Weakly informative priors and prior-data conflict checking for likelihood-free inference

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Bayesian likelihood-free inference, which is used to perform Bayesian inference when the likelihood is intractable, enjoys an increasing number of important scientific applications. However, many aspects of a Bayesian analysis become more challenging in the likelihood-free setting. One example of this is prior-data conflict checking, where the goal is to assess whether the information in the data and the prior are inconsistent. Conflicts of this kind are important to detect, since they may reveal problems in an investigator's understanding of what are relevant values of the parameters, and can result in sensitivity of Bayesian inferences to the prior. Here we consider methods for prior-data conflict checking which are applicable regardless of whether the likelihood is tractable or not. In constructing our checks, we consider checking statistics based on prior-to-posterior Kullback-Leibler divergences. The checks are implemented using mixture approximations to the posterior distribution and closed-form approximations to Kullback-Leibler divergences for mixtures, which make Monte Carlo approximation of reference distributions for calibration computationally feasible. When prior-data conflicts occur, it is useful to consider weakly informative prior specifications in alternative analyses as part of a sensitivity analysis. As a main application of our methodology, we develop a technique for searching for weakly informative priors in likelihood-free inference, where the notion of a weakly informative prior is formalized using prior-data conflict checks. The methods are demonstrated in three examples.

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1. INTRODUCTION

It is often natural to translate scientific knowledge into an appropriate statistical model through specification of a generative process for the data, and this leads to models defined in terms of a simulation algorithm rather than through an

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explicit mathematical formulation. For these kinds of models, computation of the likelihood may be intractable, and then likelihood-free inference methods, which simulate from the model as a surrogate for likelihood evaluations, can be used. Perhaps the two most popular Bayesian likelihoodfree inference approaches are approximate Bayesian computation (ABC) [43, 6, 49] and synthetic likelihood [50, 42], and the further development of these and other likelihoodfree inference algorithms is an active topic of current research. The purpose of the current paper is to develop some tools for checking for prior-data conflict which are applicable when the likelihood is intractable. This means developing checks which can be computed using only simulation from the model, without requiring evaluation of the likelihood. As a main application of our methodology, a technique for searching for a weakly informative prior with respect to an elicited prior is also developed, where the notion of a weakly informative prior is formalized using prior-data conflict checks.

For complex models, a challenging aspect of any Bayesian analysis is specification of the prior distribution, since an inadequate elicitation process may result in a prior distribution that is informative in ways that are unintended. If an informative prior has been used, one approach to guarding against undesirable prior sensitivity is to check for the existence of prior-data conflicts, which occur when the prior puts all its mass out in the tails of the likelihood. Priordata conflicts are important to detect, since they indicate a lack of understanding in setting up the model. Furthermore, prior sensitivity of inferences will increase with the severity of the conflict [2]. A difficulty with many prior-data conflict checking methods, however, is that the required computations are demanding, even when the likelihood is tractable.

It is especially important in the context of Bayesian likelihood-free inference to develop prior-data conflict checking methods, since alternative techniques for investigating prior sensitivity or exploring conflicts are usually unavailable. For example, objective Bayes methods [7] which specify a prior as a reference for comparison usually cannot be implemented, since determining these involves computations using the likelihood. Here we develop an approach to prior-data conflict checking which is applicable whether the likelihood is tractable or not. We consider the conflict checks recently suggested in [35], which use prior-toposterior divergences as checking statistics. To make computations tractable, we use mixture approximations to the posterior distribution, which makes repeated computations of posterior distributions for different datasets feasible. These together with closed form approximations of the Kullback-Leibler divergence for mixtures can be used to calculate tail probabilities for calibration of the checks in a computationally tractable way.

When prior-data conflicts occur, it can be helpful to consider an alternative analysis using a weakly informative prior which retains some of the original prior information but resolves the conflict, in order to see how this affects conclusions of interest. [17], inspired by [23], developed a formalization of the notion of a weakly informative prior relative to a base prior which uses a prior-data conflict check in the definition. As a main application of our methodology, we develop convenient methods for searching for weakly informative priors in the sense of [17]. While these weakly informative priors are a useful tool for exploring prior sensitivity, the goals of prior-data conflict checking and development of associated weakly informative priors do not relate solely to Bayesian sensitivity analysis, for which there is a large existing literature ([33], [29], [12], [51], [46], among many others). See [2] for further discussion of the relationship between prior sensitivity and prior-data conflict.

