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A note on approximate Bayesian credible sets based on modified loglikelihood ratios

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ABSTRACT

Higher-order asymptotic arguments for a scalar parameter of interest have been widely investigated for Bayesian inference. In this paper the theory of asymptotic expansions is discussed for a vector parameter of interest. A modified loglikelihood ratio is suggested, which can be used to derive approximate Bayesian credible sets with accurate frequentist coverage. Three examples are illustrated.

1. Introduction

The aim of this contribution is to discuss recent advances in approximate Bayesian inference based on the asymptotic theory of modified loglikelihood ratios. This theory provides asymptotic formulas for approximate credible regions for a multidimensional parameter with accurate frequentist coverage.

Approximate credible intervals for a scalar parameter based on modifications of the likelihood root have been widely discussed in the Bayesian literature; see, among others, DiCiccio et al. (1990), Sweeting (1995, 1996, 1999), Ventura et al. (2013), and the references therein. One appealing feature of these higher-order results is that they may routinely be applied for Bayesian inference, since they require little more than standard likelihood quantities for their implementation, and hence they may be available at little additional computational cost over simple first-order approximations.

In this paper we indicate how approximate Bayesian credible sets may be derived for a vector parameter of interest. As is the case with the approximations for a scalar parameter, the proposed results are based on the asymptotic theory of modified loglikelihood ratios (Skovgaard, 2001), they require only routine maximization output for their implementation, and they are constructed for arbitrary prior distributions.

The paper is organized as follows. Section 2 reviews higher-order Bayesian approximations for a scalar parameter of interest. Section 3 indicates how these ideas generalize to the multiparameter case. Section 4 illustrates some numerical examples. Finally, some concluding remarks are given in Section 5.

2. Preliminaries and background

Consider a sampling model $f(y;\theta)$ with scalar parameter $\theta \in \Theta \subseteq \mathbb{R}$, and let $L(\theta) = L(\theta; y) = \exp\{\ell(\theta)\}$ denote the likelihood function based on data y. Given a prior density $\pi(\theta)$ for θ, Bayesian inference is based on the posterior density $\pi(\theta|y) \propto \pi(\theta)L(\theta)$.

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Let $\hat{\theta}$ be the maximum likelihood estimator (MLE) of θ, and let $r(\theta) = \text{sign}(\hat{\theta} - \theta)W(\theta)^{1/2}$ be the likelihood root, where $W(\theta) = 2(\ell(\hat{\theta}) - \ell(\theta))$ is the loglikelihood ratio statistic. Furthermore, let $q(\theta) = \ell'(\theta)|j(\hat{\theta})|^{-1/2}\frac{\pi(\hat{\theta})}{\pi(\theta)}$, where $\ell'(\theta)$ is the score function and $j(\theta)$ is the observed information. For Bayesian inference under the prior $\pi(\theta)$, the modified likelihood root is given by (see Sweeting, 1996; Brazzale et al., 2007; Ventura et al., 2013)

$$r^*(\theta) = r(\theta) + \frac{1}{r(\theta)} \log \frac{q(\theta)}{r(\theta)}, \tag{1}$$

whose posterior distribution is standard normal to $O(n^{-3/2})$. Note that, for Jeffreys' prior $\pi(\theta) \propto i(\theta)^{1/2}$, with $i(\theta)$ expected information, (1) coincides with the modified likelihood root discussed in Barndorff-Nielsen and Chamberlin (1994).

The modified likelihood root (1) can be derived following the three-step procedure discussed in Skovgaard (2001); see also Davison (2003, Chapter 11), and the references therein.

Step 1: Consider the Laplace expansion of $\pi(\theta|y)$, given by

$$\pi(\theta|y) \doteq \frac{1}{\sqrt{2\pi}} |j(\hat{\theta})|^{1/2} \frac{\pi(\theta)}{\pi(\hat{\theta})} \exp\left\{-\frac{1}{2} r(\theta)^2\right\}, \tag{2}$$

where the symbol "$\doteq$" indicates that the approximation is accurate to order $O(n^{-1})$.

