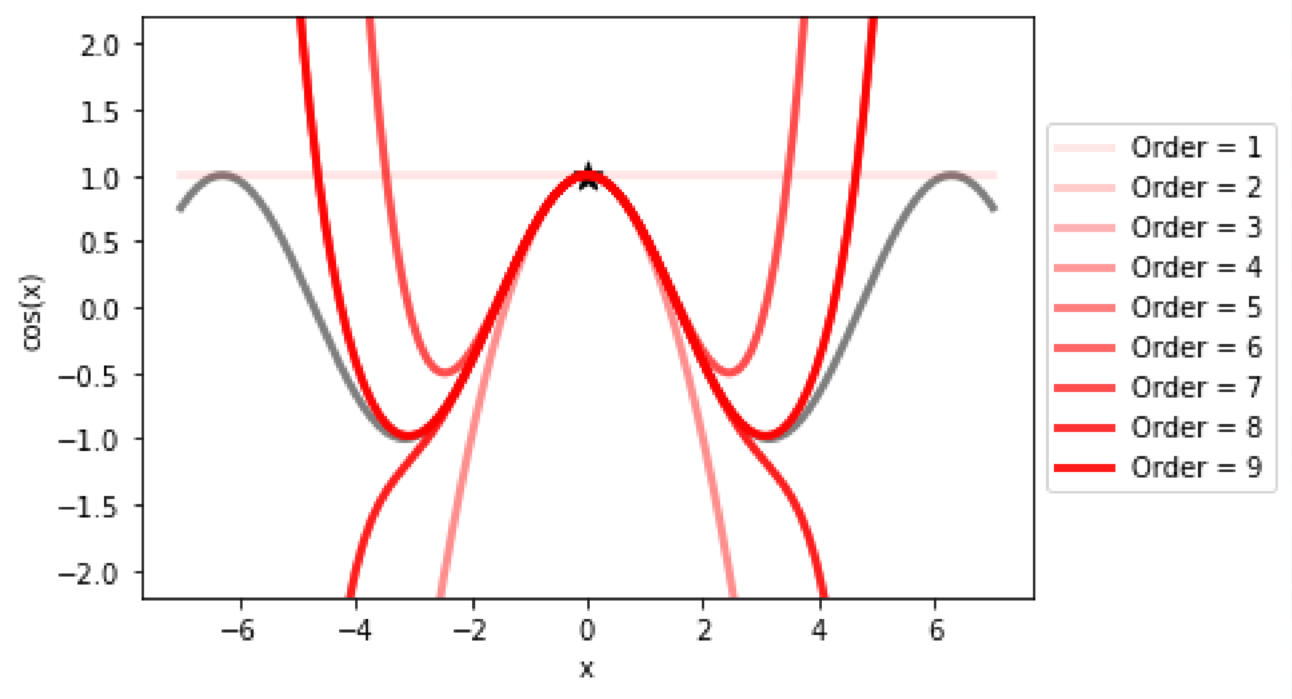

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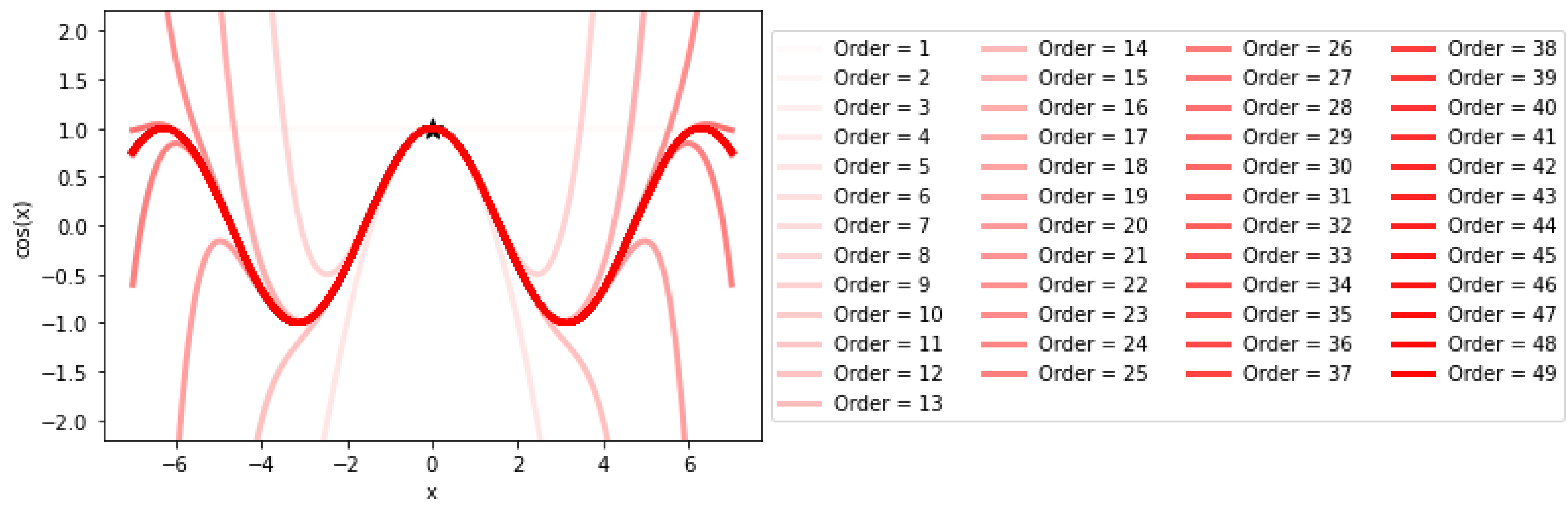
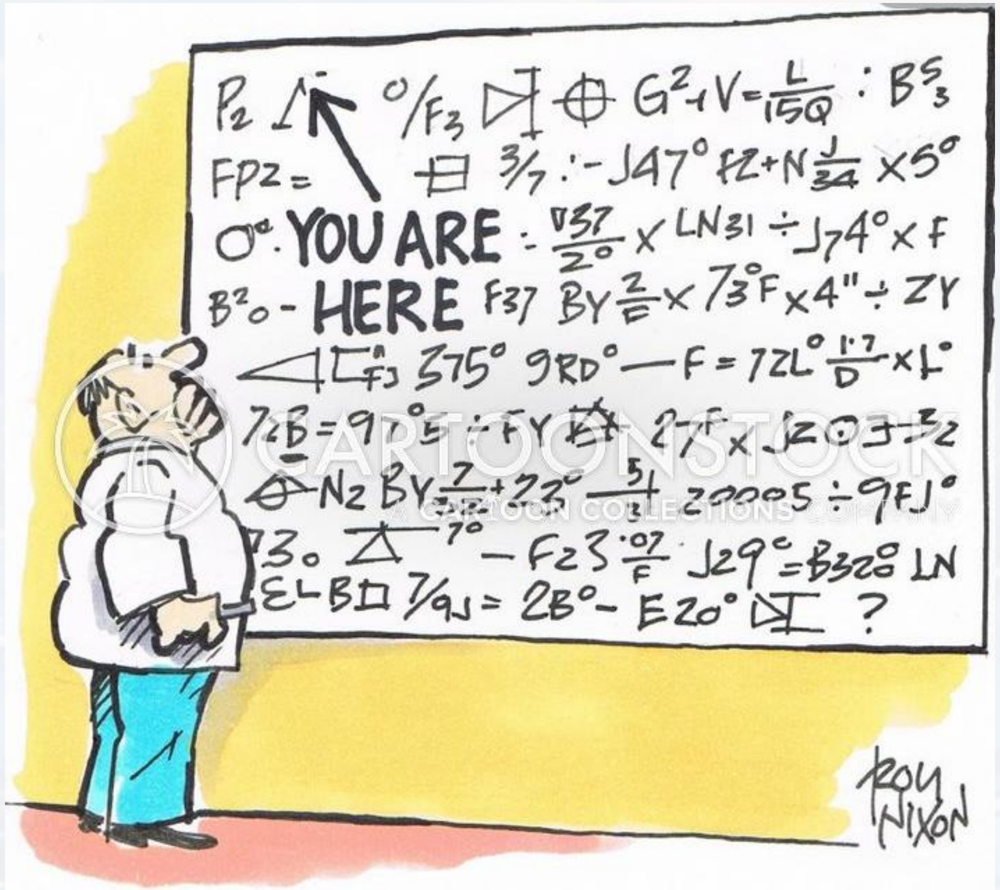




