

PSCB57 - PROF. HANNO REIN

EXAM PREPARATION

GENERAL TIPPS

- I will test your understanding of concepts, not memorization.
- Be able to transfer existing knowledge to a new area.
- Everything from the lectures, the assignments, and tutorials, can be on the final exam.

GENERAL TIPPS

- No complicated calculations, i.e. no calculator needed.
- If a calculation gets difficult, that might be an indication that you made a mistake.
- If there are many questions, answer the questions that you know first. Keep track of the time.

GENERAL TIPPS

- Don't get confused if a question uses a different symbol than the one we used in the lecture!

GENERAL TIPPS

- It's ok not to answer a question.
- If you do not understand a question or are unsure what is asked for, raise your hand and ask for clarification. Others might have the same problem.

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PYTHON

PYTHON

- You should be comfortable with reading short python programs
- Understand control structures (`if/for/while`), variables, lists, built-in functions such as `len`, `print`, etc.

PYTHON

```
def x(l):  
    N = len(l)  
    r = -1e307  
    for i in range(N):  
        if r < l[i]:  
            r = l[i]  
    return r
```

PYTHON

- No need to know detailed syntax for functions
- No need to worry about getting indices on matrices right
- You're not expected to code up any significant program on paper

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NUMBER FORMATS

INTEGERS

- Fixed number of bits to represent an integer number
- Typical: 16, 32, 64 bits
- Finite ranges:
 $0..2^{16}-1, 0..2^{32}-1, 0..2^{64}-1$ (unsigned)
 $-2^{15}..2^{15}-1, 2^{31}..2^{31}-1, 2^{63}..2^{63}-1$ (signed)

INTEGERS

- Python 3 does something special:
It automatically increases the number of bits if you run over the range.
- Other programming languages
(including earlier versions of python)
behave differently

INTEGERS

What do you use integers for?

- Counters
- Exact calculations

INTEGERS

What are integers **not** good for?

- Calculations with a large dynamic range (i.e. most scientific applications!)

FLOATING POINT NUMBERS

- Fixed number of bits (64 for double precision that we focussed on)
- Be able to decode simple binary representations of floating point numbers

FLOATING POINT NUMBERS

64 bits



↑
52 bits for the mantissa

↑
11 bits for the exponent

↑
1 bit for the sign

$$x = (-1)^s \cdot 2^{e-1023} \cdot (1 + m)$$

FLOATING POINT NUMBERS

Important numbers to remember:

- Range: $\sim -1e-308 \dots 1e+308$
- Precision: $\sim 1e-16$

FLOATING POINT NUMBERS

When do operations become problematic?

- $1e+30 + 3.4 = 1e+30$

- $1e-16 + 1e-19 = 1.001e-16$

FLOATING POINT NUMBERS

How to prepare for the exam?

- Look at the Jupyter notebooks in the course repository.
- Try to convert a few floating point numbers by hand.
- Try to come up with floating point expressions that barely work.

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ALGORITHMIC COMPLEXITY

ALGORITHMIC COMPLEXITY

Idea:

- The time the algorithm takes to complete a calculation depends on some number N
- N can be size of your dataset, number of steps in an integration, or the number of outputs.
- How does the runtime *scale* for large N ?

ALGORITHMIC COMPLEXITY

$O(1)$	Constant
$O(\log(N))$	Logarithmic
$O(N)$	Linear
$O(N \log(N))$	Log Linear
$O(N^2)$	Quadratic
$O(N^3)$	Cubic
$O(2^N)$	Exponential

ALGORITHMIC COMPLEXITY

How to determine the complexity of a given piece of code:

- Is it recursive? How many times does it call itself?
- Closely look at for/while loops. Are they nested?
- Focus on the big picture, ignore details.

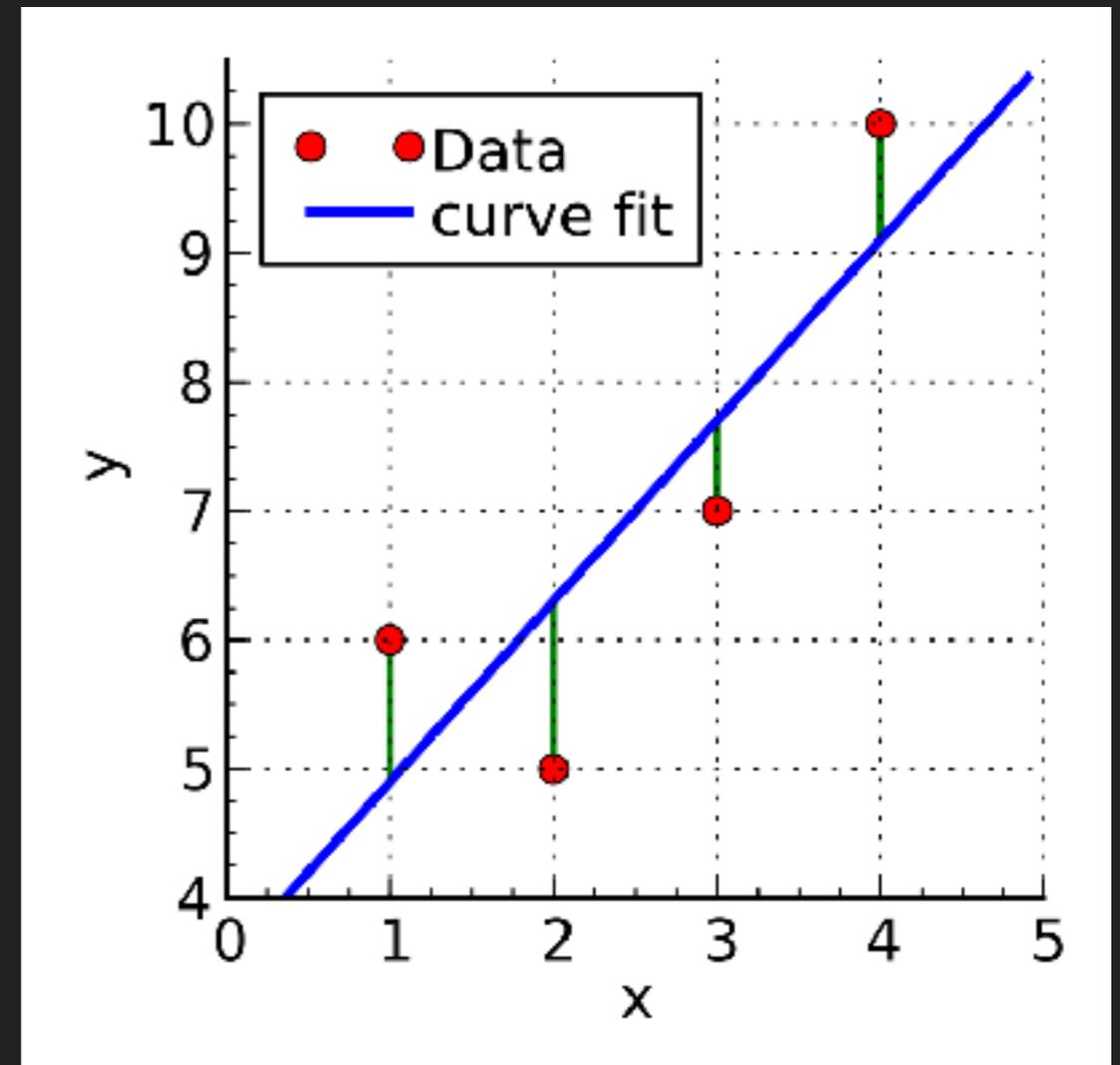
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LINEAR LEAST SQUARE FIT

