Lecture 01:

Introduction

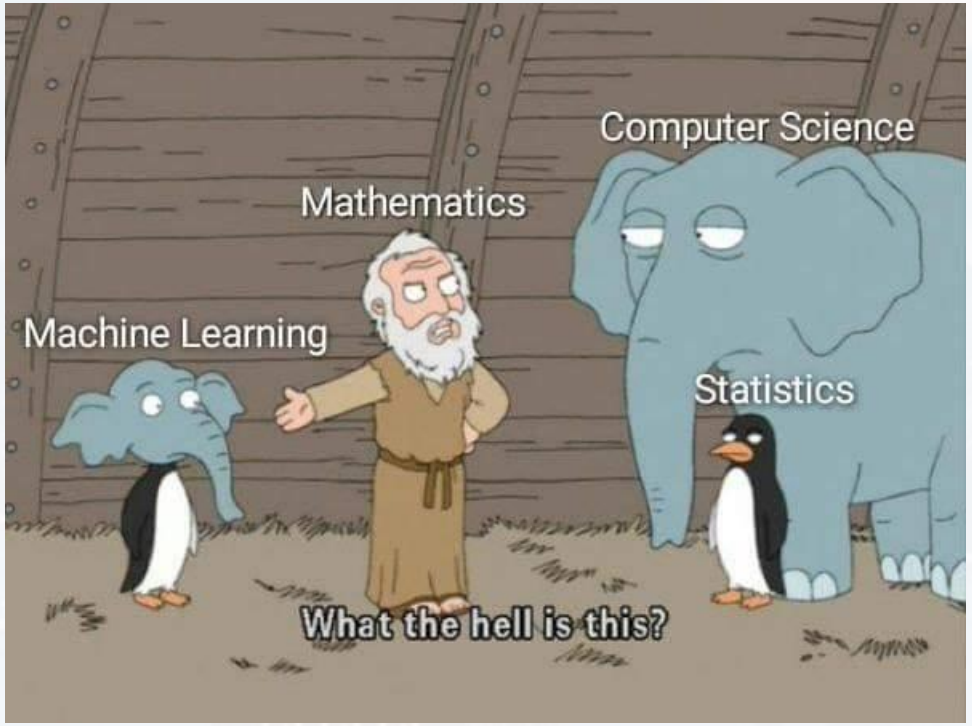
Markus Hohle

University California, Berkeley

Machine Learning Algorithms

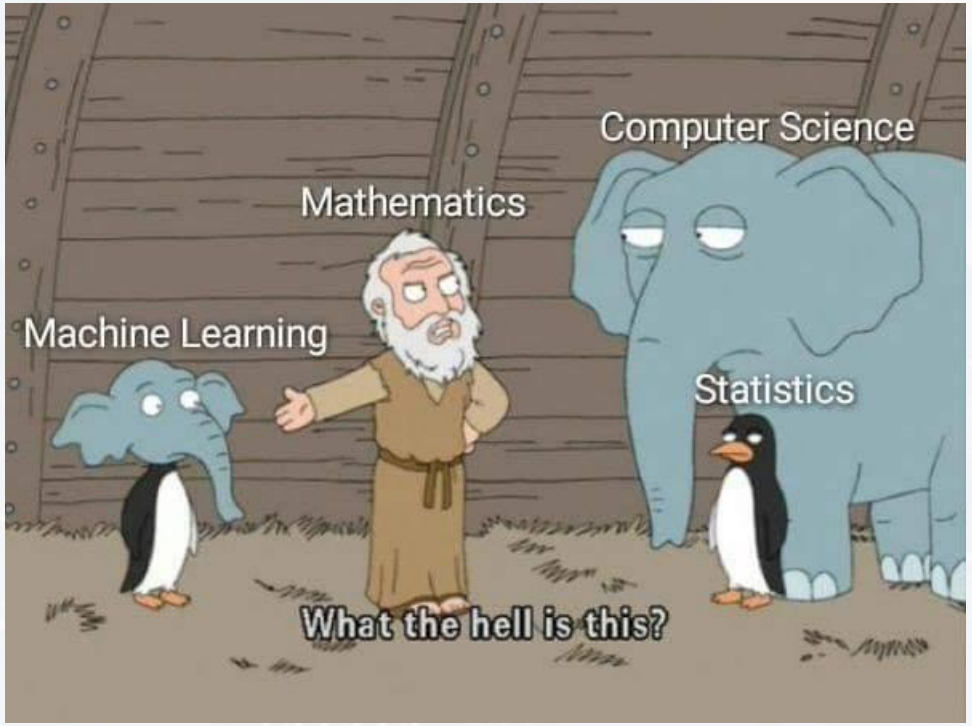
MSSE 277B, 3 Units

Berkeley MSSE
MOLECULAR SCIENCE & SOFTWARE ENGINEERING



Outline

- Motivation
- What is Machine Learning?
- The Lecture
- Course Map



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Why Machine Learning?