Step 2: Change the variable from θ to $r = r(\theta)$. A motivation for considering such a transformation is that, in terms of r^2, the quantity $\exp(-r^2/2)$ in (2) is the kernel of the standard normal density. The Jacobian is $dr(\theta)/d\theta = -\ell'(\theta)/r(\theta)$, and thus

$$\pi(r|y) \doteq \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2} r^2 + \log b(r)\right\},$$

where the positive quantity $b(r) = |j(\hat{\theta})|^{1/2} \frac{\pi(\theta)}{\pi(\hat{\theta})} \frac{r(\theta)}{\ell'(\theta)}$ is regarded as a function of r.

Step 3: Change of variable from r to $r^* = r^*(\theta) = r - r^{-1} \log b(r)$, so that

$$-(r^*)^2 = -r^2 + 2 \log b(r) - \left(r^{-1} \log b(r)\right)^2. \tag{3}$$

The Jacobian of the transformation and the third term in (3) contribute only to the error, and it can be shown that (see Sweeting, 1995, 1996, Severini, 2000, Chapter 2)

$$\pi(r^*|y) \ddot{=} \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(r^*)^2\right\}, \tag{4}$$

where the symbol "$\ddot{=}$" indicates that the approximation is accurate to order $O(n^{-3/2})$.

Note that from (4) the following tail area approximation can be derived:

$$\int_{-\infty}^{\theta_0} \pi(\theta|y)\, d\theta \ddot{=} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{r_0^*} \exp\left\{-\frac{1}{2}(r^*)^2\right\} dr^* = \Phi(r_0^*), \tag{5}$$

where $\Phi(\cdot)$ is the standard normal distribution function and $r_0^* = r^*(\theta_0)$. Formula (5) gives an explicit expression for the posterior quantiles, and $1-\Phi(r_0^*)$ is the Bayesian survivor probability. Moreover, (5) gives rise to a simple simulation scheme (Ruli et al., in press), alternative to MCMC, for Bayesian computation of posterior distributions.

From (4) an approximate credible interval for θ can be computed as $CI = \{\theta : w^*(\theta) \le \chi^2_{1,1-\alpha}\}$, where $w^*(\theta) = r^*(\theta)^2$ and $\chi^2_{1,1-\alpha}$ is the $(1-\alpha)$-quantile of the χ^2_1 distribution. Equivalently, CI can be computed as

$$CI = \left\{\theta : |r^*(\theta)| \le z_{1-\alpha/2}\right\}, \tag{6}$$

where $z_{1-\alpha/2}$ is the $(1-\alpha/2)$-quantile of the standard normal distribution. Note that (6) defines a third-order equi-tailed credible interval for θ with frequentist accurate coverage.

3. Approximate Bayesian computation for multidimensional parameters

Suppose that $\theta \in \Theta \subseteq \mathbb{R}^d$, with $d > 1$. Paralleling results in Section 2, in this section we study asymptotic expansions based on modifications of the loglikelihood ratio. As in the scalar parameter case, the derivation of these asymptotic expansions can be based on the following three steps (see Skovgaard, 2001):

Step 1: computation of the Laplace approximation of $\pi(\theta|y)$, given by

$$\pi(\theta|y) \doteq (2\pi)^{-d/2} |j(\hat{\theta})|^{1/2} \frac{\pi(\theta)}{\pi(\hat{\theta})} \exp\left\{-\frac{1}{2} W(\theta)\right\};$$

Step 2: change of the variable of integration from θ to $r_m = r_m(\theta)$, such that for the loglikelihood ratio we have $W(\theta) = 2\left(\ell(\hat{\theta}) - \ell(\theta)\right) = r_m(\theta)^\top r_m(\theta)$;

Step 3: change of the variable of integration from r_m to a more accurate version of the form $r_m^* = r_m^*(\theta) = r_m - \delta(r_m)$, with $\delta = \delta(r_m)$ chosen to satisfy $r_m^\top \delta(r_m) = \log g(r_m)$ for a suitably defined term $g(r_m)$, so that $(r_m - \delta)^\top (r_m - \delta) = r_m^\top r_m - 2\log g(r_m) + O(n^{-2})$ is asymptotically χ^2_d.

