On Reparameterization Invariant Bayesian Point Estimates and Credible Regions

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September 23, 2021

Abstract

This paper considers reparameterization invariant Bayesian point estimates and credible regions of model parameters for scientific inference and communication. The effect of intrinsic loss function choice in Bayesian intrinsic estimates and regions is studied with the following findings. A particular intrinsic loss function, using Kullback-Leibler divergence from the full model to the restricted model, has strong connection to a Bayesian predictive criterion, which produces point estimates with the best predictive performance. An alternative intrinsic loss function, using Kullback-Leibler divergence from the restricted model to the full model, produces estimates with interesting frequency properties for at least some commonly used distributions, that is, unbiased minimum variance estimates of the location and scale parameters.

Keywords: Bayesian inference, point estimation, credible interval, intrinsic estimation, predictive criterion, model selection

1 Introduction

In the Bayesian approach, the optimal way of making inference is to describe all the uncertainties with probabilities and probability distributions and obtain the posterior distribution of the quantity of interest by marginalizing over all other unknowns. If there is uncertainty in the model structure, the optimal Bayesian approach is to integrate also over the model space (considering models as discrete parameters). After taking into account everything we can think of, we have the full (encompassing) model $M_*$ describing optimally our knowledge of the phenomenon (see, e.g., O’Hagan and Forster, 2004; Vehtari and Ojanen, 2012). Adequacy of the full model $M_*$ should be assessed, for example, using external validation with new data, simulating external validation via cross-validation (e.g., Vehtari and Ojanen, 2012) or using various posterior consistency checks (see, e.g., Dey et al., 1994; Gelman et al., 1996; Gelman et al., 2013, Ch. 6).

Sometimes it may be helpful to use point estimates for some of the quantities, for example, to reduce future computational load, or as a necessary part of reporting results. Related problems are estimation of credible regions (or intervals in one dimension), hypothesis testing and model selection. Credible regions are natural extension of point estimates. Hypothesis testing can be used to test whether a particular unknown could be fixed to a particular value, for example, whether a covariate related parameter could be fixed to zero. Model selection may be thought as point estimation in the model space.
In view of having the full model, all these problems can be considered as model reduction problems, in which there is some desire for using a reduced restricted model $M_R$ instead of the full model $M_*$. Model reduction can be considered as a decision problem, in which there is some utility associated to the performance of the model or loss associated to the divergence from the full model. There may also be associated measurement and computation costs. Preferably one should use an application specific utility (or loss or cost) function. Sometimes this utility is not readily available and it would then be useful to be able to use a generic reference utility. See Vehtari and Ojanen (2012) for further discussion and references.

This paper concentrates on the point and credible region estimation for pure scientific inference and communication using generic reference utilities. Connection to hypothesis testing and model selection is discussed in the end. Specifically the purpose of the paper is to compare the properties of the estimates and credible regions obtained using the following methods.

- Intrinsic estimation with the symmetric intrinsic loss function as proposed by Bernardo and Juárez (2003) and Bernardo (2005b).
- Intrinsic estimation with Kullback-Leibler divergence from the full model to the restricted model. Bernardo (1999) used this loss function in Bayesian Reference Criterion before it was replaced with symmetric version by Bernardo and Rueda (2002).
- Intrinsic estimation with Kullback-Leibler divergence from the restricted model to the full model. This loss function is part of the symmetric version, but it has not been previously used alone.
- Predictive criterion. This is based on a predictive model selection criterion proposed by San Martini and Spezzaferri (1984), which has not been previously used for point or credible region estimation.

This paper shows a connection, including equality in special case, between intrinsic estimation with Kullback-Leibler divergence from the full model to the restricted model and the predictive criterion. Examples demonstrate that the intrinsic estimation with Kullback-Leibler divergence from the restricted model to the full model has interesting frequency properties, that is, it produces unbiased minimum variance estimates for certain models with commonly used parameterization. Furthermore, it is illustrated that the symmetric intrinsic loss function advocated by Bernardo and Rueda (2002), Bernardo and Juárez (2003) and Bernardo (2005c,b) is a compromise between these two.

To illustrate the interesting properties, this paper focuses on simple models for which we can compute the solutions analytically or with low dimensional quadrature. The predictive criterion approach is closely connected to the projective predictive approach which replaces the exact criterion with an approximation that is computationally faster (Piironen et al., 2020; Catalina et al., 2020, 2021).

Section 3 reviews the point estimation as a decision problem and preferable properties for a generic utility (loss) function for pure scientific inference and communication. Section 4 reviews the predictive model selection criterion, shows how it can be used in point estimation and builds up for the connection to intrinsic estimation. Section 5 reviews intrinsic estimation and different intrinsic loss functions used in this paper, shows the connection of intrinsic estimation with a particular loss function to the predictive criterion, and discusses properties of other loss functions used in this paper. Section 6 reviews credible regions, and show how point estimation methods discussed in this paper are extended to estimation of credible regions. Section 7 illustrates the properties of the methods in several examples. Derivations of the estimates are given. In the simplest examples, the point estimates can be solved analytically and for the rest solutions require partial numerical computation. Numerical examples are used for further illustration. Conclusion of the results and additional discussion are presented in Sections 8 and 9.
2 Point estimation

In the Bayesian approach, the uncertainties are presented with distributions. To fully describe the information presented by the distribution the whole distribution has to be presented (see, e.g., Bernardo and Smith, 1994, Ch. 2 and 3). Point estimates may be used to summarize the distributions for simpler communication, they may be necessary if the action in decision problem requires stating a single value (e.g., in control), or they may be used to simplify the model.

Loss function can be used to measure the consequences of using a point estimate instead of the full distribution and the point estimate is then obtained using the decision theory.

We follow the notation by Vehtari and Ojanen (2012). Let $y_{(1:n)} = (y_1, \ldots, y_n)$ denote the observed data, $\tilde{y}$ denote the not yet observed future observation. We assume here the $M$-completed view (Bernardo and Smith, 1994; Vehtari and Ojanen, 2012), and assume that the posterior predictive distribution using the full model $M$,

$$p(\tilde{y}|y_{(1:n)}, M_\ast) = \int p(\tilde{y}|\theta, M_\ast)p(\theta|y_{(1:n)}, M_\ast)d\theta$$  (1)

is our best description of the unknown true distribution $p_\ast(y)$ (see Vehtari and Ojanen, 2012, for further discussion on this assumption).

In some cases, we may want to summarise some of the parameters $\theta$ by point estimates. The most commonly used Bayesian point estimates for $\theta$ are the posterior mean, median, and mode (see, e.g., Bernardo and Smith, 1994, Ch. 5; Robert, 2001, Ch. 4; Gelman et al., 2013, Ch. 2; Press, 2003, Ch. 8). These correspond to using squared, absolute and zero-one loss functions respectively and the expectation is taken over the marginal posterior of $\theta$ given the observations $y$

$$\hat{\theta} = \arg\min_{\theta} \int l(\theta, \tilde{\theta})p(\theta|y_{(1:n)}, M_\ast)d\theta. $$  (2)

In some cases these loss functions may be justified by the application, but most often they are simply used to summarize the location of the marginal distribution. Problem is that posterior mean and mode are not invariant under reparameterization and median is not easily generalizable to more than one dimension.

We also consider cases where we form point estimates only for subset of parameters. Let $p(y|\theta, \lambda, M_\ast)$ be the full model with additional parameters $\lambda$, and $p(y|\tilde{\theta}, \lambda, M_R)$ be the restricted model in which $\theta$ is estimated with $\tilde{\theta}$. Now there are a few alternatives how to define the decision problem. For clarity, in this paper models conditional on covariates $p(y|x, \theta, \lambda, M)$ are not considered, since not having explicit model for the distribution of $x$ complicates the analysis (see Vehtari and Ojanen, 2012, for related discussion). Such analysis will be presented in a forthcoming paper.

3 Loss functions

There are several well justified desirable properties for loss functions in pure scientific inference. Bernardo (1979a) and Bernardo and Smith (1994, Sec. 2.7 and 3.4) argue that the loss function should be proper local score function. Robert (1996) argues that loss function should be invariant to reparameterization. Bernardo and Juárez (2003) elaborate that invariance to reparameterization is necessary since in a purely inferential context, the loss function should not measure the discrepancy between parameter values, but directly measure the discrepancy between the models they label. A loss function comparing models directly $l(p, \tilde{p})$ is called an intrinsic loss (Robert, 1996). Not all intrinsic loss functions are equally well suited, and Bernardo (2005b) gives additional preferred condition of invariancy under reduction of
the data to sufficient statistics. See Robert (1996), and Bernardo (2005c,b) for further discussion and references.

Robert (1996), Bernardo and Juárez (2003), and Bernardo (2005c,b) consider parameterization invariant loss functions based on comparing models \( p(\tilde{y}|\theta, \lambda, M_e) \) and \( p(\tilde{y}|\theta, \lambda, M_R) \). However, parameterization invariant loss functions can also be achieved by comparing predictive distributions of the models \( p(\tilde{y}|y(1:n), M_e) \) and \( p(\tilde{y}|y(1:n), M_R) \). The predictive model selection criterion based point estimation is introduced in Section 4 and intrinsic estimation, based on intrinsic loss functions for models, is reviewed in Section 5. Extension of point estimates to credible regions is reviewed in Section 6.

