



SIMULATION, MODELING, AND AI

INSTRUCTOR: MICHELLE MILLER

WHO AM I?

- Graduated with ScB in Astrophysics from Brown University
 - Enrolled in part-time distant masters in Accelerator Physics through Indiana U – US Particle Accelerator School
- Switching fields and now I'm working full time in a neuroscience lab at Columbia
 - I've done research in a variety of subfields in physics including astrophysics, particle physics, accelerator physics and now neurophysics!

WHAT EXACTLY IS THIS COURSE?

- There will be two courses you will partake in:
 - Simulation and Modeling Processes on Coursera
 - Artificial Intelligence A to Z on Udemy
- There is one auxiliary I will recommend to those who want to solidify their python:
 - Python for Data Science and Artificial Intelligence

WHAT EXACTLY IS THIS COURSE?

- I will generally try to expose or teach you the math or fundamental ideas that you will need in order to understand the upcoming weeks
- I will answer questions from what you had from the past weeks
- I will expose you to other applications of these codes in the real world even beyond just science but in sociology, finance, etc.

WHEN WILL WE MEET?

There are two days in the week I am considering to have sessions:

- Wednesdays:

- 5pm
- 6pm
- 7pm
- 8pm

- Thursdays:

- 5pm
- 6pm
- 7pm
- 8pm

SO WHY SIMULATION, MODELING, AND ARTIFICIAL INTELLIGENCE?

- These are topics and fields that are quite transcendent when considering the applications of the tools you will learn
- Upon completion of this course you should:
 - Have a foundational knowledge computational methods for simulation including numerical methods, sampling methods, machine learning algorithms, etc.
 - Develop a stronger mathematical foundation and intuition; some calculus will be used but is broken down in code in a way that the calculus knowledge is not essential
 - Feel comfortable writing your own simulations and code for non-trivial questions and problems in the real world
 - Produce a final project with a partner(s) that you feel proud of!

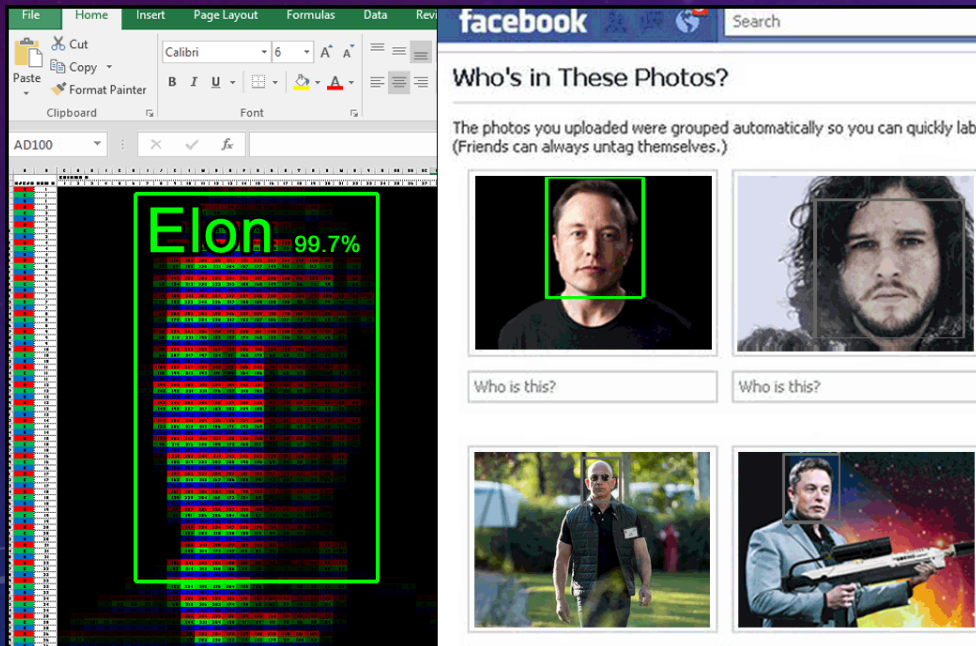
THESE TOOLS HAVE APPLICATIONS ALL AROUND THE WORLD

- Example: Stock Price Prediction using Time Series Recurrent Neural Networks
- We can build models that learn patterns over time that can then learn to predict the future steps of a process →
 - A major application of this is the stock market! People want to earn big!



