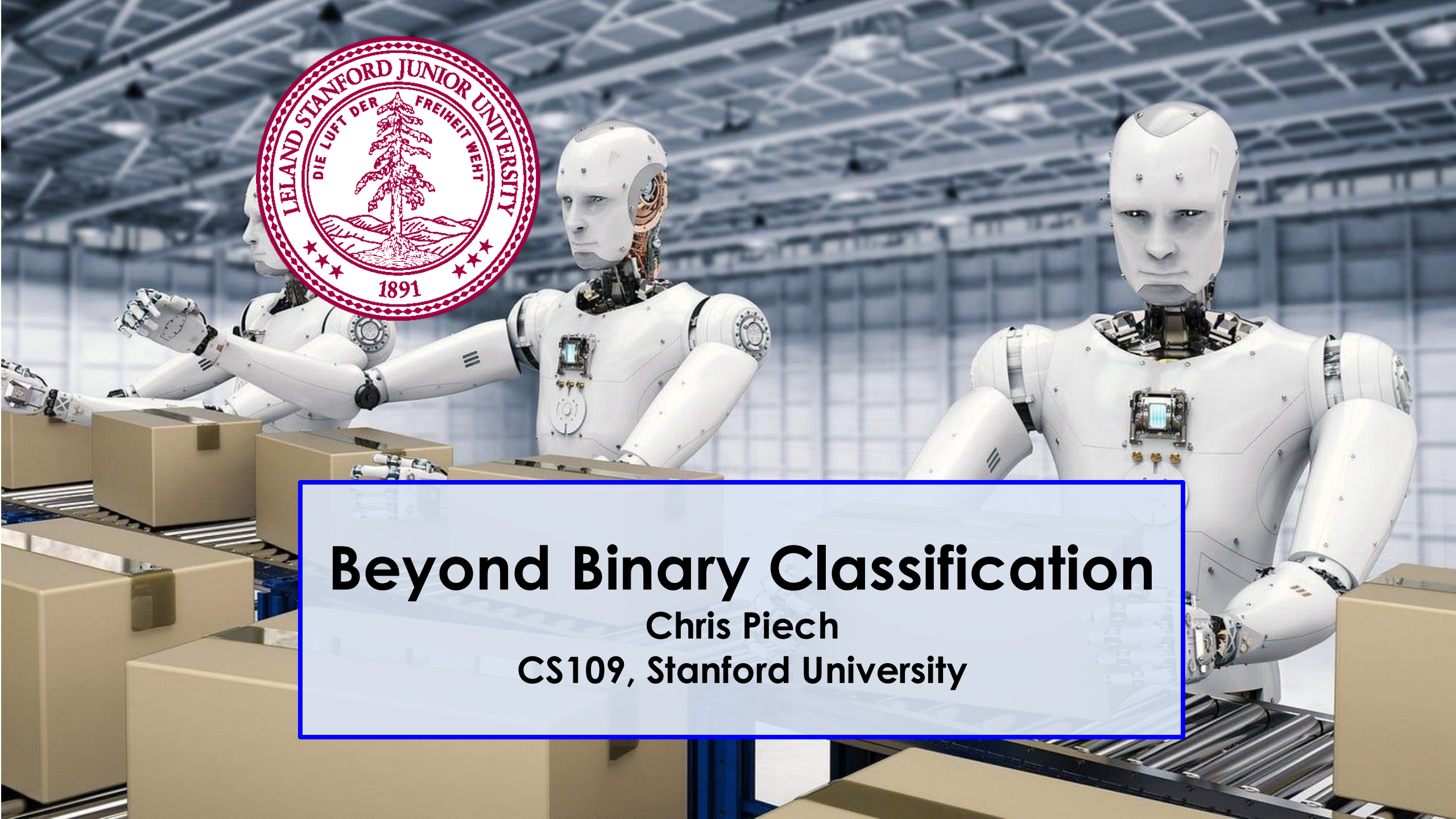
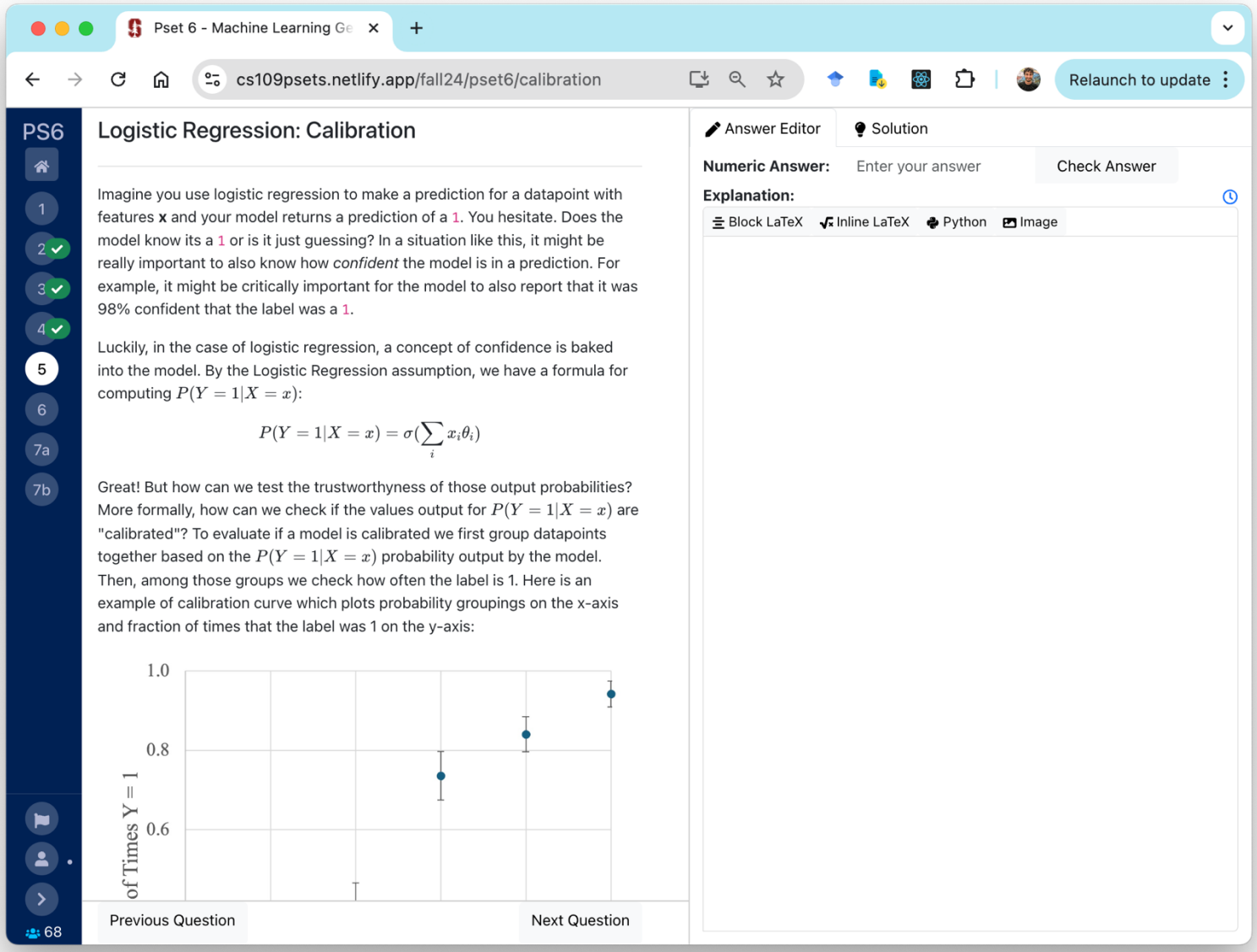


Beyond Binary Classification

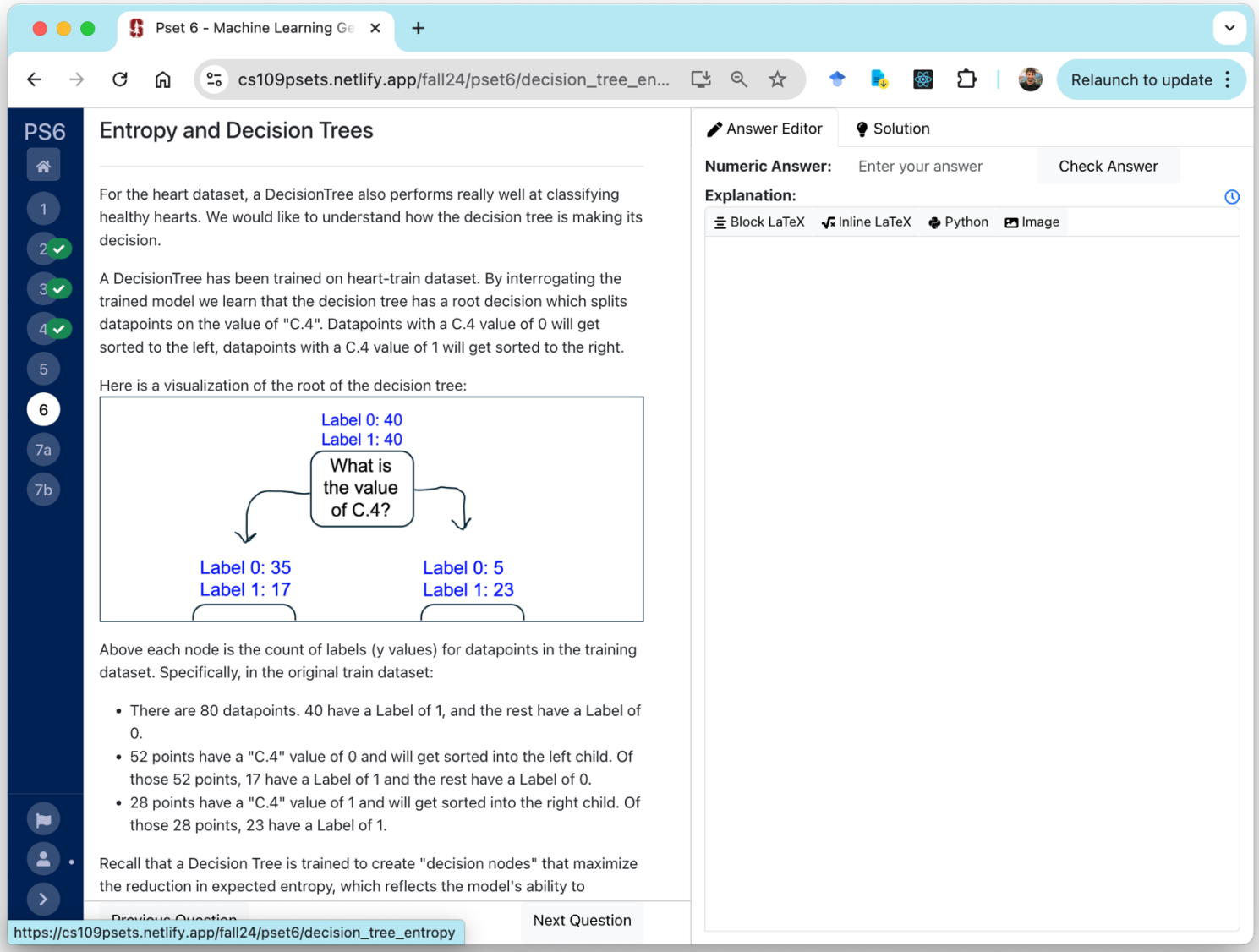
Chris Piech
CS109, Stanford University

Review

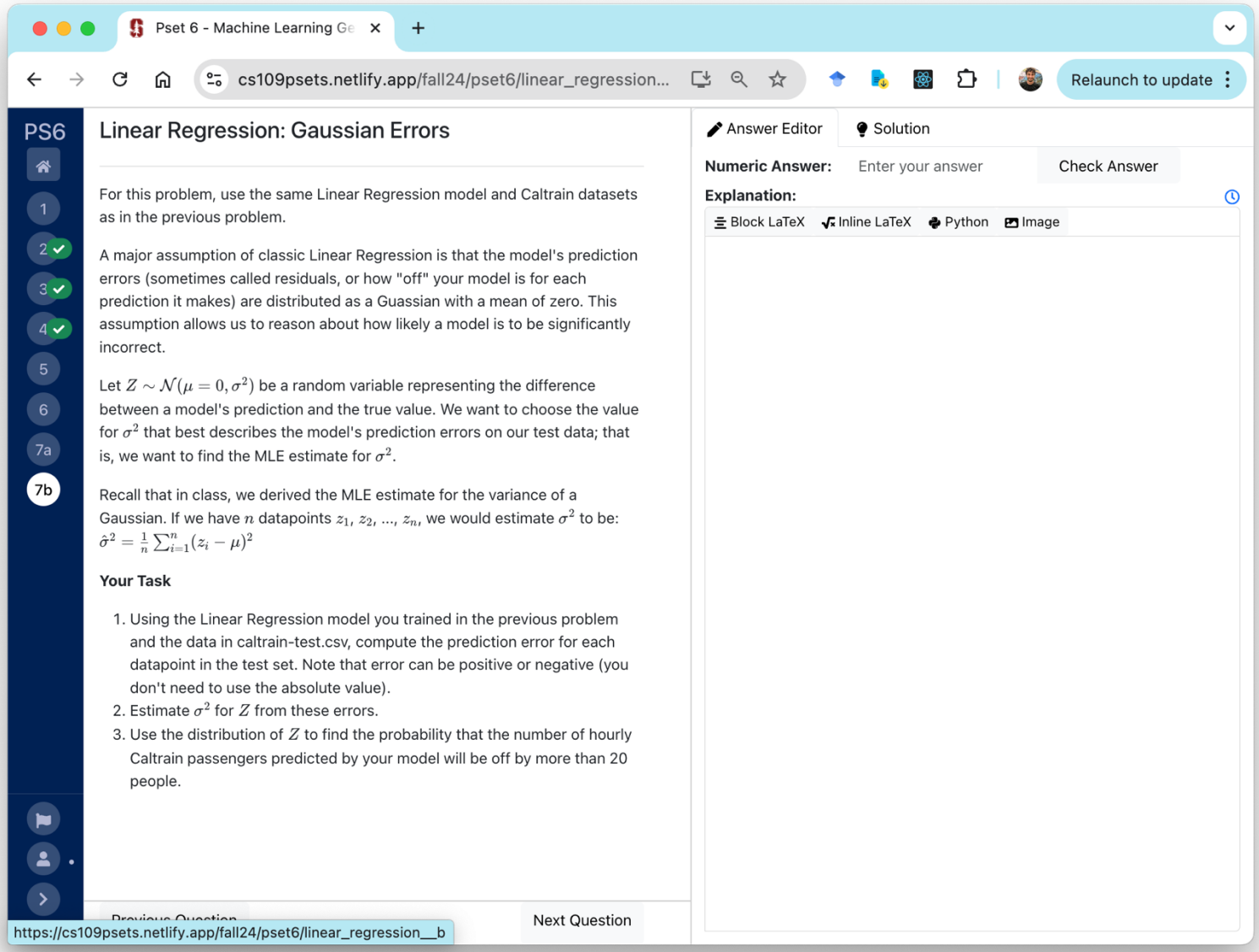
Whats new on PSet7?



Whats new on PSet7?

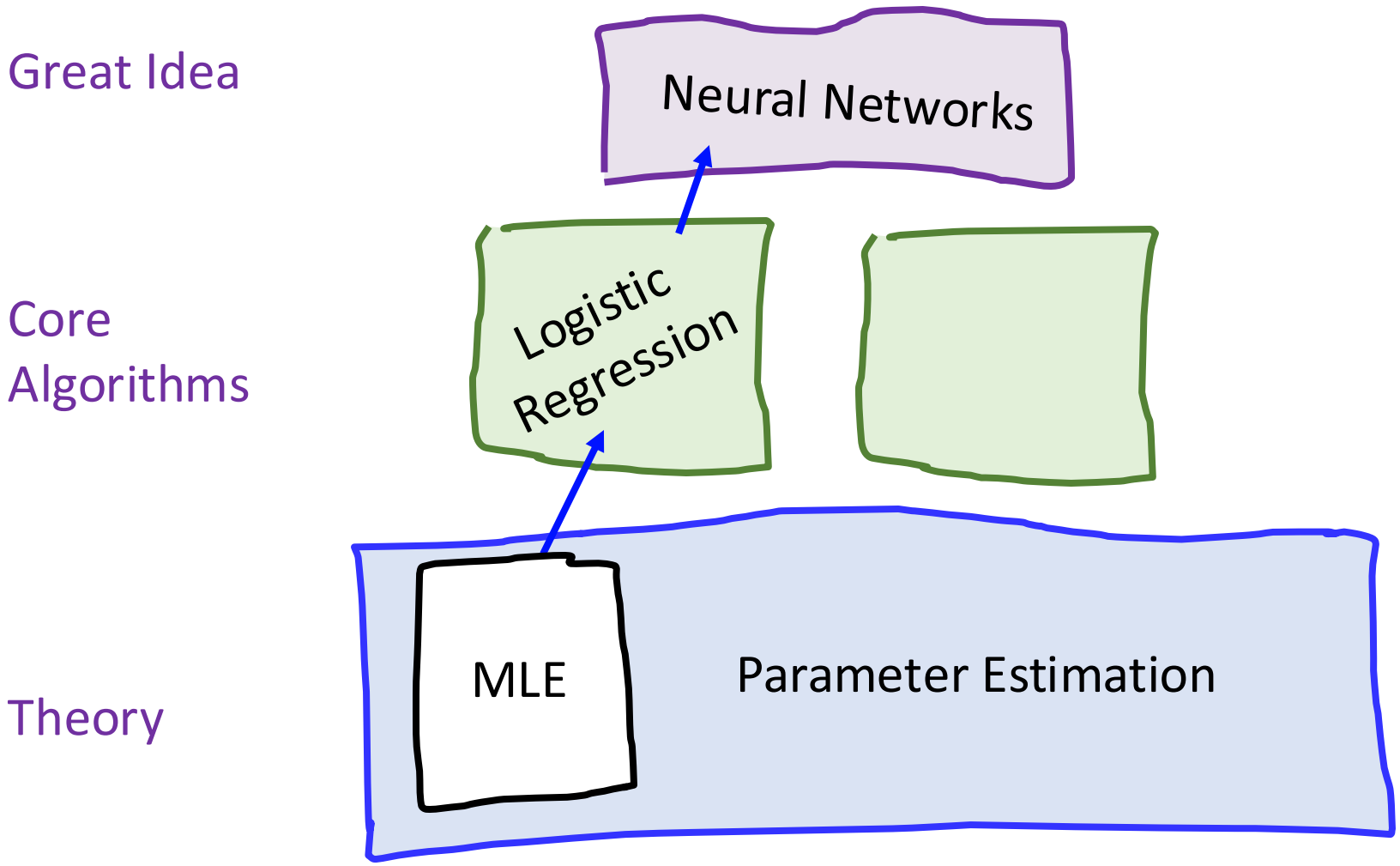


Whats new on PSet7?