LINEAR LEAST SQUARE FIT

Definition: minimize the "sum of squares"

$$S = \sum_{i=0}^{N-1} e_i^2$$



LINEAR LEAST SQUARE FIT

- ▶ We have a function with a set of free parameters a .
- ▶ Want to parameters a to minimize S .
- ▶ This lead us to the matrix equation:

$$\underbrace{C^T \cdot y}_b = \underbrace{(C^T C)}_A \cdot a$$

LINEAR LEAST SQUARE FIT

- ▶ Where the matrix C depends on the function we want to fit and the datapoints. For example:

$$f(t) = a_0 + a_1 \sin\left(\frac{t}{24}2\pi\right) + a_2 \cos\left(\frac{t}{24}2\pi\right)$$

$$\begin{pmatrix} 1 & \sin\left(\frac{x_0}{24}2\pi\right) & \cos\left(\frac{x_0}{24}2\pi\right) \\ 1 & \sin\left(\frac{x_1}{24}2\pi\right) & \cos\left(\frac{x_1}{24}2\pi\right) \\ \vdots & \vdots & \vdots \\ 1 & \sin\left(\frac{x_{N-1}}{24}2\pi\right) & \cos\left(\frac{x_{N-1}}{24}2\pi\right) \end{pmatrix}$$

LINEAR LEAST SQUARE FIT

- ▶ You should be able to construct the matrix C , as well as the vector b and matrix A for arbitrary functions and datapoints.
- ▶ You are expected to then solve the linear system of equations *only* if the number of parameters is ≤ 2 .

LINEAR LEAST SQUARE FIT

- ▶ What does the term *linear* refer to?

$$f(t) = a_0 + a_1 \sin\left(\frac{t}{24}2\pi\right) + a_2 \cos\left(\frac{t}{24}2\pi\right)$$

- ▶ Know when you cannot fit a function using a *linear* least square fit.

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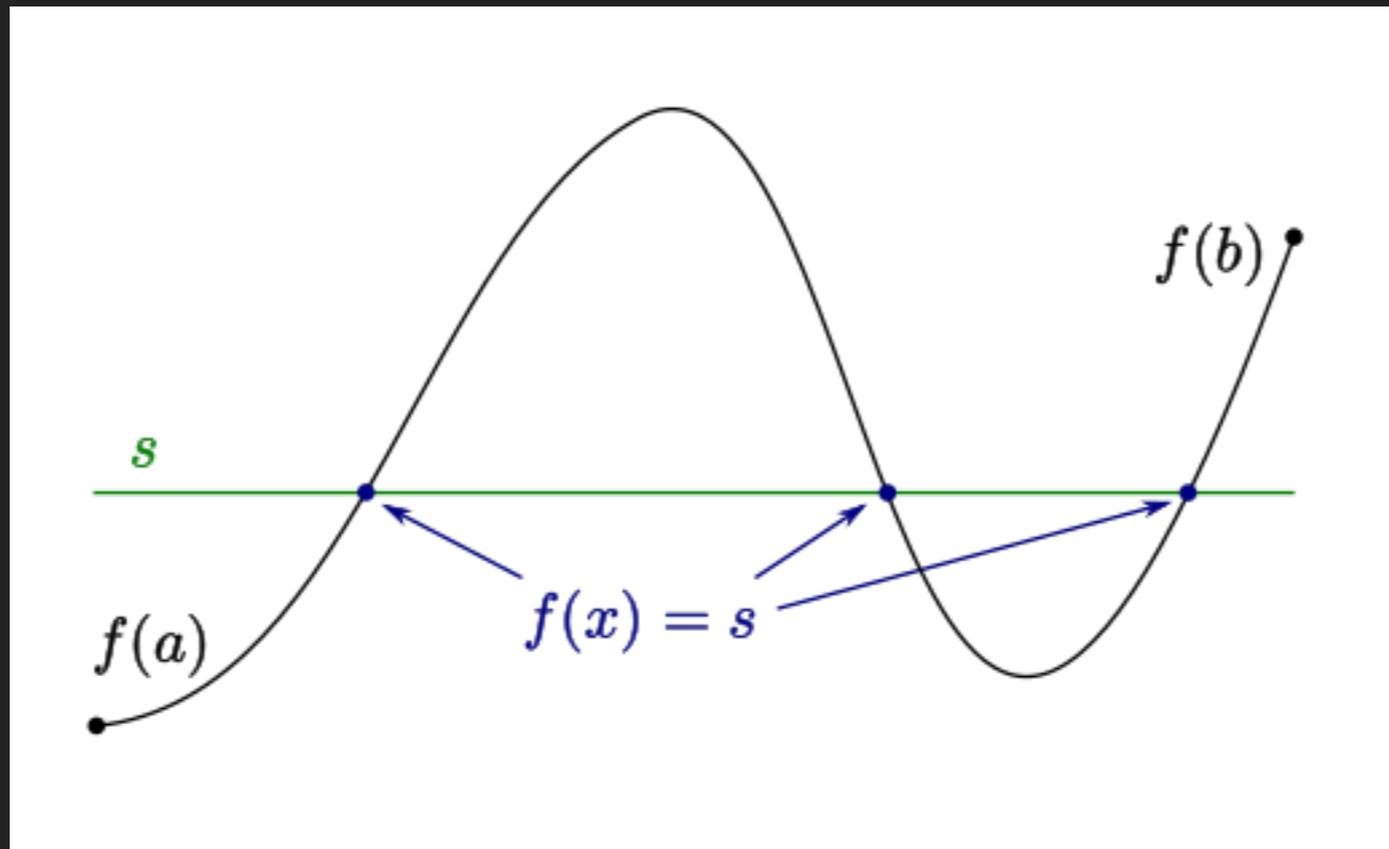
ROOT FINDING METHODS

ROOT FINDING METHODS

- ▶ Where do we encounter root finding?
- ▶ Least Square Fit
- ▶ Optimization methods
- ▶ Constrained equations

ROOT FINDING METHODS

- ▶ Intermediate value theorem.



- ▶ Guarantees existence of a root.

ROOT FINDING METHODS

- ▶ Intermediate value theorem directly leads to the bisection method
- ▶ Bisection method always works!
- ▶ Needs starting interval
- ▶ Reduces interval by half at each step

ROOT FINDING METHODS

- ▶ How many times do you have to iterate the bisection method when using double floating point precision?
- ▶ At most 52 times!

