



Parameter Estimation

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MACHINE LEARNING



<Review>

General “Inference”



General “Inference”

WebMD Symptom Checker BETA

INFO

SYMPOMS

QUESTIONS

CONDITIONS

DETAILS

TREATMENT

Add more symptoms

Type your main symptom here

AGE 30

GENDER Male

MY SYMPTOMS

cough ×

throat irritation ×

sneezing ×

or Choose common symptoms

bloating

cough

diarrhea

dizziness

fatigue

fever

headache

muscle cramp

nausea

throat irritation

Results Strength: MODERATE



Previous

Info

Continue



Conditions that match your symptoms

UNDERSTANDING YOUR RESULTS

Influenza (flu) adults



 Moderate match

Pneumococcal infections



 Moderate match

H1N1 Flu Virus (Swine Flu)



 Moderate match

Bacterial Pneumonia



 Moderate match

Sepsis (blood infection)



 Moderate match

Gender Male

Age 30

Edit

My Symptoms

Edit

fever 103f to 104f, dizziness,

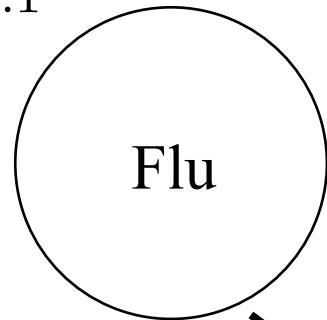
throat irritation, migraine headache



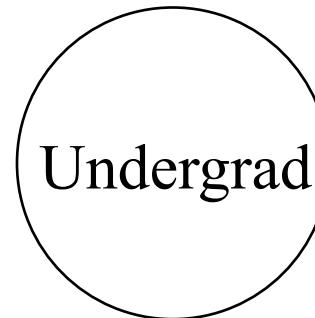
Start Over

Probabilistic Model

$$P(Fl = 1) = 0.1$$



$$P(U = 1) = 0.8$$



$$Fev|Flu = 0 \sim N(100.0, 1.81)$$

$$Fev|Flu = 1 \sim N(98.25, 0.73)$$



$$P(T = 1|Flu = 0, U = 0) = 0.1$$

$$P(T = 1|Flu = 0, U = 1) = 0.8$$

$$P(T = 1|Flu = 1, U = 0) = 0.9$$

$$P(T = 1|Flu = 1, U = 1) = 1.0$$



If you know the probability of each random variables given the ones that directly cause it, you can joint sample!

Alg #1: Joint Sampling

```
3 N_SAMPLES = 100000
4
5 # Program: Joint Sa
6 #
7 # we can answer any
8 # with multivariate
9 # where conditioned
10 def main():
11     obs = getObservation()
12     print 'Observation =', obs
13
14     samples = sample(N_SAMPLES)
15     prob = probFluGivenSamples(samples, obs)
16     print 'Pr(Flu | Obs) =', prob
```

[0, 0, 0, 0]
[0, 1, 0, 1]
[1, 0, 1, 0]
[1, 1, 1, 1]
[0, 1, 0, 1]
[0, 1, 0, 0]
[0, 0, 0, 0]
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[1, 1, 1, 1]
[0, 0, 0, 0]
[0, 0, 0, 0]
[1, 1, 1, 1]
[0, 1, 0, 0]
Observation = [None, None, None, 1]
Pr(Flu | Obs) = 0.140635888502
>

Each one of
these is one
posterior
sample:

[Flu, Ugrad, Fever, Tired]

Alg #2: MCMC

```
webkit -- bash -- 10x20
[1, 1, 101.0, 1]
[1, 1, 101.0, 1]
[0, 1, 101.0, 0]
[0, 0, 101.0, 0]
[1, 0, 101.0, 1]
[1, 0, 101.0, 0]
[1, 0, 101.0, 1]
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[1, 1, 101.0, 1]
[1, 0, 101.0, 1]
[1, 1, 101.0, 1]
[1, 1, 101.0, 1]
Pr(Flu) = 0.9773
>
```

MCMC is a way to sample
with conditioned variables
fixed

Each one of
these is one
posterior
sample:

[Flu, Undergrad, Fever, Tired]



</ Review>

BAE's Theorem?

$$P(A \mid B E) = \frac{P(\textcolor{blue}{B} \mid A E) P(A \mid E)}{P(B \mid E)}$$



Alg #3: Straight Math

Know: $P(\text{symptom} \mid \text{flu, undergrad})$ $P(\text{flu})$ $P(\text{undergrad})$

Flu is independent of undergrad

Tired and fever are conditionally independent given flu, undergrad

$$\begin{aligned} & P(F = 1 \mid \text{all other rvs}) \\ &= P(F = 1 \mid \text{symptoms}, U = u) \\ &= \frac{P(\text{symptoms} \mid F = 1, U = u)P(F = 1 \mid U = u)}{P(\text{symptoms} \mid U = u)} \\ &\propto P(\text{symptoms} \mid F = 1, U = u)P(F = 1 \mid U = u) \\ &\propto P(F = 1)P(\text{symptoms} \mid F = 1, U = u) \\ &\propto P(F = 1) \prod_i P(\text{symptom}_i \mid F = 1, U = u) \end{aligned}$$

$P(F = 1 \mid \text{all other rvs})$

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$$P(F = 1 | \text{all other rvs}) \propto P(F = 1) \prod_i P(\text{symptom}_i | F = 1, U = u)$$

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121     f1 = getFluPr1(sample)
122     f0 = getFluPr0(sample)
123     p1 = f1 / (f1 + f0)
124     return bern(p1)
125
126 def getFluPr0(sample):
127     _, und, fev, tir = sample
128     pFlu0 = 0.9
129     pFev = getPrFeverX(fev, flu=0)
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See you soon!

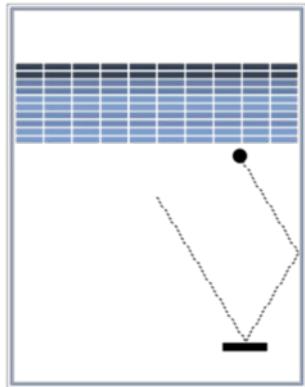
Summary

General Inference Summary



- **Straight Math** is fast, but can be prohibitively hard for complex models (see hw).
- **Joint Sampling** is really easy to program but fails for continuous variables (and when what you are conditioning on is rare)
- **MCMC** works well when conditioning on rare events, but is *much* harder to code / derive.
- All sampling is **slow**.

Insight



Let x be a student's program

Let y be student mistakes

Label Console

✓ Num Done: 8273

Strategy

- Beeper Boundary (most people do this)
- Triangle Strategy
- Recursive Strategy

Looping

- Correct use of looping
- Doesn't use a while
- Doesn't have correct stop condition
- Body is missing statements
- Body has extra statements
- Body order is incorrect
- Sets up initial precondition
- Does not get nesting
- Loop post condition doesn't match precondition
- Repetition of bodies

Feedback task:

$$P(y|x)$$

Hard for humans
Hard for computers

Joint sample:

$$(\hat{x}, \hat{y}) \sim P(x, y)$$

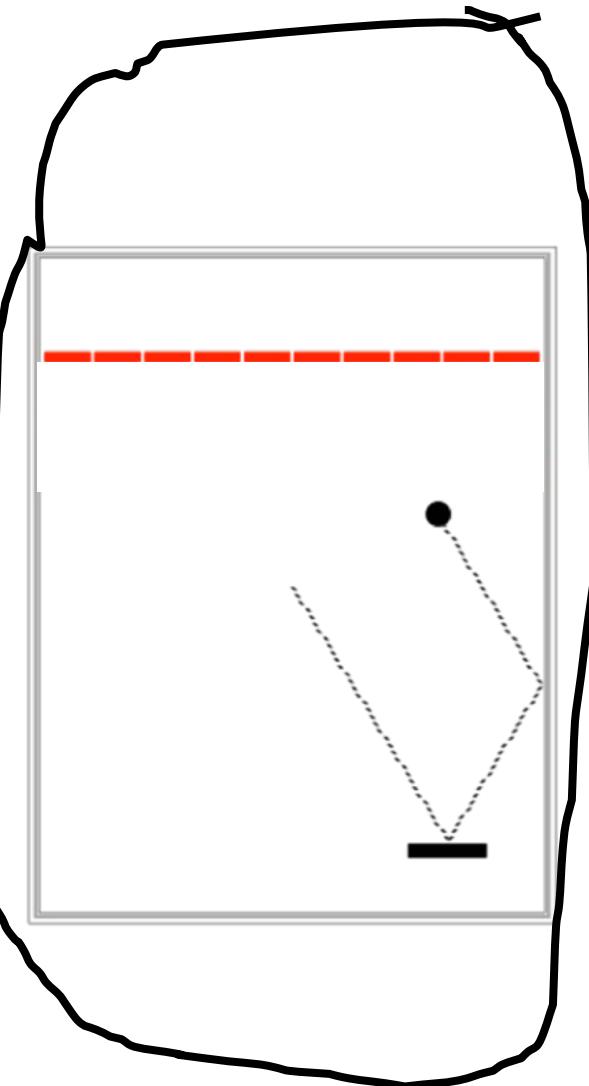
Easy for humans



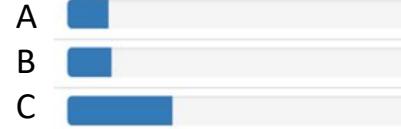
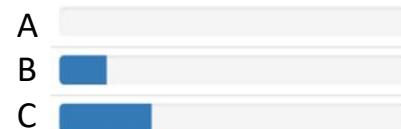
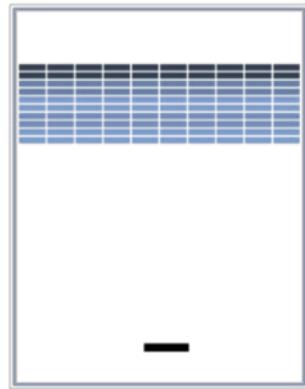
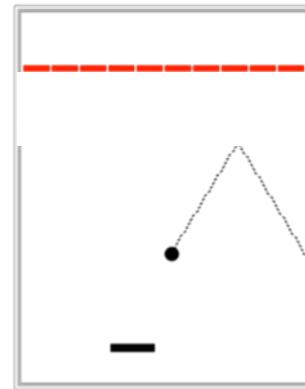
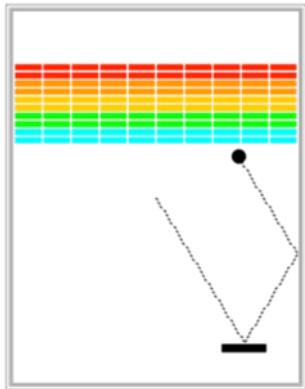
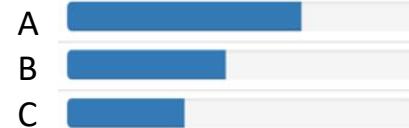
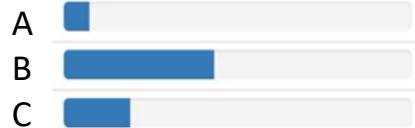
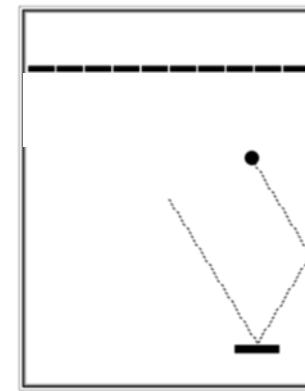
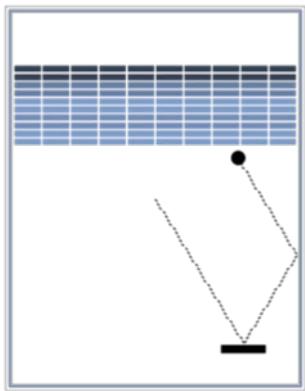
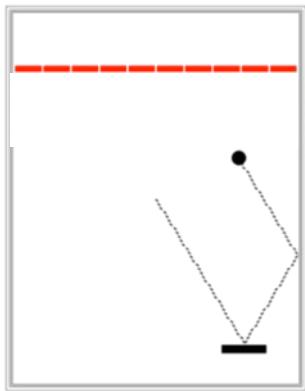
Imagine Students

$$(\hat{x}, \hat{y}) \sim P(x, y)$$

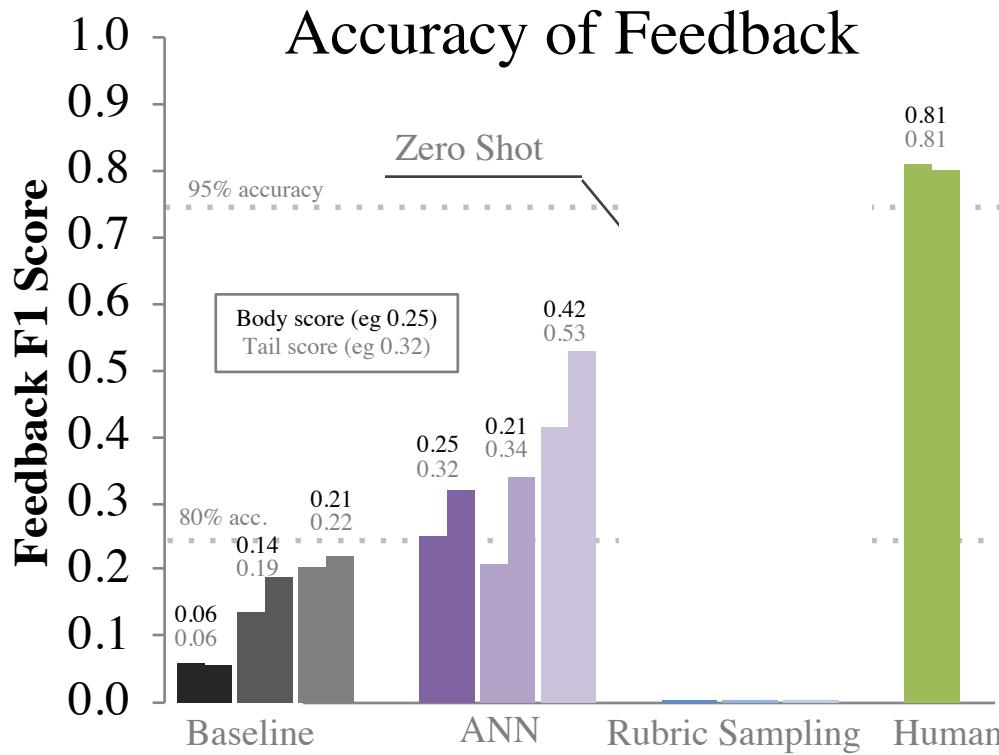
- Struggle with double for loops
- Confuses logic for deleting bricks



Start Imagining Students



Zero Shot Learning



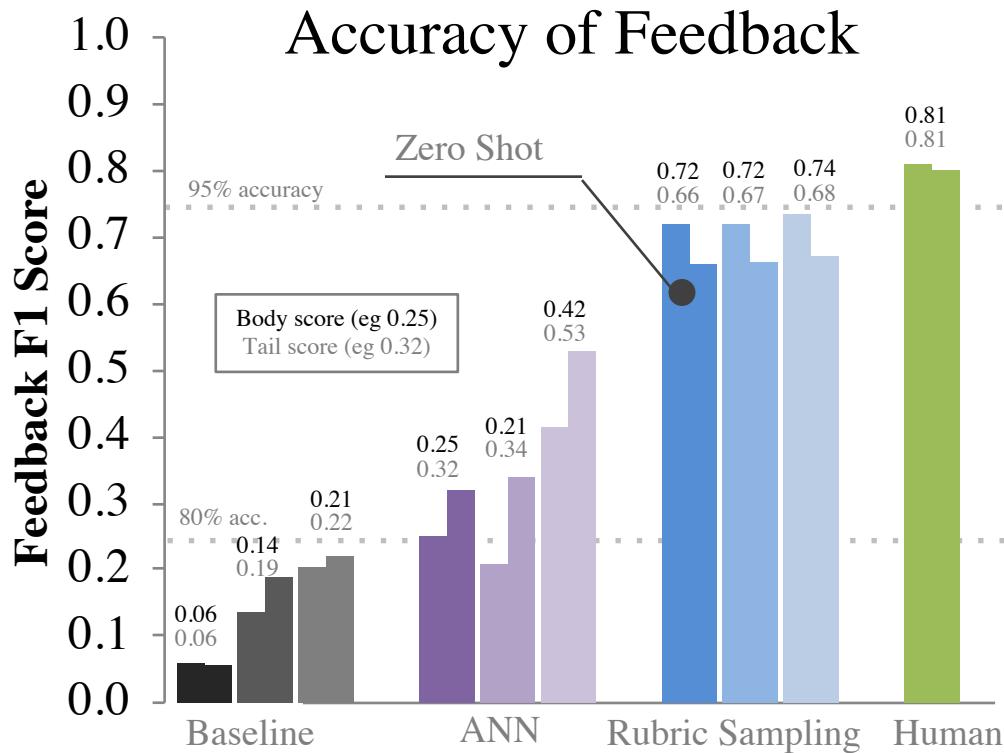
- Majority Vote
- Syntactic Analysis
- Program Output *

- FNN
- RNN
- MVAE

Expert Human



Zero Shot Learning



■ Majority Vote
■ Syntactic Analysis
■ Program Output *

■ FNN
■ RNN
■ MVAE
■ Rubric Sampling, Zero shot
■ Rubric Sampling, Learned θ
■ Rubric Sampling, MVAE

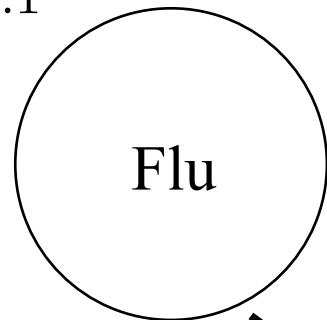
■ Expert Human

Model	Amount of Correct Feedback
Predicting from output	1,483,157 (86.0%)
Rubric sampling with MVAE	1,610,020 (93.7%)
Expert human	1,658,162 (96.2%)

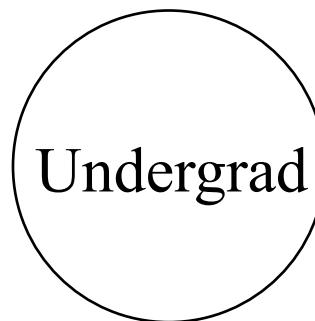


Where Do The Numbers Come From?

$$P(Fl = 1) = 0.1$$

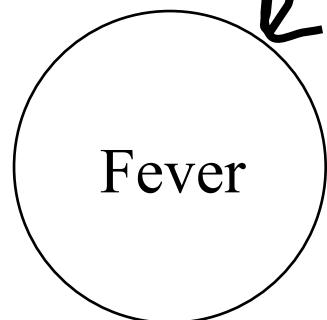


$$P(U = 1) = 0.8$$



$$Fev|Flu = 0 \sim N(100.0, 1.81)$$

$$Fev|Flu = 1 \sim N(98.25, 0.73)$$



$$P(T = 1|Flu = 0, U = 0) = 0.1$$

$$P(T = 1|Flu = 0, U = 1) = 0.8$$

$$P(T = 1|Flu = 1, U = 0) = 0.9$$

$$P(T = 1|Flu = 1, U = 1) = 1.0$$

Pedagogical Pause

At this point, if you are given a *model*,
with all the involved probabilities, you
can make predictions

But what if you want to *learn* the probabilities in the model?

But what if you want to *learn* the probabilities in the model?

Oh can we also learn the *structure* of the model too?

But what if you want to *learn* the probabilities in the model?

