

# Advanced Bayesian Methods: Theory and Applications in R

Principles of Bayesian Inference

Nikolaus Umlauf https://nikum.org/abm.html

## Principles of Bayesian Inference

#### Aims of sections 1-4:

- Introduce the foundations of Bayesian inference and compare it to frequentist maximum likelihood.
- Motivate how Markov chain Monte Carlo (MCMC) simulations provide numerical access to the posterior distributions.
- Discuss practical aspects of working with MCMC simulations.

#### Bayes' Theorem

- Two central components of a Bayesian model formulation.
  - Observation model  $p(\mathbf{y}|\theta)$ , which describes how the data  $\mathbf{y}$  are generated for given model parameters  $\theta$ .
  - Prior distribution p( heta) representing prior beliefs about the parameter vector heta
- Bayesian learning updates prior beliefs on  $\theta$  based on information in the data  $\mathbf{y}$  using Bayes' theorem

$$p(\theta|\mathbf{y}) = rac{p(\mathbf{y}|\theta)p(\theta)}{p(\mathbf{y})} = rac{p(\mathbf{y}|\theta)p(\theta)}{\int p(\mathbf{y}|\theta)p(\theta)d\theta},$$

where  $p(\mathbf{y})$  is the marginal density of the data.

- Data  $y \stackrel{i.i.d.}{\sim} Be(\pi)$  with unknown success probability  $\pi \in (0, 1)$ .
- We consider n = 10 trials with one success (1) and nine failures (0).
- The likelihood is the product of each the probabilities of each individual Bernoulli trial

$$\mathcal{L}(\pi|\mathbf{y}) = \prod_{i=1}^{n} p(\pi|y_i) = \prod_{i=1}^{n} \pi^{y_i} (1-\pi)^{1-y_i} = \pi^{\sum_{i=1}^{n} y_i} (1-\pi)^{n-\sum_{i=1}^{n} y_i}.$$

• For the prior distribution of  $\pi$ , we use a Beta distribution with parameters a > 0 and b > 0:

$$\pi \sim \mathsf{Beta}(\pmb{a}, \pmb{b})$$

• The density function of the Beta distribution is:

$$p(\pi|a,b)=rac{\pi^{a-1}(1-\pi)^{b-1}}{B(a,b)}, ext{ where } B(a,b)=rac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}.$$

Here,  $\Gamma(\cdot)$  is the Gamma function.

• The posterior distribution combines the likelihood function and the prior

$$egin{aligned} p(\pi|\mathbf{y}) &\propto & \mathcal{L}(\pi|\mathbf{y}) \cdot p(\pi|a,b) \ &= & \left(\prod_{i=1}^n \pi^{y_i} (1-\pi)^{1-y_i} 
ight) \cdot \pi^{a-1} (1-\pi)^{b-1} \ &= & \pi^{\sum_{i=1}^n y_i + a - 1} (1-\pi)^{n - \sum_{i=1}^n y_i + b - 1} \end{aligned}$$

• Hence, this is the kernel of a Beta distribution. Therefore, the posterior distribution for  $\pi$  is:

$$\pi | \mathbf{y} \sim \mathsf{Beta}\left( a + \sum_{i=1}^n y_i, b + n - \sum_{i=1}^n y_i 
ight).$$

• We can express the parameters of the posterior Beta distribution as:

$$\tilde{a} = a + \sum_{i=1}^{n} y_i, \ \tilde{b} = b + n - \sum_{i=1}^{n} y_i.$$

```
In R:
R > v < - c(1, rep(0, 9))
R> prior <- function(p, a, b, ...) {
+ p^{(a - 1)} * (1 - p)^{(b - 1)} / beta(a, b)
+ }
R> likelihood <- function(p, ...) {</pre>
     p^{(sum(y))} * (1 - p)^{(length(y) - sum(y))}
+
+ }
R> posterior <- function(p, a, b, nc = TRUE, ...) {</pre>
     if(nc) {
+
       a < -a + sum(y)
+
       b \le b + length(y) - sum(y)
+
       pv \leftarrow p^{(a - 1)} * (1 - p)^{(b - 1)} / beta(a. b)
+
     } else {
+
       pv <- likelihood(p) * prior(p, a, b)</pre>
+
     3
+
     return(pv)
+
+
```



## Relation to Maximum Likelihood Estimation

• If the prior distribution is flat, i.e.

