

### 3. Parametric Density Estimation

Dongwoo Kim

[dongwookim.ac.kr](mailto:dongwookim.ac.kr)

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# Motivation

We have a coin, and a probability to get a head of the coin is  $\mu$ .

- ▶ We flipped the coin 10 times and observed 7 heads and 3 tails.
- ▶ Q: what would be the most plausible value of  $\mu$  given these observations?

# Motivation

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  - ▶ A:  $\mu = 0.7$

# Motivation

We have a coin, and a probability to get a head of the coin is  $\mu$ .

- ▶ We flipped the coin 10 times and observed 7 heads and 3 tails.
- ▶ Q: what would be the most plausible value of  $\mu$  given these observations?
  - ▶ A:  $\mu = 0.7$
- ▶ Where did you get this number? Are there any other answers?
- ▶ How can we formalize this process (observation  $\rightarrow$  parameter) in a **principled way**?

# Statistical Model: a Set of Probabilistic Models

One way to extract **patterns** from data is to find **the most likely probability model** generating observed data  $\mathcal{D}$  among a set of probabilistic models (or statistical model):

- ▶ Supervised learning
  - ▶ Use samples of input  $x$  and output  $y$ , i.e.,  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$
  - ▶ Learn a mapping from input to output under a probabilistic model of  $p(y | x)$ , e.g., a **parameterized** model  $p(y | x, \theta)$
- ▶ Unsupervised learning (today; for simplicity)
  - ▶ Use samples of input  $x$ , i.e.,  $\mathcal{D} = \{x_i\}_{i=1}^n$
  - ▶ Learn an explanation using a probabilistic model of  $p(x)$ , e.g., a **parameterized** model  $p(x | \theta)$

# Application of Statistical Model

- ▶ Predicting the expectation  $\mathbb{E}[X]$  or variance  $\text{Var}[X]$ 
  - ▶ c.f., considering  $(x, y)$  as a sample  $x'$ , the learned joint distribution  $p(x' = (x, y))$  allows us to predict  $\mathbb{E}[Y | X]$
- ▶ Predicting the tail distribution  $\inf\{a : p(X \geq a) \leq 0.1\}$ , ... <sup>1</sup>
- ▶ Detecting outliers (a.k.a. ood; out-of-distribution) by checking likelihood  $p(X = x_*)$
- ▶ ...

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<sup>1</sup>[https://en.wikipedia.org/wiki/Infimum\\_and\\_supremum](https://en.wikipedia.org/wiki/Infimum_and_supremum)

# A Typical Setup for Statistical Model (1)

- ▶ Let  $X_1, \dots, X_n$  be  $n$  independent copies of  $X$ , i.e.,  $X_i$ 's are drawn from a single distribution independently (i.i.d.)
- ▶ The goal of statistics is to learn the distribution of  $X$



# A Typical Setup for Statistical Model (1)

- ▶ Let  $X_1, \dots, X_n$  be  $n$  independent copies of  $X$ , i.e.,  $X_i$ 's are drawn from a single distribution independently (i.i.d.)
- ▶ The goal of statistics is to learn the distribution of  $X$
- ▶ e.g., survey on the number of siblings:

0, 2, 0, 1, 2, 3, 0, 1, ...

- ▶ We could make no assumption and try to learn the pmf:

x	0	1	2	3	4	5	$\geq 6$
$p(X = x)$	$p_0$	$p_1$	$p_2$	$p_3$	$p_4$	$p_5$	$p_{6+} = \sum_{i \geq 6} p_i$

where we need to learn 7 parameters (count & normalize)

## A Typical Setup for Statistical Model (2)

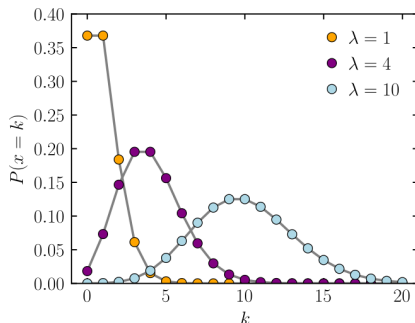


Figure: PMF of Poisson distribution

- Instead, we could assume that  $X \sim \text{Poisson}(\lambda)$  with single parameter<sup>2</sup>