- **automating workflows**

  → face recognition, identification/authentication tools
  → **manufacturing processes, quality control**
  → **repetitive, standardized workflows**

- **handling large data sets**

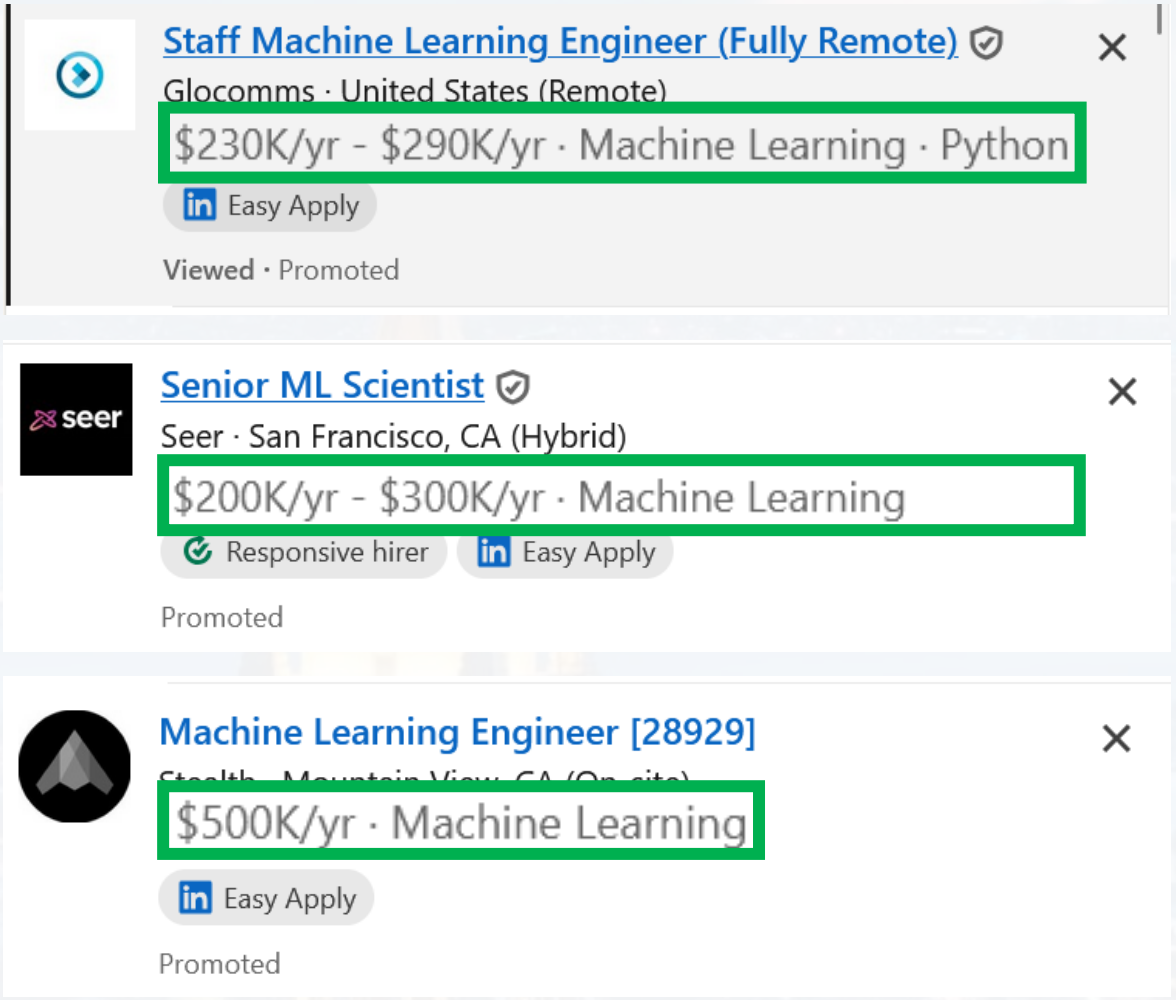
  → **epigenetic data for drug development**
  → traffic management
  → **disease control**
  → stock market dynamics

- **generating new data**

  → **new materials (semiconductor, superconductor)**
  → AI generated images/videos

Why Machine Learning?

LinkedIn: 1st three Job Postings, Jan 10th 2025

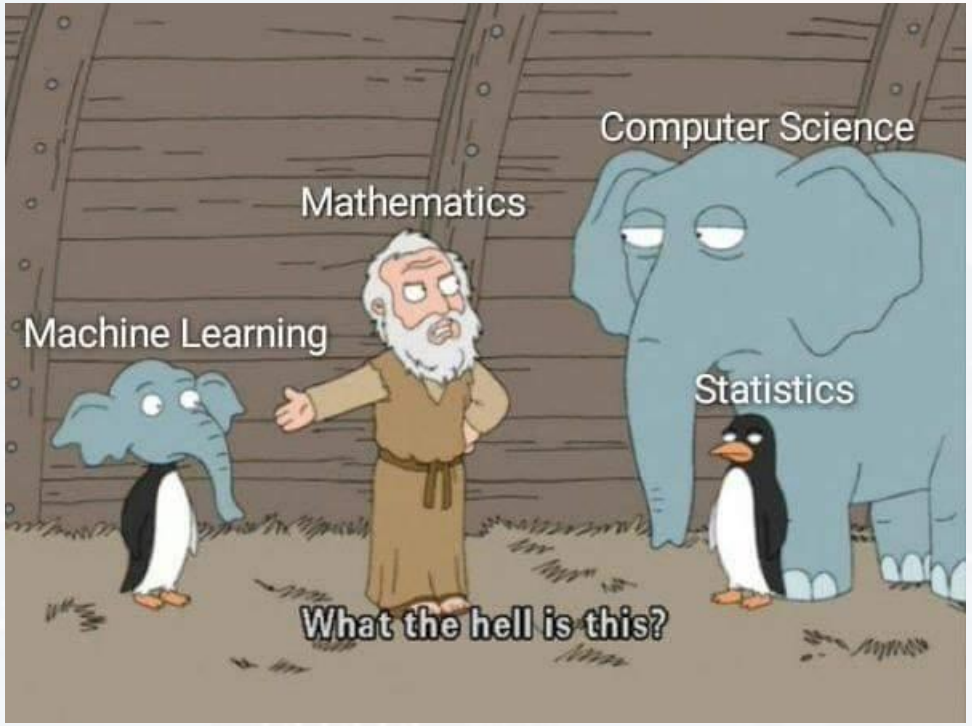


Why Machine Learning?