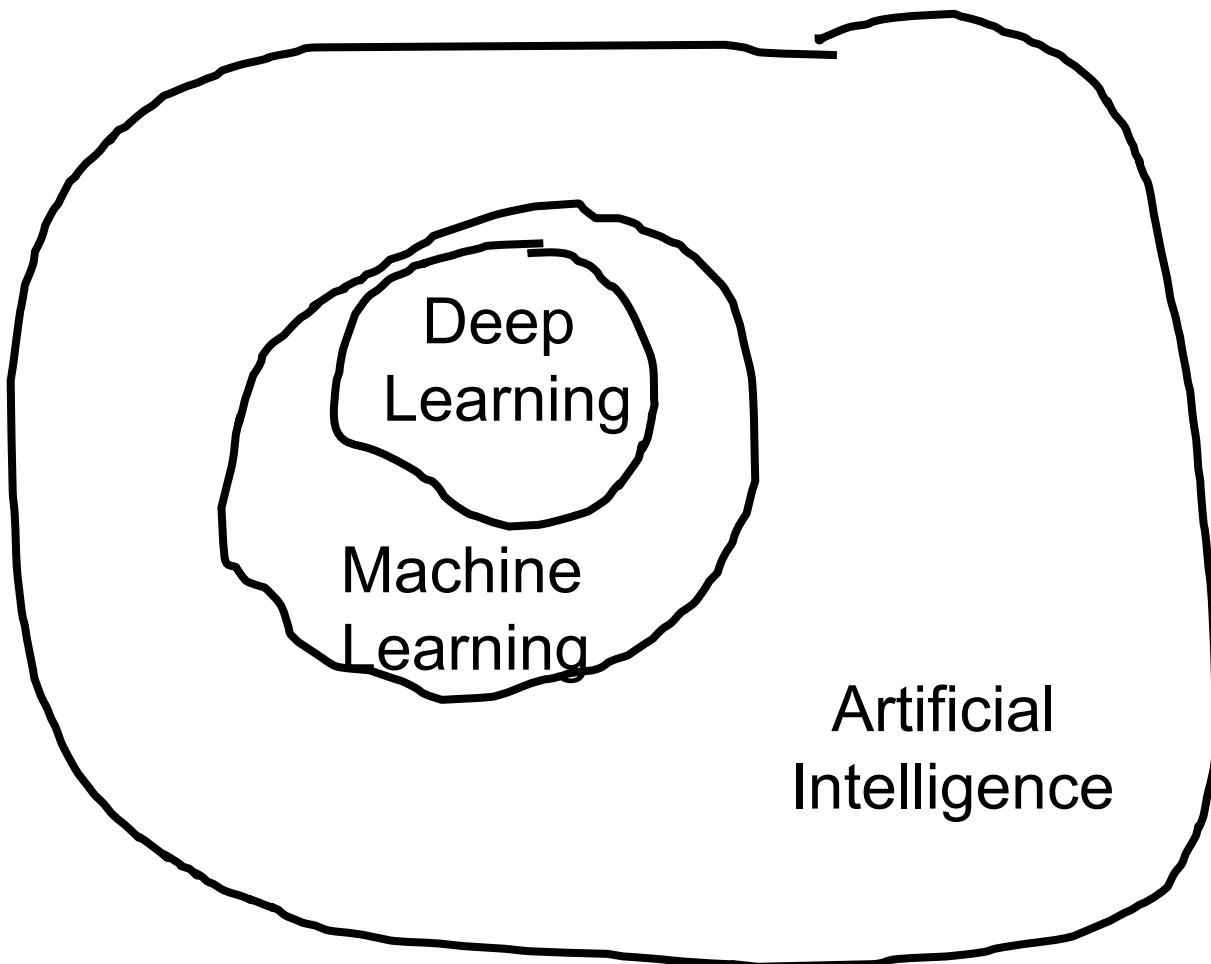
~~Oh can we also learn the *structure* of
the model too?~~

I wish. Another day ☺

But what if you want to *learn* the probabilities in the model?

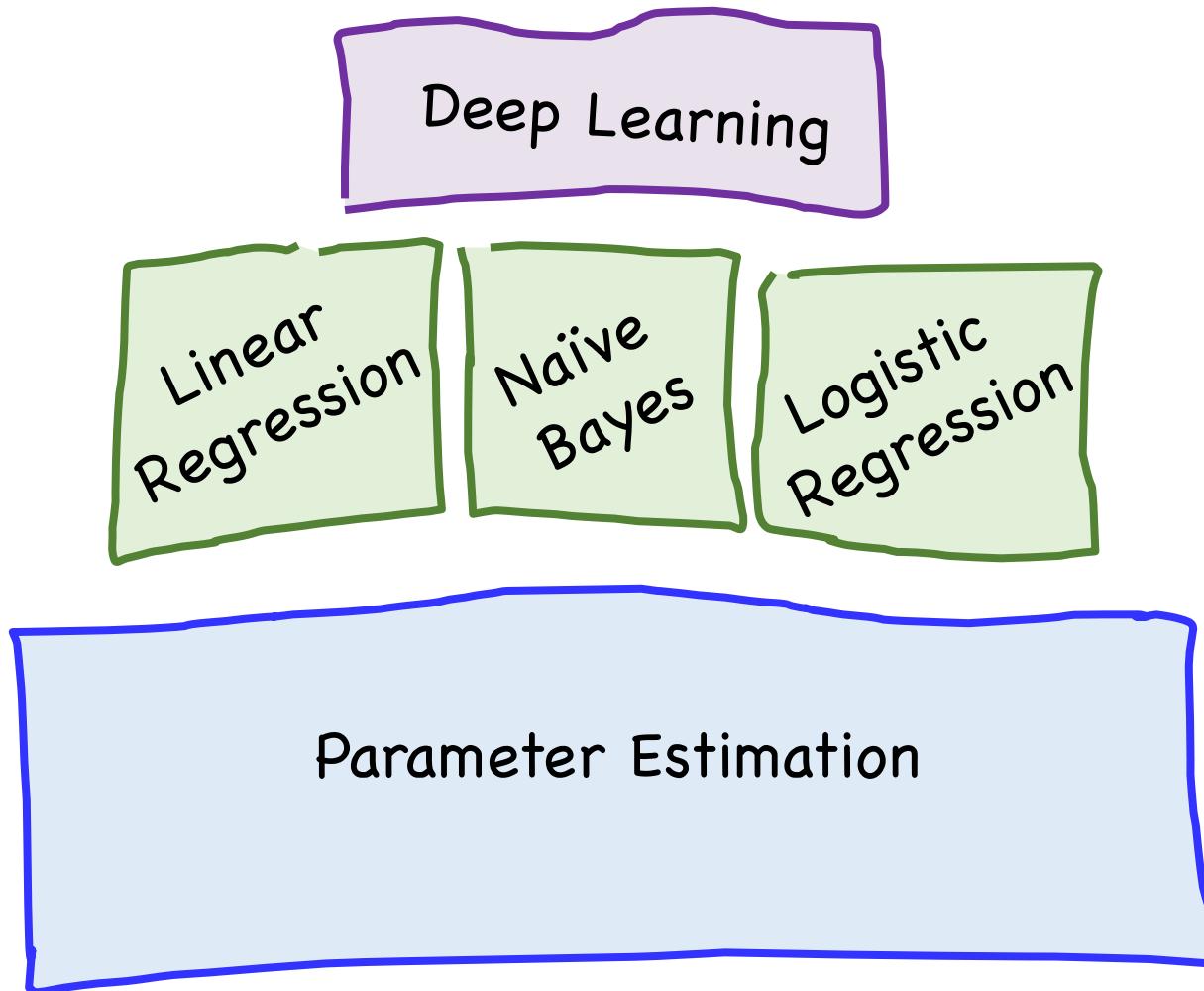
Machine Learning

AI and Machine Learning

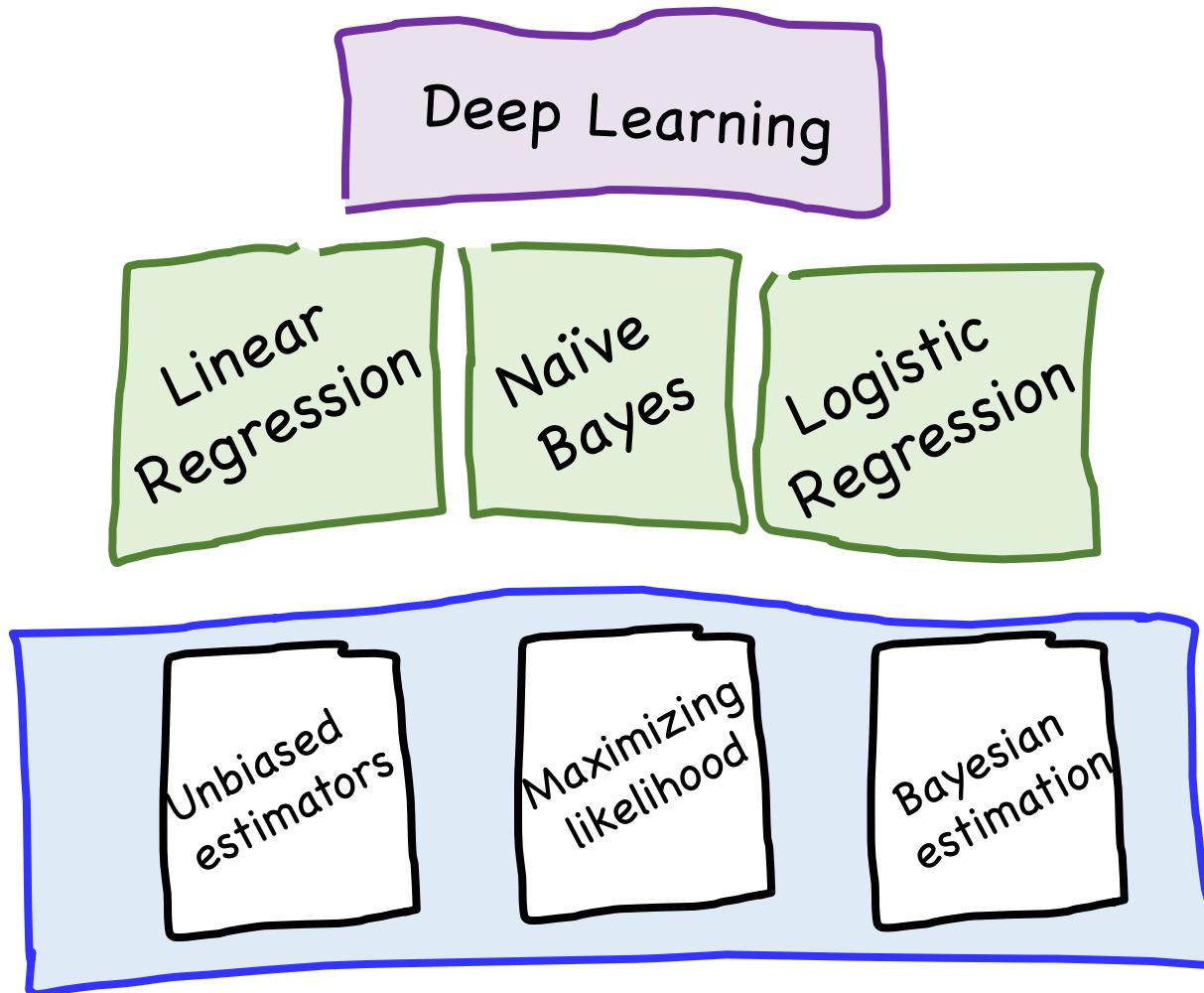


ML: Rooted in probability theory

Our Path



Our Path



Jump Straight to Deep Learning?

Tensor Flow



Jump Straight to Deep Learning?



Understand the theory to help you debug

But another reason...

Machine Learning Uses a Lot of Data



One Shot Learning

Single training example:

କୁ

Test set:

ଏ	ଶ	ଅ	ଶ
କୁ	ଅ	ପ୍ର	କୁ
ମ	ବୁ	ଇ	ବୁ
ମ	ଅ	କୁ	ମୁ

One Shot Learning

Single
training
example:



Computers struggle...