SOCIAL APPLICATIONS

- Facial recognition as seen used by facebook and governments these days:



POLITICAL RAMIFICATIONS

- Around this time last year, the government of Sri Lanka misidentified an American Muslim college student as being responsible for the Easter terrorist attacks
- They later admitted to their mistake after realizing it was a fault in their facial recognition system

American Student Misidentified as Sri Lanka Suspect Faces Backlash

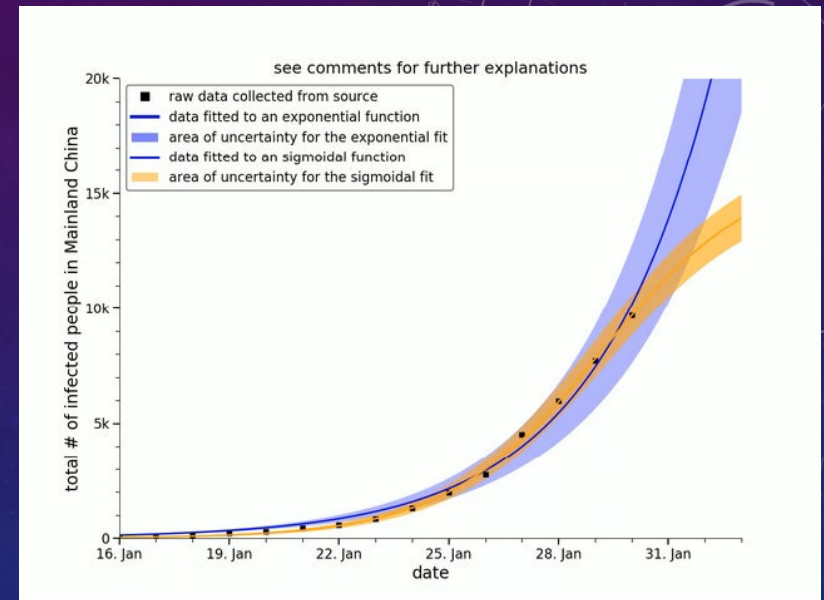
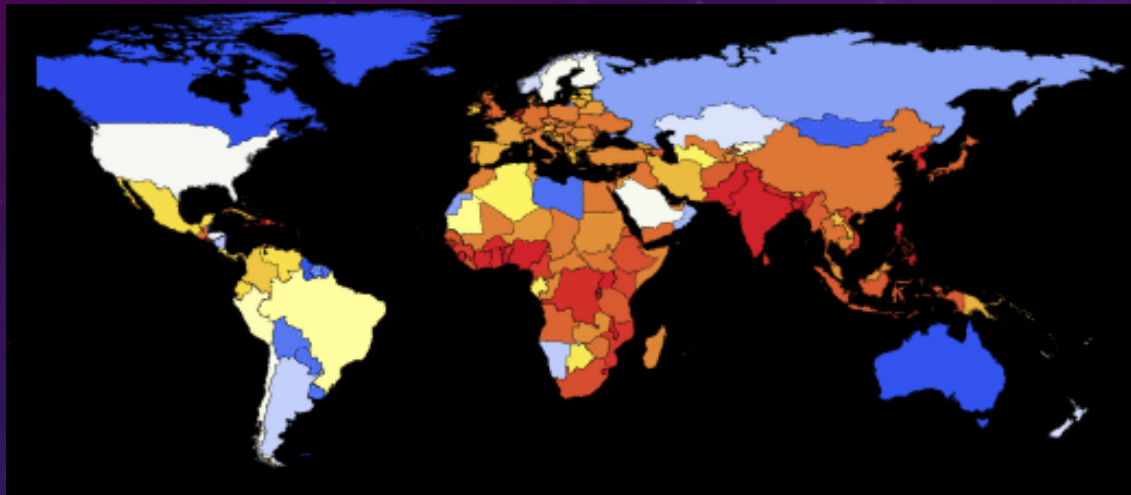


Amara Majeed, a student at Brown University and a prominent Muslim activist in the United States, heard from relatives in Sri Lanka that her photo was mistakenly included in a Sri Lankan police alert.