Listen up son, there are three languages you need to learn in order to become successful:

- *English*
- *Math*
- *Python *)*

*) or C++



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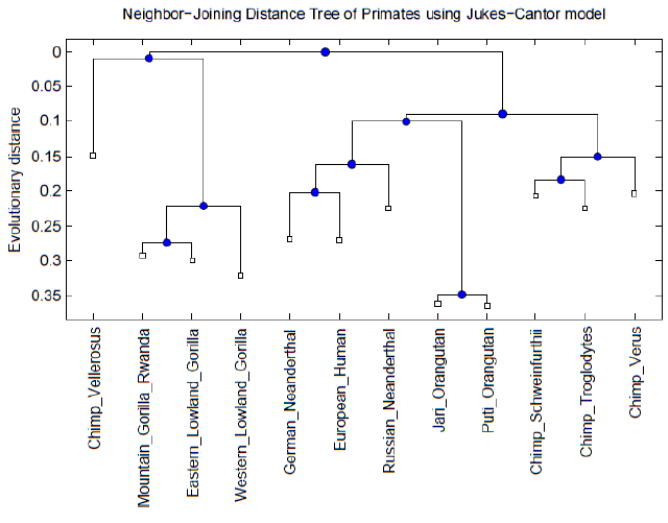
Wiki says:

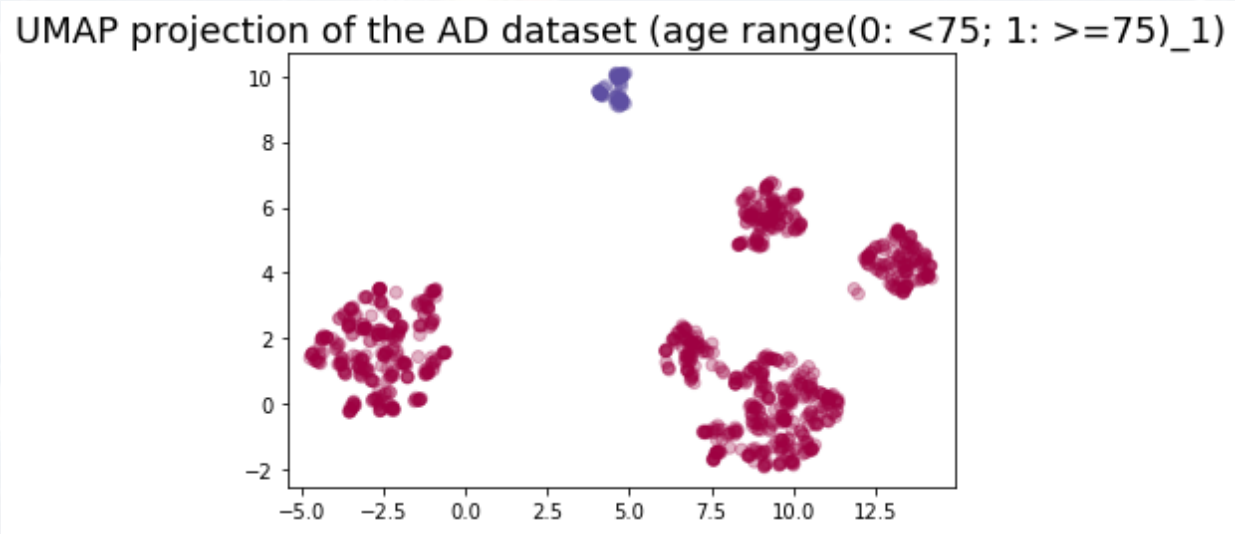
*"**Machine learning** (**ML**) is a field of study in **artificial intelligence** concerned with the development and study of **statistical algorithms** that can learn from data and generalize to unseen data, and thus perform tasks **without explicit instructions**"*

→ **more flexible than standard programs**

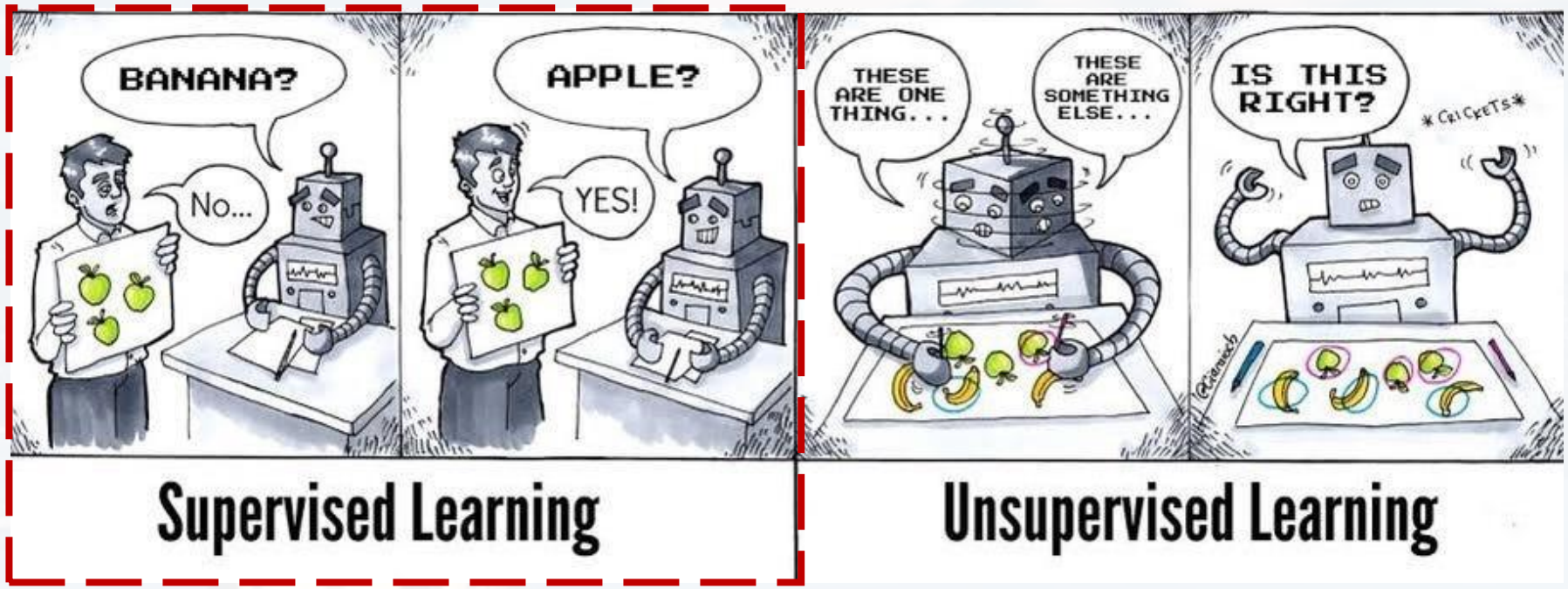
- *artificial intelligence*
- *statistics*