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<sup>2</sup>[https://en.wikipedia.org/wiki/Poisson\\_distribution](https://en.wikipedia.org/wiki/Poisson_distribution)

# Density Estimation

- ▶ The density estimation is the problem of modeling a probability density function  $p(x)$  given a finite number of data points,  $\{x_i\}_{i=1}^n$  drawn from that density function
- ▶ Approaches to density estimation
  - ▶ **Parametric estimation** (this lecture) assumes a specific functional form for density model governed by a set of parameters, and finds the most likely parameters that explain the data.
  - ▶ **Nonparametric estimation** has no specific function form, and allows the form of the density to be determined entirely by the data, e.g., histogram<sup>3</sup>, kernel density estimation.

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<sup>3</sup><https://en.wikipedia.org/wiki/Histogram>

# Parameter Estimation (1)

## Definition (Parametric statistical model)

Let the observed outcome of a statistical experiment be a sample  $X_1, \dots, X_n$  of  $n$  i.i.d. random variables in some measurable space  $\Omega$  (usually  $\Omega \subseteq \mathbb{R}$  and denote by  $p$  their common distribution. A statistical model associated to that statistical experiment is a pair

$$(\Omega, (p_\theta)_{\theta \in \Theta}) ,$$

where

- ▶  $\Omega$  is sample space
- ▶  $(p_\theta)_{\theta \in \Theta}$  is a family of probability measures on  $\Omega$ , e.g., Bernoulli, Gaussian, ...
- ▶  $\Theta \subseteq \mathbb{R}^d$  is parameter set (for some  $d \geq 1$ )

# Parameter Estimation (2)

- ▶ Usually, we will assume that the statistical model is well specified, i.e.,  $\exists \theta_* \in \Theta$  s.t.  $p = p_{\theta_*}$
- ▶ This particular  $\theta_*$  is called the **true parameter**, and is unknown
- ▶ The aim of the statistical experiment is to estimate  $\theta_*$ , or check it's properties when they have a special meaning, e.g.,  $\theta > 1$ ? or  $\theta \neq 1/2$ ?, ...
- ▶ But, the fundamental problem is finding  $\hat{\theta} \approx \theta_*$ , where the quality of approximation is often measured<sup>5</sup> by
  - ▶ Bias  $(\mathbb{E}_D[\hat{\theta}] - \theta_*)$  and variance  $\mathbb{E}_D[(\mathbb{E}_D[\hat{\theta}] - \hat{\theta})^2]$
  - ▶ Note that if  $\Theta \subseteq \mathbb{R}$ ,  $\text{risk} = \text{bias}^2 + \text{variance}$

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<sup>4</sup>hat (^) indicates an estimated value in general.

<sup>5</sup>Note that  $\hat{\theta}$  is a random variable.

## Additional Slides: Bias-Variance Tradeoff

To measure the quality of estimator, we use  $\text{Risk} = \text{Bias}^2 + \text{Variance}$ . Where does this come from?

From mean squared error of an estimator,

$$\begin{aligned}\mathbb{E}[(\hat{\theta} - \theta_*)^2] &= \mathbb{E}[\hat{\theta}^2 - 2\theta_* \cdot \hat{\theta} + \theta_*^2] \\&= \mathbb{E}[\hat{\theta}^2] - 2\theta_* \mathbb{E}[\hat{\theta}] + \theta_*^2 \\&= \mathbb{E}[\hat{\theta}^2] - 2\theta_* \mathbb{E}[\hat{\theta}] + \theta_*^2 + \mathbb{E}^2[\hat{\theta}] - \mathbb{E}^2[\hat{\theta}] \\&= \underbrace{(\mathbb{E}[\hat{\theta}] - \theta_*)^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}[\hat{\theta}^2] - \mathbb{E}^2[\hat{\theta}]}_{\text{Var}(\hat{\theta})}\end{aligned}$$

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# Maximum Likelihood Estimation (MLE)