Barbara Haddock Taylor/The Baltimore Sun, via Associated Press

Amara now works in DC as a paralegal and in an advocacy group. She plans to testify in front of Congress on the implications that come with using facial recognition software

EPIDEMIOLOGICAL MODELS OF DISEASE PROPAGATION



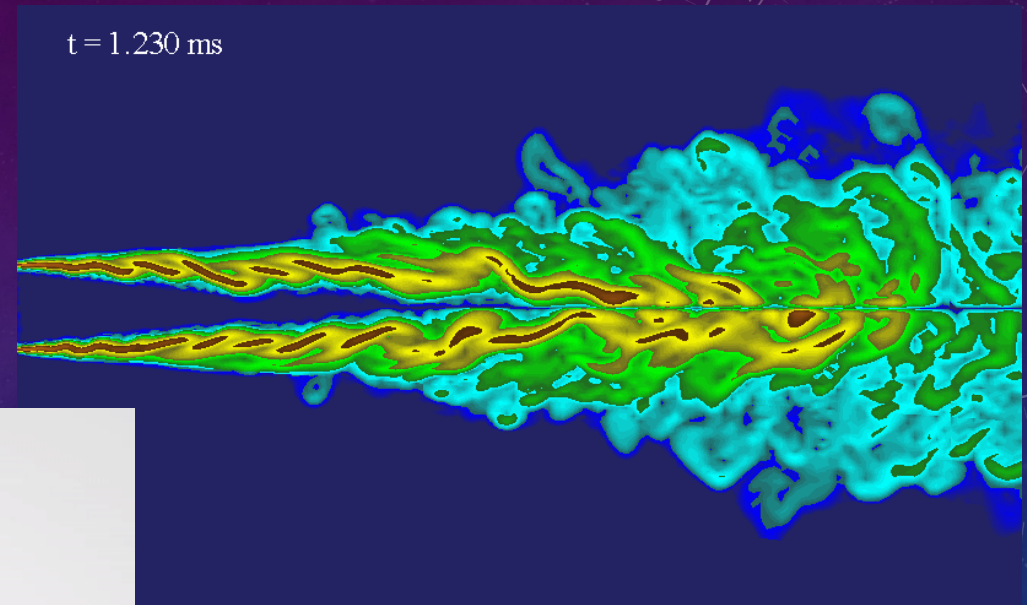
<https://blog.wolfram.com/2014/11/04/modeling-a-pandemic-like-ebola-with-the-wolfram-language/>

$$\begin{aligned}\frac{dS}{dt} &= \frac{\beta_I SI + \beta_H SH + \beta_F SF}{N} \\ \frac{dE}{dt} &= \frac{\beta_I SI + \beta_H SH + \beta_F SF}{N} - \alpha E \\ \frac{dI}{dt} &= \alpha E - [\gamma_H \theta_1 + \gamma_I (1 - \theta_1)(1 - \delta_1) + \gamma_D (1 - \theta_1) \delta_1] I \\ \frac{dH}{dt} &= \gamma_H \theta_1 I - [\gamma_{DH} \delta_2 + \gamma_M (1 - \delta_2)] H \\ \frac{dF}{dt} &= \gamma_D (1 - \theta_1) \delta_1 I + \gamma_{DH} \delta_2 H - \gamma_F F \\ \frac{dR}{dt} &= \gamma_I (1 - \theta_1)(1 - \delta_1) I + \gamma_M (1 - \delta_2) H + \gamma_F F\end{aligned}$$