Outline:

- Derivatives
- Taylor Series
- **Integrals**
- Diffusion Example

motivation:

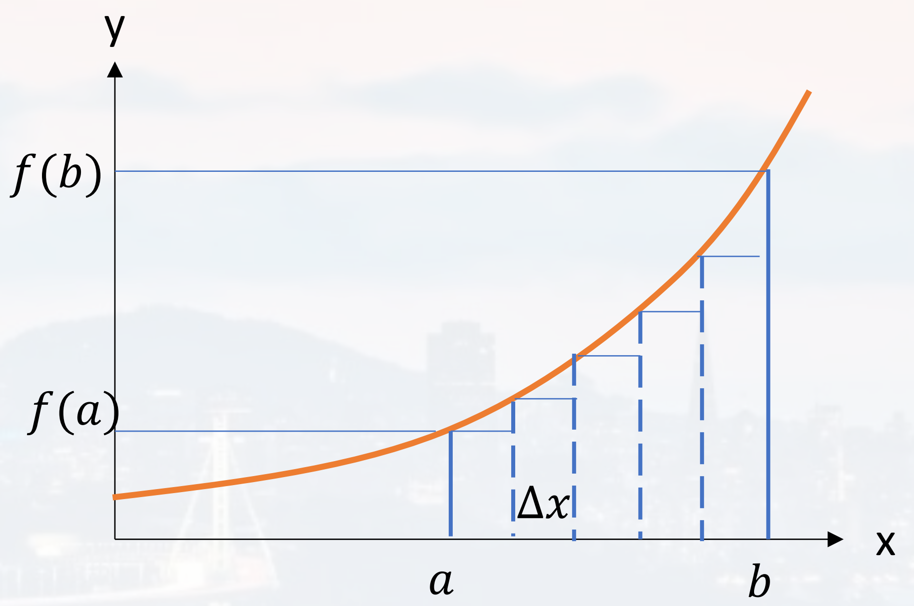
- deriving probabilities from likelihood functions
- normalization tools
- calculating volumes, areas, flow, energy, etc….
- sums → integral

area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx}$$



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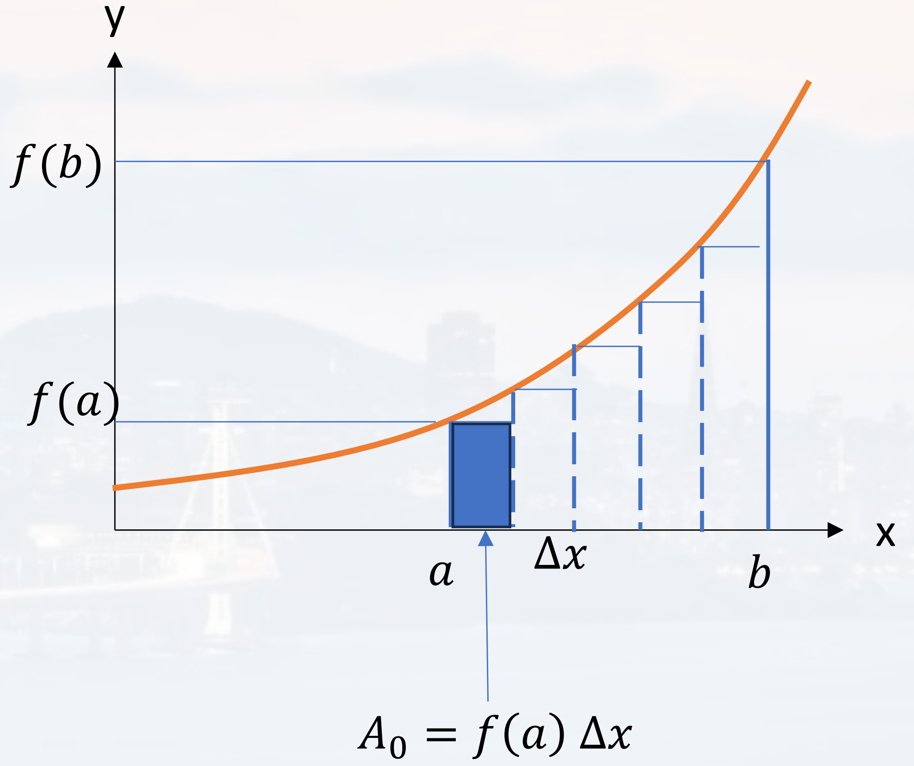
$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a)\,\Delta x$$

