

On a Class of Objective Priors from Scoring Rules

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Abstract. Objective prior distributions represent an important tool that allows one to have the advantages of using a Bayesian framework even when information about the parameters of a model is not available. The usual objective approaches work off the chosen statistical model and in the majority of cases the resulting prior is improper, which can pose limitations to a practical implementation, even when the complexity of the model is moderate. In this paper we propose to take a novel look at the construction of objective prior distributions, where the connection with a chosen sampling distribution model is removed. We explore the notion of defining objective prior distributions which allow one to have some degree of flexibility, in particular in exhibiting some desirable features, such as being proper, or log-concave, convex etc. The basic tool we use are proper scoring rules and the main result is a class of objective prior distributions that can be employed in scenarios where the usual model based priors fail, such as mixture models and model selection via Bayes factors. In addition, we show that the proposed class of priors is the result of minimising the information it contains, providing solid interpretation to the method.

Keywords: calculus of variation, differential entropy, Euler–Lagrange equation, Fisher information, invariance, objective Bayes, proper scoring rules.

1 Introduction

With the ever increasing popularity of Bayesian methods, attributable largely to the advent of Markov chain Monte Carlo methods and other sampling techniques, the need for default, otherwise known as objective or noninformative, priors is also in demand. Model based objective priors, such as the reference prior (Berger et al., 2009) and Jeffreys prior (Jeffreys, 1961), are commonly used when available. However, as models become larger and more complex, so it is that such priors are becoming more difficult to obtain, if not altogether unavailable. Indeed, it is our contention that model based objective priors have now reached their natural ceiling with little progress or advances in recent years.

Our observation is that limits to the progress in the research on objective priors is connected to their improperness. In fact, with very few exceptions, objective priors are improper. Although this may not represent a problem, as long as the posterior is

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proper, it causes severe limitations to the use of objective prior distributions. Indeed, the impropriety of objective priors is the main motivation which brought us to investigate a novel approach to derive objective priors. A thorough discussion of the problems that improper priors cause can be found in Kass and Wasserman (1996), where they illustrate issues such as incoherence, strong inconsistencies and nonconglomerability, dominating effect of the prior, inadmissibility, marginalisation paradoxes and improper posteriors. Although all points are undoubtedly important, it is probably the last issue that requires careful consideration. The main concern is that, as of today, general results that allow one to assess if a given improper prior yields a proper posterior are yet to be found. Research has progressed on a case by case basis; for example, see Ibrahim and Laud (1991) for the use of Jeffreys prior in generalised linear models, extended to overdispersed models of the same kind by Dey et al. (1993), Natarajan and McCulloch (1995), Berger and Strawderman (1993), and Yand and Chen (1995). More recently, Rubio and Steel (2018) describe general conditions to use improper priors for linear mixed models with longitudinal and survival data. As one would expect, the task of assessing posterior propriety becomes more onerous the more complex the model is. But, even for simple models, the risk is high; as, for example, the discussion in Vallejos and Steel (2013) about the use of the Jeffreys rule prior for the Student- t regression model, derived in Fonseca et al. (2008), shows.

In this paper, we investigate constructing objective prior distributions that are not model dependent and based on the sole knowledge of the parameter space, say, Θ . As such, the connection between the prior distribution, $p(\theta)$, and the likelihood function, $f(\cdot|\theta)$, is limited to the common parameter space only.

Therefore, the prior $p(\theta)$ using only Θ loses the connection with the subjective component $f(\cdot|\theta)$ and could be argued as a consequence to be *more objective*. Conversely, model based priors, such as the Jeffreys prior (Jeffreys, 1946, 1961) or the reference prior (Berger et al., 2009), necessarily include the subjective choice of the model. In fact, models are by and large misspecified and, consequently, model based priors are propagating this misspecification. So, while a model based prior reinforces the connection between the misspecified model and the prior itself, a prior that depends on the parameter space loses only the connection.

The method we propose to derive a novel class of objective priors is based on defining a scoring rule as a combination of the *log-score* and of the *Hyvärinen* score (Parry et al., 2012). We then seek a prior such that the above score, say $S(\theta, p)$, is constant, that is

$$S(\theta, p) = \text{constant} \quad \forall \theta \in \Theta. \quad (1)$$

We show in Section 3 that the density p satisfying (1) identifies a class of objective priors. Furthermore, we show in Section 4 that the density $p(\theta)$ solving (1) minimises the information in the prior as measured by a combination of the Shannon information and the Fisher information. As a result of these equivalent approaches, we show that the objective prior $p(\theta)$ is obtained by solving the following differential equation:

$$\frac{p''(\theta)}{p(\theta)} - \frac{1}{2} \left\{ \frac{p'(\theta)}{p(\theta)} \right\}^2 = 1 + \log p(\theta). \quad (2)$$

Our prior is the class of solutions to the differential equation (2). The class allows us to include constraints such as properness, convexity and being decreasing, among others.

The development of objective priors is thoroughly reviewed in Consonni et al. (2018). The idea is that in a scenario where prior elicitation is not feasible, or not desirable, a prior distribution can be formed through structural or formal rules (Kass and Wasserman, 1996). The most popular objective prior is Jeffreys prior (Jeffreys, 1946, 1961), who proposed a prior distribution for continuous parameter spaces which is invariant for one-to-one transformations of the parameter space. Although in scenarios where there is only one parameter of interest, Jeffreys prior yields sensible posterior distributions. However, in cases where the parameter space has a dimension of two or more, the prior is known to yield posteriors with poor performance (sometimes giving paradoxical results, such as the marginalisation paradox, see Stone and Dawid (1972)). In such cases the priors are taken to be independent. Although other more general invariance priors have been proposed, such as in Dawid (1983), Hartigan (1964) and Jaynes (1968), the reference prior of Bernardo (Berger et al., 2009) represents an alternative to Jeffreys prior. A limitation of reference priors is sensitivity to the order of importance of parameters; this issue and possible solutions have been discussed in Berger et al. (2015). Other objective priors proposed include that of Box and Tiao (1973), based on data-translated likelihoods, and maximum entropy priors, see, for example, Jaynes (1957, 1968). As discussed in Kass (1990), these priors turn out to be very restrictive. Another important class of objective priors are the probability matching priors, first proposed in Welch and Peers (1963). The aim is to obtain a prior distribution under which the posterior probabilities of certain regions coincide with their coverage probabilities, either exactly or approximately. Recent developments of this method can be found in Sweeting et al. (2006) and Sweeting (2008). A different method, based on information theoretical concepts, has been proposed by Zellner and Min (1993), giving the so called maximal data information prior. Possibly, the most recent development in defining prior distributions, although not strictly in an objective sense, is discussed in Simpson et al. (2017). The idea is to identify the parts in a complex model that require subjective input, while the remaining parts can be associated with non-informative priors. It is important to point out that objective priors derived from scoring rules have been proposed in the recent work of Giummolè et al. (2018). A final consideration is reserved for discrete parameter spaces, whose systematic discussion can be seen to be generated by the paper of Rissanen (1983). The lack of general methods, due to the challenges that discreteness imposes, has been filled by Berger et al. (2012) first, and by Villa and Walker (2015) later.

It is known that for a mixture model Jeffreys prior can only be found under specific conditions, as studied in Grazian and Robert (2018), for reasons identified, in part, by Titterton et al. (1985). Also, standard objective priors are problematic in model comparison since Bayes factors depend on the arbitrary normalizing constants of improper prior. Though, special solutions have been proposed, for example, by O'Hagan (1995) and Berger and Pericchi (1996). Further discussion of these contexts is contained in Sections 6.1 and 6.2, where solutions provided by our approach are explored. There are other examples where the use of improper priors is challenging. For example, Kass and Wasserman (1996) discuss some issues related to their use in hierarchical modelling. Also, paradoxical results may appear, such as the marginalisation paradox (Stone and

Dawid, 1972) or the Stein’s paradox (Bernardo and Smith, 1994). For more examples, see Stone (1976) and Syversveen (1998).

The paper is structured as follows. In Section 2 we give an outline of the idea and discuss a simple introductory example. In Section 3 we introduce the foundations of the proposed prior on the basis of scoring rules and their properties. An interesting aspect of the prior based on scoring rules is its interpretation in terms of the information content carried by the prior itself. This aspect is explored in Section 4. In Section 5 we present the objective priors concentrating on $\Theta = (0, 1)$, $(0, \infty)$, $(-\infty, +\infty)$ and $(-M, M)$, for a finite M , as well as on a multidimensional space. The implementation of the prior for some specific applications is presented in Section 6 where, in addition, we explore some properties of the proposed prior. Finally, Section 7 is dedicated to some concluding remarks.

2 Outline of the idea

Here we illustrate two key motivating examples, in particular in relation to the use of improper priors, and give an intuitive description of the core ideas of this work.

The key to our idea is to consider a loss function $l(\theta, p(\theta))$ which penalizes for each $\theta \in \Theta$ a choice of a prior density $p(\theta)$. The objective criterion is then based on the idea of finding the class of p which makes $l(\theta, p(\theta))$ constant. For obvious reasons, the loss function should have the following property

$$\int l(\theta, p(\theta))q(\theta) d\theta \geq \int l(\theta, q(\theta))q(\theta) d\theta, \quad (3)$$

for all q ’s representing a density for the θ . In other words, if a “true” density for θ exists, the expected loss should be minimised when such a density is chosen. The condition in (3) identifies a particular class of loss functions, known as *proper scoring rules*. One way of interpreting (proper) scoring rules is as loss functions that measure the quality of a quoted density p for an uncertain quantity θ ; see, for example, Parry et al. (2012). We indicate a proper scoring rule by $S(\theta, p)$, and we ask it to be constant for all $\theta \in \Theta$. So we set

$$S(\theta, p) = \text{constant} \quad \forall \theta \in \Theta,$$

and the densities satisfying the above equality identify a class of objective priors. We set the constant to 1 and show later that this choice is without loss of generality. The criterion defining this class of priors is clearly objective, for if the scoring rule were not constant, some parts of the space Θ would be given preference above others.

As discussed in Parry et al. (2012) a scoring rule is defined as *local* if it depends on the density function $p(\cdot)$ only through its value at θ , that is $p(\theta)$. Holding the above definition, we have that any *proper local* scoring rule is equivalent to the *log score*, $-\log p(\theta)$, also known as the self information loss function. However, the above scoring rule is not suitable to us, for if we set $-\log p(\theta) = \text{constant}$, we only achieve $p(\theta) \propto 1$, and the result is not interesting. Hence, we extend the score function to include the first and second derivatives of $p(\theta)$; a natural extension, in our opinion.

Thus, we consider additionally the Hyvärinen scoring rule (Hyvärinen, 2005) which makes use of the first two derivatives of p , written as p' and p'' . We then have a scoring

rule $S(\theta, p)$ which has two components; the log score and the Hyvärinen score. Finding solutions to $S(\theta, p) = 1$ will now involve solving a second order differential equation and we obtain the class of prior through the two constants connected with the two derivatives. Multivariate versions of the scoring rule criterion we are proposing, and corresponding solutions, are discussed in Section 3.

Parry et al. (2012) describe a larger class of score based on the first two derivatives; see (39) in their paper. In the second order case these are based on an Euler–Lagrange equation which itself is based on a measure of information of the form $\int [p'(\theta)]^k / [p(\theta)]^{k-1} d\theta$ for $k = 2, 3, \dots$. The only widely recognised information occurs with $k = 2$; the Fisher information and the corresponding score coincides with the Hyvärinen score. Hence, we use this. A connection between our scoring rule criterion and information is made through an alternative formulation through variational methods, which is discussed in Section 4.

3 Priors from scoring rules

Let us consider a quantity of interest, θ , which can take values in the space $\Theta \subset \mathbb{R}^k$. The fundamental argument behind objective prior distributions is that they should represent a state of actual or alleged prior ignorance about the true value of θ . Several criteria have been proposed to select such a prior, all of which assume that a probabilistic model generating the data (given θ) has been chosen. What we propose is to avoid this choice and derive a prior depending on Θ only. The idea is to measure the quality of the prior p with a proper scoring function, say $S(\theta, p)$, and require it to be constant, as discussed in the Introduction.

Definition 1. *A density p with respect to the Lebesgue measure on Θ , is objective (in accordance with commonly accepted meaning of the expression) if $S(\theta, p) = \text{constant}$ for all $\theta \in \Theta$, where S is a proper scoring rule.*

The constant here is unimportant and we can take it as 0. Any constant works – effectively it becomes 0 once the normalizing constant for p has been established.