ROOT FINDING METHODS

- ▶ Other root finding methods: Newton's method
- ▶ Even faster than bisection
- ▶ Needs a starting point (no interval)
- ▶ Need to know the derivate of the function.
- ▶ Might not converge!

ROOT FINDING METHODS

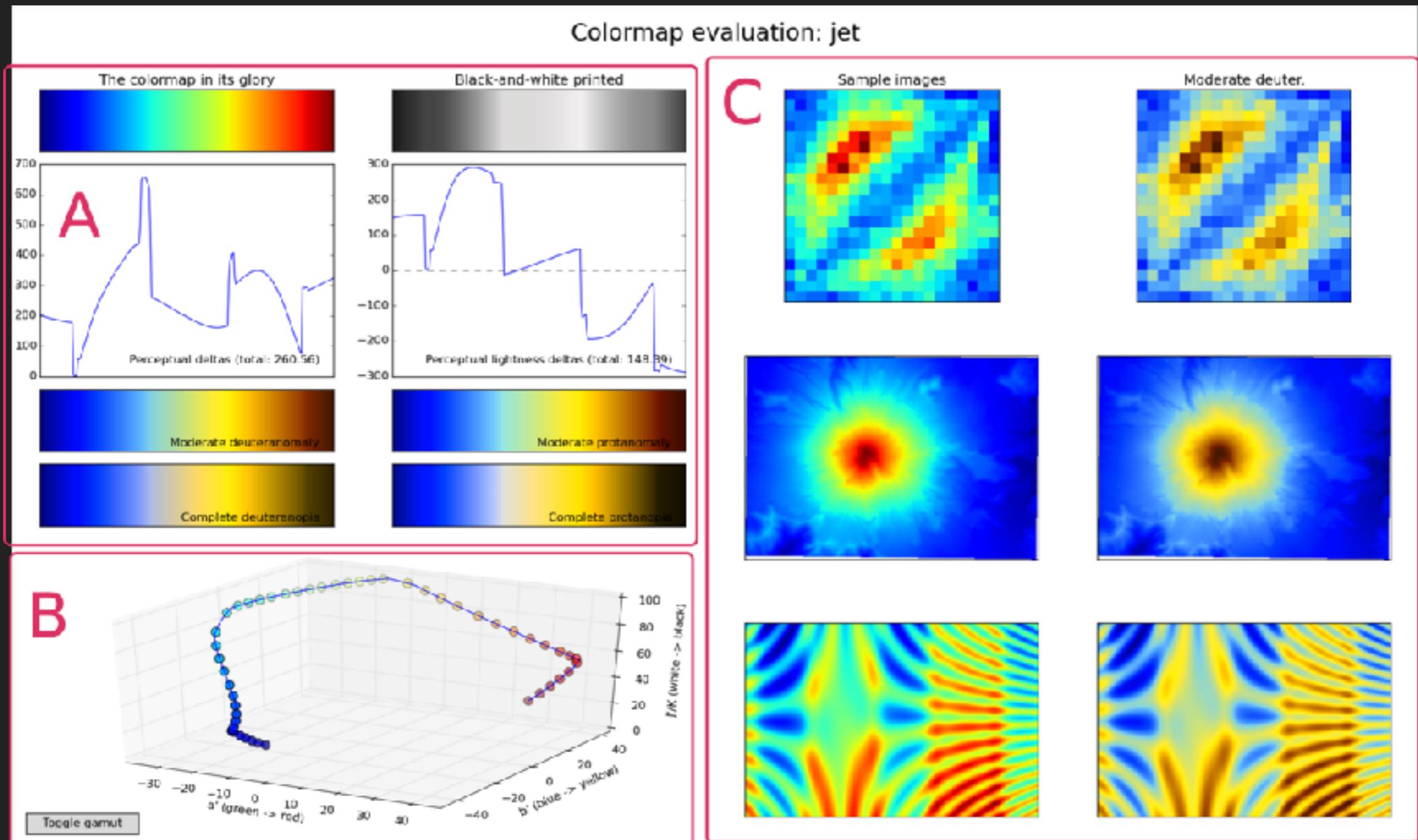
- ▶ Root finding is a very large topic.
- ▶ We just scratched the surface.
- ▶ Our methods work well for 1D
- ▶ High dimensional problems are **MUCH** harder

