

# Chapter 4: Bayesian Inference

## 강의 목표

- ▶ 베이지안 추론의 이해
  - Likelihood Method
  - Bayesian Method

## Statistical Models: Main Focus

- ▶ Inference about parameters, based on data.

## Notations and Settings: Distributions

- ▶ Denote an unobserved parameter of interest as  $\theta$ .
- ▶ Denote our data as  $\mathbf{D}$ .
- ▶ Our probability model for the data, given a value of  $\theta$ , is denoted  $P(\mathbf{D} \mid \theta)$ .
- ▶ 가정: 주어진 데이터  $D$  혹은  $X$ 는 확률 변수  $\mathbf{X}$ 의 관측치이며  $\mathbf{X}$ 의 분포는 unknown parameter  $\theta$ 에 의존하는 density function  $f(\cdot \mid \theta)$ 를 가진다.

e.g.: Normal distribution  $N(\mu, \sigma^2)$

## Notations and Settings: Data

- ▶ Suppose we observe an iid sample of data  $X = (X_1, \dots, X_n)$ .
- ▶ Now  $X$  is considered fixed and known.
- ▶ Denote our data as the  $n \times k$  matrix  $X$ .
- ▶ We denote the parameter(s) of interest to be the vector  $\theta$ .

## Likelihood Theory

- ▶ The **likelihood function**:  $L(\theta | X) = f(X | \theta)$ .
- ▶  $L(\theta | X)$  is a function of  $\theta$  that shows how “likely” are various parameter values  $\theta$  to have produced the data  $X$  that **were observed**.

## Likelihood Principle

- ▶ Mathematically, if the data  $X$  represent iid observations from probability distribution  $p(X | \theta)$ , then

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

where  $X_1, \dots, X_n$  are the  $n$  data vectors.

## Likelihood Theory

- ▶ 목표: Parameter  $\theta$
- ▶ 주어진 정보: 데이터  $X$
- ▶ 데이터  $X$ 가  $\theta$ 정보를 가지고 있으므로  $X$ 를 통해  $\theta$ 를 추측.
- ▶ 주의해야 할 점:  $\theta$ 가  $X$ 의 분포를 결정.  $X$ 가  $\theta$ 를 결정하는 것이 아님.



## Maximum Likelihood Estimator (MLE)

- ▶ In classical statistics, the specific value of  $\theta$  that maximizes  $L(\theta | X)$  is the maximum likelihood estimator (MLE) of  $\theta$ .
- ▶ e.g., 동전을 100회 던졌을때 앞면이 100회 연속 나왔다고 가정하자. 동전을 던졌을때 앞면이 나올 확률  $p$ 는 다음 중 어느 것이 더 가능성이 있을까?
  1.  $p = 0$
  2.  $p = 0.5$
  3.  $p = 1$

## Likelihood Limitations

In many common probability models, when the sample size  $n$  is large,

- ▶  $L(\theta | X)$  is unimodal in  $\theta$ .
- ▶  $L(\theta | X)$  is strictly concave.
- ▶ Unlike  $P(\theta | X)$ ,  $L(\theta | X)$  does not necessarily obey the usual laws for probability distributions.
- ▶ In the classical framework, all the randomness within  $L(\theta | X)$  is attached to  $X$ , not to  $\theta$

## Likelihood Example

- ▶ 성공확률이  $\theta$ 인 베르누이 시행을 10번 독립적으로 반복했을 때 성공횟수  $\mathbf{X}$ 는 이항분포  $B(10, \theta)$ 를 따른다.  $\mathbf{X}$ 의 관측치로  $X = 3$ 을 얻었다면  $\theta$ 의 Likelihoods는

$$L(\theta \mid X = 3) = f(3 \mid \theta) = \binom{10}{3} \theta^3 (1 - \theta)^7$$

## Likelihood Example

- ▶ The first derivative of the log likelihood  $\ell(\theta \mid X = 3)$  is as follows:

$$\frac{\partial \ell(\theta \mid X = 3)}{\partial \theta} = 3 \frac{1}{\theta} - 7 \frac{1}{1 - \theta}.$$

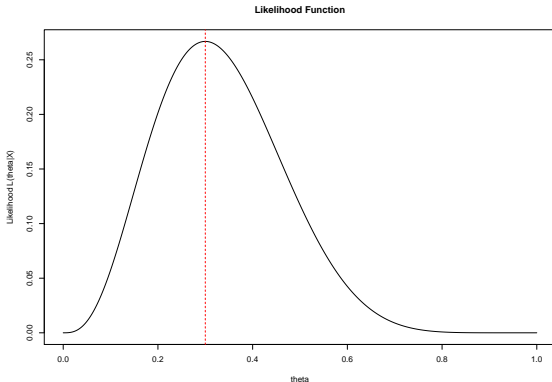
- ▶ From the first order optimality condition,

$$3(1 - \theta) - 7\theta = 0$$

- ▶ Hence MLE:  $\hat{\theta} = 0.3$ .

# Likelihood Example

```
> theta = seq(0,1, length = 1000)
> ltheta = choose(10,3)*theta^3*(1-theta)^7
> plot(theta, ltheta, type = "l", main = "Likelihood Function",
      ylab = "Likelihood L(theta|X)")
> abline(v = 0.3, lty = 2, col=2 )
```



## Likelihood Example: Negative Binomial

- ▶ 성공확률이  $\theta$ 인 베르누이 시행을 3번째 성공이 나올 때까지 실험을 계속하기로 한다면 실패횟수  $\mathbf{X}$ 는 음이항 분포  $NB(3, \theta)$ 를 따르게 된다. 관측치  $X = 7$ 이라고 하자.

$$L(\theta \mid X = 7) = f(3 \mid \theta) = \binom{3 + 7 - 1}{7} \theta^3 (1 - \theta)^7$$

- ▶ MLE:  $\hat{\theta} = 0.3$ .