Before proceeding we provide a brief discussion on scoring rules. Scoring rules are *proper* if $\int_{\Theta} S(\theta, p) q(\theta) d\theta$ is minimized at $p = q$ and *local* if it depends on p only through the value $p(\theta)$. The unique proper local scoring rule is the log score, defined as

$$S_L(\theta, p) = -\log p(\theta).$$

Parry et al. (2012) extend the local property to m -local, in that now $S(\theta, p)$ depends also on the l -derivative $p^{(l)}(\theta)$, for $0 \leq l \leq m$. In particular, for $m = 2$, there is the Hyvärinen scoring rule, (Hyvärinen, 2005), given by

$$S_H(\theta, p) = \Delta \log p(\theta) + \frac{1}{2} |\nabla \log p(\theta)|^2.$$

In Section 4 we will illustrate the connection of the Hyvärinen scoring rule to Fisher information. Our choice of scoring rule following our reasoning in Section 2, and with

the weighting factor, is

$$\begin{aligned} S(\theta, p) &= w S_L(\theta, p) + S_H(\theta, p) \\ &= -w \log p(\theta) + \sum_{j=1}^k \frac{\partial^2 p / \partial \theta_j^2}{p}(\theta) - \frac{1}{2} \sum_{j=1}^k \left(\frac{\partial p / \partial \theta_j}{p}(\theta) \right)^2. \end{aligned}$$

That this is a proper scoring rule is derived from the fact that it is the sum of two proper scoring rules. It is also clearly 2-local. Previously, priors have been sought based solely on $\log p$; for example, the reference prior, and the math becomes unnatural as a consequence. On the other hand, including higher derivatives yields well defined solutions to optimization procedures. That we set this score to 1 for all θ is done without loss of generality, as we shall see later on. That we understand this to be an objective procedure is evident from the fact that no part of Θ is being given preference; the *loss* at θ for our choice of $p(\theta)$ is the same for all θ . For, if $S(\theta, p)$ did depend on θ then we argue that this could only be driven by *information*; i.e. parts of Θ space are preferential to others.

Predominantly, throughout the paper, we will be using the choice of $w = 1$. After all the value of w is a calibration issue between the two scores; i.e. to put them on a comparable scale. The reason for $w = 1$ is that for the benchmark standard normal density function, i.e. $p(\theta) \propto e^{-\frac{1}{2}\theta^2}$, the difference between the scores S_L and S_H is a constant (i.e. does not depend on θ), and so one does not end up dominating the other, only for $w = 1$.

Hence, we see that the objective prior, $p(\theta) \propto \exp\{-u(\theta)\}$, is obtained by solving the following differential equation:

$$\sum_{j=1}^k \frac{\partial^2 u}{\partial \theta_j^2} - \frac{1}{2} \sum_{j=1}^k \left(\frac{\partial u}{\partial \theta_j} \right)^2 = wu. \quad (4)$$

To derive the solution, we have the following result.

Theorem 3.1. *The solution to (4) is given by, for $j = 1, \dots, k$,*

$$\frac{\partial u}{\partial \theta_j} = \pm \sqrt{c_j e^{u(\theta)} - 2w(1 + u(\theta))}/k, \quad (5)$$

for some suitable constants $c = (c_j)$ and a specified value of u at some point; e.g. $u(0, \dots, 0)$.

Proof. Solving the differential equation (4) is equivalent to solving the following differential equation;

$$\sum_{j=1}^k v_j \frac{\partial v_j}{\partial u} = \frac{1}{2} \sum_{j=1}^k v_j^2 + uw, \quad (6)$$

having defined $v_j = \partial u / \partial \theta_j$. It is now seen the solution is given by (5). This follows since

$$v_j \frac{\partial v_j}{\partial u} = v_j \frac{1}{2} \frac{1}{v_j} (c_j e^u - 2w/k)$$

and note that $c_j e^u - 2w/k = v_j^2 + 2wu/k$. Therefore (6) holds. \square

The missing pieces in (5) are $c = (c_j)$ and say $u(0)$, the constants of integration. Note that, the initial value $u(0)$ (together with the constant c) is required to ensure the existence and uniqueness of the solution. We will see how to complete these when we look at illustrations in Section 4. In general, as the solution depends on the above arbitrary constants, our method provides a class of solutions, where some are proper and some are improper and, more general, where the priors will have some assigned properties via specification of $(c, u(0))$.

We also note here that we do not need the normalizing constant for p and neither do we need to find an explicit solution for u , and p , beyond (5). The reason for this is that we can find an accurate solution via numerical methods; i.e. if we have $u(\theta)$ at a particular θ value, then we can evaluate

$$u(\theta + \varepsilon) = u(\theta) + \varepsilon' \frac{\partial u}{\partial \theta}(\theta) + \frac{1}{2} \varepsilon' \frac{\partial^2 u}{\partial \theta^2}(\theta) \varepsilon + o(|\varepsilon|^2)$$

for small ε , and the $\partial u / \partial \theta$ and $\partial^2 u / \partial \theta^2$ are available explicitly, combined with the ease of obtaining higher derivatives if needed. From here we can evaluate $p(\theta)$.

To ease the reader into the proposed prior, we illustrate the following simple example, where the parameter space is $\Theta = (-M, +M)$. Here we discuss an explicit solution to the equation $u'(\theta) = \pm \sqrt{ce^{u(\theta)} - 2(1 + u(\theta))}$, which is (5) where we have set $w = 1$ and, as the parameter space is unidimensional, $k = 1$. If we set $c = 0$ then for a solution to exist we must have $1 + u$ to be negative. Consider a prior on $\Theta = (-M, +M)$ for some finite M . With $c = 0$ we have the solution for u in the form $1 + u(\theta) = -\frac{1}{2}(\theta - \mu)^2$ for some μ . Hence, $p(\theta) \propto \exp\{\frac{1}{2}(\theta - \mu)^2\}$, which will provide a proper density on Θ .

A more general solution $p(\theta) \propto \exp\{\frac{1}{2}w(\theta - \mu)^2\}$ arises when we take the more general form of score function; i.e. $S(\theta, p) = w S_L(\theta, p) + S_H(\theta, p)$, providing interpretation for the score weighting parameter in this case. Plots of such $p(\theta)$ depending on w are presented in Figure 1, with $M = 2$.

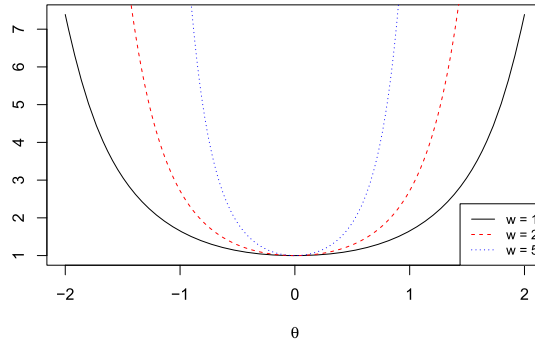


Figure 1: Prior for the parameter space $(-2, 2)$ with weights $w = 1$ (continuous black line), $w = 2$ (dashed red line) and $w = 5$ (dotted blue line).

4 Variational problems and solutions

Here we provide an alternative derivation of (4) using information theory, specifically entropy information and Fisher information. We show that the p solving (4) can also be regarded as a density carrying minimal local information. This material then is to provide support for the solution to (4) being an objective prior.

The entropy information (negative entropy) of a density function p is given by $I_E(p) = \int p(\theta) \log p(\theta) d\theta$, which is related to Shannon's entropy and is equal to negative the expected self-information loss. In addition to $I_E(p)$, we consider a measure of the information in the density p known as Fisher information, given by

$$I_F(p) = \int \frac{p'(\theta)^2}{p(\theta)} d\theta = \int p(\theta) \left\{ \frac{\partial}{\partial \theta} \log p(\theta) \right\}^2 d\theta.$$

See, for example, Bobkov et al (2014).

Now consider $I(p) = I_E(p) + \frac{1}{2}I_F(p)$ and the aim is to find the p which minimizes $I(p)$. Recalling variational methods (Rustagi, 1976), if we wish to minimise $\int_a^b L(\theta, p, p') d\theta$, a necessary condition for a local extremum of the integral of the Lagrangian $L(\theta, p, p')$ is that

$$\frac{\partial L}{\partial p} = \frac{d}{d\theta} \frac{\partial L}{\partial p'}. \quad (7)$$

Minimising $\int_a^b L(\theta, p, p') d\theta$ reduces to the classical calculus of variation problem where we want to extremize the integral of the function

$$L(\theta, p, p') = \frac{1}{2} \frac{p'(\theta)^2}{p(\theta)} + p(\theta) \log p(\theta).$$

The solution to the extremal problem, if it exists, is obtained from the Euler–Lagrange equation, given by (7). According to page 44 of Rustagi (1976), if $L(p, p')$ is strictly convex on $(0, \infty) \times (-\infty, +\infty)$, and p satisfies the Euler equation, then p is a minimum of $\int_a^b L(\theta, p, p') d\theta$. Now $L(p, p')$ is strictly convex if the matrix

$$H = \begin{pmatrix} \partial^2 L / \partial p^2 & \partial^2 L / \partial p \partial p' \\ \partial^2 L / \partial p \partial p' & \partial^2 L / \partial (p')^2 \end{pmatrix}$$

is positive definite.

Theorem 4.1. *A minimum satisfying the Euler–Lagrange equations is given by the p solving the differential equation $p' = \pm p \sqrt{c/(ep) + 2 \log p}$, for some suitable c .*

Proof. Calculations give

$$H = \frac{1}{p} \begin{pmatrix} \kappa^2 + 1 & -\kappa \\ -\kappa & 1 \end{pmatrix},$$

where $\kappa = p'/p$. This is easily seen to be a positive definite matrix; the eigenvalues are given by

$$\frac{1}{p} \left[\frac{1}{2}(2 + \kappa^2) \pm \sqrt{\frac{1}{4}(2 + \kappa^2)^2 - 1} \right],$$

which are positive.

Then (7), after some elementary algebra and differentiation, leads to the differential equation (2), which we report here for convenience,

$$\frac{p''(\theta)}{p(\theta)} - \frac{1}{2} \left\{ \frac{p'(\theta)}{p(\theta)} \right\}^2 = 1 + \log p(\theta),$$

which is the same as (4). □

This differential equation has the solution derived in the previous section. It is interesting that the Euler–Lagrange equations are solved by precisely the same p solving (4).

It might be thought that we would need the constraint $\int p(\theta) d\theta = 1$, that is to consider $L(\theta, p, p') + \lambda(p)$, i.e. to include a Lagrange multiplier. However, any ensuing differences are covered by our note in Section 5.

5 Illustrations

Before proceeding with some illustrations and applications, it is important that we discuss two aspects of the proposed class of priors within the boundaries of *Objective Bayes*: i.e. uniqueness and invariance.

It is important to discuss uniqueness and flexibility associated with objective priors. It is widely acknowledged that a prior representing total ignorance is elusive, and it might not even be possible to obtain in principle, see Bernardo and Smith (1994). As a consequence, any prior distribution, objective or not, must out of necessity provide some knowledge about something, and this “something” is not necessarily unique. For example, given a particular problem, the corresponding objective prior over a given parameter space could be proper or improper; differentiable everywhere or not; convex; log-concave; etc. In other words, a prior can be objective and exhibit desirable features of choice without impinging on subjective components relating to information.

So while we will be introducing a Bayesian objective prior criterion, it does not lead to a unique prior, rather to a class of priors, where some desirable features may or may not be included. We believe that this level of flexibility is a point of strength of the proposed approach, making it adaptable to different scenarios, including those where model based priors do not work.

Another fundamental point of discussion about prior distributions and, in particular, objective prior distributions, is invariance. Indeed, Jeffreys’ rule to derive a prior distribution for the parameters of a given model is based on an invariance requirement,

in particular on invariance under one-to-one reparameterisations. Also, other common objective priors, such as reference priors, have been shown to be invariant and the same apply, for example, to the priors in Simpson et al. (2017).

Here we discuss invariance from two opposite perspectives: that it is not important, and that it is important. Before discussing this apparent contradiction, we need to point out that we define the objective prior by setting the scoring rule equal to a constant, that is $S(\theta, p(\theta)) = \text{constant}$, is invariant under location transformations.

The question is whether lack of invariance has any practical implications given that only one parameterisation will be used. Current model based objective procedures are bound to throw away some coherence properties to achieve invariance, see Kass and Wasserman (1996). However, our point is that there is no practical consequence of any relevance arising from the lack of invariance, given that, as mentioned above, a single parameterisation will be used. For example, in the case the chosen model is the normal density, one either considers the precision parameter or the variance parameter, not both. And whichever parameterisation is used, our claim is that the corresponding objective prior is adequate for the purpose to which it has been assigned.

The above points of discussion are concerned with the perspective that invariance is not important. To consider the opposite point of view let us assume that there is a canonical parameterisation for the model $f(\cdot|\theta)$. Certainly, for most models the set of parameters for which priors would be assigned is obvious. For example, the exponential family has

$$f(x|\theta) = h(x) \exp \left\{ \sum_{j=1}^p \theta_j T_j(x) - A(\theta) \right\}$$

with $\theta = (\theta_1, \dots, \theta_p)$ being the canonical parameterisation. We can then define the canonical objective prior for statistical model $f(\cdot|\theta)$, $\theta \in \Theta$, as $p_{\Theta}(\theta) = \prod_{j=1}^p p_{\Theta_j}(\theta_j)$, where $\Theta = \otimes_{j=1}^p \Theta_j$. Then, any transformed prior can be obtained in the usual way involving variable transformations; that is $p(\phi) = |J| p_{\Theta}(\theta(\phi))$, where J is the Jacobian matrix for the transformation.