In the next section we give an introduction to some of the existing literature on Bayesian model checking, and consider in some detail the proposal of [35] for prior-data conflict checks based on prior-to-posterior divergences. We also develop an implementation of this procedure for the likelihoodfree case, based on mixture posterior approximations and closed-form approximations to Kullback-Leibler divergences for mixtures. Similar approximate checks were considered in [35] for the case of a tractable likelihood where mixture variational approximations were used for posterior computations. Because their variational approximation methods require evaluations of the likelihood, they do not apply in the likelihood-free setting. Hence, mixture approximations need to be obtained in a different way in the case of an intractable likelihood, and that is achieved here by fitting mixture models to approximate the joint density of summary statistics and model parameters. Once the approximation to the joint density is obtained, approximations to the posterior density for the parameters given summary statistics can be induced for different values of the summary statistics at negligible additional computational cost. This is crucial to the computational tractability of our approach to searching for weakly informative priors, which is described in Section 3. Section 4 considers a number of examples and Section 5 gives some concluding discussion.

2. PRIOR-DATA CONFLICT CHECKING

2.1 Basic ideas of prior-data conflict checking

Let θ be a parameter, y be data, $p(\theta)$ be a prior density for θ , $p(y|\theta)$ be the sampling density for y given θ and

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 $p(\theta|y)$ be the posterior density. In a Bayesian analysis, priordata conflict occurs when the prior density puts all its mass out in the tails of the likelihood, so that the information in the data about θ and the information in the prior are in conflict. Various methods have been developed for checking for prior-data conflict ([36, 32, 18, 26, 16, 41, 35], among many others). However, many of these methods are difficult to apply in the case of a model with an intractable likelihood. A prior-data conflict checking method is applicable with intractable likelihood if the check can be conducted using only simulation of data from the model, without evaluation of the likelihood. One method that can be applied in a likelihood-free setting is described in [34] who considered a certain implementation of the approach of [18]. However, the method of [34] relies on kernel density estimation of a vector summary statistic, which is difficult when the dimension of the summary statistic is moderately large. The method of [18] also lacks a desirable parametrization invariance property in the case of a continuous parameter where the check can depend on the choice of sufficient statistic. Further discussion of the statistical properties of the checks of [35] and [18], which are the basis for the likelihood-free versions of those checks in the present work and in [34] respectively, is given in [35].

A prior-data conflict check is a special kind of Bayesian predictive check of the kind used for Bayesian model criticism. See, for example, [25], [5] and [15] for general overviews of Bayesian model checking. A Bayesian predictive check involves the choice of a statistic and reference distribution. Write T = T(y) for a scalar statistic, and suppose that we wish to criticize the model by determining whether the observed value t_{obs} of T is surprising under some reference distribution m(t). As a measure of surprise, a Bayesian predictive p-value can be computed as

(1)
$$p = P(T \ge t_{\rm obs}),$$

where $T \sim m(t)$ and it has been assumed above that T is defined in such a way that a large value indicates a possible model failure. Note that the purpose of (1) is to locate where $t_{\rm obs}$ lies with respect to the distribution of T. [18] consider the question of what are logical requirements on the statistic T and the reference distribution m(t) when the goal is to check for prior-data conflict. They answer this question by generalizing a decomposition of the joint model for (y, θ) due to [11], and consider the terms in the decomposition as playing different roles in the analysis. For prior-data conflict checks, T plays the role of summarizing the likelihood, and T should not depend on aspects of y that are irrelevant to the likelihood; this means that T should be a function of a minimal sufficient statistic. Furthermore, any check based on a T which is a function of a minimal sufficient statistic should be invariant to the minimal sufficient statistic chosen. For detecting an inconsistency between the likelihood and prior, we want to see whether the observed likelihood (summarized

by the observed value t_{obs} of T) is unusual compared to what is expected under the prior. This means that the reference distribution m(t) should be the prior predictive distribution of T, which we write as $p(t) = \int p(t|\theta)p(\theta) d\theta$, where $p(t|\theta)$ denotes the sampling distribution of T given θ .

The prior-data conflict checks considered in [18] are not invariant to the choice of minimal sufficient statistic, and a modified version which is invariant but difficult to apply is discussed in [16]. [18] also consider conditioning on ancillary statistics, and extensions to separately checking components of hierarchical priors, but we do not consider this further here. One way to obtain a statistic that is a function of any sufficient statistic and invariant to its choice is to consider some function of the posterior distribution itself. [35] consider an approach of this kind, where the statistic T is a prior-to-posterior Rényi divergence, and it is a further development of this approach that is the focus of the current work.