## 4 Predictive criterion estimation

In prediction problems, the question in model selection is whether some of the unknowns in the model \( M_e \) could be fixed without losing information in predictive inference. The proposed problem may formally be described as a decision problem with two alternating actions. One action is to predict with the full model \( M_e \) and alternative action is to use a restricted model \( M_R \) with some parameters fixed. Point estimation can then be considered as a decision problem where values for fixed parameters are chosen to maximize the expected utility (or minimize the expected loss). See Vehtari and Ojanen (2012) for further discussion.

Let \( u(\hat{\rho}(\bar{y}), \tilde{y}) \) be a utility function associated with the choice of \( \hat{\rho}(\bar{y}) \) as the predictive distribution of the future distribution, where \( \bar{y} \) is the true unknown future value. The true expected utility is computed by integrating over true distribution \( p_t(\tilde{y}) \)

\[
\int u(\hat{\rho}(\bar{y}), \tilde{y}) p_t(\tilde{y}) d\tilde{y},
\]

where \( p_t(\tilde{y}) \) describes the uncertainty in future value of \( \bar{y} \). Since the full model \( M_e \) describes our knowledge of the phenomenon, it is natural that \( p(\bar{y}) \) is replaced with the predictive distribution of the full model \( p(\tilde{y}|y(1:n), M_e) \). Thus, the expected predictive performance of the restricted model is estimated using the full model \( M_e \) as approximate “true” belief model.

Early account of using this approach is described in an article by Lindley (1968), in which the goal was covariate selection. The analysis was made using a Gaussian linear model and quadratic loss function, which facilitates analytic solution. Instead of point estimation, part of the parameters in a restricted model were fixed to zero (thus removing their effect in the model).

Bernardo (1979a) and Bernardo and Smith (1994, Ch. 2 and 3) argued that in a pure scientific inference and communication context it is most appropriate to use a logarithmic score function, which among other good properties is also related to the information theoretic measure of the information in the distribution. Expected utility is then

\[
\int \log \hat{\rho}(\bar{y}) p(\tilde{y}|y(1:n), M_e) d\tilde{y},
\]

which was called predictive model selection criterion by San Martini and Spezzaferri (1984). To take into account the point estimation, credible regions, and hypothesis testing, we call this simply a predictive criterion. The predictive criterion for a model \( M_R \) is defined as

\[
\int \log p(\tilde{y}|y(1:n), M_R) p(\tilde{y}|y(1:n), M_e) d\tilde{y}.
\]
The optimal values for the fixed unknowns are obtained by maximizing this predictive criterion and the predictive point estimate of \( \theta \) is obtained simply as

\[
\hat{\theta}_p = \arg \max_{\theta} \int \log p(\tilde{y}|y_{1:n}), \tilde{\theta}, M_R)p(\tilde{y}|y_{1:n}), M_* d\tilde{y}.
\]

This estimate provides the best predictive distribution given the restriction that \( \theta \) is fixed instead of integrating over it.

The predictive criterion estimation approach can be considered as a comparison of the predictive distribution of the restricted model \( M_R \) to future observations generated by the belief model \( M_* \). This is obvious if one considers the Monte Carlo approximation of (5),

\[
\frac{1}{L} \sum_{l=1}^{L} \log p(y_l^{rep}|y_{1:n}), M_R),
\]

where \( y_l^{rep} \) are samples from the predictive distribution \( p(y|y_{1:n}), M_* \), which can be considered as proxy for future observations.

For simpler models (e.g. one-parameter distributions in exponential family) these estimates can be evaluated analytically. For more complex models, generic approach is to use Monte Carlo sampling for the posterior distribution and then the predictive distribution can be approximated as a mixture distribution with components having parameter values from the posterior samples. The Monte Carlo approximation (7) can generally be improved, for example, via partial use of analytic or numerical integration. Section 7 shows examples for both simpler and more complex models. For more complex models a fast approximate projection predictive approach can be used (Piironen et al., 2020; Catalina et al., 2020, 2021).

A useful loss function view of the approach is obtained if the predictive criterion of the full model \( M_* \) is computed

\[
\int \log p(y|y_{1:n}), M_*)p(y|y_{1:n}), M_*)dy,
\]

and (5) is subtracted from that to get

\[
\int p(y|y_{1:n}), M_*) \log \frac{p(y|y_{1:n}), M_*)}{p(y|y_{1:n}), M_R)},
\]

which is the Kullback-Leibler divergence from the predictive density of the full model \( p(y|y_{1:n}), M_* \) to the predictive density of a restricted model \( p(y|y_{1:n}), M_R) \). Thus the use of the predictive criterion corresponds to minimizing the loss related to consequence of using \( M_R \) instead of \( M_* \) and

\[
\hat{\theta} = \arg \min_{\theta} \int k[p(y|y_{1:n}), M_*), p(y|y_{1:n}), M_R)]p(y|y_{1:n}), M_*)dy,
\]

where \( k[p(y|y_{1:n}), M_*), p(y|y_{1:n}), M_R) \) is the Kullback-Leibler divergence (9). From the information theoretic point of view, the best point estimate for the fixed unknown is such that minimum amount of information is lost in the predictive distribution when replacing the full model with the restricted model. The amount of information lost could be used in hypothesis testing to make decision whether restricted model \( M_R \) can be accepted to be used instead of the full model \( M_* \). See Bernardo (1979a) and Bernardo and Smith (1994, Ch. 2 and 3) for discussion about value of information, and Bernardo (1999) and Bernardo and Rueda (2002) for discussion about calibration of that value for hypothesis testing. The predictive distribution is naturally associated to a next single observation in time. Alternatively, we can consider prediction where all \( n \) measurements were to be repeated again, which adds multiplication by \( n \).
to logarithmic score used. The calibration of this utility is then related to the calibration of traditionally used likelihood-ratio. For notational and computational convenience, in this paper the computations have been made without multiplication by \( n \), specially as it does not have any effect on point estimates and intervals.

Laud and Ibrahim (1995) proposed minimization of the symmetric Kullback-Leibler divergence

\[
    k\{p(y|y_{1:n}, M_*), p(y|y_{1:n}, M_R)\} + k\{p(y|y_{1:n}, M_R), p(y|y_{1:n}, M_*)\},
\]

where the second term is the Kullback-Leibler divergence from the predictive density of a restricted model \( p(y|y_{1:n}, M_R) \) to the predictive density of the full model \( p(y|y_{1:n}, M_*) \). The first term has a predictive interpretation since it differs from (5) just by a constant (8). The second term does not have this interpretation since entropy is not constant when optimizing the parameters of the restricted model. Thus sum of these terms does not have a predictive interpretation.

There are also other approaches (e.g., Laud and Ibrahim, 1995; Gelfand and Ghosh, 1998; Gutiérrez-Peña and Walker, 2001) which are predictive approaches, but which are not based on estimating the expected predictive performance of the restricted model using the full model \( M_* \) as an approximate true belief model.

## 5 Intrinsic estimation

Intrinsic estimation is a likelihood-based method, where the focus is in the likelihood instead of the predictive distribution. Intrinsic estimation is related to the Bayesian reference criterion (Bernardo, 1999; Bernardo and Rueda, 2002). Bernardo (1999) proposed to use a directed Kullback-Leibler divergence, while Bernardo and Rueda (2002) and Bernardo and Juárez (2003) proposed to use a symmetric Kullback-Leibler divergence. Bernardo (2005c,b) provides additional discussion and examples on intrinsic estimation and regions.

Intrinsic estimation by Bernardo and Juárez (2003) is based on the intrinsic discrepancy, which belongs to the class of intrinsic loss functions (Robert, 1996). The intrinsic discrepancy \( \delta\{p_1, p_2\} \) between two distributions is defined by Bernardo and Rueda (2002) and Bernardo and Juárez (2003) as

\[
    \delta\{p_1, p_2\} = \min \left\{ \int p_1(y) \log \frac{p_1(y)}{p_2(y)} dy, \int p_2(y) \log \frac{p_2(y)}{p_1(y)} dy \right\},
\]

which is the minimum of two Kullback-Leibler divergences: one from \( p_1 \) to \( p_2 \) and another from \( p_2 \) to \( p_1 \). The intrinsic discrepancy \( \delta\{M_1, M_2\} \) between two models is defined as the minimum intrinsic discrepancy between their elements

\[
    \delta\{M_1, M_2\} = \inf_{\theta_1, \theta_2} \delta\{p(y|\theta_1, M_1), p(y|\theta_2, M_2)\}. \tag{13}
\]

For intrinsic estimation consider the full model \( p(y|\theta, \lambda, M_*) \) and a restricted model \( p(y|\hat{\theta}, \lambda, M_R) \), where \( \lambda \) may be considered as nuisance parameter. The intrinsic estimator is obtained by minimizing the reference posterior expectation of the intrinsic discrepancy

\[
    \hat{\theta}_1 = \arg\min_{\theta} \int \int \min_{\lambda} \delta\{p(y|\hat{\theta}, \lambda, M_R), p(y|\theta, \lambda, M_*)\} p(\theta, \lambda|y_{1:n}, M_*) d\theta d\lambda. \tag{14}
\]

If the Kullback-Leibler divergence (discrepancy) minimization view of the predictive approach is considered (see (10)), the similarity to intrinsic estimation is obvious. In the predictive approach the unknown not fixed parameters are integrated out for each model, and posterior predictive distributions are
compared directly, while in intrinsic estimation the discrepancy of likelihoods is evaluated first and the expectation is computed by integrating over the posterior of $\theta$ and $\lambda$ given the full model $M_*$. Estimator (14) may be generally more difficult to compute than (6), since this requires minimization inside the integration, although for simpler models this minimization is solvable analytically, but more complex models require numerical integration.

