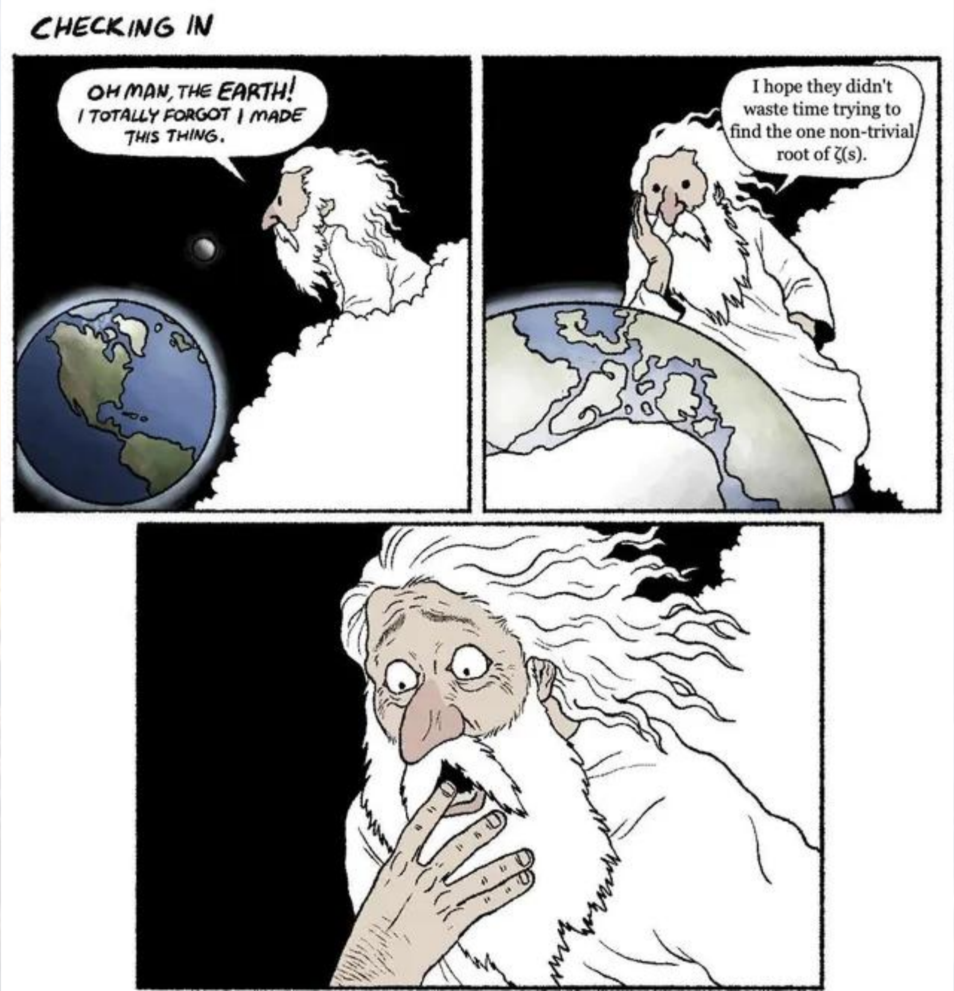
M. Hohle:

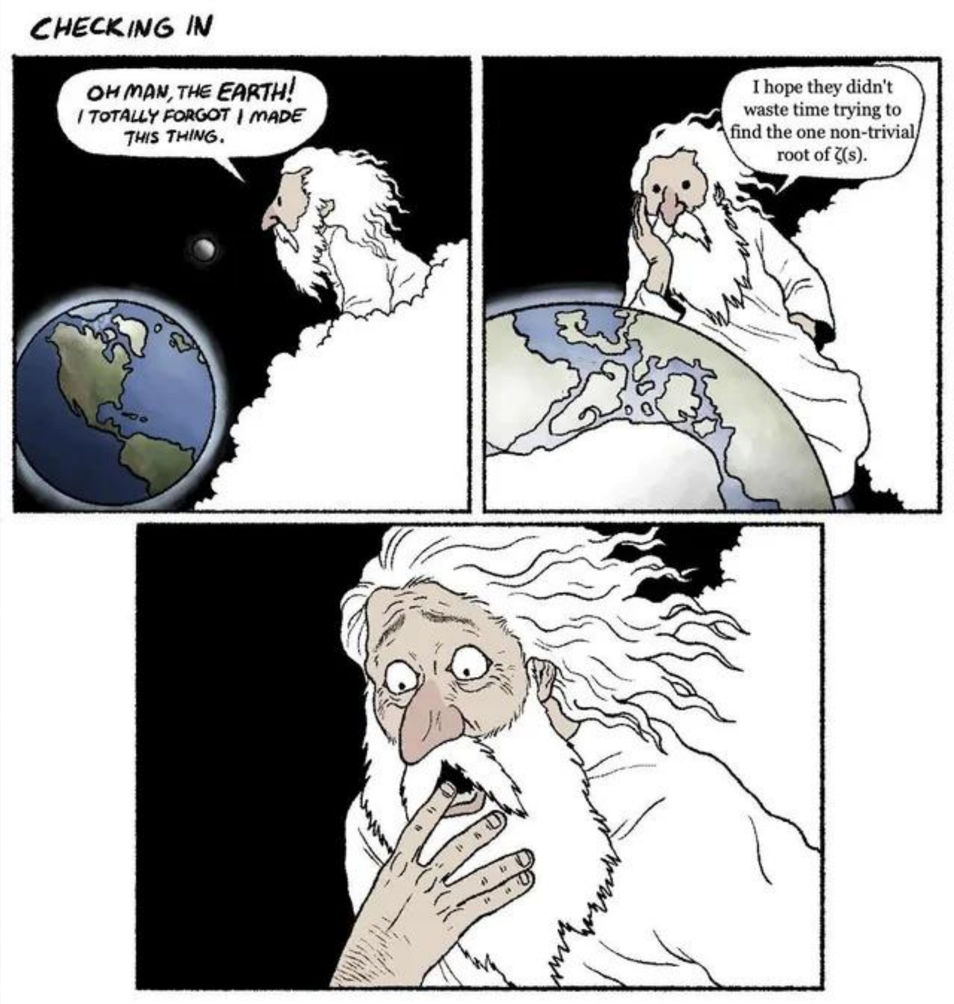
Physics 77: Introduction to Computational Techniques in Physics



Berkeley UNIVERSITY OF CALIFORNIA

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



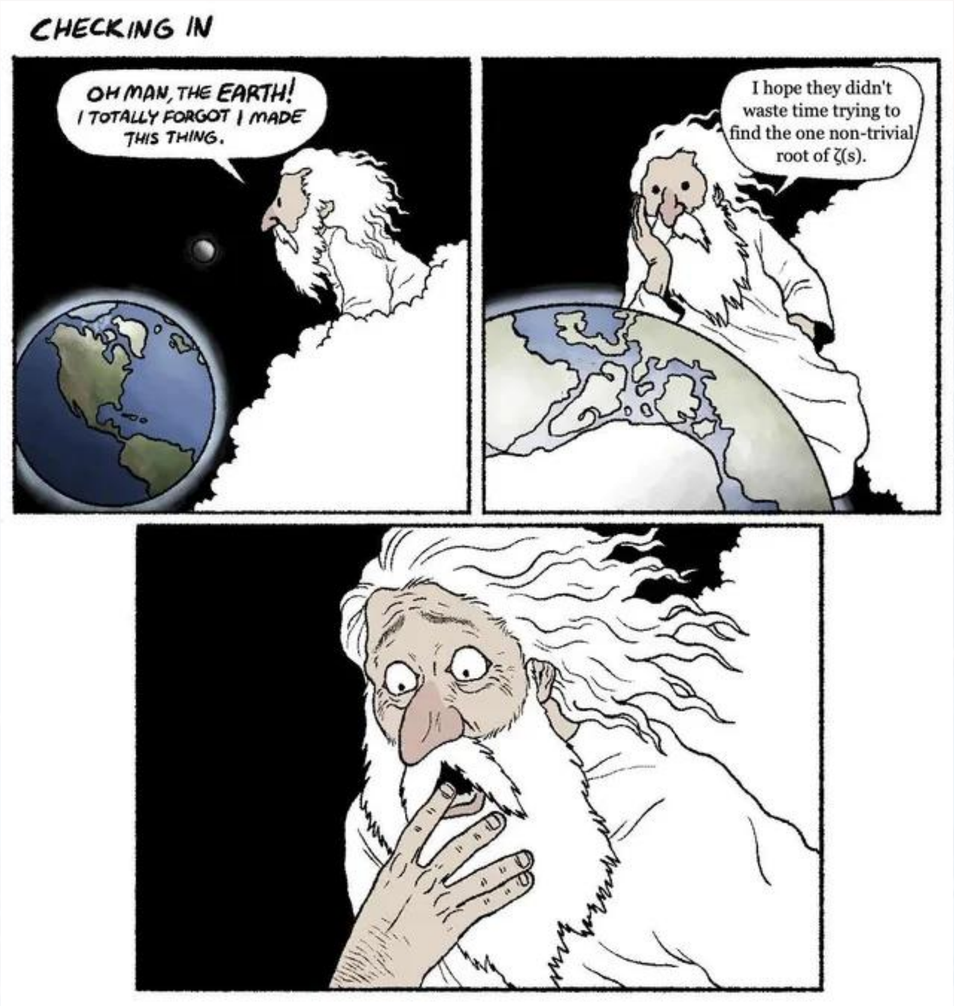
Outline

root finding

- The Problem
- Newtons Method
- Bisection

interpolation

- Lagrange Polynomials
- Interpolation techniques
- Smoothing



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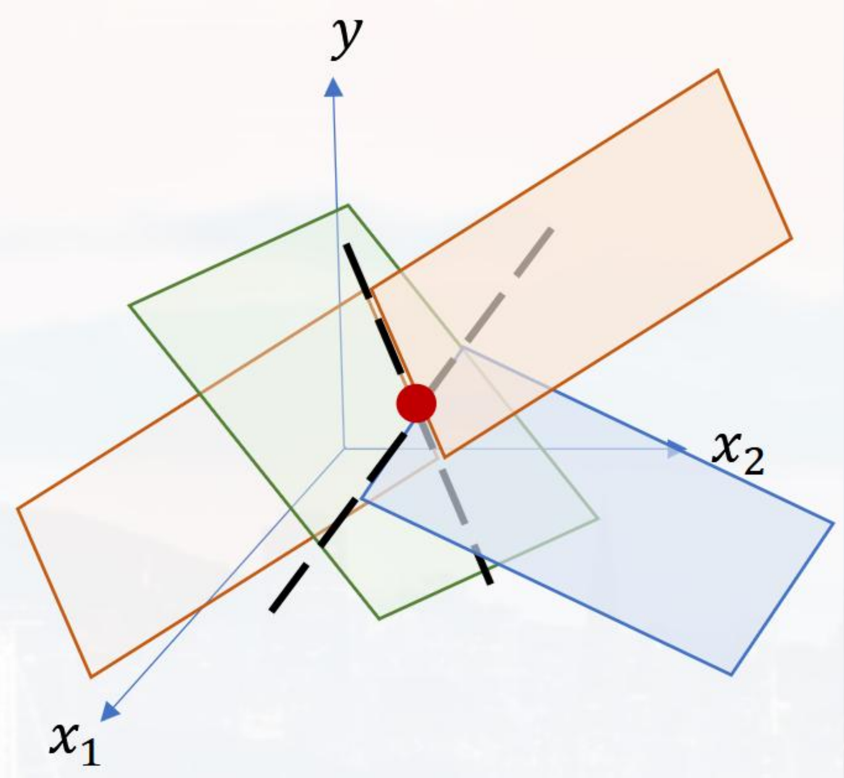
We know how to solve a set of linear equations (**see also next lecture**!):

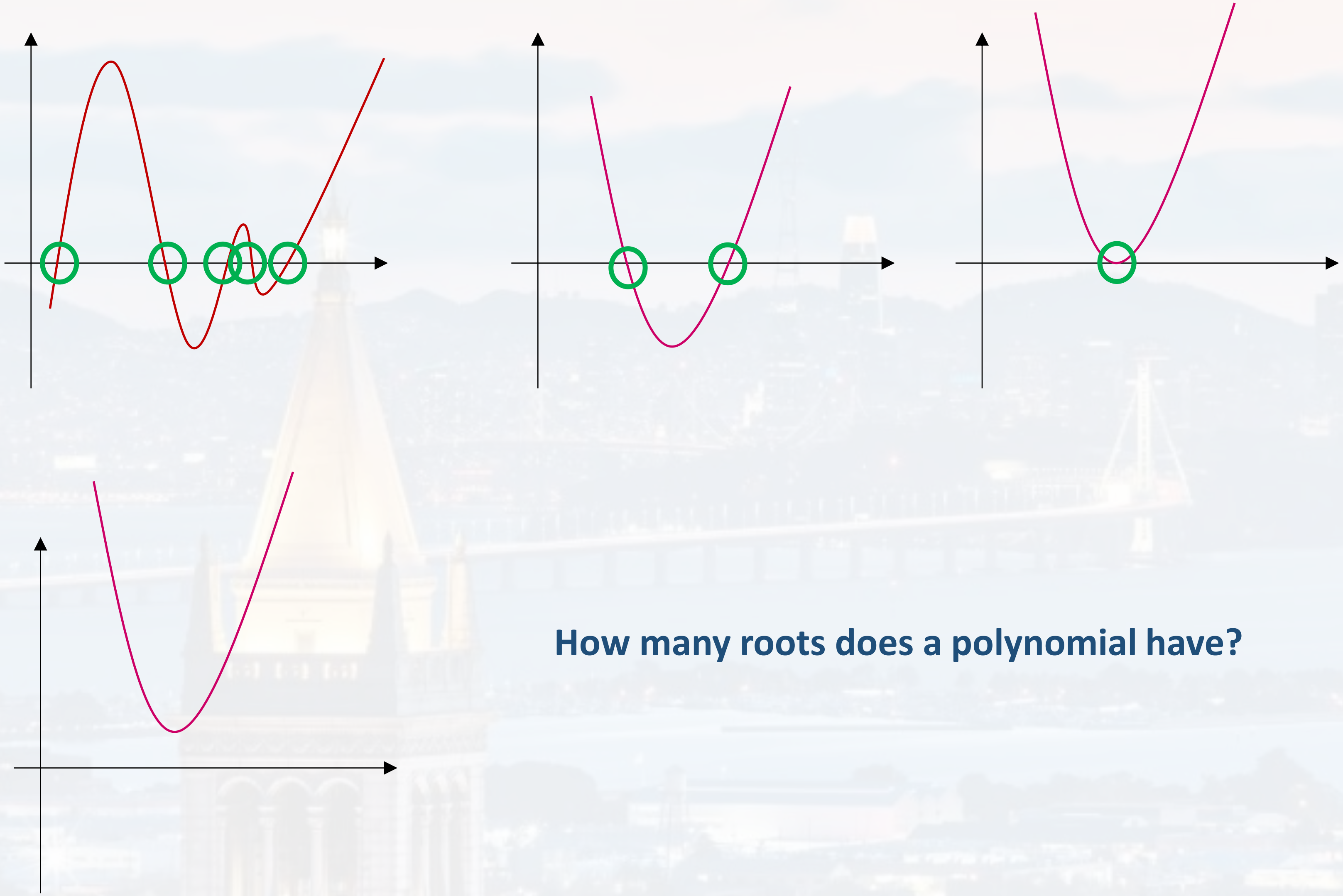
$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}}_{\vec{x}} = \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_m \end{bmatrix}}_{\vec{c}}$$

$$\boxed{A\vec{x} = \vec{c}}$$



However: what about non-linear equations?!

root finding: finding the **zeros** of a polynomial



How many roots does a polynomial have?

