



香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 9

Naive Bayes, MLE, MAP

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Oct 8, 2024

Recap: Generative Models

Recap: Generative Models



X

$$p(y | x)$$

Discriminative

Cat Y

Recap: Generative Models

$$P(x, y)$$



X

$$p(y | x)$$

Discriminative

Cat Y

Cat Y $p(y)$

Generative

$$p(x | y)$$



X

Recap: Generative Models

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

$$p(y) \quad p(x|y)$$

$$p(x) = \sum_y p(x,y) = \sum_y p(x|y)p(y)$$

$$p(y|x)$$

If our goal is to predict y , the distribution is often written as:

$$\begin{aligned} p(y|x) &\propto p(x|y)p(y) \\ \arg \max_y p(y|x) &= \arg \max_y \frac{p(x|y)p(y)}{p(x)} \\ &= \arg \max_y p(x|y)p(y). \end{aligned}$$

Recap: Generative Models Compared to Discriminative Models

Pros:

- Generative models can generate data (generation, data augmentation)
- Inject prior information through the prior distribution $P(y)$
- May be learned in an unsupervised way when y is not available
- Modeling data distribution is a fundamental goal in AI

Cons:

- Often underperforms discriminative models on discriminative tasks because of stronger assumptions on the data

Naive Bayes

Binary classification: $y \in \{0,1\}$, x is discrete

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if an email contains the j -th word of the dictionary, then we will set $x_j = 1$; otherwise, we let $x_j = 0$

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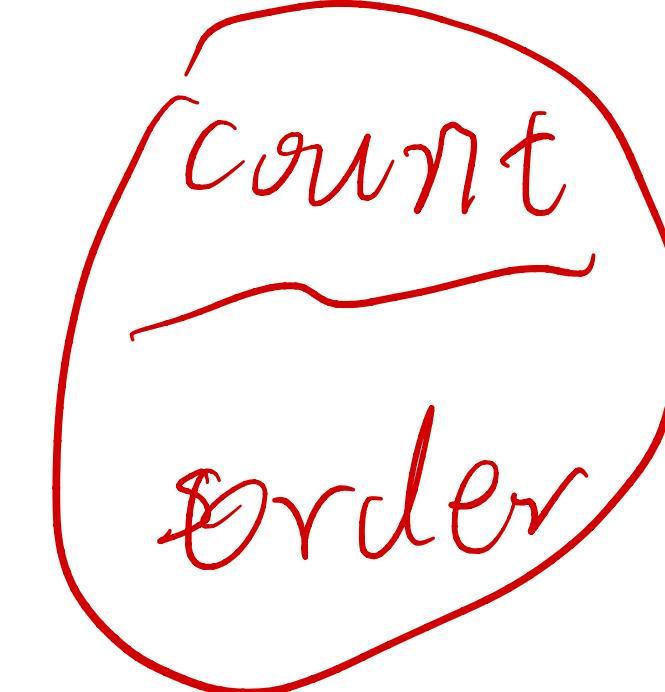
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$$x = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \quad \begin{array}{l} \text{a} \\ \text{aardvark} \\ \text{aardwolf} \\ \vdots \\ \text{buy} \\ \vdots \\ \text{zygmurgy} \end{array}$$

dictionary



count
order

Naive Bayes

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Dimension is the size of the dictionary

juvo

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vocabulary

Dimension is the size of the dictionary

Email Spam Classification

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$P(y)$ $P(x|y)$
binary ↓

Email Spam Classification

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Suppose the dictionary has 50000 words,
how many possible x ?

2^{50000} possibilities

$$P(x|y)$$

$$P(x|y=0)$$

$\checkmark x$

$$P(x|y=1)$$

$\times x$

$2^{50000} \times 2$

parameters

Email Spam Classification

$$x = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \quad \begin{array}{l} a \\ \text{aardvark} \\ \text{aardwolf} \\ \vdots \\ \text{buy} \\ \vdots \\ \text{zygmurgy} \end{array}$$

Suppose the dictionary has 50000 words,
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Naive Bayes assumption: x_i 's are conditionally independent given y

Email Spam Classification

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Suppose the dictionary has 50000 words,
how many possible x ?

$$P(x_i | y=1) \neq P(x_i | y=0, x_j)$$

Naive Bayes assumption: x_i 's are conditionally independent given y

For any i and j , $p(x_i | y) = p(x_i | y, x_j)$

$x_i = \text{whether "computer" appears}$ $P(x_i | y)$ $P(y=1)$
 $x_j = \text{whether "software" appears}$ x_j

Email Spam Classification

Email Spam Classification

$$\begin{aligned} p(x_1, \dots, x_{50000} | y) &= p(x_1 | y)p(x_2 | y, x_1)p(x_3 | y, x_1, x_2) \cdots p(x_{50000} | y, x_1, \dots, x_{49999}) \\ &= p(x_1 | y)p(x_2 | y)p(x_3 | y) \cdots p(x_{50000} | y) \\ &= \prod_{j=1}^d p(x_j | y) \end{aligned}$$

chain rule
conditional independence

Email Spam Classification

$$\begin{aligned} p(x_1, \dots, x_{50000} | y) && \text{Autoregressive} \\ = & p(x_1 | y) p(x_2 | y, x_1) p(x_3 | y, x_1, x_2) \cdots p(x_{50000} | y, x_1, \dots, x_{49999}) \\ = & p(x_1 | y) p(x_2 | y) p(x_3 | y) \cdots p(x_{50000} | y) \\ = & \prod_{j=1}^d p(x_j | y) \end{aligned}$$

Email Spam Classification

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Parameters

$$\phi_{j|y=1} = p(x_j = 1 | y = 1), \quad \phi_{j|y=0} = p(x_j = 1 | y = 0), \quad \phi_y = p(y = 1)$$