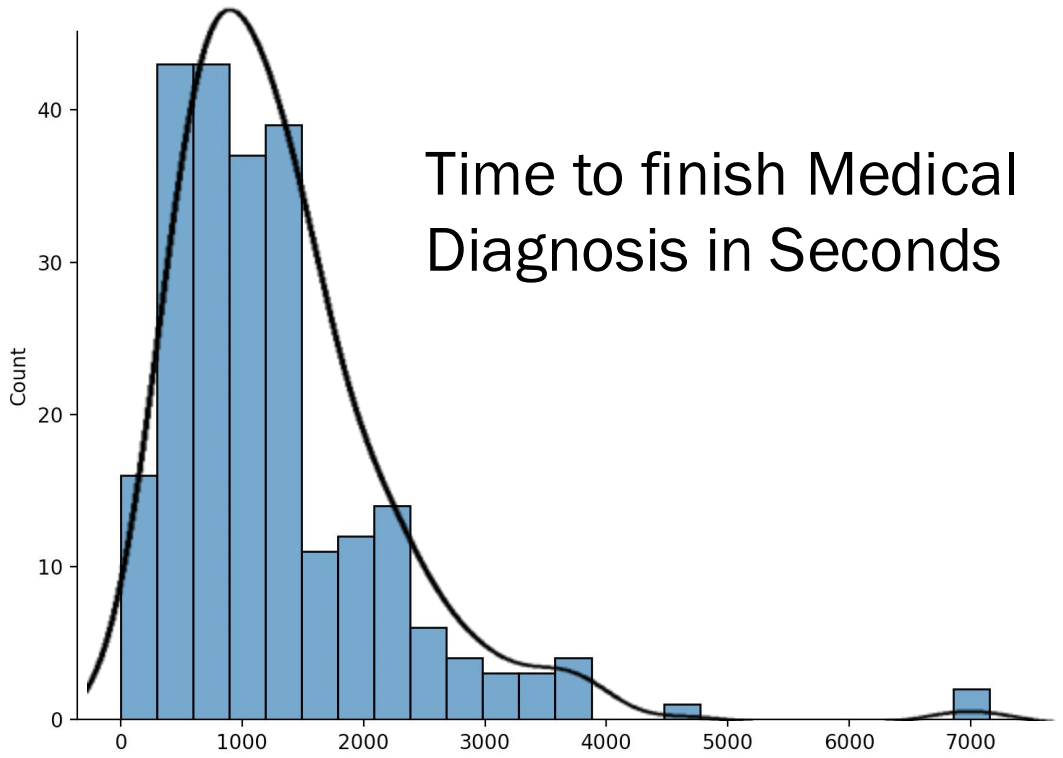
Review

Machine Learning in CS109



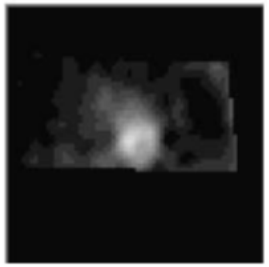
MLE of Erlang

```
[3.002, 0.983, 2.186, 1.624, 3.997, 1.777,
2.809, 0.42, 0.515, 1.582, 0.948, 0.458, 1.
066, 0.8, 2.398, 0.794, 2.561, 2.61, 0.
595, 3.897, 1.852, 1.182, 3.043, 0.905, 1.
45, 0.405, 0.445, 2.103, 1.425, 3.12, 0.
973, 1.056, 3.715, 2.952, 1.817, 2.686, 4.
173, 0.358, 2.185, 2.581, 7.134, 0.206, 2.
049, 0.896, 2.095, 4.39, 2.199, 3.434, 5.
696, 0.819, 0.416, 1.571, 1.337, 2.79, 2.
701, 3.061, 4.677, 0.671, 1.594, 3.586, 2.
708, 1.417, 1.799, 1.137, 1.771, 2.12, 0.
93, 6.835, 3.213, 2.541, 2.505, 1.257, 1.
99, 1.5, 0.014, 3.856, 0.979, 2.413, 2.
596, 1.653, 0.881, 4.457, 0.717, 3.305, 2.
456, 3.462, 1.737, 0.968, 0.528, 0.18, 1.
626, 2.224, 1.466, 1.6, 1.572, 0.12, 2.86,
1.062, 2.139, 1.217]
```



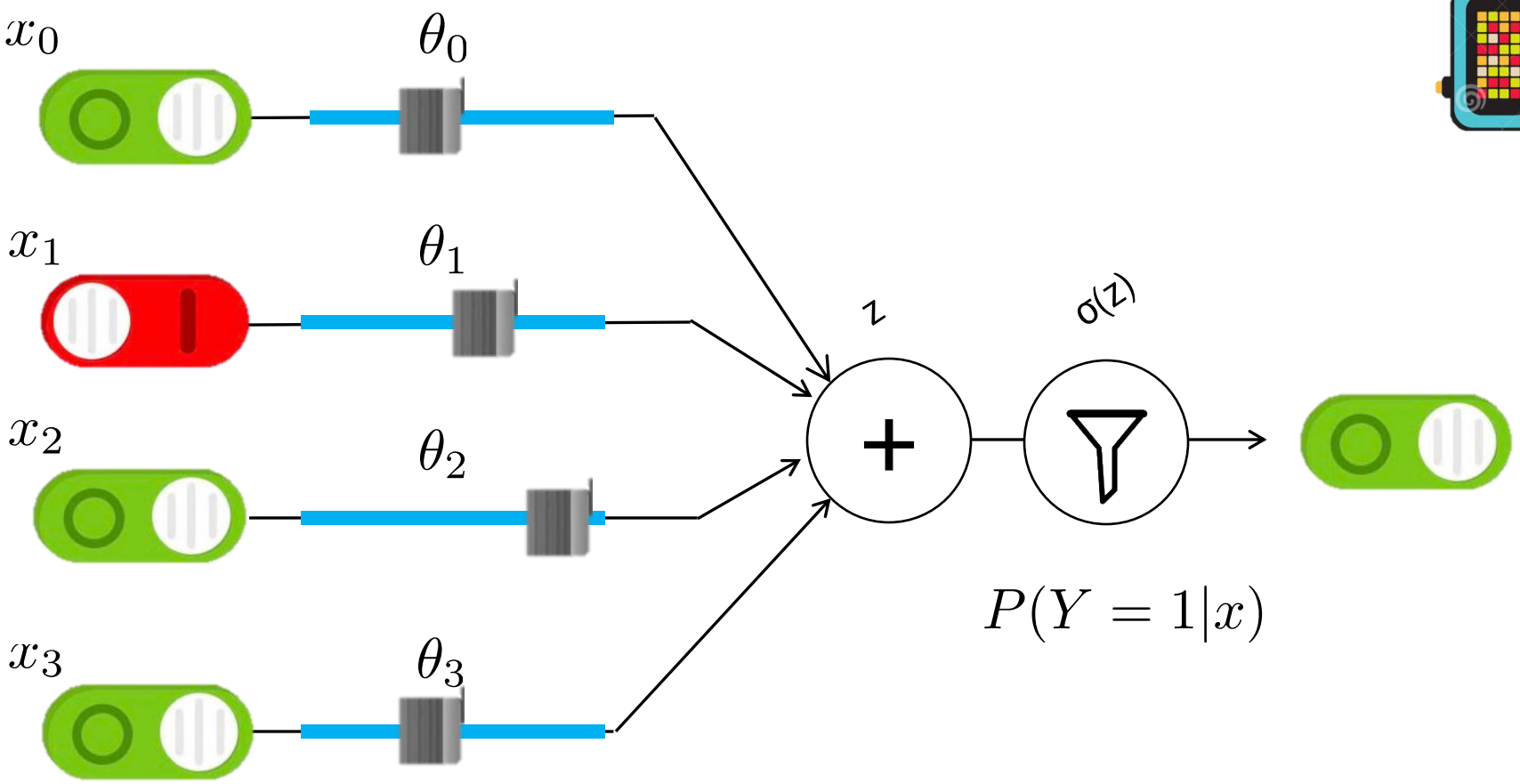
$$f(x) = \frac{\lambda^k x^{k-1} e^{-\lambda x}}{(k-1)!} = \frac{\lambda^k x^{k-1} e^{-\lambda x}}{\Gamma(k)}$$

Healthy Heart Classifier

	ROI 1	ROI 2	...	ROI *m*	Output
					
Heart 1	0	1		1	0
Heart 2	1	1		1	0
⋮					⋮
Heart *n*	0	0		0	1

$(\mathbf{x}^{(2)}, y^{(2)})$

Logistic Regression



$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\Big(\sum_i \theta_i x_i\Big)$$

Logistic Regression

1 Make logistic regression assumption

$$P(Y = 1|X = \mathbf{x}) = \sigma(\theta^T \mathbf{x})$$
$$P(Y = 0|X = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$$

Often call this $\hat{y}$

2 Calculate the log probability for all data

$$LL(\theta) = \sum_{i=0}^{n} y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)})]$$

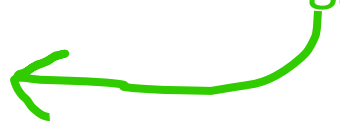
3 Get derivative of log probability with respect to thetas

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

Accuracy Comparison

Model	Train Accuracy	Test Accuracy
Baseline	0.6138	0.6300
Logistic Regression	0.7300	0.7200
Naive Bayes	0.7275	0.7200
Decision Tree	0.7975	0.6150
Random Forest	0.7950	0.7100
Gradient Boosting	0.7738	**0.7250**
AdaBoost	0.7588	0.7100

The Kaggle Champion



The **Gradient Boosting** is by far the most successful single model. Especially the package XGB is used in pretty much every winning (and probably top 50%) solution. XGB has essentially become the first model you try and the best performing single model by the end.

Kaggle
https://www.kaggle.com › general

What machine learning approaches have won most ... - Kaggle

XGB is for extreme gradient boosting

Wednesday: Three Guiding Questions

1. What are other models for classification?

2. For a dataset, how do you tell which one is best?

3. What are other validation metrics I might care about?

How **well calibrated** are my probabilities?

Measuring if Probabilities are Calibrated

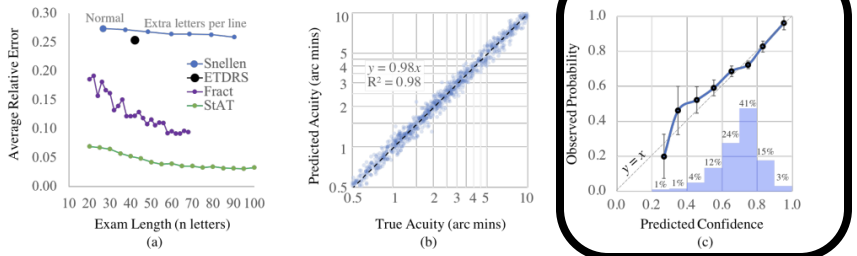


Figure 4: (a) The tradeoff between length of exam and error for the different algorithms. (b) A visualization of the predictions made by StACT. (c) Calibration test: StACT confidences correspond to how often it is correct.

4.2 Baseline Acuity Tests

We use the following baselines and prior algorithms to compare against the StACT algorithm.

Const Policy. This policy always predicts the most common visual acuity in our data i.e. the mode of the visual acuity prior. This serves as a true null model because it doesn't take patient responses into account at all.

Snellen and ETDRS. The Revised 2000 Series ETDRS charts and the Traditional Snellen Eye Chart were programmed so that we could simulate their response to different virtual patients. Both exams continue until the user incorrectly answers questions for more than half of the letters on a line. ETDRS has a function for predicted acuity score that takes into account both the last line passed, and how many letters were read on the last line not-passed. Both charts use 19 unique optotypes.

FrACT. We use an implementation of the FrACT algorithm (Bach and others 1996), with the help of code graciously shared by the original author. We also included the ability to learn the "s" parameter as suggested by the 2006 paper (Bach 2006), and verified that it improved performance.

	μ Acuity Error	μ Test length
Const	0.536	0
Snellen†	0.264	27
ETDRS†	0.254	42
FrACT	0.212	20
StACT	**0.069**	20
StACT-noSlip	0.150	20
StACT-greedyMAP	0.132	20
StACT-logistic	0.125	20
StACT-noPrior	0.090	20
StACT-goodPrior	**0.047**	20
StACT-star	**0.038**	63

Table 1: Average relative error for each algorithm. Except for Snellen each test was allowed 20 letters. Results are average relative error after 1000 tests. † Snellen and ETDRS used 19 unique optotypes.

5 Results and Evaluation

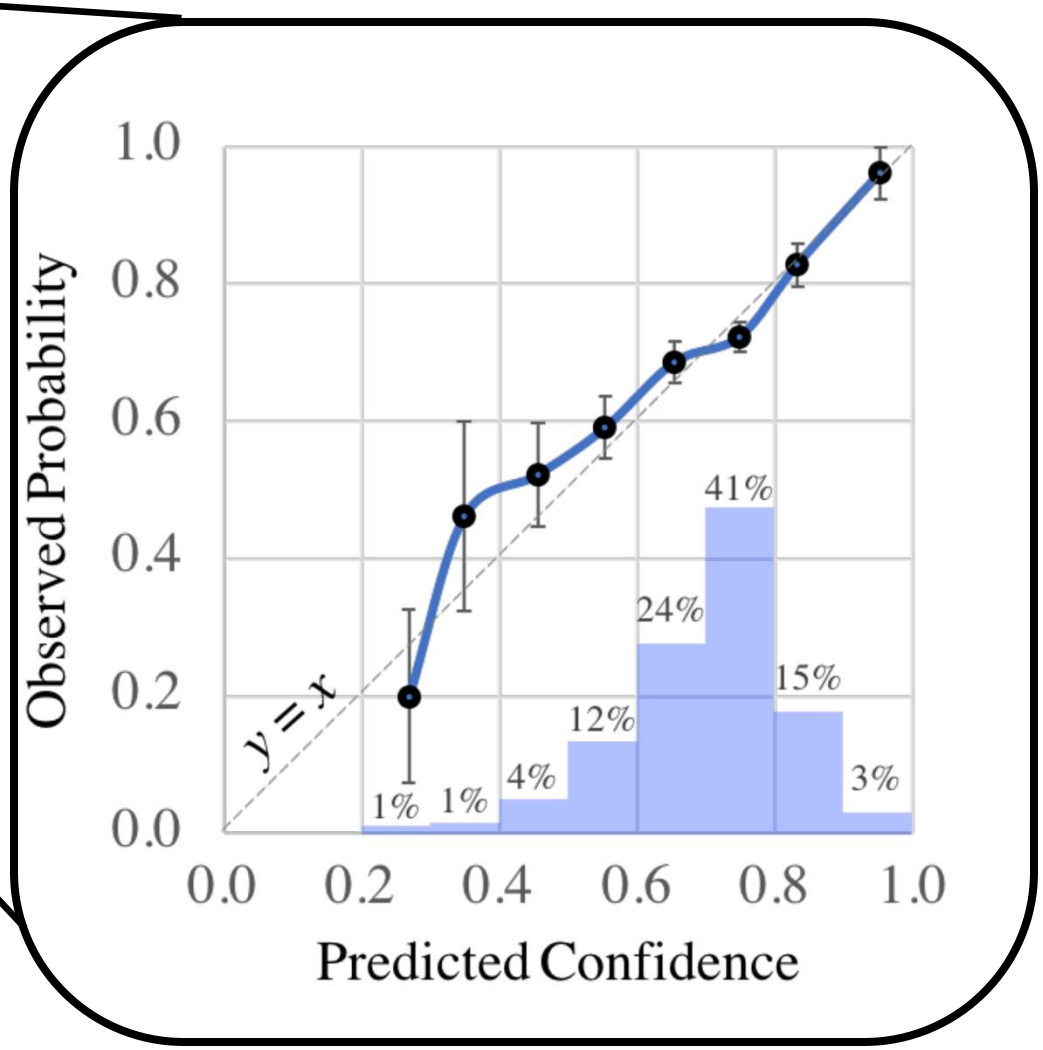
The results of the experiments can be seen in Table 1.