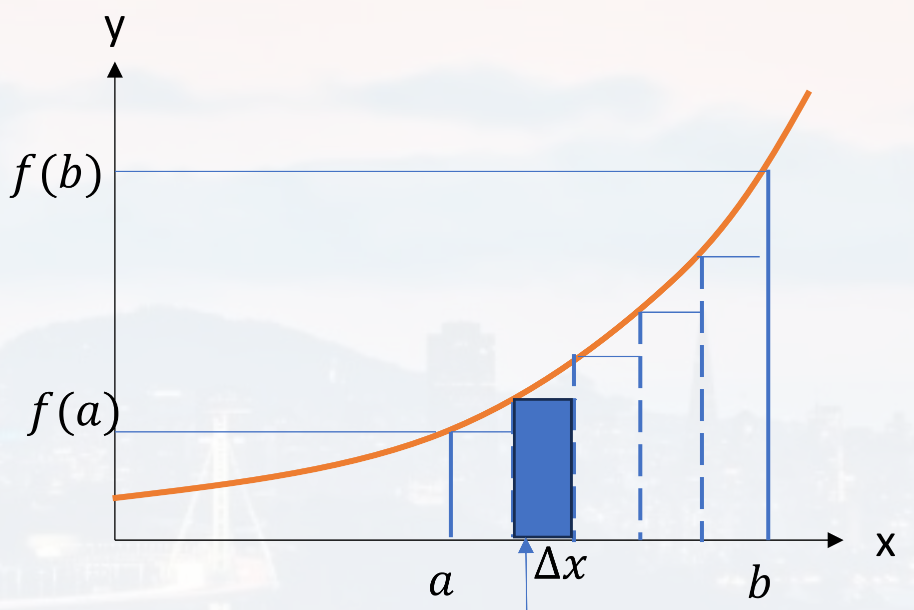


area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b-a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a)\,\Delta x + f(a+\Delta x)\,\Delta x$$



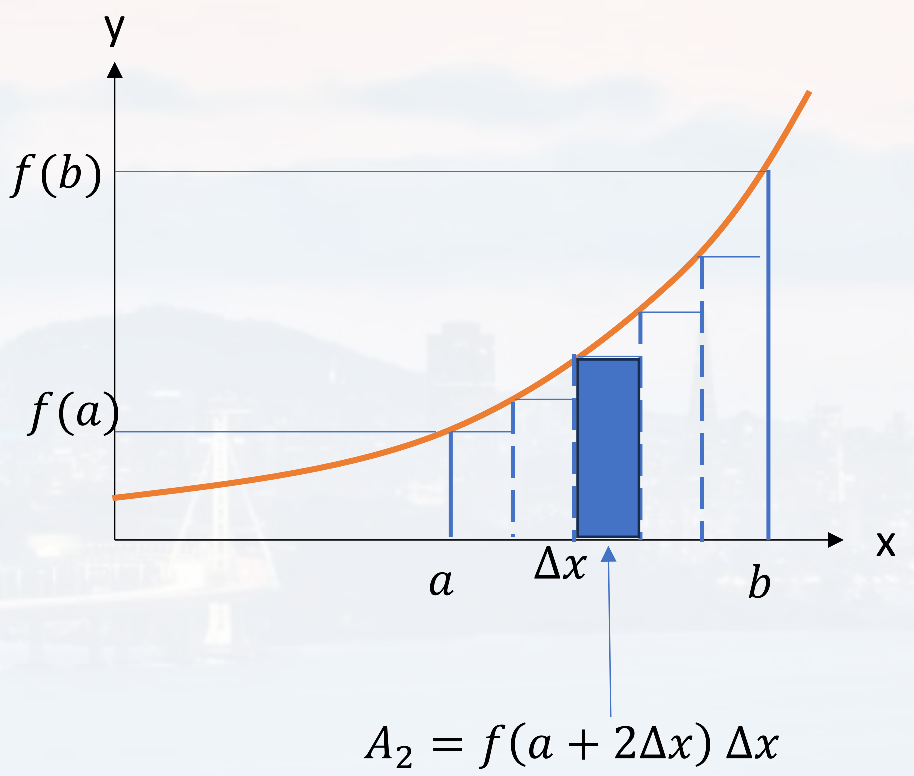
$A_1 = f(a+\Delta x)\,\Delta x$

area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a)\,\Delta x + f(a + \Delta x)\,\Delta x + f(a + 2\Delta x)\,\Delta x$$