$$p(j=0) = \frac{1}{1 + p(j=1)}$$

50000

Email Spam Classification

shared NN x_1, x_2, \dots, x_K, y

↓

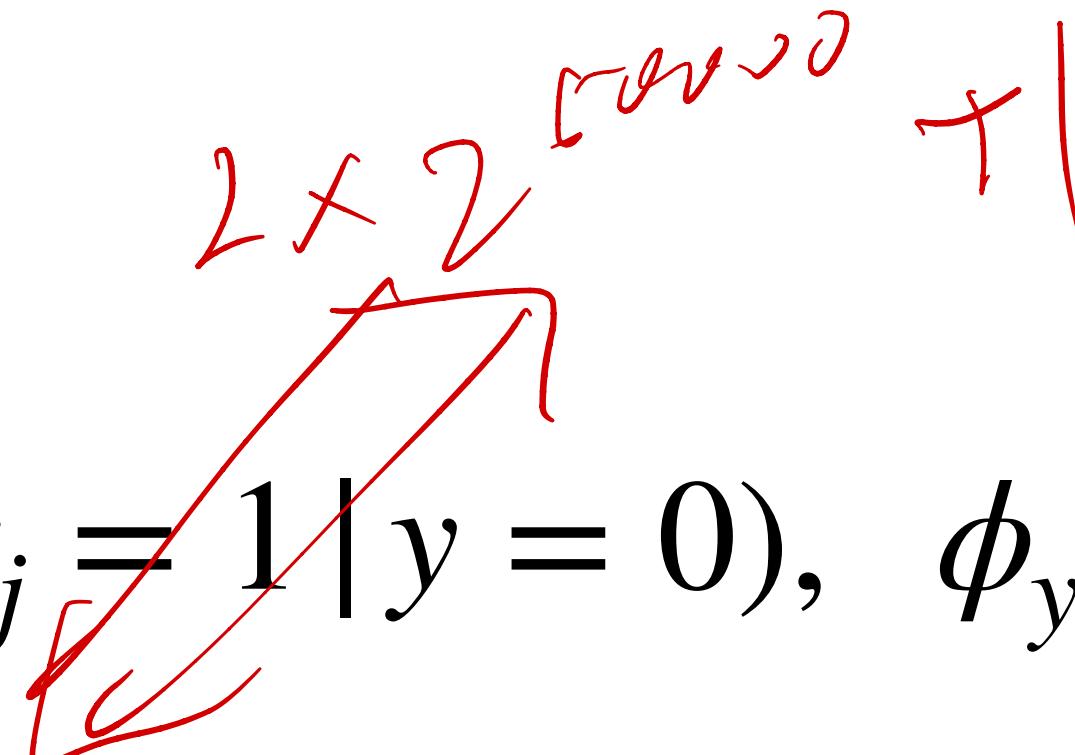
$$\begin{aligned} p(x_1, \dots, x_{50000} | y) &= p(x_1 | y) p(x_2 | y, x_1) p(x_3 | y, x_1, x_2) \cdots p(x_{50000} | y, x_1, \dots, x_{49999}) \\ &= p(x_1 | y) p(x_2 | y) p(x_3 | y) \cdots p(x_{50000} | y) \\ &= \prod_{j=1}^d p(x_j | y) \end{aligned}$$

Autoregressive

Parameters

$$\phi_{j|y=1} = p(x_j = 1 | y = 1), \quad \phi_{j|y=0} = p(x_j = 1 | y = 0), \quad \phi_y = p(y = 1)$$

50000 x 2 + 1 parameters (dict size is 50000)



Maximum Likelihood Estimation

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$$\mathcal{L}(\phi_y, \phi_{j|y=0}, \phi_{j|y=1}) = \prod_{i=1}^n p(x^{(i)}, y^{(i)})$$

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$$\phi_y = \frac{\sum_{i=1}^n 1\{y^{(i)} = 1\}}{n}$$

n : # all emails

Maximum Likelihood Estimation

$$\mathcal{L}(\phi_y, \phi_{j|y=0}, \phi_{j|y=1}) = \prod_{i=1}^n p(x^{(i)}, y^{(i)})$$

$$\begin{aligned}\phi_{j|y=1} &= \frac{\sum_{i=1}^n 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 1\}}{\sum_{i=1}^n 1\{y^{(i)} = 1\}} \\ \phi_{j|y=0} &= \frac{\sum_{i=1}^n 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 0\}}{\sum_{i=1}^n 1\{y^{(i)} = 0\}} \\ \phi_y &= \frac{\sum_{i=1}^n 1\{y^{(i)} = 1\}}{n}\end{aligned}$$

Count the occurrence of x_j in spam/
non-spam emails and normalize



Prediction

Prediction

$$\begin{aligned} p(y=1|x) &= \frac{p(x|y=1)p(y=1)}{p(x)} \\ &= \frac{\left(\prod_{j=1}^d p(x_j|y=1) \right) p(y=1)}{\left(\prod_{j=1}^d p(x_j|y=1) \right) p(y=1) + \left(\prod_{j=1}^d p(x_j|y=0) \right) p(y=0)} \end{aligned}$$

p_{cy})

$p_{cx|y})$

Prediction

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Naive Classifier

no greed

$$P(y=1|x) \propto P(x|y=1) P(y=1)$$

sample

$$P(y=0|x) \propto P(x|y=0) P(y=0)$$

denominator

Laplace Smoothing

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What if we never see the word “learning” in training data but “learning” exists in the test data?

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Suppose the index in the dictionary for
“learning” is q

$$p(x_q = 1 | y = 1) = 0$$
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↖

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$$= \frac{0}{0}$$

Laplace Smoothing

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Take the problem of estimating the mean of a multinomial random variable z taking values in $\{1, \dots, k\}$. Given the independent observations $\{z^{(1)}, \dots, z^{(n)}\}$

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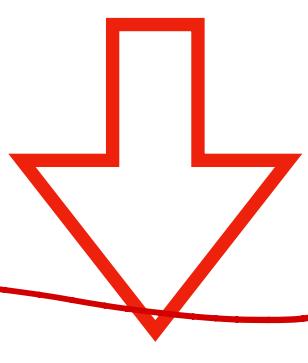
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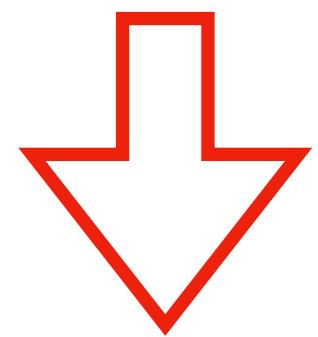
$$\phi_j = \frac{1 + \sum_{i=1}^n 1\{z^{(i)} = j\}}{k + n}$$


Laplace Smoothing

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Why adding k to the denominator?

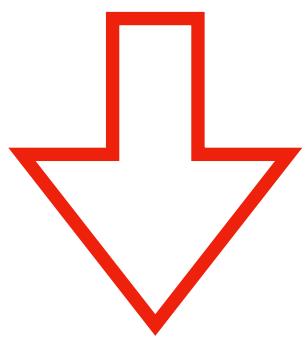
$$\left[\sum_{j=1}^K \phi_j = 1 \right]$$

Laplace Smoothing

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Why adding k to the denominator?