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PLOTTING

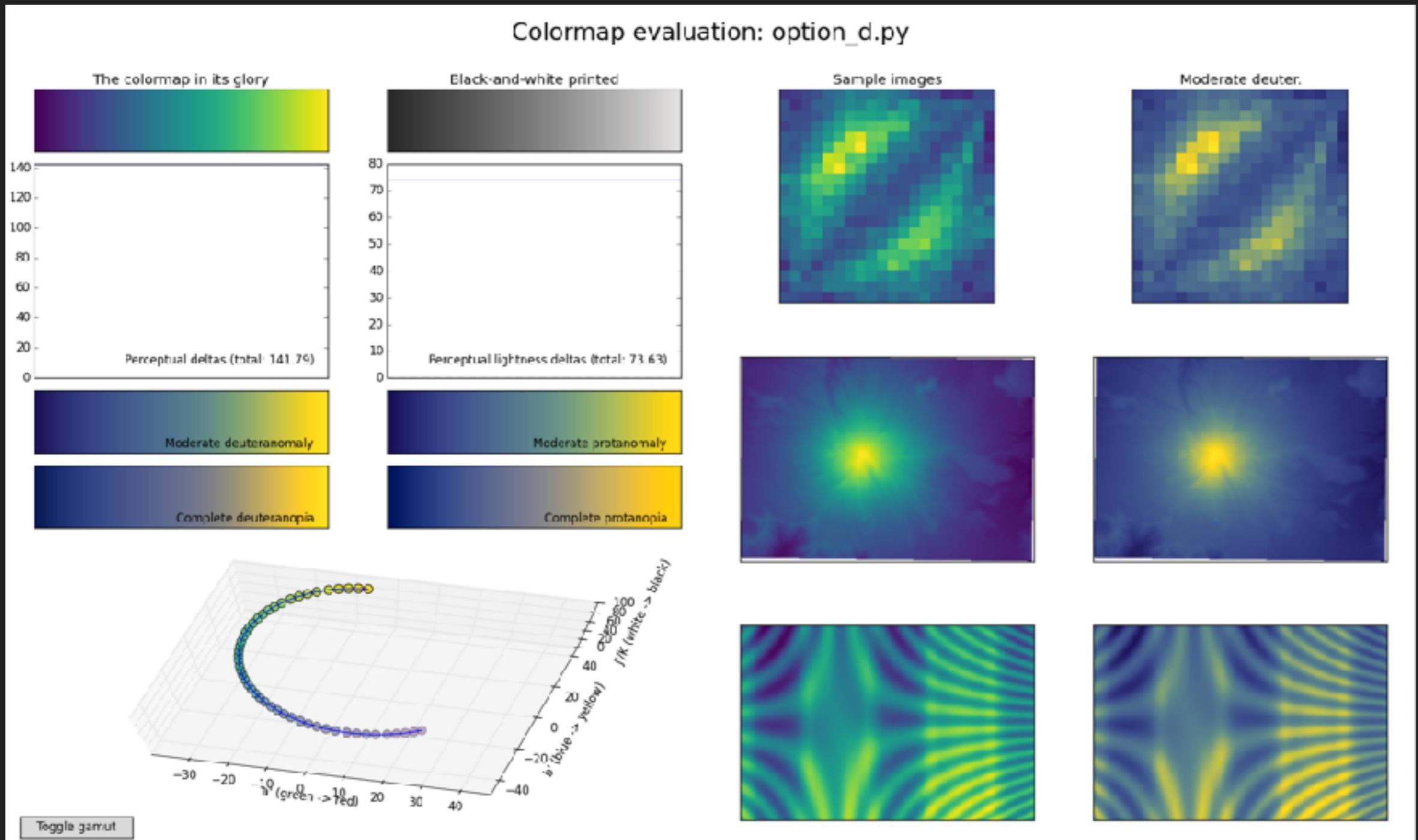
PLOTTING

► Non-perceptually uniform colour map



PLOTTING

► Perceptually uniform colour map



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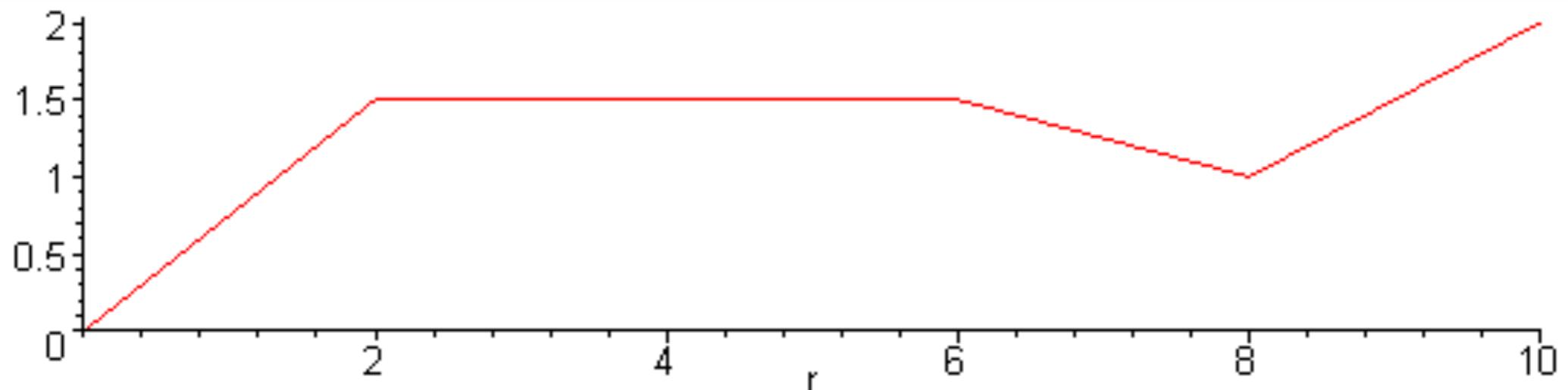
INTERPOLATION METHODS

INTERPOLATION METHODS

- ▶ Difference between interpolation and fit
- ▶ Interpolation goes through all data points, independent of any model
- ▶ Note that plotting data points and connecting them by lines is already an interpolation

INTERPOLATION METHODS

- ▶ Nearest neighbour / constant interpolation / Voronoi mesh
- ▶ Piece-wise linear interpolation



INTERPOLATION METHODS

▶ Lagrange interpolation

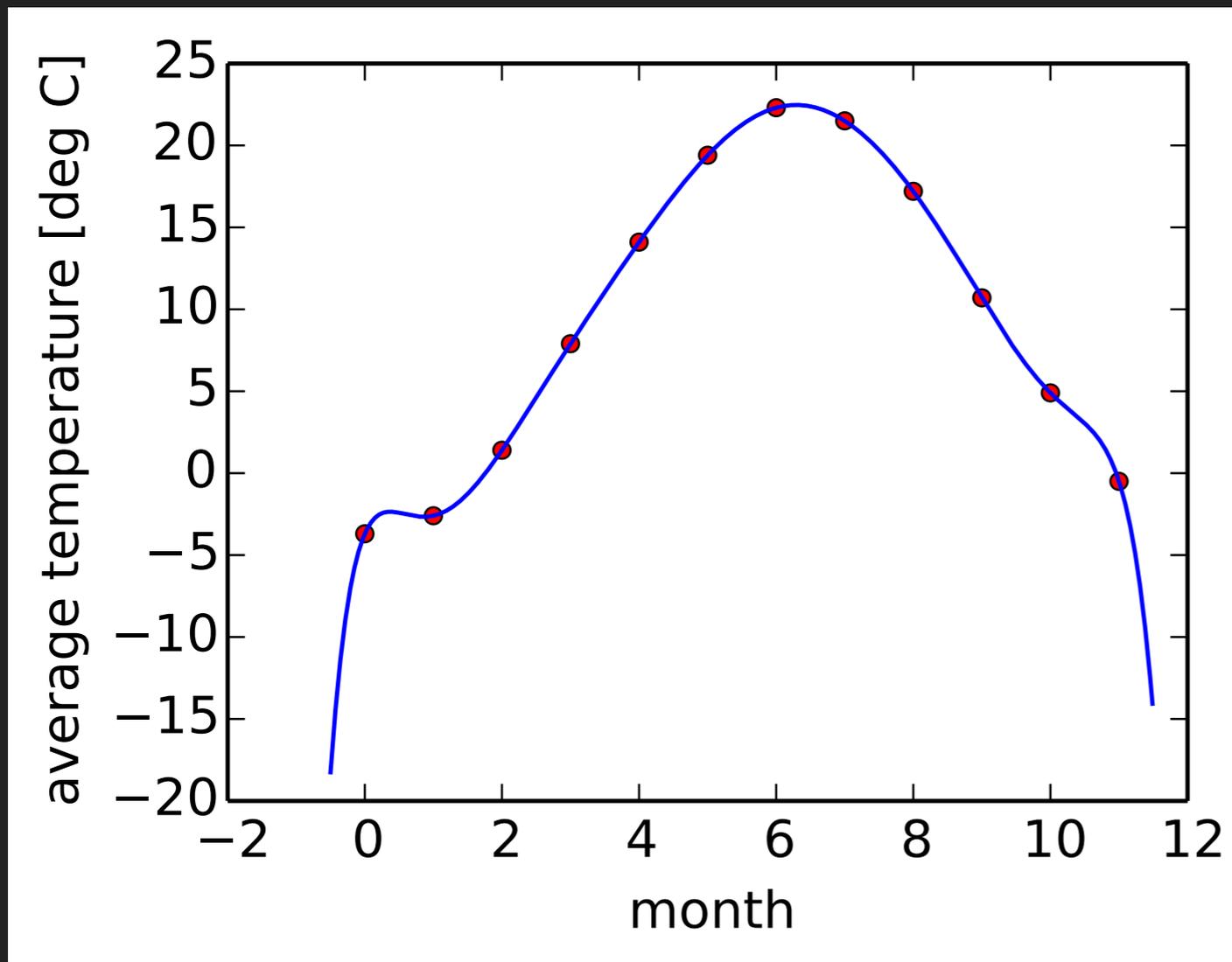
$$L(x) = \sum_{j=0}^{N-1} y_j \ell_j(x)$$