Intrinsic estimation is not directly applicable for hyperparameters in hierarchical models. The intrinsic discrepancy (13) does not have reference to hyperparameters as the discrepancy is computed using only the likelihood part of the model. To use intrinsic estimation, one has to compute the marginal likelihood by integrating over all lower level parameters, which may be difficult for complex hierarchical models. Trevisani and Gelfand (2003) discuss a problem of focus in hierarchical models when using likelihood-based methods. Intrinsic estimation does not have this problem since the focus is determined by which parameters are going to be estimated.

In this paper, three intrinsic discrepancy loss functions compared are:

$$\delta_1(\hat{\theta}, \theta) = k(\hat{\theta} | \theta)$$
$$\delta_2(\hat{\theta}, \theta) = k(\theta | \hat{\theta})$$
$$\delta_3(\hat{\theta}, \theta) = \min \{k(\hat{\theta} | \theta), k(\theta | \hat{\theta})\}$$

where $k(\hat{\theta} | \theta)$ and $k(\theta | \hat{\theta})$ are shorthand notations for $k[p(y|\hat{\theta}, M_R), p(y|\theta, M_*)]$ and $k[p(y|\theta, M_*), p(y|\hat{\theta}, M_R)]$ respectively. $\delta_1$ was used by Bernardo (1999), $\delta_3$ by Bernardo and Rueda (2002) and Bernardo and Juárez (2003), and $\delta_2$ has not been used before, but it has some interesting frequency properties as illustrated later. $\delta_1$ was also used by Goutis and Robert (1998) and Dupuis and Robert (2003), but using approximate Kullback-Leibler projections of the full model parameters to a restricted parameter space (see also later development of this approach by Piironen et al., 2020, Catalina et al., 2020, and Catalina et al., 2021).

Likelihood $p(y|\cdot)$ for several observations is a form $\prod_{i=1}^n p(y_i|\cdot)$. Discrepancies are equal for each $i$, and thus total discrepancy is $n$ times single discrepancy. Since this scaling does not affect point and interval estimation, multiplication by $n$ is omitted for notational and computational convenience. For calibration of the discrepancy to the likelihood-ratio scale multiplication by $n$ is used.

Intuitively, the intrinsic discrepancy $\delta_1$ is related to the predictive approach, since the Kullback-Leibler divergence is computed from the full model to the restricted model. If the point estimate is made for all the likelihood parameters (no nuisance parameters $\lambda$ in (14)), then relation is exact. This can be seen by rearranging the terms in the expected intrinsic discrepancy as

$$\iint p(y|\theta, M_*) \log \frac{p(y|\theta, M_*)}{p(y|\theta, M_R)} d\theta \mu(y_{(1:n)}, M_*) d\theta$$

$$= \iint p(y|\theta, M_*) \log p(y|\theta, M_*) p(\theta|y_{(1:n)}, M_*) d\theta - \iint p(y|\theta, M_*) \log p(y|\hat{\theta}, M_R) p(\theta|y_{(1:n)}, M_*) d\theta d\theta$$

$$= C - \iint p(y|\theta, M_*) p(\theta|y_{(1:n)}, M_*) d\theta \log p(y|\hat{\theta}, M_R) d\theta$$

$$= C - \iint p(y|y_{(1:n)}, M_*) \log p(y|\hat{\theta}, M_R) dy. \quad (18)$$

The second term is equal to the negative predictive criterion with $n$ predictions (see previous section). The first term is constant $C$, which is not dependent on $\hat{\theta}$. In the predictive criterion the corresponding term is the predictive criterion of the full model $M_*$ (8), but since the order of integration and logarithmic function is changed, the terms produce different values. Difference up to a constant does not have effect for the shape of the loss function given $\theta$, and thus, in this special case, both methods produce exactly the same point estimate.
If point estimate is computed only for some of the parameters, the minimization over \( \hat{\lambda} \) in (14) makes relation more complex. In the predictive approach the predictive distribution of the restricted model \( M_R \) is obtained simply by integrating over the posterior distribution \( p(\lambda|\bar{y}, y_{1:n}, M_R) \). In the intrinsic approach, taking the infimum of the discrepancy over \( \lambda \) (see (14)) corresponds to replacing the restricted model \( M_R \) with Kullback-Leibler projection of the full model, where the distribution of the \( \lambda^\perp \) is the Kullback-Leibler projection of the distribution \( p(\lambda|y_{1:n}, M_\perp) \). Using projection changes the restricted model and thus the decision problem is not exactly same in these two approaches. Point estimates and credible regions can still be similar as illustrated in Section 7.1.4 with normal model with variance as a nuisance parameter. For further discussion and examples of defining submodels as the Kullback-Leibler projections of the full model, see papers by Piironen et al. (2020), Catalina et al. (2020), and Catalina et al. (2021).

In the case of the intrinsic discrepancy \( \delta_2 \), the divergence is computed from the restricted model to the full model. Thus, for given values of \( \hat{\theta} \), it is assumed that the restricted model is the “true” model. This case differs from the case of computing the Kullback-Leibler divergence from the predictive distribution of the restricted model to the predictive distribution of the full model, since the expectation is still taken over the posterior distribution of \( \theta \) given the full model \( M_\perp \). This approach could be interpreted as trying to find a restricted “truth” which optimally agrees with the posterior information of the full model. This is related to the frequentist view of assuming that there is a true value which generated the data. In section 7, it is demonstrated that at least in the case of three regular problems with specific commonly used parameterizations, \( \delta_2 \) produces estimates which have frequency properties equal to unbiased minimum variance estimates. Equality is valid only for specific parameterizations, since unbiased estimates are not invariant under reparameterization. Note that, here unbiasedness is a side effect instead of an actual design goal. For general criticism against unbiasedness as a design goal for generic estimates, see O’Hagan and Forster (2004, Ch. 5). For advocacy of frequentist evaluation of the Bayesian methods, see, for example, Bayarri and Berger (2004) and Bernardo (2005a).

Bernardo and Rueda (2002) introduced the use of the symmetric discrepancy \( \delta_3 \) (13). They claim that it addresses two “unwelcome” features of directed Kullback-Leibler divergence; it is not symmetric, and it diverges if the support of \( p_2(y) \) is a strict subset of the support of \( p_1(y) \). In the predictive approach, it is obvious that the symmetric Kullback-Leibler divergence is in conflict with the use of the full model as an approximate “true” belief model for future observations. In intrinsic estimation, this is not as clear since the expectation of the discrepancy is still taken over the posterior of the parameters of the full model. Examples in Section 7 demonstrate that at least in four regular problems, the symmetric divergence produces results which are exactly or approximately average of results obtained with two directed divergences. Bernardo and Rueda (2002) and Bernardo and Juárez (2003) argue that important feature of the symmetric divergence is that it does not diverge if the support of \( p_2(y) \) is a strict subset of the support of \( p_1(y) \). Bernardo and Juárez (2003) illustrate this with a non-regular problem, where the directed Kullback-Leibler divergences diverge. Although providing an estimate in non-regular problem, a convincing justification of the symmetric divergence seems to be missing. In Section 7.4 the non-regular problem used by Bernardo and Juárez (2003) is reviewed and used to illustrate additional discussion on this topic.

6 Credible regions

Credible regions are natural extension of point estimates summarizing which values are close to a point estimate and thus describe the associated uncertainty in the posterior distribution.

Most commonly used Bayesian credible regions are the central interval and highest posterior density
(HPD) region (see, e.g., Bernardo and Smith, 1994, Ch. 5; Robert, 2001, Ch. 4; Gelman et al., 2003, Ch. 2; Press, 2003, Ch. 8). Central interval is defined so that there is equal amount of probability mass outside of both ends of the interval. This is not sensible, for example, if maximum of the posterior is at the edge of the parameter space or there is very low posterior density in the center of the interval. Furthermore, central interval is not generalizable to several dimensions. HPD region is defined so that inside the region the posterior density is everywhere higher than outside the region. The problem is that HPD region is not invariant under reparameterization. For further illustration of the problems of these two credible regions see Bernardo (2005b).

Decision theoretic approach for point estimates can be naturally extended to regions. Bernardo (2005c,b) proposed selecting credible regions as a lowest posterior loss (LPL) regions, where all points in the region have smaller posterior expected loss than all points outside. These regions are form

\[ C_q = \{ \tilde{\theta}; d(\tilde{\theta}|y_{1:n}) \leq l(q) \}, \]  

such that

\[ \int_{C(q)} p(\theta|y_{1:n}) d\theta = q. \]  

Bernardo (2005c,b) defines intrinsic credible region as the lowest posterior loss region with respect to the intrinsic discrepancy loss, and the appropriate reference prior.

