

Handout 12: Credible sets

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Aim: To explain and produce credible regions in the Bayesian framework.

References:

- Berger, J. O. (2013; Section 4.3.2). Statistical decision theory and Bayesian analysis. Springer Science & Business Media.
- Robert, C. (2007; Section 5.5). The Bayesian choice: from decision-theoretic foundations to computational implementation. Springer Science & Business Media.
- Bernardo, J. M., & Smith, A. F. (1994). Bayesian theory (Vol. 405). John Wiley & Sons.

Web applets:

- https://georgios-stats-1.shinyapps.io/demo_CredibleSets/

1 Set-up and aim

Notation 1. Consider a Bayesian model

$$\begin{cases} y|\theta & \sim F(y|\theta) \\ \theta & \sim \Pi(\cdot) \end{cases}$$

where $y := (y_1, \dots, y_n) \in \mathcal{Y}$ is a sequence of observables, assumed to be generated from the parametric sampling distribution $F(y|\theta)$ with pdf/pmf $f(y|\theta)$ and labeled by an unknown parameter $\theta \in \Theta$ with a prior distribution $\Pi(\theta)$ with pdf/pmf $\pi(\theta)$. Also assume a sequence of m future outcomes $z = (y_{n+1}, \dots, y_{n+m})$.

AIM: Instead of just reporting a point value for θ (or z) and the associated standard error, it is often desirable and clearer to report sets of values $C_a \subseteq \Theta$ (or $C_a \subseteq \mathcal{Z}$) with a specified probability a reflecting Your believe that $\theta \in C_a$ (or $z \in C_a$).

Note 2. Recall that

- Posterior degree of believe about uncertain parameter $\theta \in \Theta \subseteq \mathbb{R}^d$ is quantified via the posterior distribution $\Pi(\theta|y)$;

$$d\Pi(\theta|y) = \pi(\theta|y)d\theta$$

with cdf $\Pi(\theta|y)$ and pdf/pmf $\pi(\theta|y)$.

- Degree of believe about a future sequence of outcomes $z = (y_{n+1}, \dots, y_{n+m}) \in \mathcal{Z}$ is quantified via the predictive distribution $G(z|y)$;

$$dG(z|y) = g(z|y)dz$$

with cdf $G(z|y)$ and pdf/pmf $g(z|y)$.

Notation 3. We present the parametric and predictive credible intervals in a unified framework. Consider unknown random quantity $x \in \mathcal{X} \subseteq \mathbb{R}^k$ following a distribution $Q(x|y)$;

$$dQ(x|y) = q(x|y)dx$$

with cdf $Q(x|y)$ and pdf/pmf $q(x|y)$. These are dummies for the following:

- In parametric inference, we have $x \equiv \theta$, $Q \equiv \Pi$, $q \equiv \pi$, and $k = d$.
- In predictive inference, we have $x \equiv z$, $Q \equiv G$, $q \equiv g$, and $k = m$.
- Note that x can also be any function of θ or z .

2 Credible Sets

Definition 4. A set $C_a \subseteq \mathcal{X}$ is called ‘ $100(1 - a)\%$ ’ posterior credible set for x , with respect to the posterior distribution $Q(x|y)$ if

$$1 - a \leq P_Q(x \in C_a|y) = \int 1(x \in C_a) dQ(x|y)$$

Note 5. In Bayesian stats (unlike frequentist stats) we can correctly say that the $(1 - a)100\%$ credible set C_a of unknown parameter θ means that the probability that θ is in C_a is $(1 - a)100\%$. This is theoretically correct as everything unknown/uncertain is a random quantity following a distribution reflecting Your degree of believe.

Note 6. Note that different sets may satisfy Definition 4 and hence we are interested in using the most useful credible set for our application. This is addressed by imposing additional restrictions.

3 Highest probability density Credible sets¹

Note 7. Often it is useful to consider credible sets C_a which contain values of x that correspond to the highest pdf/pmf $q(x|y)$ (aka the most likely values of x). Then we can impose the restriction $q(x|y) \geq q(x'|y)$ for all $x \in C_a$, $x' \in C_a^c$, in Definition 4 which leads to Definition 8, the definition of the highest probability density (HPD) set.