▶ With basis polynomials

$$\ell_j(x) = \prod_{\substack{0 \leq m \leq N-1 \\ m \neq j}} \frac{x - x_m}{x_j - x_m} = \frac{(x - x_0) \dots (x - x_{j-1}) (x - x_{j+1}) \dots (x - x_{N-1})}{(x_j - x_0) \dots (x_j - x_{j-1}) (x_j - x_{j+1}) \dots (x_j - x_{N-1})}$$

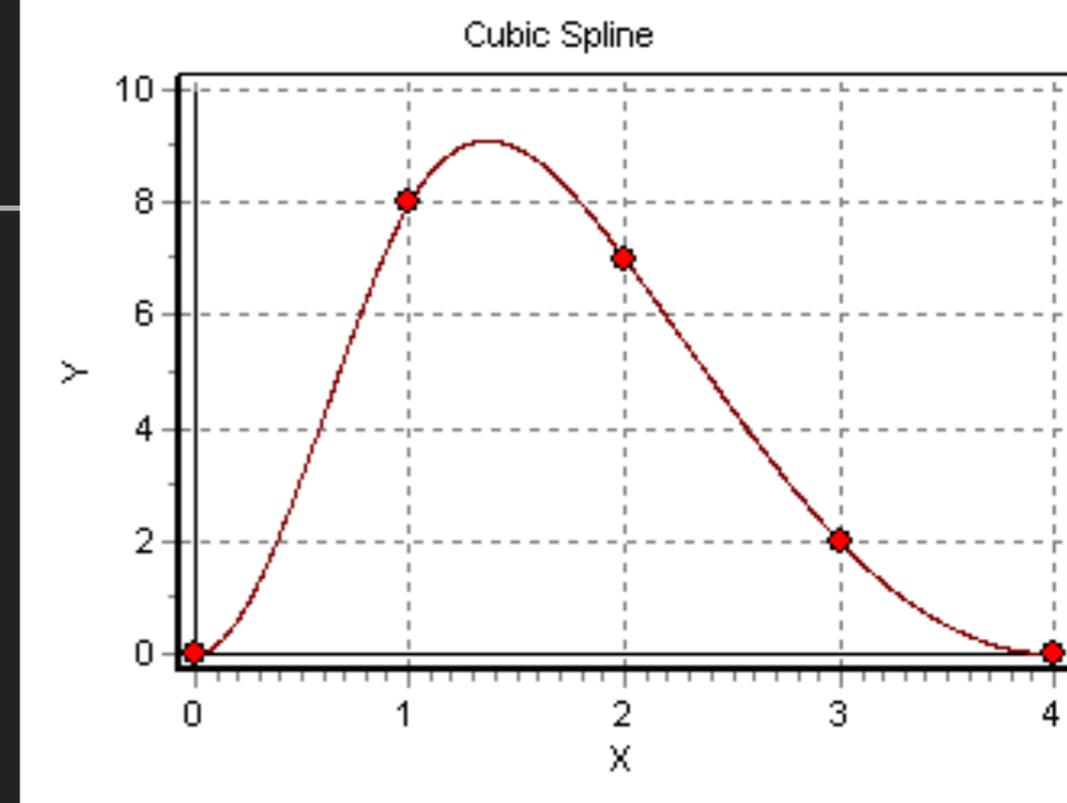
INTERPOLATION METHODS

- ▶ Problems with Lagrange interpolation



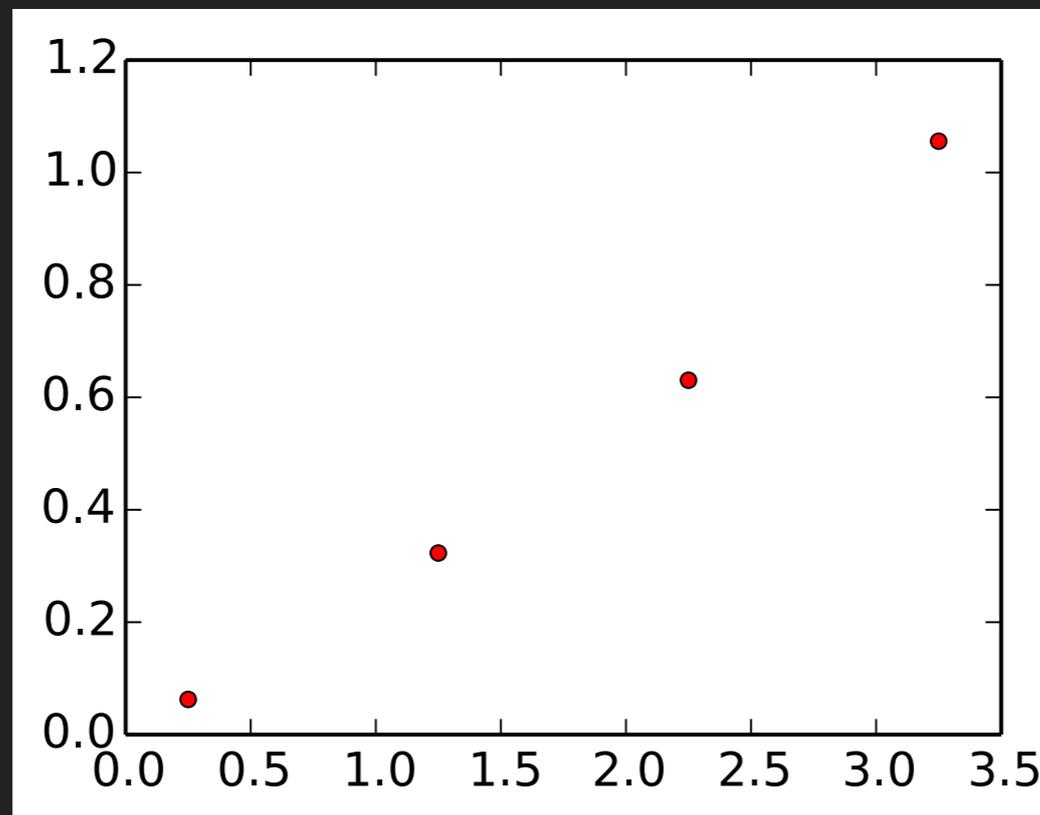
INTERPOLATION METHODS

- ▶ Cubic Spline
- ▶ Know the definition: a piecewise cubic polynomial that goes through all datapoints, matched derivatives at datapoints to make it smooth
- ▶ You do not need to know: how to derive matrix and how to solve it.