cluster and/or categorize data and understand relations/interactions, find pattern





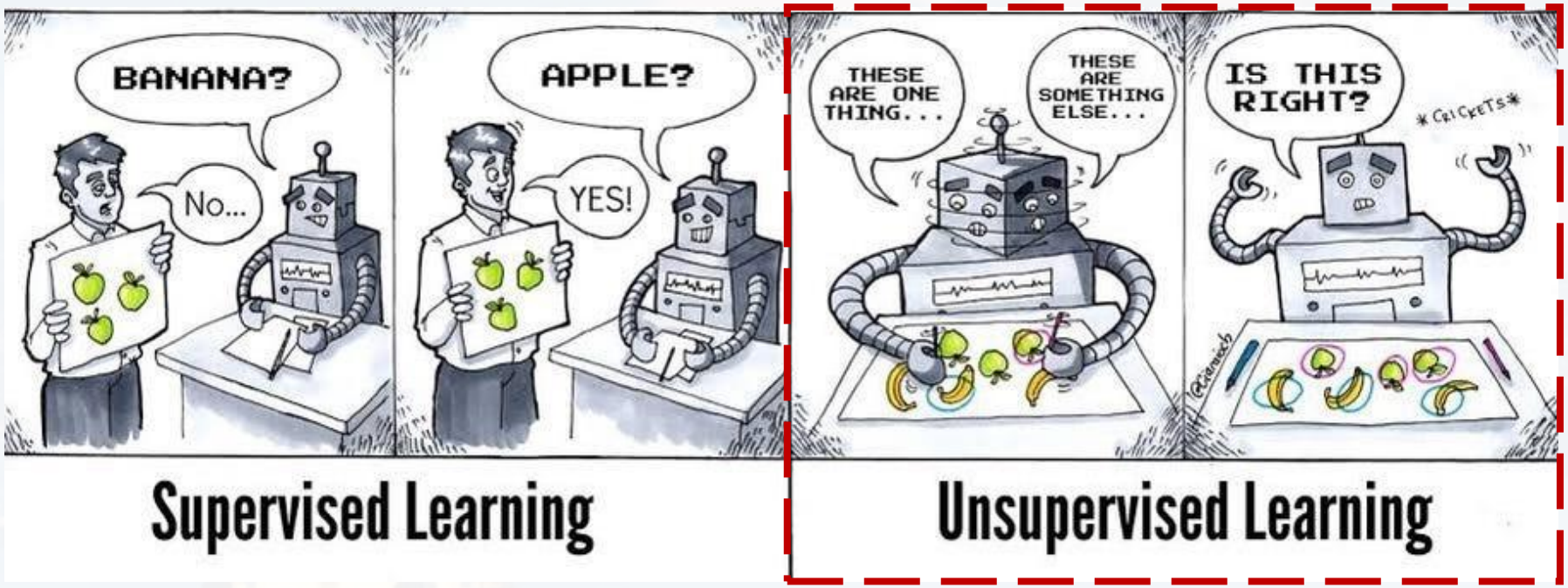
curve fitting, linear/logistic models:
training data set and a **test** data set…



- **S**upport **V**ector **M**achine
- K-nearest
- ANNs

curve fitting, linear/logistic models:
training data set and a **test** data set…

no training data set required – we can start right away!