To illustrate the proposed method we consider three common parameter spaces in the unidimensional case and one in the multidimensional case. In particular, we consider the space for a parameter representing a probability, that is $\Theta = (0, 1)$, the space $\Theta = (0, \infty)$, usually representing the support of scale parameters, and the support for (location) parameters $\Theta = (-\infty, +\infty)$. The space $\Theta = (-M, M)$, for some finite M , has been illustrated in Section 3. As an illustration for the multidimensional case, we consider the bidimensional parameter space $(0, \infty)^2$.

5.1 One dimensional parameter space

The aim here is to solve (7) for particular motivated choices of $(c, u(0))$, equivalently, $(c, p(0))$ or $(p'(0), p(0))$. In fact, the solutions to the Euler–Lagrange equations are many, and the choice of the two constants $(c, u(0))$ will then determine a unique solution.

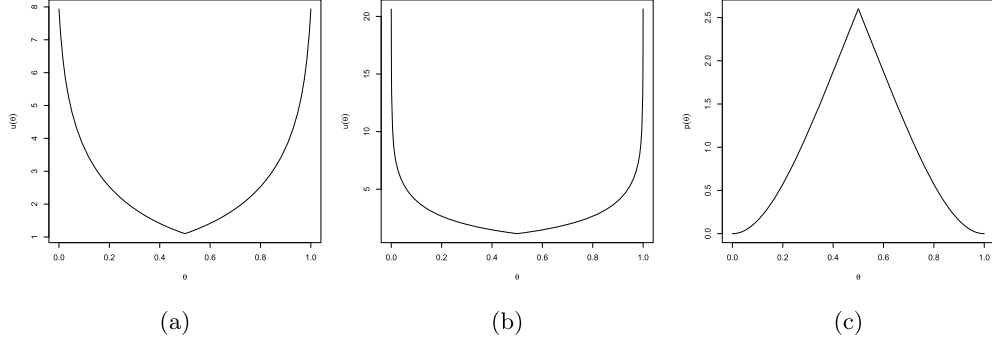


Figure 2: Plot of numerical solutions for u , panels (a) and (b) with, respectively, $u(\frac{1}{2}) = 1.1$ and $u(\frac{1}{2}) = 1.14$; plot of the normalised prior density obtained by setting $u(\frac{1}{2}) = 1.14$ (c).

Now there is the flat solution for all Θ in (4) given by $p(\theta) \propto 1$. This is achieved by setting $c = 2$ and $u(0) = 0$. However, in each of the settings of Θ considered we can find alternate priors with particular features. So, e.g. for $\Theta = (0, 1)$ we ask that $p(0) = p(1) = 0$ and for $\Theta = (0, \infty)$ we ask that p is convex and decreasing.

Case $\Theta = (0, 1)$ Here we consider the u function, recall $p \propto e^{-u}$, and so for $p(0) = p(1) = 0$ we require $u(0) = u(1) = \infty$. For additional symmetry, we can take $u(\frac{1}{2}) > 0$ and taking $c = 2$ as the extremal value, we have

$$\begin{aligned} u' &= \sqrt{2}\sqrt{e^u - 1 - u} & \theta > \frac{1}{2}, \\ u' &= -\sqrt{2}\sqrt{e^u - 1 - u} & \theta < \frac{1}{2}. \end{aligned}$$

Note there is a discontinuity in the derivative of u at $\theta = \frac{1}{2}$. As $u(\frac{1}{2})$ increases it is that $u(0)$ and $u(1)$ got to ∞ . A plot of u is given in Figure 2a for $u(\frac{1}{2}) = 1.1$ and for $u(\frac{1}{2}) = 1.14$ in Figure 2b. For these figures we used a grid of 1000 either side of $\theta = \frac{1}{2}$ to obtain the numerical solutions. In the latter case, the corresponding density for p is presented in the right plot of Figure 2c.

It is also possible to obtain a prior that mimics Jeffreys'; that is, a distribution that has spikes at $\theta = 0$ and $\theta = 1$ with the lowest value at $\theta = \frac{1}{2}$. This is done by simply inverting u : i.e. set $u = -u$ in the above prior.

Case $\Theta = (0, \infty)$ For a prior defined on the space $(0, \infty)$ we require a specific shape property for p (convex and decreasing) and then take extremal values for the c and $u(0)$. This property is common to most objective priors on $(0, \infty)$. Thus, since $p' < 0$ we require $u' > 0$ and so $u' = \sqrt{ce^u - 2(1 + u)}$, and for u' to exist for all u we must have $c \geq 2$. Thus, as an extremal value, we take $c = 2$.

For the prior to be convex we require $p'' \geq 0$. Now $p' = -u'p$ implying $p'' = p\{(u')^2 - u''\}$. Therefore, p is convex when $(u')^2 \geq u''$. From (6) and (5) we have $(u')^2 = ce^u - 2(1 + u)$ and $u'' = \frac{1}{2}ce^u - 1$, and hence we are interested in the $u(0)$ for

which $c = 2 \geq 2(1 + 2u)e^{-u}$ for all u ; i.e. $(1 + 2u)e^{-u} \leq 1$ for all u . Given that the function $(1 + 2u)e^{-u}$ is maximum, with a value of 1.31, at $u = \frac{1}{2}$, and u is increasing, since $u' > 0$, we need $u(0) > \frac{1}{2}$ and $(1 + 2u(0))e^{-u(0)} = 1$, again as an extremal value. Solving this gives a value for $u(0)$ of approximately 1.31.

In the next result we show that u' is bounded away from 0, and this will have important consequences for the properness of p .

Lemma 1. *It is that u' is bounded away from 0.*

Proof. To show this we need to show that $e^u - 1 - u$ is bounded away from 0 for $u \geq u(0)$. This follows trivially since $e^u - 1 - u \geq \frac{1}{2}u^2 \geq \frac{1}{2}u(0)^2$. \square

The result of Lemma 1 has also the implication that p is a proper density function. To show this, we require Gronwall's inequality (Gronwall, 1919). This inequality states that, if f and g are real valued functions on $\Theta = (0, \infty)$, g is differentiable on $\text{int}(\Theta)$, and $g'(t) \leq g(t) f(t)$ for all $t \in \Theta$ then $g(t) \leq g(0) \exp\{\int_0^t f(s) ds\}$.

Lemma 2. *If $p(0) < \infty$, it is that $p(\theta) \leq p(0) e^{-\epsilon\theta}$, and hence p is proper.*

Proof. Since $p' = -u'p$ and we have $u' \geq \epsilon$ for some $\epsilon > 0$, it is that $p' \leq -\epsilon p$. From Gronwall's lemma, with $f(t) = -\epsilon$ and $g = p$, we have that

$$p(\theta) \leq p(0) \exp\left\{-\int_0^\theta \epsilon ds\right\},$$

and hence the proof is complete. \square

To have a graphical image, in Figure 3a we plot the prior using the approximation available via a numerical solution to the differential equation for p . Note that this is the unnormalised p .

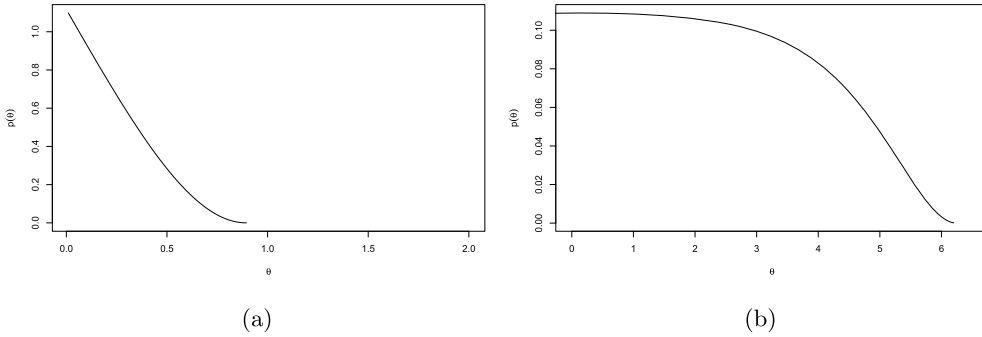


Figure 3: Plots of the prior on $(0, \infty)$ with $c = 2$ and $u(0) = 1.31$ (a). Plot of the positive half of the prior on $(-\infty, \infty)$, obtained by symmetrising the first one and make it differentiable at the origin (b). Both densities are normalised.

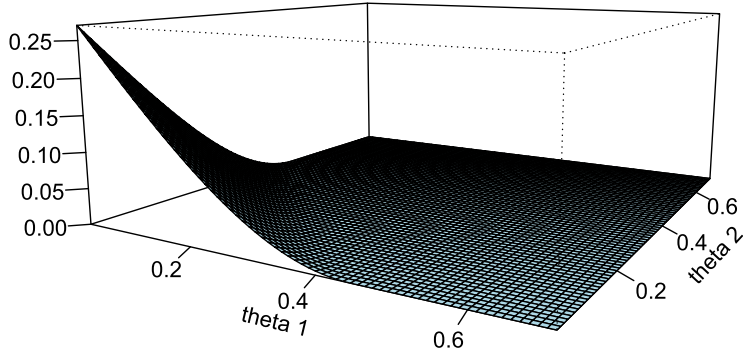


Figure 4: Surface plot of the prior for the bidimensional parameter space $\Theta = (0, \infty)^2$.

Case $\Theta = (-\infty, +\infty)$ A solution here is a symmetric version of the case $\Theta = (0, +\infty)$, which will represent a proper prior. On the other hand, if we ask that p is smooth at the origin, i.e. $p'(0) = 0$, then we need $u'(0) = 0$ and hence we must take $(c, u(0))$ to satisfy $ce^{u(0)} = 2 + 2u(0)$. If now we take $c = 2$, then $u(\theta)$ is a constant, resulting in a flat (improper) prior for p .

For a proper prior here one could take $u(0)$ to be small, say $u(0) = 0.01$ and then to take $c = 2\{1 + u(0)\}/\exp\{u(0)\}$. We computed numerically the right side; i.e. the $(0, \infty)$ side, for p , which is shown in Figure 3b.

To make the value of $u(0)$ more diverted, we could equally set a motivated choice for $p(0) = 1/(\sigma\sqrt{2\pi})$, corresponding to a normal density with zero mean and variance σ^2 .

5.2 Multidimensional parameter space

Here we consider the bidimensional parameter space $\Theta = (0, \infty)^2$, thus $\boldsymbol{\theta} = (\theta_1, \theta_2)$. As discussed in Section 3, the prior will have the solution $p(\boldsymbol{\theta}) \propto \exp\{-u(\boldsymbol{\theta})\}$, with the partial derivatives as in (5) and additional parameters c_1 and c_2 . It is sensible to expect the marginal priors $p_1(\theta_1)$ and $p_2(\theta_2)$ to be as the prior for the $\theta = (0, \infty)$ case discussed above. We can then set $u(0, 0) = (1.31, 1.31)$ and $c_1 = c_2 = 2$. The bidimensional prior is obtained using the bivariate Taylor expansion and, by applying the algorithm described in Appendix A of the Supplementary Material (Leisen et al., 2019), we obtain the prior for $(0, \infty)^2$, which surface is plotted in Figure 4.

6 Applications

The proposed class of priors is illustrated through a simulation study and the discussion of some practical implementation. Besides two initial simple examples, this section is dedicated to show the behaviour of the prior for cases where improper priors cannot be used (i.e. mixture models and model comparison via Bayes factors), while simula-

tion studies and a real data example are illustrated, respectively, in Appendix B and Appendix C in the Supplementary Material.

Although we do not have an explicit form for $p(\theta)$, we can use (5) to calculate it numerically quite easily. In particular, if we know $p(\theta)$ then we calculate $p(\theta + \delta\theta)$ for small $\delta\theta$, hence setting up the possibility of a posterior estimation process via Metropolis–Hastings sampling. The algorithm employed is detailed in Appendix A of the Supplementary Material.

To be specific, suppose we are currently at θ and the proposal value is θ' . The acceptance probability is

$$\alpha = \min \left\{ 1, \frac{l(\theta') p(\theta') q(\theta|\theta')}{l(\theta) p(\theta) q(\theta'|\theta)} \right\}, \quad (8)$$

where $l(\theta)$ is the likelihood function, and $q(\theta'|\theta)$ is the proposal density. The evaluation of $p(\theta')/p(\theta)$ in (8) does not represent any particular challenge. In fact, we have $p(\theta')/p(\theta) = \exp\{-[u(\theta') - u(\theta)]\}$, where u is the solution of the differential equation

$$u' = \sqrt{ce^u - 2(1 + u)}. \quad (9)$$

Equation (9) allows us to evaluate $u(\theta') - u(\theta)$ numerically, via

$$u(\theta') \approx u(\theta) + (\theta' - \theta)u'(\theta) + \frac{(\theta' - \theta)^2}{2}u''(\theta) + \frac{(\theta' - \theta)^3}{6}u'''(\theta),$$

where the derivatives are $u'(\theta) = \sqrt{ce^{u(\theta)} - 2(1 + u(\theta))}$, $u''(\theta) = \frac{1}{2}ce^{u(\theta)} - 1$, and $u'''(\theta) = \frac{1}{2}ce^{u(\theta)}\sqrt{ce^{u(\theta)} - 2(1 + u(\theta))}$, and so on. Depending on how far θ' is from θ we can either use the direct approximation just given or otherwise get from θ to θ' using smaller step sizes.