2.2 Conflict checks using prior-to-posterior divergence

The prior-data conflict checks of [35] use a prior-toposterior Rényi divergence as the checking statistic. Here we consider the special case of the Kullback-Leibler divergence, resulting in the checking statistic

(2)
$$G = \mathrm{KL}(p(\theta|y)||p(\theta))$$
$$\stackrel{\mathrm{def}}{=} \int \log \frac{p(\theta|y)}{p(\theta)} p(\theta|y) \, d\theta.$$

To calibrate the observed value of this statistic we use a tail probability (Bayesian predictive p-value)

(3)
$$p_{\rm KL} = P(G \ge G_{\rm obs}),$$

where $G \sim p(g)$ with p(g) the prior-predictive density of G, and $G_{\rm obs}$ denotes the observed value. It is possible in principle to replace the Kullback-Leibler divergence with other divergences in the check (2), but using the Kullback-Leibler divergence is convenient computationally here, allowing us to make use of closed-form approximations for Kullback-Leibler divergences between Gaussian mixture distributions. This is described later and allows approximate versions of the check (2) to be implemented rapidly, which is particularly important in our application to searching for weakly informative priors.

If we are to use the above check in likelihood-free inference problems, we need to implement it using only simulation from the model, without requiring evaluation of the likelihood. Before we describe how this can be done, however, it is useful to give some context about why likelihood-free inference is used. The earliest applications of likelihood-free inference arose in population genetics in the form of ABC algorithms [43], but these and similar methods are now used in a wide range of problems where the likelihood is intractable due to complex observation models or difficulty in integrating out complex latent processes. There are other more specific motivations in particular applications. For example, in developing the synthetic likelihood method. [50] considered time series models for ecological data with chaotic dynamics and low environmental noise. In these models the likelihood may be difficult to evaluate using methods relying on state estimation for state space models – see [20] for further elaboration and Section 4.3 for an example of this kind considered in [21]. Another motivation for using likelihood-free methods is to robustify Bayesian analyses with tractable likelihood by basing information only on (possibly complex) summary statistics. The summary statistic likelihood is often intractable, but considering an insufficient statistic which discards information can be useful in the case of misspecified models - see [30] for a recent discussion of the statistical motivation here, although the authors focus on applications to linear models and do not use likelihood-free methods for computation. [49] is a recent comprehensive overview of likelihood-free inference methods discussing a wide range of methods and applications.

To implement a check based on the statistic (2) in the likelihood-free setting, we make several approximations. The first is to consider replacing the posterior distribution $p(\theta|y)$ with the posterior distribution given a summary statistic, say z = z(y) in (2). Most likelihood-free inference methods, such as ABC and synthetic likelihood, make use of reduced dimension summary statistics for the data since they use empirical methods based on simulated data to estimate the distribution of the summary statistics for likelihood estimation. For example, the ABC approach can be regarded as estimating the likelihood based on a kernel density estimate of the summary statistic density, and there is a curse of dimensionality associated with the use of kernel methods, so that a low-dimensional summary statistic is desirable. Ideally the summary statistic is sufficient, so that no information about θ is lost, but non-trivial sufficient summary statistics will not usually be available. See [8] and [40] for further discussion of the issue of summary statistic choice in likelihood-free inference.

The dimension reduction achieved by using summary statistics is useful for implementing our next approximation, which is to use a mixture model to estimate the posterior distribution of the parameters given summary statistic values. Mixture approximations have been used in the ABC context before. For example, [10] consider mixture modelling of parameter and summary statistics jointly and the induced conditional distribution for the parameters as a form of nonlinear regression adjustment. [9] consider similar mixture approximations within sequential Monte Carlo ABC schemes, and [19] consider an approach to estimating the likelihood using mixtures of experts and copulas. [22] use mixture of experts approximations to the posterior distribution directly, and use their mixture estimates to define discrepancy measures in distribution space for ABC analyses. [27] have recently considered variational approximation of the posterior

density using a mixture family in likelihood-free inference problems. The method considered below is the method considered in [10]. The great advantage of this approach here is that it can allow us to produce repeated posterior approximations for different data at low computational cost, which is important for approximating the reference distribution of the conflict check in computing (2). This is also important in the application of our checks to searching for weakly informative priors in the next section.