- **S**upport **V**ector **M**achine
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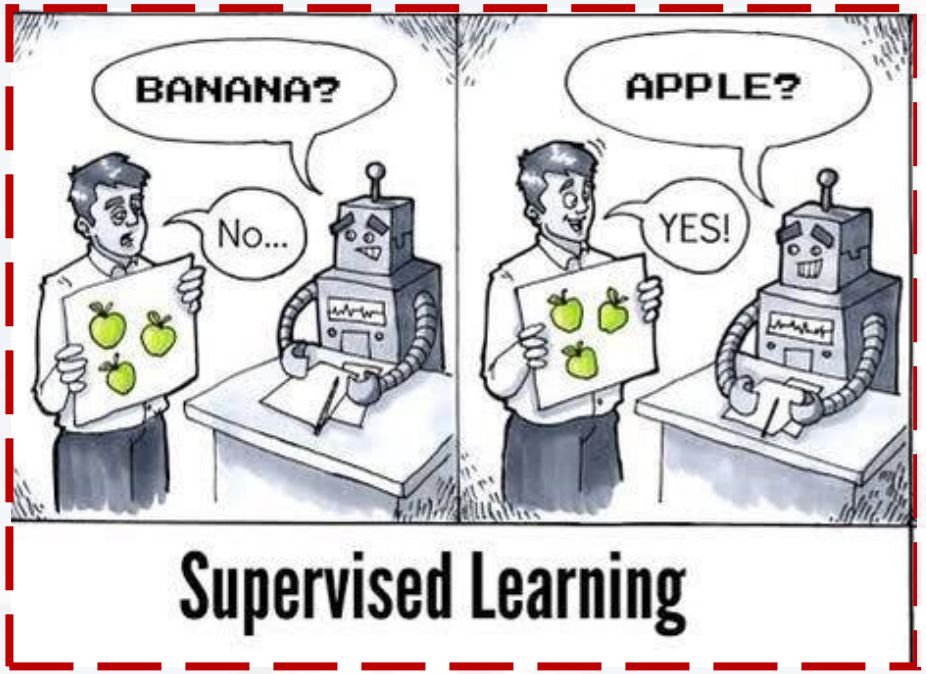
- K - means
- GMM
- trees

curve fitting, linear/logistic models:
training data set and a **test** data set…



- **S**upport **V**ector **M**achine
- K-nearest
- ANNs

1) creating the model:

```
my_model = library.method(argument1 = 'arg1'
                                    , … )
```

2) training the model

```
out = my_model.fit(xtrain, ytrain)
```

3) evaluation

```
ypred = out.predict(xeval)
accur = (ypred == yeval).sum()/len(yeval)
```

4) prediction (actual application)

```
ypred = out.predict(xnew)
```

no training data set required – we can start right away!

1) creating the model:

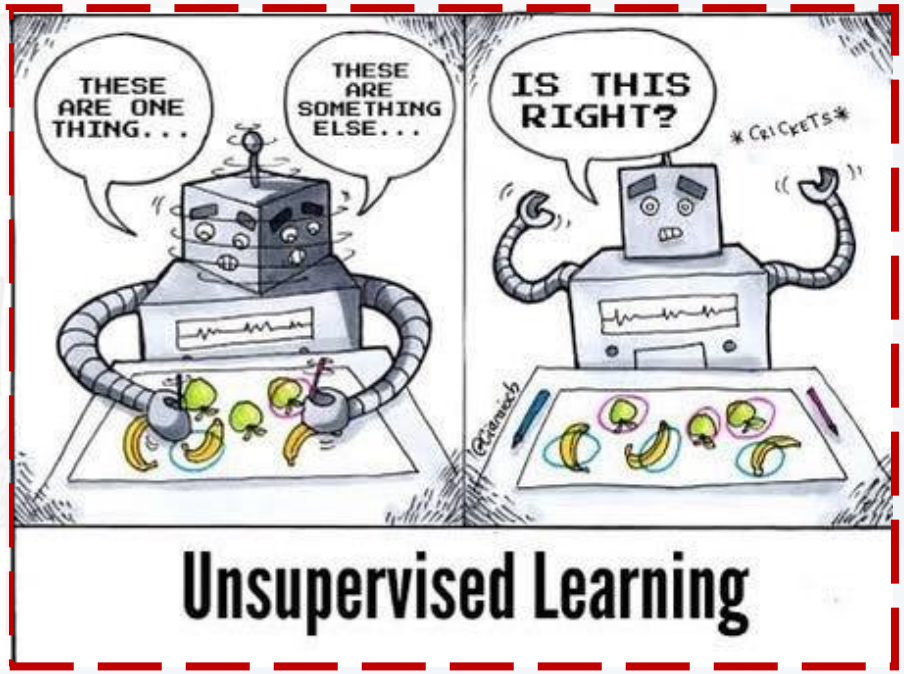
```
my_model = library.method(argument1 = 'arg1'
                                    , … )
```

3) evaluation (***if*** y is known)

```
ypred = out.predict(xeval)
accur = (ypred == yeval).sum()/len(yeval)
```