## Maximum Likelihood Estimator (MLE)

- ▶ MLE는 분포의 **kernel**에 의존한다.
- ▶ Binomial Dist:  $\theta^3(1 - \theta)^7$
- ▶ Negative Binomial Dist:  $\theta^3(1 - \theta)^7$

## Likelihood Principle

- ▶ The Likelihood Principle of Birnbaum states that (given the data) **all** of the evidence about  $\theta$  is contained in the likelihood function.
- ▶ 통계적 실험에서 데이터가 가지고 있는  $\theta$ 의 추론에 관한 정보는 Likelihood function에 모두 포함되어 있다.
- ▶ Likelihood Principle implies: Two experiments that yield equal (or proportional) likelihoods should produce equivalent inference about  $\theta$ .



## Likelihood Ratio

- ▶ What if  $L(\theta \mid X)$  is not differentiable?
- ▶ How to compare two values for  $\theta$ ?
- ▶ Likelihood Ratio:

$$f(X \mid \theta_a)/f(X \mid \theta_b) = L(\theta_a \mid X)/f(\theta_b \mid X)$$

## Likelihood Ratio Example

$X = X_1, \dots, X_n$  이  $N(\theta, 1)$ 을 따를  $\theta_a$ 와  $\theta_b$ 의 Likelihood Ratio (LR)를 구하여라.

▶ 정의에 따르면 LR은 다음과 같다.

$$\begin{aligned} L(\theta_a | X) / L(\theta_b | X) &= \frac{(2\pi)^{n/2} \exp(-\sum_{i=1}^n (X_i - \theta_a)^2 / 2)}{(2\pi)^{n/2} \exp(-\sum_{i=1}^n (X_i - \theta_b)^2 / 2)} \\ &= \frac{\exp(-\sum_{i=1}^n (X_i - \theta_a)^2 / 2)}{\exp(-\sum_{i=1}^n (X_i - \theta_b)^2 / 2)} \\ \ell(\theta_a | X) - \ell(\theta_b | X) &\propto \sum (2\theta_a X_i - \theta_a^2) - \sum (2\theta_b X_i - \theta_b^2) \\ &= 2n(\theta_a - \theta_b)\bar{X} - n(\theta_a^2 - \theta_b^2) \end{aligned}$$

## Likelihood Ratio Example

Consider  $\theta_a = 0$  and  $\theta_b = 1$ . If  $n = 10, \bar{x} = 0.1$

▶ 정의에 따르면 LR은 다음과 같다.

$$\begin{aligned}\ell(\theta_a | X) - \ell(\theta_b | X) &\propto 2n(\theta_a - \theta_b)\bar{X} - n(\theta_a^2 - \theta_b^2) \\ &= 2 \times 10(0 - 1)0.1 - 10(0 - 1) \\ &= -2 + 10 = 8\end{aligned}$$

## Sufficient Statistics

- ▶ Sufficient Statistics (충분통계량):  
 $\mathbf{X}$ 가 밀도함수  $f(\mathbf{X} | \theta)$ 를 갖는다고 하자.  $T(\mathbf{X})$ 가 주어졌을 때  $\mathbf{X}$ 의 조건부 분포가  $\theta$ 에 의존하지 않으면  $T(\mathbf{X})$ 를  $\theta$ 의 충분통계량이라고 한다.
- ▶  $T(\mathbf{X})$ :  $\theta$ 의 모든 정보를 가진 통계량
- ▶ 위 Normal 분포의 예의 경우 충분통계량은  $\bar{X}$ .
- ▶ 충분통계량  $T(\mathbf{X})$ 의 예:  $\bar{X}, \sum X, \sum (X_i - \bar{X})^2, \max X, \min X$

## Sufficient Statistics

- ▶ Likelihood Principle에 따르면,  $\theta$ 의 모든 정보는  $X$ 에 포함되어 있다.
- ▶ Sufficient Statistics에 따르면,  $\theta$ 의 모든 정보는  $T(X)$ 에 포함되어 있다.
- ▶ Hence,  $T(X)$  is sufficient to estimate  $\theta$ .
- ▶ 데이터가 가진  $\theta$ 의 정보가  $T(X)$ 에 모두 포함되어 있으므로  $T(X)$ 만 알면 더 이상 데이터의 다른 내용은 몰라도 충분하다.

## Ancillary Statistics

- ▶ Ancillary Statistics (보조 통계량): 통계량의 분포가  $\theta$ 와 무관하여  $\theta$ 에 대한 정보를 전혀 가지고 있지 않은 통계량
- ▶ Sufficient Statistics의 반대 개념

## Ancillary Statistics

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- ▶ Sufficient Statistics의 반대 개념
- ▶ i.e., 보조 통계량은  $\theta$ 의 정보가 없으므로  $\theta$ 의 추정에 아무런 도움이 안된다.

## Ancillary Statistics Example

두 변수  $X_1, X_2$ 는 모두  $U(\theta - 1, \theta + 1)$ 의 Uniform 분포를 따른다.  
이때 두 변수의 차이  $X_1 - X_2$ 는  $\theta$ 의 정보를 전혀 갖지 않는다.



## Ancillary Statistics Example

두 변수  $X_1, X_2, \dots, X_n$ 는 모두 iid  $N(\theta, 1)$ 의 분포를 따른다. 이때 sample variance ( $s^2$ )는  $\theta$ 의 정보를 전혀 갖지 않는다.

$$s^2 = \frac{1}{n-1} \sum (X_i - \bar{X})^2$$

## Review

- ▶ The main difference between Bayesian and Frequentist is how to consider  $\theta$ .
  - ▶ Constant:  $P(\theta = 0) = 1$  or  $0$ .
  - ▶ Variable: there exists a distribution for  $\theta$ .