How many roots does a polynomial have?

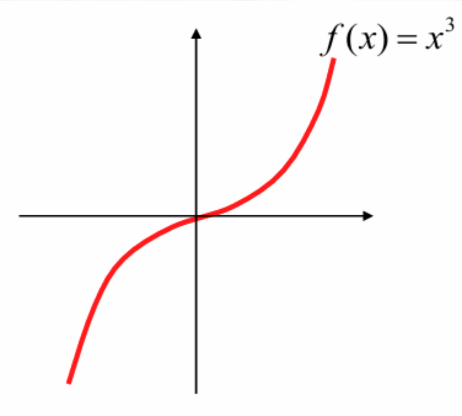
$$f_N(x) = \sum_{i=0}^{N} a_i x^i = \alpha \prod_{i=1}^{N} (x - x_i)$$

factored form

x_i : zeros

- a polynomial of **Nth order** has **N roots** (real & complex)
- for N $\geq$ 5: no analytical solutions
- for N is odd: at least one real zero

$$f(x) = x^3 = (x - x_1)(x - x_2)(x - x_3)$$



zeros: $x_1 = x_2 = x_3 = 0$

one zero with multiplicity m = 3

Calculate the **n-th** root of ***1*** and ***i***. Use Euler's identity and revisit the set of solutions for *sin(x)* and *cos(x).*

How many roots does a polynomial have?

$$f_N(x) = \sum_{i=0}^{N} a_i x^i = \boxed{\alpha \prod_{i=1}^{N} (x - x_i)}$$

factored form

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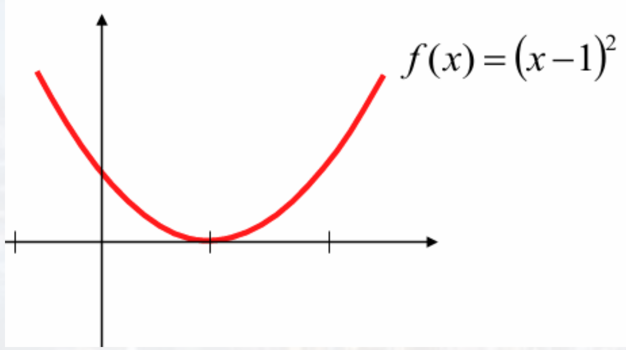


zeros: $x_1 = x_2 = 1$

one zero with multiplicity m = 2

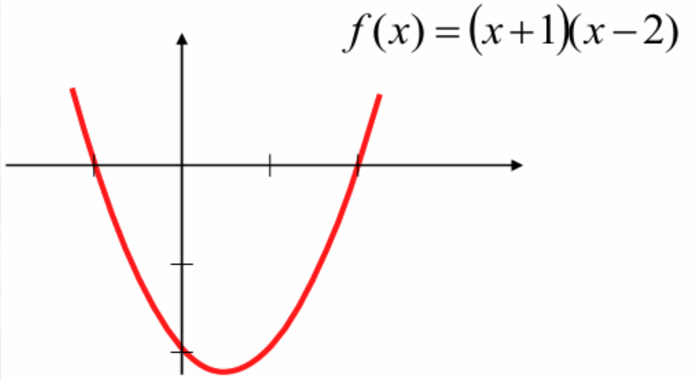
How many roots does a polynomial have?

$$f_N(x) = \sum_{i=0}^{N} a_i x^i = \alpha \prod_{i=1}^{N} (x - x_i)$$

factored form

x_i : zeros

- a polynomial of **Nth order** has **N roots** (real & complex)
- for N ≥ 5: no analytical solutions
- for N is odd: at least one real zero



zeros: $x_1 = 2,\ x_2 = -1$

two zeros with multiplicity m = 1 each

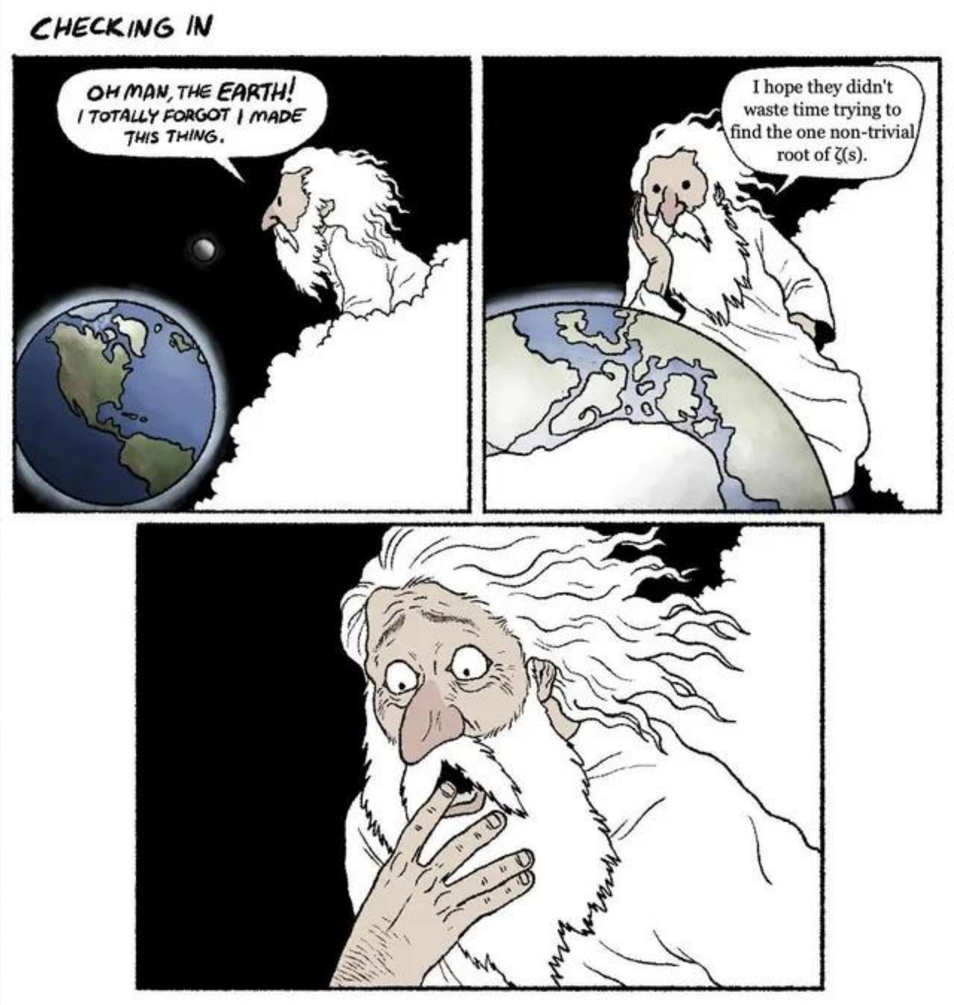
methods:

Root finding [edit]

Main article: Root-finding algorithm

- Bisection method
- False position method: and Illinois method: 2-point, bracketing
- Halley's method: uses first and second derivatives
- ITP method: minmax optimal and superlinear convergence simultaneously
- Muller's method: 3-point, quadratic interpolation
- Newton's method: finds zeros of functions with calculus
- Ridder's method: 3-point, exponential scaling
- Secant method: 2-point, 1-sided

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$



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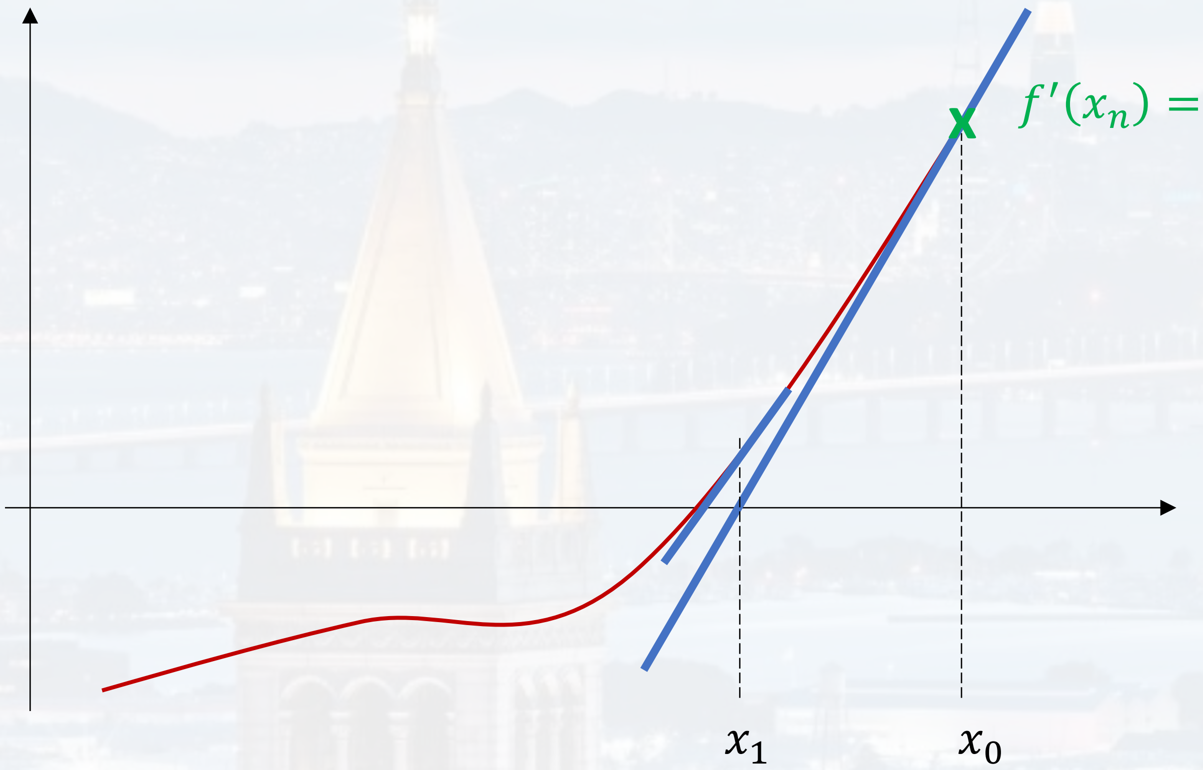
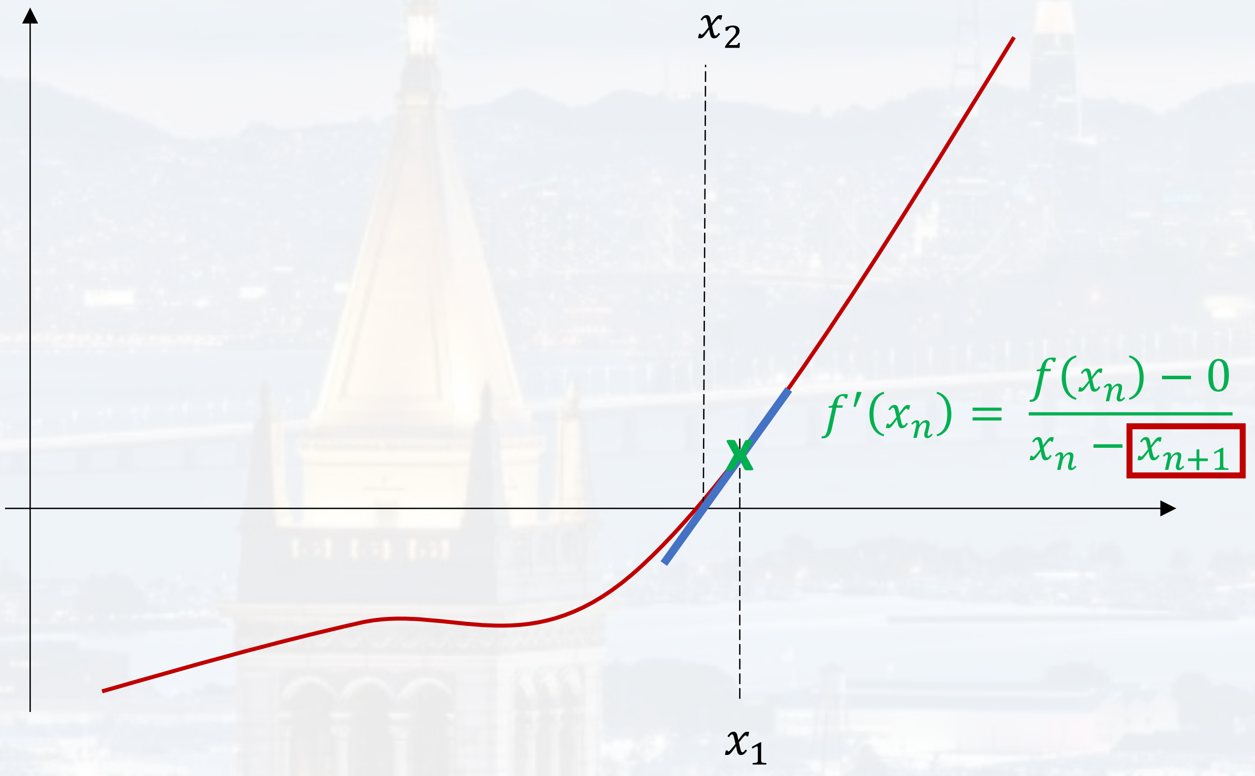
Newton's method:

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$



$$f'(x_n) = \frac{f(x_n) - 0}{x_n - \boxed{x_{n+1}}}$$

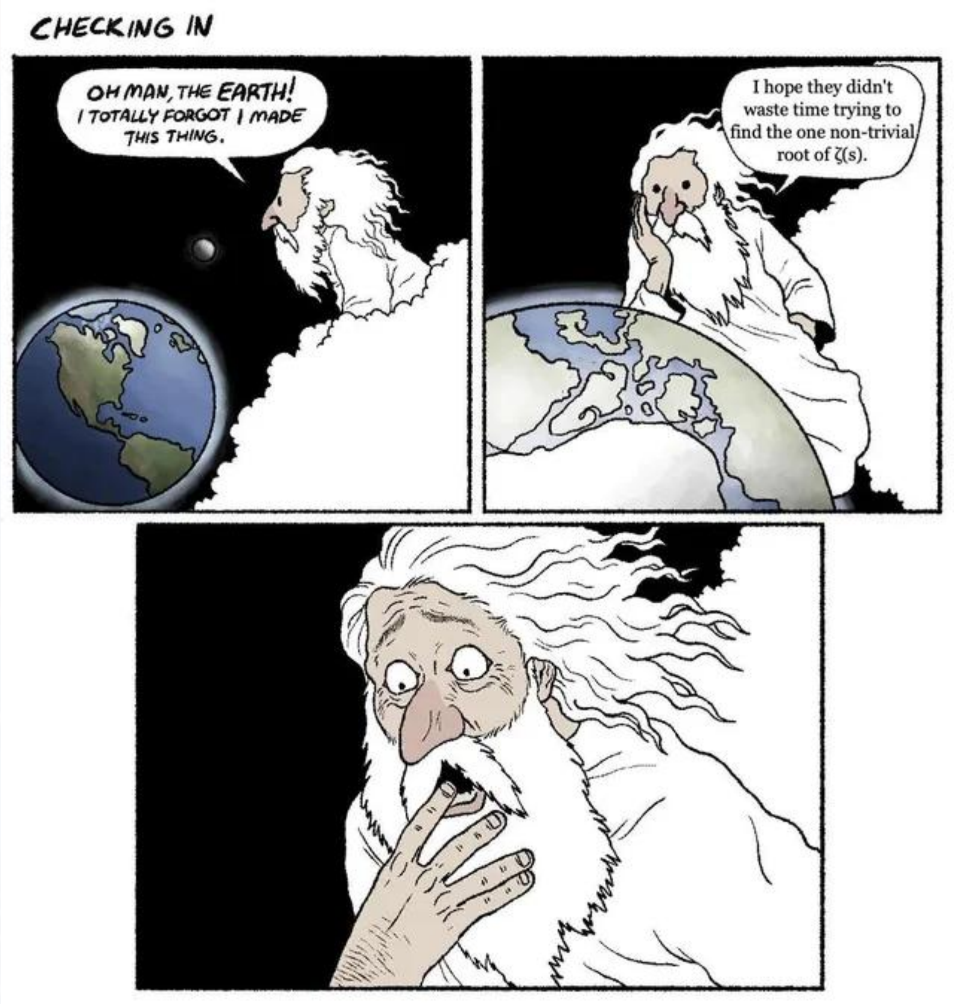
$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$



Newton's method:

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$

- since slope of the function points to next x_{n+1} → converges quadratically
- needs derivative → evaluation numerically
- convergence depends on initial guess → might not converge!