In similar way, the predictive criterion credible region can be defined as the highest posterior utility region with respect to the predictive criterion. Note that, if there is no nuisance parameters \( \lambda \), the intrinsic credible region with loss function \( k(\tilde{\theta}|\theta) \) is equal to the predictive criterion region. This follows from the relation of the corresponding expected intrinsic loss and the predictive criterion as discussed in the previous section.

Intrinsic credible regions and predictive criterion credible regions have corresponding good properties as the respective point estimates, such as invariancy under reparameterization. One way to evaluate credible regions is to examine their frequentist coverage. Bernardo (2005b) shows that for certain models all reference posterior credible regions are exact frequentist confidence regions, that is, their frequentist coverage is exact. Thus, for such models (with reference prior) all intrinsic credible regions and predictive criterion credible regions are exact confidence regions. Some of these models are presented in Section 7. Furthermore, in Section 7.2, binomial model is used to illustrate the frequentist coverage of credible regions in case for which exact confidence regions generally do not exist.

7 Examples

The discussion is illustrated with five examples: Normal model with unknown mean and variance (joint estimation and estimation under presence of nuisance parameter), Binomial model, Exponential model, Uniform model (non-regular model), and two-level hierarchical Normal model.

Examples illustrate the strong relation of intrinsic estimation with loss function \( k(\tilde{\theta}|\theta) \) to estimation with the predictive criterion, the relation of intrinsic estimation with loss function \( k(\theta|\tilde{\theta}) \) to minimum variance unbiased estimates, and that the symmetric intrinsic loss function advocated by Bernardo and Rueda (2002), Bernardo and Juárez (2003) and Bernardo (2005c,b) is a compromise between these two.

7.1 Normal model with unknown mean and variance

Let data \( y_{1:n} = \{ y_1, \ldots, y_n \} \) be a random sample from a Normal distribution \( N(y|\mu, \sigma^2) \), where both \( \mu \) and \( \sigma \) are unknown, and consider the problem of point estimation of \( \mu \) and \( \sigma \). As a numerical illustration
an example by Bernardo (2005b) is used, with \( n = 25, y(\bar{y}, n) = 0.024 \), and \( \frac{1}{n} \sum_{i=1}^{n} (y_i - \bar{y})^2 = 1.077 \). The reference prior is \( 1/\sigma^2 \) (Bernardo, 1979b).

### 7.1.1 Predictive criterion estimation

The predictive distribution for the full model is

\[
t_{n-1}(y|y(\bar{y}, n), (1 + 1/n)s^2),
\]

where \( s^2 = \frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})^2 \). The predictive distribution of the restricted model is

\[
N(y|\tilde{\mu}, \tilde{\sigma}^2).
\]

The predictive criterion to maximize is

\[
\int \log N(y|\tilde{\mu}, \tilde{\sigma}^2)t_{n-1}(y|y(\bar{y}, n), (1 + 1/n)s^2)dy,
\]

which can be efficiently evaluated given \( \tilde{\mu} \) and \( \tilde{\sigma}^2 \), for example, with adaptive quadrature methods.

### 7.1.2 Intrinsic estimation

For Normal model, Kullback-Leibler divergences are

\[
k(\tilde{\mu}, \tilde{\sigma}|\mu, \sigma) = \int N(y|\mu, \sigma^2) \log \frac{N(y|\mu, \sigma^2)}{N(y|\tilde{\mu}, \tilde{\sigma}^2)}dy
\]

\[
= \frac{1}{2} \left[ \frac{(\mu - \tilde{\mu})^2}{\tilde{\sigma}^2} \frac{\sigma^2}{\tilde{\sigma}^2} + \log \frac{\tilde{\sigma}^2}{\sigma^2} - 1 \right],
\]

and

\[
k(\mu, \sigma|\tilde{\mu}, \tilde{\sigma}) = \int N(y|\tilde{\mu}, \tilde{\sigma}^2) \log \frac{N(y|\mu, \sigma^2)}{N(y|\tilde{\mu}, \tilde{\sigma}^2)}dy
\]

\[
= \frac{1}{2} \left[ \frac{(\tilde{\mu} - \mu)^2}{\sigma^2} \frac{\tilde{\sigma}^2}{\sigma^2} + \log \frac{\sigma^2}{\tilde{\sigma}^2} - 1 \right].
\]

The intrinsic discrepancy to minimize is

\[
d(\tilde{\theta}, y(\bar{y}, n)) = \int \delta(\tilde{\theta}, \theta)p(\theta|y(\bar{y}, n))d\theta,
\]

which can be approximated using Monte Carlo

\[
d(\tilde{\theta}, y(\bar{y}, n)) \approx \frac{1}{T} \sum_{t=1}^{T} \delta(\tilde{\theta}, \theta^{(t)}),
\]

where \( \theta^{(t)} \) are samples from \( p(\theta|y(\bar{y}, n)) \).
### 7.1.3 Results

Table 1 shows point estimates of $\mu$ and $\sigma$ obtained with different methods. Note that, predictive criterion and intrinsic estimation methods are invariant under reparameterization and thus, for example, $\sigma^* = \sqrt{\sigma^2}$, but unbiased estimate of $\sigma^2$ is not unbiased estimate of $\sigma$.

Predictive criterion estimation and intrinsic estimation with directed divergence $k(\tilde{\theta}|\theta)$ give exactly the same estimate (see section 5). Both methods assume that $\mu$ and $\sigma$ are unknown and one is interested to find out the best single proxy values for these parameters so that the description of the future uncertainty (predictive distribution) changes as little as possible. Intrinsic estimation with $k(\tilde{\theta}|\theta)$ can be made in following steps

$$k(\tilde{\mu}, \tilde{\sigma}|\mu, \sigma)$$

is minimized wrt. $\tilde{\mu}$ setting $\tilde{\mu} = \mu$  

integrating over the posterior gives $\mu^* = E[\mu] = 0.024$ (31)

using above, $k(\tilde{\mu}, \tilde{\sigma}|\mu, \sigma)$ is minimized wrt. $\tilde{\sigma}$ setting $\tilde{\sigma}^2 = \sigma^2 + (\mu - \mu^*)^2$  

integrating over posterior gives $\sigma^* = \sqrt{E[\sigma^2 + (\mu - \mu^*)^2]} \approx 1.171$, (33)

that is, the estimate for $\sigma$ combines the posterior information about $\sigma$ and posterior uncertainty about $\mu$.

The frequentist minimum variance unbiased estimate is based on the assumption that there exists a true fixed value. Intrinsic estimation with directed $k(\tilde{\theta}|\theta)$ makes a similar assumption by assuming that the true belief model is the restricted model. These two methods give same result (up to a Monte Carlo error).

Intrinsic estimation with the symmetric divergence gives an estimate which is between these, and more specifically for the precision $1/\sigma^2$ the estimate is approximately arithmetic average of Bayesian predictive estimate and minimum variance unbiased estimate.

Figure 1 shows the credible regions with different methods. Predictive criterion and intrinsic credible regions with directed divergence $k(\tilde{\theta}|\theta)$ are exactly the same and shown in same subplot. Credible regions reflect the same properties as the respective point estimates. Note that in this case, all these regions are exact confidence regions (see Bernardo, 2005b).

### 7.1.4 Estimation under presence of nuisance parameter

Point estimation may be used also only for some of the parameters and the rest may be considered as nuisance parameters. In such case, the predictive criterion and the expected intrinsic discrepancy with $k(\tilde{\theta}|\theta)$ are not generally equal as in (14). As illustration, the same Normal model example is used, except only the mean in the restricted model is estimated and variance is considered as a nuisance parameter.
Figure 1: Point estimates (solid dot) and credible regions (50% and 95%) for $\mu$ and $\sigma$: (a) Predictive criterion estimation and intrinsic estimation with directed $k(\hat{\theta}|\theta)$, (b) Intrinsic estimation directed $k(\theta|\tilde{\theta})$, (c) Intrinsic estimation symmetric $\min\{k(\hat{\theta}|\theta), k(\theta|\tilde{\theta})\}$.

The posterior distribution of the $\sigma^2$ is (using notation by Gelman et al. (2003))

$$\text{Inv-}\chi^2(n, \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu})^2),$$  (34)

the predictive distribution of the restricted model is

$$t_n(y|\tilde{\mu}, \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu})^2),$$  (35)

and the predictive criterion to maximize is

$$\int \log t_n(y|\tilde{\mu}, \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{\mu})^2) t_{n-1}(y|\tilde{y}_{(1:n)}, (1 + 1/n)s^2) dy. $$  (36)

In intrinsic estimation parameters, which are not to be estimated, are chosen so that the intrinsic loss between models is minimized. The directed intrinsic discrepancy (25) is minimized by setting

$$\tilde{\sigma}^2 = (\tilde{\mu} - \mu)^2 + \sigma^2.$$  (37)

This can be considered as Kullback-Leibler projection of $\sigma^2$ of the full model. It is easy to see that distribution of this projection is different than (34). The intrinsic discrepancy is

$$\frac{1}{2} \log \left( \frac{(\mu - \tilde{\mu})^2}{\sigma^2} + 1 \right),$$  (38)

and it’s expection can be estimated numerically.