... especially for **human** problems.

Understand the theory
to push on the **grand challenges**

A silhouette of the iconic Disney castle is positioned behind the text, its spires and towers reaching towards the top of the frame.

WALT DISNEY
PICTURES



Once upon a time...

...there was parameter estimation

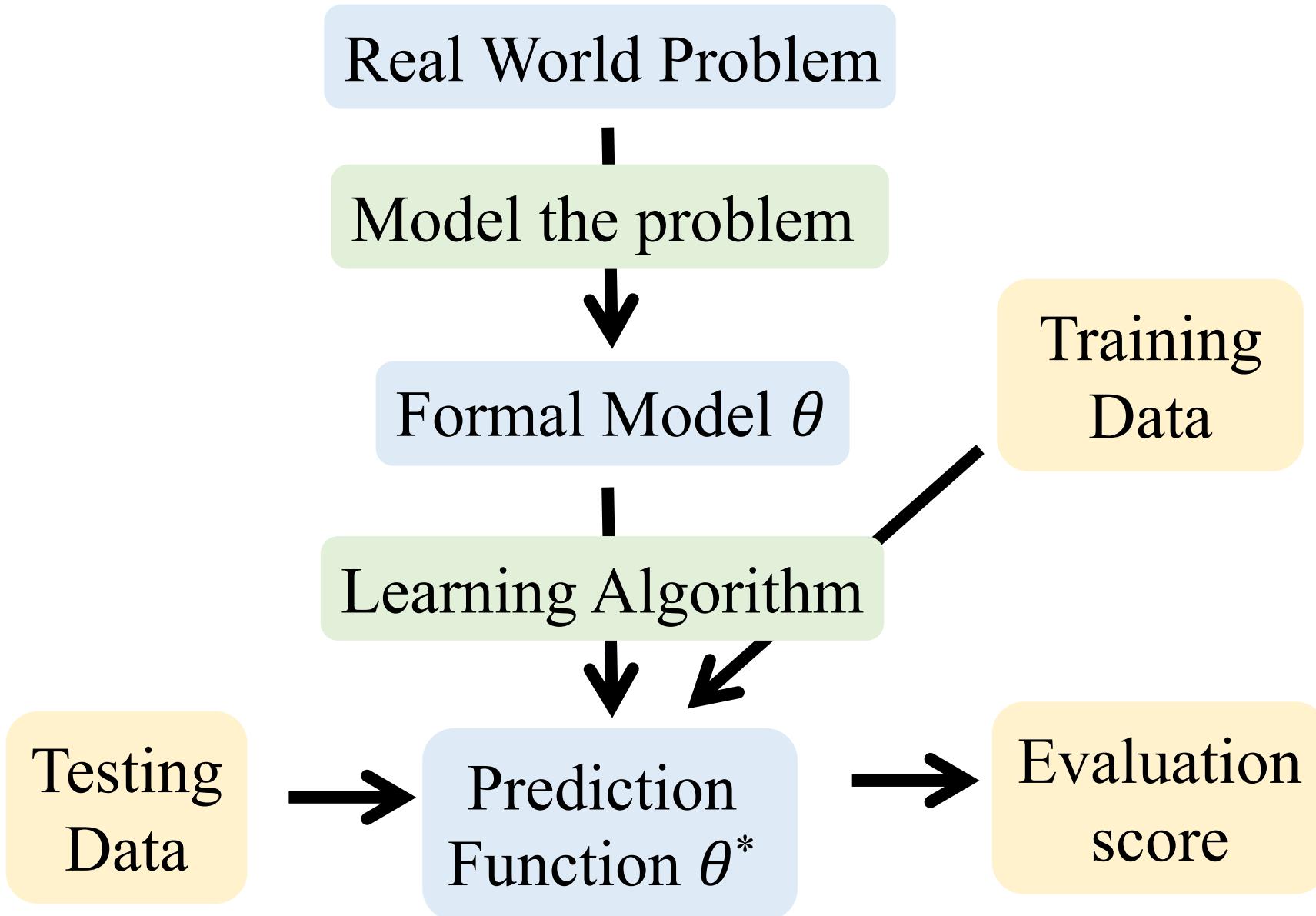
What are Parameters?

- Consider some probability distributions:
 - $\text{Ber}(p)$ $\theta = p$
 - $\text{Poi}(\lambda)$ $\theta = \lambda$
 - $\text{Uni}(\alpha, \beta)$ $\theta = (\alpha, \beta)$
 - $\text{Normal}(\mu, \sigma^2)$ $\theta = (\mu, \sigma^2)$
 - $Y = mX + b$ $\theta = (m, b)$
 - etc...
- Call these “parametric models”
- Given model, **parameters** yield actual distribution
 - Usually refer to parameters of distribution as θ
 - Note that θ that can be a vector of parameters

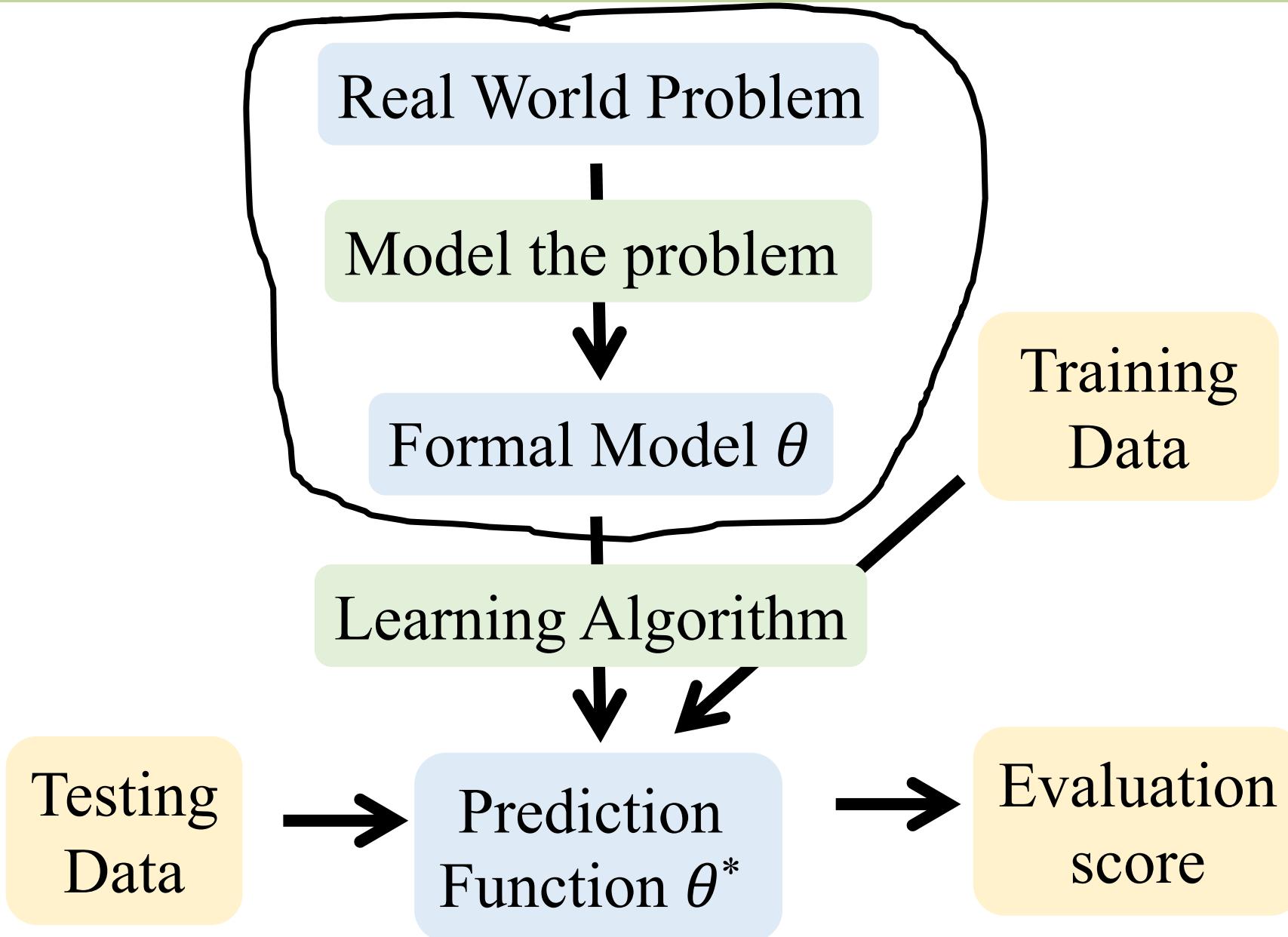
Why Do We Care?

- In real world, don't know "true" parameters
 - But, **we do get to observe data**
 - E.g., number of times coin comes up heads, lifetimes of disk drives produced, number of visitors to web site per day, etc.
 - Need to estimate model parameters from data
 - "Estimator" is random variable estimating parameter
- Estimate of parameters allows:
 - Better understanding of process producing data
 - Future **predictions** based on model
 - Simulation of processes