- ▶ The **likelihood function**  $\mathcal{L}(\theta; \mathcal{D}) := p(\mathcal{D} \mid \theta) = p_{\theta}(\mathcal{D})$  expresses how probable the observation is for different values of parameter  $\theta$
- ▶ MLE finds the parameters  $\hat{\theta}_{\text{MLE}}$  **maximizing the likelihood function**, i.e.,

$$\hat{\theta}_{\text{MLE}} := \arg \max_{\theta} \mathcal{L}(\theta; \mathcal{D}) .$$



# Maximum log-Likelihood Estimation (MLE)

The log-likelihood  $\ell(\theta; \mathcal{D}) := \log(\mathcal{L}(\theta; \mathcal{D}))$  is often used

- ▶ Since that log is monotonically increasing, we have

$$\hat{\theta}_{\text{MLE}} := \arg \max_{\theta} \mathcal{L}(\theta; \mathcal{D}) = \arg \max_{\theta} \ell(\theta; \mathcal{D}) .$$

- ▶ Suppose each point of  $\mathcal{D} = \{x_1, \dots, x_n\}$  is drawn **independently** from  $p(\cdot \mid \theta)$ . Then, we have  $p(\mathcal{D} \mid \theta) = \prod_{i=1}^n p(x_i \mid \theta)$  and thus

$$\ell(\theta; \mathcal{D}) = \sum_{i=1}^n \log(p(x_i \mid \theta)) .$$

## An Example of MLE: Binomial distribution

Assume we have observed  $x$  heads out of  $n$  trials of a coin flip from  $\text{Bin}(x|\mu, n)$  with unknown  $\mu$ . Then, MLE solution maximizes the following loss function:

$$\begin{aligned}\ell_{\text{MLE}}(\mu) &= \log p(x|\mu) \\ &= \log \binom{n}{x} \mu^x (1 - \mu)^{n-x} \\ &\propto x \log \mu + (n - x) \log(1 - \mu)\end{aligned}$$

Then, it follows from solving  $\frac{\partial \ell_{\text{MLE}}}{\partial \mu} = 0$  that

$$\hat{\mu}_{\text{MLE}} = \frac{x}{n}.$$

## An Example of MLE: Gaussian (1)

Suppose that we wish to estimate  $\mu$  from its noisy observation  $x_i \underset{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, \sigma^2)$  for  $i = 1, \dots, n$

- ▶ Estimator 1: takes the first sample only, i.e.,  $\hat{\mu} = x_1$ , then

$$\mathbb{E}[\hat{\mu}] = \mu, \quad \text{and} \quad \text{Var}(\hat{\mu}) = \sigma^2,$$

- ▶ Estimator 2: takes the average, i.e.,  $\bar{\mu} = \frac{1}{n} \sum_{i=1}^n x_i$ , then

$$\mathbb{E}[\bar{\mu}] = \mu, \quad \text{and} \quad \text{Var}(\bar{\mu}) = \frac{\sigma^2}{n},$$

Both estimators are **unbiased**, i.e.,  $\mathbb{E}[\hat{\mu}] = \mathbb{E}[\bar{\mu}] = \mu$ , but

$$\text{Var}(\bar{\mu}) \leq \text{Var}(\hat{\mu}),$$

i.e., the risk of  $\bar{\mu} = 0^2 + \sigma^2/n$  is smaller than the risk of  $\hat{\mu} = 0^2 + \sigma^2$

## An Example of MLE: Gaussian (2)

- ▶ It turns out that the empirical mean  $\bar{\mu} = \mu_{\text{MLE}}$  .
- ▶ From now on, we will obtain the MLE solution  $\hat{\theta}_{\text{MLE}}$  s.t.

$$\hat{\theta}_{\text{MLE}} = (\hat{\theta}_{\text{MLE},1}, \hat{\theta}_{\text{MLE},2}) \approx \theta = (\theta_1, \theta_2) = (\mu, \sigma^2)$$