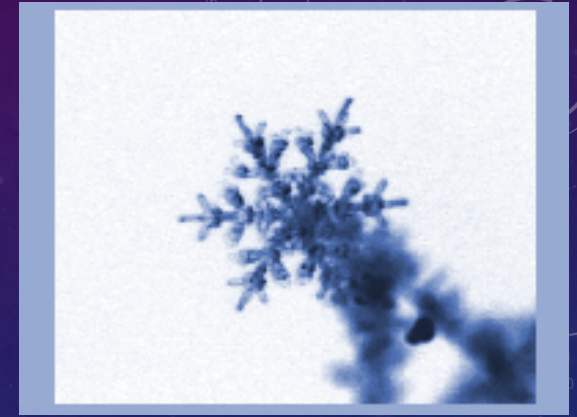
The population is divided into six compartments: Susceptible (S), Exposed (E), Infectious (I), Hospitalized (H), Funeral (F) – indicating transmission from handling a diseased patient's body, and Recovered/Removed (R). Note that λ is a composite of all β transmission terms

PHYSICS (OBVIOUSLY!)

- Example: Fluid dynamics in physics

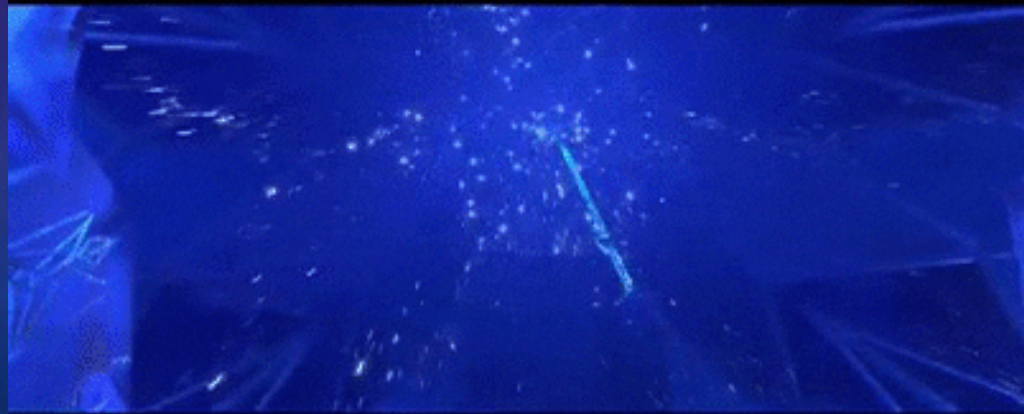


THIS HAS APPLICATIONS TO ART AND ANIMATION!



- Example: Frozen franchise

<https://www.youtube.com/watch?v=2YqldhUhlU4>



LAWS OF PROBABILITY TELL US:

1. The probability of any event is between 0 and 1 :

$$0 \leq p(x_i) \leq 1$$

2. The sum of all possible probabilities must add to 1 :

$$\sum_{i=1} p(x_i) = 1$$

3. If A and B are mutually exclusive, then the probability of A and B occurring is the sum of their individual probabilities (

$$P(A \text{ and } B) = P(A) + P(B)$$

PROBABILITY MODELS AND RULES OF PROBABILITY

- The **sample space S** of a chance process is the set of all possible outcomes.

$$P(S) = 1$$

- A **probability model** describes chance behavior by listing the possible outcomes in the **sample space S** and giving the probability that each outcome occurs.
- To find the probability of two events occurring

$$P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$$

- Two events are mutually exclusive if they have no outcomes in common (one cannot occur if the other does:

$$P(A \text{ or } B) = P(A) + P(B)$$

- Probability of two events happening in subsequent order:

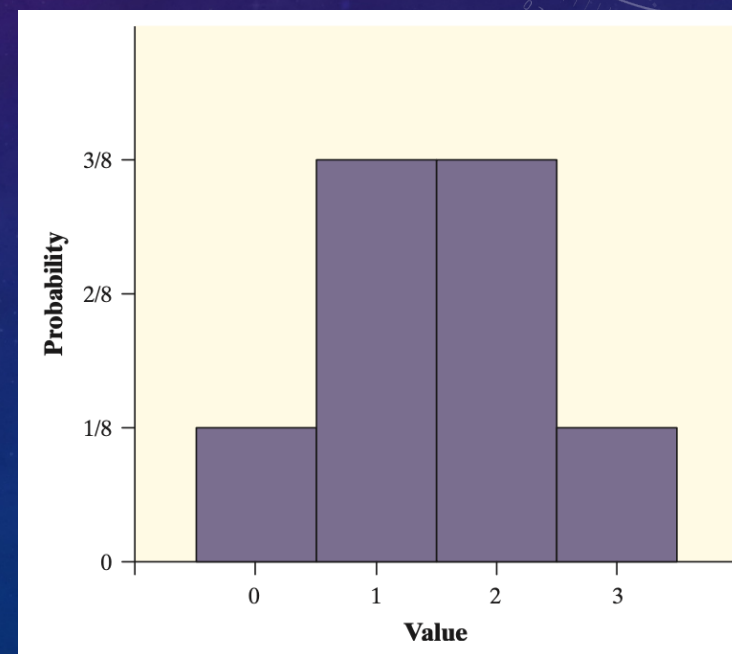
$$P(A \text{ and } B) = P(A)P(B)$$

BINOMIAL DISTRIBUTION

- When you are trying to determine the probability of an set of outcomes, given the fact that there are two possibilities on each trial
 - Example: Say we have a coin and we are flipping it three times. What is the probability of getting 3 heads?

$X = 0$: TTT
 $X = 1$: HTT THT TTH
 $X = 2$: HHT HTH THH
 $X = 3$: HHH

Value:	0	1	2	3
Probability:	$1/8$	$3/8$	$3/8$	$1/8$



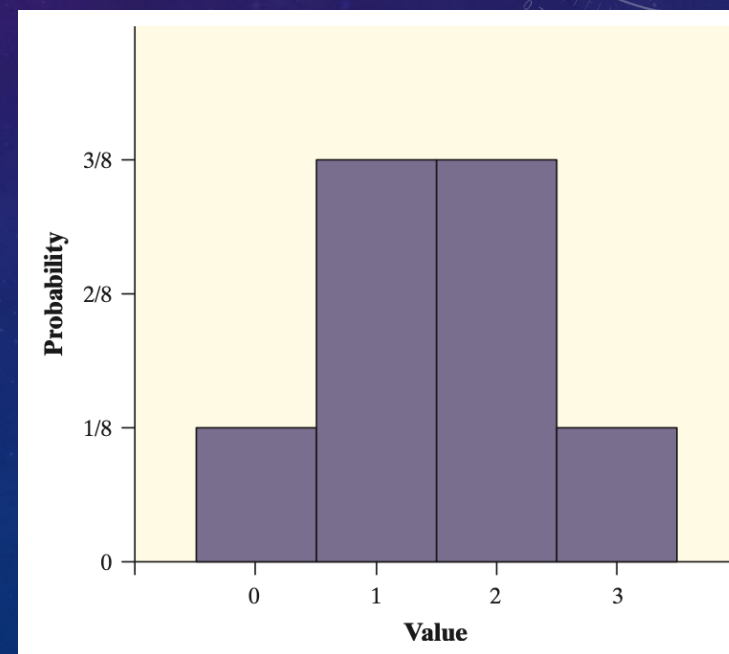
BINOMIAL DISTRIBUTION

- We can do the math:

- $P(3 \text{ heads}) = P(3 \text{ heads}) \cdot P(0 \text{ heads}) = \left(\frac{1}{2}\right) \cdot \left(\frac{1}{2}\right) \cdot \left(\frac{1}{2}\right) \cdot \left(1 - \frac{1}{2}\right)^0 = \left(\frac{1}{2}\right)^3$

X = 0: TTT
X = 1: HTT THT TTH
X = 2: HHT HTH THH
X = 3: HHH

Value:	0	1	2	3
Probability:	1/8	3/8	3/8	1/8



BINOMIAL DISTRIBUTION

- What if we want 2 heads and 1 tail?