Accuracy and error. As can be seen from Table 1, the StACT test has substantially less error than all the other baselines. After 20 optotype queries, our algorithm is capable of predicting acuity with an average relative error of 0.069. This prediction is a 74% reduction in error from our implementation of the ubiquitous Snellen test (average error = 0.276), as well as a 67% reduction in error from the FrACT test (average error = 0.212). One possible reason for the improvement over FrACT is that the simulations used in our evaluations are based off the Floored-Exponential model that StACT uses. However, even when we evaluate StACT on simulations drawn from the FrACT logistic assumption we still achieve a 41% reduction. The improved accuracy of the StACT algorithm suggests our Bayesian approach to measuring acuity is a fruitful proposal both because of our introduction of the floored exponential as well as our Thompson-sampling inspired algorithm to chose a next letter size.

Figure 4 (b) visualizes what StACT's small relative error means in terms of predictions. Each point in the plot is a single patient. The x-axis is the true acuity of the patient and the y-axis is the predicted accuracy. We can qualitatively observe that the predictions are often accurate, there are no truly erroneous predictions, and that the exam is similarly accurate for patients of all visual acuities.

Moreover, as seen in Figure 4 (a), StACT's significant improvement in error rate holds even when the length of the exam is increased. It is also evident that increasing exam length reduces our error rate: if we increase the exam length to 200 letters, the average error of StACT falls to 0.020. While this is highly accurate, its far too long an exam, even for patients who need to know their acuity to high precision.

StACT Star Exam. Our primary experiments had a fixed

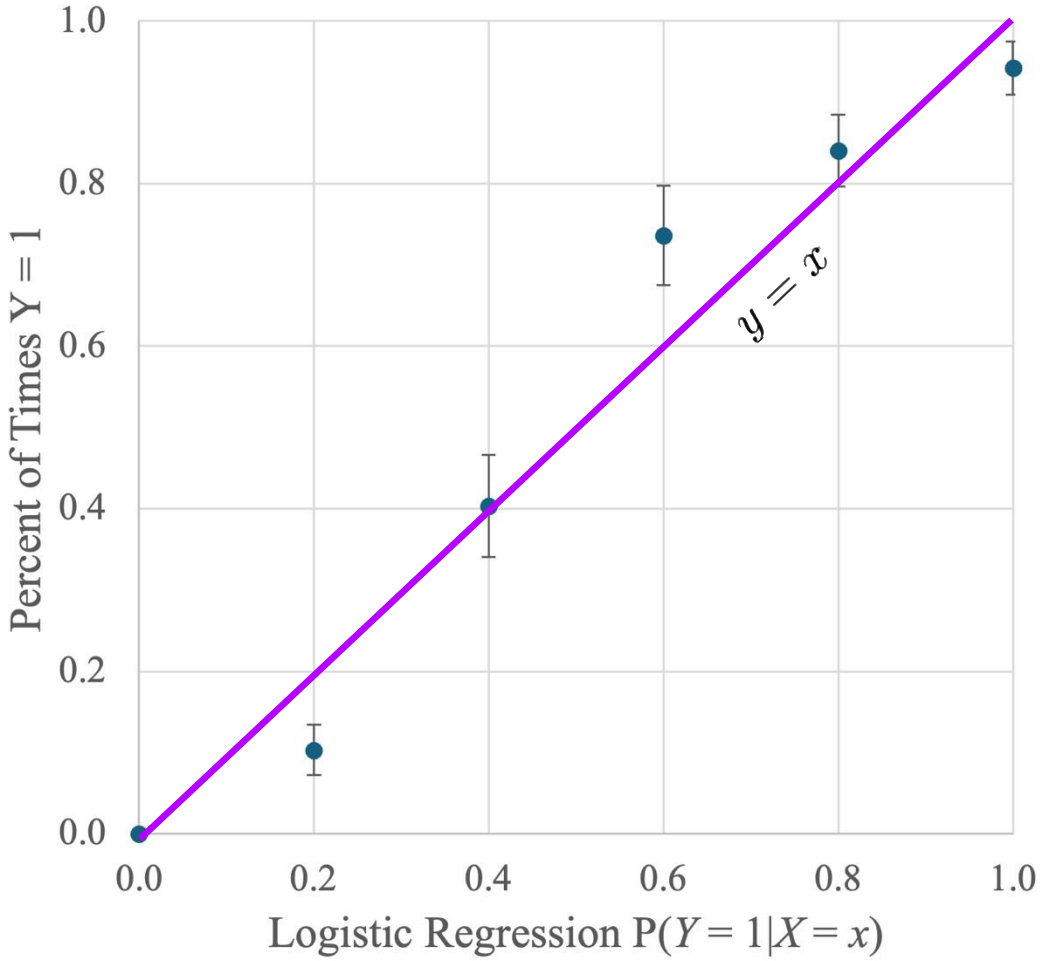


Logistic Regression Calibration Curve

$x_1 \quad x_2 \quad x_{19} \quad y$

$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

	A	B	T	U	V
1	col1	col2	col19	Label	LogRegPr
2	1	0	1	0	0.237
3	1	1	1	1	0.928
4	1	0	0	1	0.541
5	1	0	1	0	0.003
6	1	0	0	0	0.914
7	1	0	0	1	0.432
8	1	0	1	0	0.001
9	1	0	1	1	0.530
10	0	0	1	0	0.090
11	1	0	1	0	0.439
12	1	0	1	0	0.032
13	1	0	1	0	0.114
14	0	0	1	1	0.848
15	1	0	1	0	0.025
16	1	0	1	0	0.180
17	0	0	1	1	0.672
18	1	0	1	1	0.531
19	1	0	1	0	0.012
20	1	0	1	1	0.560
21	1	0	1	1	0.502



End Review

One Final Measure….

Is the Model Fair?

Two Philosophic Values of Fairness

Procedural Fairness:

Focuses on the decision-making or classification *process*, ensures that the algorithm does not rely on unfair features.

Distributive Fairness:

Focuses on the decision-making or classification *outcome*, ensures that the distribution of good and bad outcomes is equitable.

Two Philosophic Values of Fairness

Procedural Fairness:

Focuses on the decision-making or classification *process*, ensures that the algorithm does not rely on unfair features.

Distributive Fairness:

Focuses on the decision-making or classification *outcome*, ensures that the distribution of good and bad outcomes is equitable.

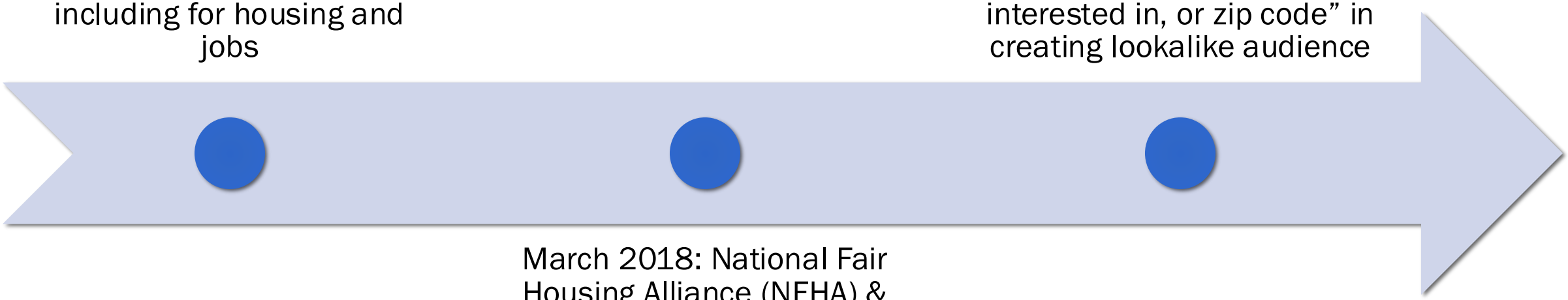
Fairness through unawareness

Case Study: Facebook Ads & Job/Housing Recommendations

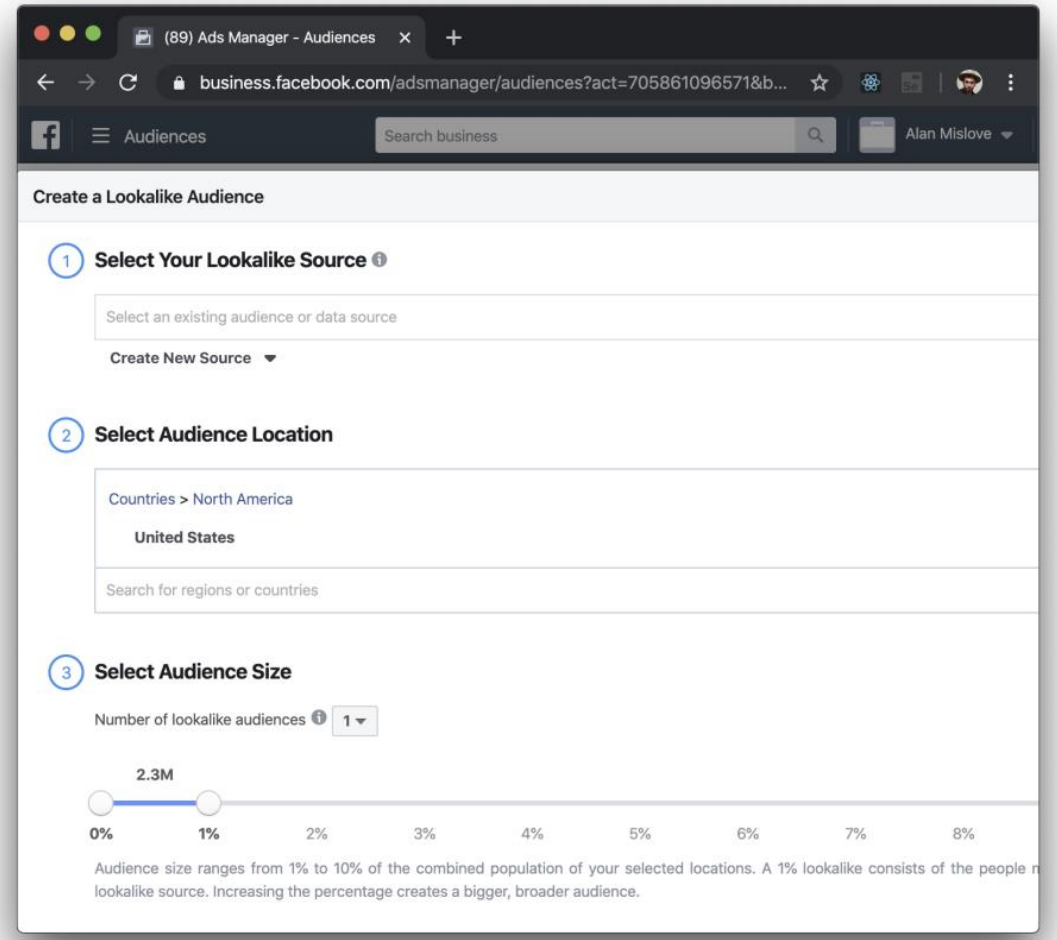
Facebook creates “Lookalike” feature for advertisers: upload a “source list” and find users with “common qualities” to target ads, including for housing and jobs

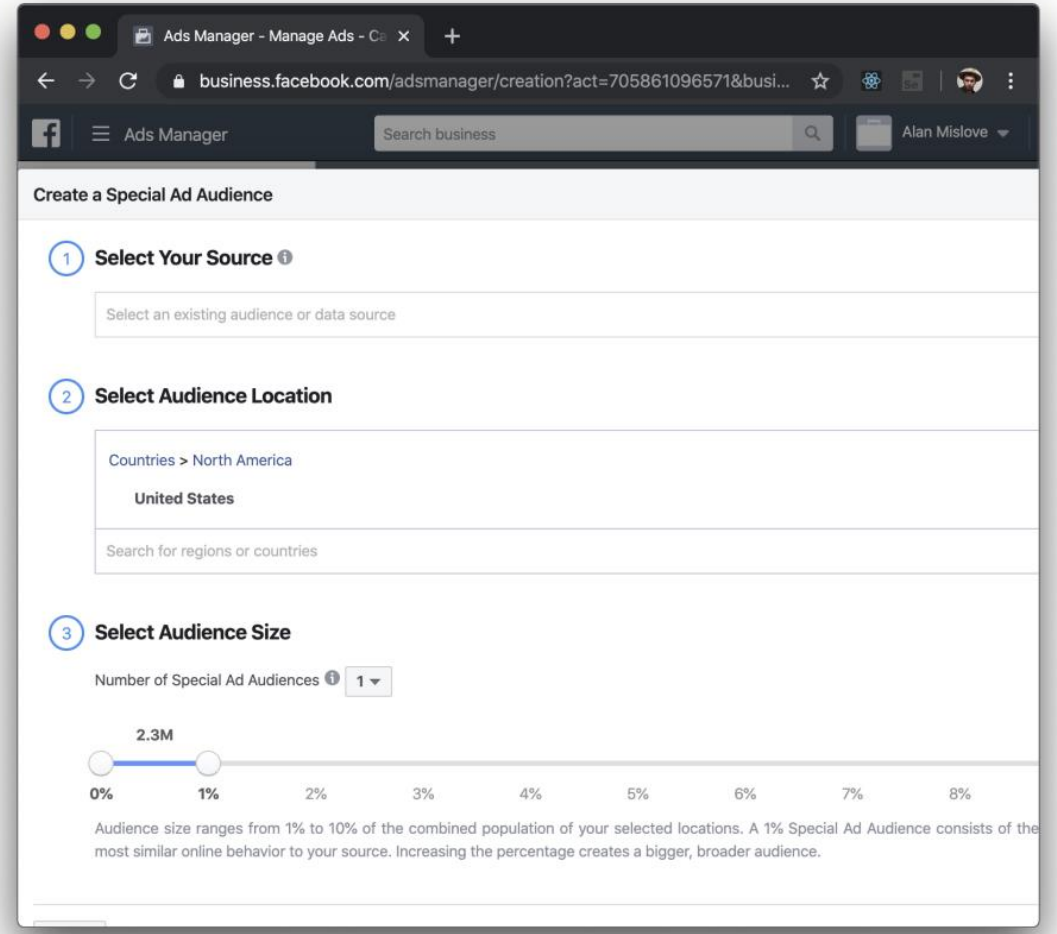
March 2018: National Fair Housing Alliance (NFHA) & other civil rights groups sue Facebook over violations of the Fair Housing Act

March 2019: As part of settlement, Facebook agrees not to use “age, gender, relationship status, religious views, school, political views, interested in, or zip code” in creating lookalike audience



Facebook Input Lookalikes





New "Special Ad" Audiences Still Biased

Gender: Equally Biased

Age: Almost as Biased

Race: more difficult to measure given the tools provided but still somewhat biased