Definition 8. The $100(1 - a)\%$ highest probability density (HPD) set for $x \in \mathcal{X}$ with respect to the posterior distribution $Q(x|y)$ is the subset C_a of Θ such that

1. $P_Q(x \in C_a|y) \geq 1 - a$, and
2. $q(x|y) \geq q(x'|y)$ for all $x \in C_a$, $x' \in C_a^c$.

Note 9. Credible sets are considered as ‘set estimators’, and hence, they can be produced as Bayes decision rules under a specified loss function.

Fact 10. [Minimal size region property] Let random quantity x follows $Q(x|y)$, let $\mathcal{D} = \{C; P_Q(x \in C|y) \geq 1 - a\}$ be the decision space containing all possible $(1 - a)$ credible sets of x , and let the loss function be

$$\ell(x, C) = \kappa \|C\| - I(x \in C), \quad \forall C \in \mathcal{D}, \forall x \in \mathcal{X}, \forall \kappa > 0, \quad (1)$$

where $\|\cdot\|$ denotes a size of an area. Then:

1. The Bayes rule (estimator) \hat{C} has the minimum size among credible sets in \mathcal{D} .
2. \hat{C} is the Bayes rule if and only if it is the $100(1 - a)\%$ highest probability density (HPD) set as defined in Definition 8.

¹Web applet: https://georgios-stats-1.shinyapps.io/demo_CredibleSets/

Proof. The proof is omitted. (1.) is straightforward; while (2.) is just tricky calculus. \square

Note. HPD credible sets are credible sets with the minimum size (by Fact 10). Clearly, loss (1) considers a trade off between two components: $\|C\|$ measuring the size of the credible set (the smaller the better), and $1(x \in C)$ indicating coverage of the credible set.

Remark 11. HPD credible sets are not, in general, invariant to transformations. If one has computed the HPD set for $x \sim Q(x|y)$, the HPD set for $\varphi = g(x)$ does not necessarily result by converting HPD set for x . To compute the HPD set for φ , one has to compute the posterior distribution

$$dQ(\varphi|y) = \underbrace{q(g^{-1}(\varphi)|y) \left| \frac{d}{d\varphi} g^{-1}(\varphi) \right|}_{=\pi(\varphi|y)} d\varphi,$$

and then compute the HPD set by implementing Definition 8.

3.1 General discussions

Definition 8 can be re-written equivalently as in Corollary 12, which provides a easier manner to compute credible regions in practice.

Corollary 12. *The $100(1 - a)\%$ highest probability density (HPD) set for $x \in \mathcal{X}$ with respect to the posterior distribution $Q(x|y)$ is the subset C_a of Θ of the form*

$$C_a = \{x \in \mathcal{X} : q(x|y) \geq k_a\} \quad (2)$$

where k_a is the largest constant such that

$$1 - a \leq P_Q(x \in C_a|y)$$

Proof. It is straightforward to show equivalence of (2) and Definition 8(2). \square

Algorithm 13. *Based on Corollary 12, a (not-that-efficient) algorithm to compute HPD credible sets with a computer²*

1. *Create a routine which computes all the solutions x^* to the equation $q(x|y) = k_a$, for a given k_a . Typically, $C_a = \{x \in \mathcal{X} : q(x|y) \geq k_a\}$ can be constructed from those solutions.*
2. *Create a routine which computes*

$$P_Q(x \in C_a|y) = \int 1(x \in C_a) dQ(x|y) \quad (3)$$

3. *Sequentially solve the equation*

$$P_Q(x \in C_a|y) = 1 - a$$

by increasing incrementally k_a from zero to larger, and stop just before (3) drops below $1 - a$.

²Web-applet https://georgios-stats-1.shinyapps.io/demo_CredibleSets/



Figure 1: Schematic of Theorem 15 (in Fig. 1(1a)) and Algorithm 13 (in Fig. 1(1a) & Fig. 1(1b))

Note 14. For the simple 1D case, $x \in \mathcal{X}$ with $\dim(\mathcal{X}) = 1$, the following theorem can be used to compute HPD credible sets.

