Bayesian Statistics III/IV (MATH3341/4031) Michaelmas term, 2019

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 intervals

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

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

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. HPD credible sets are credible sets with the minimum size (length, volume, area, etc...). In the decision theory framework, the HPD set is the Bayes estimator (Bayes rule) of the credible set under the loss

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

[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`

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

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*

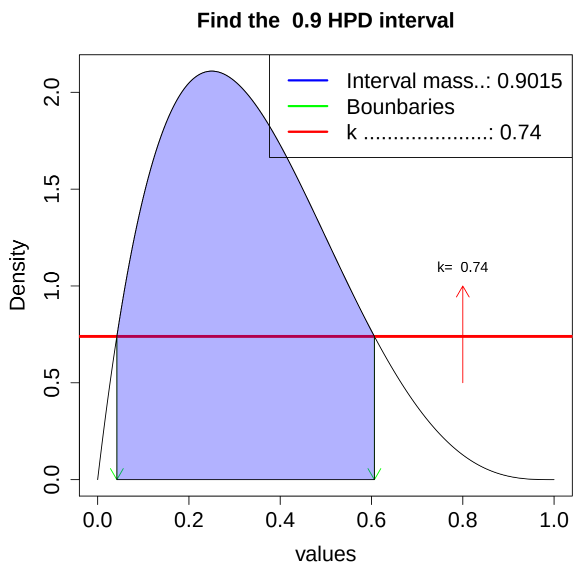
1. $\int_L^U q(x|y)dx = 1 - a$*,*
2. $q(U) = q(L) > 0$*, and*
3. $x_{mode} \in (L, U)$*, where* x_{mode} is the mode of $q(x|y)$*,*

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

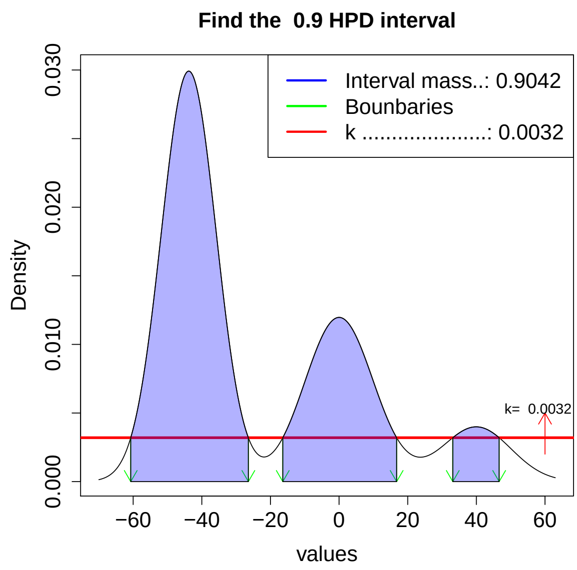
Proof. Out of scope. Use of the mean values theorem to prove. See, Casella, G., & Berger, R. L. (2002; pp. 441-443). Statistical inference (Vol. 2). Pacific Grove, CA: Duxbury. ☐

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

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

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,

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

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

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

- 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,

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

  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. 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
```

Practice

Question 18. *To practice try to work on the Exercise 64 from the Exercise sheet.*