M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics

syllabus:

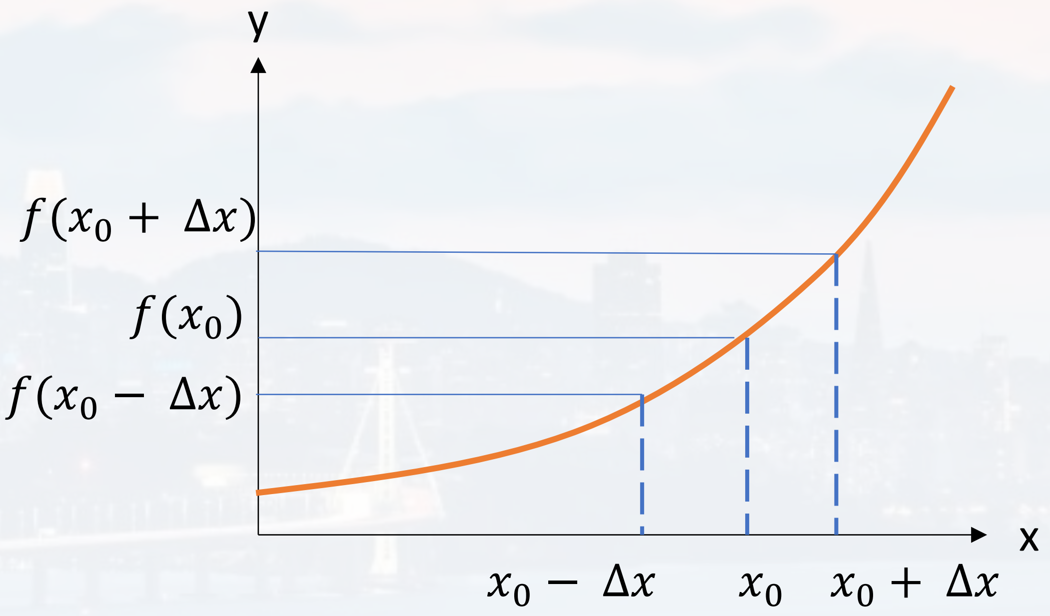
- Introduction to Unix & Python	(week 1 - 2)
- Functions, Loops, Lists and Arrays	(week 3 - 4)
- Visualization	(week 5)
- Parsing, Data Processing and File I/O	(week 6)
- Statistics and Probability, Interpreting Measurements	(week 7 - 8)
- Random Numbers, Simulation	(week 9)
- Numerical Integration and Differentiation	**(week 10)**
- Root Finding, Interpolation	(week 11)
- Systems of Linear Equations	(week 12)
- Ordinary Differential Equations	(week 13)
- Fourier Transformation and Signal Processing	(week 14)
- Capstone Project Presentations	(week 15)

short recap:

slope of a function at $x = x_0$

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

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



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

1st derivative at $x = x_0$

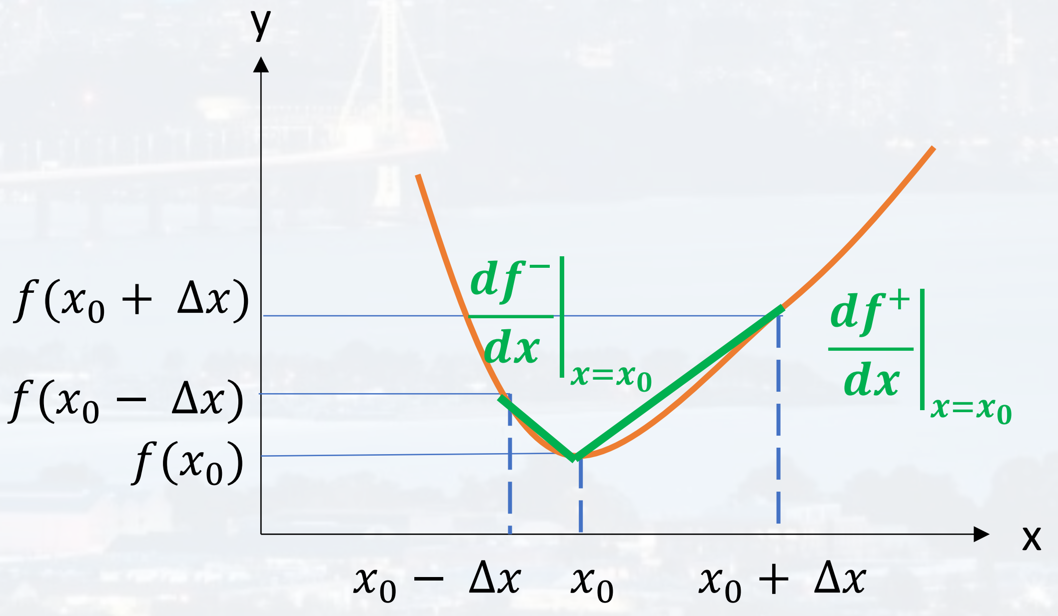
<u>short recap:</u>

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

1st derivative at $\mathbf{x} = x_0$

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

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



short recap:

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

1st derivative at $x = x_0$

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

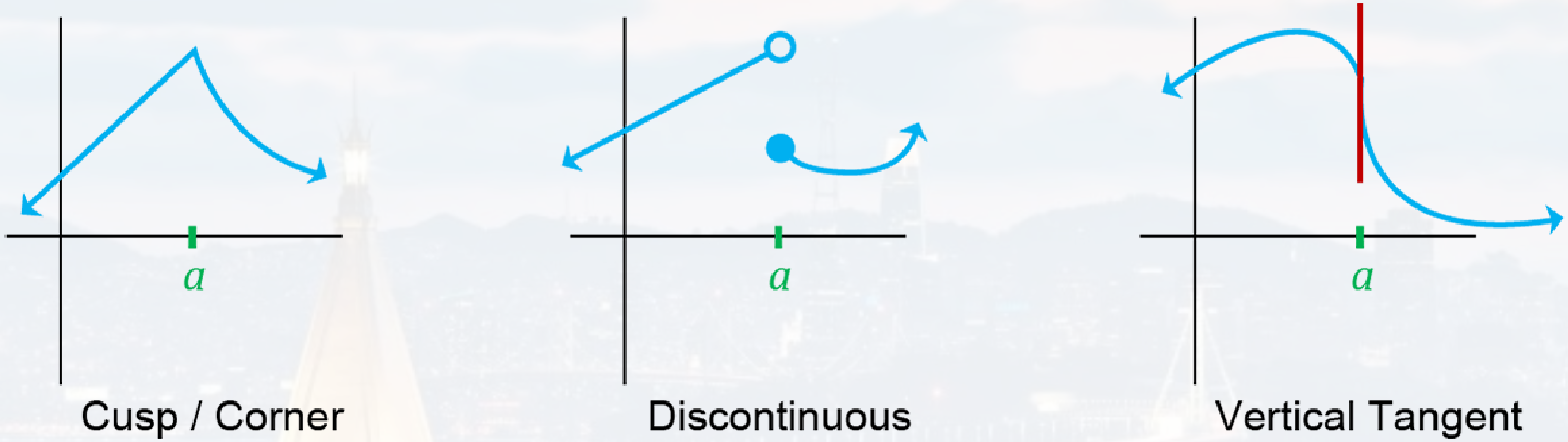
$$\left.\frac{d^2f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x\to 0}\frac{1}{\Delta x}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} - \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x\to 0}\frac{f(x_0+\Delta x)-2f(x_0)+f(x_0-\Delta x)}{\Delta x^2}$$