Theorem 15. Let $x \in \mathbb{R}$ be a continuous random variable following distribution $Q(x|y)$ with unimodal density $q(x|y)$. If the interval $C_a = [L, U]$ satisfies

1. $\int_L^U q(x|y)dx = 1 - a$,
2. $q(U) = q(L) > 0$, and
3. $x_{\text{mode}} \in (L, U)$, where x_{mode} is the mode of $q(x|y)$,

then it is the HPD interval of x with respect to $Q(x|y)$.

Proof. Use of the mean values theorem to prove. See, Casella, G., & Berger, R. L. (2002; pp. 441-443). Statistical inference (Vol. 2). Pacific Grove, CA: Duxbury. \square

Remark 16. Theorem 15 suggests a procedure to find the boundaries of C_a in 1D cases. As is Figure 1a, we can imagine a horizontal bar which moves from the maximum of the density to zero, and intersects the density at locations which are the potential boundaries of C_a . The limits of the credible set are where the density above the two points the intersection take place (shaded area) is equal to $1 - a$. This mechanism is also described in the algorithm in suggested in Algorithm 13 and hence can also be used in multimodal densities (Figure 1b) or multivariate ones.

4 Examples

Example 17. Consider a Bayesian model

$$\begin{cases} y_i | \mu & \stackrel{\text{iid}}{\sim} \mathcal{N}_d(\mu, \Sigma), & i = 1, \dots, n \\ \mu & \sim \mathcal{N}_d(\mu_0, \Sigma_0) \end{cases}$$

where uncertain $\mu \in \mathbb{R}^d$, $d \geq 1$, and known Σ , μ_0 , Σ_0 . Find the C_a parametric HPD credible set for μ .

Hint-1: If $z = (z_1, \dots, z_d)^\top$ such as $z_j \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$ for $j = 1, \dots, d$, and $\xi = z^\top z = \sum_{j=1}^d z_j^2$, then $\xi \sim \chi_d^2$

Hint-2: It is

$$\begin{aligned} -\frac{1}{2} \sum_{i=1}^n (x - \mu_i)^\top \Sigma_i^{-1} (x - \mu_i) &= -\frac{1}{2} (x - \hat{\mu})^\top \hat{\Sigma}^{-1} (x - \hat{\mu}) + C(\hat{\mu}, \hat{\Sigma}) \quad ; \\ \hat{\Sigma} &= \left(\sum_{i=1}^n \Sigma_i^{-1} \right)^{-1}; \quad \hat{\mu} = \hat{\Sigma} \left(\sum_{i=1}^n \Sigma_i^{-1} \mu_i \right); \\ C(\hat{\mu}, \hat{\Sigma}) &= \frac{1}{2} \underbrace{\left(\sum_{i=1}^n \Sigma_i^{-1} \mu_i \right)^\top \left(\sum_{i=1}^n \Sigma_i^{-1} \right)^{-1} \left(\sum_{i=1}^n \Sigma_i^{-1} \mu_i \right) - \frac{1}{2} \sum_{i=1}^n \mu_i^\top \Sigma_i^{-1} \mu_i}_{=\text{independent of } x} \end{aligned}$$

Solution. I will use the Definition 8.

- First, I compute the posterior of μ . It is

$$\begin{aligned} \pi(\mu | y) &\propto f(y | \mu) \pi(\mu) = \prod_{i=1}^n \mathcal{N}_d(y_i | \mu, \Sigma) \mathcal{N}_d(\mu | \mu_0, \Sigma_0) \\ &\propto \exp \left(-\frac{1}{2} \sum_{i=1}^n (y_i - \mu)^\top \Sigma^{-1} (y_i - \mu) - \frac{1}{2} (\mu - \mu_0)^\top \Sigma_0^{-1} (\mu - \mu_0) \right) \\ &\propto \exp \left(-\frac{1}{2} (\mu - \hat{\mu}_n)^\top \hat{\Sigma}_n^{-1} (\mu - \hat{\mu}_n) \right) \end{aligned}$$

where

$$\hat{\Sigma}_n = (n\Sigma^{-1} + \Sigma_0^{-1})^{-1}; \quad \hat{\mu}_n = \hat{\Sigma}_n (n\Sigma^{-1}\bar{y} + \Sigma_0^{-1}\mu_0)$$

