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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Recap: Generative Models

X

$p(y|x)$ Discriminative

Cat Y

Cat Y $p(y)$

Generative $p(x|y)$

X

Recap: Generative Models

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

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

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

$$p(y\,|\,x) \propto p(x\,|\,y)p(y)$$

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

Recap: Generative Models Compared to Discriminative Models

Pros:

- Generative models can generate data (generation, data augmentation)
- Inject prior information through the prior distribution
- 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

Consider an email spam detection task, to predict whether the email is spam or not

How to represent the text?

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

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

vocabulary

Dimension is the size of the dictionary

Email Spam Classification

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

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

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

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

Email Spam Classification

Autoregressive

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

Parameters

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

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

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

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

Naive Classifier

Laplace Smoothing

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

$$\phi_{j|y=1} = \frac{\sum_{i=1}^{n} 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 1\}}{\sum_{i=1}^{n} 1\{y^{(i)} = 1\}}$$

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

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

$$p(x_q = 1 \,|\, y = 1) = 0$$

$$p(x_q = 1 \,|\, y = 0) = 0$$

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

Laplace Smoothing

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

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

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

Why adding k to the denominator?

In the email spam classification case:

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

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

Parameter Estimation: MLE and MAP

Maximum Likelihood Estimation (MLE)

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

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

In practice:

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

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

Monte Carlo Estimation of Expectation

Why can we make this approximation?

Monte Carlo Estimation of Expectation

$$\mathbb{E}_{x\sim p(x)} f(x) \Leftarrow \frac{1}{n}\sum_{i=1}^{n} f(x^{(i)}), \quad x^{(i)} \sim p(x)$$

In practice, n is often small, like 1 sample

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

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

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

MLE is Approximating the Real Distribution

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

What is the optimal p_{model} ?

MLE is equivalent to

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

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

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

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

Biased/Unbiased Estimator

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

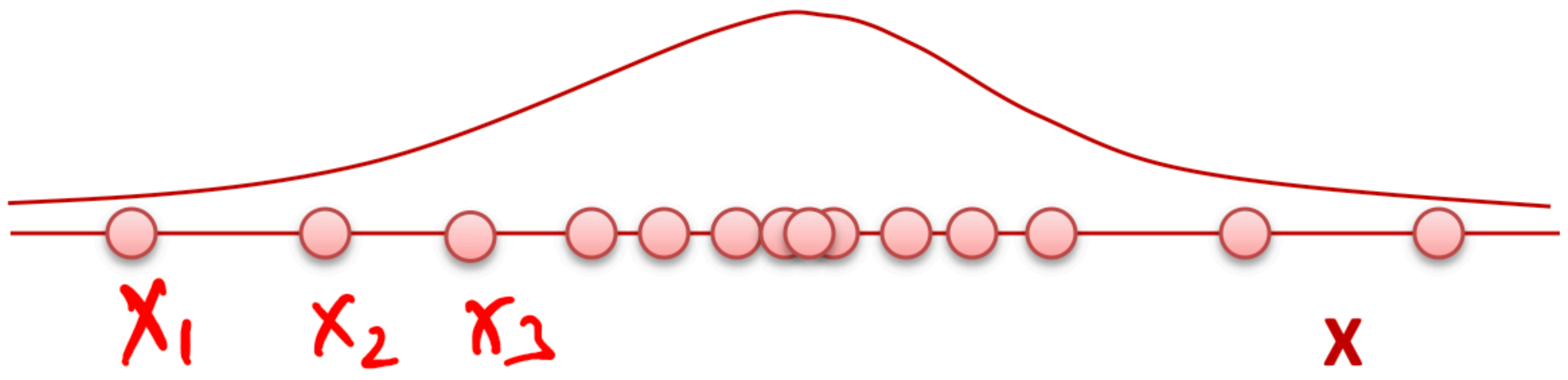
$$bias = \mathbb{E}(\hat{\theta}) - \theta*$$