The frequentist performances are illustrated in a thorough simulation study, which is presented in Appendix B of the Supplementary Material. There, we also show the complete analysis for two single i.i.d. samples, that is where we obtain data from a Poisson distribution and from a normal density with unknown mean and known variance.

6.1 Mixture models

In this section we discuss the application of the proposed method to a scenario where objective priors have been notoriously challenging, namely mixture models. Due to their flexibility, mixtures of probability distributions allow models suitable for complex data by building on simple components. As an example, consider a mixture of normal densities,

$$f(x) = \sum_{j=1}^k \omega_j N(x|\mu_j, \sigma_j^2), \quad (10)$$

where k is a positive integer, including ∞ , and the $(\omega_j, \mu_j, \sigma_j)$ are the collection of parameters. Even under the scenario when k is known, the reference prior for model (10)

has yet to be derived, and Jeffreys prior can only be obtained under specific conditions; see Grazian and Robert (2018). Furthermore, this type of model is subject to other issues related to non-identifiability and unbounded likelihoods, among others. The issues mainly arise from the fact that improper priors may not be appropriate as we might not observe outcomes from every component of the mixture (Titterington et al., 1985). For example, Grazian and Robert (2018) show that Jeffreys prior is suitable for mixtures of normal densities only in certain circumstances; that is, when the unknown parameters are the weights. If the unknown parameters are the means or the variances, then using Jeffreys prior may lead to improper posteriors. In particular, if the unknown parameters are the means only, proper posteriors exist only when the number of mixture components is at most two; while, if the unknown parameters are the variance, or the mean and the variances, then Jeffreys prior is not suitable for inference. The above issues can be generalised to apply to any type of mixture model.

Given that the objective prior we propose is proper, it allows to make inference on the parameters of a mixture density as the yielded posteriors will be proper. As an illustration, we consider a mixture of three normal densities, where the weights and the parameters of the components are unknown. In particular, we sample from the following model

$$f(y|\omega_1, \omega_2, \omega_3, \mu_1, \mu_2, \mu_3, \sigma_1^2, \sigma_2^2, \sigma_3^2) = \sum_{i=1}^3 \omega_i N(\mu_i, \sigma_i^2), \quad (11)$$

with weights $\omega_1 = 0.25$, $\omega_2 = 0.35$ and $\omega_3 = 0.40$, means $\mu_1 = -3.5$, $\mu_2 = 0$ and $\mu_3 = 2.5$, and variances $\sigma_1^2 = 0.5$, $\sigma_2^2 = 0.1$ and $\sigma_3^2 = 1.2$. Note that we have chosen mixture components that are reasonably distant, so not to be forced to impose any constraint to overcome identifiability, as the focus of the paper is not in this sense. However, the implementation of constraints in that sense is straightforward. For the parameters we have chosen prior independence, where each prior is the prior on the space $(0, 1)$ for the weights, on the space $(-\infty, \infty)$ for the means and on the space $(0, \infty)$ for the variances, in agreement with Section 5. The prior on $(-\infty, \infty)$ is the symmetrised version from $\Theta = (0, \infty)$. To ensure properness of the priors for the means and variances, we have set $c = 2$ and $u(0) = 1.31$ (as discussed in Section 5).

We have performed the analysis on two data sets of size $n = 100$ and $n = 250$. The whole details, including histograms of the sample data, description of the algorithm implemented, as well as convergence diagnostics are reported in Appendix D of the Supplementary Material.

6.2 Model comparison

Another simple case where objective priors are problematic is in model comparison (or selection) via Bayes factors. So, if we wish to compare model $M_1 = \{f_1(x|\boldsymbol{\theta}_1), p_1(\boldsymbol{\theta}_1)\}$ to model $M_2 = \{f_2(x|\boldsymbol{\theta}_2), p_2(\boldsymbol{\theta}_2)\}$, where both $\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$ are vector of parameters with some elements not in common, then the Bayes factor

$$BF_{12} = \frac{\int f_1(x|\boldsymbol{\theta}_1) p_1(\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{\int f_2(x|\boldsymbol{\theta}_2) p_2(\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2},$$

is, in general, meaningful if the priors assigned to non-common parameters are proper. If not, then the arbitrary multiplicative constant up to which they are defined do not cancel and the Bayes factor depends on an arbitrary constant. Solutions to the issue have been proposed, see, for example, O’Hagan (1995) and Berger and Pericchi (1996), however, the resulting procedures are still quite tedious to implement and are limited to simple models. By and large the above issue stays; however, Berger et al. (1998) give an exception of the issue. Furthermore, in Dawid and Musio (2015) and Dawid et al. (2017) the authors propose to make use of homogeneous scoring rules that circumvent the problem of using improper priors on the parameters.

An example on the application of the proposed prior in model selection is discussed in Appendix E of the Supplementary Material. There, a Poisson distribution and a geometric distribution are compared, where the priors are, respectively, of a parameter space $(0, \infty)$ and $(0, 1)$. As proprieness is necessary in this context, we have set $c = 2$ and $u(0) = 1.31$.

Nested models

When models under comparison are nested, there are particular considerations which are needed to be taken into account; see, for example, Consonni et al. (2013). The point is that a diffuse type prior for the larger model will end up lacking focus so that the mass assigned to the smaller model is too much. However, our argument is that if two nested models are under comparison, it is essential, at least from a coherent point of view, to center the larger prior on the fixed part of the smaller one. Let us elaborate.

Suppose $f(y|\theta)$ for $\theta \in \Theta_1$ is the larger model and the smaller one is given by $\theta \in \Theta_0$ where $\Theta_0 \subset \Theta_1$. Typically Θ_1 will be a higher dimension to Θ_0 and to get the latter from the former one fixes a particular value in the higher dimension. To make this concrete, let us consider Example 2.1 from Consonni et al. (2013), where $M_0 : f(y|\theta_0)$ is binomial(n, θ_0), with $\theta_0 = 1/4$ fixed, and $M_1 : f(y|\theta)$ is binomial(n, θ), for which a prior for θ , $p(\theta)$, is required. Given the nature of the comparison it is our argument that $p(\theta)$ must be centered on θ_0 .

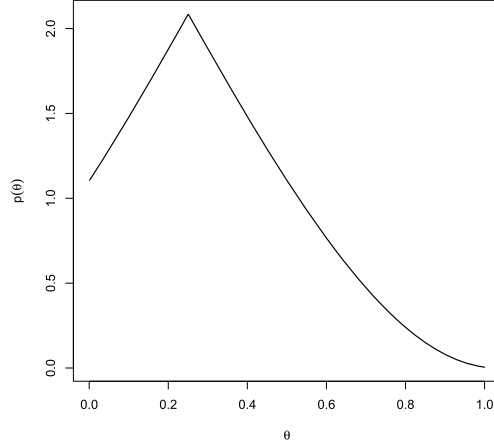
We can adapt quite easily the prior obtained in Section 4, the $\Theta = (0, 1)$, to be centered on $1/4$ rather than $\frac{1}{2}$. Without repeating the mathematics, we can take $u(1/4) = w$ and $c = 2$ and then

$$\begin{aligned} u' &= \sqrt{2}\sqrt{e^u - 1 - u} & \theta > 1/4, \\ u' &= -\sqrt{2}\sqrt{e^u - 1 - u} & \theta < 1/4. \end{aligned}$$

For the illustration of the prior $p(\theta)$, obtained numerically from u , in Figure 5 we took $w = 1.5$.

The proposed prior, centered at $\theta_0 = 0.25$, is compared with the intrinsic prior in Consonni et al. (2013), that is

$$p^I(\theta|b, t) = \sum_{x=0}^t \text{Beta}(\theta|b+x, b+t-x) \text{Bin}(x|t, \theta_0),$$

Figure 5: Numerical solution for normalized p with $w = 1.5$.

where $b = 1$ and $t = 8$. The intrinsic prior defined above is centered at $w\theta_0 + (1-w)\frac{1}{2}$, where $w = t/(2b+t)$, and has behaviour similar to the one in Figure 5, giving the Intrinsic Bayes Factor in favour of M_1

$$BF_{10}^I = \sum_{x=0}^8 \frac{B(1+x+y, 1+t-x+n-y)}{B(1+x, 1+t-x)\theta_0^y(1-\theta_0)^{n-y}},$$

where $n = 12$. A relatively small sample size allows to better capture differences in the performance of the two priors. Figure 6 shows the posterior probability for M_1 , i.e. $P(M_1|y) = (1 + 1/BF_{10}^I)^{-1}$. The priors yield model probabilities that are similar; in fact in both cases the lowest point is at $\theta = \theta_0$ and, the more θ moves away from θ_0 the higher the posterior probability for M_1 .

6.3 Further properties of the prior

It is important to illustrate how the choices of the constraints $u(0)$ and c impact the prior; in particular, in terms of mean, variance and tail behaviour.

As a general result, if we need to center the prior at a particular θ_0 , we can simply set

$$\begin{aligned} u' &= \sqrt{ce^u - 2(1+u)} & \theta > \theta_0, \\ u' &= -\sqrt{ce^u - 2(1+u)} & \theta < \theta_0. \end{aligned}$$

See Section 6.2.1. In some cases, for example, when nested models are compared, one wishes to have a prior distribution with tails that are as heaviest as it is possible; i.e. suitable for alternative priors. This is achieved by aiming to have a prior for which u' is as small as possible, thus we can set c to the smallest value for which we can solve the equation, which is $c = 2$, if $u(0) < 0$, and $c = 2(1+u(0))e^{-u(0)}$, if $u(0) > 0$.

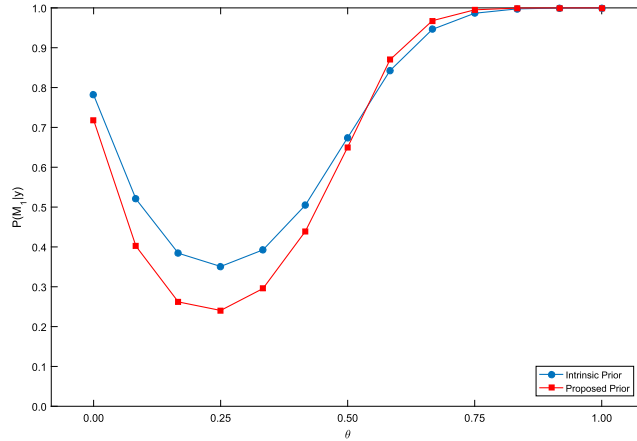


Figure 6: Small sample evidence for the Binomial example. The graph shows the posterior probability for model $f(y|\theta) = \text{Bin}(n = 12, \theta)$ using the proposed prior (squares) and the intrinsic prior (circles).

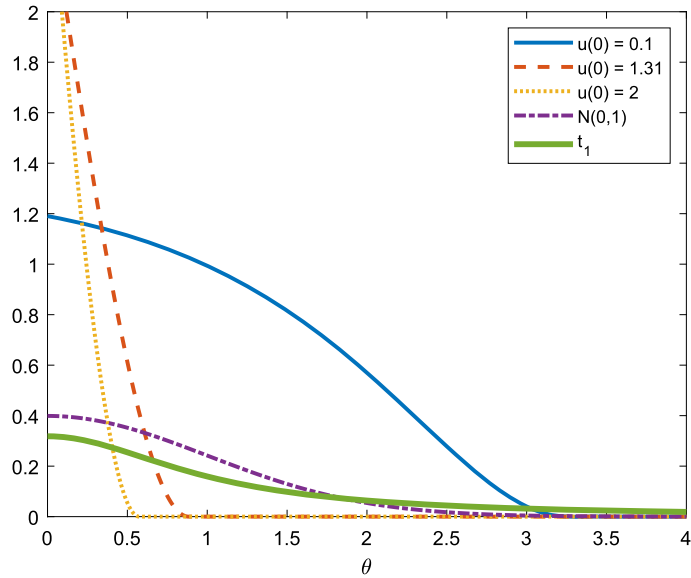


Figure 7: Comparison of the prior tail, with $c = 2$ and different values of $u(0)$, to the standard normal and the Student- t with 1 degree of freedom.

As an illustration, let us consider the case $\Theta = (-\infty, \infty)$, and compare the tail of the prior distribution to the tails of a normal density and a Student- t with 1 degree of freedom. For simplicity, we consider only the positive half of the real line. Figure 7 shows

the comparison of the prior based on scoring rules for $c = 2$ and for $u(0) = (0.1, 1.31, 2)$. When compare to both the standard normal and the Student- t with 1 degree of freedom, the proposed prior appears to have lighter tails for relatively large values of $u(0)$. In particular, the higher the value the quicker the prior drops towards 0. On the other hand, should we select a small value of the initial condition $u(0)$, then the proposed prior has a more gentle decrease to zero.