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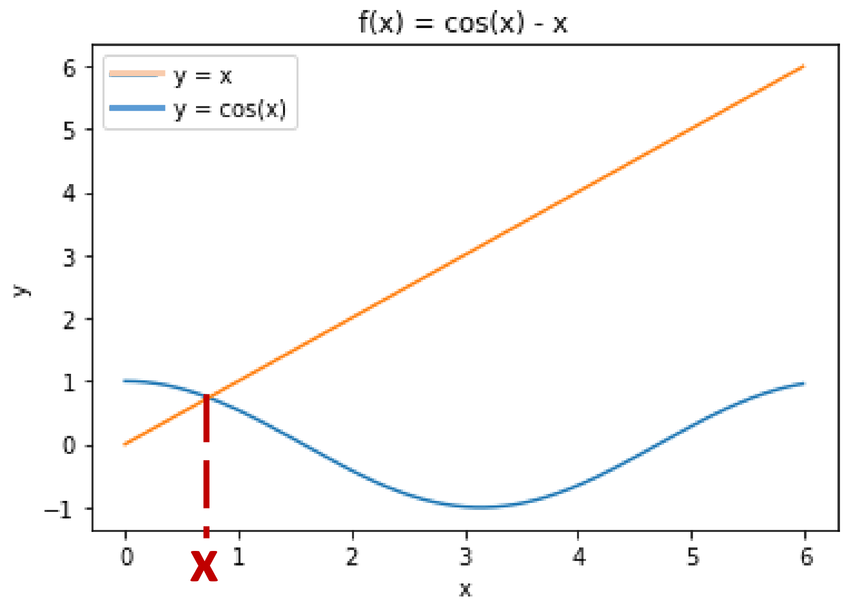
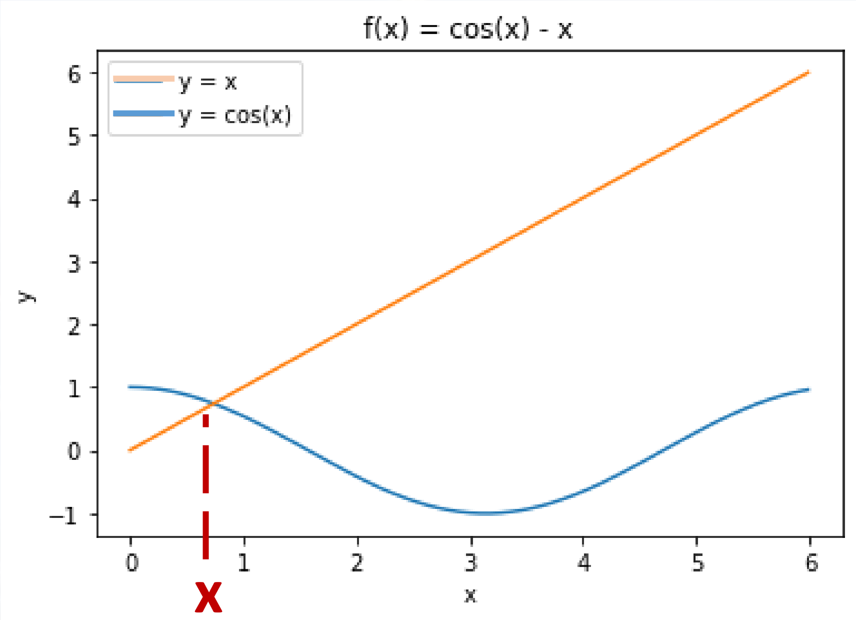
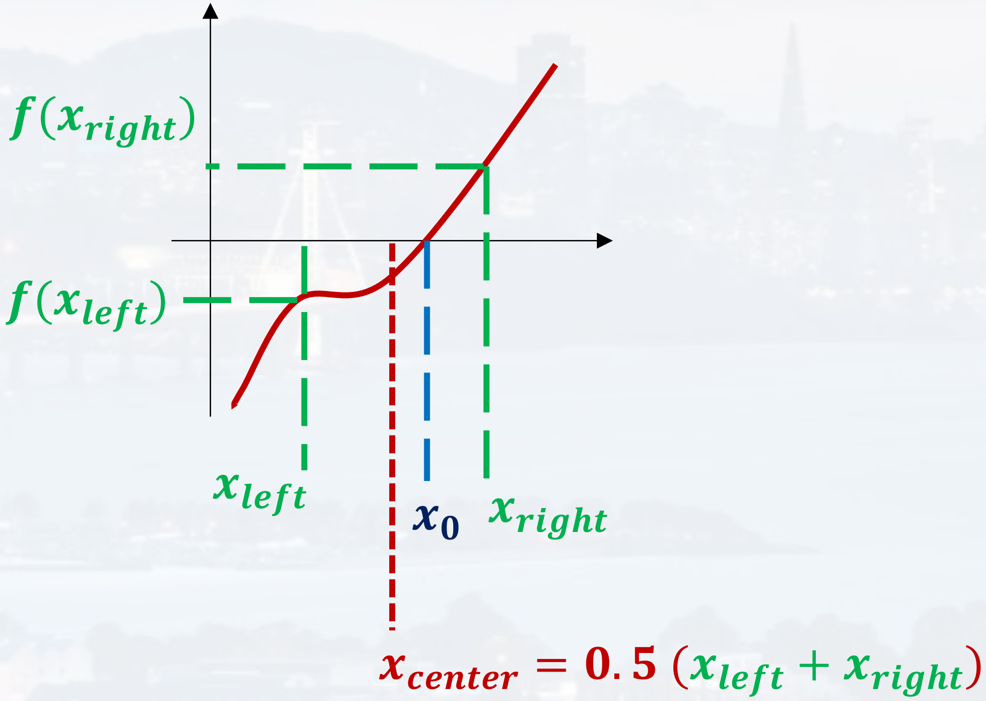
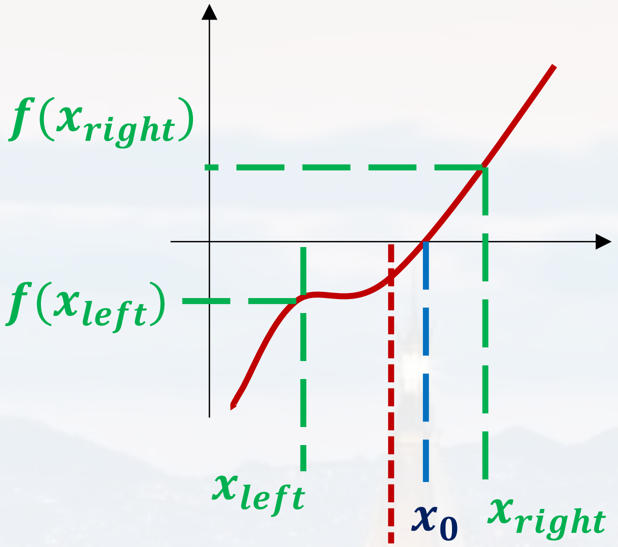


Bisection:

<u>assumption:</u> root is within interval $[x_{left}, x_{right}]$



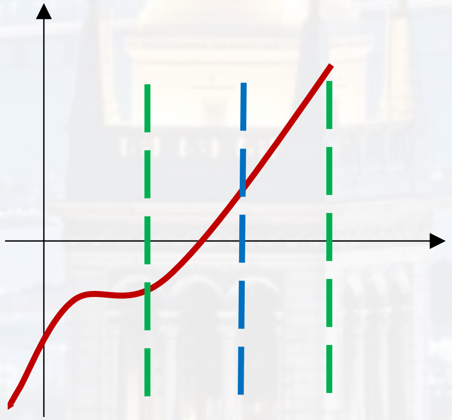


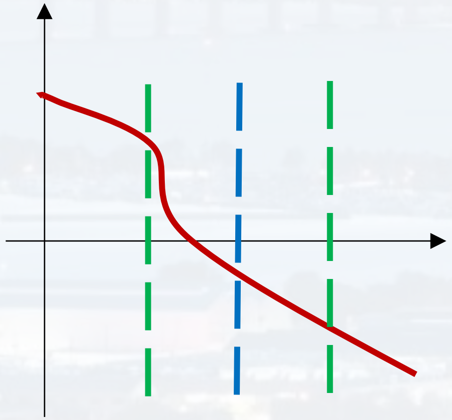


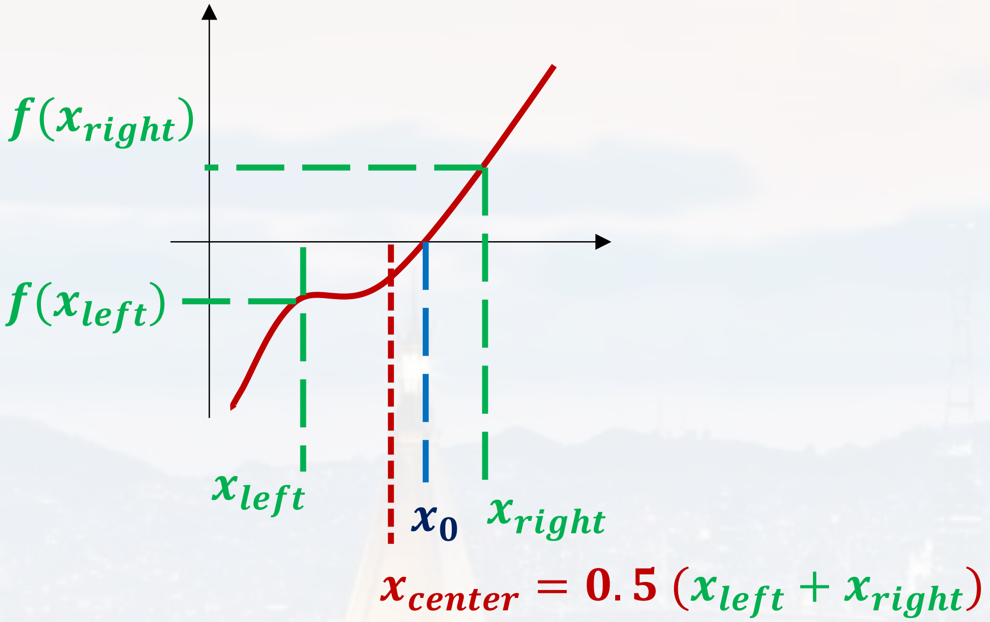
$x_{center} = 0.5\,(x_{left} + x_{right})$

if $f(x_{center}) \cdot f(x_{left}) < 0$

- $x_{left} \rightarrow x_{left}$
- set x_{right} to x_{center}
- reset $x_{center} = 0.5\,(x_{left} + x_{right})$







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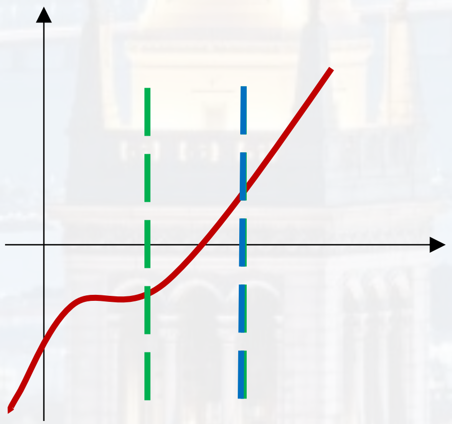