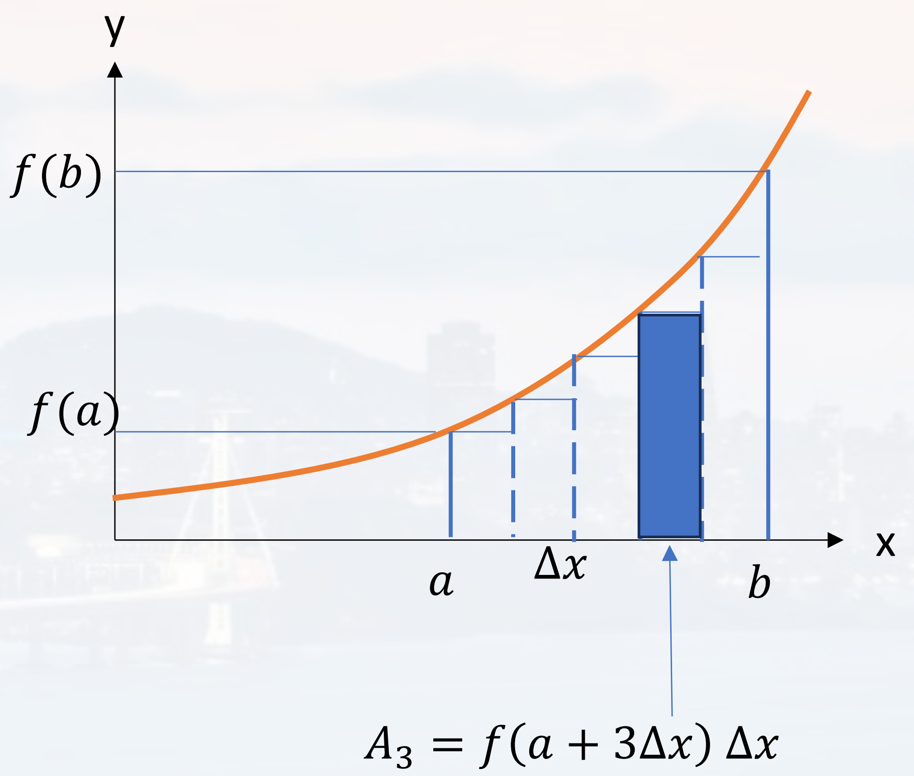


area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b-a}{\Delta x}$$

$$\boxed{A_{tot}} \approx f(a)\,\Delta x + f(a+\Delta x)\,\Delta x + f(a+2\Delta x)\,\Delta x + f(a+3\Delta x)\,\Delta x$$



area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a + \mathbf{0}\Delta x)\,\Delta x$$

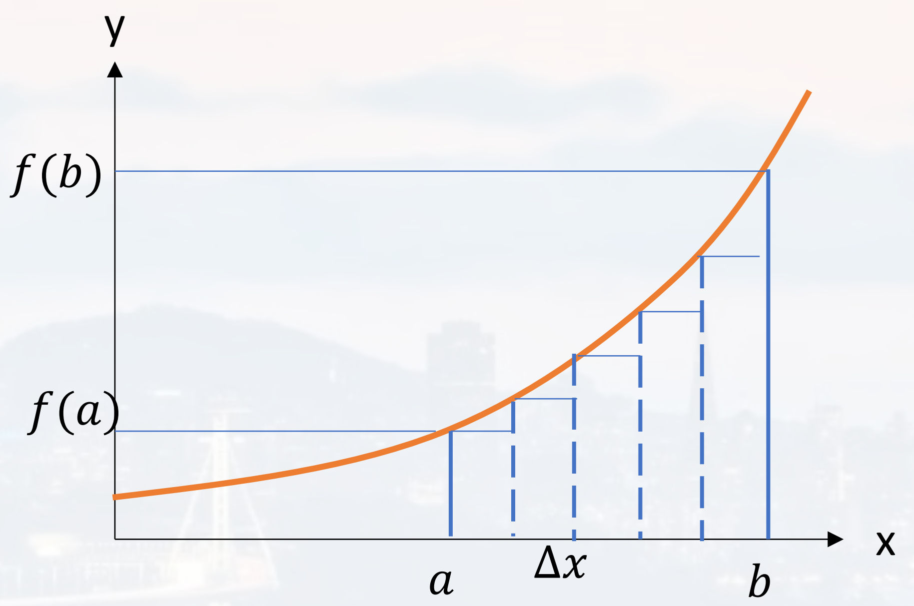
$$+ f(a + \mathbf{1}\Delta x)\,\Delta x$$

$$+ f(a + \mathbf{2}\Delta x)\,\Delta x$$

$$+ f(a + \mathbf{3}\Delta x)\,\Delta x$$

$$+ f(a + \mathbf{4}\Delta x)\,\Delta x$$

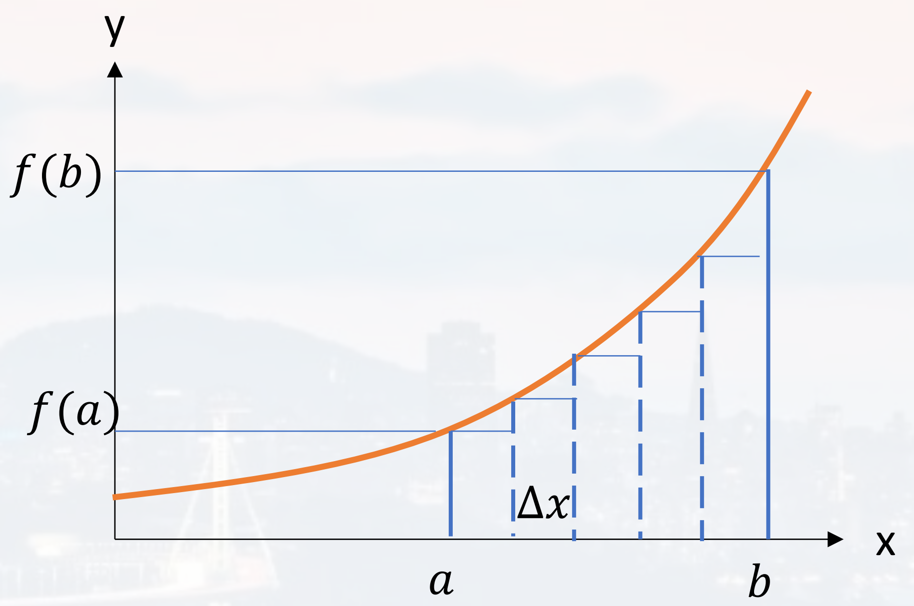
$$+ \cdots \qquad = \sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x$$



area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x$$

$$N = \frac{b-a}{\Delta x}$$



more accurate:

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} [f(a + i\,\Delta x) + f(a + (i+1)\,\Delta x)]\,\frac{\Delta x}{2}$$

trapezoidal rule

error (for large N):

$$\varepsilon = -\frac{(b-a)^2}{12\,N^2}\,[f'(b) - f'(a)] + O(N^{-3})$$

$$\int_a^b f(x)\,dx = \lim_{\Delta x\to 0} \sum_{i=0}^{N-1} [f(a + i\,\Delta x) + f(a + (i+1)\,\Delta x)]\,\frac{\Delta x}{2} \qquad N = \frac{b-a}{\Delta x}$$

example: $f(x) = x^2$

$$\int_a^b x^2\,dx = \lim_{\Delta x\to 0} \sum_{i=0}^{N-1} [(a + i\,\Delta x)^2 + (a + (i+1)\,\Delta x)^2]\,\frac{\Delta x}{2}$$

$$= \lim_{\Delta x\to 0} \sum_{i=0}^{N-1} [2a^2 + i^2\Delta x^2 + 2ai\Delta x + a^2 + (i+1)^2\Delta x^2 + 2a(i+1)\Delta x]\,\frac{\Delta x}{2}$$

$$= \lim_{\Delta x\to 0} \sum_{i=0}^{N-1} [2a^2 + i^2\Delta x^2 + 2ai\Delta x + i^2\Delta x^2 + \Delta x^2 + 2i\Delta x^2 + 2ai\Delta x + 2a\Delta x]\,\frac{\Delta x}{2}$$

example: $f(x) = x^2$

$$N = \frac{b-a}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} [2a^2 + i^2\Delta x^2 + 2ai\Delta x + i^2\Delta x^2 + \Delta x^2 + 2i\Delta x^2 + 2ai\Delta x + 2a\Delta x] \frac{\Delta x}{2}$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \sum_{i=0}^{N-1} i^2 + 2a\Delta x^2 \sum_{i=0}^{N-1} i + \frac{\Delta x^3}{2} N + \Delta x^3 \sum_{i=0}^{N-1} i + a\Delta x^2 N \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \sum_{i=0}^{N-1} i^2 + 2a\Delta x^2 \sum_{i=0}^{N-1} i + \Delta x^3 \sum_{i=0}^{N-1} i \right]$$

$$N = \frac{b-a}{\Delta x}$$

example: $f(x) = x^2$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \sum_{i=0}^{N-1} i^2 + 2a\Delta x^2 \sum_{i=0}^{N-1} i + \Delta x^3 \sum_{i=0}^{N-1} i \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{N(N+1)(2N+1)}{6} + a\Delta x^2 N(N+1) + \Delta x^3 \frac{N(N+1)}{2} \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{N(N+1)(2N+1)}{6} + a\Delta x^2 N(N+1) \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{(N^2+N)(2N+1)}{6} + a\Delta x^2 N^2 + a\Delta x^2 N \right]$$

$$N = \frac{b - a}{\Delta x}$$

example: $f(x) = x^2$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{(N^2 + N)(2N + 1)}{6} + a\Delta x^2 N^2 + a\Delta x^2 N \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{2N^3 + 3N^2 + N}{6} + a\Delta x^2 N^2 \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 \frac{b - a}{\Delta x} + \Delta x^3 \frac{2\left(\frac{b - a}{\Delta x}\right)^3 + 3\left(\frac{b - a}{\Delta x}\right)^2 + \frac{b - a}{\Delta x}}{6} + a\Delta x^2 \left(\frac{b - a}{\Delta x}\right)^2 \right]$$

$$= a^2(b - a) + \frac{(b - a)^3}{3} + a(b - a)^2 = \frac{(b - a)^3}{3}$$

$$\int_a^b x^2\, dx = \frac{(b - a)^3}{3}$$

$a, c \in \mathbb{C}$
$n \in \mathbb{R}$

rules:

$$\int \frac{d}{dx} f(x)\, dx = \int df(x) = f(x) + c$$

therefore: an integral is an **anti derivative!**

$$\int a x^n\, dx = a \frac{1}{n+1} x^{n+1} + c \quad n \neq -1$$

$$\int f(x) + g(x)\, dx = \int f(x)\, dx + \int g(x)\, dx + c$$

sum rule: integrals are linear

$$\int f(x) \frac{d}{dx} g(x)\; dx = f(x) g(x) + \int \frac{d}{dx} f(x) \cdot\; g(x) dx + c$$

product rule

$a, c \in \mathbb{C}$
$n \in \mathbb{R}$

special integrals

$$\int e^x \, dx = e^x + c$$

$$\int a^x \, dx = \frac{a^x}{\ln(a)} + c$$

$$\int \frac{1}{\mathrm{x}} dx = \ln(|x|) + c$$

$$\int log_b(x) \, dx = x log_b(x) - \frac{x}{\ln(b)} + c$$

$$\int cos(x) \, dx = \sin(x) + c$$

$$\int sin(x) \, dx = -\cos(x) + c$$

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x \qquad N = \frac{b-a}{\Delta x}$$

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} [f(a + i\,\Delta x) + f(a + (i+1)\,\Delta x)]\,\frac{\Delta x}{2}$$

trapezoidal rule

even more accurate:

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} [f(a + i\,\Delta x) + f(a + (i+1)\,\Delta x) + 4\,f(a + i\,\Delta x/2)]\,\frac{\Delta x}{6}$$

Simpson rule

Note: there are different Simpson rules, depending on how many subintervals are included