4) prediction (actual application)

```
ypred = out.predict(xnew)
```



- K - means
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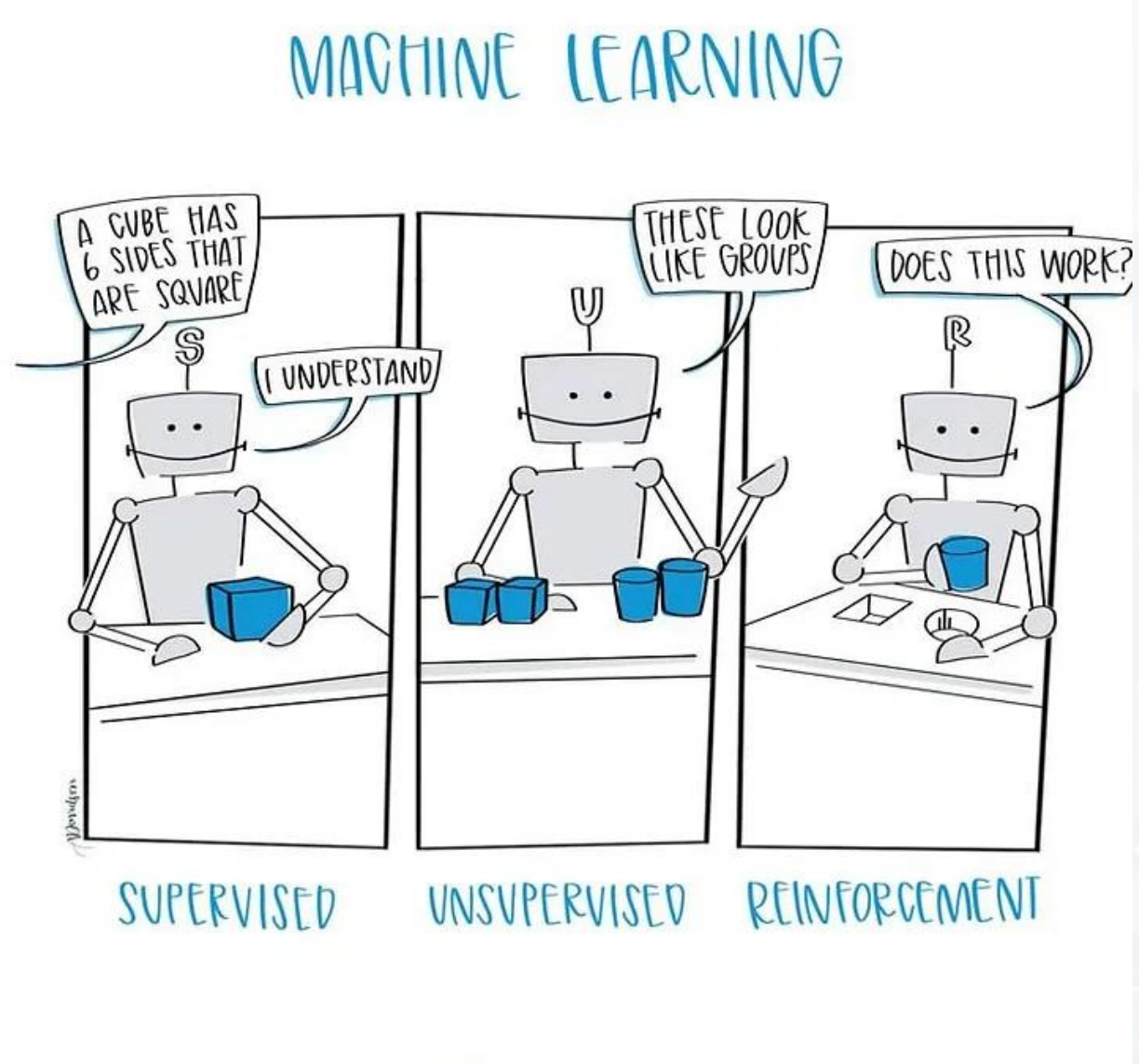
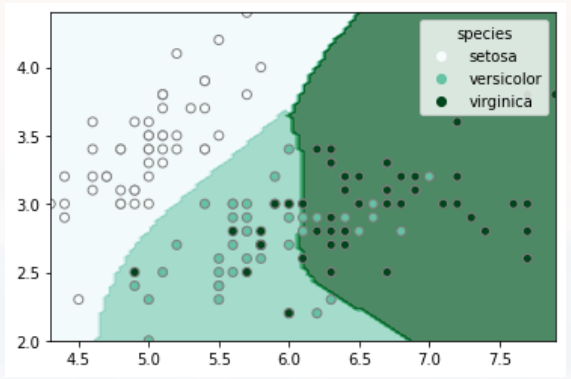

MACHINE LEARNING
A CUBE HAS 6 SIDES THAT ARE SQUARE
S
I UNDERSTAND
U
THESE LOOK LIKE GROUPS
DOES THIS WORK?
R
SUPERVISED
UNSUPERVISED
REINFORCEMENT

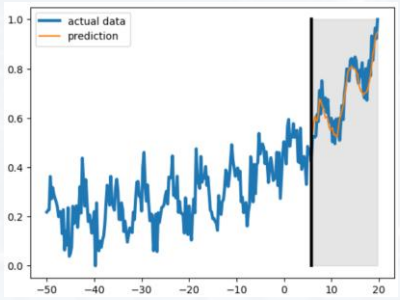
tasks:

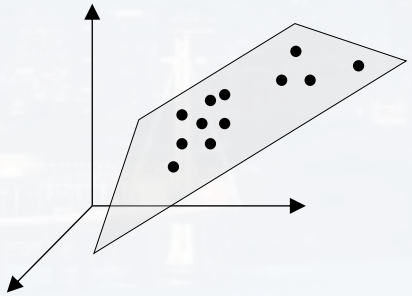
optimizing an *objective* function

- classification

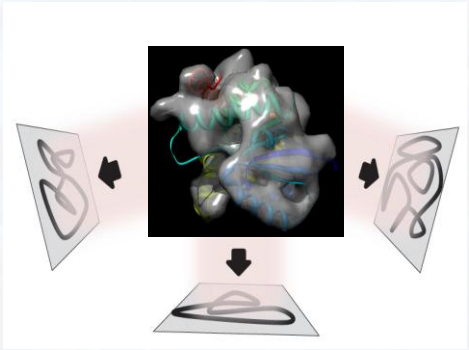


- regression





- generation



tasks:

- classification

Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	label
0	341.704	2.65585	3.09407	2	9.11147	Toxic
1	335.951	3.22262	2.89039	7	8.92848	Toxic
2	235.203	2.44115	2.48203	1	6.49731	Non-Toxic
3	246.505	2.76656	2.71547	7	7.45089	Non-Toxic
4	437.939	3.4801	3.59569	3	10.9156	Non-Toxic