- ▶ The parameterized density  $p(x | \theta)$  is given by

$$p(x | \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right) .$$

- ▶ The log-likelihood with  $\theta = (\theta_1, \theta_2) = (\mu, \sigma^2)$  is given as

$$\ell(\theta) = \sum_{i=1}^n \log p(x_i | \theta) = \sum_{i=1}^n \left[ -\frac{1}{2} \log(2\pi\theta_2) - \frac{1}{2\theta_2} (x_i - \theta_1)^2 \right]$$

## An Example of MLE: Gaussian (3)

We find stationary points by solving  $\nabla_{\theta} \ell(\theta) = 0$ :

$$\frac{1}{\theta_2} \sum_{i=1}^n (x_i - \theta_1) = 0, \quad \text{and} \quad -\sum_{i=1}^n \frac{1}{2\theta_2} + \sum_{i=1}^n \frac{(x_i - \theta_1)^2}{2\theta_2^2} = 0.$$

This leads to the following MLE solution:

$$\hat{\theta}_{\text{MLE},1} = \frac{1}{n} \sum_{i=1}^n x_i \approx \mu, \quad (\text{sample mean})$$

$$\hat{\theta}_{\text{MLE},2} = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\theta}_{\text{MLE},1})^2 \approx \sigma^2. \quad (\text{sample variance})$$

## Additional Slide: An Interpretation of MLE (1)

Suppose that each sample of dataset  $\mathcal{D} = \{x_i\}_{i=1}^n$  is drawn independently from an underlying distribution  $p(x | \theta)$ , i.e.,

- ▶ Empirical distribution  $\tilde{p}(x) = \frac{1}{n} \sum_{i=1}^n \delta(x - x_i)$  and model  $p(x | \theta)$ , where  $\delta(\cdot)$  is Dirac-delta function
- ▶ Dirac-delta function has the following characteristics<sup>6</sup>:
  - ▶  $\delta(x) = \begin{cases} \infty, & x = 0 \\ 0, & x \neq 0 \end{cases}$
  - ▶  $\int_{-\infty}^{\infty} \delta(x) dx = 1$

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<sup>6</sup>The Dirac delta is not a function in the traditional sense.

## Additional Slide: An Interpretation of MLE (2)

- ▶ Model fitting can be done by minimizing a distance between the empirical distribution and model.
- ▶ A famous distance **Kullback-Leibler (KL) divergence**:

$$\text{KL}(p\|q) := \int p(x) \log \frac{p(x)}{q(x)} dx$$

- ▶ When KL divergence is selected, we have the correspondence between MLE and KL matching

$$\arg \min_{\theta} \text{KL}(\tilde{p}\|p_{\theta}) = \hat{\theta}_{MLE} .$$

# Proof of “MLE = KL Matching”

- ▶ Empirical distribution:  $\tilde{p}(x) = \frac{1}{n} \sum_{i=1}^n \delta(x - x_i)$
- ▶ Model:  $p(x \mid \theta) = p_\theta(x)$

$$\begin{aligned}\arg \min_{\theta} \text{KL}(\tilde{p} \| p_{\theta}) &= \arg \min_{\theta} \int \tilde{p}(x) \log \frac{\tilde{p}(x)}{p_{\theta}(x)} dx \\&= \arg \min_{\theta} \left[ -H(\tilde{p}) - \int \tilde{p}(x) \log p_{\theta}(x) dx \right] \\&= \arg \max_{\theta} \frac{1}{n} \int \sum_{i=1}^n \delta(x - x_i) \log p_{\theta}(x) dx \\&= \arg \max_{\theta} \frac{1}{n} \sum_{i=1}^n \log p_{\theta}(x_i) =: \hat{\theta}_{\text{MLE}}\end{aligned}$$



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# Motivation

We have a coin, and a probability to get a head of the coin is  $\mu$ .

- ▶ We flipped the coin 10 times and observed 7 heads and 3 tails.
- ▶ Q: what would be the most plausible value  $\mu$  given these observations?
  - ▶ A:  $\hat{\mu}_{\text{MLE}} = 0.7$
- ▶ However, we know that a coin is fair in general (i.e.  $\mu = 0.5$ ). So, the result from MLE may be just because of the small number of experiments.
  - ▶ How can we encode such belief (a coin is fair) into our statistical framework?