In the email spam classification case:

$$\begin{aligned}\phi_{j|y=1} &= \frac{1 + \sum_{i=1}^n 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 1\}}{2 + \sum_{i=1}^n 1\{y^{(i)} = 1\}} \\ \phi_{j|y=0} &= \frac{1 + \sum_{i=1}^n 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 0\}}{2 + \sum_{i=1}^n 1\{y^{(i)} = 0\}}\end{aligned}$$

Parameter Estimation: MLE and MAP

Maximum Likelihood Estimation (MLE)

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Suppose $\underline{p_{data}(x)}$ is the real data distribution, $\underline{p_{model}(x; \theta)}$ is our model parameterized by θ

Maximum Likelihood Estimation (MLE)

Suppose $p_{data}(x)$ is the real data distribution, $p_{model}(x; \theta)$ is our model parameterized by θ

$$\arg \max_{\theta} \mathbb{E}_{x \sim p_{data}(x)} p_{model}(x; \theta)$$

intractable

The handwritten diagram illustrates the MLE formula. A large red bracket encloses the entire expression $\arg \max_{\theta} \mathbb{E}_{x \sim p_{data}(x)} p_{model}(x; \theta)$. Inside this bracket, a red circle highlights the expectation operator \mathbb{E} . A red arrow points from this circle to a separate rectangular box containing the term $P_{data}(x)$. Another red arrow points from the circle to the word "intractable" written below the main formula.

Maximum Likelihood Estimation (MLE)

Suppose $p_{data}(x)$ is the real data distribution, $p_{model}(x; \theta)$ is our model parameterized by θ

$$\arg \max_{\theta} \mathbb{E}_{x \sim p_{data}(x)} p_{model}(x; \theta)$$

In practice:

$$\arg \max_{\theta} \frac{1}{n} \sum_i^n p_{model}(x^{(i)}; \theta)$$

MLE



n



.

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$x^{(i)}$ are i.i.d. (independent and identically distributed) samples from $p_{data}(x)$

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Monte Carlo Estimation of Expectation

$E_{x \sim q(x)} f(x)$

unbiased estimator

approximate

$$\frac{1}{N} \sum_{i=1}^N f(x_i)$$

$n \rightarrow$

$q(x)$: easy to sample from
expectation cannot incomplete

$$x_i \sim q(x_i)$$

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Monte Carlo Estimation of Expectation

Why can we make this approximation?

Central limit theorem

Monte Carlo Estimation of Expectation

$$\mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n f(x^{(i)})\right] = \mathbb{E}_{x \sim p(x)} f(x)$$

$$Var\left[\frac{1}{n} \sum_{i=1}^n f(x^{(i)})\right] = \frac{Var(f(x))}{n}$$

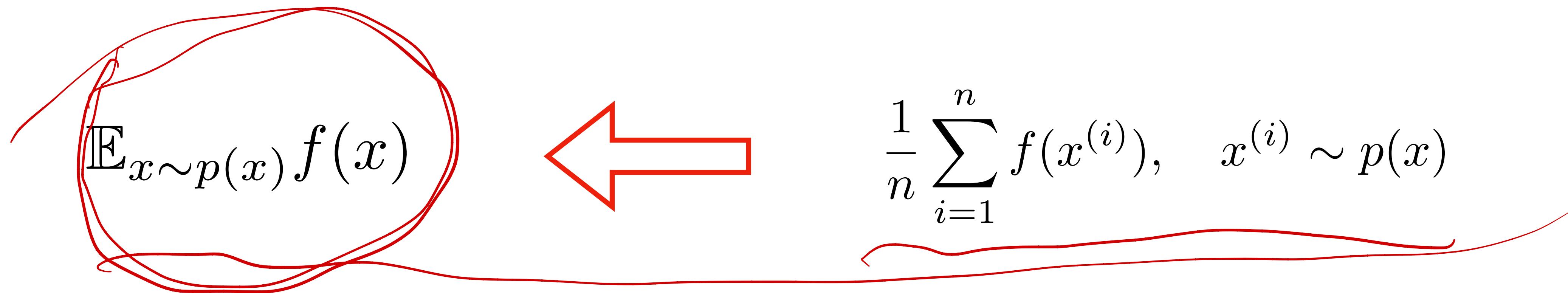
Monte Carlo Estimation of Expectation

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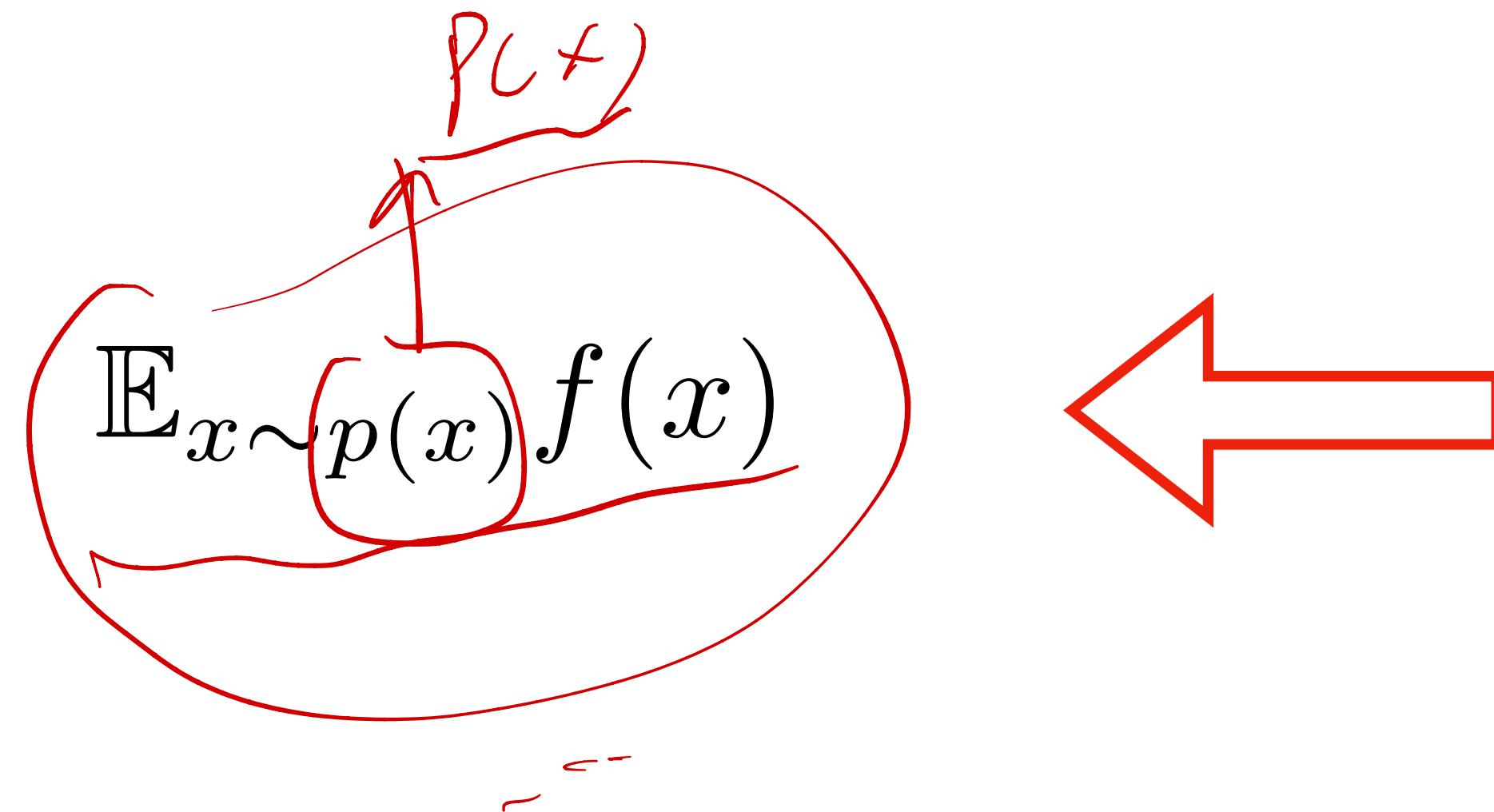
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Monte Carlo Estimation of Expectation