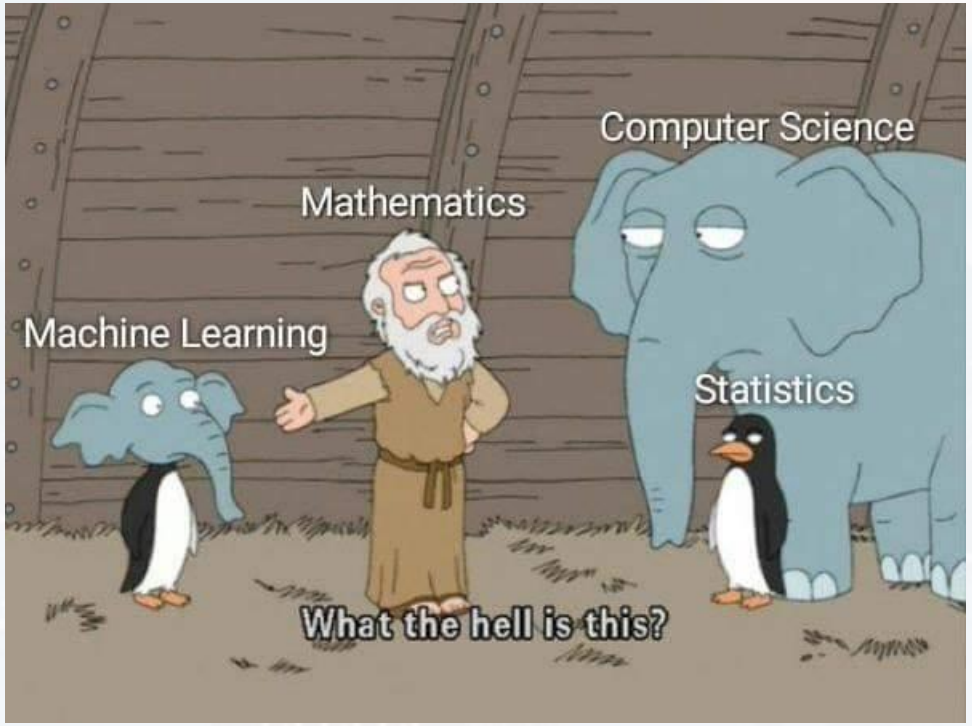
- regression

Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	toxicity_score
0	341.704	2.65585	3.09407	2	9.11147	80.9281
1	335.951	3.22262	2.89039	7	8.92848	83.4911
2	235.203	2.44115	2.48203	1	6.49731	61.8406
3	246.505	2.76656	2.71547	7	7.45089	57.0538
4	437.939	3.4801	3.59569	3	10.9156	131.326

- generation

“create a molecule with the properties XYZ, such that it is non-toxic”

carrier proteins (drug development)



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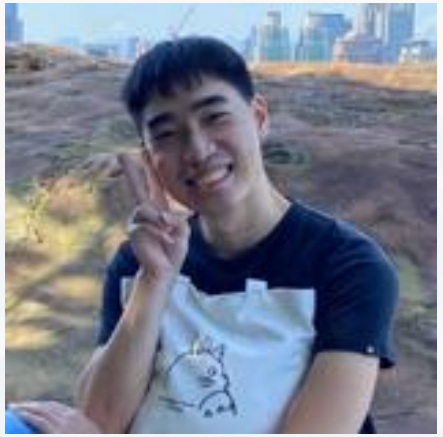
GSI: Eric Chung-Yueh Yuan

Grad Student at

Teresa Head- Gordon Lab

UC Berkeley



Lecturer: Markus Hohle

Lecturer at UC Berkeley &

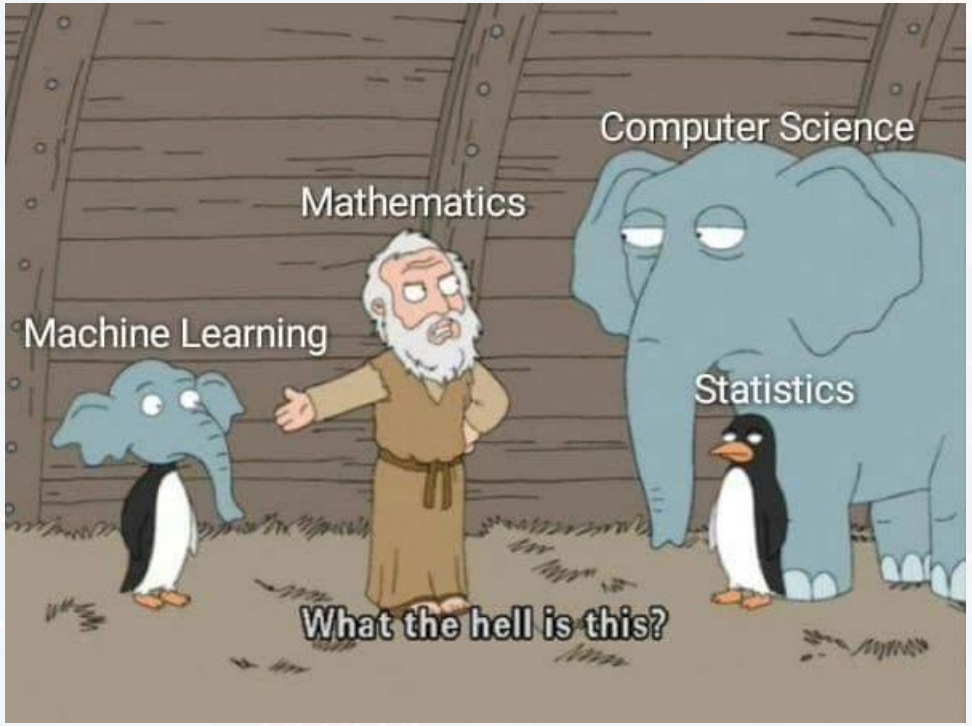
Data Analysis Consultant

PhD Physics

Lecture:	Monday	3:00 – 4:00pm PT
Discussion (Eric/Markus):	Thursday	1:00 – 2:30pm PT
Office Hours (Markus):	Friday	5:00 – 7:00pm PT