# Maximum A Posteriori (MAP)

- ▶ As MLE does, MAP has a probability model  $p(\mathcal{D} \mid \theta)$  generating data  $\mathcal{D}$  from parameter  $\theta$ ; but assumes a **a priori distribution**  $p(\theta \mid \alpha)$  of parameter additionally.
  - ▶ The **hyper-parameter**  $\alpha$  defines the prior.
  - ▶ The Latin phrases: "a priori" = "from the earlier" and "a posteriori" = "from the later"
- ▶ MAP finds the parameters  $\hat{\theta}_{\text{MAP}}$  maximizing a **posteriori distribution**  $p(\theta \mid \mathcal{D})$ , i.e.,

$$\hat{\theta}_{\text{MAP}} := \arg \max_{\theta} p(\theta \mid \mathcal{D})$$

## MAP vs. MLE

$$\begin{aligned}\hat{\theta}_{\text{MAP}} &:= \arg \max_{\theta} p(\theta \mid \mathcal{D}) \\ &= \arg \max_{\theta} \frac{p(\mathcal{D} \mid \theta)p(\theta)}{p(\mathcal{D})} \\ &= \arg \max_{\theta} p(\mathcal{D} \mid \theta)p(\theta) \\ &= \arg \max_{\theta} [\log p(\mathcal{D} \mid \theta) + \log p(\theta)] .\end{aligned}$$

- ▶ The prior  $p(\theta)$  plays a critical role in protecting against overfitting.
- ▶ If our belief says the function should be smooth, then the prior plays like an **regularizer**, which penalizes too complex models, and values simple ones.

## An Example of MAP: Beta-Binomial (0)

Recap the beta distribution

- ▶ Beta distribution is a distribution over  $[0, 1]$ .
- ▶ p.d.f, mean, and variance of  $\text{Beta}(\mu|\alpha, \beta)$  are  $(\alpha, \beta > 0)$

$$p(\mu|\alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \mu^{\alpha-1} (1 - \mu)^{\beta-1}$$
$$\mathbb{E}[\mu] = \frac{\alpha}{\alpha + \beta}$$

where  $\Gamma(\cdot)$  is a gamma function

$$\Gamma(t) := \int_0^{\infty} x^{t-1} \exp(-x) dx, \quad t > 0$$
$$\Gamma(t + 1) = t\Gamma(t)$$

## An Example of MAP: Beta-Binomial (1)

Assume we have observed  $x$  heads out of  $n$  trials of a coin flip from  $\text{Bin}(x|\mu, n)$  with unknown  $\mu$ . Use a prior  $\text{Beta}(\mu|\alpha, \beta)$ . Then, MAP solution maximizes the following loss function:

$$\begin{aligned}\mathcal{L}_{MAP}(\mu) &= \log p(x|\mu) + \log p(\mu) \\ &= \log \binom{n}{x} \mu^x (1 - \mu)^{n-x} + \log \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \mu^{\alpha-1} (1 - \mu)^{\beta-1} \\ &\propto x \log \mu + (n - x) \log(1 - \mu) \\ &\quad + (\alpha - 1) \log \mu + (\beta - 1) \log(1 - \mu)\end{aligned}$$

Then, it follows from solving  $\frac{\partial \mathcal{L}_{MAP}}{\partial \mu} = 0$  that

$$\hat{\mu}_{MAP} = \frac{\alpha + x - 1}{\alpha + \beta + n - 2}.$$

## An Example of MAP: Beta-Binomial (2)

$$\hat{\mu}_{\text{MAP}} = \frac{\alpha + x - 1}{\alpha + \beta + n - 2}$$

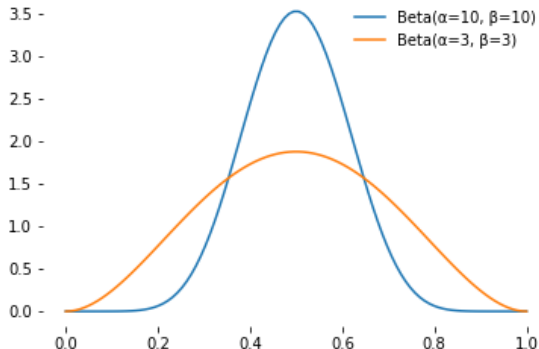
- ▶ Let  $\alpha = \beta = 3$ ,  $x = 7$  and  $n = 10$ , then

$$\hat{\mu}_{\text{MAP}} = \frac{9}{14} = 0.64 \dots < 0.7 = \hat{\mu}_{\text{MLE}}$$