Top plot of the Figure 2 shows the predictive criterion and the expected intrinsic discrepancy for different values of $\tilde{\mu}$(). Bottom plot of the Figure 2 shows the difference of these two. For comparison purposes the predictive criterion has been subtracted from the predictive criterion of the full model. Both discrepancies have been scaled by $n$. Functions are very similar, where most of the difference is due to constant term difference (see Section 5. Despite the difference, since functions are symmetric and minimum is in same point, the point estimate and the LPL-interval are equal.
7.2 Binomial model

Let $y_{(1:n)} = \{y_1, \ldots, y_n\}$, be a random sample from the Binomial distribution with parameter $\theta$. As a numerical illustration an example by Bernardo (2005b) is used, with $n = 10$ and $r = 0$. The reference prior is Beta($\frac{1}{2}, \frac{1}{2}$).

7.2.1 Predictive criterion estimation

Predictive probability that the next observation is 1 for the full model is

$$
\Pr(\tilde{y} = 1|y_{(1:n)}) = \int_0^1 \Pr(\tilde{y} = 1|\theta, y_{(1:n)}) p(\theta|y_{(1:n)}) d\theta
$$

(39)

$$
= \int_0^1 \theta^r (1-\theta)^{n-r} d\theta = \frac{r + 1/2}{n + 1},
$$

(40)

and for the restricted model

$$
\Pr(\tilde{y} = 1|\theta) = \tilde{\theta}.
$$

(41)

Taking into account the corresponding probabilities for $\Pr(\tilde{y} = 0|\cdot)$ the predictive criterion to maximize is

$$
\int \log \Pr(\tilde{y} = y|\tilde{\theta}) \Pr(\tilde{y} = y|y_{(1:n)}) dy = \log \tilde{\theta} \left( \frac{r + 1/2}{n + 1} \right) + \log (1 - \tilde{\theta}) \left( \frac{n - r + 1/2}{n + 1} \right),
$$

(42)

which is maximized by

$$
\tilde{\theta} = \frac{r + 1/2}{n + 1},
$$

(43)

that is, the posterior mean of $\theta$. 

---

Figure 2: Top plot (a) The predictive criterion (solid line) and the expected intrinsic discrepancy with directed $k(\tilde{\theta}|\theta)$ (minus $C$, dashed line) for different values of $\tilde{\mu}$. Bottom plot (b) The difference of the above two discrepancies.
### 7.2.2 Intrinsic estimation

Directed Kullback-Leibler divergences are

\[
k(\tilde{\theta}|\theta) = \theta \log[\theta/\tilde{\theta}] + (1 - \theta) \log[(1 - \theta)/(1 - \tilde{\theta})],
\]
and

\[
k(\theta|\tilde{\theta}) = \tilde{\theta} \log[\tilde{\theta}/\theta] + (1 - \tilde{\theta}) \log[(1 - \tilde{\theta})/(1 - \theta)].
\]

The symmetric intrinsic discrepancy between \(p(y_{(1:n)}|\tilde{\theta})\) and \(p(y_{(1:n)}|\theta)\) is

\[
\delta_3(\tilde{\theta}, \theta) = \begin{cases} 
  k(\theta|\tilde{\theta}) & \theta \in (\tilde{\theta}, 1 - \tilde{\theta}), \\
  k(\tilde{\theta}|\theta) & \text{otherwise}.
\end{cases}
\]

The expected posterior intrinsic discrepancy is

\[
d(\tilde{\theta}, y_{(1:n)}) = \int_0^1 \delta(\tilde{\theta}, \theta) \text{Beta}(\theta| r + 1/2, n - r + 1/2) d\theta.
\]

For the directed discrepancy \(k(\tilde{\theta}|\theta)\) this can be easily solved by taking out the terms independent of \(\tilde{\theta}\) to obtain

\[
- \int_0^1 [\theta \log(\tilde{\theta}) + (1 - \theta) \log(1 - \tilde{\theta})] \text{Beta}(\theta| r + 1/2, n - r + 1/2) d\theta \\
= - \log \tilde{\theta} \left( \frac{r + 1/2}{n + 1} \right) - \log(1 - \tilde{\theta}) \left( \frac{n - r + 1/2}{n + 1} \right),
\]

which is proportional to the negative predictive criterion (42) and minimized by

\[
\tilde{\theta} = \frac{r + 1/2}{n + 1}.
\]

There is analytical solution also for the directed discrepancy \(k(\theta|\tilde{\theta})\) given by Bernardo and Juárez (2003)

\[
\hat{\theta} = \frac{\exp[\psi(r + 1/2)]}{\exp[\psi(r + 1/2)] + \exp[\psi(n - r + 1/2)]},
\]

where \(\psi(\cdot)\) is the digamma function. This can be quite well approximated with

\[
\hat{\theta} \approx \begin{cases} 
  r + 1/2/n^{2/3} & r = 0, r = n \\
  r/n & \text{otherwise}.
\end{cases}
\]

The expectation of the symmetric discrepancy can be solved numerically. Bernardo (2005c) proposed also the following linear approximation

\[
\hat{\theta} \approx \frac{r + 1/3}{n + 2/3}.
\]
Table 2: Point estimates and 95%-credible intervals (CI) of $\theta$ of Binomial model with different methods.

| Approach                                      | $\hat{\theta}$ | CI              |
|-----------------------------------------------|----------------|-----------------|
| Predictive criterion estimation               | 0.045          | (0.0, 0.305)    |
| Intrinsic estimation directed $k(\bar{\theta}|\theta)$ | 0.045          | (0.0, 0.305)    |
| Intrinsic estimation directed $k(\theta|\bar{\theta})$ | 0.014          | (0.0, 0.171)    |
| Intrinsic estimation symmetric min $\{k(\bar{\theta}|\theta), k(\theta|\bar{\theta})\}$ | 0.031          | (0.0, 0.171)    |
| Minimum variance unbiased estimate            | 0              |                 |

7.2.3 Results

Table 2 shows point estimates and credible intervals of $\theta$ obtained with different methods. Since data are discrete, exact confidence interval does not generally exist, and thus credible intervals produced can only be approximate confidence intervals. There are many proposed approximations with different desired properties but no consensus of which one should be preferred (Brown et al., 2001), and thus comparison to them is not included.

Predictive criterion estimation and intrinsic estimation with the directed discrepancy $k(\bar{\theta}|\theta)$ give exactly the same point estimate (see (43) and (49)) and also exactly the same credible interval.

The intrinsic estimation with the directed discrepancy $k(\theta|\bar{\theta})$ gives a much lower estimate, but not exactly same as the minimum variance unbiased estimate, which can be explained by the influence of the prior. If the prior Beta$(a, a)$ is used and $a \to 0$ intrinsic estimate with the directed discrepancy $k(\theta|\bar{\theta})$ goes to 0. If using the reference posterior, but with $r = 1$, the estimate is 0.103 which is quite close to the corresponding minimum variance unbiased estimate 0.1. In fact, the approximation $\hat{\theta} \approx r/n$ is very good except for $r = 0$ and $r = n$.

Intrinsic estimation with the symmetric divergence gives an estimate which is between the directed estimates, and more specifically the estimate is approximately the arithmetic average of the directed estimates. Bernardo and Juárez (2003) use this average as an approximation to the exact result with the symmetric discrepancy, without commenting the relevance of the estimates obtained with directed discrepancies.

Further comparison of the methods is made by comparing the frequentist coverage of intervals. Since $y$ is discrete, exact confidence intervals do not exist and coverage is bound to differ from the target value for most values of true $\theta$. Figure 3 shows the frequentist coverage for different methods. Predictive criterion estimation and intrinsic estimation with the directed discrepancy $k(\bar{\theta}|\theta)$ provide exactly the same result (results shown in the same subplot). Intrinsic estimation with the directed discrepancy $k(\theta|\bar{\theta})$ and intrinsic estimation with the symmetric discrepancy min $\{k(\bar{\theta}|\theta), k(\theta|\bar{\theta})\}$ provide very similar results. Bernardo (2005b) speculates that intrinsic credible intervals with the symmetric min $\{k(\bar{\theta}|\theta), k(\theta|\bar{\theta})\}$ might possibly provide the best available solution for this particular problem, but considering discussion in Brown et al. (2001) there is no consensus on which properties should be preferred. For example, some discussants preferred intervals whose coverage is always larger than the target value. None of the methods discussed in this paper achieve that completely, although predictive criterion estimation and intrinsic estimation with the directed discrepancy $k(\bar{\theta}|\theta)$ produce the best result in this sense. As further illustration, Figure 4 shows the average coverage for different values of $n$ with different methods. These plots can be compared to plots of other methods shown in Brown et al. (2001). With all the methods average coverage converges close to the target value.
Figure 3: Frequentist coverage of binomial 95%-credible intervals: (a) Predictive criterion estimation and intrinsic estimation with directed $k(\hat{\theta}|\theta)$, (b) Intrinsic estimation directed $k(\theta|\hat{\theta})$, (c) Intrinsic estimation symmetric $\min\{k(\hat{\theta}|\theta), k(\theta|\hat{\theta})\}$.

