Handout 12: Credible sets [a]

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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.
- The Matrix Cookbook (Section 7) `http://matrixcookbook.com`

Web applets:

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

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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 $y := (y_1, ..., y_n) \in \mathcal{Y}$ 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 $\pi(\theta)$.

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 $\Pi(\theta|y)$;
$$\mathrm{d}\Pi(\theta|y) = \pi(\theta|y)\mathrm{d}\theta$$
with cdf $\Pi(\theta|y)$ and pdf/pmf $\pi(\theta|y)$.
- Degree of believe about a future sequence of outcomes $z = (y_{n+1}, ..., y_{n+m}) \in \mathcal{Z}$ is quantified via the predictive distribution $G(z|y)$;
$$\mathrm{d}G(z|y) = g(z|y)\mathrm{d}z$$
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 $Q(x|y)$;

$$\mathrm{d}Q(x|y) = q(x|y)\mathrm{d}x$$

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

$$1 - a \leq \mathsf{P}_Q(x \in C_a|y) = \int 1\left(x \in C_a\right) \mathrm{d}Q(x|y)$$

Note 5. In Bayesian stats (unlike frequetist stats) we can speak correctly and meaningfully say that the $(1-a)100\%$ credible set C_a of unknown parameter θ implies that the probability that θ in 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 intervals[1]

Note 7. Often it is useful to consider credible sets C_a which contain values of x that correspond to the highest pdf/pmf $g(x|y)$ (aka the most likely values of x). Then Definition 4 can be restricted by essentially imposing an extra restriction that: $g(x|y) \geq g(x'|y)$ for all $x \in C_a, x' \in C_a^{\complement}$. This leads to 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 of the form

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

where k_a is the largest constant such that

$$1 - a \leq \mathsf{P}_Q(x \in C_a|y)$$

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

Note 10. In the decision theory framework, the HPD set is the Bayes estimator (Bayes rule) of the credible set under the loss

$$\ell(x, \delta) = c\,\|\delta\| - 1(x \in \delta), \quad \forall \delta \in \mathcal{D},\ \forall x \in \mathcal{X},\ \forall c > 0. \tag{1}$$

where $\mathcal{D}$ is the set of all credible sets in Definition 4. Hence, interpreting (1), HPD credible sets are credible sets with the minimum size (length, volume, area, etc...).

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

4 General discussions

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

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

and then compute the HPD set by implementing Definition 8.

Note 12. [2]A (not-that-efficient) algorithm to compute HPD credible sets with a computer is as follows:

1. `Create a routine which computes all 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`

$$\mathsf{P}_Q(x \in C_a|y) = \int 1\left(x \in C_a\right)\mathrm{d}Q(x|y) \tag{2}$$

3. `Sequentially solve the equation`

$$\mathsf{P}_Q(x \in C_a|y) = 1 - a$$

`by increasing incrementally` k_a `from zero to larger, and stop just before (2)` drops below $1 - a$.

Note 13. 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 14. *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*