 $p(\theta) \propto \text{const},$ 

the posterior is proportional to the likelihood:

$$p( heta|\mathbf{y}) = rac{p(\mathbf{y}| heta)p( heta)}{p(\mathbf{y})} \propto p(\mathbf{y}| heta)p( heta) \propto p(\mathbf{y}| heta).$$

• Hence, the mode of the posterior coincides with the maximum likelihood estimate.

#### Relation to Maximum Likelihood Estimation

```
R> p <- seq(0, 1, length = 100)
R> par(mar = c(4, 4, 1, 1))
R> plot(likelihood(p), posterior(p, a = 1, b = 1))
R> abline(lm(posterior(p, a = 1, b = 1) ~ likelihood(p)))
```



## Relation to Maximum Likelihood Estimation

In general,

- the likelihood is a central part of Bayes' theorem that quantifies the information coming from the data and
- the posterior forms a compromise between data (likelihood) and prior beliefs (prior).

#### Prior Beliefs and Prior Elicitation

- Main conceptual difference between likelihood-based and Bayesian inference: Coming up with a sensible prior distribution.
- The prior should reflect your prior beliefs about the parameter of interest.
- Very common practice:
  - Pick a mathematically convenient class of distributions for the prior and
  - only decide on the parameter of this prior distribution.
- For example, one can formulate belief statements such as

$$\mathsf{P}(c_1 \leq \theta \leq c_2) = 1 - \alpha,$$

where  $c_1$  and  $c_2$  are pre-specified constants from which the prior parameters are determined.

• It is also very common to run analyses for a variety of different priors to study prior sensitivity.

#### Prior Beliefs and Prior Elicitation

Example in R:

```
R > foo <- function(par, level = 0.9) {
     p <- pbeta(0.7, par[1], par[2]) - pbeta(0.5, par[1], par[2])</pre>
+
  (p - level)^2
+
  7
+
R> opt <- optim(c(1, 1), fn = foo, method = "L-BFGS-B", lower = 1, upper = 100)
R > a <- opt par[1]; b <- opt par[2]
R> print(a)
[1] 38,34065
R> print(b)
[1] 25.81303
R > p <- seq(0, 1, length = 200)
R > par(mar = c(4, 4, 1, 1))
R > plot(p, prior(p, a, b), type = "l", lwd = 2)
```

#### Prior Beliefs and Prior Elicitation



## Noninformative Prior Specifications

• Flat priors

#### $f( heta) \propto {\sf const}$

are a popular choice to implement noninformative priors (no value of the parameter is favored a priori).

- Conceptual difficulties:
  - For non-bounded parameter spaces, flat priors are not actual probability distributions.
  - Flat priors are not invariant under transformations of the parameter of interest.

## Noninformative Prior Specifications

- An alternative are reference priors for which the prior has the smallest possible influence on the posterior (i.e., it maximizes the Kullback-Leibler discrepancy between the prior and the posterior for given data).
- Another option is Jeffreys' invariant prior:

 $p( heta) \propto \sqrt{|F( heta)|}$ 

with expected Fisher information  $F(\theta)$ .

• For scalar parameters, Jeffreys' prior is equivalent to the reference prior approach.

## Bernoulli Experiment: Likelihood and Log-Likelihood

- Consider a Bernoulli experiment where the outcome y is 1 (success) with probability  $\theta$  and 0 (failure) with probability  $1 \theta$ .
- The likelihood function for the parameter  $\theta$  given the outcome y is:

$$p(y \mid \theta) = \theta^y (1 - \theta)^{1-y}.$$

• The log-likelihood function  $\ell(\theta)$  is:

$$\ell(\theta) = \log p(y \mid \theta) = y \log \theta + (1 - y) \log(1 - \theta).$$

• Compute the first derivative of the log-likelihood function:

$$rac{\partial \ell( heta)}{\partial heta} = rac{{\mathsf y}}{ heta} - rac{{\mathsf 1}-{\mathsf y}}{{\mathsf 1}- heta}.$$

• Compute the second derivative of the log-likelihood function:

$$rac{\partial^2 \ell( heta)}{\partial heta^2} = -rac{ extsf{y}}{ heta^2} - rac{ extsf{1}- extsf{y}}{( extsf{1}- heta)^2}.$$

• The Fisher information  $F(\theta)$  is the negative expected value of the second derivative:

$$F(\theta) = -\mathbb{E}\left[rac{\partial^2 \ell(\theta)}{\partial \theta^2}
ight].$$

• Substituting the second derivative:

$${ extsf{F}}( heta) = \mathbb{E}\left[rac{y}{ heta^2} + rac{1-y}{(1- heta)^2}
ight].$$