I recognize that $\pi(\mu | y) = \mathcal{N}_d(\mu | \hat{\mu}_n, \hat{\Sigma}_n)$, and hence $\mu | y \sim \mathcal{N}_d(\hat{\mu}_n, \hat{\Sigma}_n)$

- Now let's implement Definition 8. So,

$$\begin{aligned} C_a &= \{ \mu \in \mathbb{R}^d : \pi(\mu | y) \geq k_a \} \\ &= \{ \mu \in \mathbb{R}^d : \mathcal{N}_d(\mu | \hat{\mu}_n, \hat{\Sigma}_n) \geq k_a \} \\ &= \left\{ \mu \in \mathbb{R}^d : (\mu - \hat{\mu}_n)^\top \hat{\Sigma}_n^{-1} (\mu - \hat{\mu}_n) \leq \underbrace{-\log(2\pi \det(\hat{\Sigma}_n))}_{=\bar{k}_a} k_a \right\} \end{aligned} \quad (4)$$

and I want the smallest constant \tilde{k}_a (aka the largest constant k_a) such that

$$\begin{aligned} P_{\Pi}(\mu \in C_a | y) &\geq 1 - a \iff \\ P_{\Pi} \left(\underbrace{(\mu - \hat{\mu}_n)^{\top} \hat{\Sigma}_n^{-1} (\mu - \hat{\mu}_n)}_{=\xi} \leq \tilde{k}_a \right) &\geq 1 - a \end{aligned} \quad (5)$$

- I need to find quantile \tilde{k}_a . This requires to find the distribution of ξ . I know that

$$\xi = (\mu - \hat{\mu}_n)^{\top} \hat{\Sigma}_n^{-1} (\mu - \hat{\mu}_n) \sim \chi_d^2 \quad (6)$$

because $\xi = z^{\top} z = \sum_{j=1}^n z_j^2$ with $z = L^{-1}(\mu - \hat{\mu}_n) \sim N_d(0, I_d)$ where L is the lower matrix of the Cholesky decomposition of $\hat{\Sigma}_n = L^{\top} L$.

Hence Eq. 5, (due to Eqs. 4, 6) becomes

$$P_{\chi_d^2}((\mu - \hat{\mu}_n)^{\top} \hat{\Sigma}_n^{-1} (\mu - \hat{\mu}_n) \leq \tilde{k}_a) = 1 - a \quad (7)$$

which means that, \tilde{k}_a is the $1 - a$ quantile of the χ_d^2 distribution, aka $\tilde{k}_a = \chi_{d,1-a}^2$

- Hence, the C_a parametric HPD credible set for μ is

$$C_a = \{\mu \in \mathbb{R}^d : (\mu - \hat{\mu}_n)^{\top} \hat{\Sigma}_n^{-1} (\mu - \hat{\mu}_n) \leq \chi_{d,1-a}^2\}$$

Example 18. Consider an exchangeable sequence of observables $y := (y_1, \dots, y_n) \in \mathbb{R}^n$ from model

$$\begin{cases} y_i | \theta & \stackrel{\text{iid}}{\sim} \text{Br}(\theta), & i = 1, \dots, n \\ \theta & \sim \text{Be}(a, b) \end{cases}$$

where $a = b = 2$, $n = 30$, and $\sum_{i=1}^{30} y_i = 15$. Find the 2-sides C_a parametric HPD credible interval for θ . Consider $a = 0.05$.

Solution.

- The posterior distribution of θ is $\text{Be}(a + n\bar{y}, b + n - n\bar{y})$, because

$$\pi(\theta | y) \propto \prod_{i=1}^n \text{Br}(y_i | \theta) \text{Be}(\theta | a, b) \propto \prod_{i=1}^n \theta^{y_i} (1 - \theta)^{1 - y_i} \theta^{a-1} (1 - \theta)^{b-1} \propto \theta^{n\bar{y} + a - 1} (1 - \theta)^{n - n\bar{y} + b - 1}$$

After substituting the values of the fixed parameters, I get $\pi(\theta | y) = \text{Be}(\theta | a_n = 17, b_n = 17)$.