To understand the effect of the initial conditions on mean and variance of the prior, let us start by considering the case $\Theta = (0, \infty)$. We explore options where both $u(0)$ and c have increasing values; that is,

$$u(0) = (0.01, 0.05, 0.1, 0.5, 1, 1.31, 1.5, 2, 10), \quad c = (2, 2.01, 2.05, 2.1, 2.5, 3, 5, 10, 20, 50).$$

The prior mean and variance are reported in, respectively, Table 1 and Table 2. We see that when the conditions increase, mean and variance of the prior tend to 0. This is in

c	$u(0)$								
	0.01	0.05	0.1	0.5	1	1.31	1.5	2	10
2	3.54	1.82	1.07	0.23	0.09	0.05	0.04	0.02	5.59E-06
2.01	1.63	1.23	0.90	0.23	0.09	0.05	0.04	0.02	5.57E-06
2.05	0.89	0.77	0.64	0.21	0.08	0.05	0.04	0.02	5.51E-06
2.1	0.66	0.58	0.51	0.19	0.08	0.05	0.04	0.02	5.43E-06
2.5	0.27	0.26	0.23	0.12	0.06	0.04	0.03	0.02	4.46E-06
3	0.17	0.16	0.15	0.09	0.04	0.03	0.02	0.01	3.60E-06
5	0.07	0.07	0.06	0.04	0.02	0.02	0.01	0.01	2.34E-06
10	0.03	0.03	0.03	0.02	0.01	0.01	0.01	0.00	1.11E-06
20	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	5.59E-07
50	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00E-07

Table 1: Mean of the prior distribution over $\Theta = (0, \infty)$ for different combinations of $u(0)$ and c .

c	$u(0)$								
	0.01	0.05	0.1	0.5	1	1.31	1.5	2	10
2	0.78	0.99	0.54	0.10	0.03	0.02	0.01	0.00	2.15E-08
2.01	0.88	0.63	0.45	0.10	0.03	0.02	0.01	0.00	2.14E-08
2.05	0.45	0.39	0.32	0.09	0.03	0.01	0.01	0.00	2.10E-08
2.1	0.33	0.29	0.25	0.08	0.03	0.01	0.01	0.00	2.05E-08
2.5	0.12	0.11	0.10	0.04	0.02	0.01	0.01	0.00	1.54E-08
3	0.07	0.06	0.06	0.03	0.01	0.01	0.00	0.00	1.14E-08
5	0.02	0.02	0.02	0.01	0.00	0.00	0.00	0.00	5.83E-09
10	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	2.03E-09
20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.69E-10
50	0.00	0.00	0.00	0.00	0.00	7.77E-05	5.87E-05	2.78E-05	2.07E-10

Table 2: Variance of the prior distribution over $\Theta = (0, \infty)$ for different combinations of $u(0)$ and c .

c	$u(0)$								
	0.01	0.05	0.1	0.5	1	1.31	1.5	2	10
2	10.50	3.44	1.59	0.17	0.04	0.02	0.01	0.01	2.16E-08
2.01	2.93	1.94	1.24	0.16	0.04	0.02	0.01	0.00	2.15E-08
2.05	1.21	0.97	0.75	0.14	0.04	0.02	0.01	0.00	2.10E-08
2.1	0.77	0.65	0.53	0.13	0.03	0.02	0.01	0.00	2.05E-08
2.5	0.21	0.19	0.17	0.06	0.02	0.01	0.01	0.00	1.55E-08
3	0.11	0.10	0.09	0.04	0.01	0.01	0.01	0.00	1.14E-08
5	0.03	0.03	0.02	0.01	0.01	0.00	0.00	0.00	5.84E-09
10	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	2.03E-09
20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.70E-10
50	0.00	0.00	0.00	0.00	0.00	8.07E-05	6.08E-05	2.85E-05	2.07E-10

Table 3: Variance of the prior distribution over $\Theta = (-\infty, \infty)$ for different combinations of $u(0)$ and c .

line with the tail behaviour discussed above, where the larger the value chosen for $u(0)$, the faster the prior drops to 0.

For the case $\Theta = (-\infty, \infty)$ we have chosen to center the prior at zero; although other values are easily attainable yielding similar results. Again, the prior variance (Table 3) decreases as we set the initial conditions to increasingly large values.

A final application of the proposed prior is for a Poisson regression model. The example is presented in Appendix C of the Supplementary Material, where we have worked with simulated data as well as real data. One objective of the simulation study is to show the robustness of the prior when nuisance covariates are added in the regression model; in fact, it can be seen that there is no noticeable impact on the size of the posterior credible intervals.

7 Discussion

In this paper we have introduced a new class of objective priors derived from scoring rules. A remarkable aspect is that we have been able to show that the same result can be achieved via the rigour of calculus of variations, by finding objective priors which solve the Euler–Lagrange equation for finding extremum to integrals of the type

$$\int L(\theta, p, p') d\theta.$$

If we can establish suitable choices of $L(\theta, p, p')$ which can be motivated and satisfy conditions for the existence of extremum, then new classes of objective prior can be sought. The case we have considered, which we can consider as a first step, is to use a combination of two well known measures of information in a prior density function; i.e.

$$L(\theta, p, p') = \frac{1}{2} \frac{p'(\theta)^2}{p(\theta)} + p(\theta) \log p(\theta).$$

The objective priors here defined have two desirable properties. The first is that they are somewhat detached from the choice of the sampling distribution and are dependent on the parameter space only. In other words, the information required to derive the prior is limited to the range of values that the quantity of interest can take.

The second property is that the prior can be proper. Besides the advantage of not having to check properness of the posterior, it allows to exploit the prior in scenarios where improper objective priors have been challenging. For example, as illustrated in Section 6.1, the proposed prior is used to estimate the means of a mixture of normal densities with three components. Another potential application, discussed in Section 6.2, is in model selection. In particular, the objective prior may be used to represent minimal information on the parameters that are not common to two models. In fact, the Bayes factor used to compare two models is, in general, sensitive to the proportionality constant of improper priors. While for common parameters the constant will cancel out, this is not the case if the parameter is either at the numerator or at the denominator of the ratio only. Hence, the necessity of having a proper prior assigned to this kind of parameters.

The simulation study, aimed to compare the frequentist performances of the proposed prior with the ones of the Jeffreys prior, has shown no appreciable differences, with the exception of a slightly larger Mean Squared Error (MSE) for the proposed prior; the last result is expected as it is a consequence of the smaller information used to define the proposed prior in comparison with any model based objective prior.

Future and ongoing work involves using the Fisher information alone; i.e. to minimize $\int (p')^2/p dp$ subject to p having certain constraints; for example, a zero mean or a specified variance or being log-concave. The mathematical results here would be able to provide explicit solutions including a class of non-local prior distributions (Johnson and Rossell, 2010).

Supplementary Material

On a Class of Objective Priors from Scoring Rules. Supplementary Material (DOI: [10.1214/19-BA1187SUPP](https://doi.org/10.1214/19-BA1187SUPP); .pdf). Supplement to “On a Class of Objective Priors from Scoring Rules”. The supplementary material contains the Appendixes A, B, C and D of the paper.

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Invited Discussion

Dimitris Fouskakis*

This is an interesting paper introducing a new class of objective priors, derived from scoring rules. The authors do a nice job and show that the same result can be achieved via the rigour of calculus of variations. The new defined objective priors are: (a) detached from the choice of the sampling distribution and depend only on the parameter space; (b) can be proper. Leisen, Villa & Walker measure the quality of the prior with a proper scoring function and require it to be constant; by this way they are no parts of the parameter space Θ that are “preferred”, and thus the prior is objective. Focus is given in the uniqueness and invariance of the defined priors and illustrations include the application of the proposed method in mixture models and model comparison via Bayes factor problems.

My comments below are focused on the model selection problem. The main reason for this choice is that the objective Bayes methodology for priors tailored to model selection started more recently, and its development and applications to various models have increased over the last few years; see for example Consonni et al. (2018). With my discussion below I wish to add further insights to the paper resulting in future work in the area.

Bayes factor derivation In Section 6.2 the authors consider a simple (nested) model comparison problem. The proposed prior is then compared with the intrinsic prior in Consonni et al. (2013). I would love to see some discussion on the derivation of the final Bayes factor, since the marginal likelihood is not analytical available. Is it easy, in general, to use the proposed methodology in more complicated model selection problems?

Variable selection problem One of the most common applications of model comparison is the variable selection problem for normal linear regression, as well as, generalized linear models. A variety of approaches have been proposed, such as the g -prior and its extensions (Liang et al., 2008), the robust prior (Bayarri et al., 2012), the PEP prior (Fouskakis et al., 2015, 2018) the benchmark prior (Ley and Steel, 2012) and many others (Consonni et al., 2018). Most of the priors used for variable selection problems belong to the class of “Confluent Hypergeometric Information Criterion” g -priors introduced by Li and Clyde (2018).

Furthermore, when the number of models under comparison is small, the problem can be replaced with an estimation one that focuses on the probability weight of a given model within a mixture model (Kamary et al., 2018). Using this approach, the methodology described in Section 6.1 can be applied here as well.

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To conclude with, I believe that it would be great to see an application of the proposed methodology in such problems and compare the performance of the proposed method with that of the “most established” Bayesian variable selection techniques.

Desiderata Bayarri et al. (2012) developed criteria (desiderata) to be satisfied by objective prior distributions for Bayesian model choice. A number of these criteria are applicable only in nested model comparisons. Predictive matching in particular is viewed as the most crucial aspect for objective model selection priors. Informally it says that, with a minimal sample size, one should not be able to discriminate between two models, so that the Bayes factor should be close to one, for all samples of minimal size.

I would love to see some work on this direction; i.e. check if these criteria are satisfied for the proposed prior. In Bayarri et al. (2012), first criteria meaningful for priors tailored to objective model selection were set out, and then priors satisfying them were derived. The authors could proceed in a similar manner here as well, and select constants resulting to priors that satisfying these criteria.

Selection of the constants of integration Returning back to the previous point, how the selection of the constants of integration affects the shape and the theoretical properties of the prior? Selection of different constants, results to local or non-local priors, proper or improper, with light or heavy tails. In Section 6.3 the authors illustrate how the choices of the constants impact the prior, but mostly their work is based on illustrations rather than theoretical properties. In addition, the authors are doing a great job in Section 5, by considering three common parameter spaces in unidimensional case and one in the multidimensional case, and defining a solution; but it still seems to me that the selection of the constants is a bit ad hoc. It would be nice to get a fully automatic approach, depending on the problem that the researcher faces, based on theoretical properties.

Type of prior The group invariance criterion in Bayarri et al. (2012) can be understood as a formalization of Jeffreys’ criterion for comparing nested models. This says that the prior for the specific parameter of the larger model (the alternative hypothesis) should be “centered at the simplest model”. In practice this has been implemented by assigning a continuous prior having mode at the parameter value specified by the null model, resulting to the local priors. On the other hand, Johnson and Rossell (2010) proposed the use of non-local priors in order to improve convergence rates in favor of the true null hypothesis. As mentioned above, on a previous point, it seems to me that by changing the values of the constants, the resulting priors could belong to either of these broad categories. If this is the case, would be nice to compare the non-local priors resulting by this approach with the ones that Johnson and Rossell (2010) use, under specific cases.

Model misspecification Does model misspecification affect the selection of the true model, under the proposed prior, or since the prior is detached from the choice of the sampling distribution this problem does not arise? The problem has been explored in various papers recently; see for example Rossell and Rubio (2018), and I suggest exploring this avenue.

Diffuse priors Focusing again on nested model selection problems, it is well known that if proper prior distributions with large variances are used, the resulting Bayes factors can be highly sensitive to the chosen prior variances (Bartlett, 1957). Is this the case when using particular values of the constants?

High-dimensional models Current applications of statistical methods often deal with high-dimensional models, wherein the derivation of an objective prior, defined according to a well established formal rule, like Jeffreys' or reference prior, is virtually impossible. Also in regression settings common default priors are not defined when the number of predictors p is larger than the sample size n . More generally, high-dimensional problems pose new challenges that need be addressed through novel methodologies; such as sparsity and shrinkage. These two "ideas", though distinct, are closely related as we seek for priors that do shrink strongly on noise components. On the other hand, strong signals should be clearly picked-up, and model estimates of the corresponding parameters should undergo negligible shrinkage.

How possible is to apply the proposed methodology in high-dimensional models? How the selection of the constants of integration affects the degree of shrinkage? Would be great if the authors, in a future work, explore this avenue.

Conclusion I would like to thank the authors for a thought-provoking paper on an important issue. The paper is a useful addition to the literature of objective priors. I thank also the Editor for inviting me to contribute to the discussion. All my comments above are basically associated with model selection problems, where the derivation of objective priors is a more challenging task. As a final note, will be also great if the authors create a GitHub or an Rpubs in order to share their code, to improve the visibility of the paper, and to allow reproducibility of the results. Even better, as part of a future work, an R package with an ever-increasing set of case studies and automatic tools of choosing the constants for practitioners with limited Statistics training would be great.