In order to compute Step 2, we need a statistic $r_m = r_m(\theta)$ for which $r_m^\top r_m = W(\theta)$. Let us consider the signed root loglikelihood ratio transformation defined in Sweeting (1995, 1996); see also Kharroubi and Sweeting (2010). Let $\theta = (\theta_1, \ldots, \theta_d) = (\theta^i, \theta^{(i+1)})$, where $\theta^i = (\theta_1, \ldots, \theta_i)$ is the vector of the first i components of θ and $\theta^{(i+1)} = (\theta_{i+1}, \ldots, \theta_d)$. Let $\hat{\theta}^{(i+1)}_{\theta^i}$ be the partial MLE of $\theta^{(i+1)}$ given θ^i, and let $\hat{\theta}_{j,\theta^i}$ be the jth component of $(\theta^i, \hat{\theta}^{(i+1)}_{\theta^i})$, for $j > i$. The signed root loglikelihood ratio transformation is thus defined as

$$r_m(\theta) = (r_{m1}, \ldots, r_{md}), \tag{7}$$

with

$$r_{mi} = \operatorname{sign}(\theta_i - \hat{\theta}_{i,\theta^{i-1}}) \left\{2\left[\ell\left(\theta^{i-1}, \hat{\theta}^{(i)}_{\theta^{i-1}}\right) - \ell\left(\theta^i, \hat{\theta}^{(i+1)}_{\theta^i}\right)\right]\right\}^{1/2}, \quad i = 1, \ldots, d. \tag{8}$$

Note that (8) is a function of the first i components $\theta^i = (\theta_1, \ldots, \theta_i)$ of θ. Moreover, $r_m(\theta)$ is a one-to-one data-dependent transformation of θ, such that $\exp\left\{-\frac{1}{2} r_m^\top r_m\right\} = L(\theta)/L(\hat{\theta})$. Finally, $r_m(\theta)$ is asymptotically multivariate standard normal to $O(n^{-1/2})$.

In the second step, when changing the variable of integration from θ to the statistic r_m given in (7), the Jacobian matrix $dr_m/d\theta$ is lower triangular, i.e.

$$\left|\frac{dr_m}{d\theta}\right| = \prod_{i=1}^{d} \left|\frac{\ell_i\left(\theta^i, \hat{\theta}^{(i+1)}_{\theta^i}\right)}{r_{mi}}\right|,$$

where $\ell_i(\theta)$ is the ith component of the score vector $\partial\ell(\theta)/\partial\theta$, for $i = 1, \ldots, d$.

The last step is again a change of variable. Following Skovgaard (2001), we perturb r_m to $r_m^* = r_m^*(\theta) = r_m - \delta(r_m)$, with $\delta(r_m)$ chosen to satisfy $r_m^\top \delta(r_m) = \log g(r_m)$, so that

$$-(r_m - \delta(r_m))^\top (r_m - \delta(r_m)) = -r_m^\top r_m + 2\log g(r_m) + O(n^{-2}). \tag{9}$$

In order to compute (9), we only need the existence of $\delta(r_m)$ to calculate

$$w_m^* = w_m^*(\theta) = r_m(\theta)^\top r_m(\theta) - 2\log g(r_m(\theta)), \tag{10}$$

with

$$g(r_m(\theta)) = |j(\hat{\theta})|^{1/2} \frac{\pi(\theta)}{\pi(\hat{\theta})} \left[\prod_{i=1}^{d} \left|\frac{\ell_i\left(\theta^i, \hat{\theta}^{(i+1)}_{\theta^i}\right)}{r_{mi}}\right|\right]^{-1}. \tag{11}$$

The asymptotic distribution of w_m^* is χ^2_d with relative error $O(n^{-1})$ in a large deviation region. To obtain a statistic which generalizes the scalar version (1), Skovgaard (2001) suggests to use the asymptotically equivalent approximation

$$w_m^{**} = w_m^{**}(\theta) = r_m^\top r_m \left(1 - \frac{\log g(r_m)}{r_m^\top r_m}\right)^2. \tag{12}$$

Indeed, note that, for $d = 1$, the quantity (11) reduces to $g(\theta) = r(\theta)/q(\theta)$, and thus we have $w_m^{**}(\theta) = (r - (1/r)\log b(r))^2 = (r^*)^2$.