- $P(2 \text{ heads and } 1 \text{ tail}) = P(2 \text{ heads}) \cdot P(1 \text{ heads}) = \left(\frac{1}{2}\right) \cdot \left(\frac{1}{2}\right) \cdot \left(1 - \frac{1}{2}\right)^1 = \left(\frac{1}{2}\right)^3$

X = 0: TTT		
X = 1: HTT	THT	TTH
X = 2: HHT	HTH	THH
X = 3: HHH		

Value:	0	1	2	3
Probability:	1/8	3/8	3/8	1/8

- But wait why does this not match what we see? Because we now have a **combinatorix** problem
- We have **three** possible ways in which one outcome can occur
- Because of this, we need an extra term called the combinatorial term
- # of ways arrange k items, when you have n items $= \frac{n!}{(n-k)!k!}$

BINOMIAL DISTRIBUTION

- Back to 2 heads and 1 tail:

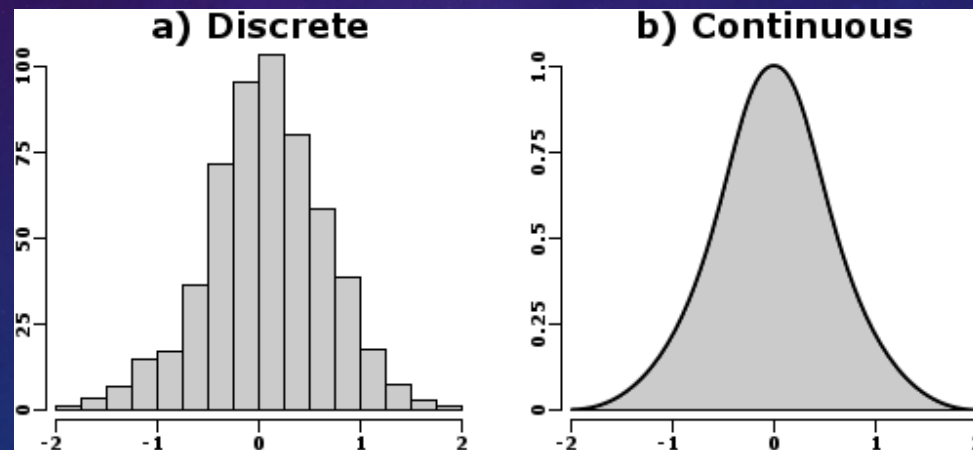
$$\begin{aligned}P(k \text{ events}) &= \frac{n!}{(n-k)!k!} P(k \text{ events}) \cdot P(n-k \text{ events}) \\&= \frac{3!}{(3-2)!2!} \cdot \left(\frac{1}{2}\right) \cdot \left(\frac{1}{2}\right) \cdot \left(1 - \frac{1}{2}\right)^1 = \frac{(1 \cdot 2 \cdot 3)}{(1) \cdot (1 \cdot 2)} \cdot \left(\frac{1}{2}\right)^3 \\&= \frac{(3)}{(1)} \cdot \left(\frac{1}{2}\right)^3\end{aligned}$$

X = 0: TTT		
X = 1: HTT	THT	TTH
X = 2: HHT	HTH	THH
X = 3: HHH		

Value:	0	1	2	3
Probability:	1/8	3/8	3/8	1/8

CALCULATING STATISTICS FROM DISCRETE DATA:

- Expectation value (mean): $\mu = \sum_{i=1} x_i \cdot P(x_i)$
- Variance (standard deviation squared) : $\sigma = \sum_{i=1} (x_i - \mu)^2 \cdot P(x_i)$



ASSIGNMENT

- Complete weeks 1 and 2 of the Simulation and Modeling course lectures and quizzes
 - Upon watching the lectures, you will discuss the Monte Carlo method
 - Some of you may not be familiar with the mathematical formulation he uses from probability – write down any questions you have about this
 - Write a piece of code in which you flip a coin 4 times and each time you consider a success to be obtaining 3 heads and one tail
 - Count up all of the successes and give the probability of obtaining this result
 - How does this compare to the theoretical result from probability? If you do not understand the theoretical probability behind it, I will explain it more in detail next time
- If you are also doing the coursework for the python coursera work, I recommend you get through the first $\frac{1}{4}$ - $\frac{1}{2}$ of that material. Some of it will overlap with week 2 of the above

ASSIGNMENT

- In your own words:
 - Explain, what is a Monte Carlo algorithm? Use the lectures or other online resources to answer this question
 - In your own words, explain in two sentences, what physical system did the professor describe when explaining the kinetic/dynamic Monte Carlo?
 - In 3 sentences, explain what is Gillespie's algorithm?