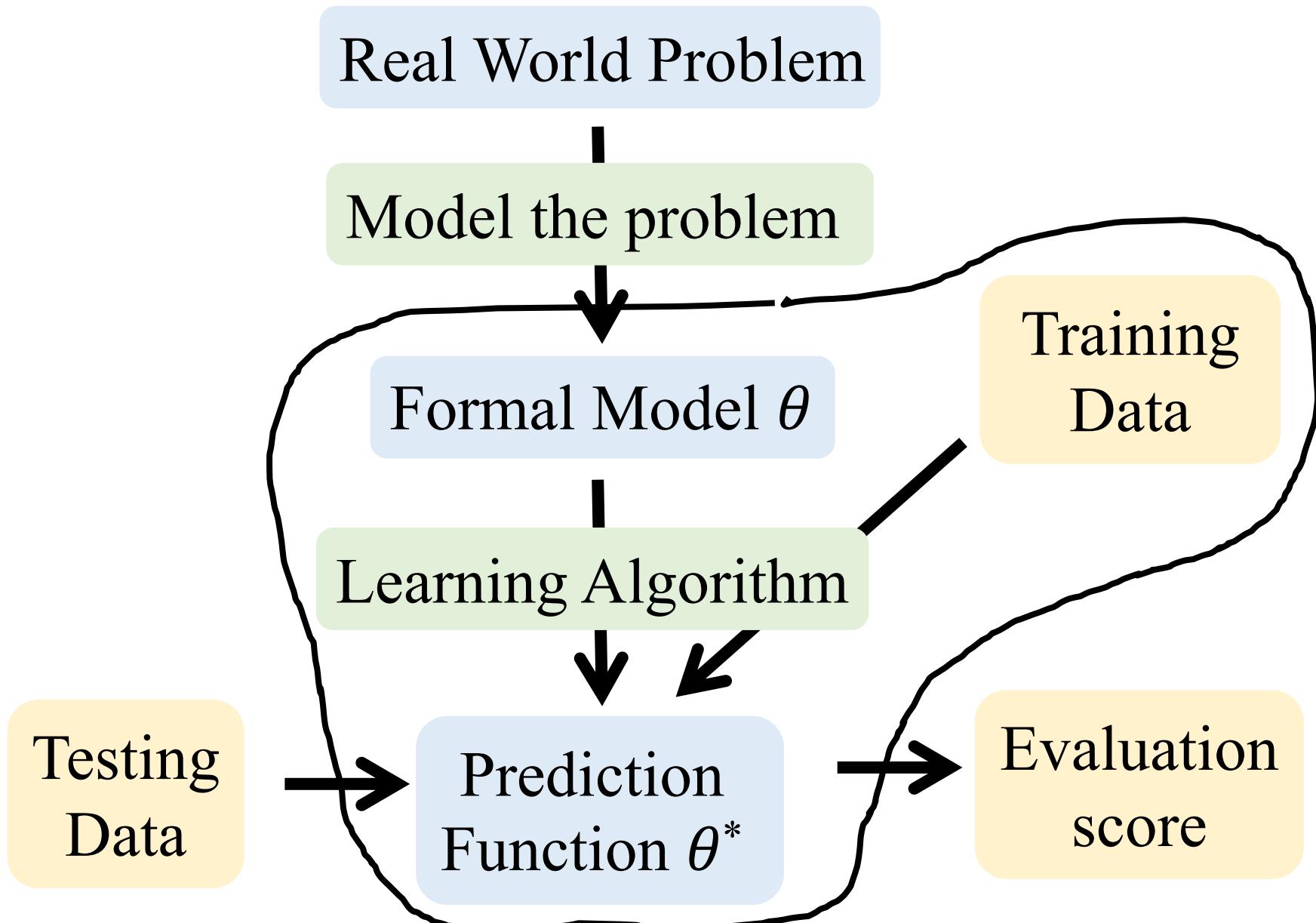
Supervised Learning



Modelling



Training



Testing

Real World Problem

Model the problem

Formal Model θ

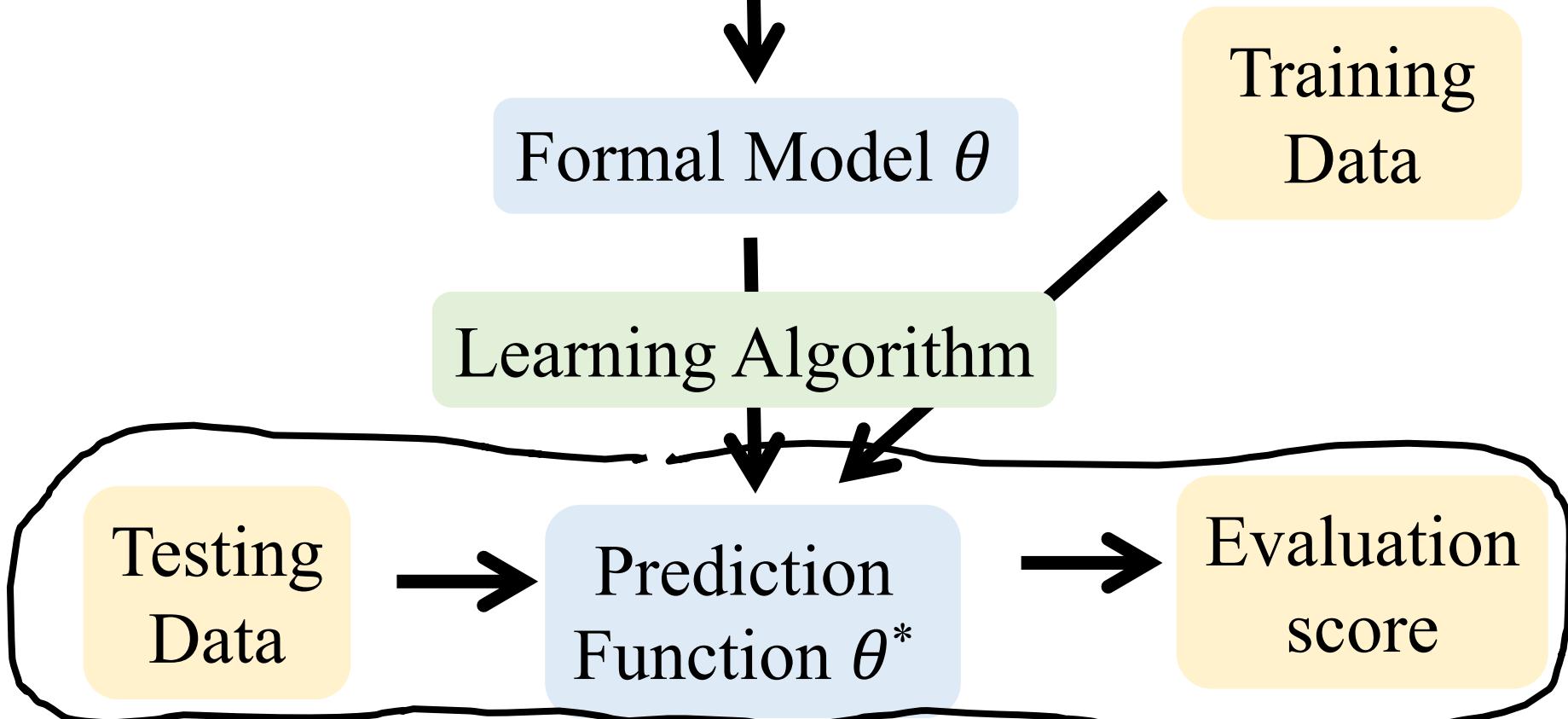
Training
Data

Learning Algorithm

Testing
Data

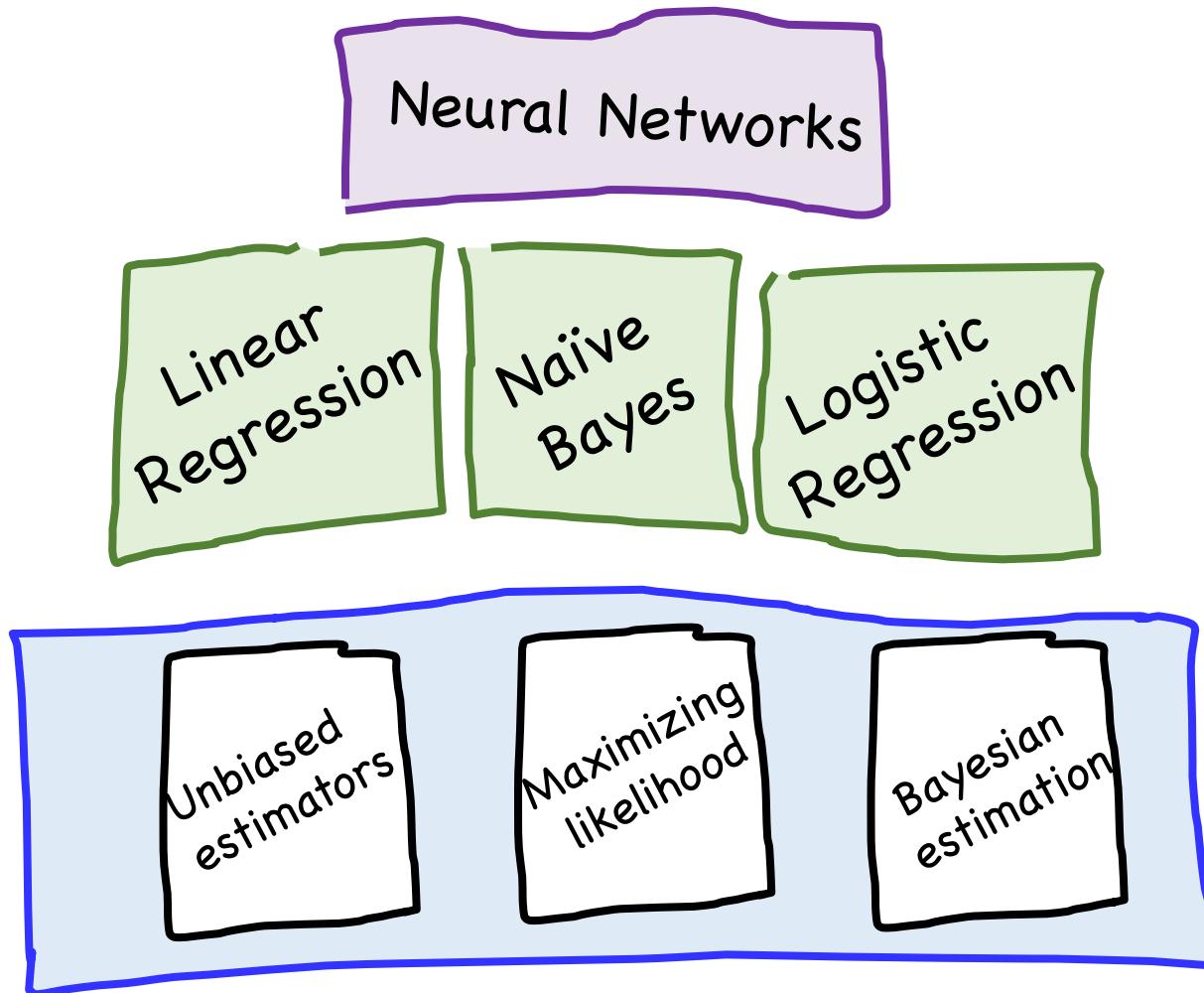
Prediction
Function θ^*

Evaluation
score

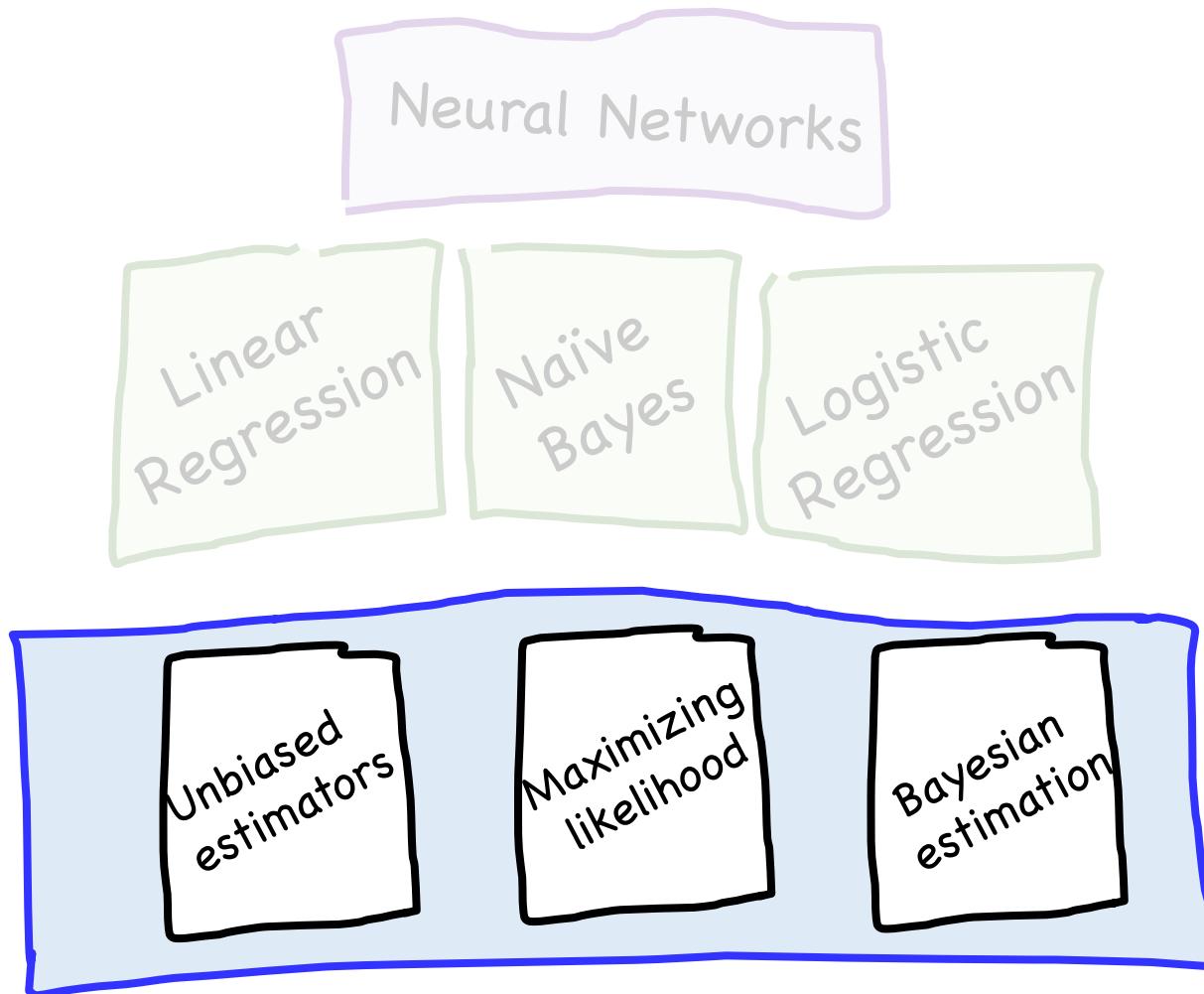


Basis for learning from data

Our Path



Parameter Estimation



Recall Sample Mean + Variance?

- Consider n I.I.D. random variables X_1, X_2, \dots, X_n
 - X_i have distribution F with $E[X_i] = \mu$ and $\text{Var}(X_i) = \sigma^2$
 - We call sequence of X_i a **sample** from distribution F
 - Recall sample mean: $\bar{X} = \sum_{i=1}^n \frac{X_i}{n}$ where $E[\bar{X}] = \mu$
$$\bar{X} \sim N\left(\mu, \frac{\sigma^2}{n}\right) \text{ as } n \rightarrow \infty$$
 - Recall sample variance:

$$S^2 = \sum_{i=1}^n \frac{(X_i - \bar{X})^2}{n-1} = \text{undefined}$$

Estimate parameters for
Bernoulli and Normal

Limited tool: how could we use that for fitting a “Mixture of Gaussians”?

Great idea in Machine Learning

Likelihood of Data

- Consider n I.I.D. random variables X_1, X_2, \dots, X_n
 - X_i is a sample from density function $f(X_i | \theta)$