From (12), or from (10), as for the scalar parameter case, an approximate credible set for θ can be computed as

$$CR = \left\{\theta : w^{**}(\theta) \le \chi^2_{d,1-\alpha}\right\}. \tag{13}$$

This credible region has $100(1-\alpha)\%$ coverage in repeated sampling with relative error $O(n^{-1})$ in a large deviation region, thus improving the first-order credible region

$$CR_N = \left\{\theta : (\theta - \tilde{\theta})^\top j_\pi(\tilde{\theta})(\theta - \tilde{\theta}) \le \chi^2_{d,1-\alpha}\right\}, \tag{14}$$

where $\tilde{\theta}$ is the posterior mode and $j_\pi(\theta) = -\partial^2 \log \pi(\theta|y)/(\partial\theta\partial\theta^\top)$, and the likelihood-type credible region

$$CR_L = \left\{\theta : -2\log\frac{\pi(\theta|y)}{\pi(\tilde{\theta}|y)} \le \chi^2_{d,1-\alpha}\right\}. \tag{15}$$

Note that, in general, first-order inference based on (14) may be questionable since it forces credible sets to have an elliptical shape; see Hills and Smith (1992) for the determination of good parameterizations in the Bayesian framework to take into account this drawback.

Table 1
Normal distribution: empirical coverage probabilities of credible regions.

$1-\alpha$	π_1			π_2		
	0.90	0.95	0.99	0.90	0.95	0.99
	$n = 10$			$n = 10$		
CR_N	0.7280	0.7830	0.8685	0.5905	0.6470	0.7402
CR_L	0.8540	0.9130	0.9770	0.7871	0.8688	0.9578
CR	0.9075	0.9510	0.9925	0.9020	0.9517	0.9904
	$n = 15$			$n = 15$		
CR_N	0.7615	0.8280	0.900	0.6698	0.7302	0.8189
CR_L	0.8485	0.9225	0.984	0.8276	0.8992	0.9738
CR	0.8935	0.9500	0.990	0.9050	0.9544	0.9916
	$n = 30$			$n = 30$		
CR_N	0.8275	0.889	0.9495	0.7688	0.8250	0.9031
CR_L	0.8775	0.936	0.9840	0.8606	0.9242	0.9824
CR	0.8980	0.948	0.9875	0.9023	0.9533	0.9888
	$n = 50$			$n = 50$		
CR_N	0.8630	0.9240	0.9730	0.8160	0.8761	0.9436
CR_L	0.8965	0.9435	0.9890	0.8791	0.9346	0.9836
CR	0.9045	0.9525	0.9890	0.9011	0.9514	0.9897

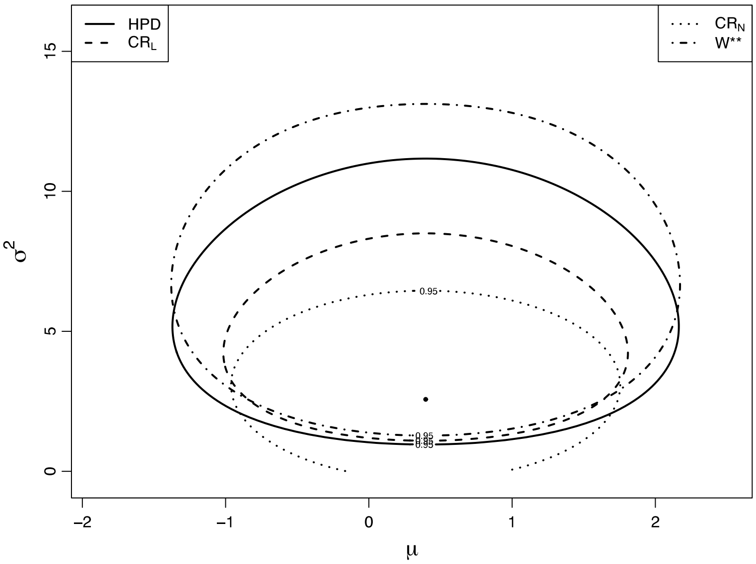

Fig. 1. Normal distribution: credible regions for (μ, σ^2).