# Bayesian Method

- ▶ Ultimate Goal: To make probability statements about  $\theta$ , given some observed data:  $p(\theta \mid \mathbf{D})$ .
- ▶ Using Bayes' Law,

$$p(\theta \mid \mathbf{D}) = \frac{p(\theta)p(\mathbf{D} \mid \theta)}{p(\mathbf{D})}.$$

- ▶ There are two challenges
  1. How to find  $p(\theta)$ ?
  2. How to find  $p(\mathbf{D})$ ?

# Prior Distribution

- ▶ How to find prior  $P(\theta)$ ?

In usual, we assume the prior distribution for  $\theta$ .

1. Informative Prior
2. Non-informative Prior

- ▶ We must specify  $P(\theta)$  based on any knowledge we have about  $\theta$  **before** observing the data.
- ▶ This could be highly specific or quite vague, depending how uncertain we are about  $\theta$ .

e.g., Albert가 아빠일 확률

## Data Distribution

### ► How to find $P(\mathbf{D})$ ?

1.  $P(\mathbf{D})$  does not depend on  $\theta$  and thus carries no information about  $\theta$ .
2. It is simply a **normalizing constant** which makes  $P(\theta | \mathbf{D})$  sum or integrate to 1.

# Posterior Distribution

- ▶ For inference about  $\theta$ , it is just as good to write.

$$p(\theta \mid \mathbf{D}) \propto p(\theta)p(\mathbf{D} \mid \theta)$$

- ▶ The LHS is called the **posterior distribution** of  $\theta$
- ▶ We can calculate the posterior distribution by
  1. Multiplying the prior by the likelihood.
  2. Normalizing the posterior at the last step.
- ▶ The posterior distribution represents a compromise between the prior information about  $\theta$  in  $p(\theta)$  and the information from the sample about  $\theta$  in  $p(\mathbf{D} \mid \theta)$ .

## Useful Statistics Using Bayes' Law

Once we obtain the posterior distribution we can use any summaries such as mean, median, variance and many others.

- ▶ **Posterior mean**

$$\mathbb{E}[\theta \mid \mathbf{D}] = \int \theta \cdot p(\theta \mid \mathbf{D}) d\theta.$$

For ease of notation,

- ▶ Posterior distribution:  $\pi(\theta \mid x), p(\theta \mid x)$ .
- ▶ Prior distribution:  $\pi(\theta), p(\theta)$ .

## Statistics Using Bayes' Law

- ▶ The **posterior variance** is

$$\begin{aligned}\text{Var}(\theta \mid \mathbf{D}) &= E \{ (\theta - E(\theta \mid \mathbf{D}))^2 \mid \mathbf{D} \} \\&= \int (\theta - E(\theta \mid \mathbf{D}))^2 1 p(\theta \mid \mathbf{D}) d\theta \\&= \int \theta^2 p(\theta \mid \mathbf{D}) d\theta - 2E(\theta \mid \mathbf{D}) \int \theta p(\theta \mid \mathbf{D}) d\theta \\&\quad + E(\theta \mid \mathbf{D})^2 \int p(\theta \mid \mathbf{D}) d\theta \\&= E(\theta^2 \mid \mathbf{D}) - E(\theta \mid \mathbf{D})^2\end{aligned}$$

- ▶ If the values of  $\theta$  are discrete, sums would replace the integrals.



## Posterior Example

성공확률이  $\theta$ 인 베르누이 시행을 10번 독립적으로 반복했을 때 성공횟수  $\mathbf{X}$ 는 이항분포  $B(10, \theta)$ 를 따른다.  $\mathbf{X}$ 의 관측치로  $X = 3$ 을 얻었다면  $\theta$ 의 Posterior를 구하시오.

- ▶ Prior Distribution (사전 분포)에 대한 정보가 없으므로  $\theta$ 의 분포를  $U(0, 1)$ 으로 가정한다.
- ▶ Posterior Distribution

$$\begin{aligned}\pi(\theta \mid X = 3) &= \frac{\binom{10}{3}\theta^3(1-\theta)^7}{\int_0^1 \binom{10}{3}\theta^3(1-\theta)^7 d\theta} \\ &= \frac{\Gamma(12)}{\Gamma(4)\Gamma(8)}\theta^3(1-\theta)^7.\end{aligned}$$

## Posterior Example

Due the joint density function or kernel  $\theta^3(1 - \theta)^7$ , the posterior distribution is Beta(4,8). Then,

- ▶ Posterior Mean:  $1/3$
- ▶ Posteiror SD: 0.13

## Principles of Bayesian Inference

- ▶  $\theta$  에 대한 이론, 경험, 과거의 자료 등 가능한 정보로부터 사전분포 (Prior)  $\pi(\theta)$ 를 구한다.
- ▶ 관측변수  $X$ 를 정하고 통계조사나 실험 등을 통하여 데이터를 얻는다. 적절한 통계 모형으로 부터  $\theta$ 가 주어졌을 때 관측데이터의 조건부 밀도함수  $f(X | \theta)$ 를 구한다.
- ▶ 베이즈 정리를 이용하요 Posterior 분포 (사후분포)를 구하고 이를 추정에 사용한다.
- ▶ 즉, Posterior Distribution이  $\theta$ 의 모든 정보를 가지고 있다.

## Binomial Distribution

If the random variable  $X$  follows the binomial distribution with parameters  $n \in \mathcal{N}$  and  $p \in [0, 1]$ , we write  $X \sim B(n, p)$ .