Figure 4: Average coverage over $\theta$ of binomial 95%-credible intervals for different $n$: (a) Predictive criterion estimation and intrinsic estimation with directed $k(\hat{\theta}|\theta)$, (b) Intrinsic estimation directed $k(\theta|\hat{\theta})$, (c) Intrinsic estimation symmetric $\min\{k(\hat{\theta}|\theta), k(\theta|\hat{\theta})\}$. 
7.3 Exponential model

Let \( y_{(1:n)} = \{y_1, \ldots, y_n\} \), be a random sample from the Exponential distribution \( \text{Ex}(y|\theta) = \theta e^{-\theta y} \). Reference prior is \( \theta^{-1} \) and corresponding posterior is Gamma \( p(\theta|y_{(1:n)}) = \text{Ga}(\theta|n, t) \), where \( t = \sum_{i=1}^{n} y_i \).

As a numerical illustration an example by Bernardo (2005a) is used, with \( n = 10 \) and \( t = 6.08 \).

7.3.1 Predictive criterion estimation

The predictive distribution for the full model is Gamma-Gamma
\[
Gg(y|n, t, 1) = \frac{\Gamma(n + 1)}{\Gamma(n)} \frac{t^n}{(t + y)^{n+1}},
\]
and the predictive distribution for the restricted model is exponential
\[
\text{Ex}(y|\tilde{\theta}) = \tilde{\theta} e^{-\tilde{\theta} y}.
\]
The predictive criterion to maximize is
\[
\int \log \text{Ex}(y|\tilde{\theta}) Gg(y|n, t, 1) dy = -t\hat{\theta}/(n - 1) + \log \hat{\theta},
\]
which is maximized by
\[
\hat{\theta} = (n - 1)/t.
\]

7.3.2 Intrinsic estimation

Directed Kullback-Leibler divergences are
\[
k(\hat{\theta} | \theta) = (\hat{\theta} / \theta) - 1 - \log(\hat{\theta} / \theta),
\]
and
\[
k(\theta | \hat{\theta}) = (\theta / \hat{\theta}) - 1 - \log(\theta / \hat{\theta}).
\]
The symmetric intrinsic discrepancy is
\[
\delta(\theta | \tilde{\theta}) = \begin{cases} (\theta / \tilde{\theta}) - 1 - \log(\theta / \tilde{\theta}) & \theta \leq \tilde{\theta} \\ (\tilde{\theta} / \theta) - 1 - \log(\tilde{\theta} / \theta) & \theta > \tilde{\theta}. \end{cases}
\]
The expected posterior intrinsic discrepancy for \( k(\hat{\theta} | \theta) \) is
\[
d(\tilde{\theta}, y_{(1:n)}) = t\tilde{\theta}/(n - 1) - \log(\tilde{\theta}) - \log(t) - 1 + \psi(n),
\]
which is ignoring the term independent of \( \tilde{\theta} \) proportional to (55). The expected discrepancy (60) is minimized by
\[
\hat{\theta} = (n - 1)/t,
\]
which is equal to (56). The expected posterior intrinsic discrepancy for \( k(\theta | \tilde{\theta}) \) is
\[
n/(t\tilde{\theta}) + \log(\tilde{\theta}) + \log(t) - 1 - \psi(n),
\]
which is minimized by
\[
\hat{\theta} = n/t.
\]
The expected posterior intrinsic discrepancy with the symmetric discrepancy does not have an analytic solution, but can be evaluated, for example, with quadrature methods. Bernardo (2005a) proposes approximation
\[
\hat{\theta} = (n - 1/2)/t,
\]
which happens to be the average of estimates obtained with directed Kullback-Leibler divergences.
7.3.3 Results

Table 3 shows point estimates and 95%-credible intervals of $\theta$ obtained with different methods. Note that, all credible intervals are in this case exact confidence intervals (see Bernardo, 2005b). Frequentist confidence intervals are central intervals. Note that, taking inverse of central interval endpoints for the scale $(1/\theta)$ does not produce exact confidence interval for the rate $\theta$.

| Approach                              | $\hat{\theta}$ | CI          |
|---------------------------------------|-----------------|-------------|
| Predictive criterion estimation       | 1.48            | (0.71, 2.68)|
| Intrinsic estimation directed $k(\hat{\theta}|\theta)$ | 1.48            | (0.71, 2.68)|
| Intrinsic estimation directed $k(\theta|\hat{\theta})$ | 1.64            | (0.89, 3.58)|
| Intrinsic estimation symmetric min{$k(\hat{\theta}|\theta), k(\theta|\hat{\theta})$} | 1.57            | (0.83, 2.95)|
| Minimum variance unbiased estimate of rate $\theta$ | 1.48            | (0.79, 2.81)|
| Inverse of minimum variance unbiased estimate of scale $(1/\theta)$ | 1.64            | (0.96, 3.43)|

Table 3: Point estimates of $\theta$ of exponential model with different methods.

Predictive criterion estimation and intrinsic estimation with the directed discrepancy $k(\hat{\theta}|\theta)$ give exactly same estimate (see (56) and (61)).

Intrinsic estimation with directed $k(\theta|\hat{\theta})$ gives higher estimate for the rate $\theta$ and lower estimate for the scale (mean wait time) $1/\theta$. Estimate for the rate is not unbiased estimate, but estimate for the scale is the minimum variance unbiased estimate for the scale. This is similar to the Normal distribution example where the intrinsic estimate with directed $k(\theta|\hat{\theta})$ is the minimum variance unbiased estimate for the scale $\sigma^2$ but not for inverse of the scale $1/\sigma^2$. This is due to a fact that that the minimum variance unbiased estimate is not, but predictive criterion and intrinsic estimates are invariant under parameterization.

Intrinsic estimation with symmetric divergence gives estimate which is between the directed estimates, and more specifically the estimate is approximately the average of the directed estimates. Bernardo (2005a) proposes this approximation without noting its connection to directed estimates.

7.4 Uniform model

The next example illustrates a non-regular problem where the directed Kullback-Leibler divergences diverge. Let $y_{(1:n)} = \{y_1, \ldots, y_n\}$, be a random sample from the Uniform distribution $\text{Un}(y|0, \theta) = \theta^{-1}, 0 < y < \theta$. Sufficient statistic is $t = \max\{y_1, \ldots, y_n\}$. As a numerical illustration an example by Bernardo and Juárez (2003) is used, with $n = 10$ and $t = 1.897$. The reference posterior distribution is the Pareto distribution (Bernardo and Juárez, 2003)

$$ p(\theta|y_{(1:n)}) = \text{Pa}(\theta|n, t) = nt^n \theta^{-(n+1)}, \quad \theta > t. \tag{65} $$

7.4.1 Predictive criterion estimation

The predictive distribution of the full model is

$$ p(y|y_{(1:n)}) = \begin{cases} \frac{t^n}{(n+1)!} & \text{if } 0 \leq y \leq t \\ \frac{nt^n}{(n+1)!} & \text{if } y > t. \end{cases} \tag{66} $$

The predictive distribution of the restricted model $\text{Un}(0, \hat{\theta})$ is

$$ p(y|\hat{\theta}) = \begin{cases} \frac{1}{\theta^n} & \text{if } y \leq \hat{\theta} \\ 0 & \text{otherwise}. \end{cases} \tag{67} $$
The problem is that the logarithmic score based predictive criterion degenerates since \( P(y|\hat{\theta}) = 0, y > \hat{\theta} \) and the support of \( P(y|y_{(1:n)}) \) is \((0, \infty)\). The logarithmic score measures the information lost when going from the full model to the restricted model. Going from any finite probability to zero probability loses an infinite amount of information, and thus it is not sensible to approximate (66) with (67) if one does not want to lose an infinite amount of information about possible values of \( y \) which may be observed.

Furthermore, consider that the predictive distribution would be used as a prior for some future inference. If the predictive distribution of the restricted model were used as prior, that prior would have zero probability for all values larger than \( \hat{\theta} \). Then, observing values larger than that would not change the posterior information. This is related to Cromwell’s Rule by Lindley (1985), which states that one should avoid using prior probability of 0.

Based on these arguments, it can be further argued that for the purposes of pure scientific inference and communication the restricted model in this problem does not make sense. On the other hand, application specific utilities can still make sense. For example, if the predictive decision problem would be reformulated as a guessing contest where the one with the closest guess wins, the best guess with the corresponding utility function would be the median of the posterior \( \hat{\theta} = 2.03 \).

### 7.4.2 Intrinsic estimation

Directed Kullback-Leibler divergences are

\[
k(\theta|\tilde{\theta}) = \begin{cases} 
\log(\theta/\tilde{\theta}) & \theta \leq \tilde{\theta} \\
\infty & \theta > \tilde{\theta}, 
\end{cases}
\]

and

\[
k(\tilde{\theta}|\theta) = \begin{cases} 
\log(\tilde{\theta}/\theta) & \theta \geq \tilde{\theta} \\
\infty & \theta < \tilde{\theta}.
\end{cases}
\]

Now directed Kullback-Leibler divergences diverge and cannot be used. Bernardo and Juárez (2003) solve this problem by using the symmetric intrinsic discrepancy by taking minimum of above directed divergences

\[
\delta(\theta|\tilde{\theta}) = \begin{cases} 
\log(\tilde{\theta}/\theta) & \theta \leq \tilde{\theta} \\
\log(\theta/\tilde{\theta}) & \theta > \tilde{\theta}.
\end{cases}
\]

Note that, not all symmetric intrinsic discrepancies have this property. For example, the sum or the average of the directed Kullback-Leibler divergences diverges too.