4. Numerical examples

Example 1 (*Normal Distribution*)**.** Consider a random sample $y = (y_1, \dots, y_n)$ from a $N(\mu, \sigma^2)$ distribution, with $\theta = (\mu, \sigma^2)$ unknown. We assume two different prior distributions of θ, i.e. the improper prior $\pi_1(\theta) \propto 1/\sigma^2$ and the normal-gamma prior $\pi_2(\theta)$. In this case, all the quantities involved in the computation of w^* and w^{**} are easy to compute.

To judge the coverage quality of the credible region (13), a simulation study based on 10000 Monte Carlo trials has been performed. Table 1 gives the empirical frequentist coverages for $(1-\alpha)$ posterior credible regions (13) in comparison to the first-order credible regions CR_N and CR_L. From Table 1 we note that, for every n, CR clearly improves on (14) and (15). Larger sample sizes would show, as one would expect, rather little differences between the results of all the procedures.

For a sample of size $n = 10$, Fig. 1 gives the contours of several credible regions for $\theta = (\mu, \sigma^2)$, i.e. CR_N, CR_L, the 95% HPD credible region, and the CR based on w_m^{**}. The posterior probability of CR_N is 0.674, of CR_L is 0.881 and of CR is 0.949. Only CR has the correct posterior probability.

Example 2 (*Gamma Distribution*)**.** Consider a random sample $y = (y_1, \dots, y_n)$ from a gamma distribution, with both the shape κ and scale σ parameters unknown. Let $\theta = (\log \sigma, \log \kappa)$. We assume two prior distributions of θ, that are $\pi_1(\theta) \propto 1$ and $\pi_2(\theta) = N(\mu, \nu) \times N(\mu, \nu)$, where (μ, ν) is a fixed hyperparameter. As in the previous example, to judge the coverage

Table 2
Gamma distribution: empirical coverage probabilities of credible regions.

$1-\alpha$	π_1			$\pi_2(\mu=0,\nu=10)$			$\pi_2(\mu=3,\nu=10)$		
	0.90	0.95	0.99	0.90	0.95	0.99	0.90	0.95	0.99
	$n=5$			$n=5$			$n=5$		
CR_N	0.8188	0.7991	0.8801	0.7642	0.8288	0.9040	0.6630	0.7324	0.8374
CR_L	0.8405	0.9084	0.9755	0.8624	0.9265	0.9837	0.7787	0.8659	0.9594
CR	0.9018	0.9500	0.9895	0.9166	0.9612	0.9933	0.8753	0.9338	0.9864
	$n=10$			$n=10$			$n=10$		
CR_N	0.8188	0.8779	0.9445	0.8281	0.8868	0.9495	0.7764	0.8381	0.9215
CR_L	0.8748	0.9336	0.9832	0.8826	0.9385	0.9854	0.8402	0.9115	0.9764
CR	0.9028	0.9519	0.9893	0.9084	0.9564	0.9908	0.8866	0.9424	0.9872

Table 3
Weibull model: empirical coverage probabilities of credible regions; the hyperparameter μ is fixed equal to $(\log 2, -1, 1, -1, 1)$ for $p=4$ and to $(\log 2, -1, 1, -1, 1, -1, 1, -1, 1, -1)$ for $p=9$.