$$\Pr(x; n, p) = \Pr(X = x) = \binom{n}{x} p^x (1 - p)^{n-x}.$$

$$\mathbb{E}(X) = np,$$

$$\text{Var}(X) = np(1 - p).$$

## Negative Binomial Distribution

베르누이 시행을 미리 정한 성공횟수  $r$  회가 될 때까지 반복 시행할 때 확률변수  $X$  (실패횟수 또는 시행횟수)가 나타내는 분포를 말한다. The probability mass function of the negative binomial distribution is

$$\Pr(X = x) = \binom{k+r-1}{k} p^r (1-p)^x \quad \text{for } k = 0, 1, 2, \dots,$$

$$\mathbb{E}(X) = \frac{pr}{1-p},$$

$$\text{Var}(X) = \frac{pr}{(1-p)^2}.$$

## Poisson

A discrete random variable  $X$  is said to have a Poisson distribution with parameter  $\lambda > 0$ , if, for  $x = 0, 1, 2, \dots$ , the probability mass function of  $X$  is given by

$$Pr(X = x) = \frac{\lambda^x e^{-\lambda}}{x!}$$

$$\mathbb{E}(X) = \lambda,$$

$$\text{Var}(X) = \lambda.$$

## Uniform

The probability density function of the continuous uniform distribution is

$$\Pr(x; \alpha, \beta) = \Pr(X = x) = \frac{1}{\beta - \alpha} \quad \text{for } \alpha \leq x \leq \beta$$

$$\mathbb{E}(X) = \frac{\beta + \alpha}{2},$$

$$\text{Var}(X) = \frac{(\beta - \alpha)^2}{12}.$$

## Gamma

The gamma distribution can be parameterized in terms of a shape parameter  $\alpha$  and an inverse scale parameter  $\beta$ , called a rate parameter. The corresponding probability density function in the shape-rate parametrization is

$$\Pr(x; \alpha, \beta) = \Pr(X = x) = \frac{1}{\Gamma(\alpha)\beta^\alpha} x^{\alpha-1} e^{-\frac{x}{\beta}} \quad \text{for } x > 0,$$

$$\mathbb{E}(X) = \alpha\beta,$$

$$\text{Var}(X) = \alpha\beta^2.$$



## Inverse Gamma

The inverse gamma distribution's probability density function is defined over the support  $x > 0$

$$\Pr(x; \alpha, \beta) = \Pr(X = x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{-\alpha-1} e^{-\frac{\beta}{x}} \quad \text{for } x > 0$$

$$\mathbb{E}(X) = \frac{\beta}{\alpha - 1},$$

$$\text{Var}(X) = \frac{\beta^2}{(\alpha - 1)^2(\alpha - 2)}.$$

## Normal

The probability density of the normal distribution is

$$\Pr(x; \mu, \sigma^2) = \Pr(X = x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad \text{for} \quad -\infty < x < \infty,$$

$$\mathbb{E}(X) = \mu,$$

$$\text{Var}(X) = \sigma^2.$$

## Student T

Student's t-distribution has the probability density function given by

$$\Pr(x; \nu) = \frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi}\Gamma(\frac{\nu}{2})} \left(1 + \frac{x^2}{\nu}\right)^{-\frac{\nu+1}{2}} \quad \text{for } -\infty < x < \infty$$

$$\mathbb{E}(X) = 0$$

$$\text{Var}(X) = \begin{cases} \frac{\nu}{\nu-2} & \text{if } \nu > 2 \\ \infty & \text{if } 1 < \nu \leq 2 \end{cases}$$

## Posterior Intervals

- ▶ The ideal summary of  $\theta$  is an interval (or region) with a certain probability of containing  $\theta$ . For some positive  $\alpha$ ,

$$\Pr(L_\alpha \leq \theta \leq U_\alpha) = 1 - \alpha.$$

- ▶ Note that a classical (frequentist) **confidence interval (CI)** does not exactly have this interpretation.

## Definitions of C.I. Coverage

- ▶ **Definition:** A random interval  $L(\mathbf{X}), U(\mathbf{X})$  has  $100(1 - \alpha)\%$  frequentist coverage for  $\theta$  if, **before** the data are gathered,

$$P[L(\mathbf{X}) < \theta < U(\mathbf{X}) \mid \theta] = 1 - \alpha.$$

(Pre-experimental  $1 - \alpha$  coverage)

- ▶ Note that if we observe  $\mathbf{X} = x$  and plug  $x$  into our confidence interval formula,

$$P(L(x) < \theta < U(x) \mid \theta) = \begin{cases} 0 & \text{if } \theta \notin (L(x), U(x)) \\ 1 & \text{if } \theta \in (L(x), U(x)) \end{cases}$$

(**Not** Post-experimental  $1 - \alpha$  coverage)

## Definitions of C.I. Coverage

- ▶ **Definition:** An interval  $(L(x), U(x))$ , based on the observed data  $\mathbf{X} = x$ , has  $100(1 - \alpha)\%$  Bayesian coverage for  $\theta$  if

$$P[L(\mathbf{X}) < \theta < U(\mathbf{X}) \mid \mathbf{X} = x] = 1 - \alpha.$$

(Post-experimental  $1 - \alpha$  coverage)

- ▶ The Frequentist interpretation is less desirable if we are performing inference about  $\theta$  based on a single interval.

## Bayesian Credible Intervals

- ▶ A **credible interval** (or a **credible set**) is the Bayesian analogue of a confidence interval (C.I.)
- ▶ A  $100(1 - \alpha)\%$  credible set  $\mathcal{C}$  is a subset of  $\Theta$  such that

$$\int_{\mathcal{C}} \pi(\theta \mid X) d\theta = 1 - \alpha.$$

- ▶ This is equivalent to

$$\Pr(\theta \in \mathcal{C} \mid x) = 1 - \alpha.$$

- ▶ If the parameter space  $\Theta$  is discrete, a sum replaces the integral.