The mixture approximations we consider are obtained in the following way. Write $x = (\theta, z)$, and suppose we sample parameter value and summary statistic pairs $x_i = (\theta_i, z_i)$, i = 1, ..., n, from $p(x) = p(\theta, z) = p(\theta)p(z|\theta)$. The posterior density of θ given z_{obs} is the conditional density of θ given $z = z_{obs}$ derived from the joint density $p(x) = p(\theta, z)$. We fit a Gaussian mixture model to $x_i, i = 1, ..., n$, to obtain a Gaussian mixture approximation to $p(\theta, z)$, which we denote by $\tilde{p}(x)$,

(4)
$$\widetilde{p}(x) = \sum_{j=1}^{J} w_j \phi_j(x),$$

where J is the number of mixture components, w_j are nonnegative mixing weights summing to one, and $\phi_j(x) = \phi(x; \mu_j, \Sigma_j)$ denotes a multivariate Gaussian density with mean vector μ_j and covariance matrix Σ_j . For a Gaussian mixture model, conditional distributions are also Gaussian mixture models having easily computed closed form expressions. So once the joint density p(x) has been approximated by $\tilde{p}(x)$, we can obtain the conditional density for θ given z, which we denote by $\tilde{p}(\theta|z)$. To give an expression for this we need some further notation. Suppose we partition μ_j and Σ_j in the same way as $x = (\theta, z)$ as $\mu_j = (\mu_{j,\theta}, \mu_{j,z})$ and

$$\Sigma_j = \left[\begin{array}{cc} \Sigma_{j,\theta} & \Sigma_{j,\theta z} \\ \Sigma_{j,z\theta} & \Sigma_{j,z} \end{array} \right].$$

Then

(5)
$$\widetilde{p}(\theta|z) = \sum_{j=1}^{J} w_{j|z} \phi_{j|z}(\theta),$$

where $\phi_{j|z}(\theta) = \phi(\theta; \mu_{j|z}, \Sigma_{j|z})$, with

$$\mu_{j|z} = \mu_{j,\theta} + \sum_{j,\theta z} \sum_{j,z}^{-1} (z - \mu_{j,z}),$$

 $\Sigma_{j|z} = \Sigma_{j,\theta} - \Sigma_{j,\theta z} \Sigma_{j,z}^{-1} \Sigma_{j,z\theta},$

and

$$w_{j|z} = \frac{w_j \phi_j(z)}{\sum_{l=1}^J w_l \phi_l(z)}$$

where $\phi_j(z) = \phi(z; \mu_{j,z}, \Sigma_{j,z}).$

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The conditional density (5) is an approximation to the posterior density of θ given z, and is easily computable for any summary statistic value z. This is important since Monte Carlo approximation of the tail probability (3) involves approximating the posterior density repeatedly for different data. To approximate (3) using Monte Carlo, we generate summary statistic values $z^{(1)}, \ldots, z^{(R)}$ from the prior predictive for z, then compute the approximate posterior densities $\tilde{p}(\theta|z_{\text{obs}})$ and $\tilde{p}(\theta|z^{(r)}), r = 1, \ldots, R$, where z_{obs} is the observed value for z. If we were able to compute the prior-to-posterior Kullback-Leibler divergences for our approximations, we would then compute the proportion of the simulated summary statistics for which the divergence was larger than that for the observed summary statistic as in (3).

To overcome the difficulty of computing the prior-toposterior Kullback-Leibler divergence, we exploit the fact that our posterior approximations are Gaussian mixtures, and assume that the prior can be approximated as a Gaussian mixture also. We write $\tilde{p}(\theta)$ for the mixture approximation to the prior. If the prior is Gaussian or a Gaussian mixture, then $\tilde{p}(\theta) = p(\theta)$, but if it is not we might simulate samples from the prior and then fit a mixture model as described to obtain $\tilde{p}(\theta)$. A closed-form approximation for the Kullback-Leibler divergence between two mixture models, due to Hershey and Olsen [28, Section 7], is then used as in [35]. For this consider two mixture densities $f(\theta)$ and $g(\theta)$,

$$f(\theta) = \sum_{j=1}^{J_f} w_{f,j} \phi_{f,j}(\theta), \quad g(\theta) = \sum_{j=1}^{J_g} w_{g,j} \phi_{g,j}(\theta),$$

where J_f and J_g are the number of mixture components for f and g respectively, $w_{f,j}$, $j = 1, \ldots, J_f$ and $w_{g,j}$, $j = 1, \ldots, J_g$ are non-negative mixing weights for the respective densities summing to one, and $\phi_{f,j}(\theta) = \phi(\theta; \mu_{f,j}, \Sigma_{f,j})$ and $\phi_{g,j}(\theta) = \phi(\theta; \mu_{g,j}, \Sigma_{g,j})$ are respective multivariate normal component densities. Then approximate the Kullback-Leibler divergence $\mathrm{KL}(g(\theta)||f(\theta))$ by