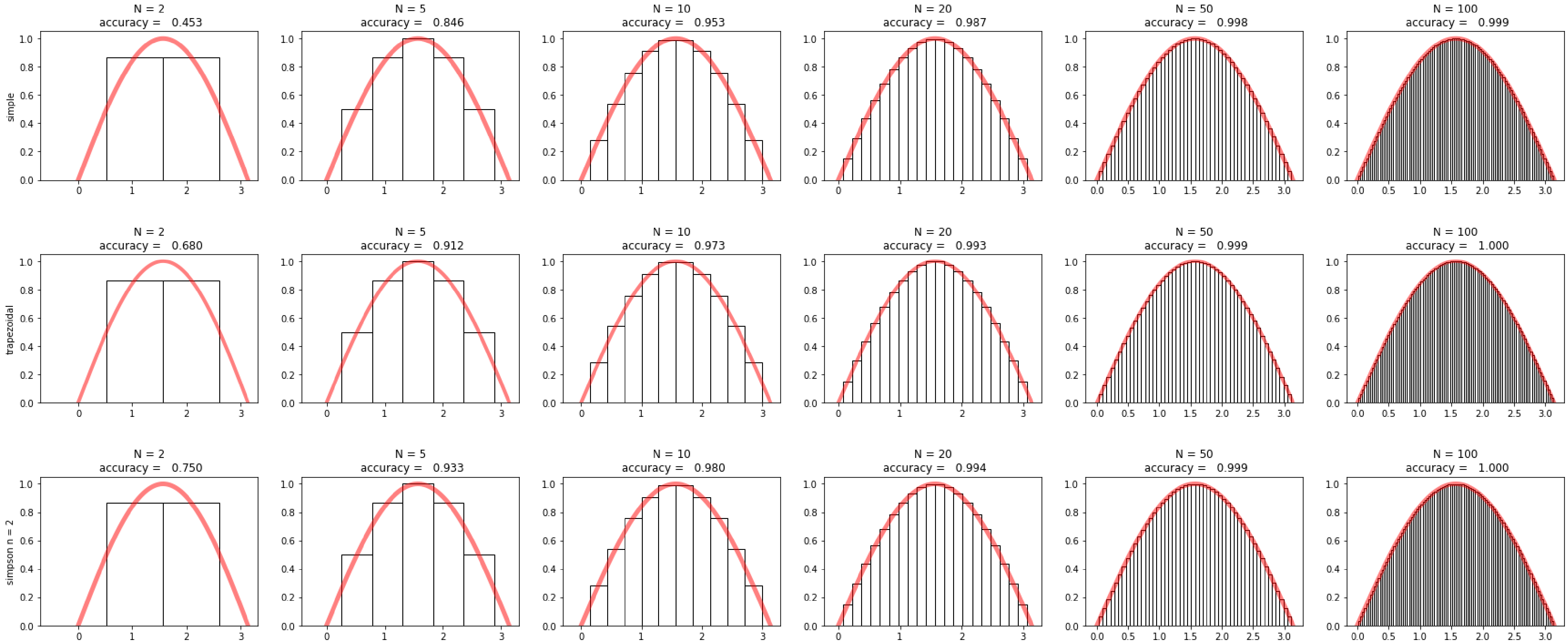
Newton-Cotes Equations

approximation	error	
$\frac{1}{2}\,\Delta x\,(f_i\ + f_{i+1})$	$\varepsilon \sim \frac{\Delta x^3}{12}$	trapezoidal
$\frac{1}{6}\,\Delta x\,(f_i\ + f_{i+2} + 4f_{i+1})$	$\varepsilon \sim \frac{\Delta x^5}{90}$	Simpson
$\frac{1}{8}\,\Delta x\,(f_i\ + 3f_{i+1} + 3f_{i+2} + f_{i+3})$	$\varepsilon \sim \frac{3\,\Delta x^5}{80}$	Simpson 3/8
$\frac{1}{90}\,\Delta x\,(7f_i\ + 32f_{i+1} + 12f_{i+2} + 32f_{i+3} + 7f_{i+4})$	$\varepsilon \sim \frac{8\,\Delta x^7}{945}$	Boole

Note: *i* here refers to subinterval **within** Δx

run the function `IntegrationAccuracy.py`

integrating sin(x)



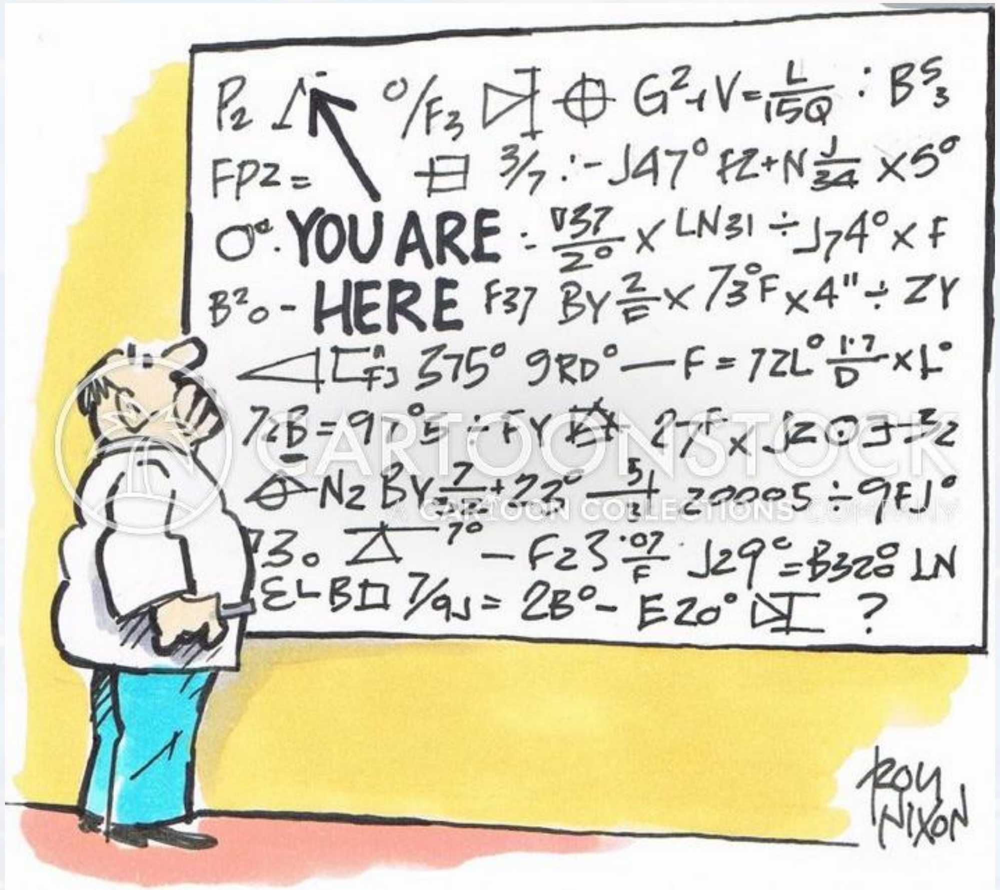
SciPy

```
from scipy.integrate import *

simpson
trapezoid
quad
```