 - Note: now explicitly specify parameter θ of distribution



Likelihood question:
How likely is the data given the samples?

$$\text{Likelihood}(\theta) = f(\text{Samples}|\theta)$$

[Demo](#)





Likelihood of Data

- Consider n I.I.D. random variables X_1, X_2, \dots, X_n
 - X_i is a sample from density function $f(X_i | \theta)$
 - Note: now explicitly specify parameter θ of distribution
 - We want to determine how “likely” the observed data (x_1, x_2, \dots, x_n) is based on density $f(X_i | \theta)$
 - Define the **Likelihood function**, $L(\theta)$:

$$L(\theta) = \prod_{i=1}^n f(X_i | \theta)$$

- This is just a product since X_i are I.I.D.
- Intuitively: what is probability of observed data using density function $f(X_i | \theta)$, for some choice of θ

Maximum Likelihood Estimator

- The Maximum Likelihood Estimator (MLE) of θ , is the value of θ that maximizes $L(\theta)$
 - More formally: $\theta_{MLE} = \arg \max_{\theta} L(\theta)$



Likelihood (of data given parameters):

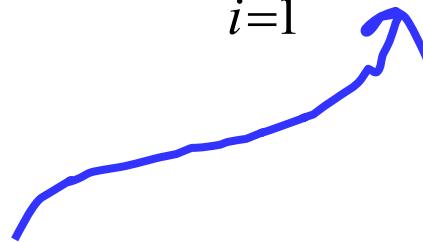
$$L(\theta) = \prod_{i=1}^n f(X_i \mid \theta)$$





Likelihood (of data given parameters):

$$L(\theta) = \prod_{i=1}^n f(X_i | \theta)$$



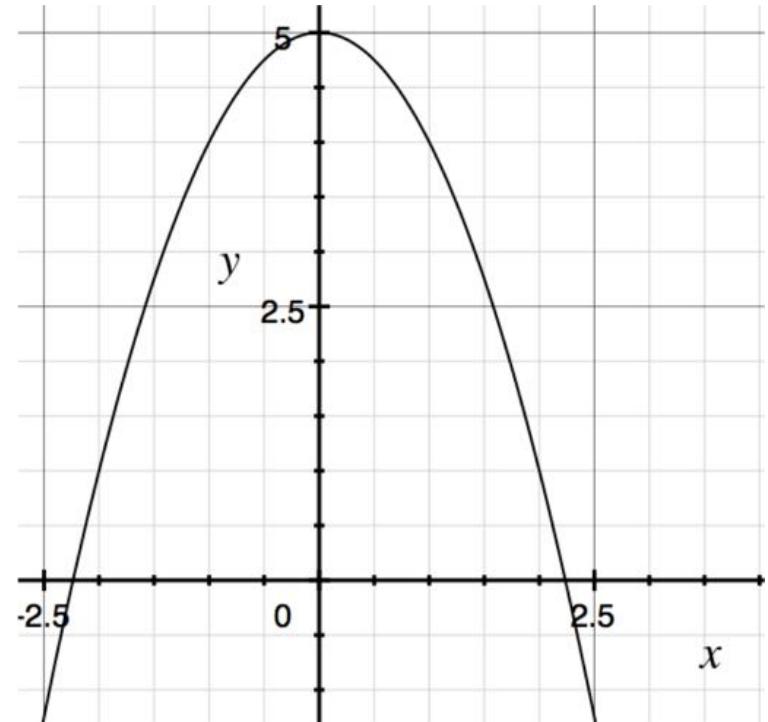
Either the
PDF (continuous) or
PMF (discrete)