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Contributed Discussion

Matteo Iacopini^{*§}, Francesco Ravazzolo[†], and Luca Rossini[‡]

We have greatly appreciated the work by Leisen, Villa and Walker, who have proposed a novel method for constructing objective prior distributions which circumvents the need to specify a statistical model and relies solely on a specific proper scoring rule.

Scoring rules are of tantamount importance in practical statistical analysis, since they encode the preferences of the stakeholder (e.g., a policymaker). In fact, since scoring rules provide a simple mean to assess the performance of a set of statistical models with respect to a specific user-defined goal, they have been widely used as a tool for evaluation, comparison and ranking of competing statistical models.

Recently, Iacopini et al. (2020) proposed the asymmetric continuous probabilistic score (ACPS), a new proper scoring rule for evaluating density forecasts according to asymmetric preferences of the stakeholder. Being the ACPS a proper scoring rule, the methodology developed by the Authors can be directly applied to derive a class of objective prior distributions. Moreover, since ACPS has one free parameter specifying the type and degree of asymmetric preferences, the ensuing class of priors would inherit this degree of freedom. Intuitively, its role would be analogous to that of the free constants, c and $u(0)$, in Section 3 of the discussed Article.

To obtain the class of objective priors stemming from the ACPS proper scoring rule, first recall its definition. Let $P : \mathcal{D} \rightarrow [0, 1]$ be a cumulative distribution function, with $\mathcal{D} \subseteq \mathbb{R}$, let $y \in \mathcal{D}$, and denote with $c \in (0, 1)$ the asymmetry parameter. Then

$$\begin{aligned} ACPS(P, y; c) &= \int_{-\infty}^y (c^2 - P(u)^2) f(P, c) du + \int_y^{+\infty} ((1-c)^2 - (1-P(u))^2) f(P, c) du \\ &= \int_{\mathbb{R}} \left[(c^2 - P(u)^2) \mathbb{I}(u < y) + ((1-c)^2 - (1-P(u))^2) \mathbb{I}(u > y) \right] f(P, c) du, \end{aligned}$$

where $f(P, c) = \mathbb{I}(P(u) > c)/(1-c)^2 + \mathbb{I}(P(u) \leq c)/c^2$. Therefore, solving for P the equation $ACPS(P, y; c) = k$, with $k \in \mathbb{R}$, would be equivalent to solve the minimization problem

$$\min_P \left| \int_{\mathbb{R}} L(u, P, P') du - k \right|, \quad (1)$$

where $L(u, P, P') = [(c^2 - P(u)^2) \mathbb{I}(u < y) + ((1-c)^2 - (1-P(u))^2) \mathbb{I}(u > y)] f(P, c)$. This minimization problem can be reconciled to a standard calculus of variations problem, as follows. First, one can obtain an approximation by substituting \mathbb{R} with a bounded

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region $(a, b) \subset \mathbb{R}$. Second, the absolute value can be removed by a suitable choice of the constant k . Since the equality $ACPS(P, y; c) = k$ can be satisfied for any arbitrary choice of $k \in \mathbb{R}$, and $ACPS(P, y; c) < +\infty$, then there exists $k^* \in \mathbb{R}$ such that $ACPS(P, y; c) - k^* > 0$. Therefore, by choosing $k = k^*$ one gets

$$ACPS(P, y; c) = k^*, \quad \text{where} \quad |ACPS(P, y; c) - k^*| = ACPS(P, y; c) - k^* > 0.$$

Putting all together one gets the following minimization problem

$$\min_P \left\{ ACPS(P, y; c) - k^* \right\} \equiv \min_P \left\{ \int_a^b L(u, P, P') \, du - k^* \right\}. \quad (2)$$

Finally, since k^* is constant, the optimum is $P^* = k^* + P^{**}$, where P^{**} is the solution of the problem

$$\min_P \int_a^b L(u, P, P') \, du,$$

for which the corresponding Euler-Lagrange equation is

$$\frac{\partial L}{\partial P} = 0.$$

Therefore, solving the minimization problem (2) yields a class of cumulative distribution functions, P^* , which depends on two free parameters: (i) the asymmetry parameter of the ACPS, c , and (ii) the constant of integration, \bar{c} .

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Contributed Discussion

F. J. Rubio* and M. F. J. Steel†

We congratulate the authors on a very interesting and thought-provoking paper. We welcome the exploration of novel ideas for producing priors using formal rules. Our comments relate to: (i) the principle for constructing the proposed priors and the role of the parameterisation; (ii) the use of the proposed priors for hypothesis testing.

On the principle

In order to make the proposed principle operational, it is necessary to select the values w , c and $u(0)$. The authors provide some guidelines on how these values could be selected, but the precise mapping between the choice of these values and the properties of the resulting prior distribution still seems to be a partly open question.

The choice of these values is crucial for determining the properties of the prior. For instance, for the prior with support on $(0, \infty)$ presented in the paper, the solution for $u(\theta)$ grows very rapidly after a threshold that depends on the values of w , c and $u(0)$. This implies that the prior density decreases at a very fast rate after this point, seemingly super-exponentially fast, making it virtually zero beyond such a threshold. Thus, the prior is close to a truncated prior and then it is clear that things like (arbitrary) choices of scaling or parameterisation will have a substantial effect on the outcome. For example, consider a simple scenario where we wish to estimate the variance $\sigma^2 = 0.25$ in the model $X_i \sim N(0, \sigma^2)$, $i = 1, \dots, 750$, using the proposed prior (with the choices recommended in the paper, see their Figure 3(a)). Figure 1(a) shows the posterior distribution obtained with a Markov Chain Monte Carlo (MCMC) sample of size 5,000. If we specify, say, a $\text{gamma}(0.01, 0.01)$ prior on σ^2 we get a similar result with the posterior concentrated around the true value. In contrast, suppose that now we are interested in estimating the precision $\tau = 1/\sigma^2 = 4$ using the same prior but now on τ . In order to implement the proposed prior for τ , we need to solve for $u(\tau)$ in a region where it grows at a fast rate, so we have discretised the prior on a grid of values of τ and obtained a numerical solution in Mathematica on that grid (R leads to numerical problems). Figure 1(b) shows the corresponding posterior, which is concentrated far from the true value of the parameter as the vanishingly thin tail of the prior dominates the posterior distribution. In contrast, Figure 1(c) shows the posterior distribution of τ obtained with a $\text{gamma}(0.01, 0.01)$ prior on τ , which is a $\text{gamma}(375.01, (1/2) \sum_{i=1}^{750} x_i^2 + 0.01)$, now concentrated around the true value of the parameter. In view of the sample size, any other prior with a tail that is not decreasing (much) faster than exponential would give a similar reasonable answer.

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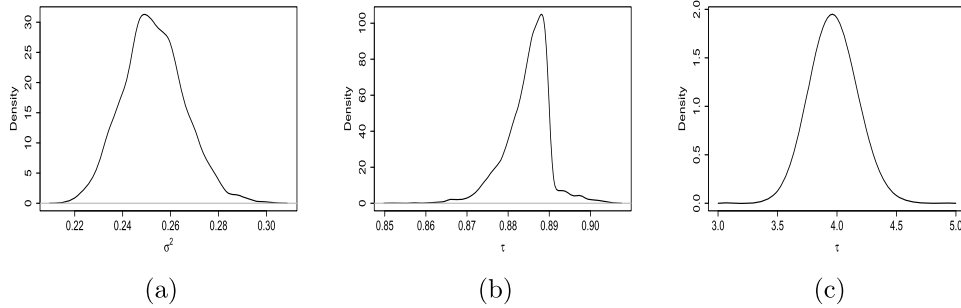


Figure 1: $X_i \sim N(0, \sigma^2)$. Posterior distribution of: (a) σ^2 using the proposed prior on σ^2 ; (b) $\tau = \sigma^{-2}$ using the proposed prior on τ ; (c) τ using a $\text{gamma}(0.01, 0.01)$ prior on τ .

The aforementioned points seem to be effects induced by the addition of the Hyvärinen scoring rule, but the gain in terms of the frequentist and Bayesian performance remains unclear. The adoption of this particular rule induces the extremely thin tails which is, for many practical purposes, akin to a prior truncation and this flies in the face of the usual “folklore” that objective priors should rather err on the side of heavy tails to avoid excluding potentially important parts of the parameter space. Heavy-tailed priors tend to induce better frequentist performance of the posterior distribution, which is a desirable property for objective priors.

In our view, the interpretation of the parameters plays a crucial role in the specification of a prior distribution. Although the initial formulation of the proposed prior is not connected with the model, the need for specifying additional properties (such as shape) leaves a choice to the user. Specifying the additional ingredients in the proposed rule to produce priors for these parameters would require some analysis of their role, thus re-establishing the connection with the model at a more subjective level. The effect of the role of the parameters may be more noticeable for parameters taking values on the same parameter space but with completely different roles, such as a scale parameter and the degrees of freedom of the Student- t distribution.

Inference versus testing

For practically important situations such as mixture models or Bayesian variable selection it is typically difficult to use automatic principles. It often seems more useful to adopt a bespoke prior framework, which is not borne out of a principle, but reflects the question one wants to address. For example, non-local priors (Johnson and Rossell, 2010) aim to control the convergence rate of the Bayes factor. We would be interested to see how we could achieve such properties using the proposed principle (as suggested in Section 7), but we expect that the priors for testing presented in the paper could have a large impact on the results due to their local nature and extremely light tails.

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Contributed Discussion

F. Llorente^{*}, L. Martino[†], and D. Delgado-Gómez[‡]

In (Leisen et al., 2018), the authors introduce a novel approach for building objective prior densities $p(\theta)$ based on proper score rules. Here we discuss some issues regarding the fact that $p(\theta)$ can only be evaluated up to a normalizing constant, and the application for model selection purposes. We also provide an additional comparison (and the corresponding code) with the intrinsic Bayes factor approach, extending the numerical experiment in Appendix E of the Supplementary Material, provided by (Leisen et al., 2018).

Introduction

We would like to congratulate the authors in (Leisen et al., 2018) for this contribution on devising objective prior densities, as we believe it will further encourage the use of the Bayesian formalism when there is little, or any, *a priori* knowledge of the parameter of interest. Only the knowledge of support domain Θ is required for the construction, hence they are “more” objective than other popular model-based approaches. To derive the objective priors, in the form of $p(\theta) \propto e^{-u(\theta)}$, the authors rely on proper score rules, which defines a second order differential equation for $p(\theta)$. Interestingly, the authors also show that the same differential equation can be obtained by minimizing the sum of entropy and Fisher information. The solution is not a unique prior density but a class of prior distributions, where some parameters can be set by the practitioner. For instance, the resulting priors can be forced to be proper. This is very useful in contexts where other objective priors are problematic, e.g., model selection via Bayes factors.

Analysis of the proposed approach

Although we believe the class of objective priors that result from this work are really useful, below we remark some critical points and suggest some possible solutions. The proposed prior densities $p(\theta) \propto e^{-u(\theta)}$ cannot be analytically obtained, but they are implicitly determined by an equation relating $u(\theta)$ and its derivative $u'(\theta)$. The authors use a Taylor expansion to evaluate $u(\theta+\epsilon)$ provided that $u(\theta)$ is known. Thus, the evaluation of $p \propto e^{-u}$ is only approximate (even if additional terms in the Taylor expansion can be included in order to increase the precision). Furthermore, the normalizing constants of the priors $p(\theta) \propto e^{-u(\theta)}$ are also unknown. These normalizing constants are not needed in the Markov chain Monte Carlo (MCMC) scheme given in Appendix A of the Supplementary Material, but it is required for the computation of Bayes factors. To solve this issue, one possibility is to modify this MCMC algorithm in order to sample from $p(\theta)$ and then use *reverse importance sampling* (RIS) (Llorente et al., 2020, Section 3). Namely,

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we first obtain a sample $\theta^{(1)}, \dots, \theta^{(T)}$ from the prior $p(\theta)$ using a modification of the MCMC algorithm from Appendix A, where the acceptance probability is replaced by

$$\alpha = \min \left\{ 1, e^{-[u(\theta') - u(\theta^{(t)})]} \frac{q(\theta^{(t)}|\theta')}{q(\theta'|\theta^{(t)})} \right\}. \quad (1)$$

Then, using an auxiliary density $\varphi(\theta)$ defined on Θ , we compute

$$\hat{c} = \left(\frac{1}{T} \sum_{t=1}^T \frac{\varphi(\theta^{(t)})}{e^{-u(\theta^{(t)})}} \right)^{-1}, \quad (2)$$

which is a consistent estimator of $\int_{\Theta} e^{-u(\theta)} d\theta$. The auxiliary density $\varphi(\theta)$ should have lighter tails than the prior $p(\theta)$ to avoid the infinite variance problem (as often occurs with the harmonic mean estimator). See the theoretical example in Section 7.1 of (Llorente et al., 2020). Since the evaluation of $p(\theta)$ is approximate, note also that the resulting MCMC algorithms fall within the noisy MCMC framework (Alquier et al., 2016; Andrieu and Roberts, 2009).