## Quantile-Based Interval

- ▶ If  $\theta_L^*$  is the  $\alpha/2$  posterior quantile for  $\theta$ , and  $\theta_U^*$  is the  $1 - \alpha/2$  posterior quantile for  $\theta$ , then  $(\theta_L^*, \theta_U^*)$  is a  $100(1 - \alpha)\%$  credible interval for  $\theta$ .
- ▶ Note that  $P(\theta < \theta_L^* | X) = \alpha/2$  and  $P(\theta > \theta_U^* | X) = \alpha/2$ .

$$\begin{aligned} P(\theta \in (\theta_L^*, \theta_U^*) | X) &= 1 - P(\theta \notin (\theta_L^*, \theta_U^*) | X) \\ &= 1 - (P(\theta < \theta_L^* | X) + P(\theta > \theta_U^* | X)) \\ &= 1 - \alpha. \end{aligned}$$



## Example: Quantile-Based Interval

- ▶ Suppose  $X_1, \dots, X_n$  are the durations of cabinets for a sample of cabinets from Western European countries.
- ▶ We assume the  $X_i$ 's follow an exponential distribution.

$$p(X_i | \theta) = \theta e^{-\theta X_i}, \quad X_i > 0,$$

$$L(\theta | X) = \theta^n e^{-\theta \sum_{i=1}^n X_i}.$$

- ▶ Suppose our prior distribution for  $\theta$  is

$$p(\theta) \propto 1/\theta, \quad \theta > 0.$$

→ Larger values of  $\theta$  are less likely a **priori**.

## Example: Quantile-Based Interval

- ▶ Then, we have

$$\pi(\theta \mid x) \propto p(\theta)L(\theta \mid x)$$

## Example: Quantile-Based Interval

► Then, we have

$$\begin{aligned}\pi(\theta \mid x) &\propto p(\theta)L(\theta \mid x) \\ &= \left(\frac{1}{\theta}\right) \theta^n e^{-\theta \sum_{i=1}^n x_i}\end{aligned}$$

## Example: Quantile-Based Interval

► Then, we have

$$\begin{aligned}\pi(\theta \mid x) &\propto p(\theta)L(\theta \mid x) \\ &= \left(\frac{1}{\theta}\right) \theta^n e^{-\theta \sum_{i=1}^n x_i} \\ &= \theta^{n-1} e^{-\theta \sum_{i=1}^n x_i}.\end{aligned}$$

## Example: Quantile-Based Interval

- ▶ Then, we have

$$\begin{aligned}\pi(\theta \mid x) &\propto p(\theta)L(\theta \mid x) \\ &= \left(\frac{1}{\theta}\right) \theta^n e^{-\theta \sum_{i=1}^n x_i} \\ &= \theta^{n-1} e^{-\theta \sum_{i=1}^n x_i}.\end{aligned}$$

- ▶ This is the kernel of a gamma distribution with "shape" parameter  $n$  and "rate" parameter  $\sum_{i=1}^n x_i$ .

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- ▶ This is the kernel of a gamma distribution with "shape" parameter  $n$  and "rate" parameter  $\sum_{i=1}^n x_i$ .
- ▶ After including the normalizing constant,

$$\pi(\theta \mid X) = \frac{(\sum x_i)^n}{\Gamma(n)} \theta^{n-1} e^{-\theta \sum_{i=1}^n x_i}, \quad \theta > 0.$$

## Example: Quantile-Based Interval

- ▶ Now, given the observed data  $x_1, \dots, x_n$ , we can calculate any quantiles of this gamma distribution.



## Example: Quantile-Based Interval

- ▶ Now, given the observed data  $x_1, \dots, x_n$ , we can calculate any quantiles of this gamma distribution.
- ▶ The 0.05 and 0.95 quantiles will give us a 90% credible interval for  $\theta$ .

## Example: Quantile-Based Interval

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$$p(\theta) = 1, \quad \theta > 1$$

(favors all values of  $\theta$  equally).

- ▶ Then our posterior is

$$\begin{aligned}\pi(\theta \mid x) &\propto p(\theta)L(\theta \mid x) \\ &= (1)\theta^n e^{-\theta \sum_{i=1}^n x_i} \\ &= \theta^n e^{-\theta \sum_{i=1}^n x_i}.\end{aligned}$$

## Example: Quantile-Based Interval

- ▶ This is the kernel of a gamma distribution with "shape" parameter  $n + 1$  and "rate" parameter  $\sum_{i=1}^n x_i$ .

## Example: Quantile-Based Interval

- ▶ This is the kernel of a gamma distribution with "shape" parameter  $n + 1$  and "rate" parameter  $\sum_{i=1}^n x_i$ .
- ▶ We can similarly find the equal-tail credible interval.

## Example: Quantile-Based Interval

- ▶ First Case:  $\mathbb{E}(\theta \mid X_1, \dots, X_n) = \frac{n-1}{\sum X_i}$ .
- ▶ Second Case:  $\mathbb{E}(\theta \mid X_1, \dots, X_n) = \frac{n}{\sum X_i}$ .

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- ▶ As  $n \rightarrow \infty$  the both becomes similar.



## Example: Quantile-Based Interval

- ▶ First Case:  $\mathbb{E}(\theta \mid X_1, \dots, X_n) = \frac{n-1}{\sum X_i}$ .
- ▶ Second Case:  $\mathbb{E}(\theta \mid X_1, \dots, X_n) = \frac{n}{\sum X_i}$ .
- ▶ As  $n \rightarrow \infty$  the both becomes similar.
- ▶ Although the priors different, the posterior distributions are similar when  $n$  is sufficiently large enough.

## Example 2: Quantile-Based Interval

- ▶ Consider 10 flips of a coin having  $\Pr(\text{Heads}) = \theta$ .

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- ▶ Consider 10 flips of a coin having  $\Pr(\text{Heads}) = \theta$ .
- ▶ Suppose we observe 2 "heads".
- ▶ We model the count of heads as binomial:

$$p(X = x \mid \theta) = \binom{10}{x} \theta^x (1 - \theta)^{10-x}, \quad x = 0, 1, \dots, 10.$$

- ▶ Let's use a uniform prior for  $\theta$ :

$$p(\theta) = 1, \quad 0 \leq \theta \leq 1.$$

## Example 2: Quantile-Based Interval

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- ▶ This is a **beta distribution** for  $\theta$  with parameters  $x + 1$  and  $10 - x + 1$ .
- ▶ Since  $x = 2$  here,  $\pi(\theta \mid x = 2)$  is beta (3, 9).