Political Views: Less Biased

Sapiezynski et. al 2019,

https://sapiezynski.com/papers/sapiezynski2019algorithms.pdf

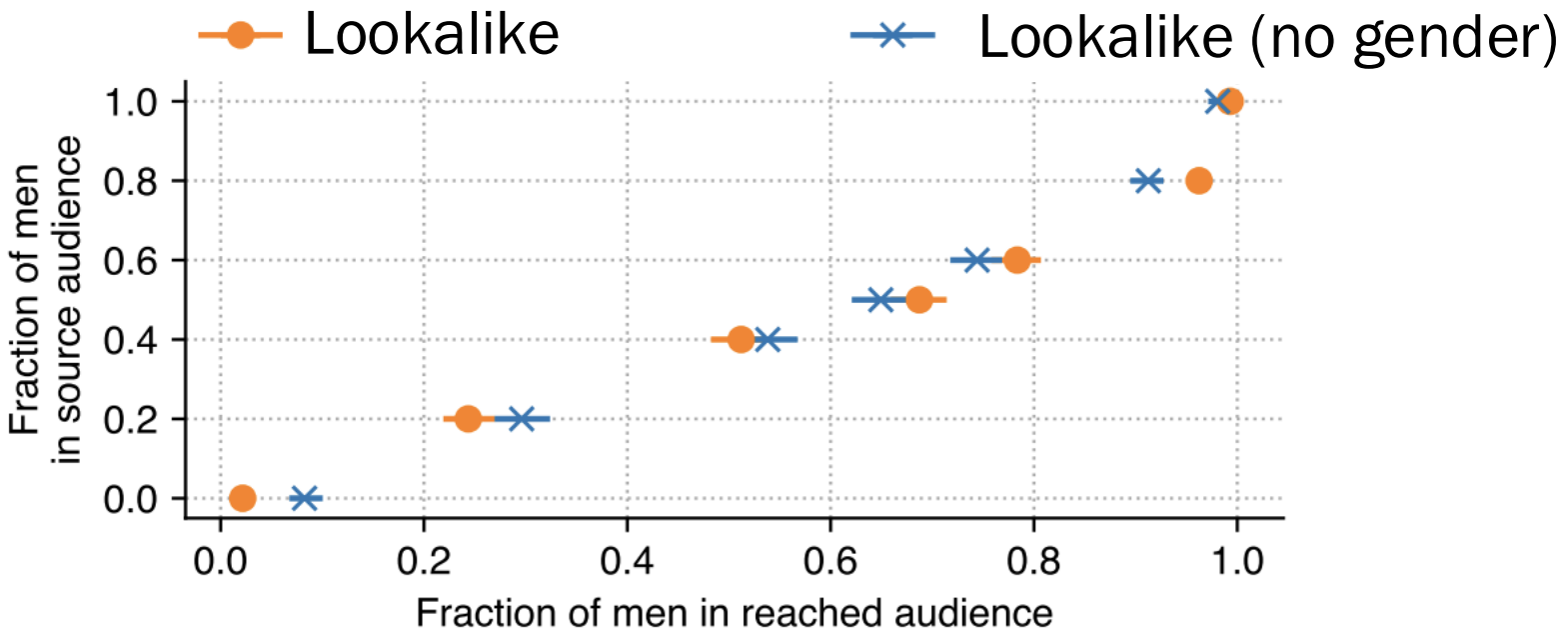
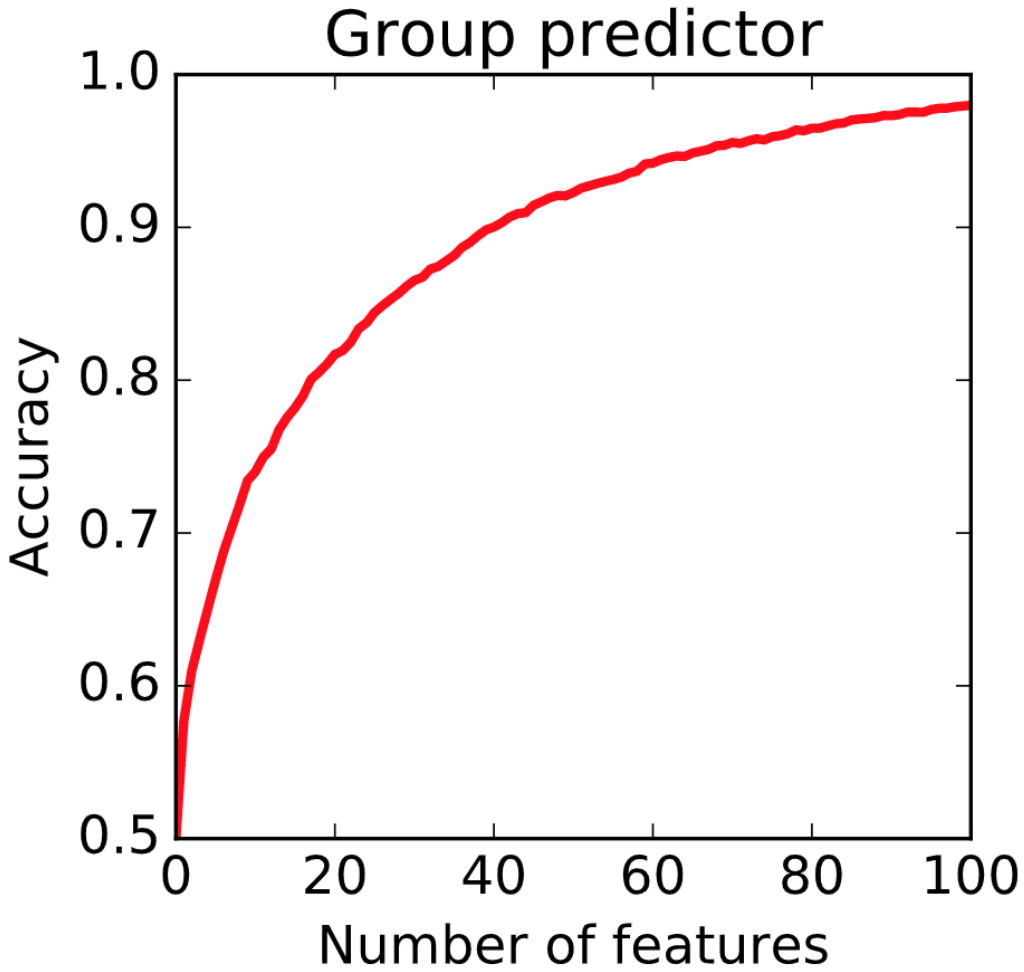


Figure 2: Gender breakdown of ad delivery to Lookalike and Special Ad audiences created from the same source audience with varying fraction of male users, using the same ad creative. We can observe that both Lookalike and Special Ad audiences reflect the gender distribution of the source audience, despite the lack of gender being provided as an input to Special Ad Audiences.

Yo, Piotr, you got your axis backwards ☺



Many Features = Accurate Group Prediction

Sensitive attributes are often “redundantly encoded” in the dataset

Many of the features or datapoints are correlated with the sensitive attribute

Two Philosophic Values of Fairness

Procedural Fairness:

Focuses on the decision-making or classification *process*, ensures that the algorithm does not rely on unfair features.

Distributive Fairness:

Focuses on the decision-making or classification *outcome*, ensures that the distribution of good and bad outcomes is equitable.

Fairness through unawareness
(facebook example shows this is hard)

Let’s Try Fairness Through Awareness!

Awareness of what?

Fairness Through Awareness Terms

D: protected demographic
G: guess of your model (aka y hat)
T: the true value (aka y)

$D = 0$

	$G = 0$	$G = 1$
$T = 0$	0.21	0.32
$T = 1$	0.07	0.28

$D = 1$

	$G = 0$	$G = 1$
$T = 0$	0.01	0.01
$T = 1$	0.02	0.08

Distributive Fairness #1: Parity

Fairness definition #1: Parity

An algorithm satisfies "parity" if the probability that the algorithm makes a positive prediction ($G = 1$) is the same regardless of begin conditioned on demographic variable.

D: protected demographic
G: guess of your model (aka y hat)
T: the true value (aka y)

$$P(G=1|D=1) = P(G = 1 \mid D = 0)$$

Distributive Fairness #2: Calibration

Fairness definition #2: Calibration

An algorithm satisfies "calibration" if the probability that the algorithm is correct ($G = T$) is the same regardless of demographics.

D: protected demographic
G: guess of your model (aka y hat)
T: the true value (aka y)

$$P(G = T|D = 0) = P(G = T|D = 1)$$

Calibration (Relaxed)

Fairness definition #2: Calibration

An algorithm satisfies "calibration" if the probability that the algorithm is correct ($G = T$) is the same regardless of demographics.

D: protected demographic
G: guess of your model (aka y hat)
T: the true value (aka y)

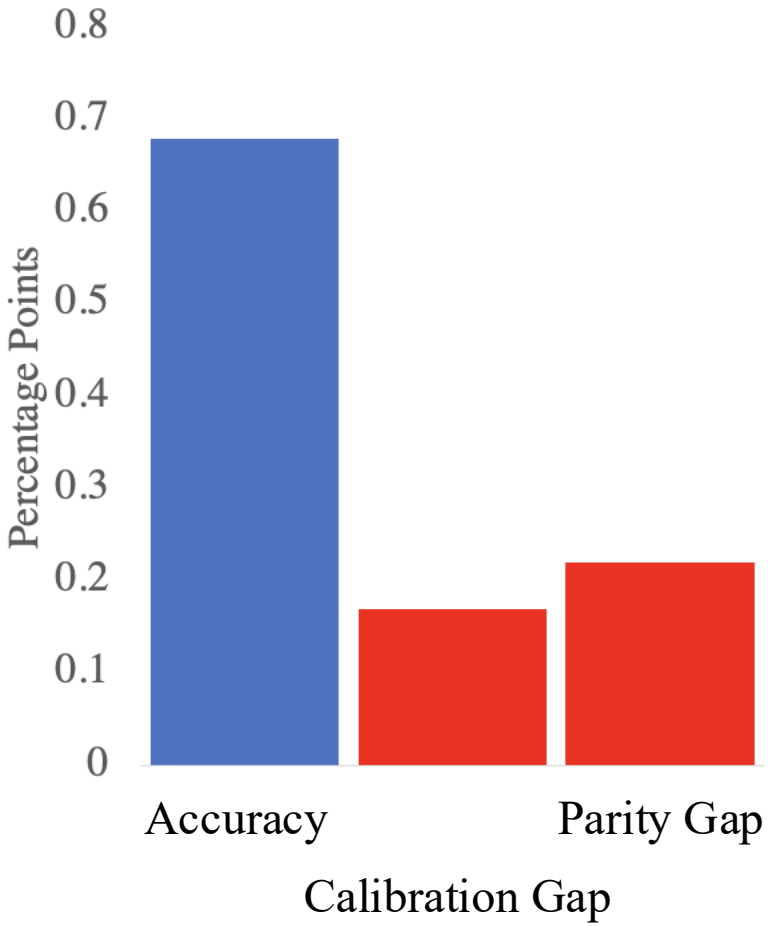
$$\frac{P(G = T|D = 1)}{P(G = T|D = 0)} \geq 1 - \epsilon$$

Where epsilon = 0.2

US legal standard: "disparate impact," also known as the 80% rule.

COMPAS: Biased Against Black Inmates

Before: Compas is Biased



Train bias out

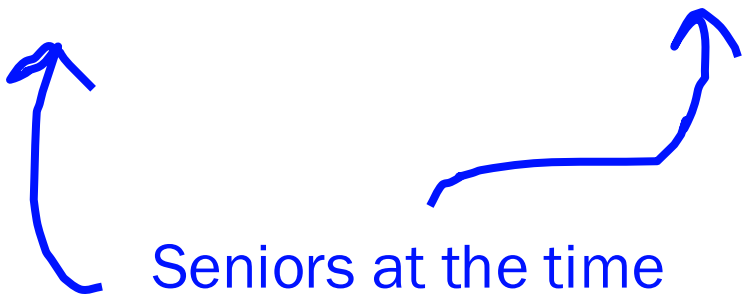
Advanced Idea: Adversarial Learning

Achieving Fairness through Adversarial Learning: an Application to Recidivism Prediction

Christina Wadsworth
Stanford University
Stanford, CA
cwads@cs.stanford.edu

Francesca Vera
Stanford University
Stanford, CA
fvera@cs.stanford.edu

Chris Piech
Stanford University
Stanford, CA
piech@cs.stanford.edu



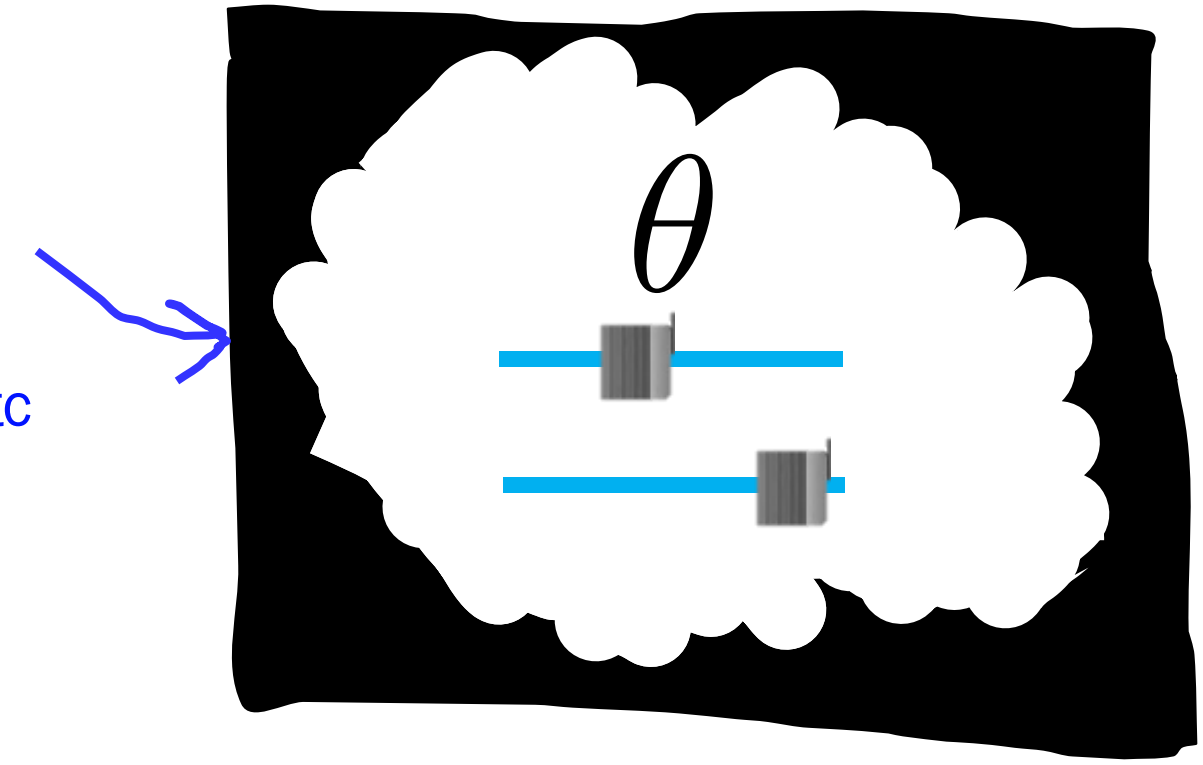
Seniors at the time they wrote it

220+ citations

COMPAS: Predicting "Recidivism"

$\mathbf{x}$

Data about an inmate:
Their zip code, past crimes, etc



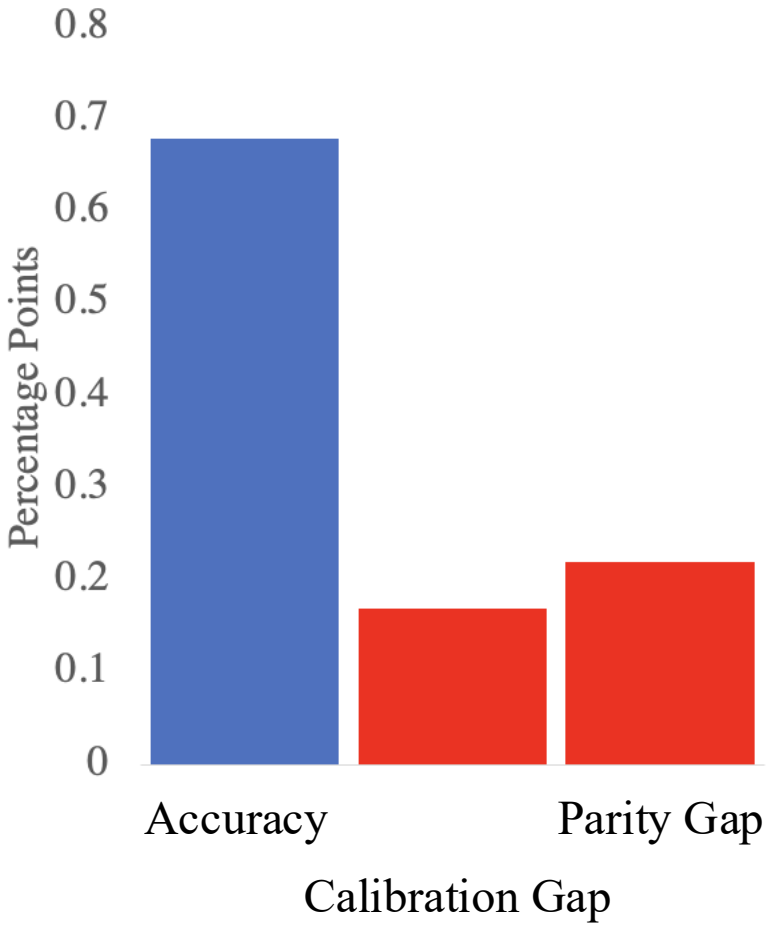
$\hat{y} = 0$

Will they commit a crime again

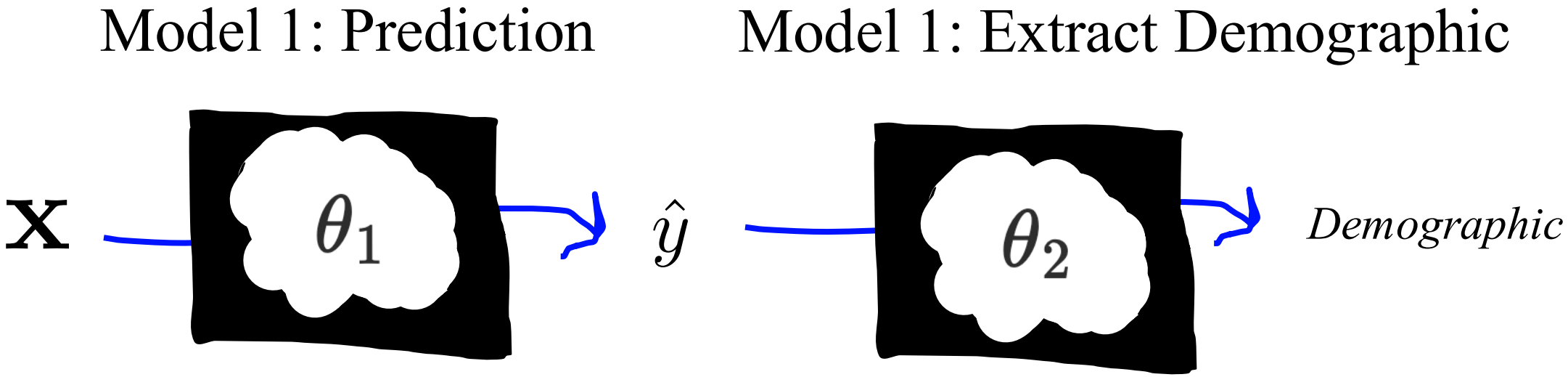
Was in use in California and Florida

COMPAS: Biased Against Black Inmates

Before: Compas is Biased



Can We Train Out Bias?