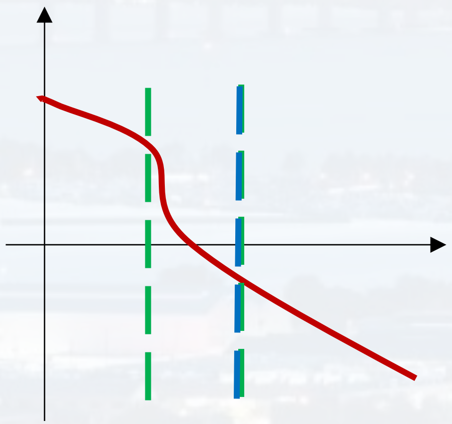

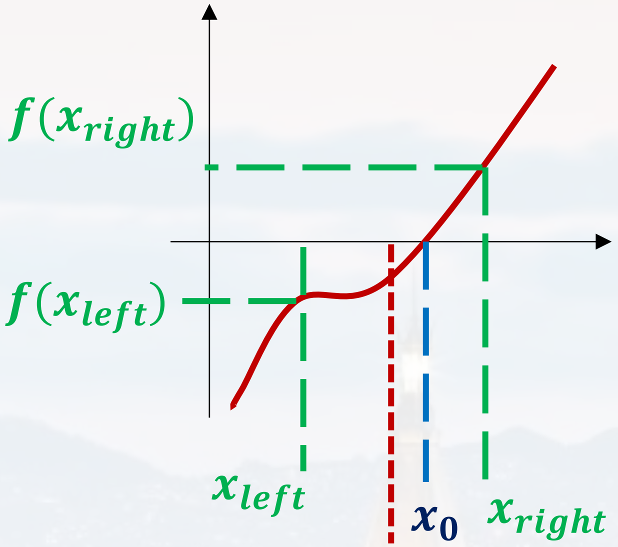

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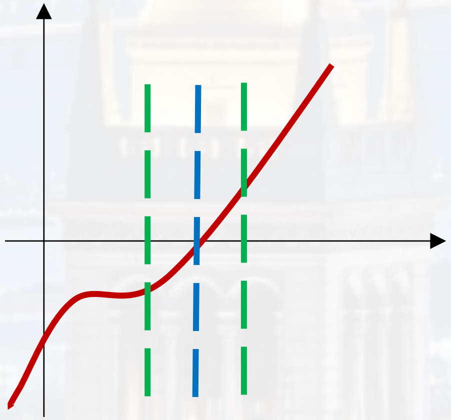
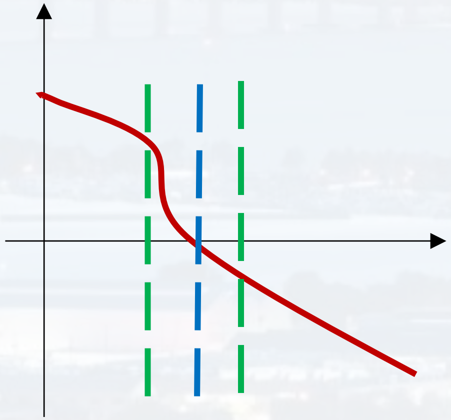
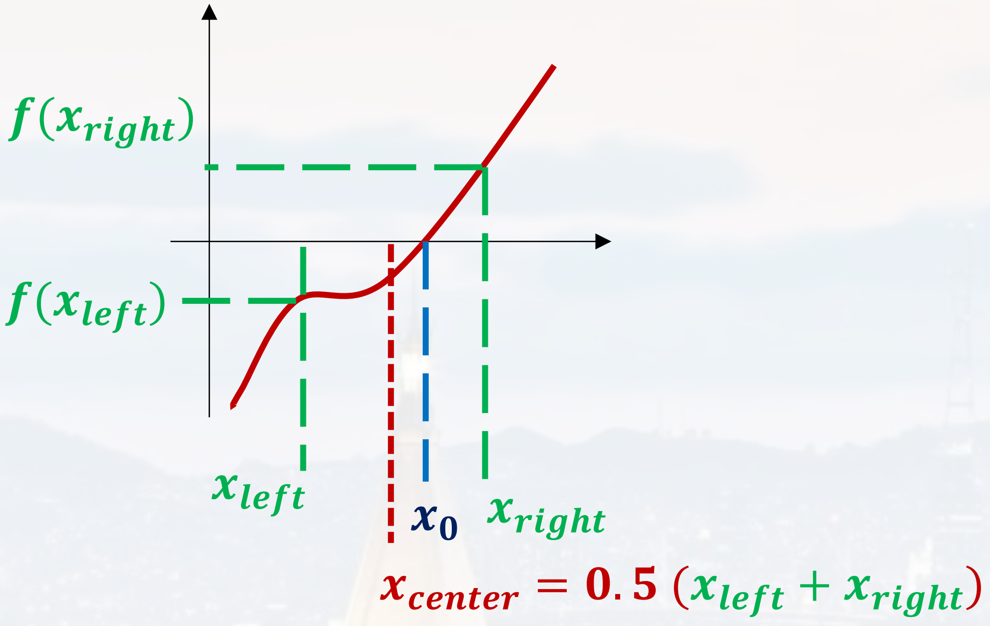




either we end up with
the same situation, or…



if $f(x_{center}) \cdot f(x_{left}) > 0$

- set x_{left} to x_{center}
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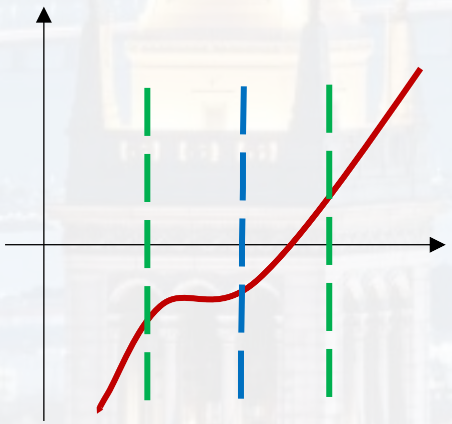

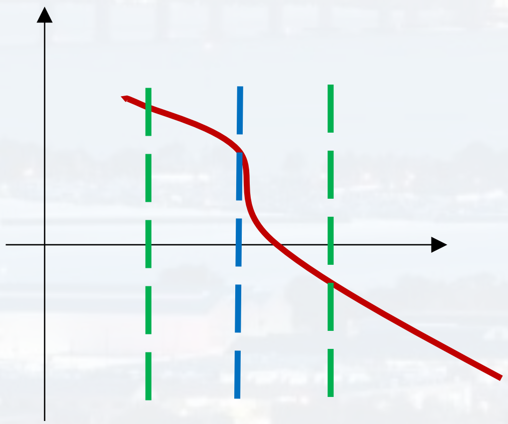

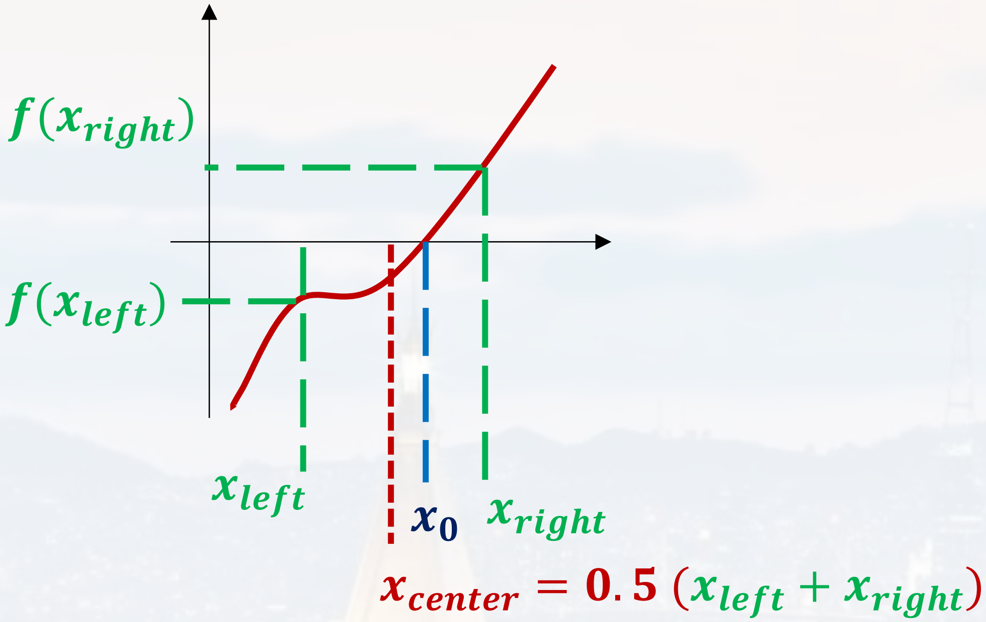

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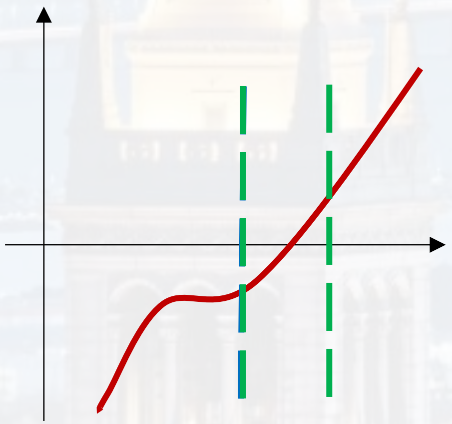

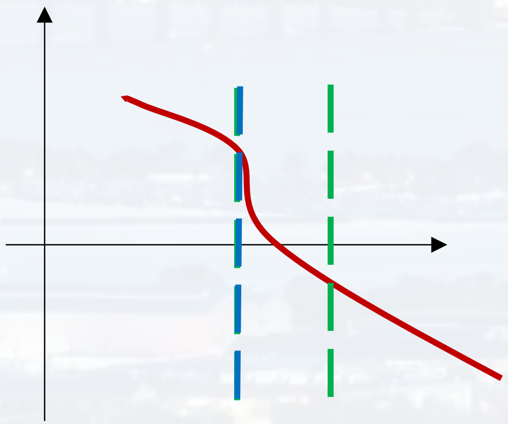

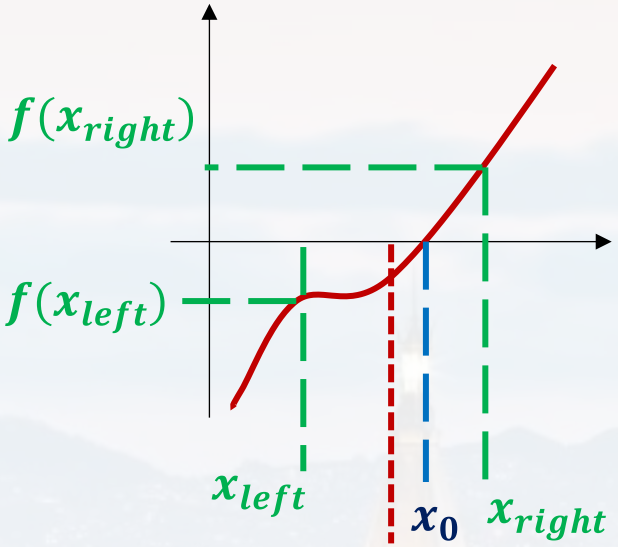

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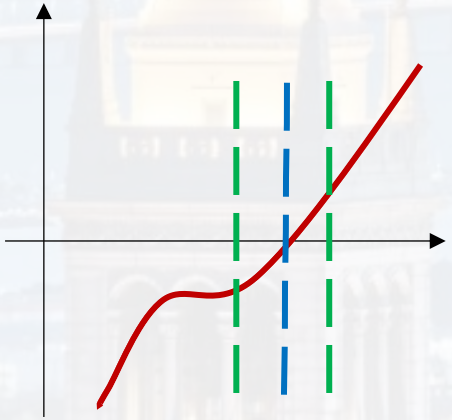
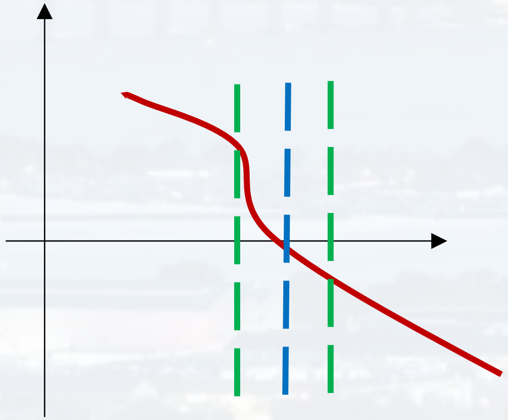
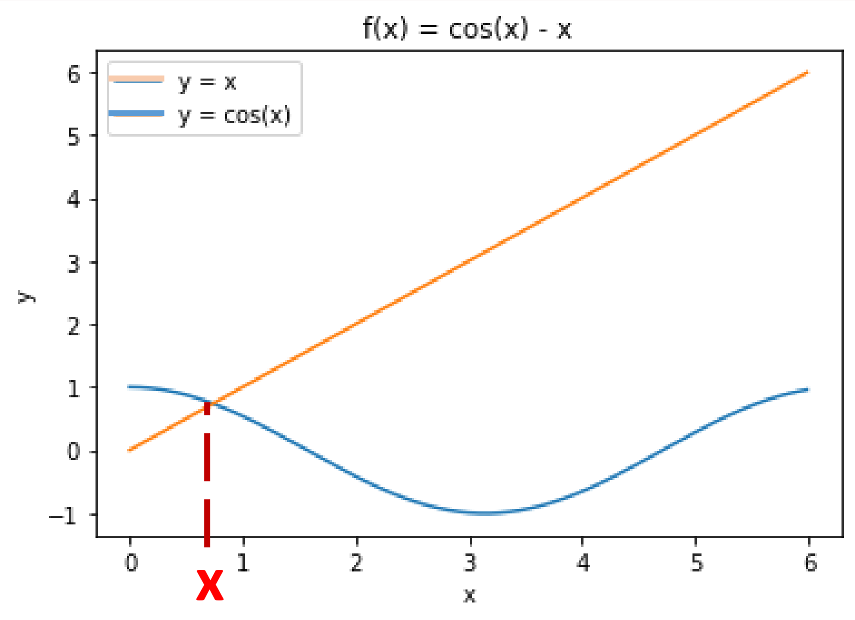
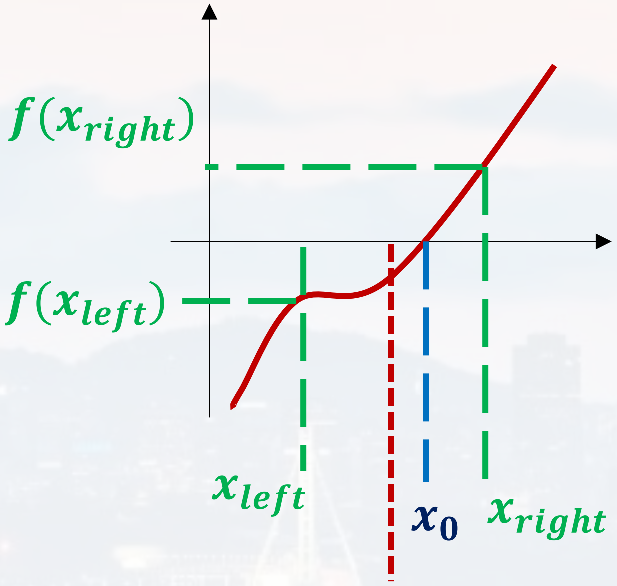




…and so on…

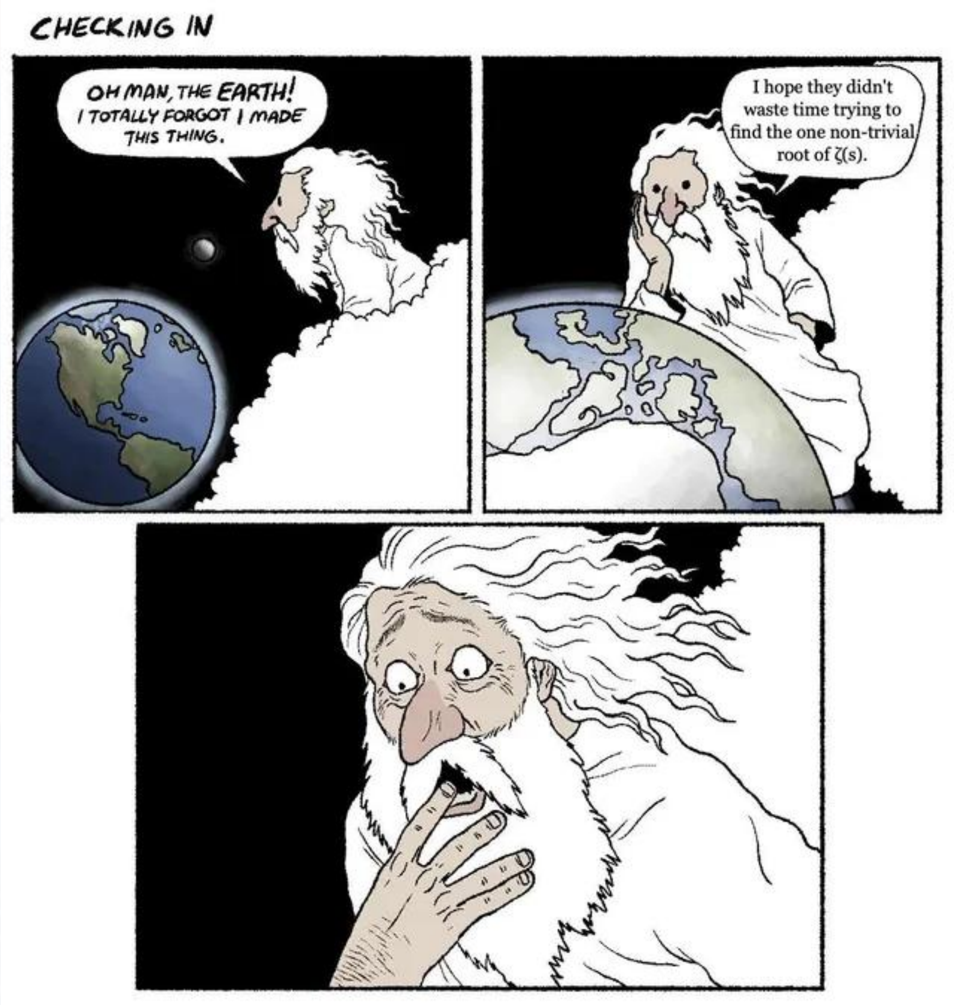
Bisection:





$$x_{center} = 0.5\,(x_{left} + x_{right})$$

- robust: always finds a root
- easy to implement (recursion), → Lecture Exercise
- slow: converges linearly **(accuracy increases by factor of 2 for each step *n*)** with *n* required for a certain accuracy