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

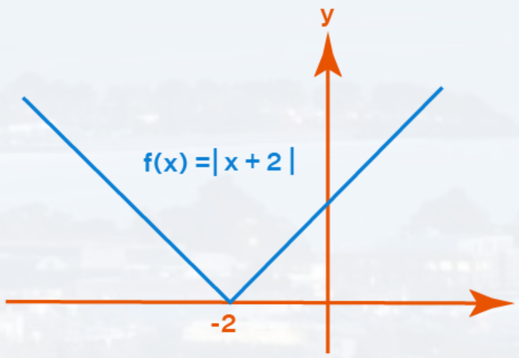
2nd derivative at $x = x_0$

…and so on

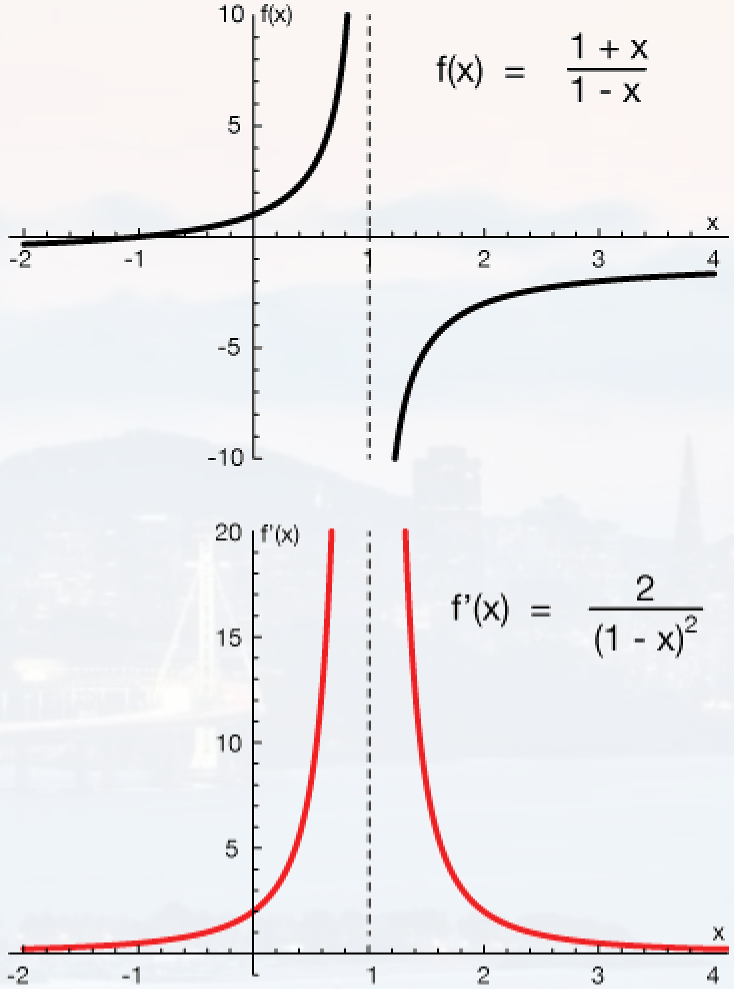
derivatives are not always defined:



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



derivatives are not always defined:



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

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

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

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

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

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

Taylor Series

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

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

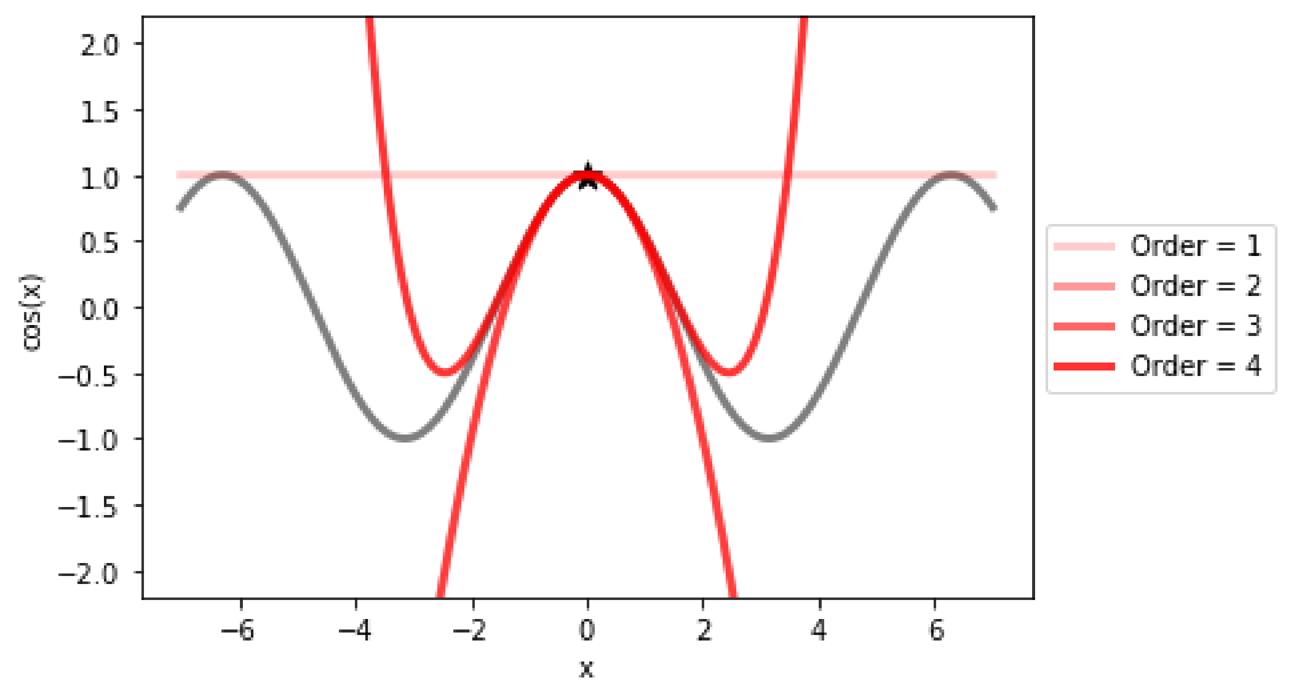
n = 1: $f(x) \approx f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} (x - x_0)$ tangent on f at $x = x_0$