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- ▶ This is a **beta distribution** for  $\theta$  with parameters  $x + 1$  and  $10 - x + 1$ .
- ▶ Since  $x = 2$  here,  $\pi(\theta \mid x = 2)$  is beta (3, 9).
- ▶ The 0.025 and 0.975 quantiles of a beta (3, 9) are (.0602, .5178), which is a 95% credible interval for  $\theta$ .

### Example 3: Quantile-Based Interval

$N(\theta, 2^2)$ 분포로부터 16개의 표본을 추출한 결과  $\bar{X} = 0.3$ 이었다.  $\theta$ 에 대한 무정보 사전분포 (non-informative)로  $\pi(\theta) = 1$ 을 가정하고, 이를  $\bar{\mathbf{X}} \mid \theta \sim N(\theta, 2^2/16)$ 과 합성하여 사후분포를 유도하여라. 그리고 대응되는 95% 베이지안 신뢰구간을 구해 보자.

### Example 3: Quantile-Based Interval

$$\pi(\theta \mid \bar{X}) \propto f(\bar{X} \mid \theta)\pi(\theta)$$

### Example 3: Quantile-Based Interval

$$\begin{aligned}\pi(\theta \mid \bar{X}) &\propto f(\bar{X} \mid \theta)\pi(\theta) \\ &\propto \exp\left(-\frac{1}{2 \times 0.25}(0.3 - \theta)^2\right).\end{aligned}$$

Hence the posterior distribution is  $\text{Normal}(0.3, 0.5^2)$

### Example 3: Quantile-Based Interval

- ▶  $\mathcal{C}$ 은 유일하지 않을 수 있다.

### Example 3: Quantile-Based Interval

- ▶  $\mathcal{C}$ 은 유일하지 않을 수 있다.
- ▶ 가장 좋은 신뢰구간은 어떤 것일까?



## Highest Posterior Density (HPD) Intervals

- ▶ Note that values of  $\theta$  around 0.3 have much higher posterior probability than values around 7.5.
- ▶ A better approach here is to create our interval of  $\theta$ -values having the **Highest Posterior Density**.

# Highest Posterior Density (HPD) Intervals

- ▶ Definition: A  $100(1 - \alpha)\%$  HPD interval for  $\theta$  is a subset  $\mathcal{C} \in \Theta$  defined by

$$\mathcal{C} = \{\theta : \pi(\theta | x) \geq k\}$$

where  $k$  is the largest number such that

$$\int_{\theta: \pi(\theta|x) \geq k} \pi(\theta | x) d\theta = 1 - \alpha.$$

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- ▶ The value  $k$  can be thought of as a horizontal line placed over the posterior density whose intersection(s) with the posterior define regions with probability  $1 - \alpha$ .

## Highest Posterior Density (HPD) Intervals

- Definition: A  $100(1 - \alpha)\%$  HPD interval for  $\theta$  is a subset  $(\theta_1, \theta_2)$  defined by

1.  $P(\theta_1 < \theta < \theta_2 \mid X) = 1 - \alpha$ .
2. 만약  $\theta_a \in (\theta_1, \theta_2)$ 이고  $\theta_b \notin (\theta_1, \theta_2)$  이면  $\Pr(\theta_a \mid x) > \Pr(\theta_b \mid x)$ .

## Highest Posterior Density (HPD) Intervals

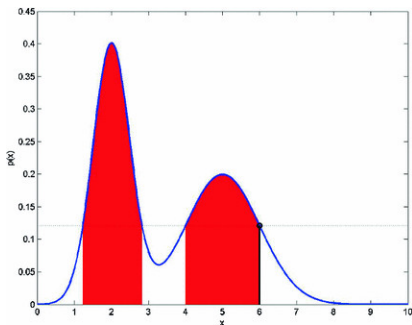
- ▶ Definition: A  $100(1 - \alpha)\%$  HPD interval for  $\theta$  is a subset  $(\theta_1, \theta_2)$  defined by
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  2. 만약  $\theta_a \in (\theta_1, \theta_2)$ 이고  $\theta_b \notin (\theta_1, \theta_2)$  이면
$$\Pr(\theta_a \mid x) > \Pr(\theta_b \mid x).$$
- ▶ 최대사후구간 (HPD Interval)은 주어진 신뢰도를 만족하는 베이지안 구간 중 최대한 Posterior density 값이 높은  $\theta$ 들의 합집합이다.

### Example 3: HPD Interval

- ▶ From the previous example, the posterior dist is  $\text{Normal}(0.3, (0.5)^2)$
- ▶ HPD Interval is  $0.3 \pm 1.96 \times 0.5 = (-0.68, 1.28)$
- ▶ For Normal distribution, the HPD interval has the minimum distance than other credible sets

## Highest Posterior Density Intervals

- ▶ The HPD region will be an interval when the posterior is unimodal.
- ▶ If the posterior is multimodal, the HPD region might be a **discontiguous** set.



## How to Find HPD Interval

- ▶ 예를 통해 보면 구간의 경계값들에서 사후밀도함수값이 동일함을 알 수 있다.
- ▶ 즉 주어진 신뢰도를 만족하는 구간 중 최대한 사후밀도함수값이 높은  $\theta$ 값을 모으기 위하여 가상의 수평 막대를 사후밀도함수의 최댓값에서 두 점차 아래로 내리면서 만나는 점들 사이의 면적을 계산하여 면적이 최초로  $(1 - \alpha)$ 와 동일 하는 구간이 HPD interval이 된다.



## How to Find HPD Interval

- ▶ 수리적으로 찾는 방법은 매우 어렵다.
- ▶ 그래서 근사적으로 찾는 방법이 권장 된다.
- ▶ 앞으로 근사적으로 HPD interval을 찾는 세가지 방법을 고려하겠다.

## Case 1: How to Find HPD Interval

- ▶ Suppose that the posterior is symmetric and unimodal.
- ▶ Then consider the  $\alpha/2$  and  $1 - \alpha/2$  percentile.
- ▶ If the posterior distributions are well-known, the existing packages can be exploited.
- ▶ Otherwise some sampling methods can be used.