$1-\alpha$	$p=4$			$p=4$			$p=9$			$p=9$		
	π_1			π_2			π_1			π_2		
	0.90	0.95	0.99	0.90	0.95	0.99	0.90	0.95	0.99	0.90	0.95	0.99
	$n=10$			$n=10$			$n=15$			$n=15$		
CR_N	0.4292	0.5054	0.6176	0.4530	0.5282	0.6424	0.0128	0.1610	0.2332	0.1380	0.1780	0.2540
CR_L	0.7322	0.8270	0.9374	0.7490	0.8432	0.9448	0.5008	0.6094	0.7992	0.5226	0.6314	0.8132
CR	0.9348	0.9700	0.9944	0.9424	0.9754	0.9962	0.9560	0.9776	0.9966	0.9634	0.9828	0.9970
	$n=20$			$n=20$			$n=20$			$n=20$		
CR_N	0.6736	0.7444	0.8496	0.6814	0.7528	0.8550	0.2656	0.3300	0.4584	0.2758	0.3332	0.4548
CR_L	0.8382	0.9114	0.9774	0.8452	0.9154	0.9792	0.6582	0.7628	0.9034	0.6592	0.7650	0.9100
CR	0.9190	0.9592	0.9920	0.9234	0.9636	0.9932	0.9472	0.9750	0.9954	0.9528	0.9796	0.9964
	$n=30$			$n=30$			$n=30$			$n=30$		
CR_N	0.7526	0.8242	0.9114	0.7564	0.8282	0.9130	0.4332	0.5134	0.6536	0.4580	0.5378	0.6694
CR_L	0.8616	0.9238	0.9794	0.8650	0.9262	0.9806	0.7562	0.8480	0.9494	0.7692	0.8516	0.9540
CR	0.9074	0.9534	0.9912	0.9104	0.9558	0.9914	0.9356	0.9686	0.9948	0.9388	0.9708	0.9954
	$n=50$			$n=50$			$n=50$			$n=50$		
CR_N	0.8058	0.8756	0.9454	0.8088	0.8768	0.9464	0.6286	0.7090	0.8290	0.6178	0.7006	0.8254
CR_L	0.8762	0.9336	0.9864	0.8784	0.9360	0.9870	0.8294	0.9044	0.9716	0.8254	0.9032	0.9756
CR	0.9052	0.9530	0.9926	0.9072	0.9534	0.9926	0.9220	0.9616	0.9928	0.9220	0.9608	0.9918

quality of CR, a simulation study based on 2000 Monte Carlo trials has been performed. Table 2 gives the empirical frequentist coverages for (13) in comparison to the first-order credible regions CR_N and CR_L. From Table 2 we note that, for every n, CR improves on (14) and (15). Observe also that for parameter values in regions of low prior density there may be, as expected, some degradation in the coverage accuracy.

Example 3 (*Weibull Model*)**.** Let us consider a random sample $(t_1, \ldots, t_n)$ from a Weibull model with shape parameter κ and scale parameter $\lambda_i = x_i^{\mathsf{T}}\beta$, where x_i is a known $p \times 1$ vector, $i = 1, \ldots, n$, and the unknown parameters are the $p \times 1$ vector β and κ. Note that $y_i = \log t_i$ follows a regression and scale model of the form $y_i = x_i^{\mathsf{T}}\beta + \sigma\varepsilon_i$, with $\sigma = 1/\kappa$ and ε_i log-Weibull or extreme-value random variable, $i = 1, \ldots, n$.

For the parameter $\theta = (\beta, \tau)$, with $\tau = \log\sigma$, we assume two prior distributions, i.e. the noninformative prior $\pi_1(\theta) \propto 1$ and the proper prior $\pi_2(\theta) = \prod_{i=1}^{p+1} N(\mu_i, 20)$, where $\mu = (\mu_1, \ldots, \mu_{p+1})$ is a fixed hyperparameter. A simulation study based on 5000 Monte Carlo trials has been performed with $p = 4$ and $p = 9$ in order to judge the coverage quality of CR in comparison to the first-order credible regions CR_N and CR_L. From Table 3 we note that, for every n and p, CR is always preferable to (14) and (15).

5. Final remarks

To obtain credible regions for a vector parameter, approximate Bayesian computations based on loglikelihood ratios provide important quantities of the posterior distribution with very little computational effort, in a fraction of the time required for a full simulation approach. Although the approximations described in this paper are derived from asymptotic considerations, they perform extremely well in small sample situations.

A key feature of the approximations discussed and developed in this paper is that they do not require the calculation of loglikelihood derivatives beyond the second order for their implementation. In this respect, higher-order expansions represent a very quick and accurate method for computing posterior quantities and they make quite straightforward to assess the effect of changing priors; see, e.g., Kass et al. (1988), Reid and Sun (2010), Ruli et al. (in press), and Ventura et al. (2013).

Finally, note that the signed root loglikelihood ratio transformation (7) in general depends on the chosen parameter order. However, in certain situations, such as the examples considered in the previous section, the results of the simulation studies do not change (results not reported here) when inverting the parameter order.

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