exercise:
- 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 ***i*** which only property is $\boldsymbol{i^2 = -1}$

Taylor Series

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

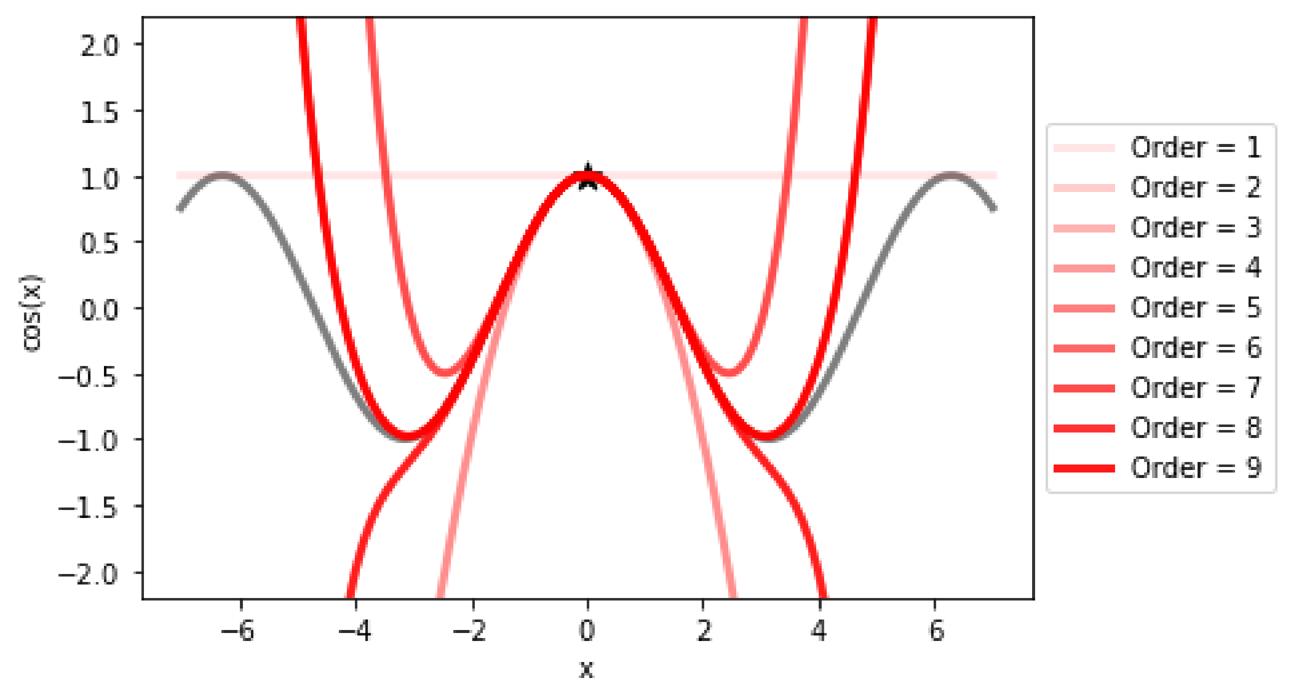
run the function `PlotTaylorSeries.py`



Taylor Series

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

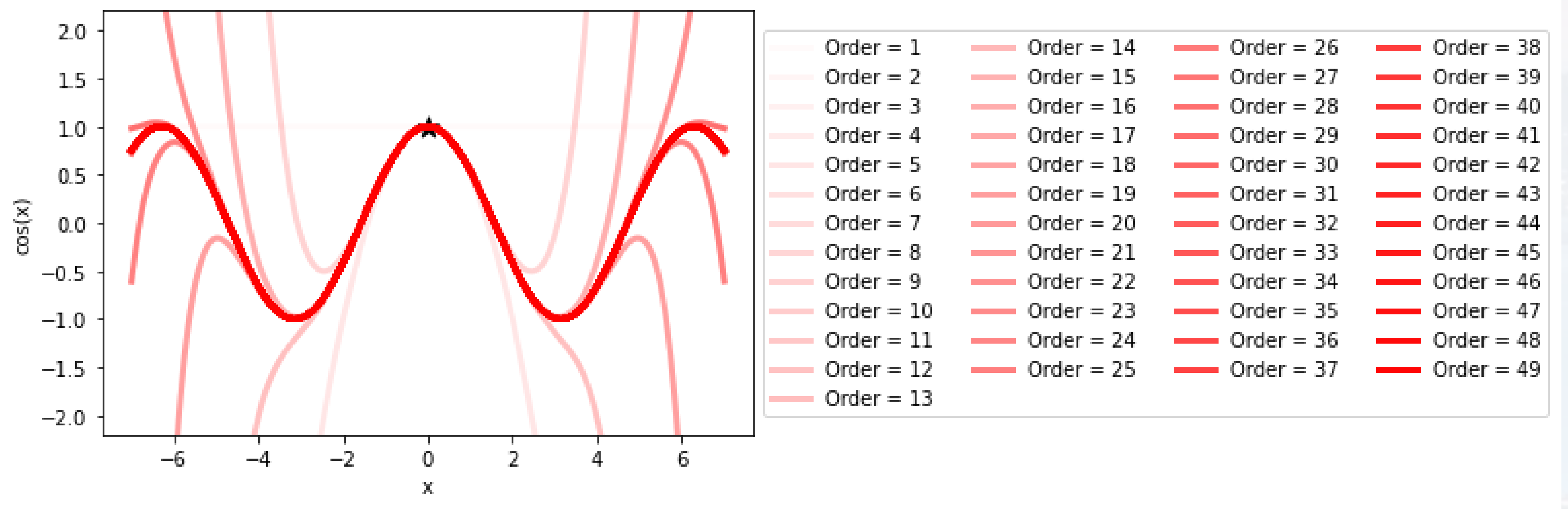
run the function `PlotTaylorSeries.py`



Taylor Series

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