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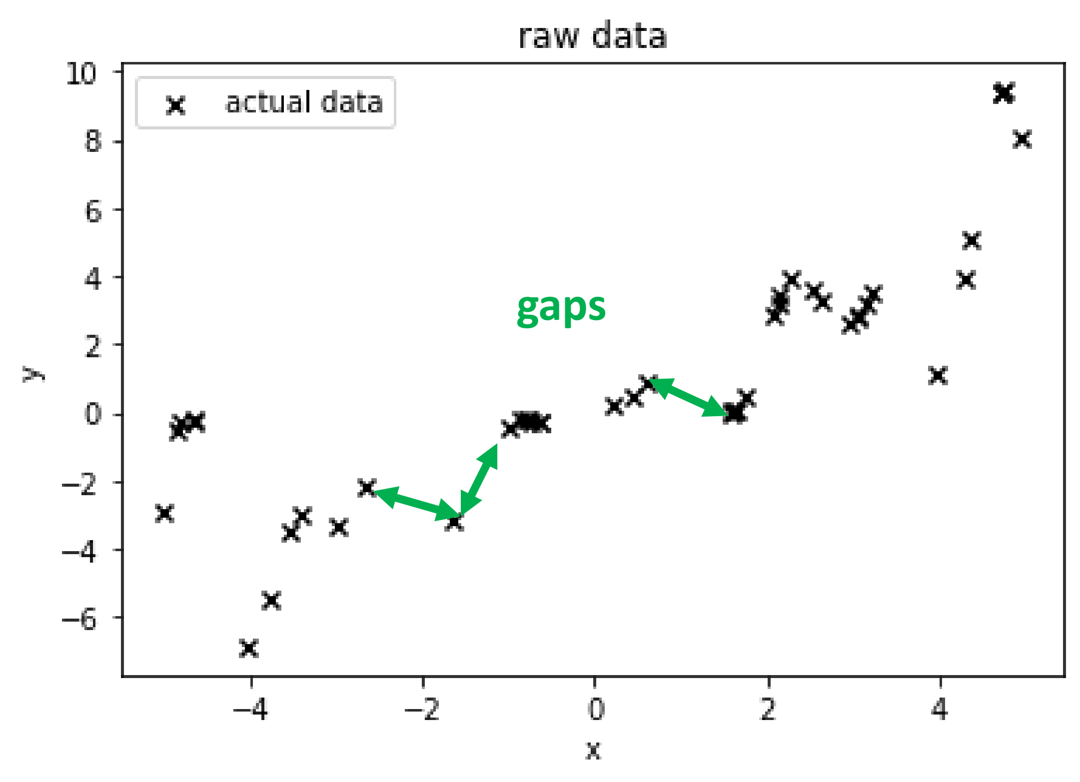
the problem:



How to interpolate?

- polynomials (1st order = linear)
- piecewise polynomials
- trigonometric functions
- exponential functions
- rational functions

called **"basis functions"**

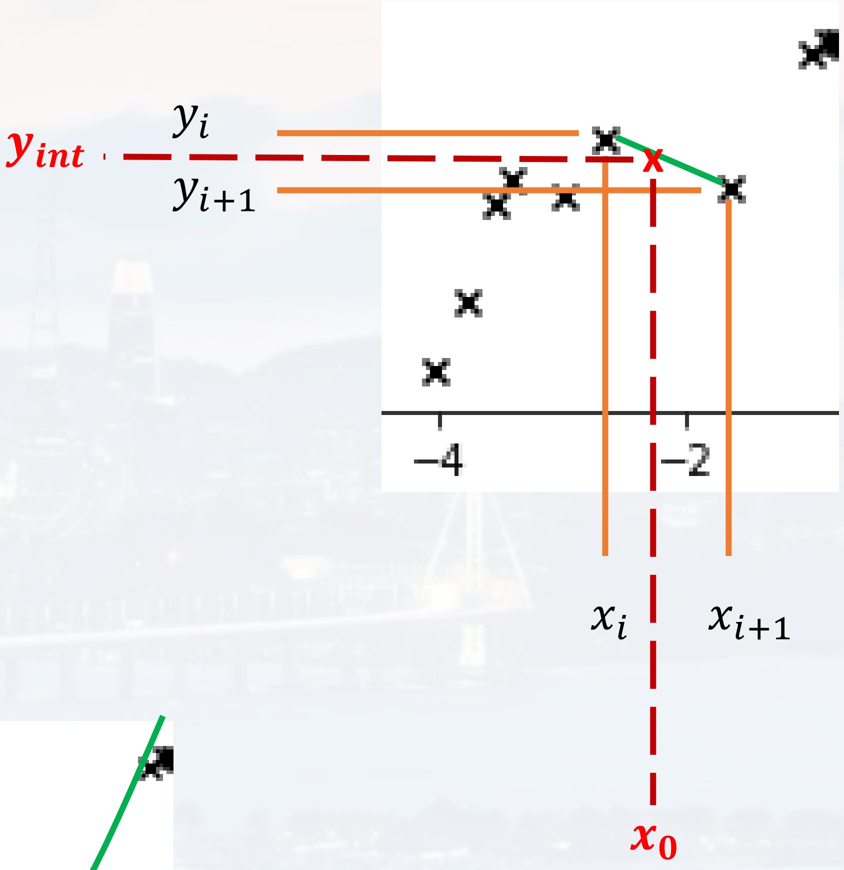
note: interpolation is not fitting!

the problem:

linear interpolation

$$y_{int} = y_i + m\,(x_0 - x_i)$$

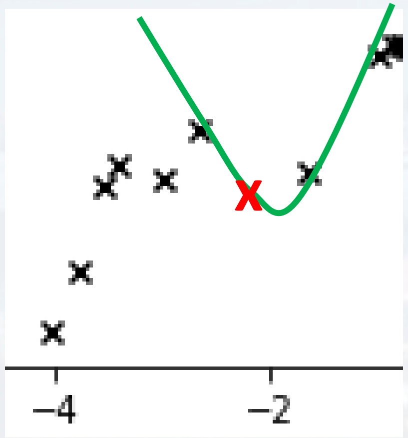
$$y_{int} = y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}\,(x_0 - x_i)$$



quadratic interpolation

$$y_{int} = y_i + m\,(x_0 - x_i) + a\,(x_0 - x_i)^2$$

this time we need **one more** reference point for calculating ***a***



the problem:

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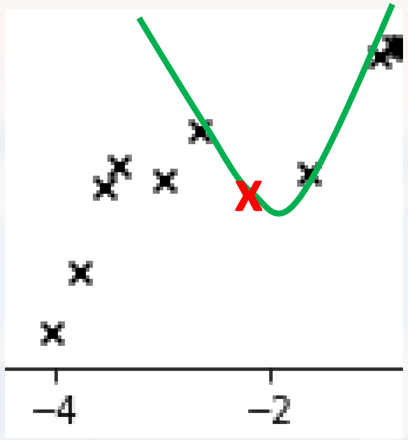


this time we need **one more** reference point for calculating ***a***

all three reference points need to fit the same parabola

$$y_i \quad = c + mx_i \quad + a\,x_i^{\,2}$$

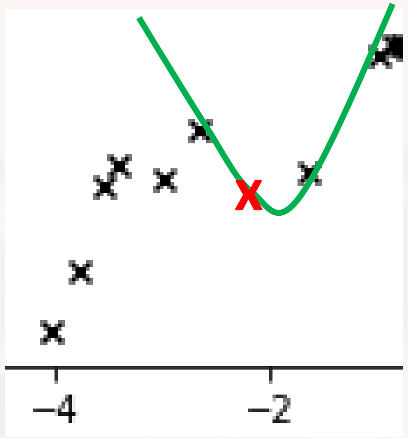
$$y_{i+1} = c + mx_{i+1} + a\,x_{i+1}^{\,2}$$

$$y_{i+2} = c + mx_{i+2} + a\,x_{i+2}^{\,2}$$

solving for c, m and a

the problem:

linear interpolation: $$y_{int} = y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}(x_0 - x_i)$$



quadratic interpolation:

$$\begin{aligned} y_i &= c + m x_i + a\, x_i^2 \\ y_{i+1} &= c + m x_{i+1} + a\, x_{i+1}^2 \\ y_{i+2} &= c + m x_{i+2} + a\, x_{i+2}^2 \end{aligned}$$

$\Rightarrow$ **solving for c, m and a**

Maybe there is a closed (= general) solution/method? → **Lagrange Polynomials**

$$\begin{aligned} y_i &= y_{int} + y'_{int}(x_i - x_0) + \mathcal{O}(\Delta x^2) \\ y_{i+1} &= y_{int} + y'_{int}(x_{i+1} - x_0) + \mathcal{O}(\Delta x^2) \end{aligned}$$

Taylor expansion

$$y_{int} = \frac{y_i(x_{i+1} - x_0)}{(x_{i+1} - x_i)} - \frac{y_{i+1}(x_i - x_0)}{(x_{i+1} - x_i)} = \boxed{y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}(x_0 - x_i)}$$

Maybe there is a closed (= general) solution/method? → **Lagrange Polynomials**

$$y_i = y_{int} + y'_{int}(x_i - x_0) + \mathcal{O}(\Delta x^2)$$

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Taylor expansion

$$y_{int} = \frac{y_i(x_{i+1} - x_0)}{(x_{i+1} - x_i)} - \frac{y_{i+1}(x_i - x_0)}{(x_{i+1} - x_i)} = \boxed{y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}(x_0 - x_i)}$$

$$y_i = y_{int} + y'_{int}(x_i - x_0) + y''_{int}(x_i - x_0)(x_i - x_0)/2 + \mathcal{O}(\Delta x^3)$$

$$y_{i+1} = y_{int} + y'_{int}(x_{i+1} - x_0) + y''_{int}(x_{i+1} - x_0)(x_{i+1} - x_0)/2 + \mathcal{O}(\Delta x^3)$$

$$y_{i+2} = y_{int} + y'_{int}(x_{i+2} - x_0) + y''_{int}(x_{i+2} - x_0)(x_{i+2} - x_0)/2 + \mathcal{O}(\Delta x^3)$$

Taylor expansion

$$y_{int} = \frac{(x_0 - x_{i+1})(x_0 - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{(x_0 - x_i)(x_0 - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{(x_0 - x_i)(x_0 - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}$$

Maybe there is a closed (= general) solution/method? → **Lagrange Polynomials**

$$y_{int} = \frac{(x_0 - x_{i+1})(x_0 - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{(x_0 - x_i)(x_0 - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{(x_0 - x_i)(x_0 - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}$$

<u>for any polynomial of n-th order:</u>

$$y_{int} = \frac{(x_0 - x_{i+1})(x_0 - x_{i+2}) \dots (x_0 - x_{i+n})}{(x_i - x_{i+1})(x_i - x_{i+2}) \dots (x_i - x_{i+n})} y_i + \frac{(x_0 - x_i)(x_0 - x_{i+2}) \dots (x_0 - x_{i+n})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2}) \dots (x_{i+1} - x_{i+n})} y_{i+1} +$$

$$\dots + \frac{(x_0 - x_i)(x_0 - x_{i+2}) \dots (x_0 - x_{i+n-1})}{(x_{i+n} - x_i)(x_n - x_{i+2}) \dots (x_{i+1} - x_{i+n-1})} y_{i+n}$$

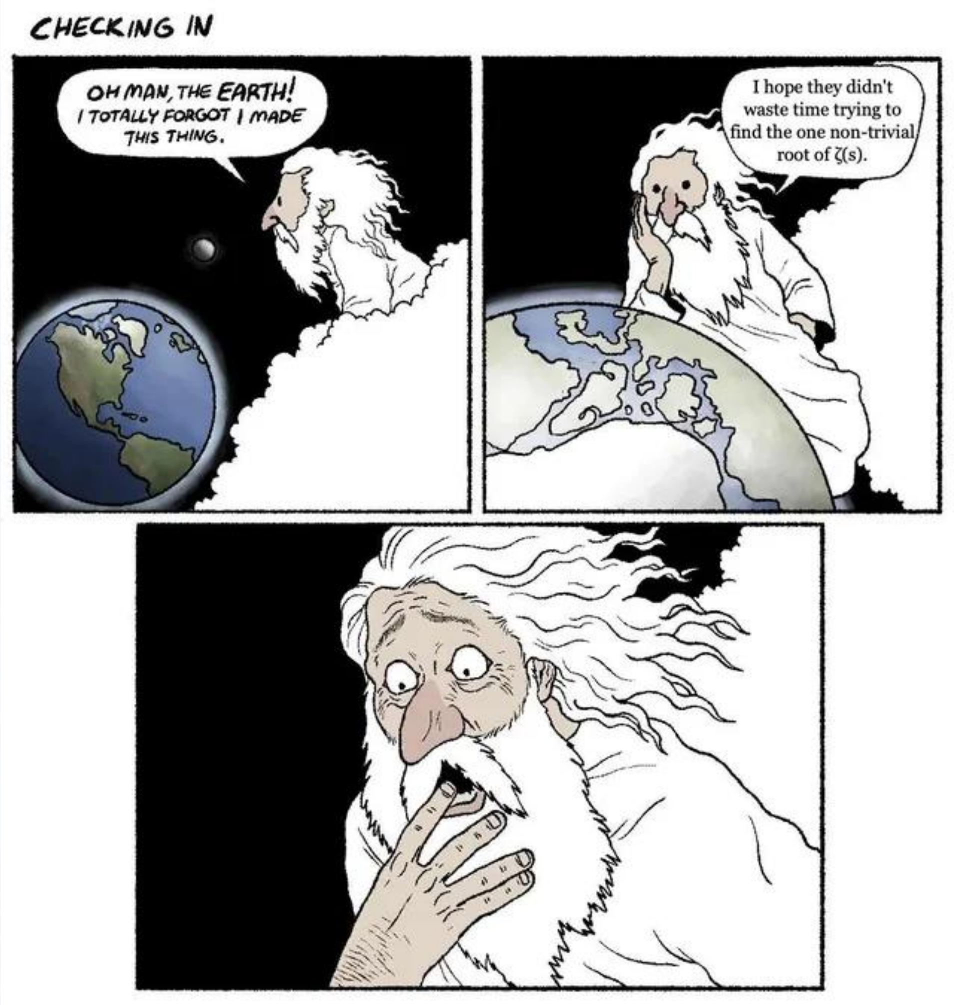
$$\boxed{y_{int} = L(x_0) = \sum_{j=0}^{n} y_j \prod_{\substack{0 \le m < n \\ m \ne j}} \frac{x_0 - x_m}{x_j - x_m}}$$

Lagrange Polynomials

$$y_{int} = L(x_0) = \sum_{j=0}^{n} y_j \prod_{\substack{0\leq m<n \\ m\neq j}} \frac{x_0 - x_m}{x_j - x_m}$$