- ▶  $\alpha$  and  $\beta$  is our prior belief about the fairness of a coin.
- ▶ As we increases  $\alpha$  and  $\beta$ ,  $\hat{\mu}_{\text{MAP}}$  approaches to one half.
- ▶ In case of  $n \gg \alpha + \beta$ , i.e., prior is weaker than data, we have

$$\hat{\mu}_{\text{MAP}} \simeq \hat{\mu}_{\text{MLE}}$$

## An Example of MAP: Beta-Binomial (3)



Beta distributions with two parameters  $\alpha$  and  $\beta$ .



## An Example of MAP: Gaussian (1)

Assume  $\mathcal{D}$  is  $n$  i.i.d. copies of univariate Gaussian random variable  $\mathcal{N}(\mu, 1)$  with **unknown**<sup>7</sup>  $\mu$ . Use a prior  $p(\mu | \alpha) \sim \mathcal{N}(0, \alpha^2)$ . Then, MAP solution maximizes the following loss function:

$$\begin{aligned}\mathcal{L}_{MAP}(\theta) &= \log p(\mathcal{D} | \theta) + \log p(\theta) \\ &\propto \left[ -\frac{1}{2} \sum_{i=1}^n (x_i - \mu)^2 - \frac{1}{2\alpha^2} \mu^2 \right]\end{aligned}$$

Then, it follows from solving  $\frac{\partial \mathcal{L}_{MAP}}{\partial \mu} = 0$  that

$$\hat{\mu}_{MAP} = \frac{1}{\left(n + \frac{1}{\alpha^2}\right)} \sum_{i=1}^n x_i .$$

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<sup>7</sup>Here we assume that we know the variance.

## An Example of MAP: Gaussian (2)

- ▶ In case of  $n \gg \frac{1}{\alpha^2}$ , i.e., prior is weaker than data, we have

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

- ▶ In case of  $n \ll \frac{1}{\alpha^2}$ , i.e., prior is stronger than data, we have

$$\hat{\mu}_{\text{MAP}} \simeq 0 .$$

If only few data points are available, the prior will bias the estimate towards the priori expected value.

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- ▶ We flipped the coin 10 times and observed 7 heads and 3 tails.
- ▶ Q: what would be the most plausible value  $\mu$  given these observations?
  - ▶ A:  $\hat{\mu}_{\text{MLE}} = 0.7$  with MLE and  $\hat{\mu}_{\text{MAP}} < 0.7$  with MAP.
- ▶ However, would it be okay to represents the results as a single number?
  - ▶ How much are we sure about the results? (**uncertainty**)

# MLE/MAP as Point-wise Estimator

MLE/MAP extracts a value of parameter  $\hat{\theta} = \hat{\theta}_{\text{MLE}}$  or  $\hat{\theta}_{\text{MAP}}$  representing dataset  $\mathcal{D}$ . From which, our prediction can be done via

- ▶ Unsupervised  $p(x_{\text{new}} \mid \mathcal{D}; \alpha)$  would be  $p(x_{\text{new}} \mid \hat{\theta})$ .
- ▶ Supervised  $p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}; \alpha)$  would be  $p(y_{\text{new}} \mid x_{\text{new}}, \hat{\theta})$ .

Again the prediction is made on a single estimated value.

Due to this property, we call MLE/MAP as a point-wise estimator.