The expected posterior intrinsic discrepancy is

\[
d(\tilde{\theta}, y_{(1:n)}) = \int_0^\infty \delta(\tilde{\theta}, \theta) \text{Pa}(\theta|n, t) d\theta = 2 \left( \frac{t}{\tilde{\theta}} \right)^n - n \log \left( \frac{t}{\tilde{\theta}} \right) - 1,
\]

which is minimized by \( \tilde{\theta} = 2^{1/n} t \), which happens to be also the median of the reference posterior. In the numerical example, the intrinsic estimate and the posterior median is \( \hat{\theta} = 2.03 \), and the minimum variance unbiased estimate is \( \hat{\theta} = (n + 1)/n \approx 2.09 \).

The symmetric intrinsic discrepancy \( \delta_3 \) provides answer in this problem, but it was achieved by changing the cost of consequences. It is not entirely clear whether taking the minimum of two directed discrepancies with different properties is well justified as a cost for consequences in pure scientific inference and communication.
7.5 Hierarchical model

So far models in the examples have been one-level models. This section demonstrate a problem with a simple two-level hierarchical normal model of data $y_{ij}$ with group level effects $\alpha_j$:

$$y_{ij} \sim N(\mu + \alpha_j, \sigma^2_\mu), \quad i = 1, \ldots, n_j, \quad j = 1, \ldots, J$$
$$\alpha_j \sim N(0, \sigma^2_\alpha), \quad j = 1, \ldots, J.$$  \hfill (72)

Data are from the 8-schools example described in Gelman et al. (2003, Ch. 5). Here, the parameters $\alpha_1, \ldots, \alpha_8$ represent the relative effects of Scholastic Aptitude Test coaching programs in eight different schools, and $\sigma_\alpha$ represents the between-school standard deviations of these effects. Gelman et al. (2003, Ch. 5) further simplify the model (72) to

$$\bar{y}_j \sim N(\mu + \alpha_j, \sigma^2_j), \quad j = 1, \ldots, J$$
$$\alpha_j \sim N(0, \sigma^2_\alpha), \quad j = 1, \ldots, J,$$  \hfill (73)

where

$$\bar{y}_j = \frac{1}{n_j} \sum_{i=1}^{n_j} y_{ij} \quad \text{and} \quad \sigma^2_j = \frac{\sigma^2_\alpha}{n_j}. \hfill (74)$$

Data are $J = 8$, $y_{i,j} = \{28, 8, -3, 7, 1, 1, 1, 8, 12\}$, and $\sigma = \{15, 10, 16, 11, 9, 11, 10, 18\}$. Uniform priors for $\mu$ and $\sigma_\alpha$ are used as recommended by Gelman et al. (2003, Ch. 5) and Gelman (2006). In this example, terms intrinsic estimation and intrinsic credible intervals are used liberally, since strictly intrinsic estimation is defined by Bernardo and Juarez (2003) only for reference posteriors obtained using reference priors, and the prior used here is not a reference prior (see Yang and Berger (1997) for reference priors for $\sigma_\alpha$). Point estimates are computed for the hyperparameters $\mu$ and $\sigma_\alpha$, that is for the common effect of the coaching and the between-school standard deviation.

The posterior distribution is not available in analytical form but it is easily estimated using Monte Carlo methods. To obtain samples from the posterior distribution the factorized simulation described in Gelman et al. (2003, p. 137) was used. The posterior can be factorized as

$$p(\alpha_j, \mu, \sigma^2_\alpha | y_{1:n}, M_s) = p(\sigma^2_\alpha | y_{1:n}, M_s) p(\mu | \sigma^2_\alpha, y_{1:n}, M_s) p(\alpha_j | \mu, \sigma^2_\alpha, y_{1:n}, M_s). \hfill (75)$$

Simulation from the marginal distribution $p(\sigma^2_\alpha | y_{1:n}, M_s)$ is performed numerically using the one dimensional grid sampling. Simulation from $p(\mu | \sigma^2_\alpha, y_{1:n}, M_s)$ and $p(\alpha_j | \mu, \sigma^2_\alpha, y_{1:n}, M_s)$ is easy as they are Normal distributions.

7.5.1 Predictive criterion estimation

There are two choices for prediction. One could predict $y_{j}$ or $y_{j+1}$. Since $\sigma^2_j$ are given as fixed, there is no proper model for predicting $\sigma^2_{j+1}$ which would be required for predicting $y_{j+1}$. Thus, $y_{j}$ are predicted. Note that, point estimate may be different depending on the predictive inference one is interested in. The predictive distribution is

$$p(\bar{y} | y_{1:n}, M_s) = \int p(\bar{y} | \alpha_j, M_s) p(\sigma^2_\alpha | y_{1:n}, M_s) p(\mu | \sigma^2_\alpha, y_{1:n}, M_s) p(\alpha_j | \mu, \sigma^2_\alpha, y_{1:n}, M_s) d\alpha_j d\mu.$$  \hfill (76)
Parameters $\alpha_j$ can be integrated out analytically to get the predictive distribution of the full model in the form

$$p(\tilde{y}|y_{(1:n)}, M_s) = \int p(\tilde{y}|\mu, \sigma^2_\alpha, M_s) p(\sigma^2_\alpha|y_{(1:n)}, M_s) p(\mu|\sigma^2_\alpha, y_{(1:n)}, M_s) d\mu d\sigma^2_\alpha,$$

(77)

which is a mixture of normal distributions. By integrating out parameters $\alpha_j$, the predictive distribution of the restricted model is

$$p(\tilde{y}|y_{(1:n)}, M_R) = p(\tilde{y}|\tilde{\mu}, \tilde{\sigma}^2_\alpha),$$

(78)

which is a normal distribution with parameters whose values can be computed given data and the values of $\tilde{\mu}$ and $\tilde{\sigma}^2_\alpha$. The value of the predictive criterion given $\tilde{\mu}$ and $\tilde{\sigma}^2_\alpha$ is easily computed using combination of Monte Carlo sampling of $\tilde{\mu}$ and $\tilde{\sigma}^2_\alpha$ and quadrature integration for the rest.

### 7.5.2 Intrinsic estimation

Intrinsic estimation is not directly applicable for hierarchical models. The intrinsic discrepancy (13) does not have reference to hyperparameters as the discrepancy is computed using only likelihood part of the model. To overcome this problem, it is possible to integrate over the parameters $\alpha_j$ and use the predictive distribution conditional on the hyperparameters

$$p(\tilde{y}|\mu, \sigma^2_\alpha),$$

(79)

which is a normal distribution with parameters whose values can be computed given data and values of $\tilde{\mu}$ and $\tilde{\sigma}^2_\alpha$. Kullback-Leibler divergence equations are given in section 7.1 and the expected discrepancy is computed over the posterior distribution of $\mu$ and $\sigma^2_\alpha$. The expectation is easily estimated using Monte Carlo simulation.

### 7.5.3 Results

Table 4 shows point estimates of $\mu$ and $\sigma_\alpha$ obtained with different methods. Note that, classical unbiased estimate based on analysis of variance fails by estimating $\sigma^2_\alpha$ to be negative (see Gelman et al., 2003, Ch. 5). As in other examples, predictive criterion estimation and intrinsic estimation with directed divergence

| Approach                              | $\mu^*$ | $\sigma^2_\alpha$ |
|---------------------------------------|---------|--------------------|
| Predictive criterion estimation       | 8.0     | 7.3                |
| Intrinsic estimation directed $k(\tilde{\theta})$ | 8.0     | 7.3                |
| Intrinsic estimation directed $k(\theta|\tilde{\theta})$ | 7.9     | 5.7                |
| Intrinsic estimation symmetric min{$k(\tilde{\theta})$, $k(\theta|\tilde{\theta})$} | 7.9     | 6.7                |

Table 4: Point estimate of $\mu$ and $\sigma_\alpha$ of two-level normal model with different methods.

$k(\tilde{\theta})$ give the same estimate. Intrinsic estimation with directed $k(\theta|\tilde{\theta})$ gives lower estimate for $\sigma_\alpha$ which is in line with results for one-level normal model in section 7.1. The predictive approach includes the uncertainty form the full model predictive inference by giving more pessimistic point estimates. As in other examples, intrinsic estimation with the symmetric divergence gives an estimate which is between directed estimates, although it is not as close to the average of the directed estimates as in the other examples.
8 Conclusion

The selection of utility function should not be arbitrary. The purpose of this paper was to examine properties of the intrinsic loss function used in intrinsic estimation and credible regions by Bernardo and Juárez (2003) and Bernardo (2005b), and compare them to the predictive criterion. Intrinsic estimation tries to provide a reference point estimate without an explicit application specific utility. If an application specific loss function were available, naturally it should be used instead of intrinsic loss function. The problem is that when application specific utility is not available, there is no unambiguous choice of intrinsic loss function.