## Case 1: How to Find HPD Interval

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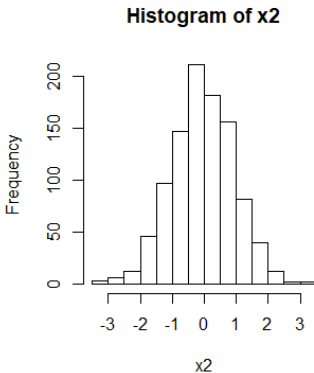
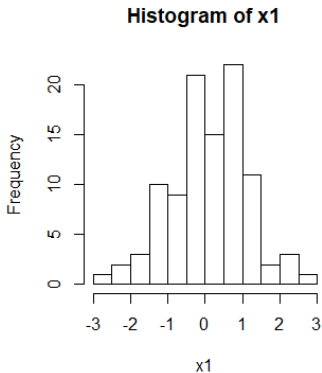
## Case 1: Example

```
> n = 100  
  
> x1 <- rnorm(n, 0, 1)  
  
> quantile(x1, c(.025, .975))  
  
2.5%      97.5%  
-1.959474  2.269712  
  
>  
  
> n = 1000  
  
> x2 <- rnorm(n, 0, 1)  
  
> quantile(x2, c(.025, .975))  
  
2.5%      97.5%  
-1.928400  1.894172
```

## Case 1: Example

```
> par(mfrow = c(1,2))
```

```
> hist(x1);hist(x2)
```



## Case 2: Grid Search Method (격자점 방법)

- ▶ Main idea: Consider  $\theta$  as  $N$  distinct values  $(\theta_1, \theta_2, \dots, \theta_N)$ .

## Case 2: Grid Search Method (격자점 방법)

- ▶ Main idea: Consider  $\theta$  as  $N$  distinct values  $(\theta_1, \theta_2, \dots, \theta_N)$ .
- ▶ Calculate

$$\hat{\pi}(\theta_i | x) = \frac{\pi(\theta_i) f(x | \theta_i)}{\sum_i \pi(\theta_i) f(x | \theta_i)}.$$

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- ▶ Calculate

$$\hat{\pi}(\theta_i | x) = \frac{\pi(\theta_i) f(x | \theta_i)}{\sum_i \pi(\theta_i) f(x | \theta_i)}.$$

- ▶ Find  $M$  such that

$$M := \min \left\{ m \mid \sum_{j=1}^m \hat{\pi}(\theta_j | x)^{\text{ordered}} \geq 1 - \alpha \right\}$$



## Case 2: Grid Search Method (격자점 방법)

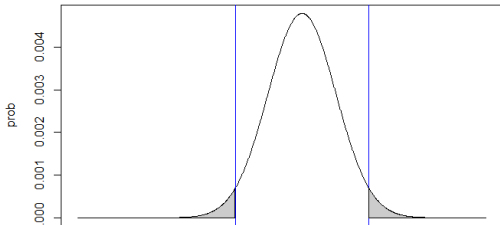
```
HPDgrid = function(prob, level = 0.95){  
  prob.sort = sort(prob, decreasing = T)  
  M = min( which(cumsum(prob.sort)>=level) )  
  height = prob.sort[M]  
  HPD.index = which( prob >= height)  
  HPD.level = sum(prob[HPD.index])  
  res = list( index = HPD.index, level = HPD.level )  
  return(res)  
}
```

## Case 2: Grid Search Method (격자점 방법)

Suppose that the posterior distributions satisfies

$$f(\theta | x) \propto \exp(-2(\theta - 0.3)^2).$$

```
> N = 1001  
> theta = seq(-3, 3, length = N)  
> prob = exp(-0.5/0.25*(theta-0.3)^2)  
> prob = prob/sum(prob)  
> alpha = 0.05; level = 1-alpha
```



## Case 2: Grid Search Method (격자점 방법)

```
HPD = HPDgrid(prob, level)
HPDgrid.hat = c( min(theta[HPD$index]),
                 max(theta[HPD$index]) )
HPDgrid.hat
-0.678  1.278
```

## Case 2: Grid Search Method (격자점 방법)

```
par(mfrow = c(1,1))  
plot(theta, prob, type = "l", ylab = "prob", xlab = "theta",  
xlim = c(-3,3))  
abline(v = HPDgrid.hat, col = 'blue')  
polygon(x = c(theta[which(theta < HPDgrid.hat[1])],  
  rev(theta[which(theta < HPDgrid.hat[1])]) ),  
  y = c(prob[which(theta < HPDgrid.hat[1])],  
  rep( 0, sum(theta < HPDgrid.hat[1]) )), col = "grey80")  
polygon(x = c(theta[which(theta > HPDgrid.hat[2])],  
  rev(theta[which(theta > HPDgrid.hat[2])]) ),  
  y = c(prob[which(theta > HPDgrid.hat[2])],  
  rep( 0, sum(theta > HPDgrid.hat[2]) )),  
  col = "grey80")  
}
```

## Case 2: Grid Search Method (격자점 방법)

Suppose that the posterior distributions satisfies

$$f(\theta | x) \propto \exp(-(\theta - 2)^2/2) + \exp(-(\theta + 2)^2/2).$$

$N = 1001$

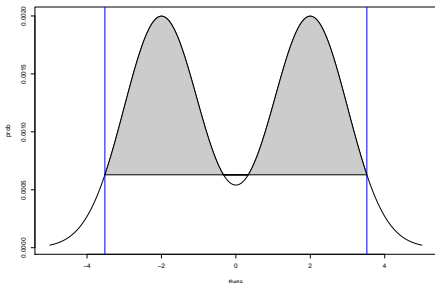
```
theta = seq(-5, 5, length = N)
```

```
#prob = exp(-0.5/0.25*(theta-0.3)^2)
```

```
prob = exp(-1/2*(theta+2)^2) + exp(-1/2*(theta-2)^2)
```

```
prob = prob/sum(prob)
```

```
alpha = 0.10; level = 1-alpha
```