…and more.
See homework assignment!

```
I = simpson(y, x)
```



Outline:

- Derivatives
- Taylor Series
- Integrals
- **Diffusion Example**

often, we need to **model diffusion processes** (heat conduction, diffusion reaction, electromagnetism etc)

$$\boxed{\frac{\partial c(x,y,z,t)}{\partial t} = D\, \Delta c(x,y,z,t)}$$

c: concentration

D: diffusion constant

$\Delta \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$: Laplace operator

numerically:

$$\frac{c(x_0,\ y_0,\ t_0 +\ \Delta t) - c(x_0, y_0,\ t_0 -\ \Delta t)}{2\Delta t} = \quad D[$$

$$\frac{c(x_0 +\ \Delta x,\ y_0, t_0)\ - 2c(x_0,\ y_0, t_0) + c(x_0 -\ \Delta x,\ y_0, t_0)}{\Delta x^2} +$$

$$\frac{c(x_0,\ y_0 +\ \Delta y, t_0)\ - 2c(x_0,\ y_0, t_0) + c(x_0,\ y_0 +\ \Delta y, t_0)}{\Delta y^2}$$

often, we need to **model diffusion processes** (heat conduction, diffusion reaction, electromagnetism etc)

$$\boxed{\frac{\partial c(x,y,z,t)}{\partial t} = D\,\Delta c(x,y,z,t)}$$

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numerically:

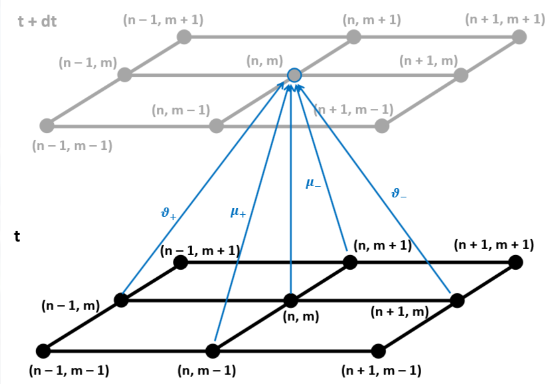
$$c(x_0, y_0, t_0 + \Delta t) =$$

We can calculate c in the ***future***

$$2\Delta t D \left[\frac{c(x_0 + \Delta x,\ y_0, t_0) - 2c(x_0,\ y_0, t_0) + c(x_0 - \Delta x,\ y_0, t_0)}{\Delta x^2} + \right.$$

by using all adjacent ***current*** values

$$\left. \frac{c(x_0,\ y_0 + \Delta y, t_0) - 2c(x_0,\ y_0\ , t_0) + c(x_0,\ y_0 + \Delta y, t_0)}{\Delta y^2} \right]$$