Intrinsic estimation with the directed discrepancy $k(\hat{\theta}|\theta)$ is strongly related to the predictive criterion approach suitable for finding a restricted model with the best predictive performance. This can also be interpreted as finding a restricted model with as similar predictive density as possible as the predictive density of the full model. This approach is useful if the restricted model is going to be used for further predictive inference. If there are no nuisance parameters the methods are equal, and with presence of nuisance parameters methods produce similar estimates. The predictive criterion is generally easier to compute for arbitrary models (e.g., with help of MCMC) and its interpretation is more obvious.

Intrinsic estimation with the directed discrepancy $k(\hat{\theta}|\theta)$ is related to the frequentist approach assuming there exists a true fixed value, which generated the data, and the goal is to find the best estimate for that value. Specially in three regular problems, estimates for the location and scale parameters were also unbiased minimum variance estimates. This approach might be useful if good frequency properties are desired, although further research is required.

Intrinsic estimation with the symmetric discrepancy $\min\{k(\hat{\theta}|\theta), k(\theta|\hat{\theta})\}$ is compromise between the estimation with the directed discrepancies. The use of the symmetric discrepancy seems to be not convincingly justified. Estimates are not as good for further predictions as estimates with the directed discrepancy $k(\hat{\theta}|\theta)$ nor do they have as good frequency properties as estimates with the directed discrepancy $k(\theta|\hat{\theta})$. Even in pure scientific inference and communication, one should probably know, which one of these properties is preferred for estimates.

9 Discussion

The results in this paper have also relevance to hypothesis testing and model selection. Intrinsic discrepancy based hypothesis testing was proposed by Bernardo and Rueda (2002) and further advocated by Bernardo (2005c). Bernardo and Rueda (2002) define hypothesis testing as a model selection problem where the full model $M_*$ is tentatively accepted, and it is desired to test whether a restricted model $M_R$ is compatible with observed data. Since in the Bayesian approach we should integrate over the model uncertainty, the full model $M_*$ should automatically include the alternative models as submodels, and all model selection matches with this definition of hypothesis testing.

In point estimation, the restricted model $M_R$ obtained by minimizing the expected discrepancy was automatically accepted. Regardless of whether $M_R$ is obtained by point estimation or by fixing $\theta$ to some value with special meaning in the model (e.g. zero), in hypothesis testing also the value of the expected discrepancy is considered. The problem is how to calibrate the discrepancy, that is, how large expected discrepancy can be accepted without rejecting the hypothesis. Bernardo (1999) and Bernardo and Rueda (2002) note the connection of the expected discrepancy to the log-likelihood ratio and propose that scale used for the log-likelihood ratio could be used. Bernardo (1999) used the directed discrepancy $k(\hat{\theta}|\theta)$ and Bernardo and Rueda (2002) the symmetric discrepancy $\min\{k(\hat{\theta}|\theta), k(\theta|\hat{\theta})\}$. With same argumentation the log-likelihood ratio scale would be suitable also for the directed discrepancy $k(\hat{\theta}|\theta)$ and the predictive criterion.
Three intrinsic discrepancies considered in this paper all give different expected discrepancies, with different minima and shapes. It seems plausible that properties in hypothesis testing would be similar to properties in point estimation, although this requires further research.

Acknowledgments

The author would like to thank Jouko Lampinen, Ilkka Kalliomäki, and Harri Valpola for helpful comments and suggestions.

References

Bayarri, M. J. and Berger, J. O. (2004). The interplay of Bayesian and frequentist analysis. *Statistical Science*, 19(1):58–80.

Bernardo, J. M. (1979a). Expected information as expected utility. *Annals of Statistics*, 7(3):686–690.

Bernardo, J. M. (1979b). Reference posterior distributions for Bayesian inference. *Journal of the Royal Statistical Society. Series B (Methodological)*, 41(2):113–147.

Bernardo, J. M. (1999). Nested hypothesis testing: The Bayesian reference criterion. In Bernardo, J. M., Berger, J. O., and Dawid, A. P., editors, *Bayesian Statistics 6*, pp. 101–130. Oxford University Press.

Bernardo, J. M. (2005a). An integrated mathematical statistics primer: Objective Bayesian construction, frequentist evaluation. *ISI Bulletin*. In press.

Bernardo, J. M. (2005b). Intrinsic credible regions: An objective bayesian approach to interval estimation. *Test*, 14(2): 317–384.

Bernardo, J. M. (2005c). Reference analysis. In Dey, D. and Rao, C. R., editors, *Handbook of Statistics*, volume 25. Elsevier. 17–90.

Bernardo, J. M. and Juárez, M. A. (2003). Intrinsic estimation. In Bernardo, J. M., Bayarri, M. J., Berger, J. O., Dawid, A. P., Heckerman, D., Smith, A. F. M., and West, M., editors, *Bayesian Statistics 7*, pp. 456–476. Oxford University Press.

Bernardo, J. M. and Rueda, R. (2002). Bayesian hypothesis testing: a reference approach. *International Statistical Review*, 70(3):351–372.

Bernardo, J. M. and Smith, A. F. M. (1994). *Bayesian Theory*. John Wiley & Sons.

Brown, L. D., Cai, T. T., and DasGupta, A. (2001). Interval estimation for a binomial proportion (with discussion). *Statistical Science*, 16(2):101–133.

Catalina, A., Bürkner, P., and Vehtari, A. (2021). Latent space projection predictive inference. *arXiv preprint arXiv:2109.04702*.

Catalina, A., Bürkner, P.-C., and Vehtari, A. (2020). Projection predictive inference for generalized linear and additive multilevel models. *arXiv preprint arXiv:2010.06994*. 
Dey, D. K., Gelfand, A. E., Swartz, T. B., and Vlachos, P. K. (1994). A simulation-intensive approach for checking hierarchical models. Technical Report tr9529, Department of Statistics, University of Connecticut.

Dupuis, J. A. and Robert, C. P. (2003). Variable selection in qualitative models via an entropic explanatory power. *Journal of Statistical Planning and Inference*, 111:77–94.

Gelfand, A. E. and Ghosh, S. K. (1998). Model choice: A minimum posterior predictive loss approach. *Biometrika*, 85:1–11.

Gelman, A. (2006). Prior distributions for variance parameters in hierarchical models (comment on article by Browne and Draper). *Bayesian Analysis*, 1(3):515–534.

Gelman, A., Carlin, J. B., Stern, H. S., Dunson, D. B., Vehtari, A., and Rubin, D. B. (2013). *Bayesian Data Analysis*. Chapman & Hall/CRC, third edition.

Gelman, A., Carlin, J. B., Stern, H. S., and Rubin, D. R. (2003). *Bayesian Data Analysis*. Chapman & Hall, 2nd edition.

Gelman, A., Meng, X.-L., and Stern, H. (1996). Posterior predictive assessment of model fitness via realized discrepancies (with discussion). *Statistica Sinica*, 6(4):733–807.

Gouïtis, C. and Robert, C. P. (1998). Model choice in generalised linear models: A Bayesian approach via Kullback-Leibler projections. *Biometrika*, 85(1):29–37.

Gutiérrez-Peña, E. and Walker, S. G. (2001). A Bayesian predictive approach to model selection. *Journal of Statistical Planning and Inference*, 93(1–2):259–276.

Laud, P. and Ibrahim, J. (1995). Predictive model selection. *Journal of the Royal Statistical Society. Series B (Methodological)*, 57:247–262.

Lindley, D. V. (1968). The choice of variables in multiple regression. *Journal of the Royal Statistical Society. Series B (Methodological)*, 30(1):31–66.

Lindley, D. V. (1985). *Making decisions*. John Wiley & Sons, 2nd edition.

O’Hagan, A. and Forster, J. (2004). *Bayesian Inference*, volume 2B of *Kendall’s Advanced Theory of Statistics*. Arnold, 2nd edition.

Piironen, J., Paasiniemi, M., and Vehtari, A. (2020). Projective inference in high-dimensional problems: Prediction and feature selection. *Electronic Journal of Statistics*, 14(1):2155–2197.

Press, S. J. (2003). *Subjective and Objective Bayesian Statistics: Principles, Models, and Applications*. John Wiley & Sons.

Robert, C. P. (1996). Intrinsic losses. *Theory and decision*, 40(2):191–214.

Robert, C. P. (2001). *The Bayesian Choice: from Decision-Theoretic Motivations to Computational Implementation*. Springer, 2nd edition.

San Martini, A. and Spezzaferri, F. (1984). A predictive model selection criterion. *Journal of the Royal Statistical Society. Series B (Methodological)*, 46(2):296–303.
Trevisani, M. and Gelfand, A. E. (2003). Inequalities between expected marginal log likelihoods with implications for likelihood-based model comparison. *The Canadian Journal of Statistics*, 31(3):239–250.

Vehtari, A. and Ojanen, J. (2012). A survey of Bayesian predictive methods for model assessment, selection and comparison. *Statistics Surveys*, 6:142 – 228.

Yang, R. and Berger, J. O. (1997). A catalog of noninformative priors. ISDS Discussion Paper 97-42, Institute of Statistics and Decision Sciences, Duke University.