$$\mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n f(x^{(i)})\right] = \mathbb{E}_{x \sim p(x)} f(x)$$

$n=1$

$$Var\left[\frac{1}{n} \sum_{i=1}^n f(x^{(i)})\right] = \frac{Var(f(x))}{n}$$

Sampling and Evaluation of Distributions

Sampling and Evaluation of Distributions

- Some distributions are easy to sample from but hard to compute the probability value (hard to evaluate)
- Monte Carlo estimation requires this kind of distribution

$$P(x) = f(x)$$

x_0

GANs

Example:

$$P(z) \sim N(0, 1)$$

$$x = f_{NN}(z)$$

$$z \sim N(0, 1) \quad x = f(z)$$

x_0

$$P(x) = \int_z P(z) P(x|z)$$

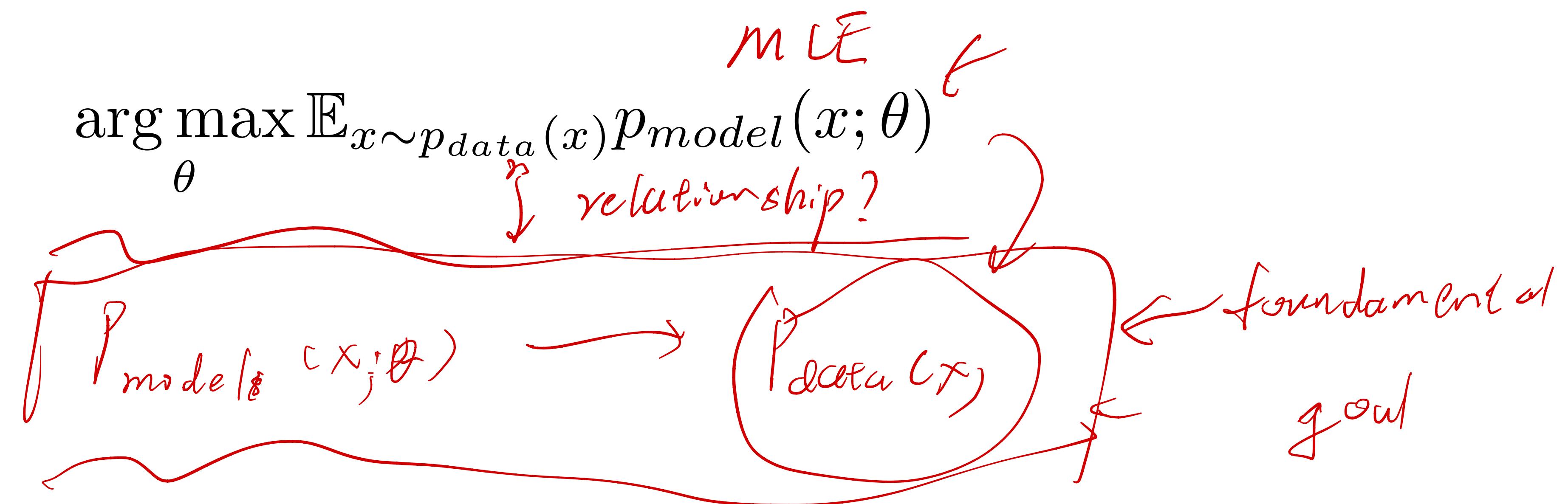
Sampling and Evaluation of Distributions

- Some distributions are easy to sample from but hard to compute the probability value (hard to evaluate)
Monte Carlo estimation requires this kind of distribution

- Some distributions are easy to compute the probability value (easy to evaluate) but hard to sample from
- How to sample from a distribution efficiently is a separate topic

$P(x)$ is continuous
 $P(x)$ is explicit
 $P(x)$ is implicit
generative models

MLE is Approximating the Real Distribution



MLE is Approximating the Real Distribution

$$\arg \max_{\theta} \mathbb{E}_{x \sim p_{data}(x)} p_{model}(x; \theta) \quad \swarrow$$

What is the optimal p_{model} ?



MLE is Approximating the Real Distribution

$$\arg \max_{\theta} \mathbb{E}_{x \sim p_{data}(x)} p_{model}(x; \theta)$$

What is the optimal p_{model} ?

MLE is equivalent to

KL divergence

$$\arg \min_{\theta} D_{KL}(p_{data}(x) || p_{model}(x; \theta))$$

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$$\arg \min_{\theta} D_{KL}(p_{data}(x) || p_{model}(x; \theta))$$

$D_{KL} \geq 0$ is a distance metric between two distributions, it is 0 when the two distributions are identical

MLE is Approximating the Real Distribution

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MLE is equivalent to

$$\arg \min_{\theta} D_{KL}(p_{data}(x) || p_{model}(x; \theta))$$

$D_{KL} \geq 0$ is a distance metric between two distributions, it is 0 when the two distributions are identical

$$D_{KL}(p(x) || q(x)) = \mathbb{E}_{p(x)} \log \frac{p(x)}{q(x)}$$

$$D_{KL}(q_{\theta(x)} || p_{\theta(x)}) = \mathbb{E}_{q_{\theta(x)}} \log \frac{q_{\theta(x)}}{p_{\theta(x)}}$$

$$\arg \min_{\theta} D_{KL}(P_{\text{data}(x)} || P_{\theta(x)})$$

$$= \arg \min_{\theta} \left(\mathbb{E}_{P_{\text{data}(x)}} \log P_{\text{data}(x)} \right) - \mathbb{E}_{P_{\text{data}(x)}} \log P_{\theta(x)}$$

constant

$$= \arg \min_{\theta} - \mathbb{E}_{P_{\text{data}}(x)} \log P_{\theta}(x)$$

$$= \arg \max_{\theta} \mathbb{E}_{P_{\text{data}}(x)} \log P_{\theta}(x) \quad \text{MLE}$$

MLE is Approximating the Real Distribution

$$\arg \max_{\theta} \mathbb{E}_{x \sim p_{\text{data}}(x)} p_{\text{model}}(x; \theta)$$

What is the optimal p_{model} ?