# MLE/MAP vs Bayesian Inference

Bayesian inference tries to estimate them directly via a **weighted average over all values of  $\theta$**  instead of choosing a specific value of parameter:

## ► Unsupervised Bayesian

$$\begin{aligned} p(x_{\text{new}} \mid \mathcal{D}; \alpha) &= \int p(x_{\text{new}} \mid \theta, \mathcal{D}; \alpha) p(\theta \mid \mathcal{D}; \alpha) d\theta \\ &= \int p(x_{\text{new}} \mid \theta) \underbrace{p(\theta \mid \mathcal{D}; \alpha)}_{\text{MAP}} d\theta . \end{aligned}$$

## ► Supervised Bayesian

$$\begin{aligned} p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}; \alpha) &= \int p(y_{\text{new}} \mid x_{\text{new}}, \theta, \mathcal{D}; \alpha) p(\theta \mid \mathcal{D}; \alpha) d\theta \\ &= \int p(y_{\text{new}} \mid x_{\text{new}}, \theta) p(\theta \mid \mathcal{D}; \alpha) d\theta . \end{aligned}$$

Therefore, we need a posterior **distribution!** (instead of a point that maximize the posterior)

# Bayesian Inference: Posterior Calculation

The posterior distribution of  $\theta$  is updated using Bayes rule, where the likelihood is given by  $p(\mathcal{D} \mid \theta) = \prod_{i=1}^n p(x_i \mid \theta)$ :

$$\begin{aligned} p(\theta \mid \mathcal{D}) &= \frac{p(\mathcal{D} \mid \theta)p(\theta)}{p(\mathcal{D})} \\ &= \frac{p(\theta) \prod_{i=1}^n p(x_i \mid \theta)}{\underbrace{\int p(\theta') \prod_{i=1}^n p(x_i \mid \theta') d\theta'}_{\text{We don't ignore anymore}}} \end{aligned}$$

**Conjugate prior:** a good choice of prior for the ease of analysis

- A prior  $p(\theta)$  which gives rise to a posterior  $p(\theta \mid \mathcal{D})$  having the same function form, given  $p(\mathcal{D} \mid \theta)$ .

## Some Conjugate Priors<sup>8</sup>

Prior $p(\theta \mid \alpha)$	Likelihood $p(\mathcal{D} \mid \theta)$	Posterior $p(\theta \mid \mathcal{D}, \alpha)$
Beta	Benoulli	Beta
Beta	Binomial	Beta
Normal	Normal	Normal
Gamma	Gamma	Gamma
Gamma	Poisson	Gamma
Normal-Gamma	Normal	Normal-Gamma

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<sup>8</sup> [https://en.wikipedia.org/wiki/Conjugate\\_prior#Table\\_of\\_conjugate\\_distributions](https://en.wikipedia.org/wiki/Conjugate_prior#Table_of_conjugate_distributions)



# Beta-Bernoulli Conjugacy (1)

Think about coin toss with observation  $x$ .

- ▶ The likelihood of observing  $x$  can be modeled with Bernoulli parameterized by  $\mu$ , i.e,  $p(x|\mu) = \text{Ber}(x|\mu)$  .
- ▶ We don't know  $\mu$ , but we can place a Beta distribution parameterized by  $\alpha, \beta$ ,. i.e  $p(\mu|\alpha, \beta) = \text{Beta}(\mu|\alpha, \beta)$ .
- ▶ Bayes rule tells us the posterior of  $\mu$  given  $x$  as

$$p(\mu|x, \alpha, \beta) = \frac{p(x|\mu)p(\mu|\alpha, \beta)}{p(x|\alpha, \beta)}$$

- ▶ Compute the posterior!