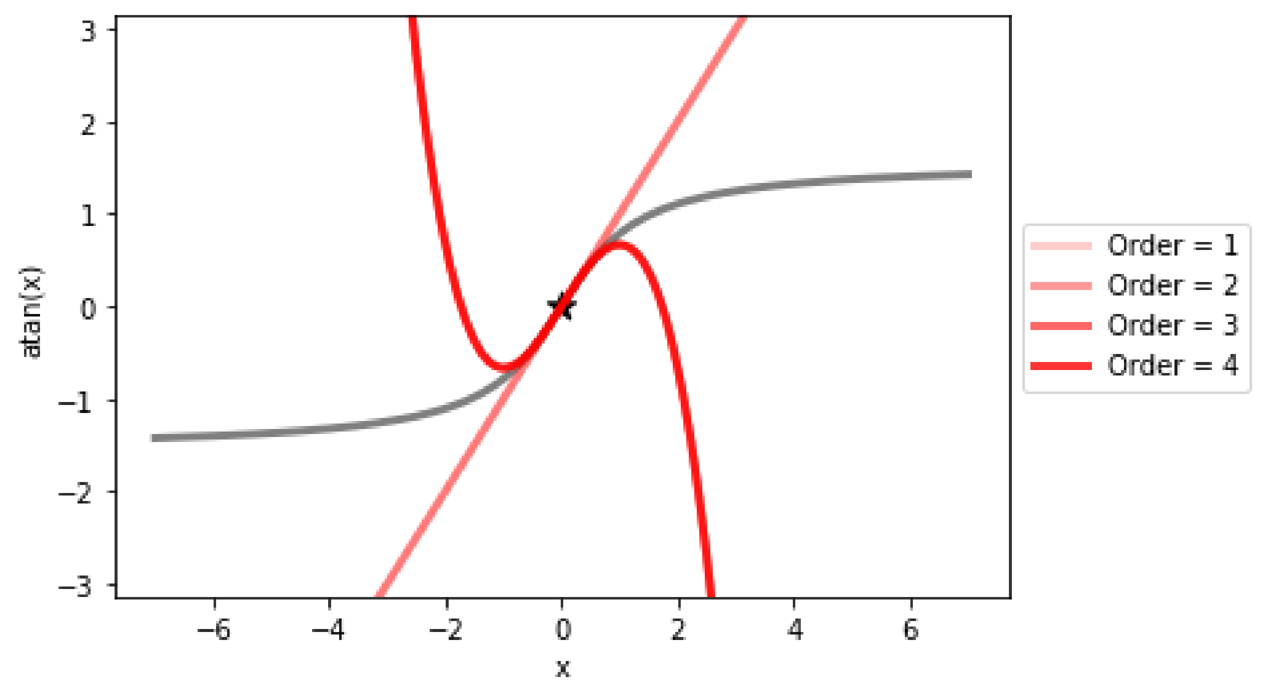
run the function `PlotTaylorSeries.py`



Taylor Series

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

run the function `PlotTaylorSeries.py`



Taylor Series

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

approximation of n-th order: error $\varepsilon = \varepsilon(\Delta x^{n+1})$

Hooke's law (approximation of a function around its extreme):

→ unknown energy function around its minimum/ground state

n = 2:

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

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

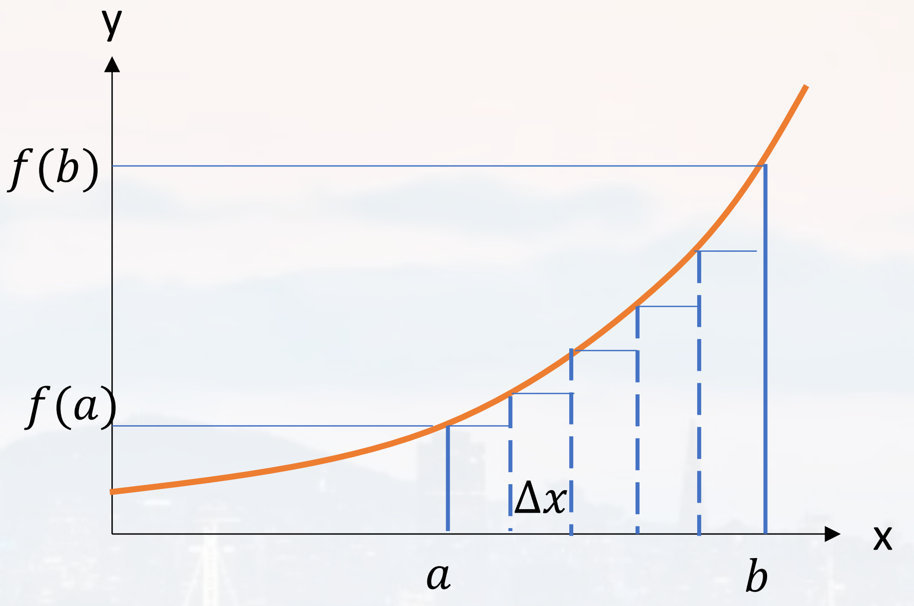
$$E(x) \approx E(x_0) + \frac{1}{2} k (x - x_0)^2$$

$$\boxed{\Delta E \approx \frac{1}{2} k \, \Delta x^2}$$

Introduction to Computational Techniques in Physics:

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

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



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):