MLE is equivalent to

$$\arg \min_{\theta} D_{\text{KL}}(p_{\text{data}}(x) \parallel p_{\text{model}}(x; \theta))$$

$$JSD = KL(p_{\text{data}} \parallel p_{\text{model}}) + KL(p_{\text{model}} \parallel p_{\text{data}})$$

$D_{\text{KL}} \geq 0$ is a distance metric between two distributions, it is 0 when the two distributions are identical

$$D_{\text{KL}}(p(x) \parallel q(x)) = \mathbb{E}_{p(x)} \log \frac{p(x)}{q(x)}$$

When data is all the data from the world, then MLE is learning a distribution for the world

$$\underset{\theta}{\operatorname{argmin}} d(P_{\text{data}}, P_{\text{model}})$$

$d(\cdot, \cdot)$ distance, KL is only one option

when $d = \underbrace{\text{KL}(\cdot, \cdot)}_{\rightarrow \text{MLE}}$

$d = \int SDC \Rightarrow \text{GAN}$

GAN

$$KL(q||p) = \underbrace{E_{q(x)} \log \frac{q(x)}{p(x)}} \quad \text{distance}$$

not symmetric

$$KL(q||p) \neq KL(p||q)$$

$$d = KL(q||p) + KL(p||q) \quad \text{symmetric}$$

$$d \geq 0$$

Biased/Unbiased Estimator

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Suppose we want to estimate a true quantity θ^* , and our estimation is $\hat{\theta}$, then we define the bias of the estimation as: $\underline{\underline{z}}$

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When does the estimation converges to the true value when we have infinite data samples?

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$bias \rightarrow 0$,

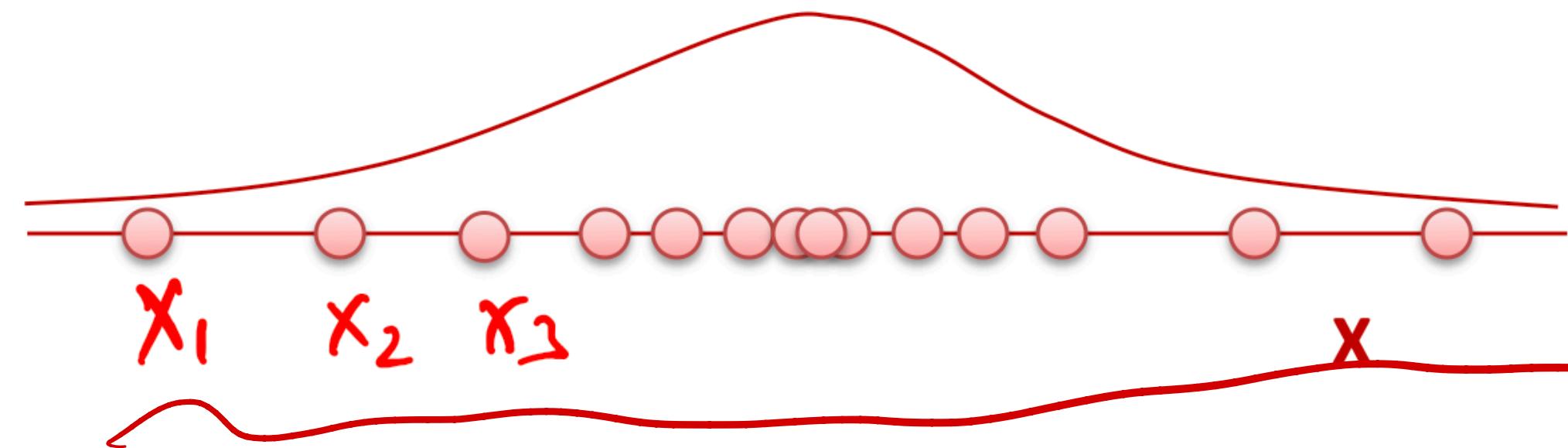
unbiased

$Var(\hat{\theta}) \rightarrow 0$


bias=0 unbiased
bias ≠ 0, bias → 0
bias = $\frac{1}{n}$

Learn Parameters from Data with MLE

Data, $D =$



Approximate the mean and variance of the data

Data are **i.i.d.**:

- **Independent** events
- **Identically distributed** according to Gaussian distribution

$$\mu, \sigma^2$$

MLE for Gaussian Mean and Variance

$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i$$

$$\hat{\sigma}_{MLE}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu})^2$$

$$\text{Var} := \mathbb{E}[(x - \mathbb{E}[x])^2]$$

MLE for Gaussian Mean and Variance

$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i$$

unbiased

$$E[\hat{\mu}_{MLE}] = \frac{1}{n} \sum_{i=1}^n E(x_i) = \frac{1}{n} \sum_{i=1}^n \mu = \mu$$

biased $\hat{\sigma}_{MLE}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu})^2$

$$E[\hat{\sigma}_{MLE}^2] \neq \sigma^2 = \mu$$

Are the estimations biased?

MLE for Gaussian Mean and Variance

$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i$$

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Are the estimations biased?

Unbiased estimator: $\hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \hat{\mu})^2$