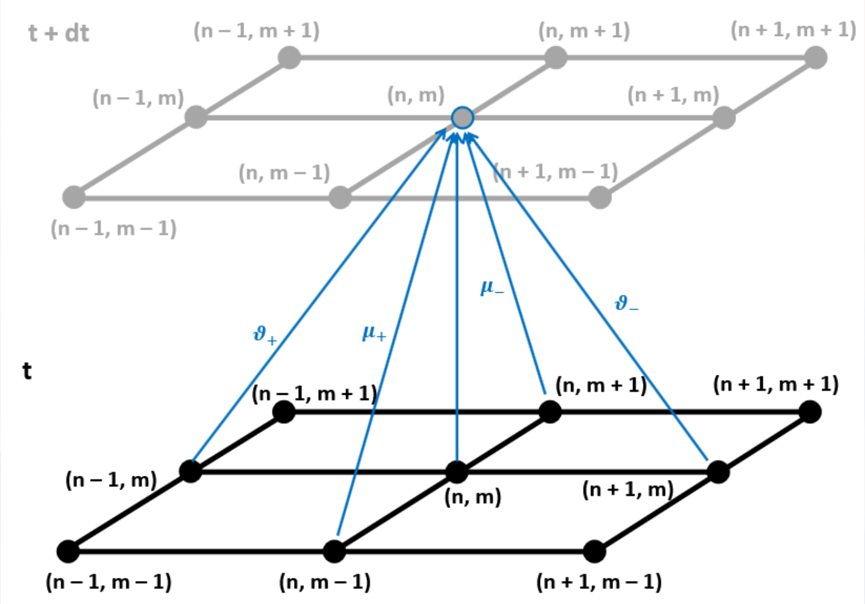


$$+\ c(x_0, y_0, t_0 -\ \Delta t)$$

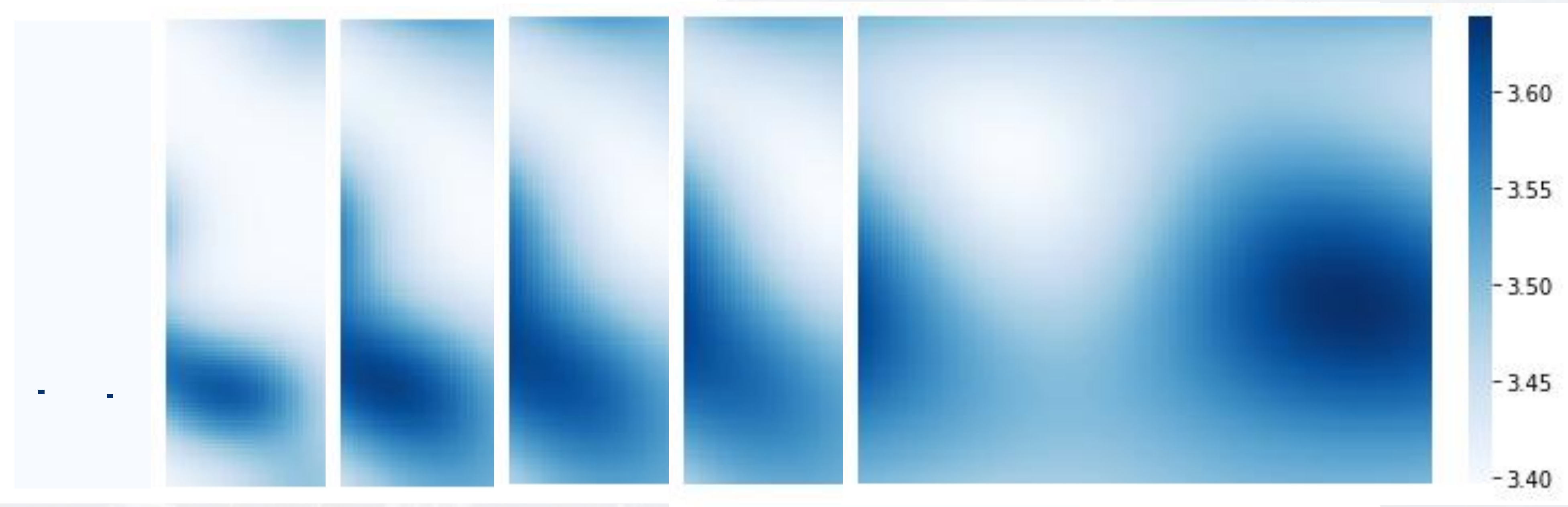
and the immediate ***past*** value

run the script Diffusion2D.py

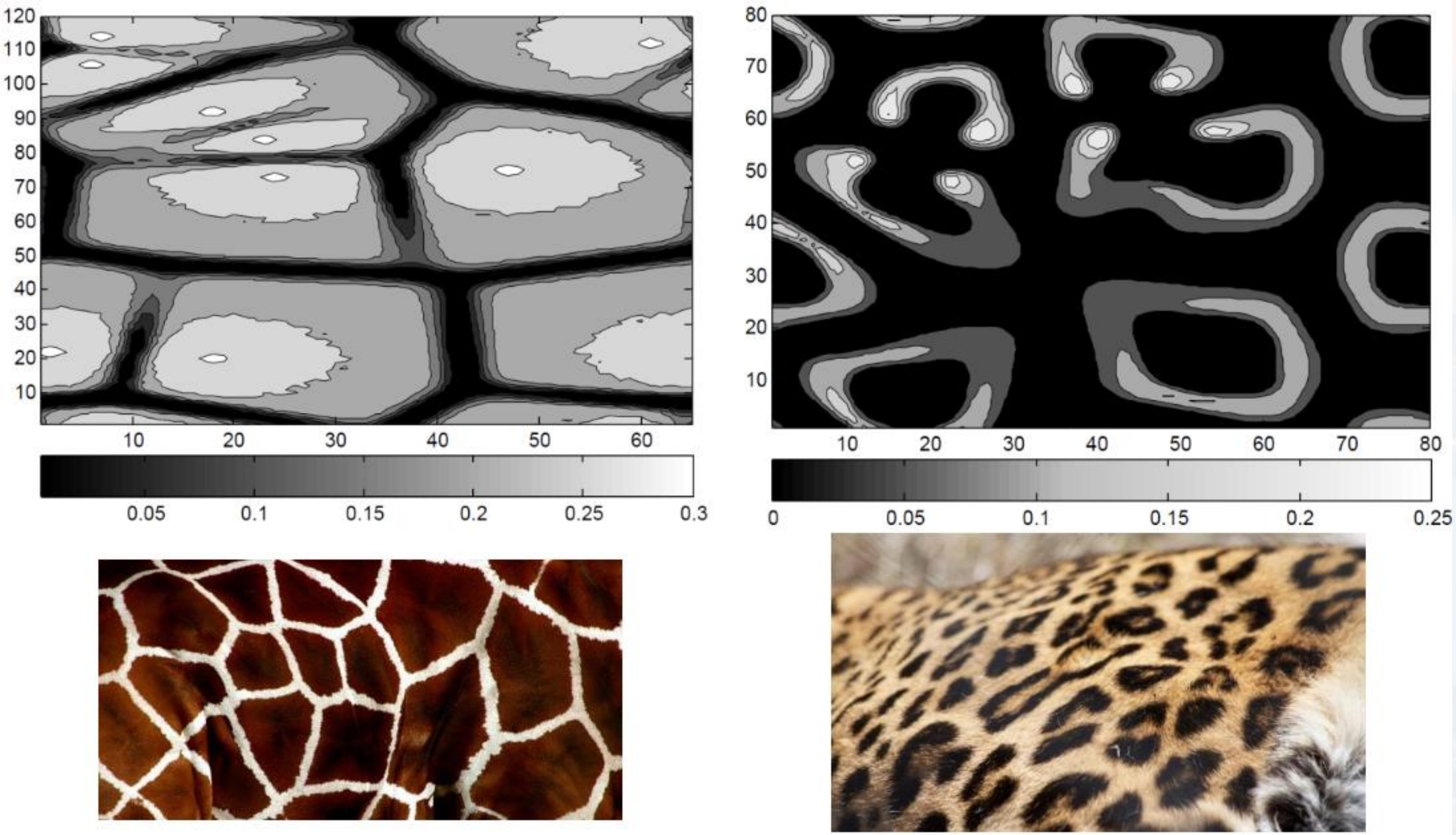
```python
from Diffusion2D import *

D = Diffusion2D()
D.RunSimulation()
```



initial condition



Possible Capstone Project: modelling fur and skin pattern:



Thank you very much for your attention!