Comparison with partial and intrinsic Bayes factors

Consider the example from Appendix E of the Supplementary Material. The goal is to compare two models by means of the Bayes factor, namely $M_1 = \{f_1(x|\theta) = \theta^x e^{-\theta}/x!, p_1(\theta)\}$ and $M_2 = \{f_2(x|\phi) = \phi(1-\phi)^x, p_2(\phi)\}$, when independent data $\mathbf{x} = (x_1, \dots, x_n)$ are generated from each of them. The authors used a uniform prior $p_2(\phi) = 1$, $\phi \in (0, 1)$, and their proposed prior for $p_1(\theta)$. Hence, the Bayes factor BF_{12} is well defined since $p_1(\theta)$ is proper. Note that the unknown normalizing constant of $p_1(\theta)$ needs to be approximated in order to compute BF_{12} . Tables 7 and 8 in the Supplementary Material give the results obtained for $n = 30$ and $n = 100$, showing the good performance in the detection of true model using the proposed objective prior $p_1(\theta)$.

Here, we aim to replicate Tables 7 and 8 using another uniform prior $p_{1,u}(\theta) \propto 1$, $\theta \in (0, \infty)$ for model M_1 instead, i.e. an improper prior. In this situation, the Bayes factor is not well-defined due to the arbitrary constant in $p_{1,u}(\theta)$. Hence, we need to resort to *partial* Bayes factors (O'Hagan, 1995, Sect. 2), where we compute the posterior of a single observation x_i (training set) under prior $p_{1,u}(\theta)$, i.e., $p_1(\theta|x_i) \propto f_1(x_i|\theta)p_{1,u}(\theta)$, and use $p_1(\theta|x_i)$ now as a proper prior in the computation of BF_{12} . In order to avoid the dependence on the training sample, we use the idea in (Berger and Pericchi, 1996), called *intrinsic* Bayes factors, that consists in averaging over all possible training samples, resulting in the following intrinsic Bayes factor

$$IBF_{12} = \frac{1}{n} \sum_{i=1}^n \frac{\int_0^\infty f_1(\mathbf{x}_{-i}|\theta) p_1(\theta|x_i) d\theta}{\int_0^1 f_2(\mathbf{x}|\phi) d\phi} = \frac{1}{n} \sum_{i=1}^n \frac{\int_0^\infty f_1(\mathbf{x}|\theta) d\theta / \int_0^\infty f_1(x_i|\theta) d\theta}{\int_0^1 f_2(\mathbf{x}|\phi) d\phi}. \quad (3)$$

Note that the cost of computing IBF_{12} increases with n . We compute IBF_{12} in 100 different runs for several true values of θ and ϕ , and we show the results in Table 1 and Table 2 for $n = 30$ and $n = 100$, respectively.¹ The results clearly show that the

¹The Matlab code is available at http://www.lucamartino.altervista.org/Code_Llorente-CommentLeisen.m.

uniform prior on θ allows for correctly selecting M_1 when it is indeed the true model, with very few exceptions as also obtained in the paper. However, when M_2 is the true model, the use of such improper prior makes probable selecting M_1 as the most likely model, as proves the 43 exceptions obtained when $\phi = 0.8$ and $n = 100$, that is, almost half of the time we would wrongly select M_1 over M_2 . This also shows the benefit of the objective priors proposed in (Leisen et al., 2018).

True model = M_1				True model = M_2			
θ	min	max	Exceptions	ϕ	min	max	Exceptions
5	6.28×10^3	3.95×10^{11}	0	0.5	5.45×10^{-9}	884.25	30
2	0.55	7.40×10^6	1	0.2	1.61×10^{-26}	9.76	2
				0.8	0.004	10.51	66

Table 1: Model comparison for $n = 30$. Minimum and maximum IBF_{12} under true model M_1 (Poisson) and M_2 (Geometric) for 100 simulations.

True model = M_1				True model = M_2			
θ	min	max	Exceptions	ϕ	min	max	Exceptions
5	2.38×10^{11}	4.52×10^{29}	0	0.5	1.98×10^{-13}	500.52	4
2	2.22×10^3	2.60×10^{14}	0	0.2	2.02×10^{-72}	3.34×10^{-18}	0
				0.8	0.003	6.69	43

Table 2: Model comparison for $n = 100$. Minimum and maximum IBF_{12} under true model M_1 (Poisson) and M_2 (Geometric) for 100 simulations.

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Invited Discussion

Guido Consonni^{*,†} and Gonzalo García-Donato^{†,‡,§}

1 General aspects

This paper is a welcome addition to the research on objective Bayes (OB) methods. The Authors (A's) summarize their main motivations under two main headings:

1) current methodology for building OB priors is predicated on the statistical model; as models grow in complexity, so does the difficulty in obtaining OB priors. A related issue is model misspecification which would naturally propagate to OB priors;

2) OB priors are often improper. This is seen by the A's as a serious concern, because of a host of difficulties. In particular assessing posterior properness becomes onerous in complex models; also improper priors cannot be used (in general) for model comparison *via* Bayes Factor due to their dependence on arbitrary normalizing constants.

Because of 1 and 2 the A's set out their program as finding OB priors which only depend on the parameter space, thus severing the connection with the model. This is a major departure from more traditional principles to formalize ignorance such as *context invariance* (Dawid, 2006) which states that only the formal structure of the distributional model of the observables should matter when specifying the prior (model-dependent priors).

The content of this discussion is as follows. In Section 1 we examine some structural aspects of the criterion proposed to define an objective prior. In Section 2 we assess a prior employed by the A's in their paper from the point of view of testing. Specifically we consider two scenarios: i) testing normality *versus* Cauchy errors in a problem with several means (a non-nested setup); ii) testing a sharp null hypothesis against an unrestricted alternative on the mean of a normal model with unknown variance (a nested setup).

The broad conclusion we reach is that the method is too general as it stands to provide useful guidelines especially in applied work. We also believe that the structure of the statistical model cannot be easily dispensed with when constructing an objective prior, and that its neglect may generate undesirable features especially in a testing scenario.

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1.1 Is the constant scoring rule criterion too weak?

The A's proposal starts with a specific proper *scoring rule*, which measures the quality of a quoted probability density p for the parameter $\theta \in \Theta$; next they look for those p 's such that the score is *constant* over Θ . The intuition is that if the score were not constant, then some parts of the parameter space would be given preferences over the remaining ones, thus violating noninformativity and objectivity.

It turns out that the solution to the above program is a whole *class* of priors (which always includes the *uniform* prior, irrespective of the nature of the parameter space, e.g. the real line, half the real line, or a bounded interval). The A's see this as an advantage, in that it adds flexibility to their method. They write (Section 5): "... given a particular problem, the objective prior over a given parameter space could be proper or improper; differentiable everywhere or not; convex; log-concave; etc. In other words, a prior can be objective and exhibit desirable features of choice without impinging on subjective components relating to information". While the above quotation encourages optimism, from a pragmatic viewpoint it is troublesome because it requires supplementing the basic criterion, based solely on a scoring rule, with additional specifications. The latter appear a critical aspect of the method, and the illustrations provided in Section 5 (A's paper) are paradigmatic.

For the case $\Theta = (0, 1)$, a possible specification is to set $p(0) = p(1) = 0$ with additionally symmetry leading to a concave function. On the other hand, it is also possible to obtain a distribution which mimics Jeffreys prior, i.e. convex and unbounded in the neighborhood of 0 and 1. Unfortunately no guidelines are available to set up these additional features, especially from an objective viewpoint. Another concern is that the resulting prior seems somewhat sensitive to numerical specifications of the base function $u(\cdot)$ at some specific points; see plot (a) and (b) in Figure 2 (A's paper) where the former holds for $u(1/2) = 1.1$ and the latter for $u(1/2) = 1.14$. It is hard to believe that one might sensibly distinguish between values of a prior density at a single point with such a high level of precision.

As another illustration the A's consider the case $\Theta = (0, \infty)$ where they require a specific shape property (convex and decreasing), the reason being that "this property is common to most objective priors on $(0, \infty)$ ". What they fail to add however is that this property usually stems from considerations involving the model, as in the Jeffreys' prior. While this is admittedly a mere illustration of their methodology, it reflects the pragmatic problem of specifying sensible additional features which are not model-dependent.

1.2 Does invariance matter?

The method proposed by the A's is not invariant to re-parametrizations. Yet they contend that this is not an issue because, for any given model, one usually works with a specific parameter throughout the analysis. However we remark that often the choice of a parametrization is conventional, as in the example they quote, namely a normal model parametrized either by the variance or the precision. An important point about invariance to re-parametrization is that the prior and posterior predictive of the observ-

ables will be unchanged whatever the parametrization; this desirable feature is lost if a method produces priors which are not probabilistically equivalent.

The A's concede that if invariance is a concern, then one can always transform by change of variable the prior obtained under one parametrization. However this begs the question of where to start from. The whole idea of invariance is that it does not matter which parameter we start with because the analysis will be equivalent in the end. In this context, they consider the natural exponential family with canonical parameter θ . Because of the special status enjoyed by θ , one could apply the method to θ , and then induce the resulting prior onto any other parameter ϕ say. However if θ is a canonical parameter, so is any affine transformation of θ ; so their method should be at least invariant to affine transformation. Is this the case? (In the paper the A's state that their method is invariant to location transformations).

2 Priors for testing

How do priors based on scoring rules (SR-priors) behave in a problem involving hypothesis testing? In this section we assess a proper SR-prior on the real line presented by the A's in two testing scenarios.

2.1 Priors for common parameters

Example 1 We consider a measurement-error model applied to k populations with unknown distinct means. For each population n independent replicates are available. Errors can be either normal or Cauchy (t_1). Specifically

$$x_{ij} = \mu_i + \varepsilon_{ij}, \quad i = 1, \dots, k, \quad j = 1, \dots, n,$$

and the testing problem is $H_0 : \varepsilon_{ij} \stackrel{iid}{\sim} N(0, 1)$ versus $H_1 : \varepsilon_{ij} \stackrel{iid}{\sim} t_1$. Notice that the unknown k -dimensional parameter $\boldsymbol{\mu} = (\mu_1, \dots, \mu_k)$ appears in both competing models, and can be regarded as a common parameter. To compute the Bayes factor of H_1 to H_0 , priors are required, and we denote them with $\pi_0(\boldsymbol{\mu})$ (under H_0) and $\pi_1(\boldsymbol{\mu})$ (under H_1). If $\pi^{SR}(\mu_i)$ denotes an objective prior based on the scoring-rule methodology for $\mu_i \in R$, a prior for the vector $\boldsymbol{\mu}$ can be constructed as

$$\pi_0^{SR}(\boldsymbol{\mu}) = \pi_1^{SR}(\boldsymbol{\mu}) = \prod_{i=1}^k \pi^{SR}(\mu_i). \quad (2.1)$$

Specifically we take π^{SR} to be the proper prior presented by the A's in Figure 3b of their paper. Notice that it is unimodal with the mode at zero.

To assess both priors, we apply the criterion of predictive matching introduced by Jeffreys (1961), and subsequently revisited by Bayarri et al. (2012). Informally it states that, for samples of minimal size, one should not be able to clearly discriminate between two models –the Bayes factor should be close to one–. In this Example, a minimal sample size is $n = 1$, that is one observation per group. Accordingly we write such minimal

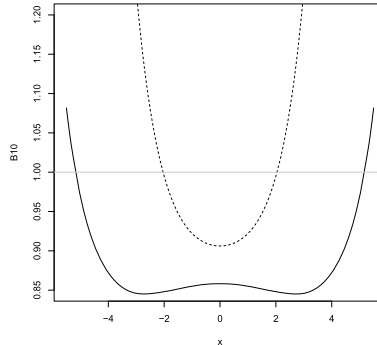


Figure 1: Example 1: Bayes factor \mathcal{B}^{SR} under SR-prior (solid line) and under $N(0,1)$ prior (dashed line).

sample as $\mathbf{x}^* = (x_{11}^*, x_{21}^*, \dots, x_{k1}^*)$. The Bayes factor associated to \mathbf{x}^* and the priors in (2.1) is

$$B_{10}^{SR}(\mathbf{x}^*) = \prod_{i=1}^k \mathcal{B}^{SR}(x_{i1}^*).$$

A plot of $\mathcal{B}^{SR}(x)$ is presented in Figure 1. For values of $|x| \leq 5$, $\mathcal{B}^{SR}(x)$ ranges in $[0.85, 1.05]$. This implies that violation of the predictive matching criterion could be large even for a moderate number of populations. For instance, if $k = 4$ and x_{i1}^* 's are small then $B_{10}^{SR}(\mathbf{x}^*) \approx 0.85^4 \approx 0.44$. We experienced computational problems when trying to study the behavior of \mathcal{B}^{SR} when the x_{i1} 's are large, because of the implicit definition of the SR prior. While this remains an open question, our conjecture is that $\mathcal{B}^{SR}(x)$ will grow to infinity as $|x|$ grows given the different nature of the tails of the t_1 and $N(0,1)$, similarly to what happens with other proper priors like the standard normal (see dashed line in Figure 1).