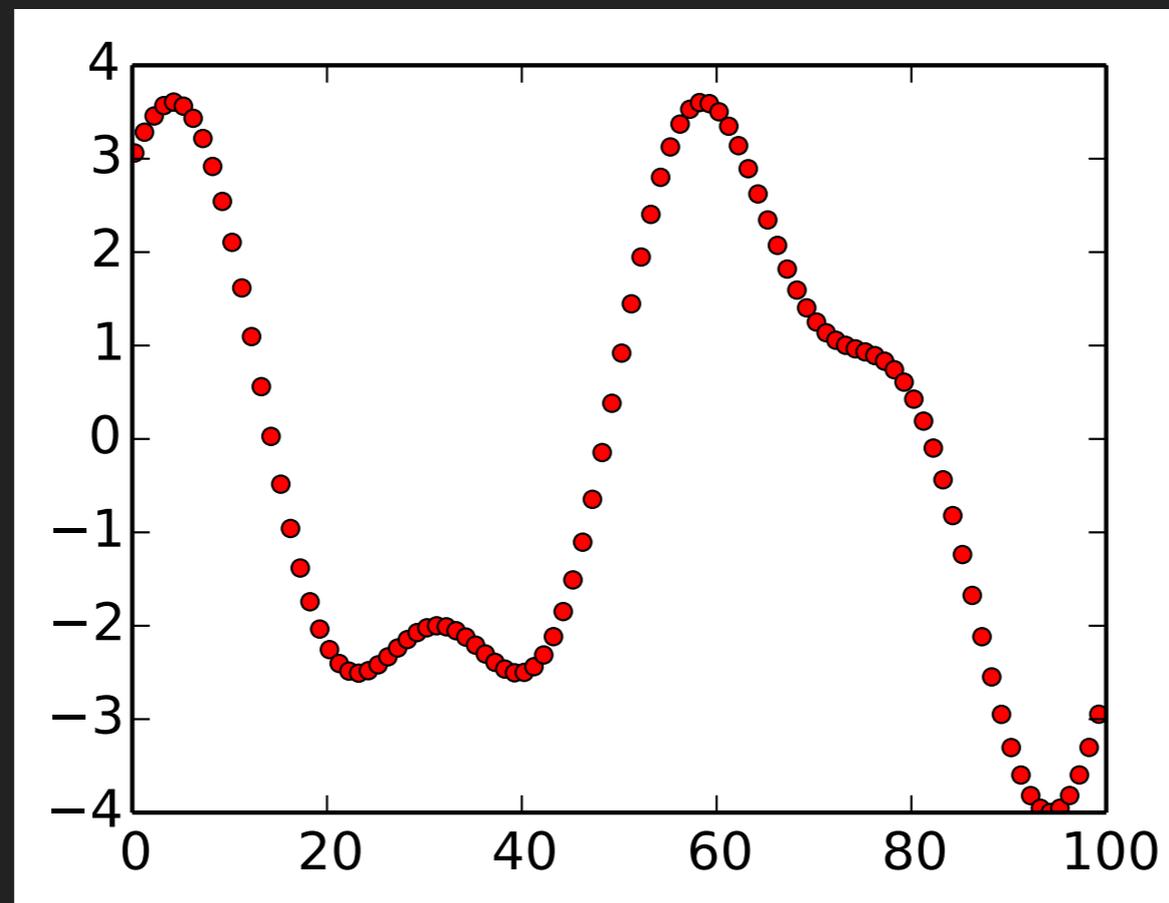
INTERPOLATION METHODS

- ▶ You should be able to choose the appropriate interpolation method!



INTERPOLATION METHODS

- ▶ You should be able to choose the appropriate interpolation method!



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DIFFERENTIAL EQUATIONS

DIFFERENTIAL EQUATIONS

- ▶ Definition: A set of equations where the solution is a function.
- ▶ We talk about ordinary differential equations in this course.
- ▶ They have an order, determined by the highest derivative.

DIFFERENTIAL EQUATIONS

- ▶ Some differential equations depend explicitly on time, others do not (autonomous)
- ▶ In general we write a first order ordinary differential equations in the form

$$y'(t) = F(y, t)$$

DIFFERENTIAL EQUATIONS

- ▶ Note that the names of the variables might differ depending on the problem at hand.
- ▶ You need to identify which is the time variable, which is the right hand side, etc

$$y'(t) = F(y, t)$$

DIFFERENTIAL EQUATIONS

- ▶ You can rewrite any high order differential equation as a set of first order differential equations.
- ▶ This is important because almost all the methods we talked about are for first order differential equations.
- ▶ Practice how to do that!

DIFFERENTIAL EQUATIONS

- ▶ Every differential equations needs initial conditions!
- ▶ First order \rightarrow 1 initial condition
- ▶ Second order \rightarrow 2 initial conditions
- ▶ Etc

DIFFERENTIAL EQUATIONS

- ▶ We talked about multiple numerical methods to solve differential equations.
- ▶ All work by splitting the time into very small timesteps dt
- ▶ The smaller the timestep, the more accurate, but also the more expensive the method