Argmax

$$f(x) = -x^2 + 5$$

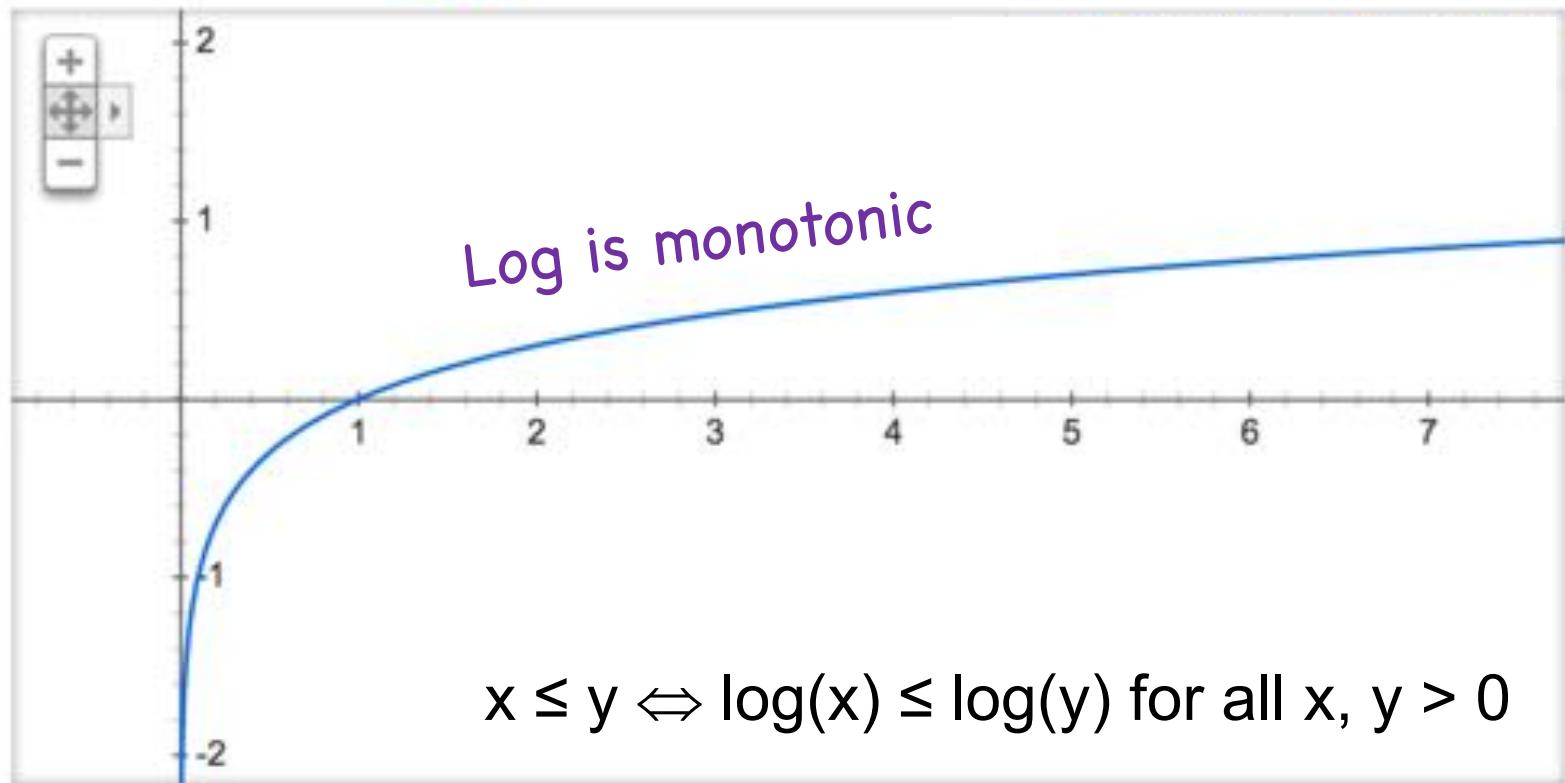
$$\max_x -x^2 + 5 = 5$$

$$\operatorname{argmax}_x -x^2 + 5 = 0$$



Argmax of Log

Graph for $\log(x)$



Claim: $\operatorname{argmax}_x f(x) = \operatorname{argmax}_x \log f(x)$

Argmax of Log

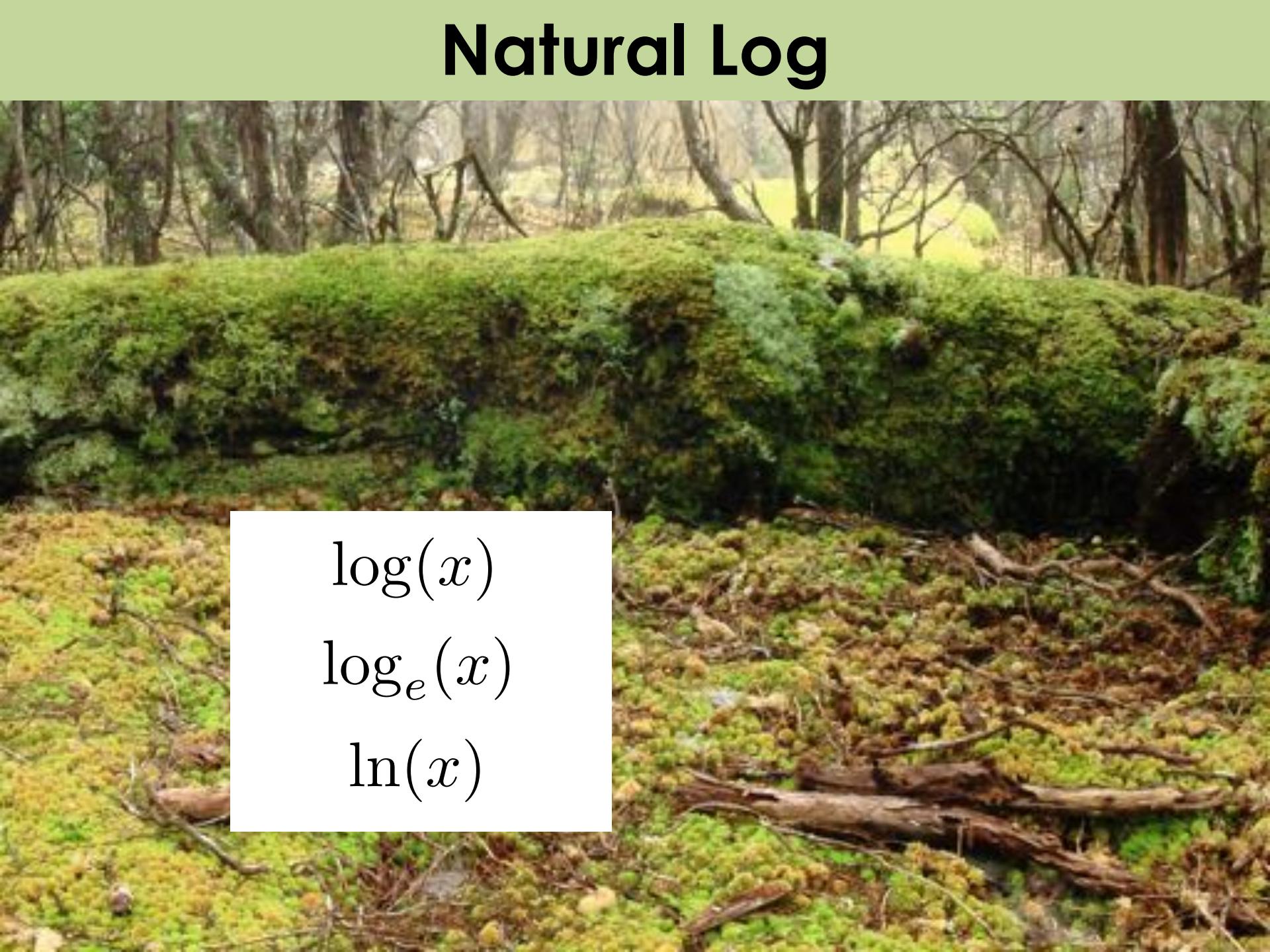


$$\operatorname{argmax}_x f(x) = \operatorname{argmax}_x \log f(x)$$

Log I Love You

$$\log(ab) = \log(a) + \log(b)$$

Natural Log



$\log(x)$
 $\log_e(x)$
 $\ln(x)$

Maximum Likelihood Estimator

- The **Maximum Likelihood Estimator** (MLE) of θ , is the value of θ that maximizes $L(\theta)$
 - More formally: $\theta_{MLE} = \arg \max_{\theta} L(\theta)$
 - More convenient to use **log-likelihood function**, $LL(\theta)$:

$$LL(\theta) = \log L(\theta) = \log \prod_{i=1}^n f(X_i | \theta) = \sum_{i=1}^n \log f(X_i | \theta)$$

- θ that maximizes $LL(\theta)$ also maximizes $L(\theta)$
 - Formally: $\arg \max_{\theta} LL(\theta) = \arg \max_{\theta} L(\theta)$
 - Similarly, for any positive constant c (not dependent on θ):

$$\arg \max_{\theta} (c \cdot LL(\theta)) = \arg \max_{\theta} LL(\theta) = \arg \max_{\theta} L(\theta)$$

Story so far: We can chose parameters by
finding the argmax of the log likelihood of our
data

Maximum Likelihood



$$L(\theta) = \prod_{i=1}^n f(X_i | \theta)$$

$$LL(\theta) = \sum_{i=1}^n \log f(X_i | \theta)$$

$$\hat{\theta} = \operatorname{argmax}_{\theta} LL(\theta)$$



But how do we compute argmax?

Option #1: Straight optimization

Computing the MLE

- General approach for finding MLE of θ
 - Determine formula for $LL(\theta)$
 - Differentiate $LL(\theta)$ w.r.t. (each) θ : $\frac{\partial LL(\theta)}{\partial \theta}$
 - To maximize, set $\frac{\partial LL(\theta)}{\partial \theta} = 0$
 - Solve resulting (simultaneous) equations to get θ_{MLE}
 - Make sure that derived $\hat{\theta}_{MLE}$ is actually a maximum (and not a minimum or saddle point). E.g., check $LL(\theta_{MLE} \pm \varepsilon) < LL(\theta_{MLE})$
 - This step often ignored in expository derivations
 - So, we'll ignore it here too (and won't require it in this class)

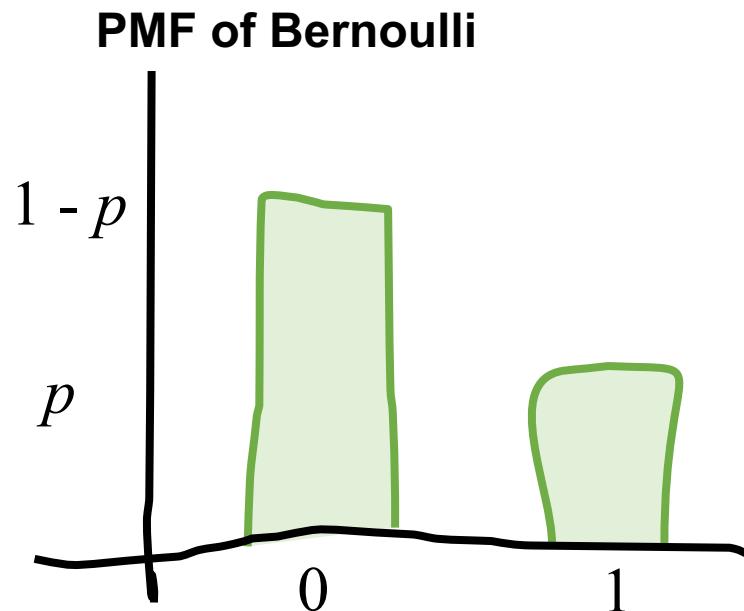
Maximizing Likelihood with Bernoulli

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim \text{Ber}(p)$
 - Probability mass function, $f(X_i | p)$:

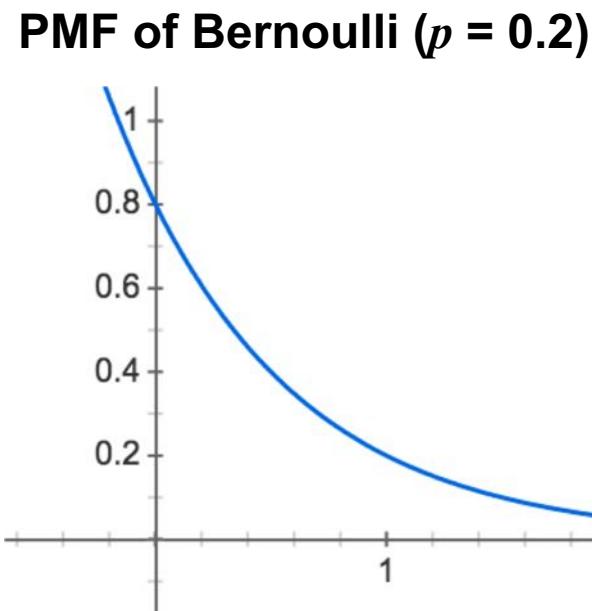


Maximizing Likelihood with Bernoulli

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim \text{Ber}(p)$
 - Probability mass function, $f(X_i | p)$:



$$f(X_i | p) = p^{x_i} (1-p)^{1-x_i}$$



$$f(x) = 0.2^x (1 - 0.2)^{1-x}$$

Bernoulli PMF

$$X \sim \text{Ber}(p)$$



$$f(X = x|p) = p^x(1 - p)^{1-x}$$

Maximizing Likelihood with Bernoulli

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim \text{Ber}(p)$
 - Probability mass function, $f(X_i | p)$, can be written as:

$$f(X_i | p) = p^{x_i} (1-p)^{1-x_i} \quad \text{where } x_i = 0 \text{ or } 1$$

- Likelihood: $L(\theta) = \prod_{i=1}^n p^{X_i} (1-p)^{1-X_i}$

- Log-likelihood:

$$\begin{aligned} LL(\theta) &= \sum_{i=1}^n \log(p^{X_i} (1-p)^{1-X_i}) = \sum_{i=1}^n [X_i (\log p) + (1-X_i) \log(1-p)] \\ &= Y(\log p) + (n-Y)\log(1-p) \quad \text{where } Y = \sum_{i=1}^n X_i \end{aligned}$$

- Differentiate w.r.t. p , and set to 0:

$$\frac{\partial LL(p)}{\partial p} = Y \frac{1}{p} + (n-Y) \frac{-1}{1-p} = 0 \quad \Rightarrow \quad p_{MLE} = \frac{Y}{n} = \frac{1}{n} \sum_{i=1}^n X_i$$

Isn't that the same as
unbiased estimator?