• Since *y* follows a Bernoulli distribution:

$$E[y] = \theta$$
 and  $E[1-y] = 1 - \theta$ ,

SO

$$F(\theta) = \frac{\theta}{\theta^2} + \frac{1-\theta}{(1-\theta)^2} = \frac{1}{\theta} + \frac{1}{1-\theta} = \frac{1}{\theta(1-\theta)}.$$

• Jeffreys' prior is proportional to the square root of the Fisher information:

 $p(\theta) \propto \sqrt{F(\theta)}.$ 

• Therefore:

$$p( heta) \propto \sqrt{rac{1}{ heta(1- heta)}}.$$

• Simplifying:

$$p( heta) \propto rac{1}{\sqrt{ heta(1- heta)}} = heta^{0.5-1}(1- heta)^{0.5-1}.$$

 This is equivalent to the Beta(0.5, 0.5) distribution, which is a noninformative prior reflecting minimal prior knowledge about θ.

Example in R:

```
R> Jeffreys <- function(p) { dbeta(p, 0.5, 0.5) }
R> p <- seq(0, 1, length = 100)
R> par(mar = c(4, 4, 1, 1))
R> plot(p, Jeffreys(p), type = "l", lwd = 2)
```



#### Priors for the Success Probability

- The beta distribution is conjugate to the Bernoulli observation model, i.e., the posterior is then also a beta distribution with updated parameters.
- Elicit the hyperparameters a > 0 and b > 0 based on prior statements, e.g., the prior expectation, variance, quantiles, probabilities, etc.
- A flat prior is  $\pi \sim U(0, 1)$ , which is also a beta distribution with a = b = 1.
- Jeffreys' prior is a beta distribution with a = b = 0.5.

## Priors for the Success Probability

- A typical discussion on Bayesian inference is that:
  - Frequentist inference assumes a true, fixed parameter value, whereas
  - *Bayesian inference* assumes the parameter to be a random variable.
- This is, in general, misleading since the prior is merely used to reflect prior (un)certainty about the parameter of interest.
- The underlying philosophical question is whether this can be done in a sensible way . . .

#### Posterior Mean and 95% Credible Interval

Model Setup:

- Likelihood:  $y \mid \theta \sim \text{Bernoulli}(\theta)$
- Prior:  $\theta \sim \text{Beta}(\alpha, \beta)$
- Posterior:  $\theta \mid y \sim \text{Beta}(y + \alpha, n y + \beta)$

Example Parameters:

- Number of trials n = 10
- Number of successes y = 7
- Prior parameters:  $\alpha = 2$ ,  $\beta = 2$

#### Posterior Mean and 95% Credible Interval

Posterior Distribution:

$$\theta \mid y \sim \text{Beta}(9,5)$$

Posterior Mean:

Mean 
$$= \frac{\alpha'}{\alpha' + \beta'} = \frac{9}{9+5} = \frac{9}{14} \approx 0.643$$

95% Credible Interval:

• Compute quantiles using the Beta distribution:

Lower Bound = 
$$Beta^{-1}(0.025; 9, 5)$$
  
Upper Bound =  $Beta^{-1}(0.975; 9, 5)$ 

#### Posterior Mean and 95% Credible Interval

• Numerical values:

```
R> qbeta(0.025, 9, 5)
[1] 0.3857383
R> qbeta(0.975, 9, 5)
[1] 0.8614207
```

Result: The 95% credible interval for  $\theta$  is approximately (0.386, 0.861).

## Challenges with Non-Conjugate Prior

#### Challenges:

- No Closed-Form Solution: What if the posterior distribution  $p(\theta | \mathbf{y})$  does not simplify to a standard form?
- **Numerical Approximation Required**: Direct calculation of posterior mean and credible intervals is not feasible.
- **MCMC Methods**: To approximate the posterior mean and credible interval, MCMC methods (e.g., Metropolis-Hastings, Gibbs sampling) must be used.

Summary: Non-conjugate priors may lead to complex posterior distributions that require advanced numerical techniques for estimation.

## Frequentist vs. Bayesian Inference

#### • Frequentist Inference:

- Assumes a **fixed, true parameter** in the population.
- Estimation through **repeated sampling**.

#### • Bayesian Inference:

- Treats the parameter as a random variable, reflecting uncertainty.
- Combines prior beliefs with observed data to update beliefs (posterior distribution).
- **Misconception**: Bayesian inference does not imply the parameter is truly random, but reflects uncertainty.
- **Role of Prior**: Encapsulates prior knowledge or uncertainty, updated with data.
- **Philosophical Debate**: How to sensibly define objective priors?