- To find the 2-sides C_a parametric HPD credible interval for θ , I use Theorem 15.

$$1 - a = \int_L^U \text{Be}(\theta | 17, 17) d\theta = P_{\text{Be}(17,17)}(\theta < U) - P_{\text{Be}(17,17)}(\theta < L)$$

I note that the posterior is symmetric around 0.5 because $a_n = b_n$. Then,

$$1 - a = P_{\text{Be}(17,17)}(\theta < U) - (1 - P_{\text{Be}(17,17)}(\theta < U)) = 2P_{\text{Be}(17,17)}(\theta < U) - 1$$

so $P_{\text{Be}(17,17)}(\theta < U) = 1 - a/2$, and hence $U = \theta_{1-\frac{a}{2}}^*$. Also,

$$\frac{1}{2} - L = U - \frac{1}{2} \implies L = 1 - U \implies L = 1 - \theta_{1-\frac{a}{2}}^*$$

Putting these together, for $a = 0.05$, the 95% posterior credible interval for θ is

$$[L, U] = [0.36, 0.64].$$

- Note that, if we follow the same procedure, the compute the 95% prior credible interval for θ is

$$[L, U] = [0.14, 0.85].$$

As expected, the posterior 95 credible interval is narrower than the corresponding posterior one. (Try to check it in R).

```
> install.packages('HDIInterval')
> library('HDIInterval')
> hdi(qbeta, 0.95, shape1=17, shape2=17)
lower upper
0.3354445 0.6645555
```

Example 19. Assume a 1-dimensional random quantity $x \sim Q(x|y)$, with unimodal density $q(x|y)$. Show that the $(1 - a)$ -credible interval $C_a = [L, U]$ for x as a Bayesian rule C_a under the loss function

$$\ell(x, C_a; L, U) = k(U - L) - 1(x \in [L, U]), \quad \text{with } k \in (0, \max_{x \in \mathbb{R}}(q(x|y)))$$

is given by $q(L) = q(U) = k$, and $P_Q(x \in [L, U]|y) = 1 - a$.

Discuss known properties of the derived credible interval.

Solution. The decision space is $\mathcal{D} = \{C_a = [L, U] : P_Q(x \in C_a|y) = 1 - a\}$. It is

$$\begin{aligned} E_Q(\ell(x, C_a; L, U)|y) &= \int (k(U - L) - 1(x \in [L, U])) dQ(x|y) \\ &= \int k(U - L)q(x|y)dx - \int_L^U q(x|y)dx = k(U - L) - \int_{-\infty}^U q(x|y)dx + \int_{-\infty}^L q(x|y)dx \end{aligned}$$

To find the critical values \hat{L} , and \hat{U} for L and U , it is

$$\begin{aligned} 0 &= \frac{d}{dL} E_Q(\ell(x, C_a; L, U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = \frac{d}{dL} \left(k(U - L) - \int_{-\infty}^U q(x|y)dx + \int_{-\infty}^L q(x|y)dx \right) \Big|_{C_a=[\hat{L}, \hat{U}]} \\ &= -k + q(\hat{L}|y) \implies q(\hat{L}|y) = k \\ 0 &= \frac{d}{dU} E_Q(\ell(x, C_a; L, U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = \dots = k - q(\hat{U}|y) \implies q(\hat{U}|y) = k \end{aligned}$$

which are minimizers because

$$\begin{aligned} \frac{d^2}{dL^2} E_Q(\ell(x, C_a; L, U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} &= \frac{d}{dL} q(L|y) \Big|_{\hat{L}} > 0; & \frac{d^2}{dLdU} E_Q(\ell(x, C_a; L, U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} &= 0 \\ \frac{d^2}{dU^2} E_Q(\ell(x, C_a; L, U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} &= -\frac{d}{dU} q(U|y) \Big|_{\hat{U}} > 0 \end{aligned}$$

So it is $C_a = [\hat{L}, \hat{U}]$ such that $q(\hat{L}|y) = q(\hat{U}|y) = k$, and $P_Q(x \in [\hat{L}, \hat{U}]|y) = 1 - a$.