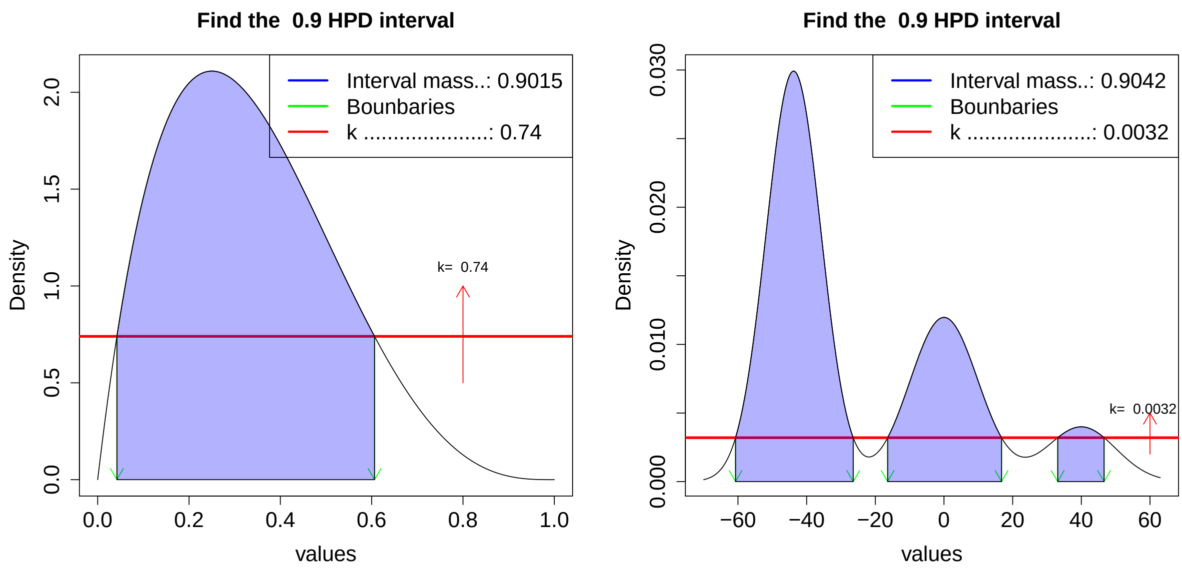
1. $\int_L^U q(x|y)dx = 1 - a$,
2. $q(U) = q(L) > 0$, *and*
3. $x_{mode} \in (L, U)$, *where* x_{mode} is the mode of $q(x|y)$,

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

Proof. Out of scope. 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. □

Remark 15. Theorem 14 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 trick can also be used in multimodal densities (Figure 1b).

[2]`https://georgios-stats-1.shinyapps.io/demo_CredibleSets/`



(a) Unimodal case; $C_a = [L, U]$ (b) Multimodal ; $C_a = [L_1, U_1] \cup [L_2, U_2]$

Figure 1: Schematic of Theorem 14 (in Fig. 1(1a)) and Note 12 (in Fig. 1(1a) & Fig. 1(1b))

5 Examples

Example 16. Consider a Bayesian model

$$\begin{cases} y_i|\mu & \overset{\text{iid}}{\sim} \mathrm{N}_d(\mu, \Sigma), \qquad i = 1, ..., n \\ \mu & \sim \mathrm{N}_d(\mu_0, \Sigma_0) \end{cases}$$

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 $z = (z_1, ..., z_d)^\top$ such as $z_j \overset{\text{iid}}{\sim} \mathrm{N}(0, 1)$ for $j = 1, ..., d$, and $\xi = z^\top z = \sum_{j=1}^{d} z_j^2$, then $\xi \sim \chi_d^2$

Hint-2: It is

$$-\frac{1}{2}\sum_{i=1}^{n}(x - \mu_i)^\top \Sigma_i^{-1}(x - \mu_i)) = -\frac{1}{2}(x - \hat{\mu})^\top \hat{\Sigma}^{-1}(x - \hat{\mu})) + C(\hat{\mu}, \hat{\Sigma}) \quad ;$$

$$\hat{\Sigma} = (\sum_{i=1}^{n} \Sigma_i^{-1})^{-1}; \quad \hat{\mu} = \hat{\Sigma}(\sum_{i=1}^{n} \Sigma_i^{-1}\mu_i);$$

$$C(\hat{\mu}, \hat{\Sigma}) = \underbrace{\frac{1}{2}(\sum_{i=1}^{n} \Sigma_i^{-1}\mu_i)^\top (\sum_{i=1}^{n} \Sigma_i^{-1})^{-1}(\sum_{i=1}^{n} \Sigma_i^{-1}\mu_i) - \frac{1}{2}\sum_{i=1}^{n} \mu_i^\top \Sigma_i^{-1}\mu_i}_{=\text{independent of } x}$$

Solution. I will use the Definition 8.