Lagrange Polynomials

- computation is simple
- but not efficient for large n
- → only considering data points close to x_0
- → reduces approximation accuracy



Outline

root finding

- The Problem

- Newtons Method

- Bisection

interpolation

- Lagrange Polynomials

- Interpolation techniques

- Smoothing

check out InterpolateExamples.py

```
from scipy import interpolate

I    = interpolate.interp1d(x, y)

xint = np.arange(left, right, 0.1)
yint = I(xint)

plt.plot(xint, yint, c = 'r', linewidth = 3, alpha = 0.3,\
                                                  label = 'interpolation')
plt.scatter(x, y, marker = 'x', c = 'k', label = 'actual data')
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.title('linear interpolation')
plt.show()
```

check out InterpolateExamples.py

```
from scipy import interpolate

I    = interpolate.interp1d(x, y)

xint = np.arange(left, right, 0.1)
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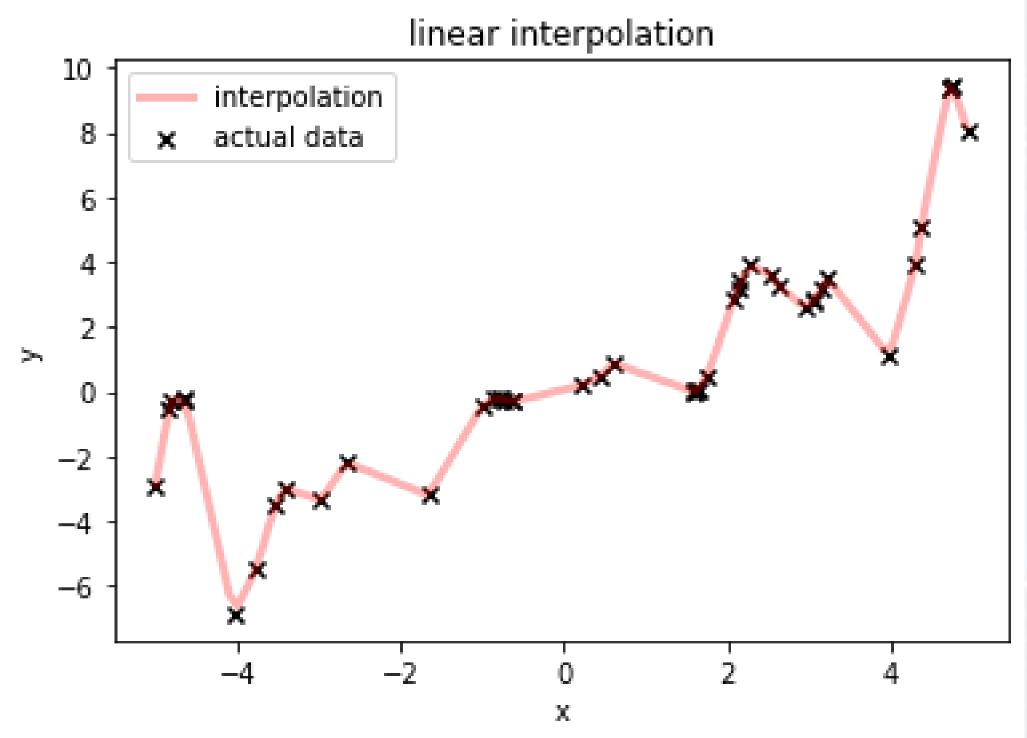

check out InterpolateExamples.py

```
from scipy import interpolate

I    = interpolate.interp1d(x, y, kind = 2)

xint = np.arange(left, right, 0.1)
yint = I(xint)

plt.plot(xint, yint, c = 'r', linewidth = 3, alpha = 0.3,\
                                          label = 'interpolation')
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plt.show()
```

quadratic interpolation

check out InterpolateExamples.py

```
from scipy import interpolate

I    = interpolate.interp1d(x, y, kind = 2)

xint = np.arange(left, right, 0.1)
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plt.scatter(x, y, marker = 'x', c = 'k',
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
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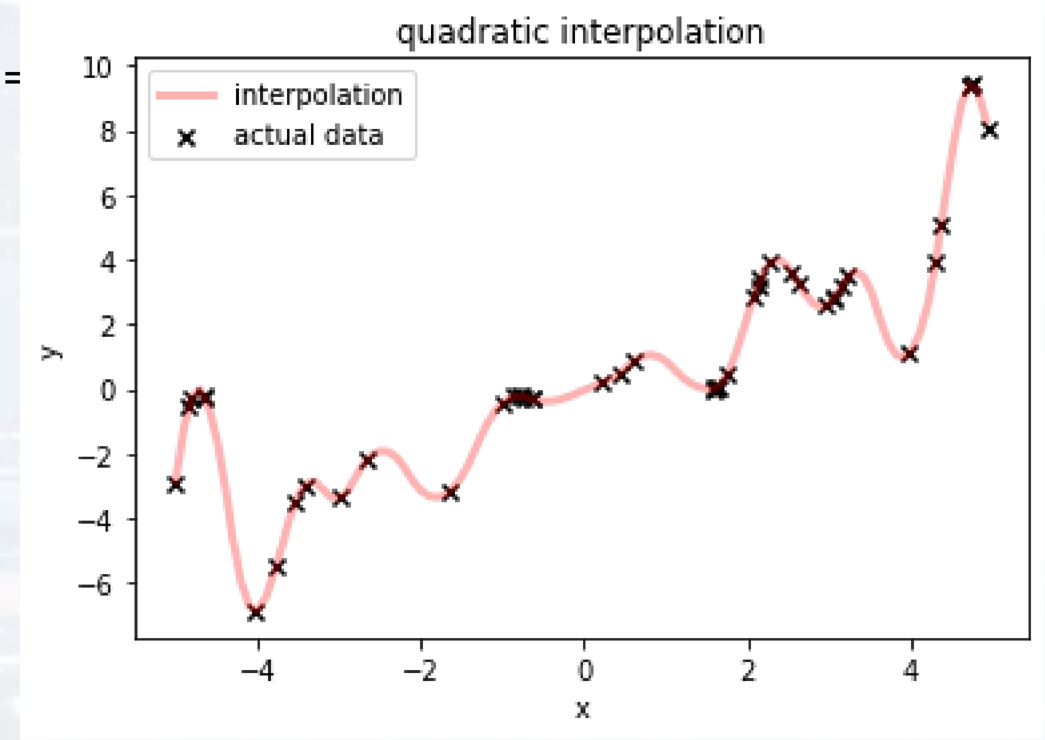
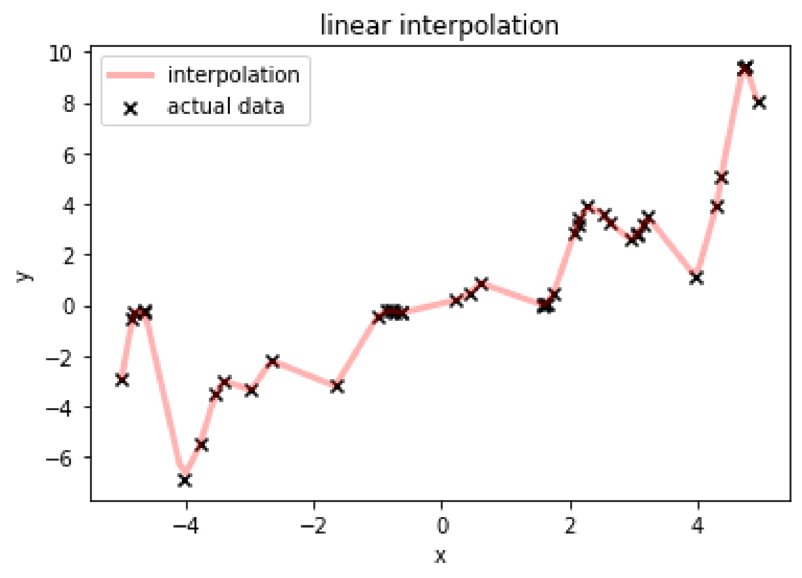
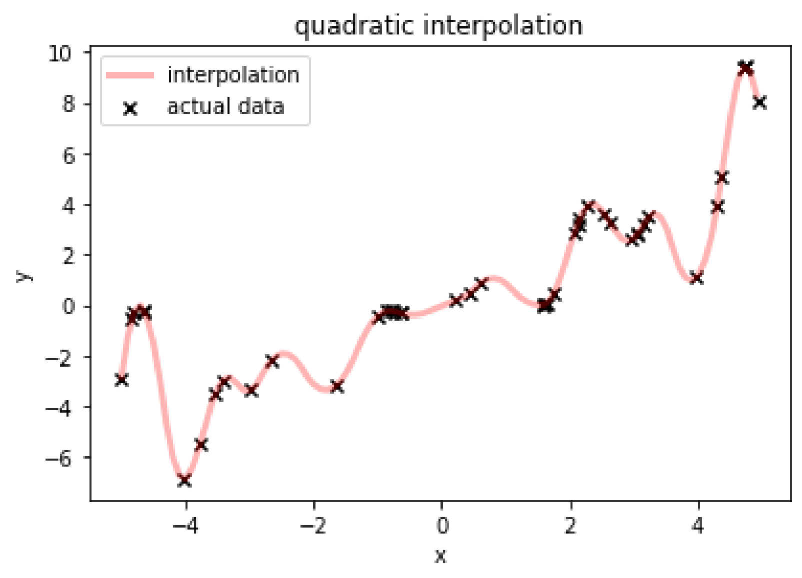
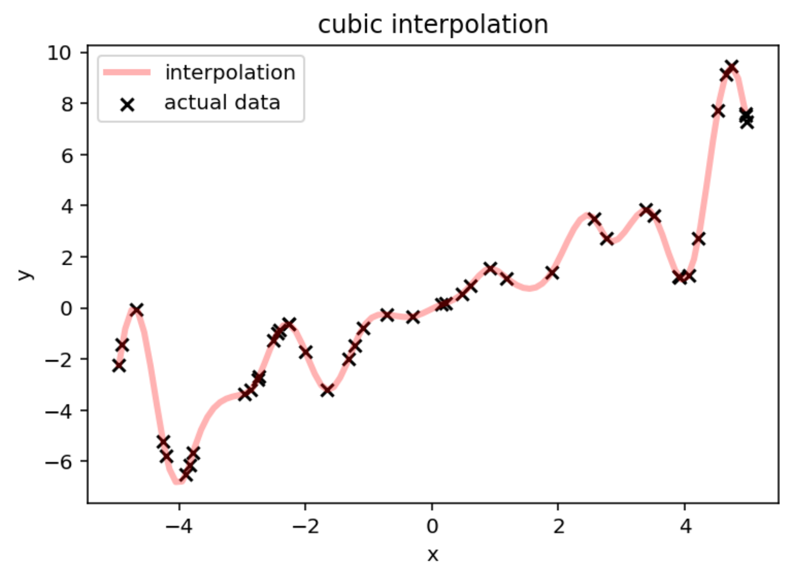
plt.show()
```

quadratic interpolation

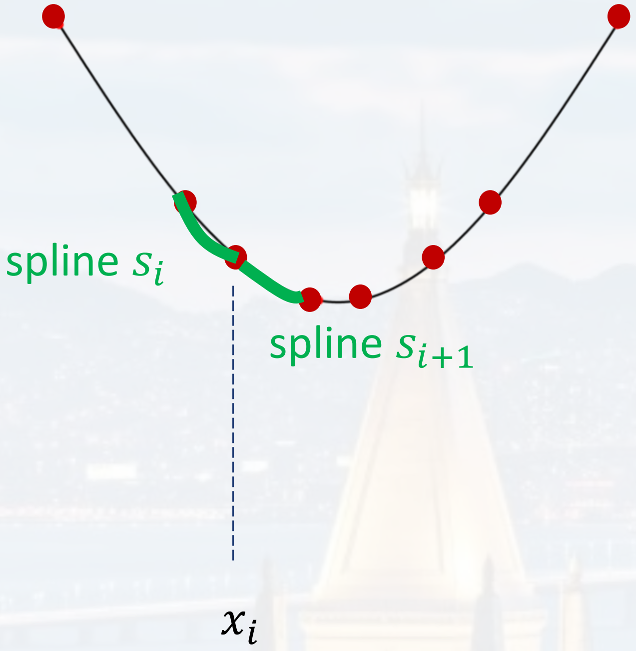



linear interpolation
interpolation
actual data
x
y


quadratic interpolation
interpolation
actual data
x
y


cubic interpolation
interpolation
actual data
x
y

spline interpolation



A shape (**piecewise** polynomials, usually cubic) that minimizes the curvature ***κ*** under the constraint of passing through all reference points

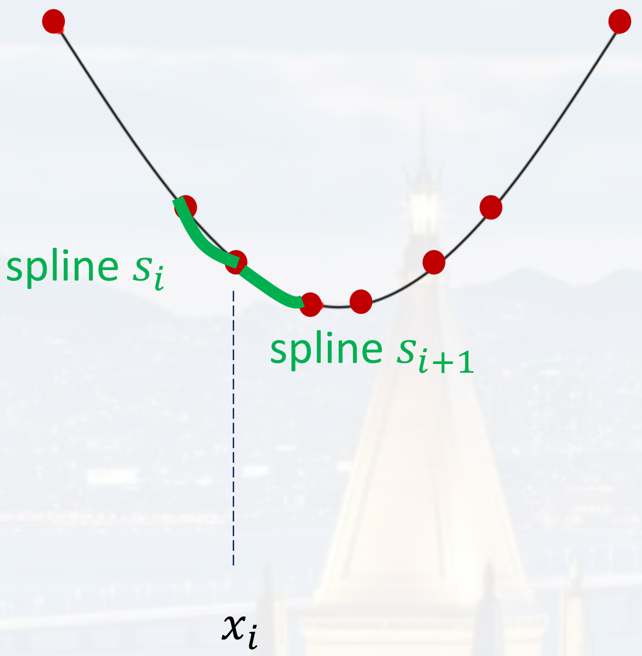
$$\kappa = \frac{\frac{d^2y}{dx^2}}{\left(1 + \left[\frac{dy}{dx}\right]^2\right)^{3/2}}$$

$$s_i(x_i) = s_{i+1}(x_i) = y_i$$

$$s_i'(x_i) = s_{i+1}'(x_i)$$

$$s_i''(x_i) = s_{i+1}''(x_i)$$

spline interpolation



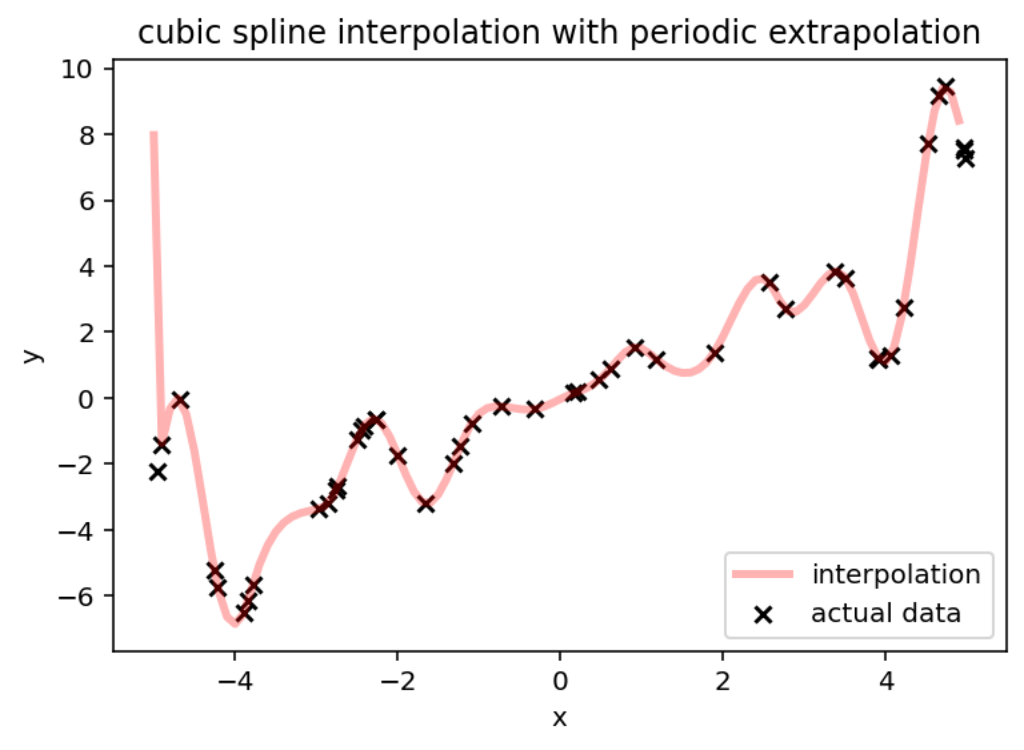
A shape (**piecewise** polynomials, usually cubic) that minimizes the curvature ***κ*** under the constraint of passing through all reference points

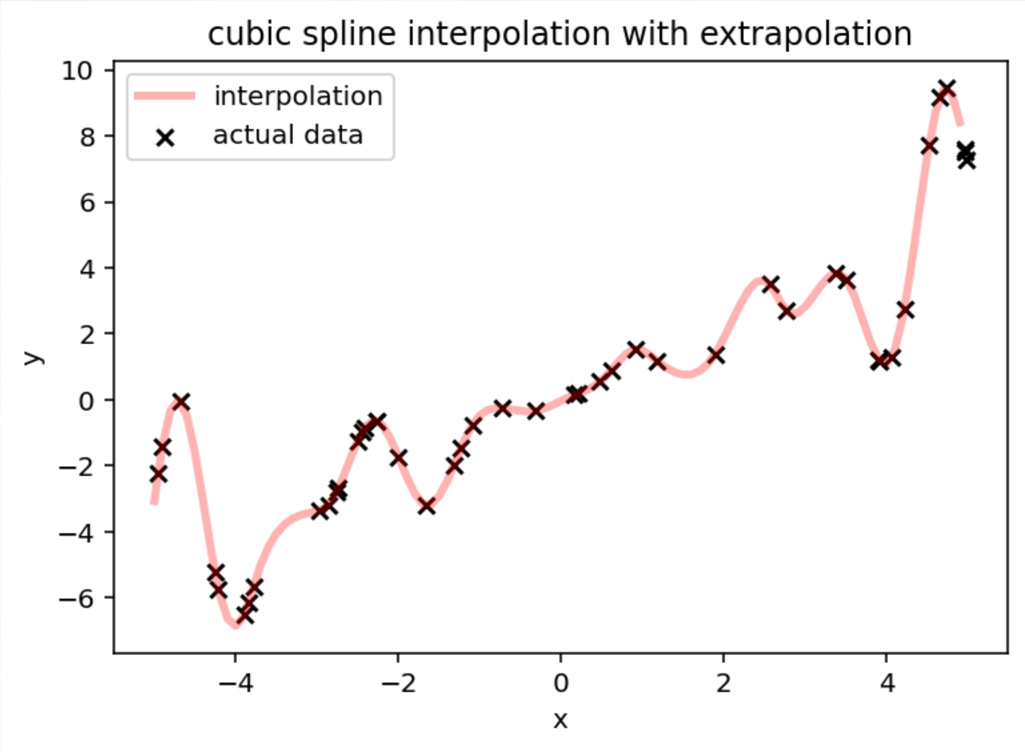
$$\kappa = \frac{\frac{d^2y}{dx^2}}{\left(1+\left[\frac{dy}{dx}\right]^2\right)^{3/2}}$$

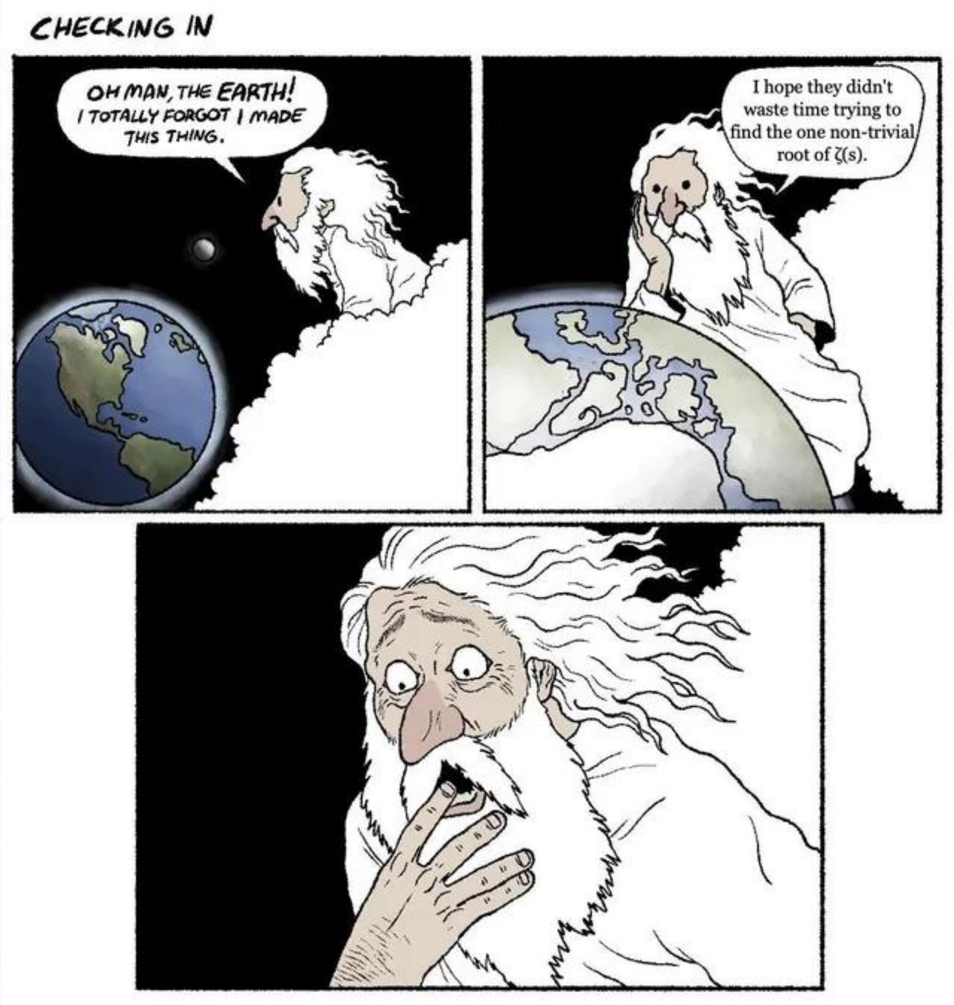
x needs to be sorted in ascending order
* stands for unpacking zipped objects