Max A Posterior (MAP) Estimation

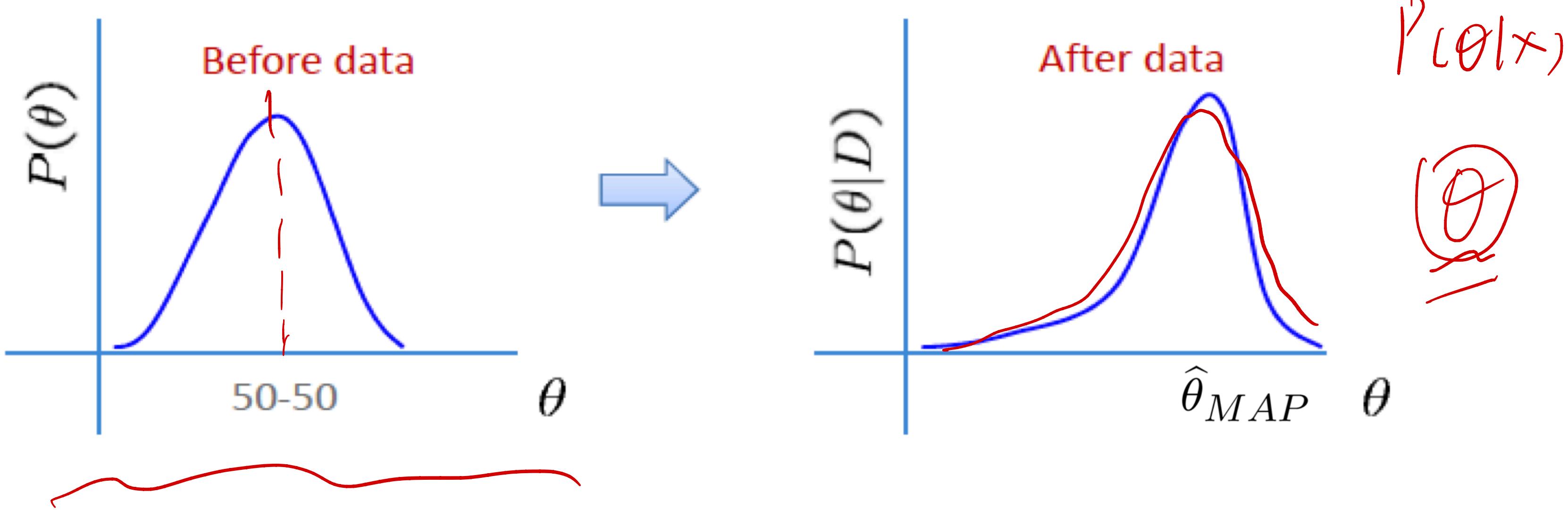
Max A Posterior (MAP) Estimation

Bring prior knowledge to the parameter, define the prior $P(\theta)$. The posterior distribution is $\underline{P(\theta | D)}$. D is the training dataset