Model 1 should be accurate

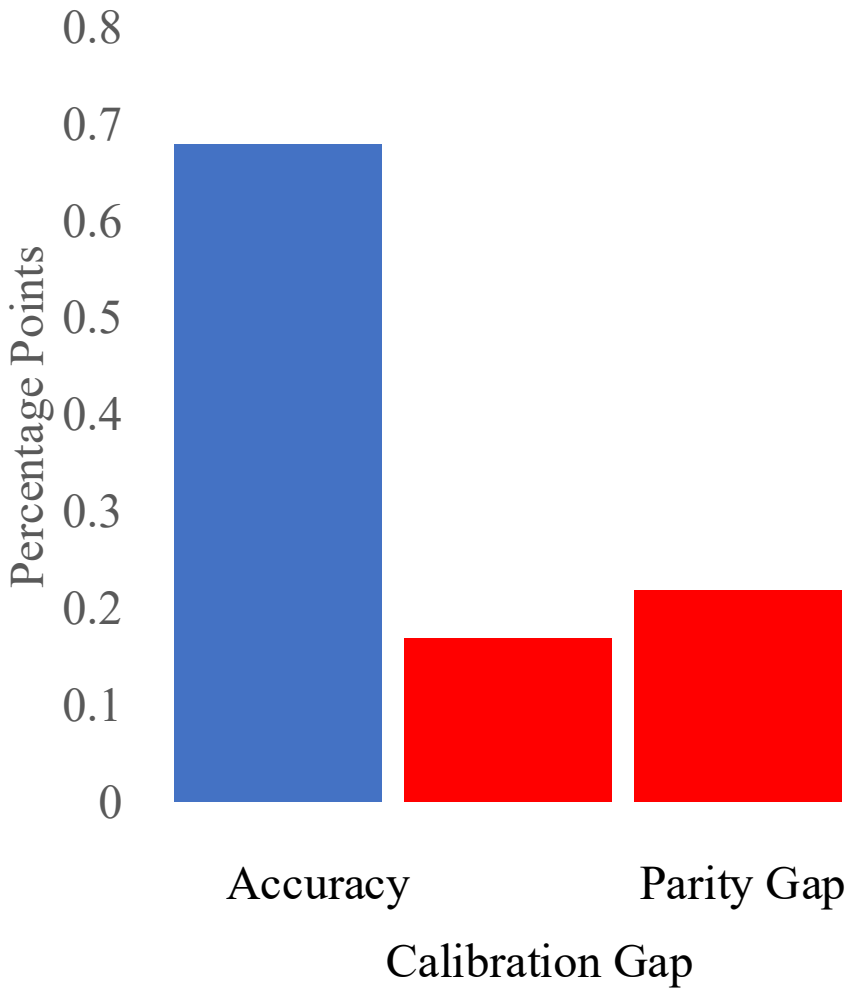
*Model 2 should be **in**accurate*

$$\theta_1 = \underset{\theta_1}{\text{argmax}}\ L_1(\theta_1) - L_2(\theta_2)$$

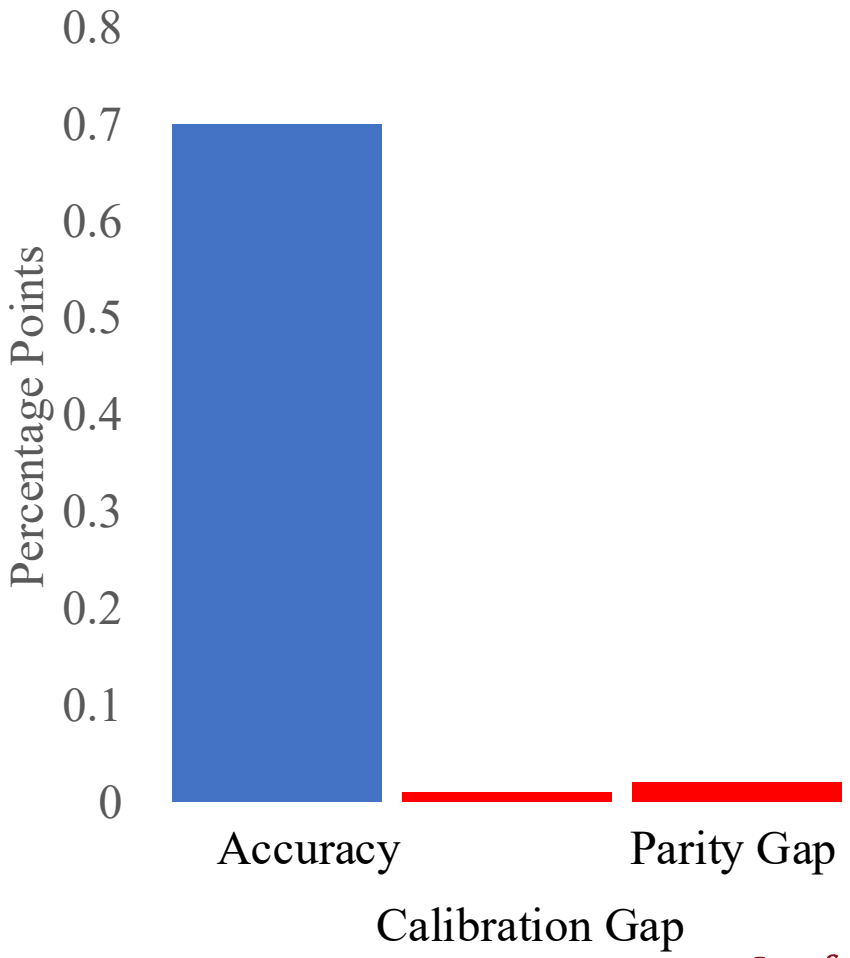
*note in the paper these were neural nets

Can We Train Out Bias?

Before: Compas is Biased



After: Gaps are reduced



Their Conclusion

DON'T USE BLACK BOX ALGORITHMS TO MAKE RECIDIVISM PREDICTIONS

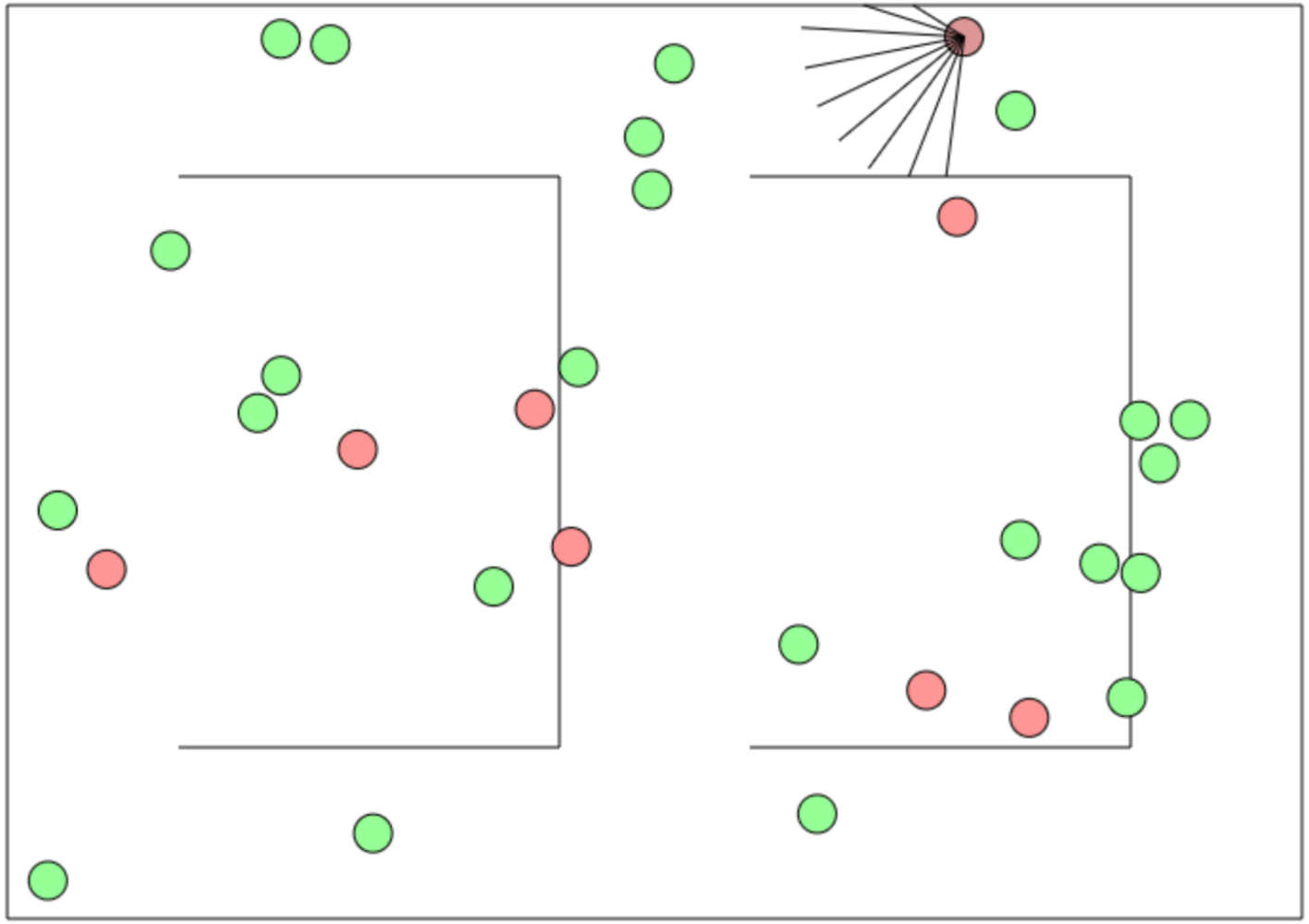
Many ways to evaluate models:

Test Accuracy!
Calibration!
Fairness!

But wait….

Is all of ML Classification?