```
sorted_pairs       = sorted(zip(x, y))
x_sorted, y_sorted = zip(*sorted_pairs)
```

```
I = interpolate.CubicSpline(x_sorted, y_sorted,\
                              extrapolate = 'periodic')
```


cubic spline interpolation with periodic extrapolation
interpolation
actual data
x
y


cubic spline interpolation with extrapolation
interpolation
actual data
x
y



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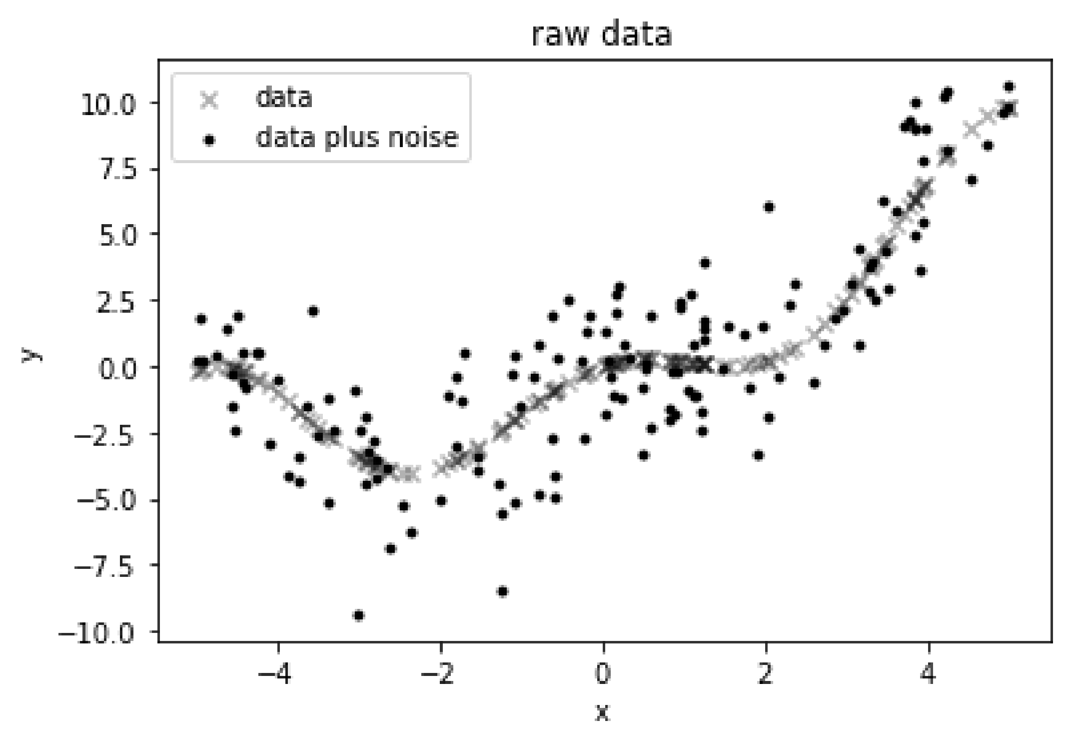
the problem:



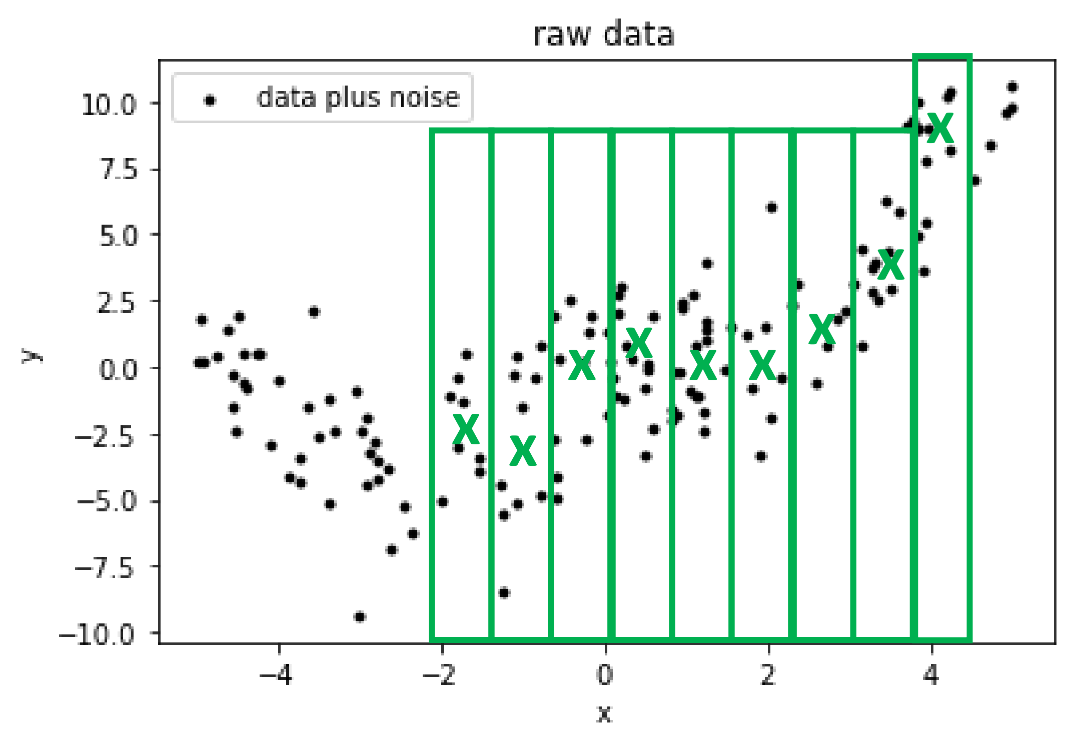
when interpolating

→ you don't want to interpolate noise

many noise filter are **low pass** filter

smoothing filter:

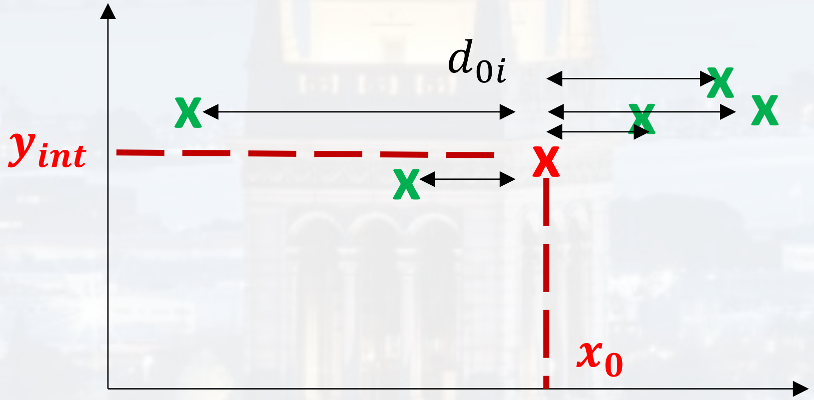
Algorithm	Overview and uses	Pros	Cons
Additive smoothing	used to smooth categorical data.		
Butterworth filter	Slower roll-off than a Chebyshev Type I/Type II filter or an elliptic filter	• More linear phase response in the passband than Chebyshev Type I/ Type II and elliptic filters can achieve. • Designed to have a frequency response as flat as possible in the passband.	• requires a higher order to implement a particular stopband specification
Chebyshev filter	Has a steeper roll-off and more passband ripple (type I) or stopband ripple (type II) than Butterworth filters.	• Minimizes the error between the idealized and the actual filter characteristic over the range of the filter	• Contains ripples in the passband.
Digital filter	Used on a sampled, discrete-time signal to reduce or enhance certain aspects of that signal		
Elliptic filter			
Exponential smoothing	• Used to reduce irregularities (random fluctuations) in time series data, thus providing a clearer view of the true underlying behaviour of the series. • Also, provides an effective means of predicting future values of the time series (forecasting).[3]		



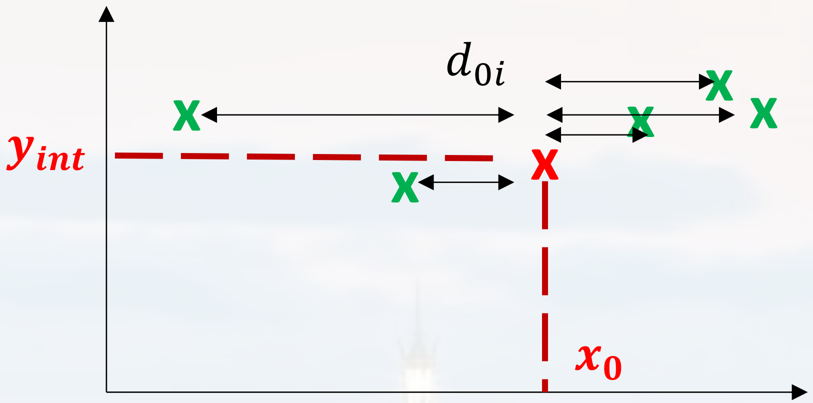
moving averages

better: → weighted average

→ data points **further away** from reference point have **lower weights** w

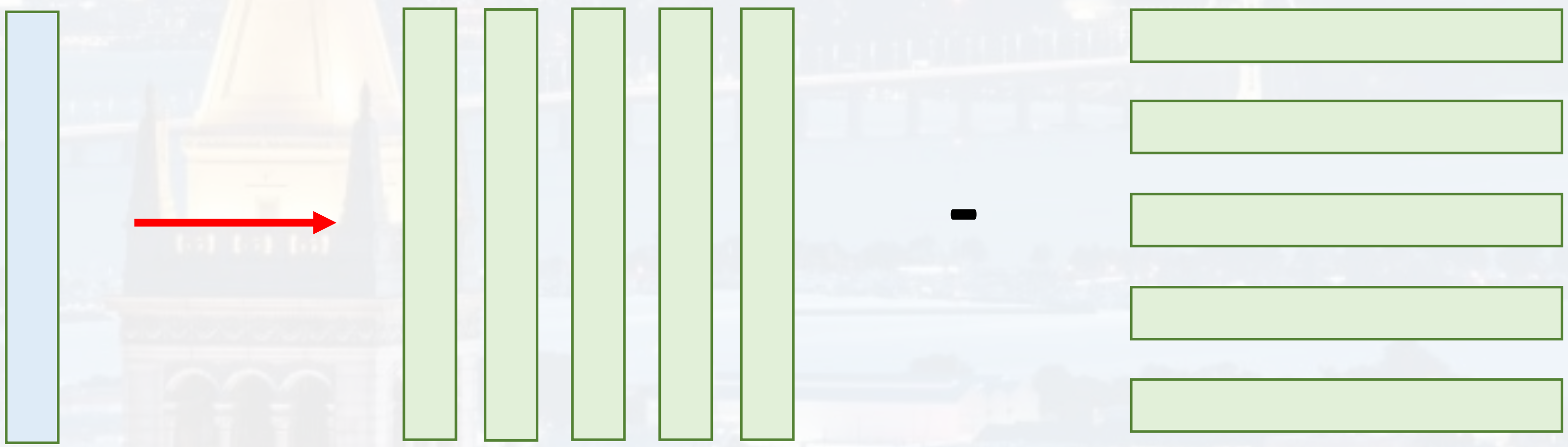


$$y_{int} \sim \sum_{i=1}^{I} w_i \, y_i \qquad w_i \sim \frac{1}{d_{0i}}$$



data points **further away** from reference point have **lower weights** w

$$y_{int} \sim \sum_{i=1}^{I} w_i \, y_i \qquad w_i \sim \frac{1}{\boxed{d_{0i}}}$$