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

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

  where

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

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

- Now let's implement Definition 8. So,

$$\begin{aligned}
C_a &= \left\{\mu \in \mathbb{R}^d : \pi(\mu|y) \geq k_a\right\} \\
&= \left\{\mu \in \mathbb{R}^d : \mathrm{N}_q(\mu|\hat{\mu}_n,\hat{\Sigma}_n) \geq k_a\right\} \\
&= \left\{\mu \in \mathbb{R}^d : (\mu-\hat{\mu}_n)^\top\hat{\Sigma}_n^{-1}(\mu-\hat{\mu}_n) \leq \underbrace{-\log(2\pi\det(\hat{\Sigma}_n)))k_a}_{=\tilde{k}_a}\right\}
\end{aligned} \tag{3}$$

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

$$\mathsf{P}_\Pi\left(\mu \in C_a|y\right) \geq 1-a \iff$$

$$\mathsf{P}_\Pi\left(\underbrace{(\mu-\hat{\mu}_n)^\top\hat{\Sigma}_n^{-1}(\mu-\hat{\mu}_n)}_{=\xi} \leq \tilde{k}_a\right) \geq 1-a \tag{4}$$

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

$$\xi = (\mu-\hat{\mu}_n)^\top\hat{\Sigma}_n^{-1}(\mu-\hat{\mu}_n) \sim \chi^2_d \tag{5}$$

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

  Hence Eq. 4, (due to Eqs. 3, 5) becomes

$$\mathsf{P}_{\chi^2_d}((\mu-\hat{\mu}_n)^\top\hat{\Sigma}_n^{-1}(\mu-\hat{\mu}_n) \leq \tilde{k}_a) = 1-a \tag{6}$$

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

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

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

Example 17. Consider an exchangeable sequence of observables $y := (y_1,...y_n) \in \mathbb{R}^n$ from model

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

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 $a = 0.95$.

Solution.

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

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

  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 14.

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

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

$$1 - a = \mathsf{P}_{\text{Be}(17,17)}(\theta < U) - \big(1 - \mathsf{P}_{\text{Be}(17,17)}(\theta < U)\big) = 2\mathsf{P}_{\text{Be}(17,17)}(\theta < U) - 1$$

  so $\mathsf{P}_{\text{Be}(17,17)}(\theta < U) = 1 - a/2$ and $L = 1 - U$. For $a = 0.95$, 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('HDInterval')
> library('HDInterval')
> hdi(qbeta, 0.95, shape1=17, shape2=17)
lower upper
0.3354445 0.6645555
```

Example 18. Assume an 1- dimensional random quantity $x \sim Q(x|y)$. In the Lecture Handout (Handout 11: Bayesian point estimation), we can say that:

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

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

  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

$$\ell(x, C_a; \varpi_L, \varpi_U) = \ell(x, L; \varpi_L) + \ell(x, U; \varpi_U) \tag{7}$$

   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 (7) 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 (7) by computing L and U.

To be presented in the revision lecture.

Solution. It is given that

$$0 = \mathrm{E}_Q\left(\ell(x, \delta; \varpi)|y\right)|_{\delta=\hat{\delta}} = \frac{\mathrm{d}}{\mathrm{d}\delta}\int \ell(x, \delta; \varpi)\mathrm{d}Q(x|y)\bigg|_{\delta=\hat{\delta}} \implies \hat{\delta} = x_{\varpi}$$

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

$$0 = \frac{\mathrm{d}}{\mathrm{d}L}\mathrm{E}_Q\left(\ell(x, C_a; \varpi_L, \varpi_U)|y\right)\bigg|_{C_a=[\hat{L},\hat{U}]} = \mathrm{E}_Q\left(\ell(x, L; \varpi_L)|y\right)|_{L=\hat{L}} \implies \hat{L} = x_{\varpi_L}$$
$$0 = \frac{\mathrm{d}}{\mathrm{d}U}\mathrm{E}_Q\left(\ell(x, C_a; \varpi_L, \varpi_U)|y\right)\bigg|_{C_a=[\hat{L},\hat{U}]} = \mathrm{E}_Q\left(\ell(x, U; \varpi_U)|y\right)|_{U=\hat{U}} \implies \hat{U} = x_{\varpi_U}$$

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

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

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 19. *To practice try to work on the Exercise 65 from the Exercise sheet.*