- **you can pick a ML/AI project**
- **work in teams of 4/5**
- **start planning after 1/3 of the course**
- **more detailed intro after ½ of the course**
- **submit proposal**
- **checkpoint**
- **presentation**

Material:	Recorded Lectures:	→ bcourses
	codes/slides	→ bcourses & GitHub
	HW assignments	→ bcourses
Grades:	HW assignments:	→ 50%
	Final Project	→ 40%
	Course Attendance	→ 10%



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Lecture 1: Course Overview and Introduction to Machine Learning

Lecture 2: Bayesian Methods in Machine Learning

Lecture 3: Dimensionality Reduction: Principal Component Analysis

Lecture 4: Linear and Non-linear Regression and Classification

Lecture 5: Unsupervised Learning: Clustering and Gaussian Mixture Models

Lecture 6: Adaptive Learning and Gradient Descent Optimization Algorithms

classic ML tools & algorithms

Lecture 7: Introduction to Artificial Neural Networks - The Perceptron

Lecture 8: Introduction to Artificial Neural Networks - Building Multiple Dense Layers

Lecture 9: Convolutional Neural Networks (CNNs) - Part I

Lecture 10: CNNs - Part II

Lecture 11: Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTMs)

Lecture 12: Combining LSTMs and CNNs

Lecture 13: Running Models on GPUs and Parallel Processing

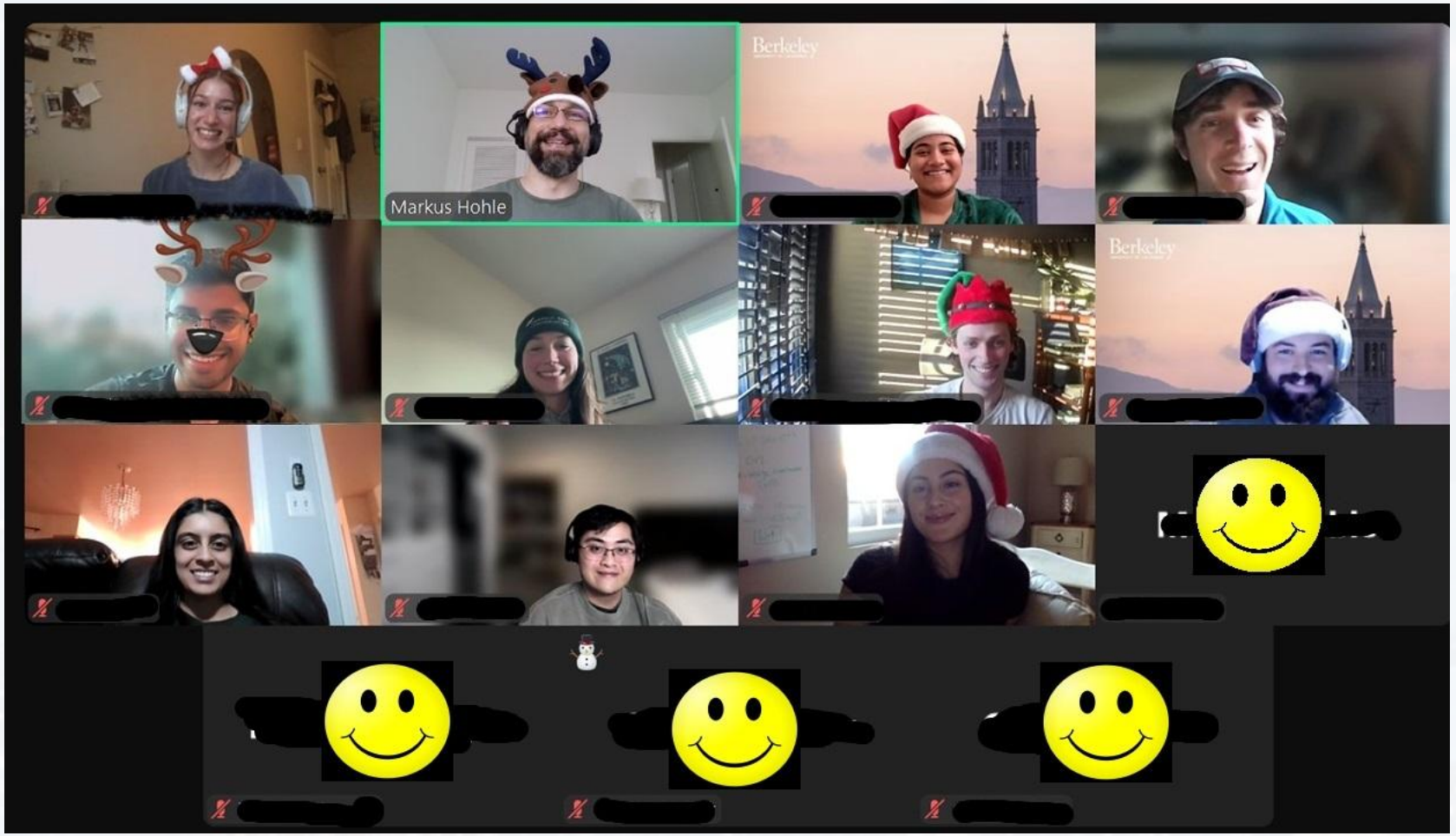
Lecture 14: Project Presentations

Lecture 15: Transformer

Lecture 16: GNN

ANNs/AI/Deep Learning

Dec 2024



Thank you very much for your attention!

?Questions?