## Beta-Bernoulli Conjugacy (2)

The marginal  $p(x | \alpha, \beta)$  can be obtained by

$$\begin{aligned} p(x | \alpha, \beta) &= \int p(x|\mu)p(\mu|\alpha, \beta)d\mu \\ &= \int \mu^x(1-\mu)^{1-x} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \mu^{\alpha-1}(1-\mu)^{\beta-1} d\mu \\ &= \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \underbrace{\int \mu^{x+\alpha-1}(1-\mu)^{\beta-x} d\mu}_{\text{Beta function}} \\ &= \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{\Gamma(\alpha+x)\Gamma(\beta-x+1)}{\Gamma(\alpha+\beta+1)} \end{aligned}$$

The posterior distribution can then be derived as

$$\frac{p(x|\mu)p(\mu|\alpha, \beta)}{p(x|\alpha, \beta)} \sim \text{Beta}(x + \alpha, \beta - x + 1)$$

## Beta-Bernoulli Conjugacy (3)

Since  $p(x|\alpha, \beta)$  is just a part of normalizing constant making  $\int p(\mu|x) d\mu = 1$ , you can directly obtain posterior from

$$\begin{aligned}\frac{p(x|\mu)p(\mu|\alpha, \beta)}{p(x|\alpha, \beta)} &\propto \mu^x(1-\mu)^{1-x} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \mu^{\alpha-1}(1-\mu)^{\beta-1} \\ &\propto \mu^{x+\alpha-1}(1-\mu)^{\beta-x} \\ &\sim \text{Beta}(x+\alpha, \beta-x+1)\end{aligned}$$

In other words, from  $\int A\mu^{x+\alpha-1}(1-\mu)^{\beta-x} d\mu = 1$  where  $A$  is a normalizing constant, we can directly obtain Beta distribution.

This result can be generalized to the Beta-Binomial case.

## Some Conjugate Priors<sup>9</sup>

Prior $p(\theta \mid \alpha)$	Likelihood $p(\mathcal{D} \mid \theta)$	Posterior $p(\theta \mid \mathcal{D}, \alpha)$
Beta	Benoulli	Beta
Beta	Binomial	Beta
Normal	Normal	Normal
Gamma	Gamma	Gamma
Gamma	Poisson	Gamma
Normal-Gamma	Normal	Normal-Gamma

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<sup>9</sup> [https://en.wikipedia.org/wiki/Conjugate\\_prior#Table\\_of\\_conjugate\\_distributions](https://en.wikipedia.org/wiki/Conjugate_prior#Table_of_conjugate_distributions)

# Bayesian Inference: Normal-Normal (1)

For a given set  $\mathcal{D} = \{x_i\}_{i=1}^n$  of  $n$  real numbers, assume that:

- ▶ (as model) each  $x_i$  is drawn independently from  $\mathcal{N}(\mu, \sigma^2)$
- ▶ (as prior)  $\sigma^2$  is known in advance, and  $\mu$  is drawn from  $\mathcal{N}(\mu_0, \sigma_0^2)$ , of which density function is denoted by  $p_0(\mu; \mu_0, \sigma_0^2)$ .

The posterior is calculated as follows:

$$p(\mu \mid \mathcal{D}) = \frac{p_0(\mu)}{p(\mathcal{D})} \prod_{i=1}^n p(x_i \mid \mu) ,$$

where

$$p(x_i \mid \mu) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{1}{2\sigma^2} (x_i - \mu)^2 \right) .$$

## Bayesian Inference: Normal-Normal (2)

After a basic calculus, we have

$$p(\mu \mid \mathcal{D}) = \frac{1}{\sqrt{2\pi\tilde{\sigma}^2}} \exp\left(-\frac{1}{2\tilde{\sigma}^2} (\mu - \tilde{\mu})^2\right),$$

where

$$\tilde{\mu} = \frac{\frac{\mu_0}{\sigma_0^2} + \sum_{i=1}^n \frac{1}{\sigma^2} x_i}{\frac{1}{\sigma_0^2} + \sum_{i=1}^n \frac{1}{\sigma^2}} \quad \text{and} \quad \frac{1}{\tilde{\sigma}^2} = \frac{1}{\sigma_0^2} + \frac{n}{\sigma^2}.$$

- ▶ When  $n = 0$ ,  $\tilde{\mu}$  reduces to the prior mean  $\mu$ .
- ▶ As  $n \rightarrow \infty$ , the posterior mean is given by the ML solution.

## Additional Reading

- ▶ Section 3 of the text book (Probabilistic Machine Learning: An Introduction)
- ▶ Supplementary material on PLMS (Bayesian\_Normal.pdf)