## Case 2: Grid Search Method (격자점 방법)

```
> HPD = HPDgrid(prob, level)
> HPDgrid.hat = c( min(theta[HPD$index]), max(theta[HPD$index]) )
> HPDgrid.hat
[1] -3.52  3.52
> theta[which(prob == min( prob[HPD$index] ) )]
[1] -0.33  0.33
```

## Case 2: Grid Search Method (격자점 방법)

```
par(mfrow = c(1,1))  
plot(theta, prob, type = "l", ylab = "prob", xlab = "theta", xlim = c(-5,5))  
abline(v = HPDgrid.hat, col = 'blue')  
polygon(x = c(theta[HPD$index]) , y = c(prob[HPD$index] ), col = "grey80")
```

## Case 2: Grid Search Method (격자점 방법)

- ▶ It is very useful for the multivariate or multimodal  $\theta$ .
- ▶ It is difficult for find the optimal HPD interval when the posterior density is wiggly.
- ▶ It is hard to calculate all possible values for  $\theta$  if  $\theta \in \mathbb{R}$ .



### Case 3: Bayesian Posterior Sampling

- ▶ Posterior sampling histogram 이 density function 과 유사하다는 성질을 이용
- ▶ 예를 들어 1000개의 사후표본이 주어졌을때, 95% CI는 950개의 표본을 포함할 것이다.
- ▶ 1000개의  $\theta$  오름차순으로 정렬하여  $(\theta_1, \dots, \theta_{1000})$ 이라고 하자.
- ▶ 이 때 가능한 신뢰구간은  $(\theta_1, \theta_{950}), (\theta_2, \theta_{951}), (\theta_3, \theta_{953}), \dots$ 이 된다.
- ▶ 이 중에 가장 짧은 구간을 근사적 HPD interval로 취할 수 있다.

## Case 3: Bayesian Posterior Sampling

```
HPDsample = function(theta, level = 0.95){  
  N = length(theta)  
  theta.sort = sort(theta)  
  M = ceiling(N*level)  
  nCI=N-M  
  CI.width = rep(0, nCI)  
  for(i in 1:nCI) CI.width[i] = theta.sort[i+M] - theta.sort[i]  
  index = which.min(CI.width)  
  HPD = c(theta.sort[index], theta.sort[index+M])  
  return(HPD)  
}
```

## Case 3: Bayesian Posterior Sampling

- ▶ Suppose that the posterior distribution is  $\theta \sim N(0, 1)$ .

```
> N = 1000  
> theta = rnorm(N, 0, 1)  
> alpha = 0.05  
> level = 1-alpha  
> HPDsample(theta)  
[1] -1.632139  2.141612
```

## Case 3: Bayesian Posterior Sampling

- Suppose that the posterior distribution is  $\theta \sim N(0, 1)$ .

```
> N = 10000  
> theta = rnorm(N, 0, 1)  
> alpha = 0.05  
> level = 1-alpha  
> HPDsample(theta)  
[1] -1.909751  1.967354
```

## Case 3: Bayesian Posterior Sampling

Pros.

- ▶ 많은 경우  $\theta$ 의 posterior distribution이 매우 복잡하여 percentile을 직접 찾을 수 없다.
- ▶ Grid search method의 경우, 도메인이 무한인 경우 사용하기 어렵다.

Cons.

- ▶ Unimodal에서만 사용 가능하다.
- ▶ 다변량 모수에 대한 다차원 사후구간을 찾는 데에 적용할 수 없다.

## Weakness of Frequentist

분산이  $\sigma^2 = 1$ 인 정규분포의 평균  $\theta$ 를 추정하고자 한다. 표본을 얻기 전에 먼저 동전을 던져 앞면이 나오면 표본을 2개만 취하고, 뒷면이 나오면 표본을 1000개 취하기로 하였다. 즉 표본크기  $n$ 은 각각 확률  $\frac{1}{2}$ 로 2, 아니면 1000이 될 것이다. 이 실험에서  $\theta$ 에 대한 추정치는 표본의 평균  $\bar{X}$ 가 적절하며  $\bar{X}$ 의 정확도를 측정하는 통계량으로는  $\bar{X}$ 의 분산이 적절 할 것이다.  $\bar{X}$ 의 분산은

$$\begin{aligned}\text{Var}(\bar{X}) &= \frac{1}{2}\text{Var}(\bar{X} \mid n = 2) + \frac{1}{2}\text{Var}(\bar{X} \mid n = 1000) \\ &= \frac{1}{2}(\sigma^2/2 + \sigma^2/1000) \approx 1/4.\end{aligned}$$

## Weakness of Frequentist

만약 동전의 결과가 뒷면이고 따라서 1000개의 표본을 취한 결과가  $\bar{X} = 0.1$ 이었다고 하자. 고전적 통계추론에 의하면  $\theta$ 에 대한 추정치는 0.1이고 추정오차는  $\sqrt{\frac{1}{4}} = 0.5$ 로 결론 짓는다. 이미 1000개의 표본을 취했다는 것을 안 상태에서, 추정오차를  $\sqrt{\frac{1}{1000}} = 0.03$ 아닌 0.5를 합리적인 추정오차라고 할 수 있겠는가?

## Weakness of Frequentist

두 변수  $X_1, X_2$ 는  $U(\theta - \frac{1}{2}, \theta + \frac{1}{2})$ 를 따른다. 고전적 통계추론에서  $\theta$ 대한 95% 신뢰구간을 구하면, 적절한 양의 상수  $C$ 에 대하여  $\bar{X} \pm C$ 의 형태를 가진다. 만약 두변수의 관측값이 각각,  $X_1 = 1, X_2 = 2$ 라면,  $\theta$ 가 1.5임이 확실하다. 이때 우리가 신뢰계수를 100%가 아닌 95%로 보아야 하는가?