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

$$bias \rightarrow 0, \quad Var(\hat{\theta}) \rightarrow 0$$

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

MLE for Gaussian Mean and Variance

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

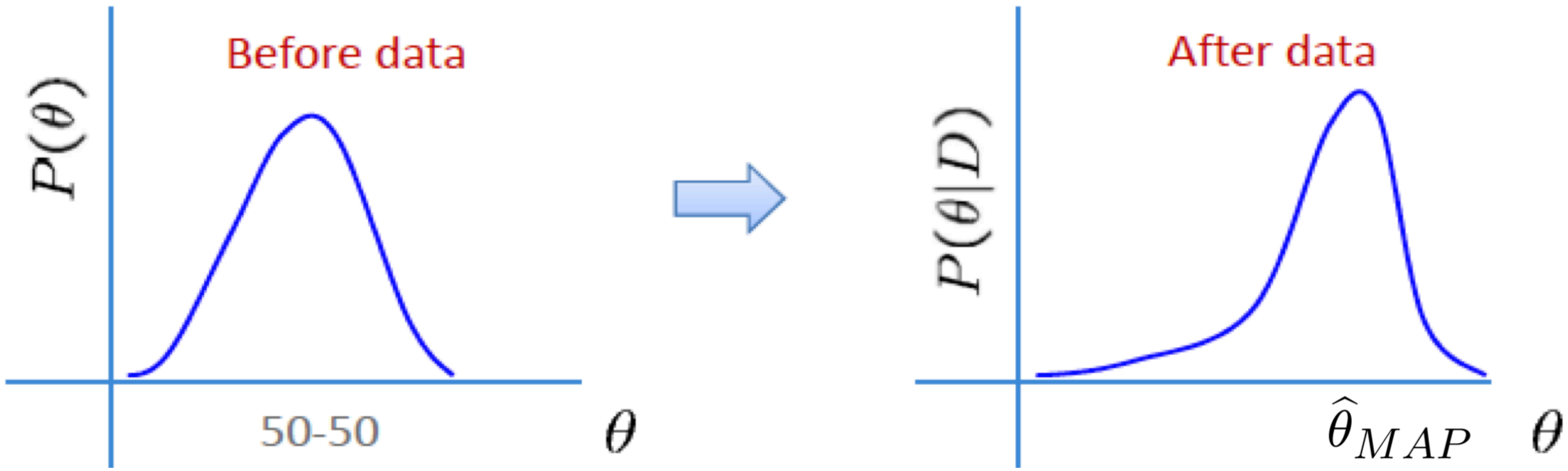
$$\hat{\sigma}^2_{MLE} = \frac{1}{n}\sum_{i=1}^{n} (x_i - \hat{\mu})^2$$

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

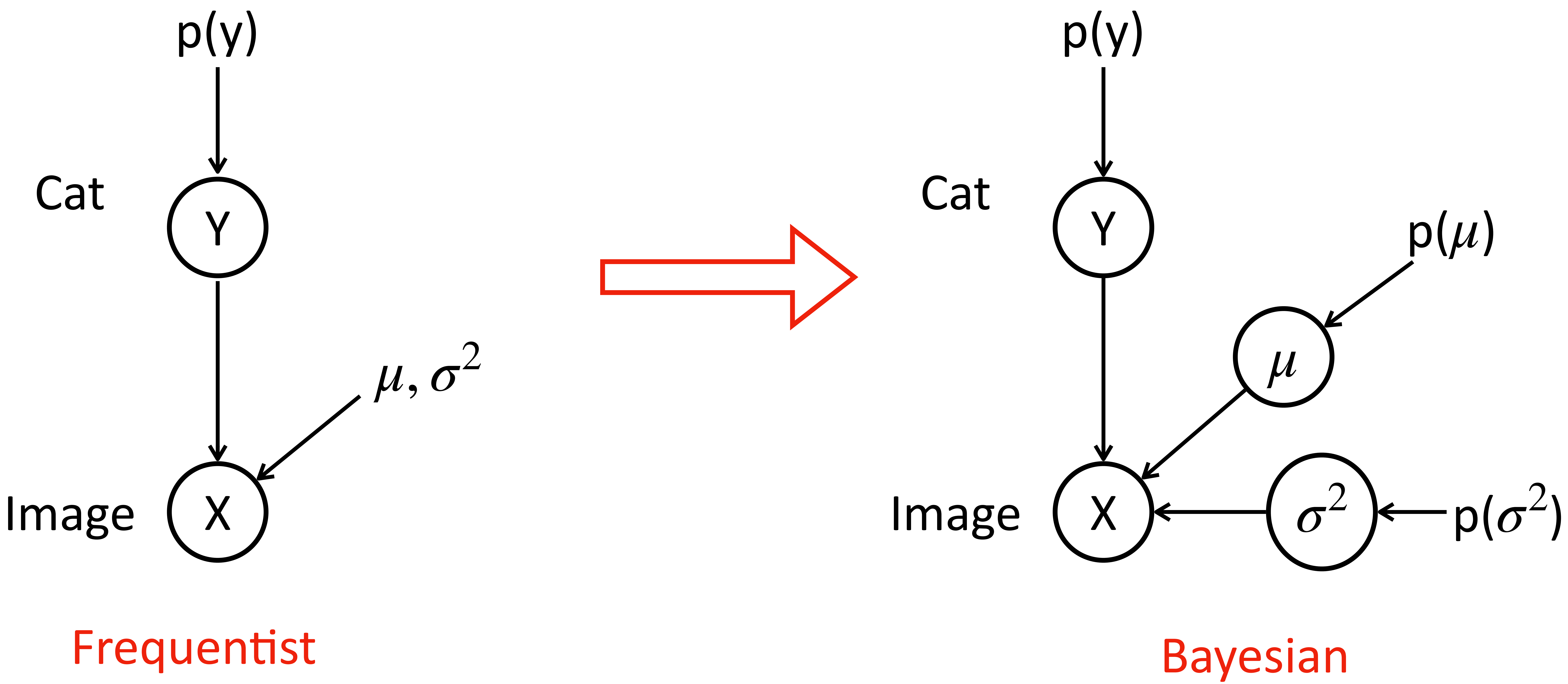
Bring prior knowledge to the parameter, define the prior $P(\theta)$. The posterior distribution is $P(\theta | D)$. D is the training dataset



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

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

Max A Posterior (MAP) Estimation



How to Choose Prior

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

- Posterior easy to compute
  - Conjugate prior

Conjugate Prior

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

$$\text{Posterior} = \text{Likelihood} \times \text{Prior}$$

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

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

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

Maximum *a posteriori* (MAP) estimation

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

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

When are they the same?

Thank You!
Q & A