On the other hand, it can be easily seen that the Bayes factor associated with the improper priors $\pi_0(\boldsymbol{\mu}) = \pi_1(\boldsymbol{\mu}) = 1$ is always unitary (independently of \mathbf{x}^*), so that they satisfy predictive matching. (Notice that the arbitrary constant inherent in the improper priors cancels out when taking ratios). An additional argument in favor of these priors connects with the family of intrinsic Bayes factors proposed by Berger and Pericchi (1996). It is a remarkable fact that if $\pi_0(\boldsymbol{\mu}) = \pi_1(\boldsymbol{\mu}) = 1$ then *all* intrinsic Bayes factors coincide and are equal to one.

In conclusion the SR-prior used by the A's in Figure 3 of their paper fails to achieve predictive matching between two models involving several common location parameters. On the other hand the standard flat improper priors achieve this goal, and the computational effort is trivial. Of course it could be argued that flat priors on the real line are also SR-priors. The issue however remains: how to decide on this choice which looks optimal in this case? Predictive matching cannot be invoked as a property to be satisfied because it involves the statistical model, thus undermining the premises set out by the A's.

2.2 Nested models

The assignment of an objective prior for a multidimensional parameter is treated only briefly in the paper. However, possibly to alleviate the burden of the computation of the SR-prior, the assumption of independence of the parameter components seems like a natural choice in their approach; see for instance the preamble of Section 5. On the other hand Section 5.2 suggests to take marginal SR-priors as inputs for the construction of the overall prior. In this subsection we discuss objective priors for vectors of parameters in the context of testing in view of assessing whether independence of the components is in general a sensible choice.

Consider the classic example of testing the mean of a normal model with unknown variance.

Example 2. Let $x_i \sim N(\mu, \sigma^2)$, independently for $i = 1, \dots, n$, and consider the testing problem $H_0 : \mu = 0$ versus $H_1 : \mu \neq 0$. Objective priors $\pi_0(\sigma)$ and $\pi_1(\mu, \sigma)$ have to be specified.

Since we want to investigate the impact of assuming independence *a priori* between (μ, σ) , we take the SR-prior to be $\pi_1^{SR}(\mu, \sigma) = \pi_1^{SR}(\mu)\pi_1(\sigma)$, where for concreteness the SR prior for $\mu \in (-\infty, \infty)$ is the proper prior we employed in the previous subsection. For the marginal priors on the common parameter σ we use for both models the standard objective prior $\pi(\sigma) = \sigma^{-1}$. This is done for simplicity and should not affect the take-home message of this example.

The Bayes factor can be expressed as the univariate integral

$$B_{10}^{SR}(\bar{x}, S) = \int \left(\frac{\bar{x}^2 + S^2}{(\bar{x} - \mu)^2 + S^2} \right)^{n/2} \pi^{SR}(\mu) d\mu,$$

(where \bar{x} and S^2 are the sample mean and sample variance). It can be shown that the minimal training sample associated with these priors is $n = 2$. We have represented, in Figure 2 (left panel) B_{10}^{SR} as a function of \bar{x} , and for $n = 2$ and a few values of S . Because of symmetry, the plot is presented only for $\bar{x} \geq 0$. We immediately conclude that $\pi_1^{SR}(\mu, \sigma)$ is not predictive matching. Nevertheless, one could argue that this is to be expected because a sample with $n = 2$ might well contain some information. What is worrisome however is the behavior of B_{10}^{SR} exhibited in the left panel of Figure 2: this is not monotone increasing in \bar{x} —for fixed S and n —and this holds as n increases; clearly an undesirable feature.

Now consider a conventional objective prior for this problem

$$\pi_0(\sigma) = \pi_1(\sigma) = \sigma^{-1}, \quad \pi_1(\mu | \sigma) = \text{Cauchy}(\mu | 0, \sigma^2). \quad (2.2)$$

This prior was first proposed by Jeffreys (1961) who derived it based on a certain desirable properties. Berger and Pericchi (2001) named it ‘conventional’ and later Bayarri and García-Donato (2008) showed that it can be obtained applying a general rule based on the Kullback-Leibler divergence. This prior leads to the Bayes factor

$$B_{10}(\bar{x}, S) = \int (1 + nt)^{(n-1)/2} \left(1 + nt \frac{S^2}{\bar{x}^2 + S^2} \right)^{-n/2} \text{IGa}(t | 0.5, 0.5) dt,$$

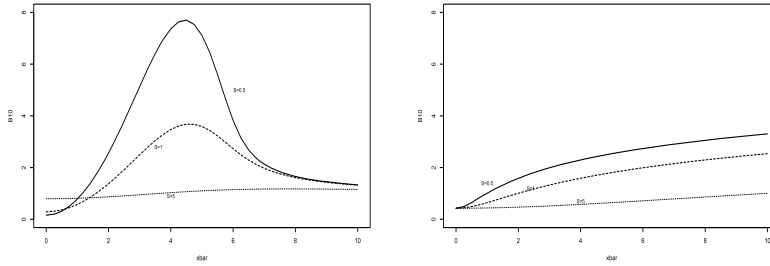


Figure 2: Example 2. B_{10}^{SR} (left) and B_{10} (right) for $n = 2$ as functions of \bar{x} and for a few values of S . (Both Bayes factors are symmetric around zero with respect to \bar{x} and only positive values are represented).

where $IGa(a, b)$ stands for the inverse gamma density with shape a and rate b . The corresponding minimal training sample size is $n = 1$, for which we obtain a unitary Bayes factor (see expression above with $S = 0$), so the conventional prior is exact predictive matching. For comparison purposes we also computed the conventional Bayes factor for $n = 2$, whose plot is reported in the right panel of Figure 2. Its behavior appears quite sensible; in particular as \bar{x} gets larger the evidence in favor of H_1 increases.

The SR-prior we used in Example 2 was constructed by assuming independence between μ and σ , which we surmise might explain the unsatisfactory behavior of B_{10}^{SR} depicted in Figure 2. A crucial feature of the conventional prior leading to its sensible testing performance in this problem is that the prior on μ scales by σ . While this seems to be a sensible option in location-scale problems, prior dependence in other problems has to be carefully assessed. Inevitably however, intrinsic features of the entertained models will come to the fore (see the invariance criterion in Bayarri et al., 2012). It would be interesting to see whether the A’s methodology could produce an SR-prior with such adaptive structural property without invoking aspects of the statistical model for its construction.

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Contributed Discussion

Zhou Lan*

The authors proposed a novel objective prior from scoring rules. For spatial statisticians, a practical example which the priors from scoring rules can be applied to, is the prior specifications of the parameters of the Matern correlation function, under the Gaussian process model. The Matern correlation function is a commonly used correlation function capturing spatial dependence. It is expressed as

$$\mathcal{K}(d|\rho, \nu) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{d}{\rho} \right)^\nu K_\nu \left(\sqrt{2\nu} \frac{d}{\rho} \right),$$

where d is the Euclidean distance, and the function of d depends on two parameters: range parameter $\rho \in (0, \infty)$ and smooth parameter $\nu \in (0, \infty)$. K_ν is the modified Bessel function of the second kind and Γ is the gamma function. The current objective priors (Berger et al., 2001) i.e., Jeffery and reference priors may be complicated. The “weakly”-informative priors are actually implemented in many practical spatial papers. Because of its convenience, the most common one is to give uniform prior such that $\nu \sim \mathcal{U}(a_\nu, b_\nu)$ and $\rho \sim \mathcal{U}(a_\rho, b_\rho)$ (e.g., Reich et al., 2010), where $\mathcal{U}(a, b)$ denotes a uniform distribution ranging from a to b , or to use log-normal distribution such that $\log \nu \sim \mathcal{N}(\mu_\nu, \sigma_\nu^2)$ and $\log \rho \sim \mathcal{N}(\mu_\rho, \sigma_\rho^2)$ (e.g., Boehm et al., 2013), where $\mathcal{N}(\boldsymbol{\mu}, \mathbf{S})$ denotes a normal distribution with mean (vector) $\boldsymbol{\mu}$ and variance (matrix) \mathbf{S} . Our discussion aims to use numerical studies to evaluate performances of the proposed prior, in comparison to the uniform prior and the log-normal prior.

Here is the specification of the Gaussian process model. Let $Y(\mathbf{s}) \in \mathbb{R}$ be the spatial response at location $\mathbf{s} \in \mathcal{D}$, where \mathbf{s} is the coordinate of a location and \mathcal{D} is a collection of locations. The model is specified as $[Y(\mathbf{s}_1), \dots, Y(\mathbf{s}_n)]^T \sim \mathcal{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\boldsymbol{\Sigma})$, where $\mathbf{X}_{n \times (p+1)}$ is the design matrix (an intercept and p covariates), $\boldsymbol{\beta}_{(p+1) \times 1}$ is the coefficients, and σ^2 is the marginal variance for each variable. $\boldsymbol{\Sigma}$ is the correlation matrix constructed by Matern such that the correlation between locations \mathbf{s} and \mathbf{s}' is $\mathcal{K}(\|\mathbf{s} - \mathbf{s}'\| | \rho, \nu)$. The Bayesian analysis of this model requires the prior specifications of the unknown parameters. We can assign conjugate priors to the coefficients $\boldsymbol{\beta}$ and the variance σ^2 : $\boldsymbol{\beta}$ follows a normal distribution with mean $\mathbf{0}$ and covariance matrix $100\mathbf{I}$; σ^2 follows a gamma distribution with shape parameter 0.01 and rate parameter 0.01. The data are generated as follows. The data is generated on a 2-dimensional map ($\mathbf{s}_i = [x_i, y_i] \in \mathcal{D} \subseteq \mathbb{R}^2$). For each replication, we generated $n = 200$ data points. Their coordinates from uniform distributions ranging from 0 to 1, denoted as $[x_i, y_i] \sim \mathcal{U}(0, 1) \times \mathcal{U}(0, 1)$. Each data point has four covariates (X_{ij} , $j = 1 : 4$, $i = 1 : 200$) and each was generated from $X_{ij} \sim \mathcal{N}(0, 1)$. Thus, the design matrix is $\mathbf{X} = [\mathbf{X}_1, \dots, \mathbf{X}_n]^T$ and $\mathbf{X}_i = [1, X_{i1}, X_{i2}, X_{i3}, X_{i4}]^T$. The coefficients vector is $\boldsymbol{\beta} = [\beta_0, \beta_1, \beta_2, \beta_3, \beta_4]^T = [1, 10, 0, 1, 2]^T$. The variance is $\sigma^2 = 0.5$. We give

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$\{\rho = 0.1, \nu = 0.5\}$ to construct the spatial correlation matrix, where the MSE is averages over all replications and the coverages are the proportions that the 95% posterior covers the true value of a parameter.

We assign the proposed priors to the two unknown parameters (ρ, ν) with $c = 2$ and $u(\theta) = 10^{-5}$. Given Figure 7 of the paper, we give $u(0) = 10^{-5}$ because thus the prior $p(\theta)$ has a gentle decay toward 0. In comparison, the uniform prior is set as $\nu \sim \mathcal{U}(0, 1000)$ and $\rho \sim \mathcal{U}(0, 1000)$, and the log-normal prior is set as $\log \nu \sim \mathcal{N}(-1, 1)$ and $\log \rho \sim \mathcal{N}(0, 100)$. For each replication, 8000 Markov chain Monte Carlo (MCMC) samples are collected after 2000 burn-ins to calculate the mean square error (MSE) of the posterior means and the 95% posterior coverage. 80 simulation replications are generated, and the MCMC chains of the three methods are checked to pass Heidelberger and Welch’s convergence diagnostic in each replication. The results are summarized in Table 1. From the results, we can find that the proposed prior performs the best.

Parameter	Proposed		Uniform		LogNormal	
	MSE	Coverage	MSE	Coverage	MSE	Coverage
ρ	0.50	0.95	0.77	0.96	0.86	0.96
ν	0.017	0.91	0.019	0.90	0.095	0.95

Table 1: Simulation results: the MSE is averages over all replications and the coverages are the proportions that the 95% posterior covers the true value of a parameter.

Although there are many concerns on the uniform prior, the uniform prior is still the most popular prior. The uniform prior is simple and “safe”. Unlike other priors (e.g., LogNormal) that you have to “guess” the best support for this prior, the uniform prior can be simply set as a very large interval. This numerical study is a preliminary result that may initiate some changes in Bayesian spatial statistics. Besides the efforts of objective priors (Berger et al., 2001), people also put some efforts to construct good priors for spatial models (e.g., Fuglstad et al., 2019). A comprehensive review and some numerical comparisons are encouraged to be given. Furthermore, there are two practical issues which may prohibit the widely use of the proposed prior: (1) how to set up C and $u(0)$ is vague to some practitioners; (2) the computation of the prior is using Taylor’s expansion is inconvenient to some practitioners, and a package or some codes are encouraged to be provided. Once the proposed prior can be implemented as easily as the uniform prior, there is no doubt that people will switch to the proposed objective prior.

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