Yes. For Bernoulli.



Maximum Likelihood Algorithm

1. Decide on a model for the distribution of your samples. Define the PMF / PDF for your sample.

2. Write out the log likelihood function.

3. State that the optimal parameters are the argmax of the log likelihood function.

4. Use an optimization algorithm to calculate argmax



Maximizing Likelihood with Poisson

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim \text{Poi}(\lambda)$
 - PMF: $f(X_i | \lambda) = \frac{e^{-\lambda} \lambda^{x_i}}{x_i!}$ Likelihood: $L(\theta) = \prod_{i=1}^n \frac{e^{-\lambda} \lambda^{X_i}}{X_i!}$
 - Log-likelihood:
$$\begin{aligned} LL(\theta) &= \sum_{i=1}^n \log\left(\frac{e^{-\lambda} \lambda^{X_i}}{X_i!}\right) = \sum_{i=1}^n [-\lambda \log(e) + X_i \log(\lambda) - \log(X_i!)] \\ &= -n\lambda + \log(\lambda) \sum_{i=1}^n X_i - \sum_{i=1}^n \log(X_i!) \end{aligned}$$
 - Differentiate w.r.t. λ , and set to 0:

$$\frac{\partial LL(\lambda)}{\partial \lambda} = -n + \frac{1}{\lambda} \sum_{i=1}^n X_i = 0 \quad \Rightarrow \quad \lambda_{MLE} = \frac{1}{n} \sum_{i=1}^n X_i$$

Its so general!

Maximizing Likelihood with Normal

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim N(\mu, \sigma^2)$
 - PDF: $f(X_i | \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(X_i - \mu)^2 / (2\sigma^2)}$
 - Log-likelihood:

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

- First, differentiate w.r.t. μ , and set to 0:

$$\frac{\partial LL(\mu, \sigma^2)}{\partial \mu} = \sum_{i=1}^n 2(X_i - \mu) / (2\sigma^2) = \frac{1}{\sigma^2} \sum_{i=1}^n (X_i - \mu) = 0$$

- Then, differentiate w.r.t. σ , and set to 0:

$$\frac{\partial LL(\mu, \sigma^2)}{\partial \sigma} = \sum_{i=1}^n -\frac{1}{\sigma} + 2(X_i - \mu)^2 / (2\sigma^3) = -\frac{n}{\sigma} + \sum_{i=1}^n (X_i - \mu)^2 / (\sigma^3) = 0$$

Being Normal, Simultaneously

- Now have two equations, two unknowns:

$$\frac{1}{\sigma^2} \sum_{i=1}^n (X_i - \mu) = 0 \quad -\frac{n}{\sigma} + \sum_{i=1}^n (X_i - \mu)^2 / (\sigma^3) = 0$$

- First, solve for μ_{MLE} :

$$\frac{1}{\sigma^2} \sum_{i=1}^n (X_i - \mu) = 0 \Rightarrow \sum_{i=1}^n X_i = n\mu \Rightarrow \mu_{MLE} = \frac{1}{n} \sum_{i=1}^n X_i$$

- Then, solve for σ^2_{MLE} :

$$-\frac{n}{\sigma} + \sum_{i=1}^n (X_i - \mu)^2 / (\sigma^3) = 0 \Rightarrow n\sigma^2 = \sum_{i=1}^n (X_i - \mu)^2$$

$$\sigma_{MLE}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \mu_{MLE})^2$$

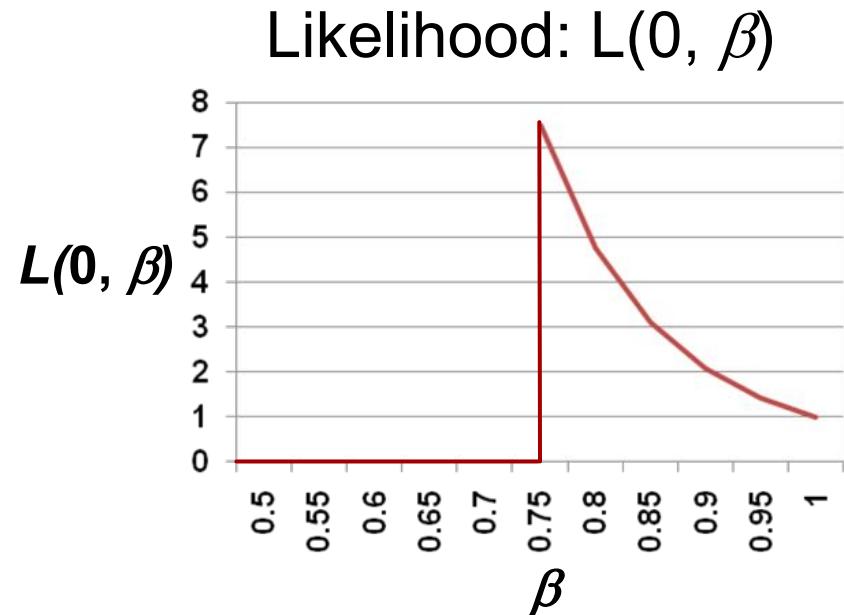
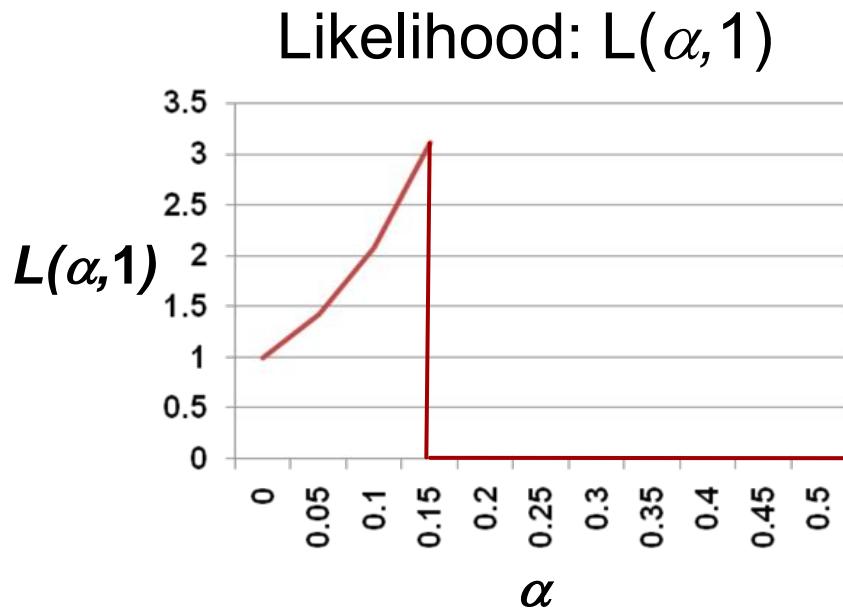
- Note: μ_{MLE} unbiased, but σ^2_{MLE} biased

Maximizing Likelihood with Uniform

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim \text{Uni}(\alpha, \beta)$
 - PDF: $f(X_i | \alpha, \beta) = \begin{cases} \frac{1}{\beta - \alpha} & \alpha \leq x_i \leq \beta \\ 0 & \text{otherwise} \end{cases}$
 - Likelihood: $L(\theta) = \begin{cases} \left(\frac{1}{\beta - \alpha}\right)^n & \alpha \leq x_1, x_2, \dots, x_n \leq \beta \\ 0 & \text{otherwise} \end{cases}$
 - Constraint $\alpha \leq x_1, x_2, \dots, x_n \leq \beta$ makes differentiation tricky
 - Intuition: want interval size $(\beta - \alpha)$ to be as small as possible to maximize likelihood function for each data point
 - But need to make sure all observed data contained in interval
 - If all observed data not in interval, then $L(\theta) = 0$
 - Solution: $\alpha_{MLE} = \min(x_1, \dots, x_n) \quad \beta_{MLE} = \max(x_1, \dots, x_n)$

Understanding MLE with Uniform

- Consider I.I.D. random variables X_1, X_2, \dots, X_n
 - $X_i \sim \text{Uni}(0, 1)$
 - Observe data:
 - 0.15, 0.20, 0.30, 0.40, 0.65, 0.70, 0.75



Small Samples = Problems

- How do small samples affect MLE?
 - In many cases, $\mu_{MLE} = \frac{1}{n} \sum_{i=1}^n X_i$ = sample mean
 - Unbiased. Not too shabby...
 - As seen with Normal, $\sigma_{MLE}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \mu_{MLE})^2$
 - Biased. Underestimates for small n (e.g., 0 for $n = 1$)
 - As seen with Uniform, $\alpha_{MLE} \geq \alpha$ and $\beta_{MLE} \leq \beta$
 - Biased. Problematic for small n (e.g., $\alpha = \beta$ when $n = 1$)
 - Small sample phenomena intuitively make sense:
 - Maximum likelihood \Rightarrow best explain data we've seen
 - Does not attempt to generalize to unseen data

Properties of MLE

- Maximum Likelihood Estimators are generally:
 - **Consistent:** $\lim_{n \rightarrow \infty} P(|\hat{\theta} - \theta| < \varepsilon) = 1$ for $\varepsilon > 0$
 - Potentially biased (though asymptotically less so)
 - **Asymptotically optimal**
 - Has smallest variance of “good” estimators for large samples
 - **Often used in practice** where sample size is large relative to parameter space
 - But be careful, there are some very large parameter spaces