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

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

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

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

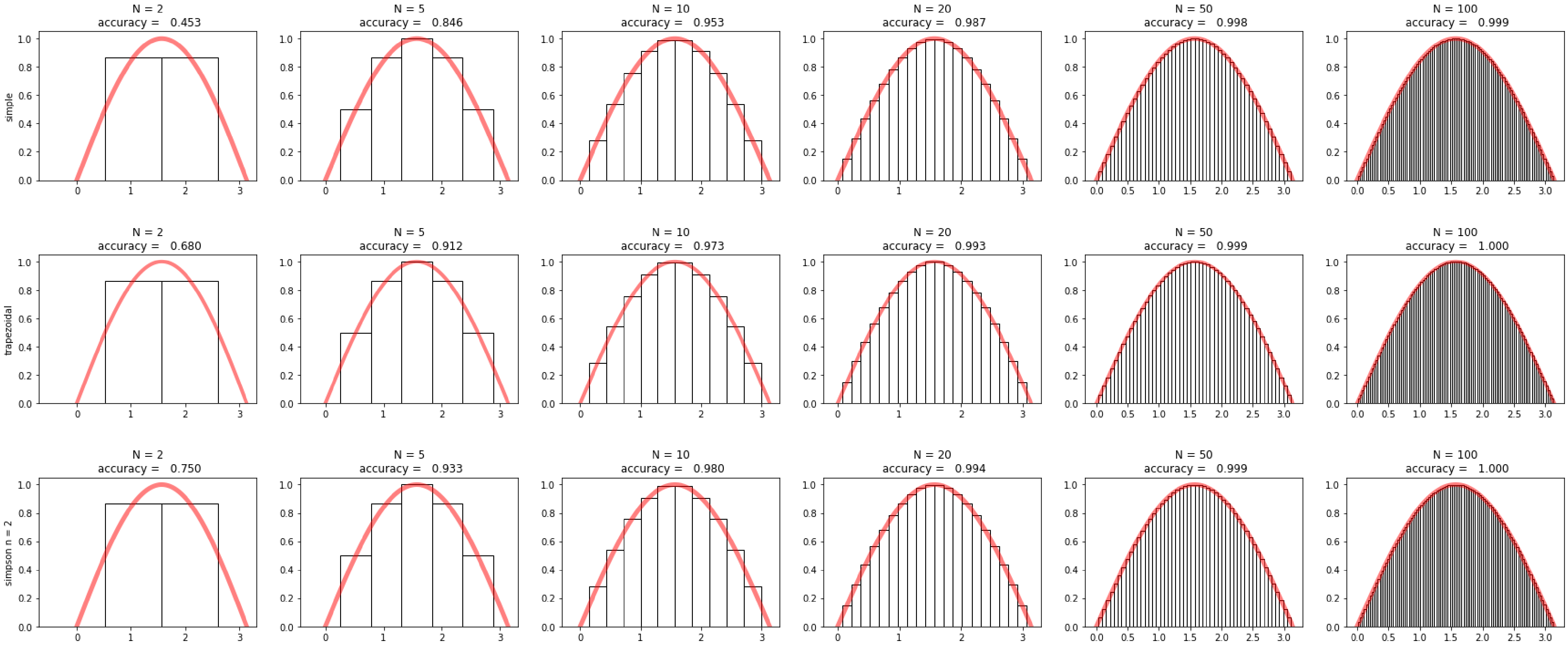
Berkeley UNIVERSITY OF CALIFORNIA

Introduction to Computational Techniques in Physics:

Integration

run the function `IntegrationAccuracy.py`

integrating sin(x)



SciPy

- **quad** – General Purpose Integration
- **dblquad** – General Purpose Double Integration
- **nquad** – General Purpose n- fold Integration
- **fixed_quad** – Gaussian quadrature, order n
- **quadrature** – Gaussian quadrature to tolerance
- **romberg** – Romberg integration
- **trapz** – Trapezoidal rule
- **cumtrapz** – Trapezoidal rule to cumulatively compute integral
- **simps** – Simpson's rule
- **romb** – Romberg integration
- **polyint** – Analytical polynomial integration (NumPy)

depreciated

```
from scipy.integrate import simpson

I = simpson(y, x)
```

Thank you very much for your attention!