Lets start training a Critter



http://cs.stanford.edu/people/karpathy/convnetjs/demo/rldemo.html

Types of Machine Learning Tasks

Muli-Class Classification

Regression

Reinforcement Learning

Generation

Types of Machine Learning Tasks

Muli-Class Classification

Regression

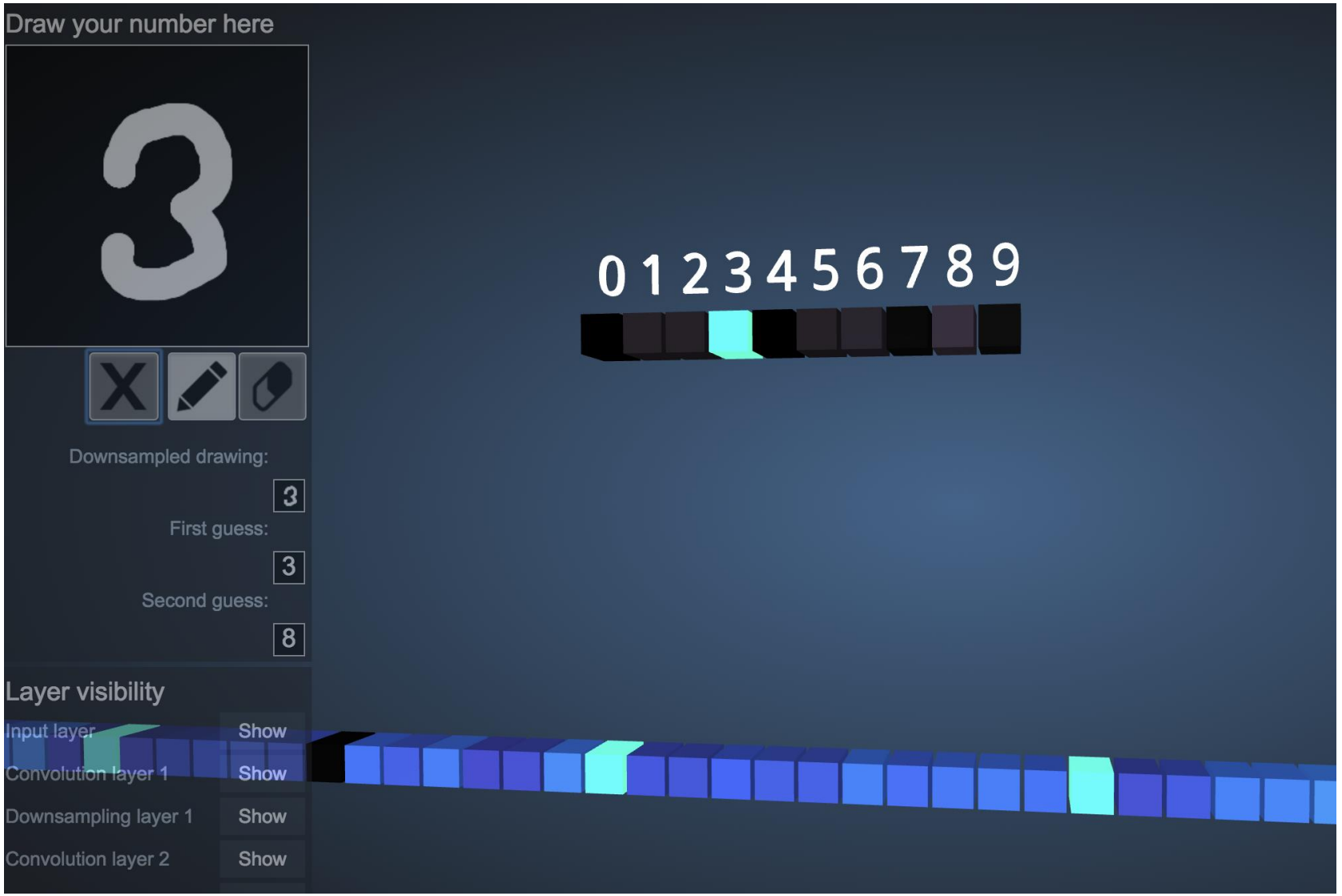
Today

Reinforcement Learning

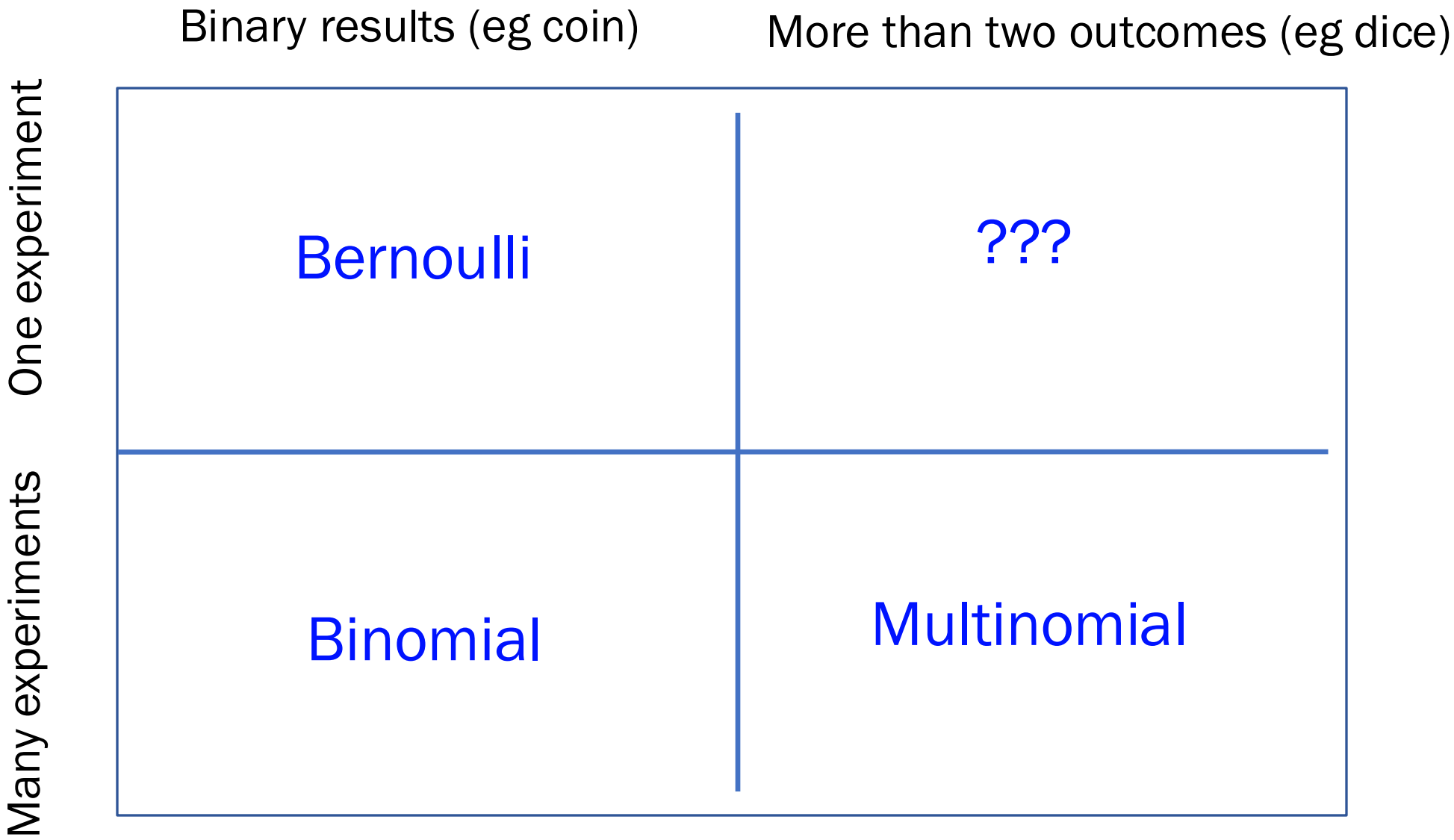
Generation

Beyond Binary Classification

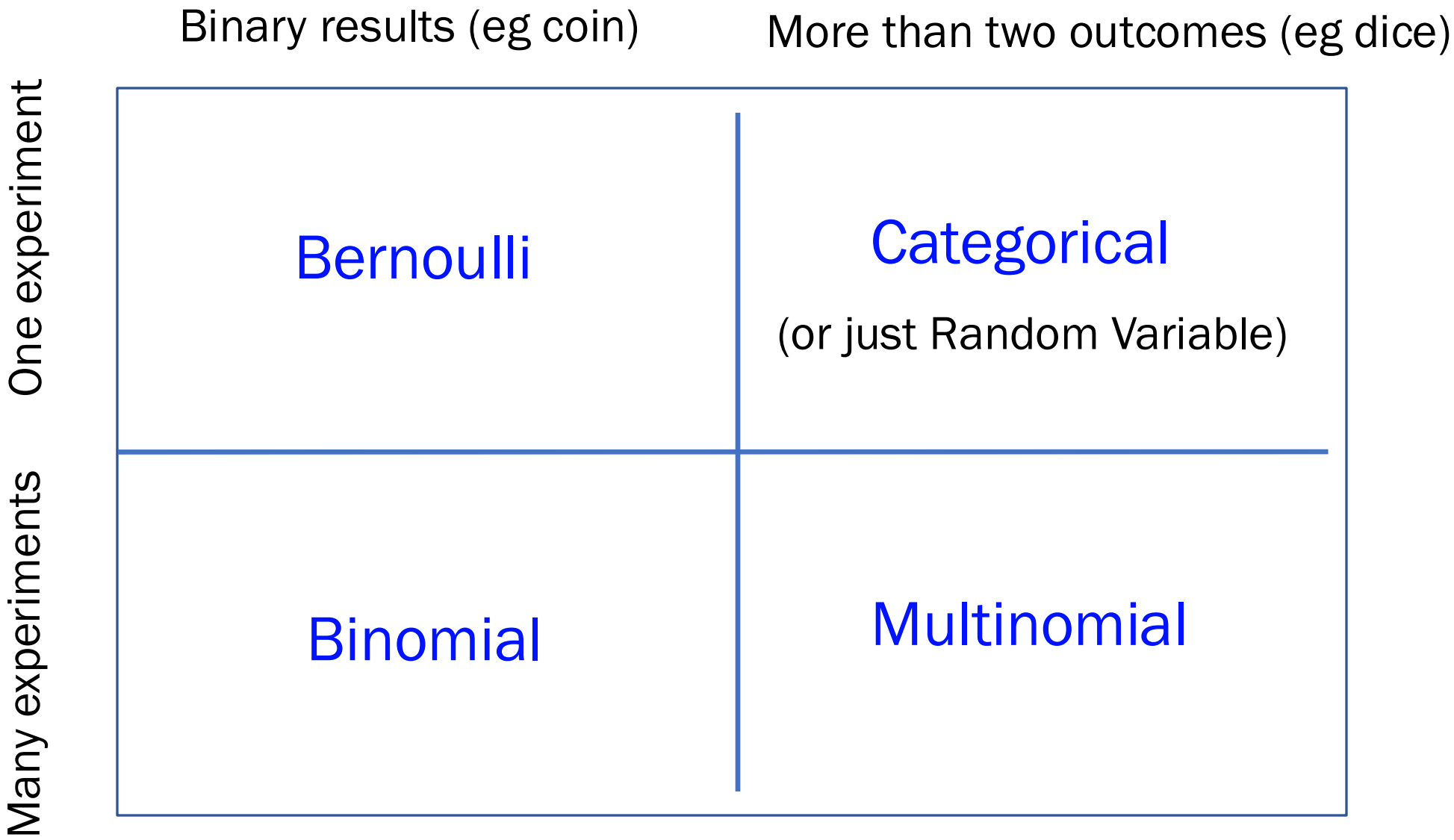
Multiple Outputs



The Categorical



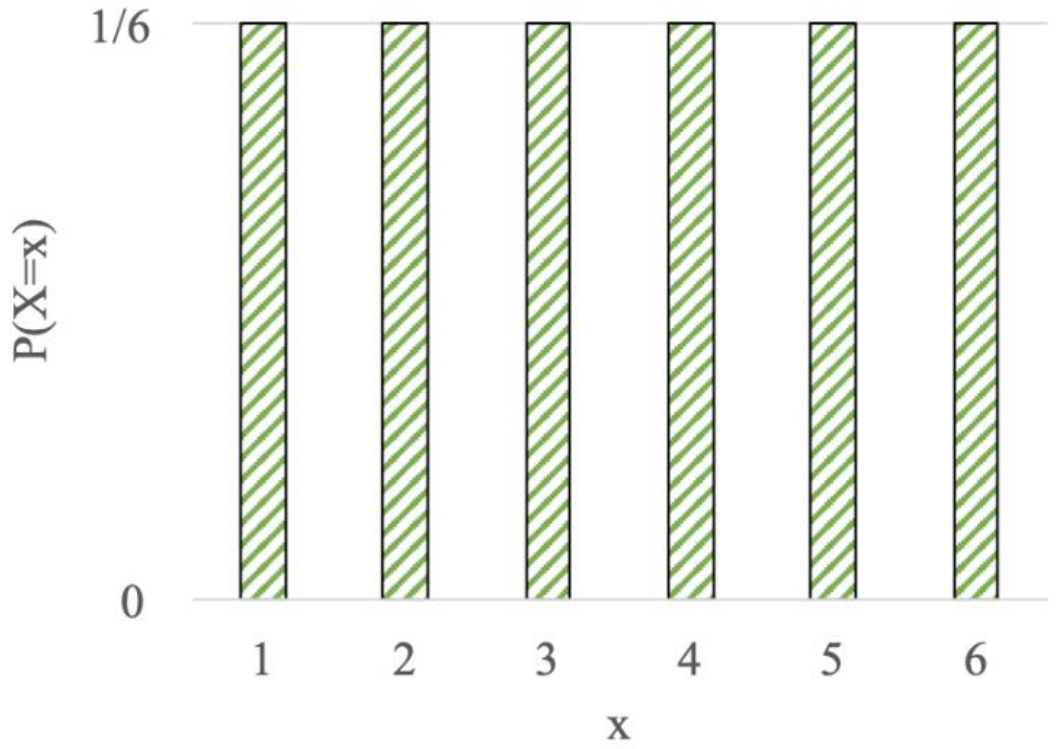
The Categorical



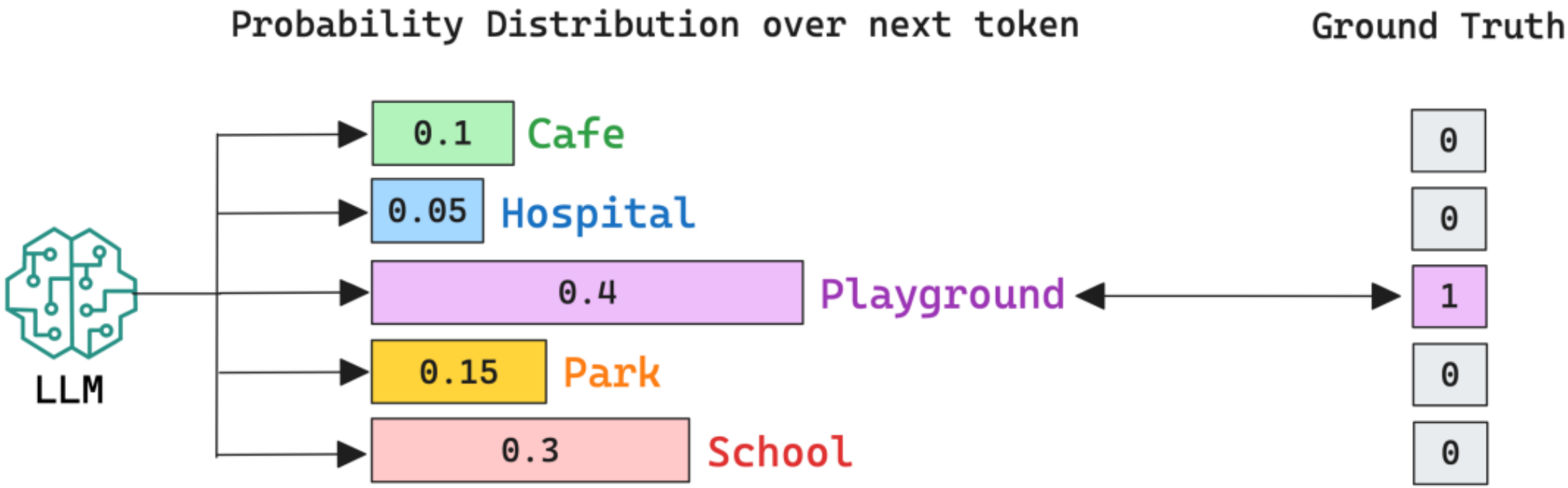
Categorial Example from Class: Thinking of an Animal

Notice that these are not numbers

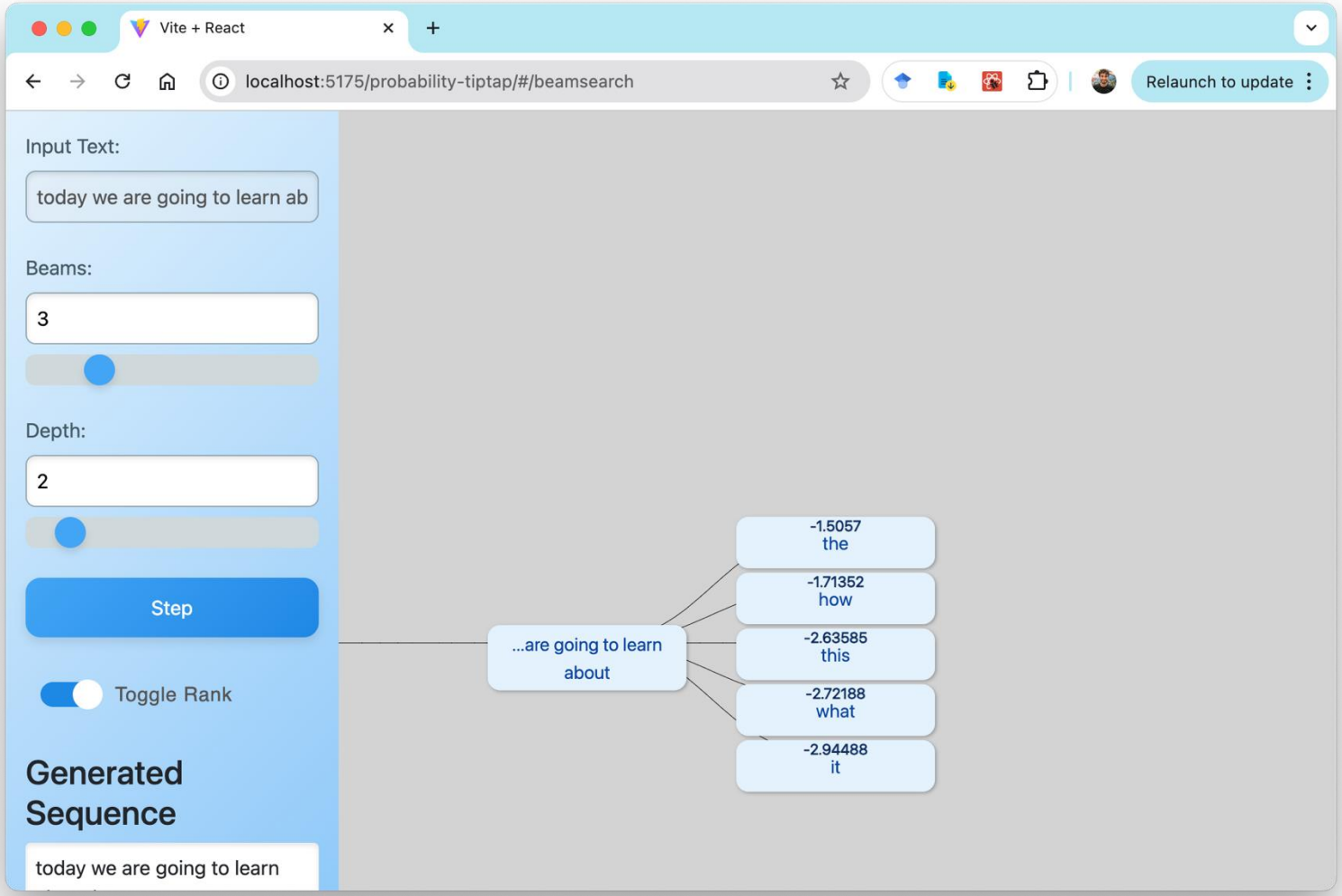
Categorial Example from Class: Single Dice Roll



Output of an LLM is a Categorical for Next Token

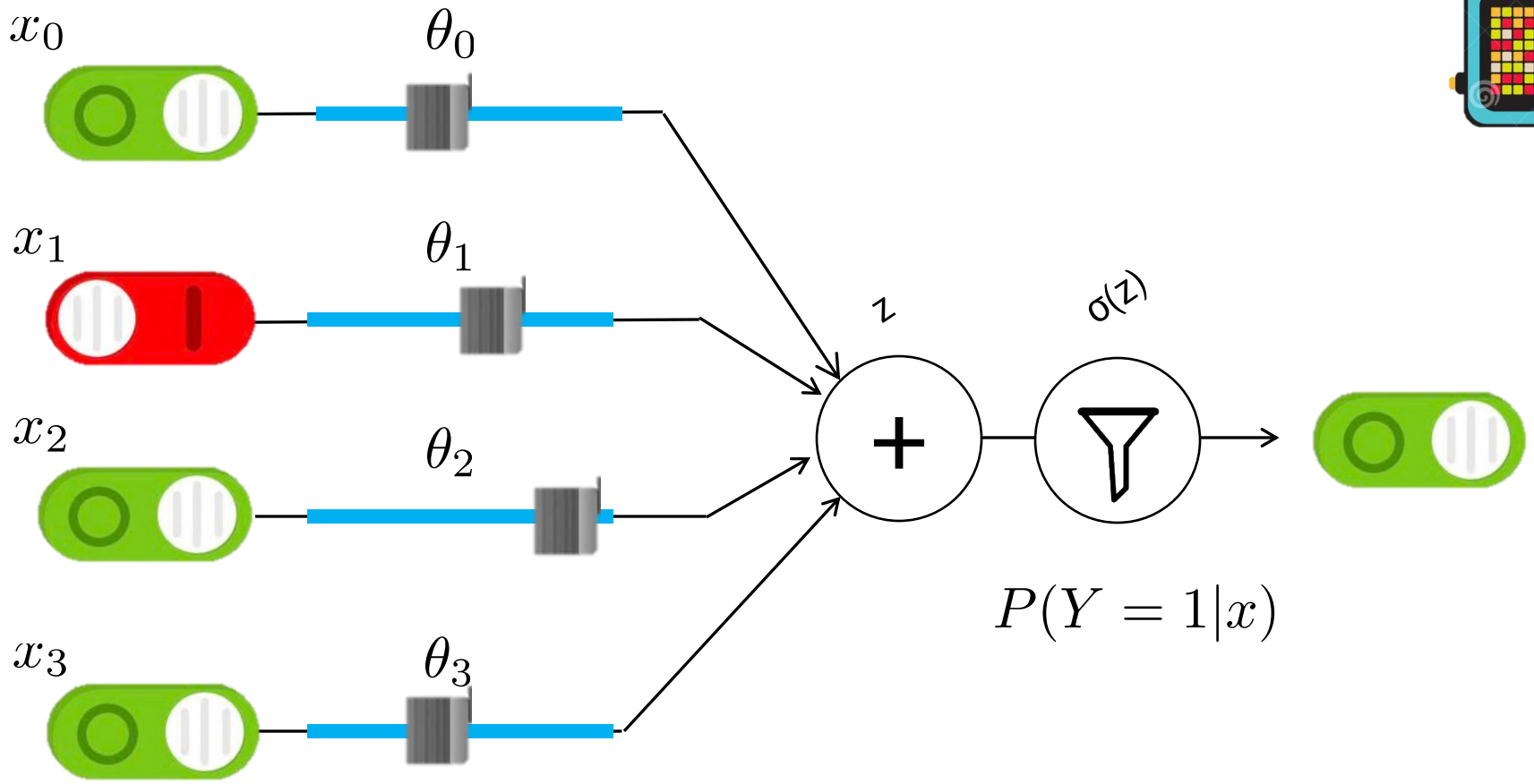


Output of an LLM is a Categorical for Next Token



Thanks to Justin Blumencranz and Adam Boswell

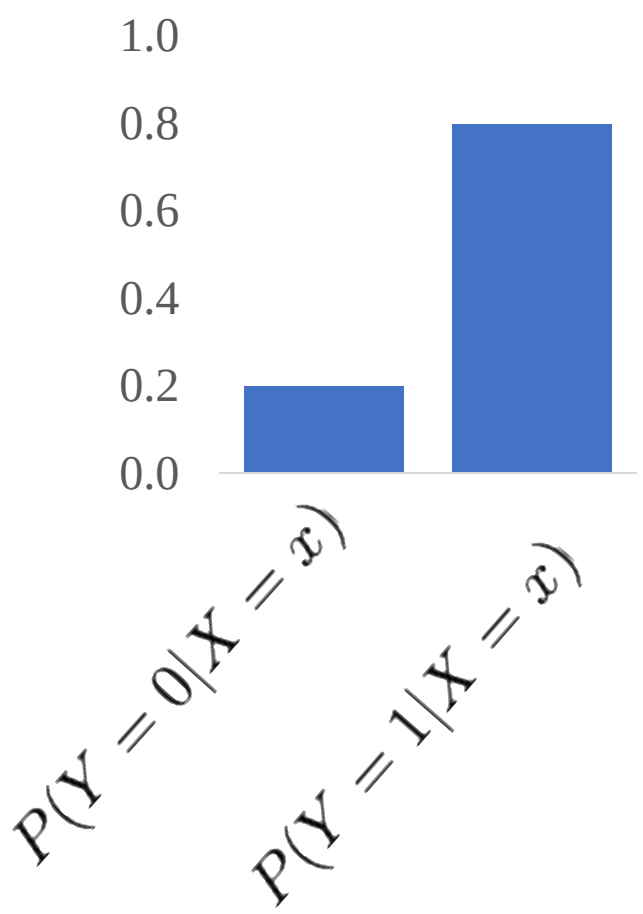
Logistic Regression to Predict a Categorical?