DIFFERENTIAL EQUATIONS

- ▶ Explicit Euler method
- ▶ Simplest method possible
- ▶ 1st order

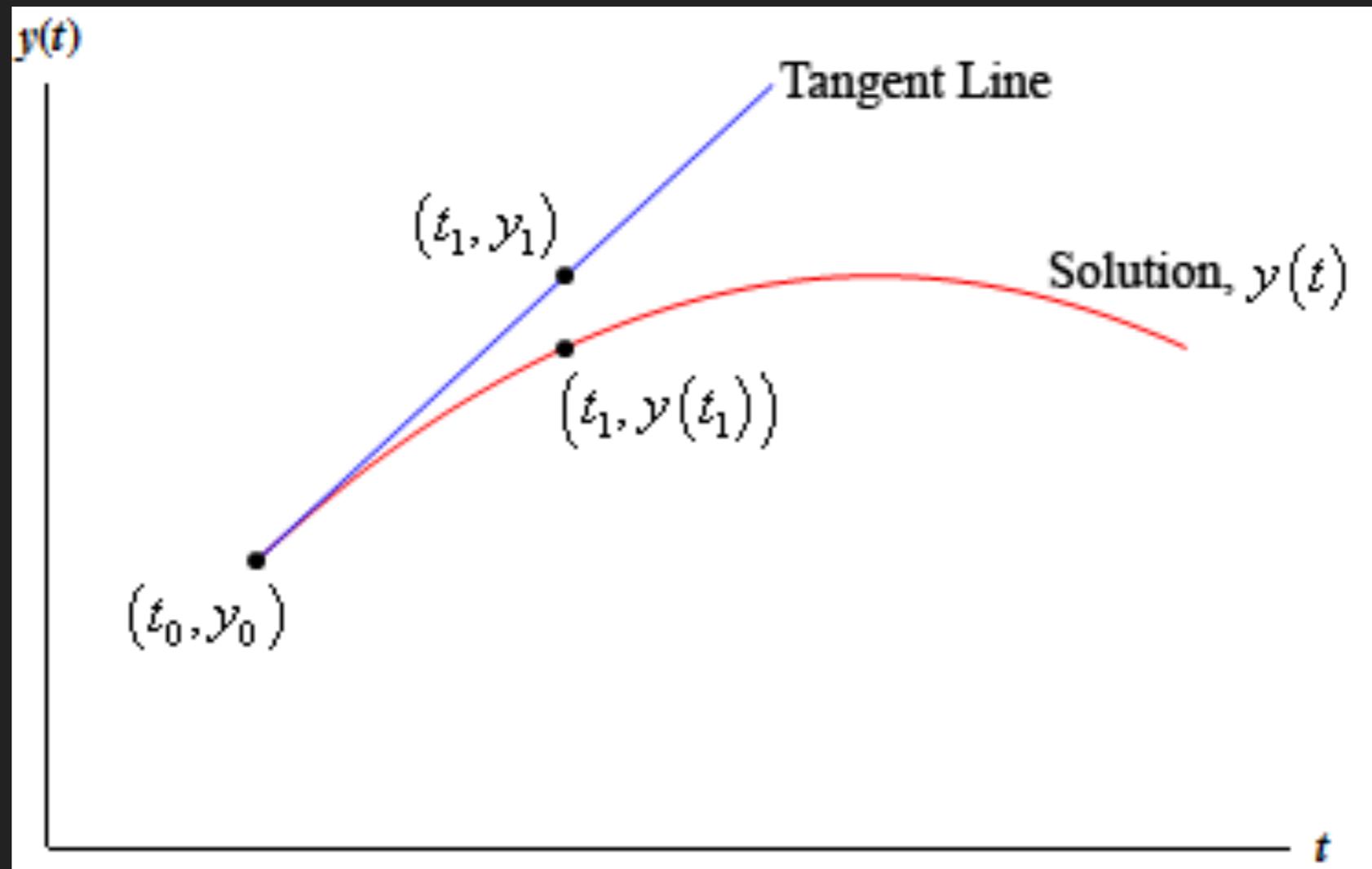
$$E \sim \frac{1}{2} dt^2 \cdot \frac{\partial^2 y}{\partial t^2}$$

DIFFERENTIAL EQUATIONS

- ▶ Explicit Euler method
- ▶ Calculate derivative (right hand side) at beginning of time step, multiply with dt , then add to value at beginning.

DIFFERENTIAL EQUATIONS

- ▶ Graphical representation of explicit Euler method

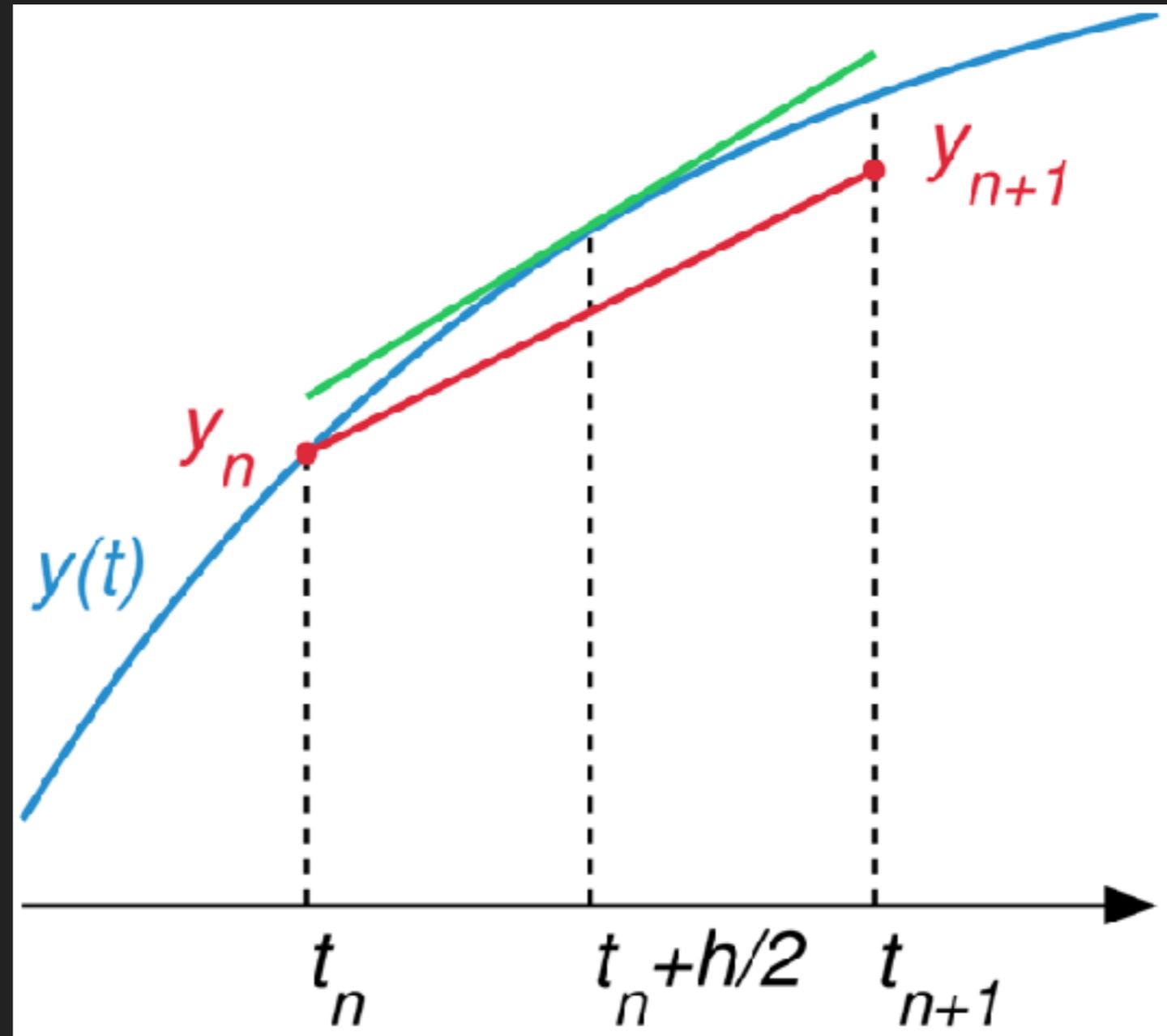


DIFFERENTIAL EQUATIONS

- ▶ Explicit Euler method is rarely ever used.
- ▶ This is because of the low order.
- ▶ Midpoint method is second order.
- ▶ Uses a sub-step, effectively combining two Euler steps

DIFFERENTIAL EQUATIONS

- ▶ Graphical representation of the midpoint method



DIFFERENTIAL EQUATIONS

- ▶ Higher order methods can be constructed.
- ▶ Often used: 4th or 5th order Runge Kutta

0				
1/2	1/2			
1/2	0	1/2		
1	0	0	1	
	1/6	1/3	1/3	1/6

DIFFERENTIAL EQUATIONS

- ▶ N-body simulations are simulations of N interacting gravitational bodies
- ▶ Need to solve a $6*N$ dimensional coupled differential equation
- ▶ Difficult because we need very high precision over long timescales

DIFFERENTIAL EQUATIONS

- ▶ N-body simulations often use advanced integration methods
- ▶ Either very high order
- ▶ Or geometric/symplectic integrators which preserve some of the underlying symmetries of the problem.