Based on Theorem 15, it is the HPD credible interval and in fact the shorter length credible interval.

Example 20. Assume an 1- dimensional random quantity $x \sim Q(x|y)$. In the Lecture Handout (Handout 11: Bayesian point estimation), discussed the following Hint:

Hint: The Bayes estimate $\hat{\delta}$ of x under the linear loss function

$$\ell(x, \delta; \varpi) = (1 - \varpi)(\delta - x)1_{x \leq \delta}(\delta) + \varpi(x - \delta)1_{x > \delta}(\delta),$$

where $\varpi \in [0, 1]$, is the ϖ -th quantile of distribution Q , let's denote it as x_{ϖ} .

1. Derive the $(1 - a)$ -credible interval $C_a = [L, U]$ for x as a Bayesian rule C_a under the loss function

$$\ell(x, C_a; \varpi_L, \varpi_U) = \ell(x, L; \varpi_L) + \ell(x, U; \varpi_U) \quad (8)$$

by computing L and U .

2. Your client is worried the same both for under-estimation and over-estimation; derive a suitable $(1 - a)$ -credible interval $C_a = [L, U]$ based on (8) by computing L , and U .
3. Your client is worried only for over-estimation; derive a suitable $(1 - a)$ -credible interval $C_a = [L, U]$ based on (8) by computing L and U .

Solution. It is given that

$$\begin{aligned} 0 &= \frac{d}{d\delta} E_Q(\ell(x, \delta; \varpi)|y) \Big|_{\delta=\hat{\delta}} = \frac{d}{d\delta} \int \ell(x, \delta; \varpi) dQ(x|y) \Big|_{\delta=\hat{\delta}} \implies \hat{\delta} = x_{\varpi} \\ &= (1 - \varpi)P_Q(\{x \leq \hat{\delta}\}|y) - \varpi P_Q(\{x \leq \hat{\delta}\}^c|y) \implies \hat{\delta} = x_{\varpi} \end{aligned}$$

1. The decision space is $\mathcal{D} = \{C_a = [L, U] : P_Q(x \in C_a|y) = 1 - a\}$. Therefore, to find the Bayes rule (or Bayes estimate) of $C_a = [L, U]$ I need to minimize the expected posterior loss $E_Q(\ell(x, C_a; \varpi_L, \varpi_U)|y)$ with respect to C_a or equivalently L, U , so

$$\begin{aligned} 0 &= \frac{d}{dL} E_Q(\ell(x, C_a; \varpi_L, \varpi_U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = E_Q(\ell(x, L; \varpi_L)|y) \Big|_{L=\hat{L}} \implies \hat{L} = x_{\varpi_L} \\ 0 &= \frac{d}{dU} E_Q(\ell(x, C_a; \varpi_L, \varpi_U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = E_Q(\ell(x, U; \varpi_U)|y) \Big|_{U=\hat{U}} \implies \hat{U} = x_{\varpi_U} \end{aligned}$$

So $x \in [x_{\varpi_L}, x_{\varpi_U}]$ where $\varpi_U + \varpi_L = 1 - a$. It is the minimum because

$$\frac{d^2}{dU^2} E_Q(\ell(x, C_a; \varpi_L, \varpi_U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = q(\hat{U}|y) > 0$$

$$\frac{d^2}{dL^2} E_Q(\ell(x, C_a; \varpi_L, \varpi_U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = q(\hat{L}|y) > 0$$

$$\frac{d}{dU} \frac{d}{dL} E_Q(\ell(x, C_a; \varpi_L, \varpi_U)|y) \Big|_{C_a=[\hat{L}, \hat{U}]} = 0$$

and hence the determinant of the Hessian is positive.

2. Then I can use the equi-tail interval: $x \in [x_{a/2}, x_{1-a/2}]$ with $\varpi_L = a/2$ and $\varpi_U = 1 - a/2$
3. Then I can use the lower-tail interval: $x \in (-\infty, x_{1-a}]$ with $\varpi_L = 0$ and $\varpi_U = 1 - a$.

Practice

Question 21. To practice try to work on the Exercises ??, and ?? from the Exercise sheet.