$$\underline{P(\theta)} \quad \underline{P(\theta | x)}$$

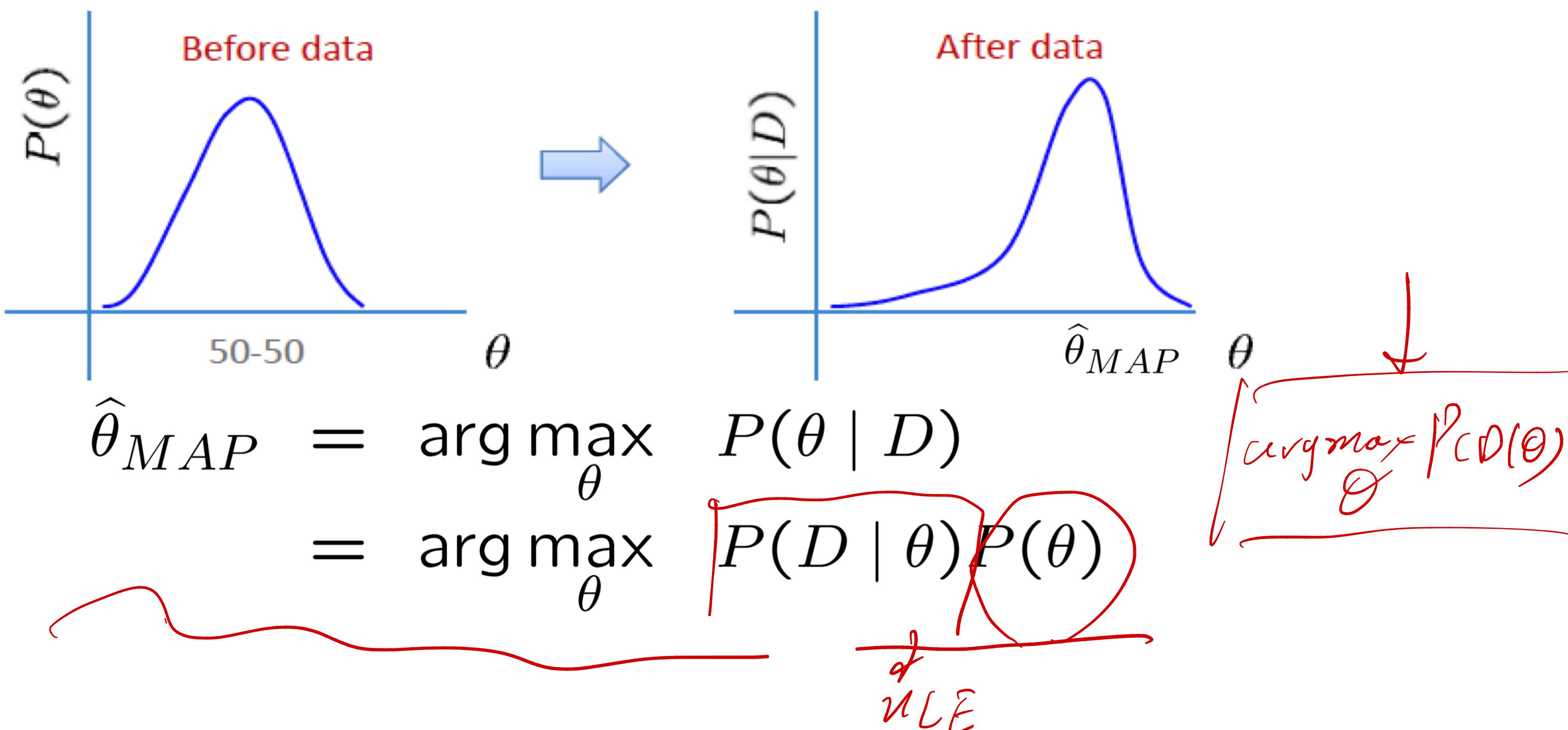
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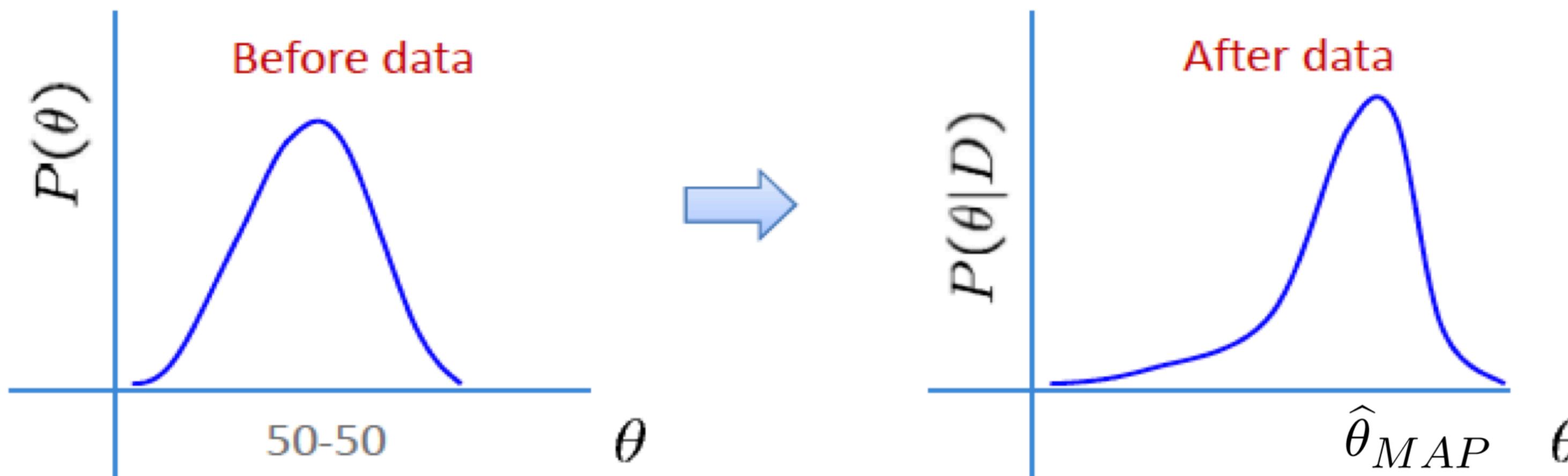
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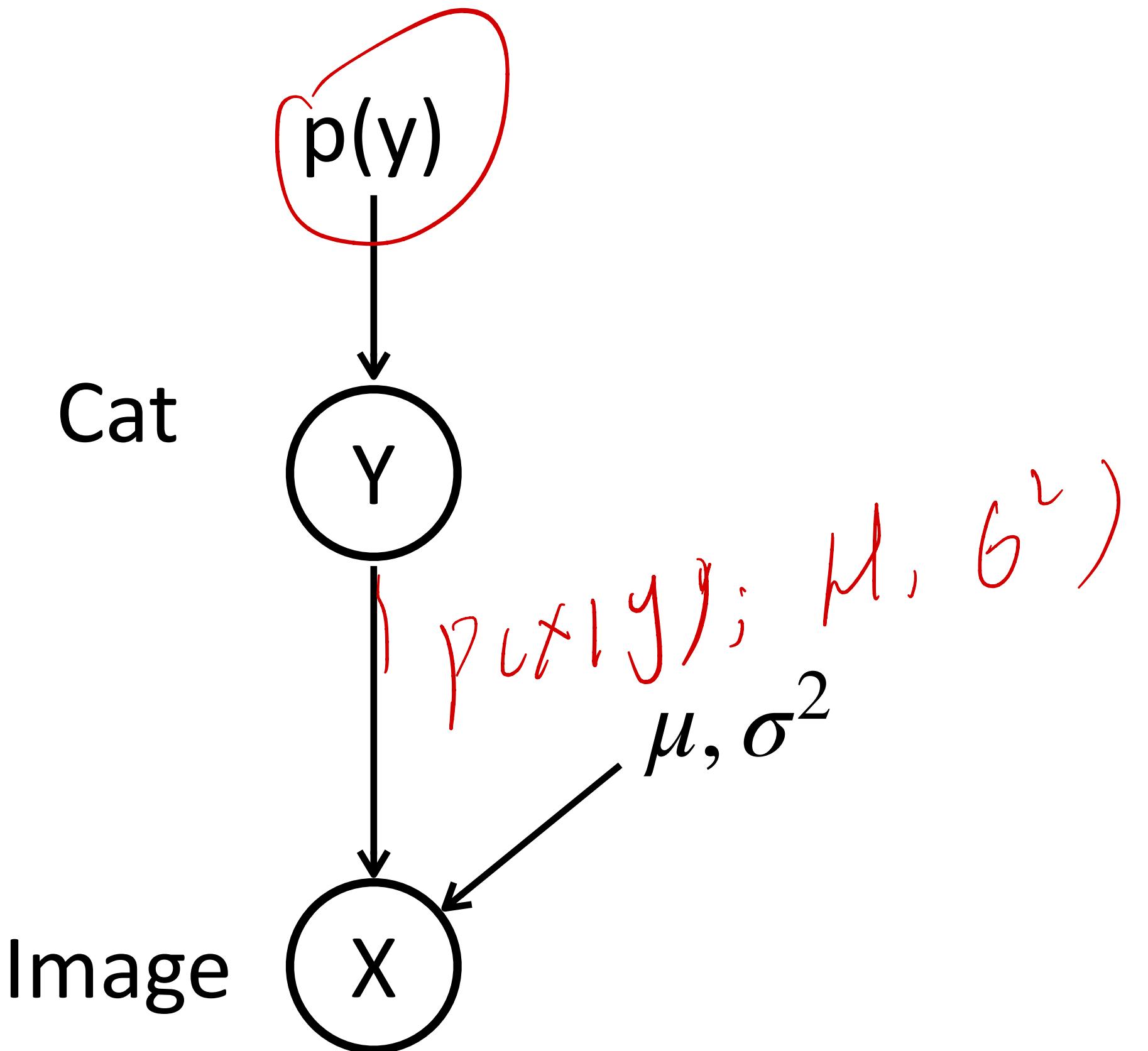