```
L = np.random.uniform(0,1,(100,1))

D = np.tile(L, (1, len(L))) - np.tile(L.transpose(), (len(L), 1))
```

check out:

```
SmoothGaussKernel.py
SmoothExamples.py
```

```
import numpy as np

def SmoothGaussKernel(x, xint, y, sigma):

    diff  = np.median(abs(x[:-1] -x[1:]))
    sigma *= diff

    Dx    = np.tile(x.transpose(), (len(xint), 1))
    Dxint = np.tile(xint.transpose(), (len(x), 1))
    D     = Dx.transpose() - Dxint

    W     = np.exp(-(D**2)/(sigma**2))
    W     = W/np.sum(W + 1e-16, axis = 0)

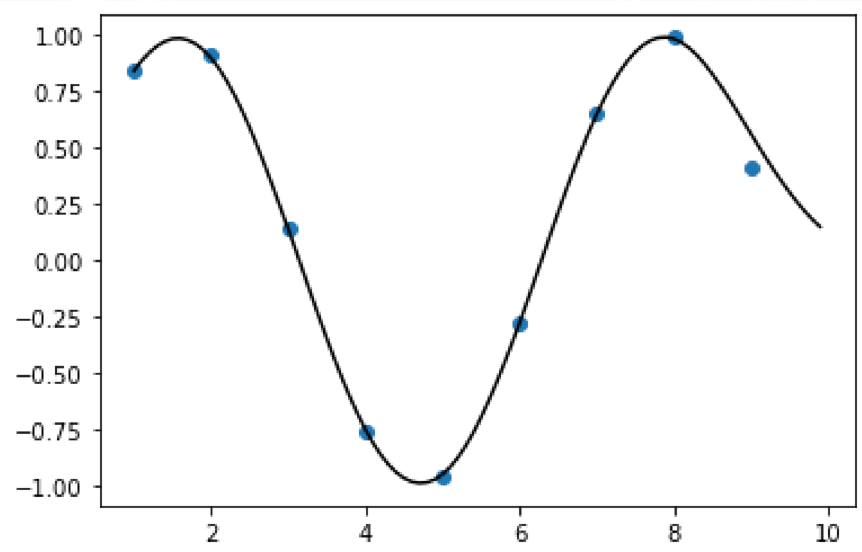
    yint  = np.dot(W.transpose(), y)

  return yint
```

scaling to dispersion of dataset

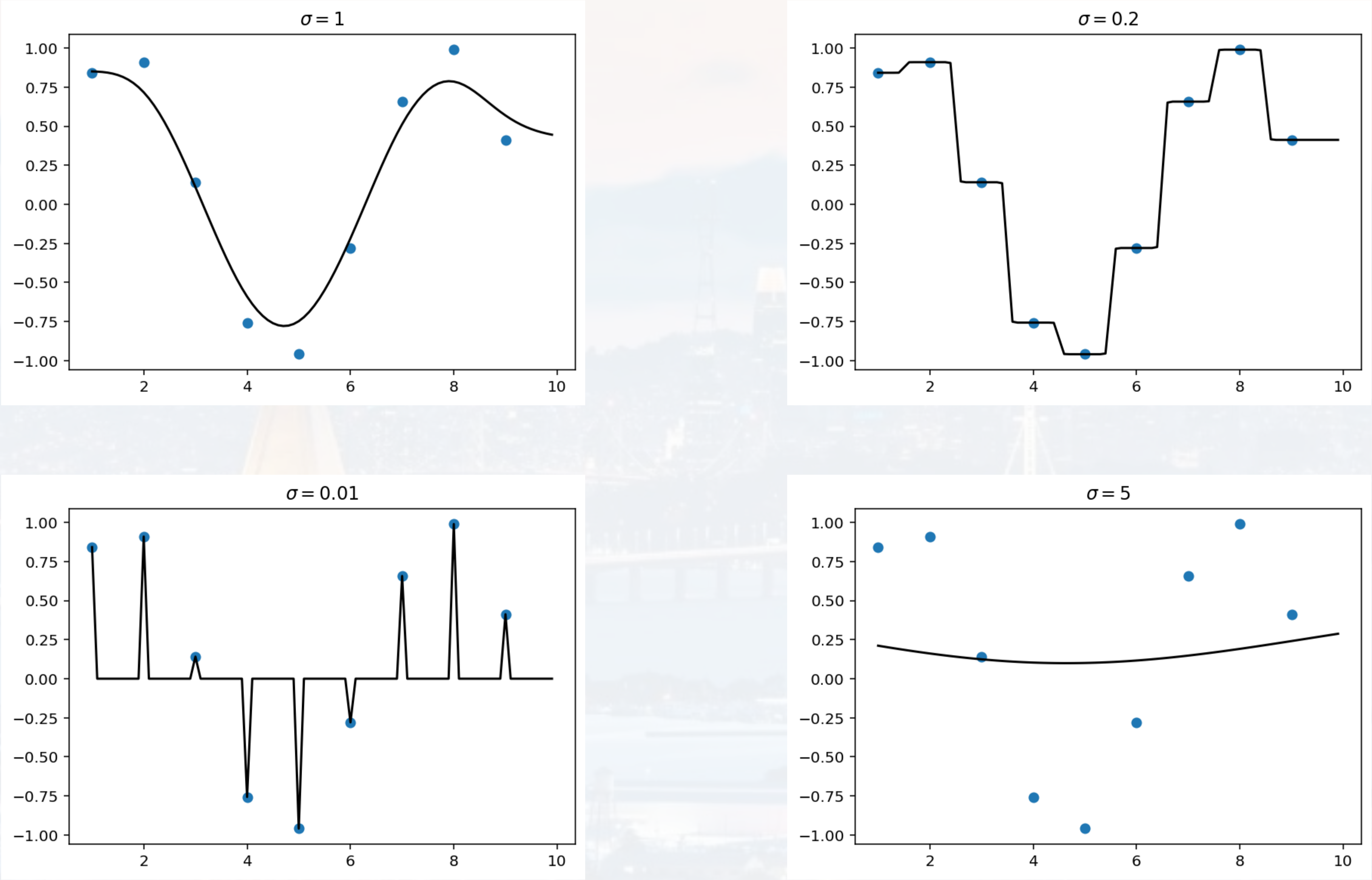
distance calculation

determining how distances are been weighted. Here: normal distribution aka **kernel**

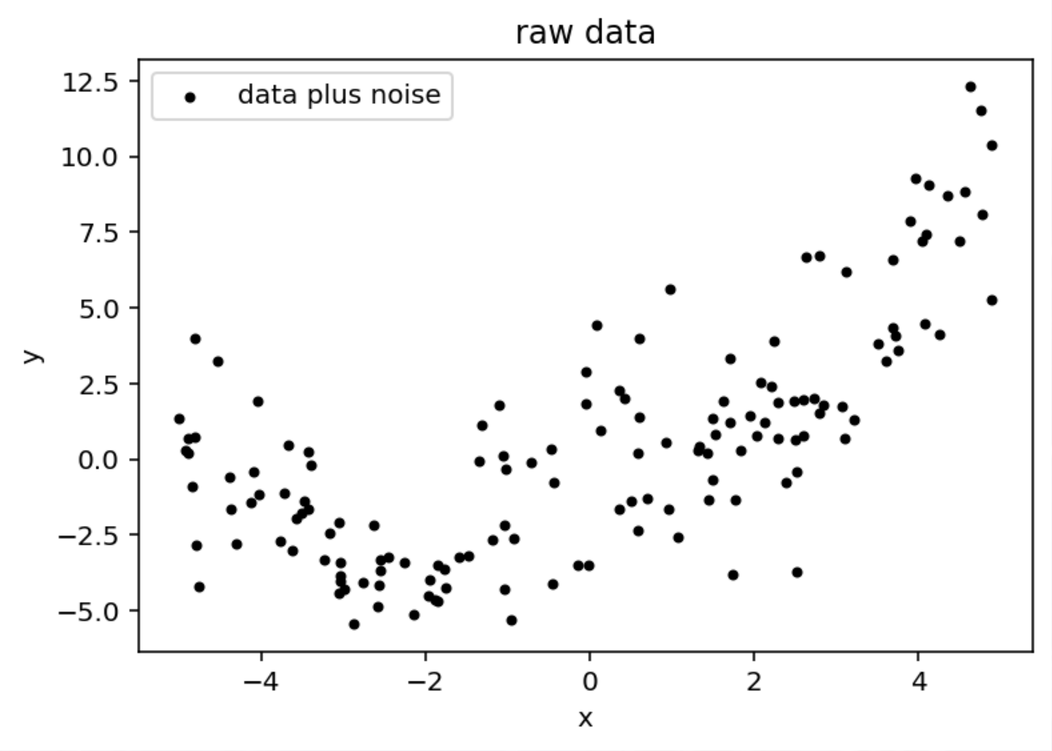


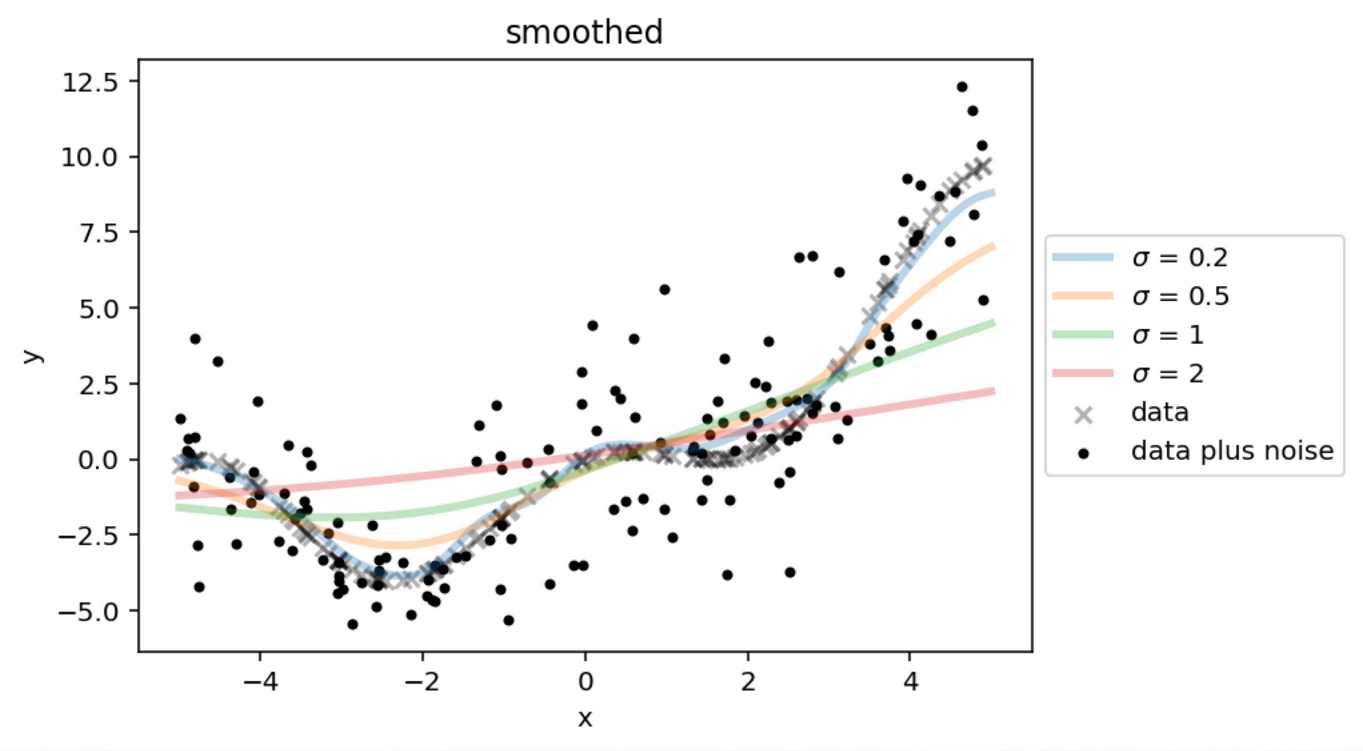
Introduction to Computational Techniques in Physics:

Smoothing



SmoothExamples.py





M. Hohle:

Thank you very much for your attention!