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MONTE CARLO METHODS

MONTE CARLO METHODS

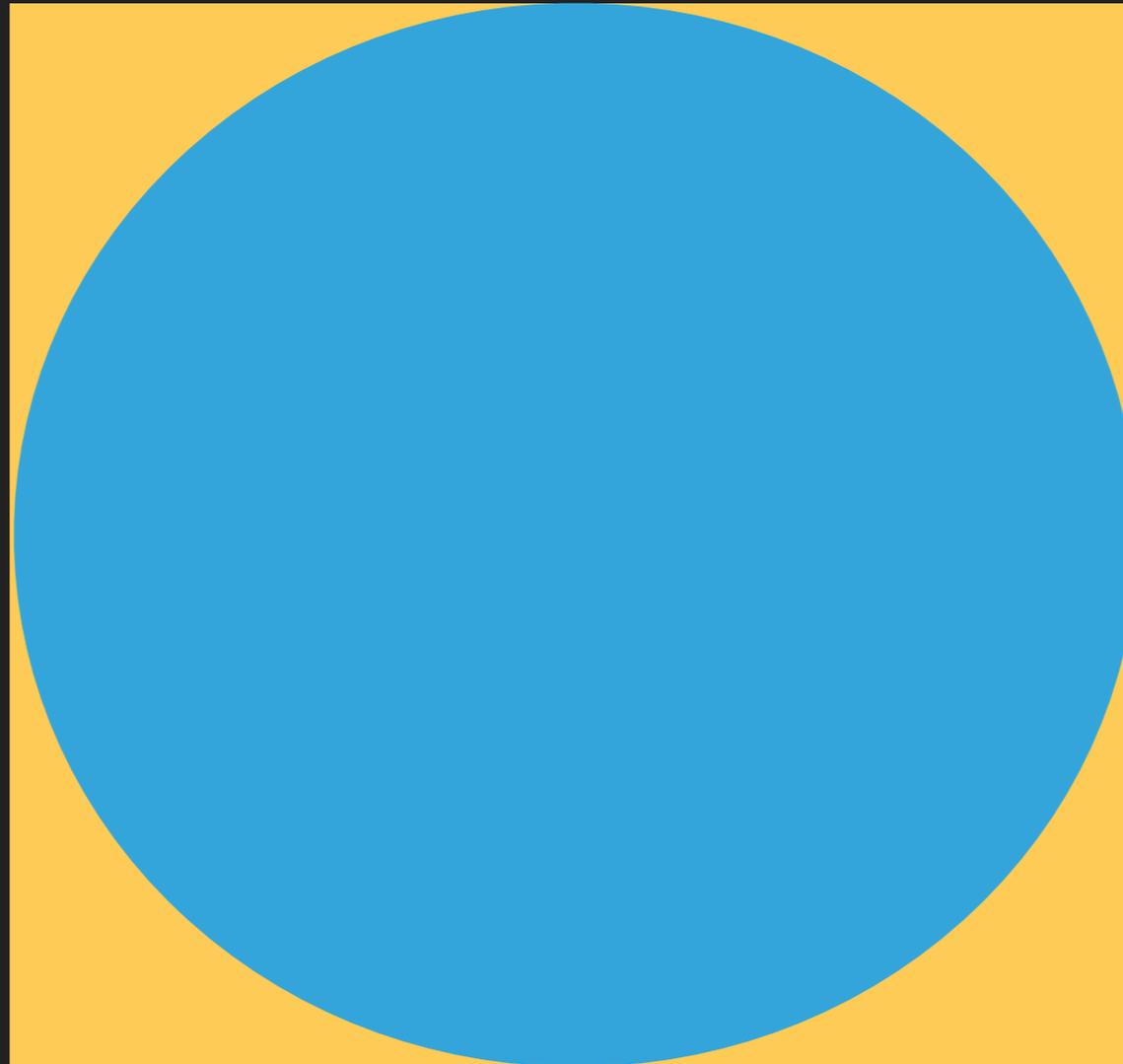
- ▶ A random number generator outputs *pseudo* random numbers on a computer
- ▶ Randomness is hard for the computer
- ▶ A good random number generator outputs uncorrelated, uniformly distributed random numbers that are hard to predict.

MONTE CARLO METHODS

- ▶ Random numbers are used in cryptography
- ▶ We use them to simplify numerical calculations!

MONTE CARLO METHODS

- ▶ Calculate pi using random numbers:



MONTE CARLO METHODS

- ▶ In general: use random numbers to calculate an integral:



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BAYES' THEOREM

BAYES' THEOREM

- ▶ Very important statistical tool.
- ▶ Derivation is very simple!

$$P(A | B) = \frac{P(B | A)P(A)}{P(B)}$$

BAYES' THEOREM

- ▶ Makes use of conditional probability.
- ▶ The syntax $P(A|B)$ means the probability that event A is true given event B is true.
- ▶ Can use Bayes' theorem to invert the equation to get $P(B|A)$

BAYES' THEOREM

- ▶ Can apply this to simple statical problems such as the *Cookie problem* or the *Monty Hall* problem.
- ▶ Make sure you know how we did those calculations!

BAYES' THEOREM

- ▶ Diachronic interpretation
- ▶ Used in relationship to testing a hypothesis in science using data
- ▶ Terms in Bayes' Theorem have names. Know them and understand their meaning!

BAYES' THEOREM

$$P(A | B) = \frac{P(B | A)P(A)}{P(B)}$$

- ▶ $P(A|B)$ = Posterior
- ▶ $P(B|A)$ = Likelihood
- ▶ $P(A)$ = Prior
- ▶ $P(B)$ = normalization constant

BAYES' THEOREM

- ▶ Using Bayes' theorem is related to solving a high dimensional integral.
- ▶ Can use Monte Carlo Methods to do that.
- ▶ We are randomly *sampling the posterior*.

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COMING UP . . .

TUTORIAL TOMORROW

- ▶ Come to get help with the project.
- ▶ Run the presentation by me, if you want.
- ▶ Also can ask questions about any other material from the course.

PROJECT REPORT

- ▶ Due on December 4th
- ▶ Can hand it in in paper form or submit it online.

PROJECT PRESENTATIONS

- ▶ Will happen on December 4th
- ▶ All project members need to be present, but not all need to take part in the presentation
- ▶ Make sure your computer works if you plan to use the projector
- ▶ Make sure you do not run over