$$\begin{aligned}\hat{\theta}_{MAP} &= \arg \max_{\theta} P(\theta | D) \\ &= \arg \max_{\theta} P(D | \theta)P(\theta)\end{aligned}$$

Bayesian statistics: there is no “parameters” in the world, all are posterior distributions to estimate

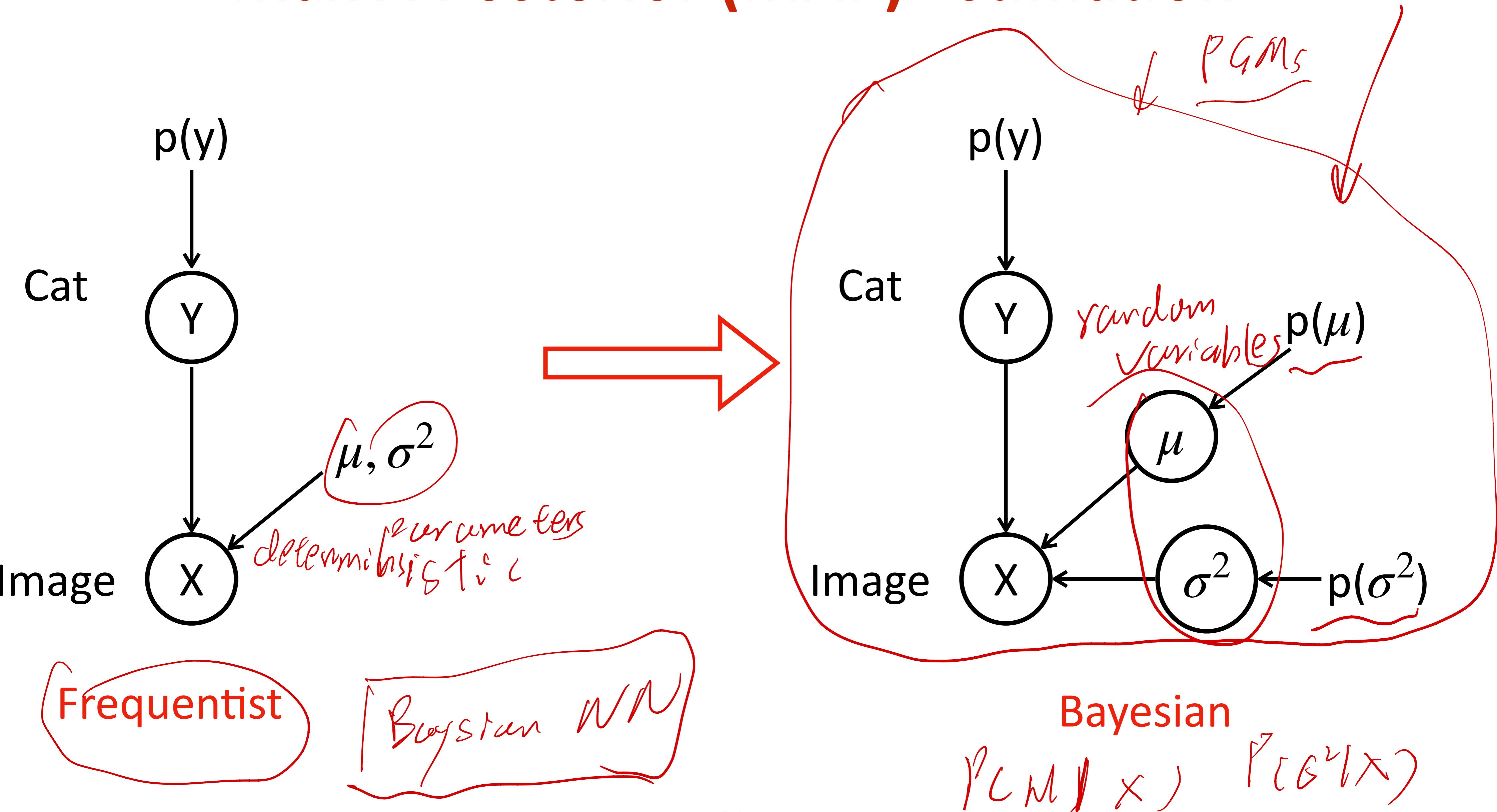
Max A Posterior (MAP) Estimation

Max A Posterior (MAP) Estimation



Frequentist

Max A Posterior (MAP) Estimation



How to Choose Prior

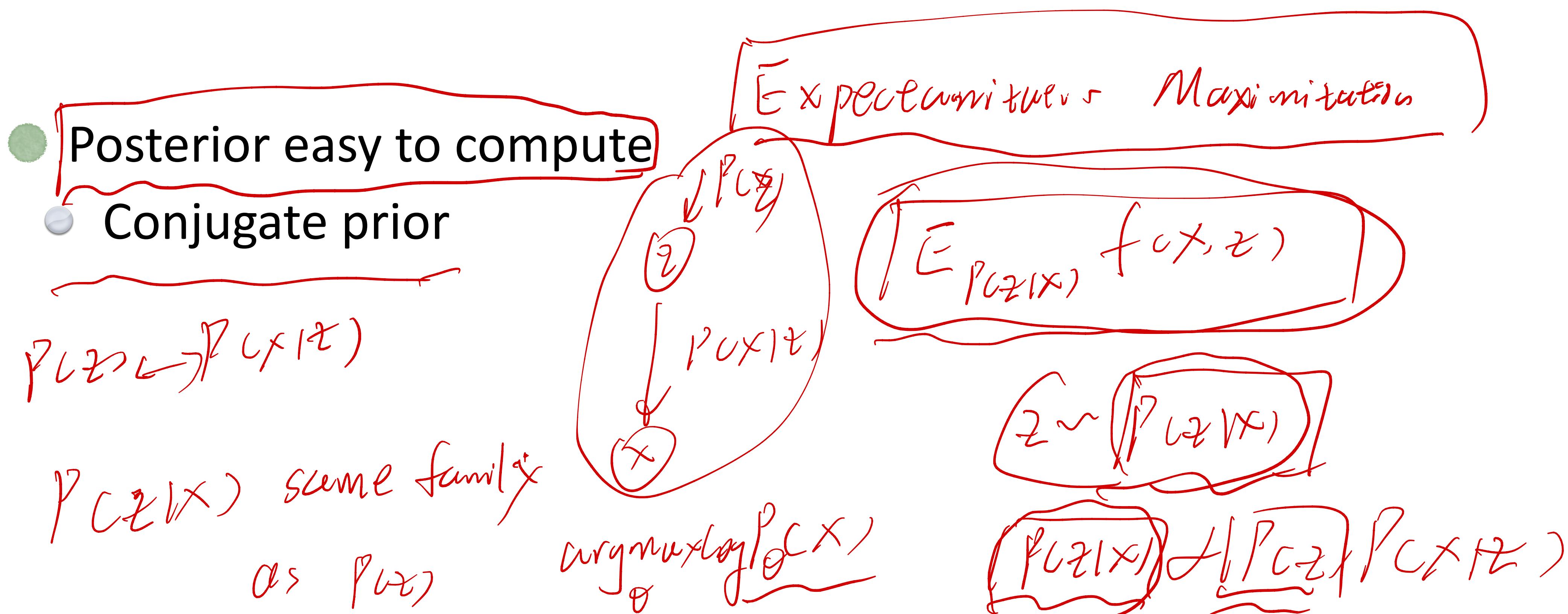
- Inject prior human knowledge to regularize the estimate
 - Could learn better if data is limited

$P(y)$ z continuous

$P(z) \sim N(0, 1)$

How to Choose Prior

- Inject prior human knowledge to regularize the estimate
 - Could learn better if data is limited



Conjugate Prior

Conjugate Prior

If $P(\theta)$ is conjugate prior for $P(D|\theta)$, then Posterior has same form as prior

Posterior = Likelihood x Prior

$$P(\theta|D) = P(D|\theta) \times P(\theta)$$

Conjugate Prior

If $P(\theta)$ is conjugate prior for $P(D|\theta)$, then Posterior has same form as prior

Posterior = Likelihood x Prior

$$P(\theta|D) = P(D|\theta) \times P(\theta)$$

P(theta)	P(D theta)	P(theta D)
Gaussian	Gaussian	Gaussian
Beta	Bernoulli	Beta
Dirichlet	Multinomial	Dirichlet

MLE vs. MAP

Maximum Likelihood estimation (MLE)

Choose value that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg \max_{\theta} P(D|\theta)$$

Maximum *a posteriori* (MAP) estimation

Choose value that is most probable given observed data and prior belief

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg \max_{\theta} P(\theta|D) \\ &= \arg \max_{\theta} P(D|\theta)P(\theta)\end{aligned}$$

When are they the same?

Thank You!
Q & A