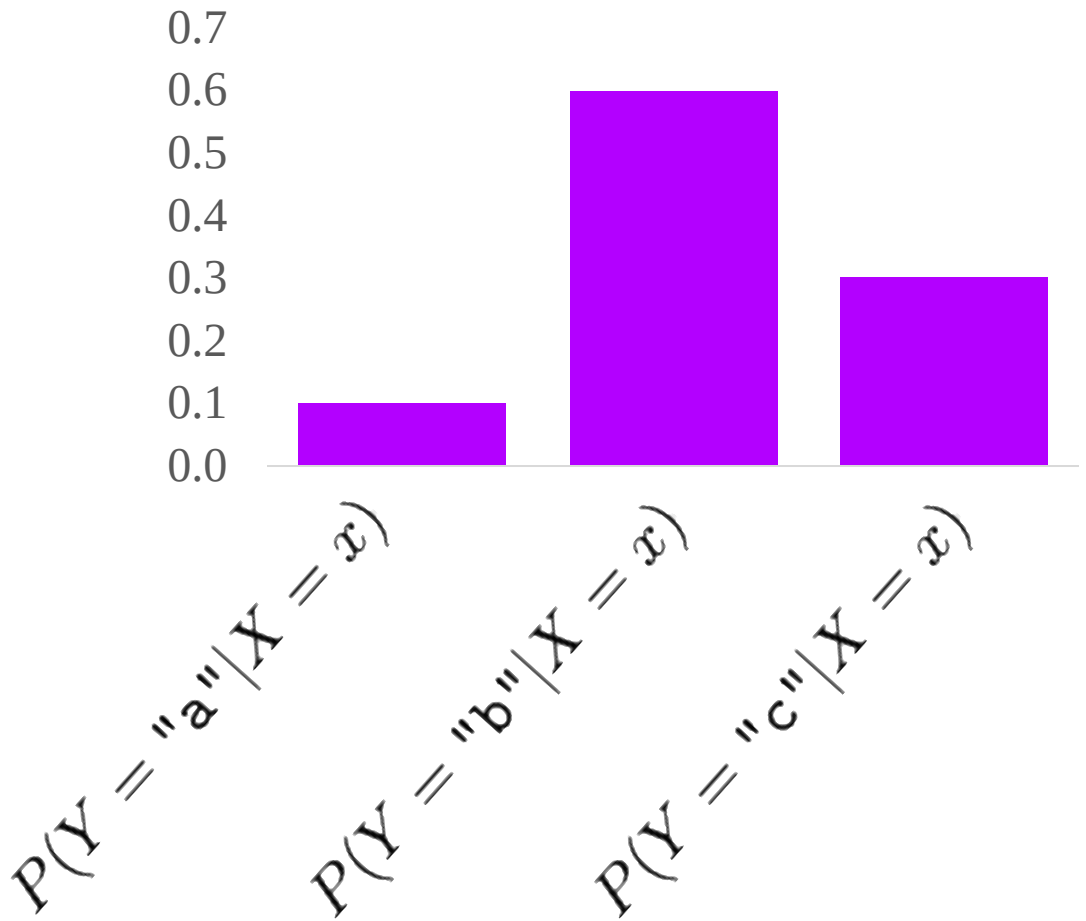
$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

Logistic Regression to Predict a Categorical?

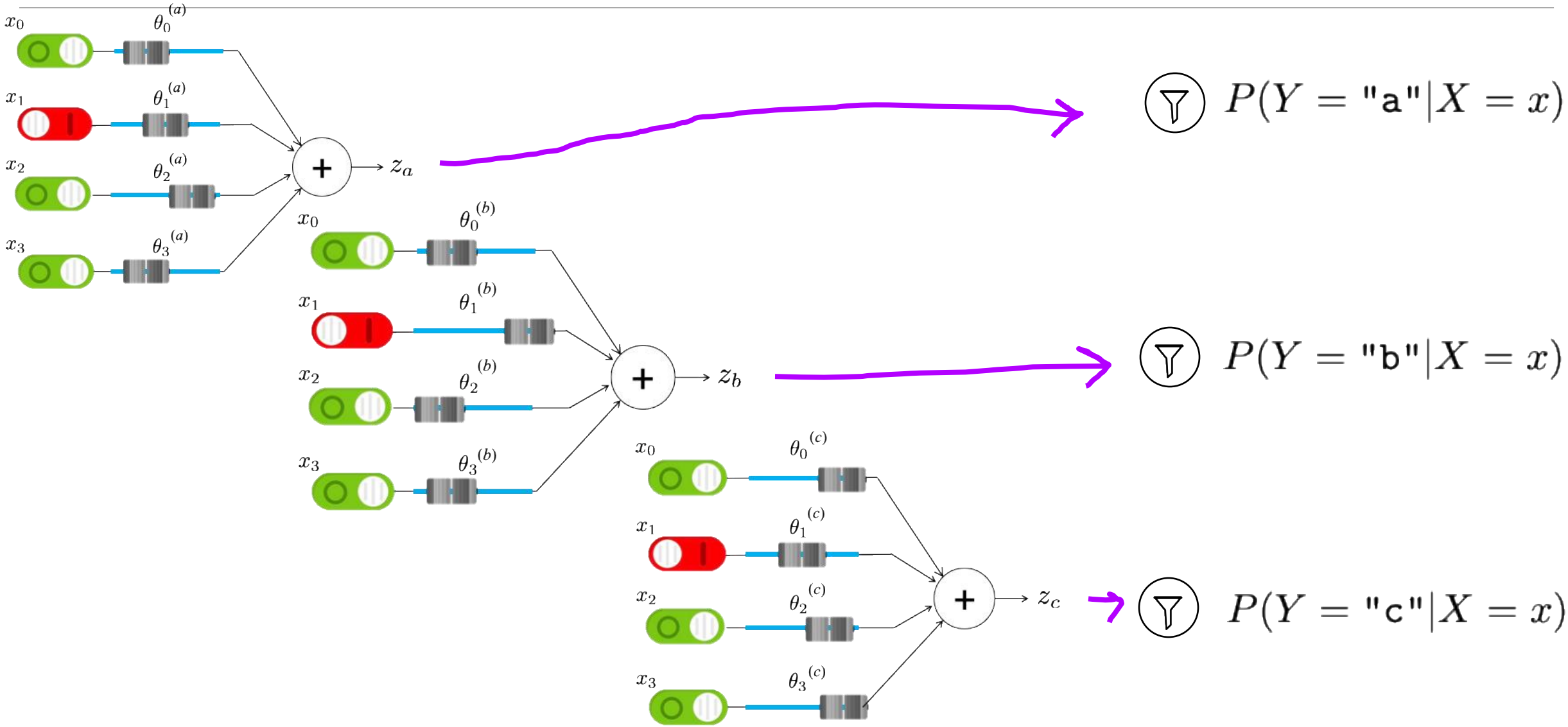
Standard Logistic Regression



Multi-Class Logistic Regression



Logistic Regression to Predict a Categorical



Categorical Classification?

Softmax is a generalization of the sigmoid function that squashes a K -dimensional vector $\mathbf{z}$ of arbitrary real values to a K-dimensional vector $\text{softmax}(\mathbf{z})$ of real values in the range [0, 1] that **add up to 1**.

$$P(Y = i|\mathbf{X} = \mathbf{x}) = \text{softmax}(\mathbf{z})_i$$

Sigmoid is to Bernoulli as Softmax is to Categorical

$$\text{softmax}(\mathbf{z})_i = \frac{\exp(z_i)}{\sum_{j=1}^{n} \exp(z_j)}$$

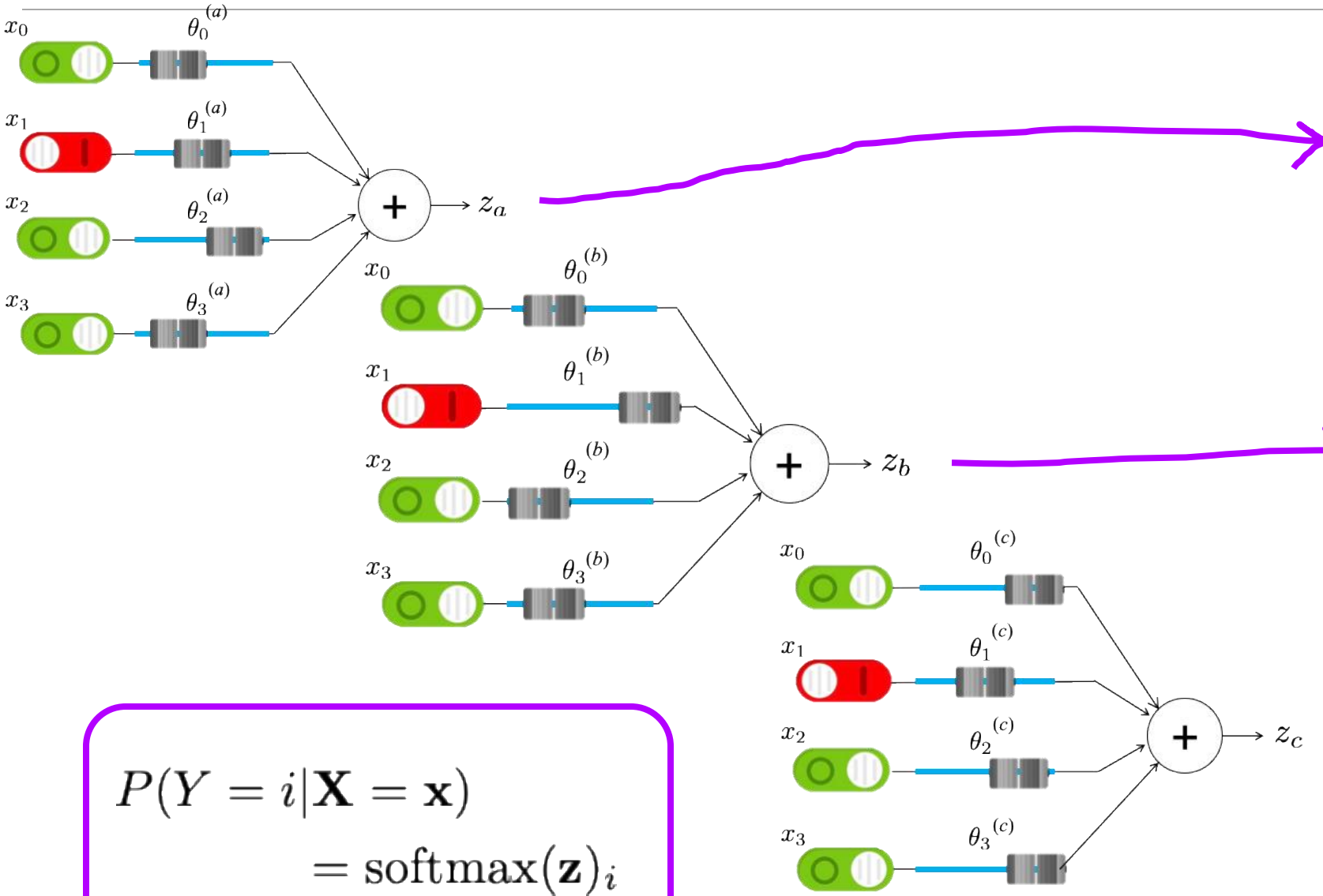
Understanding Softmax

```
 9  def softmax(list_values):
10      """
11      Compute the softmax of a list of numbers.
12      >>> softmax([1, 2, 3])
13      [0.09, 0.24, 0.67]
14      >>> softmax([5, 2, 8])
15      [0.02, 0.00, 0.98]
16      """
17
18      # take the exp of each value in the list
19      raw_exp_values = []
20      for value in list_values:
21          raw_exp_values.append(math.exp(value))
22
23      # normalize the list
24      sum_exp_values = sum(raw_exp_values)
25      softmax_values = []
26      for value in raw_exp_values:
27          softmax_values.append(value / sum_exp_values)
28
29      return softmax_values
```

List: 7 7 7 7
[0.25, 0.25, 0.25, 0.25]

List: 2 8 5 6
[0.0, 0.84, 0.04, 0.11]

What is Log Likelihood?



$$P(Y = \texttt{"a"} | X = x)$$

$$P(Y = \texttt{"b"} | X = x)$$

$$P(Y = \texttt{"c"} | X = x)$$

$$P(Y = i | \mathbf{X} = \mathbf{x}) = \text{softmax}(\mathbf{z})_i$$

What is Log Likelihood?

$$L(\theta) = \prod_i P(Y = y | X = x)$$

$$\begin{cases} P(Y = \text{'a'} | X = x) & \text{if truth is 'a'} \\ P(Y = \text{'b'} | X = x) & \text{if truth is 'b'} \\ P(Y = \text{'c'} | X = x) & \text{if truth is 'c'} \end{cases}$$

$$LL(\theta) = \sum_i \log P(Y = y | X = x)$$

$$= \sum_i \log \text{softmax}(\mathbf{z})_y$$

Types of Machine Learning Tasks

Muli-Class Classification

Regression

Reinforcement Learning

Generation

Regression: Predicting Real Numbers

	Opposing team ELO	Points in last game	...	At Home?	Output
					 # Points
Game 1	84	105		1	120
Game 2	90	102		0	95
		⋮			⋮
Game *n*	74	120		0	115

Same Notation for Training Data

Training Data: assignments all random variables **X** and Y

Assume IID data:

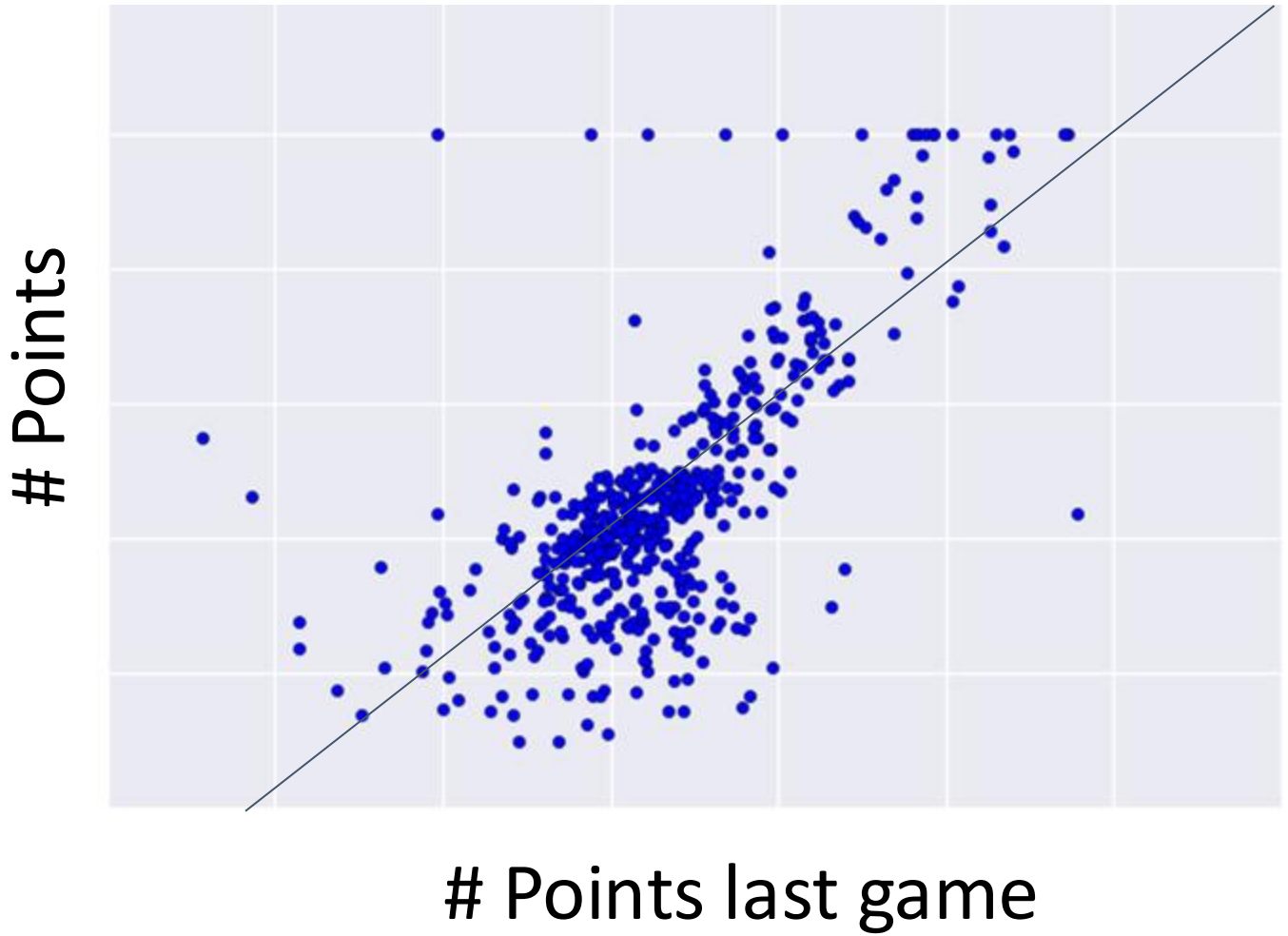
n training datapoints

$$(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots (\mathbf{x}^{(n)}, y^{(n)})$$

$$m = |\mathbf{x}^{(i)}|$$

Each datapoint has m features and a single output

Linear Regression with one Input



Linear Regression Model

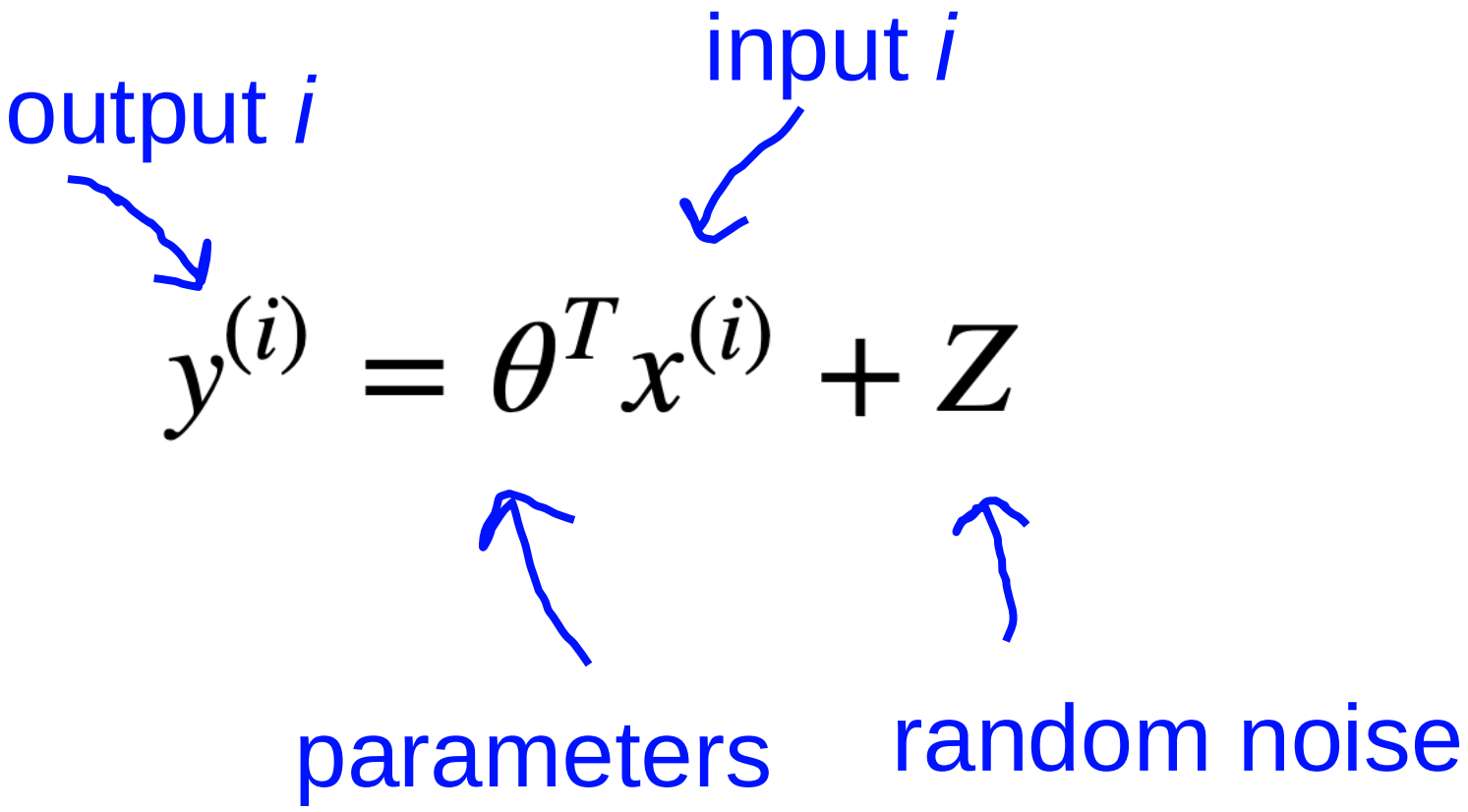
output *i*

input *i*

$$\hat{y}^{(i)} = \theta^T x^{(i)}$$

parameters

Linear Regression Model



Linear Regression Model

output *i*

input *i*

$$y^{(i)} = \theta^T x^{(i)} + Z$$

parameters

random noise

Noise is *N* with mean 0

$$Z \sim N(0, \sigma^2)$$

Linear Regression Model

output *i*

noise

$$y^{(i)} = \theta^T x^{(i)} + Z$$

noise is *N* with mean 0

$$Z \sim N(0, \sigma^2)$$

1. Linear Transform

If X is a Normal such that $X \sim N(\mu, \sigma^2)$ and Y is a linear transform of X such that $Y = aX + b$ then Y is also a Normal where:

$$Y \sim N(a\mu + b, a^2\sigma^2)$$

Linear Regression Model

output *i*

noise

$$y^{(i)} = \theta^T x^{(i)} + Z$$

noise is *N* with mean 0

$$Z \sim N(0, \sigma^2)$$

Output is normal too:

$$y^{(i)} \sim N(\theta^T x^{(i)}, \sigma^2)$$

Log Likelihood

$$y^{(i)} = \theta^T x^{(i)} + Z \qquad Z \sim N(0, \sigma^2)$$

Assume: $y^{(i)} \sim N(\theta^T x^{(i)}, \sigma^2)$

Data: $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots (\mathbf{x}^{(n)}, y^{(n)})$

$$LL(\theta) = \sum_{i=1}^{n} \log \left[f(y^{(i)}) \right]$$

$$= \sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y^{(i)}-\mu}{\sigma}\right)^2} \right]$$

Normal distribution PDF

$$= \sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y^{(i)}-\theta^T x^{(i)}}{\sigma}\right)^2} \right]$$

Substitute in the mean

$$= \sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} \right] - \frac{1}{2} \left(\frac{y^{(i)} - \theta^T x^{(i)}}{\sigma} \right)^2$$

Apply the log

Optimization

$$y^{(i)} = \theta^T x^{(i)} + Z \qquad Z \sim N(0, \sigma^2)$$

Log likelihood: $$LL(\theta) = \sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} \right] - \frac{1}{2} \left(\frac{y^{(i)} - \theta^T x^{(i)}}{\sigma} \right)^2$$

$$\begin{aligned}
\underset{\theta}{\text{argmax}}\, LL(\theta) &= \underset{\theta}{\text{argmax}} \sum_{i=1}^{n} \log \left[\frac{1}{\sigma\sqrt{2\pi}} \right] - \frac{1}{2} \left(\frac{y^{(i)} - \theta^T x^{(i)}}{\sigma} \right)^2 \\
&= \underset{\theta}{\text{argmax}} - \sum_{i=1}^{n} \frac{1}{2} \left(\frac{y^{(i)} - \theta^T x^{(i)}}{\sigma} \right)^2 \qquad \text{Simplify} \\
&= \underset{\theta}{\text{argmax}} - \sum_{i=1}^{n} \left(y^{(i)} - \theta^T x^{(i)} \right)^2 \qquad \text{Simplify}
\end{aligned}$$

Hey it's the sum of squared errors!

Derivative is Necessary for Gradient Ascent

$$\frac{\partial LL(\theta)}{\partial \theta_j} = -\sum_{i=1}^{n} \frac{\partial}{\partial \theta_j} \left(y^{(i)} - \theta^T x^{(i)} \right)^2$$

Derivative of a sum

$$= -\sum_{i=1}^{n} 2\left(y^{(i)} - \theta^T x^{(i)} \right)(-x_j^{(i)})$$

Chain rule

$$= \sum_{i=1}^{n} 2\left(y^{(i)} - \theta^T x^{(i)} \right) \cdot x_j^{(i)}$$

Simplify

Linear Regression with one Input

Types of Machine Learning Tasks

Muli-Class Classification

Regression

Reinforcement Learning

Generation

Types of Machine Learning Tasks

Muli-Class Classification

Regression

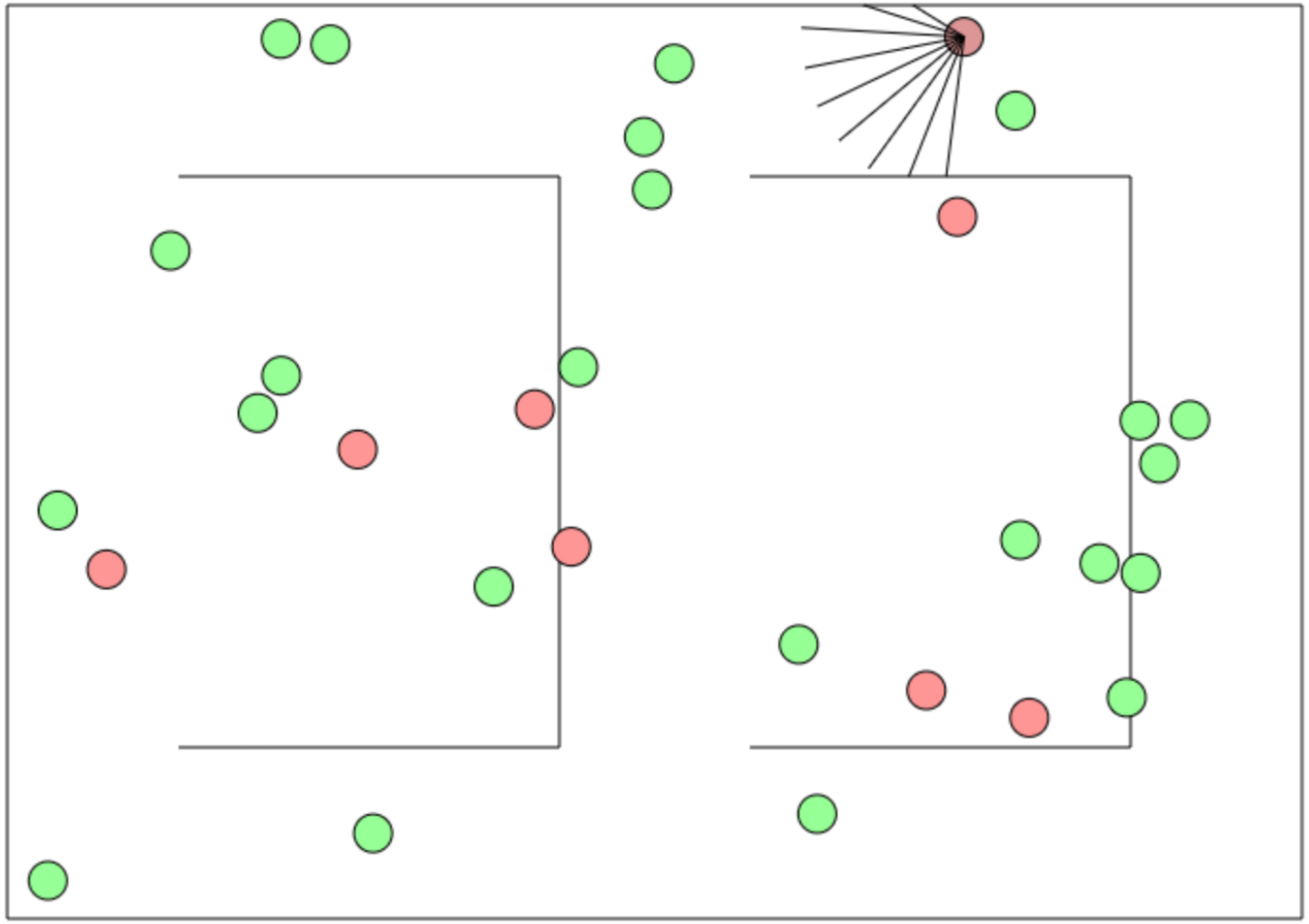
Reinforcement Learning

Generation

Making Decisions?

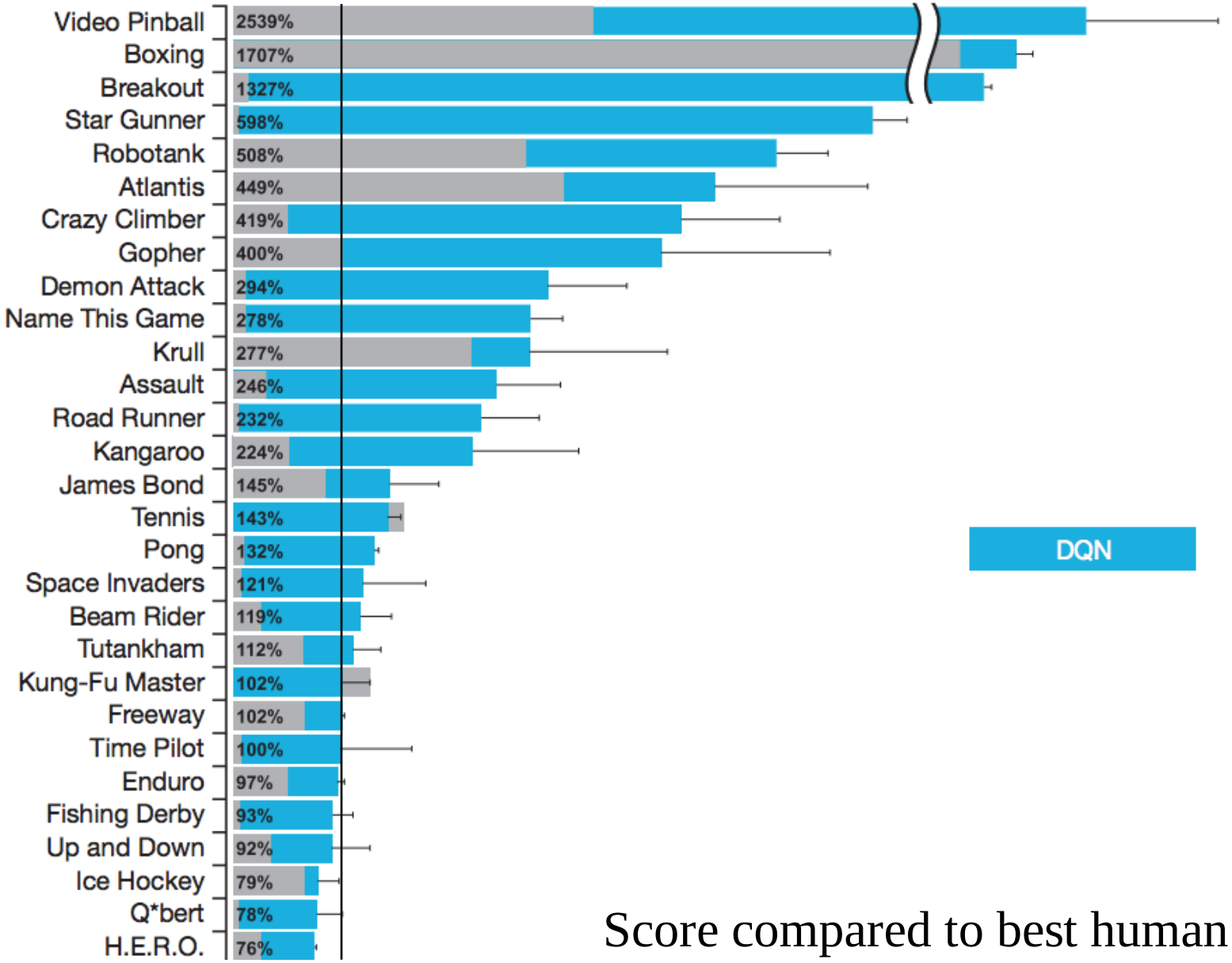
Deep Reinforcement Learning
Instead of having the output of a model be a probability you can make it an expectation.

Deep Reinforcement Learning



http://cs.stanford.edu/people/karpathy/convnetjs/demo/rldemo.html

Deep Mind Atari Games



Score compared to best human

It is time for Deep Learning!