(6)
$$\begin{split} \mathbf{K} \mathbf{\tilde{L}}(g(\theta) || f(\theta)) \\ &= \sum_{j=1}^{J_g} w_{g,j} \log \frac{\sum_{k=1}^{J_g} w_{g,k} \exp(-\mathbf{K} \mathbf{L}(\phi_{g,j} || \phi_{g,k}))}{\sum_{l=1}^{J_f} w_{f,l} \exp(-\mathbf{K} \mathbf{L}(\phi_{g,j} || \phi_{f,l}))}, \end{split}$$

where the Kullback-Leibler divergences on the right-hand side in the above expression are between multivariate normal components densities, for which there is an exact closedform expression.

Combining our normal mixture approximations to the prior and posterior and the approximation (6), an approximate version of the prior-to-posterior Kullback-Leibler divergence statistic (2) for z is then given by

(7)
$$\widetilde{G} = \widetilde{G}(z) = \widetilde{\mathrm{KL}}(\widetilde{p}(\theta|z)||\widetilde{p}(\theta))$$

Inputs:

- Prior distribution $p(\theta)$, model $p(z|\theta)$ for summary statistics z, observed summary statistic value z_{obs} .
- Training sample size n for fitting mixture approximation, number of replicates R for Monte Carlo approximation of p-value.

Output:

• Tail probability \tilde{p}_{KL} given in (8).

Initialization:

- Simulate $x_i = (\theta_i, z_i) \sim p(x), i = 1, ..., n$, and obtain a Gaussian mixture model approximation $\tilde{p}(x)$ of p(x).
- If the prior $p(\theta)$ is not Gaussian or a Gaussian mixture, obtain a Gaussian mixture approximation $\tilde{p}(\theta)$ of $p(\theta)$ by fitting to the samples θ_i , i = 1, ..., n.

Computation of tail probability \tilde{p}_{KL} :

- 1. For r = 1, ..., R,
 - Simulate $z^{(r)}$ from the prior predictive distribution p(z) for z.
 - Compute the posterior approximation $\tilde{p}(\theta|z^{(r)})$ using (5).
 - Compute $\widetilde{G}^{(r)} = \widetilde{\mathrm{KL}}(\widetilde{p}(\theta|z^{(r)})||\widetilde{p}(\theta))$ using (6).
- 2. Compute $\widetilde{p}(\theta|z_{\text{obs}})$ using (5), $\widetilde{G}_{\text{obs}} = \widetilde{\text{KL}}(\widetilde{p}(\theta|z_{\text{obs}})||\widetilde{p}(\theta))$ using (6) and then

$$\widetilde{p}_{\mathrm{KL}} = \frac{1}{R} \sum_{r=1}^{R} I(\widetilde{G}^{(r)} \ge \widetilde{G}_{\mathrm{obs}}).$$

Then our prior-data conflict checks for likelihood-free inference approximates (3) by

(8)
$$\widetilde{p}_{\mathrm{KL}} = \frac{1}{R} \sum_{r=1}^{R} I(\widetilde{G}^{(r)} \ge \widetilde{G}_{\mathrm{obs}}),$$

where $\widetilde{G}^{(r)} = \widetilde{G}(z^{(r)})$, $r = 1, \ldots, R$ are values of \widetilde{G} for independent simulations $z^{(r)}$, $r = 1, \ldots, R$, from the prior predictive distribution of z, $\widetilde{G}_{obs} = \widetilde{G}(z_{obs})$ is the value of \widetilde{G} for the observed summary statistic value z_{obs} , and $I(\cdot)$ denotes the indicator function. The computations required for our conflict check are summarized in Algorithm 1.

A similar approximate implementation of the conflict check based on prior-to-posterior divergences was considered in [35]. In that case, however, the likelihood was tractable and the mixture posterior approximations were obtained by learning variational approximations independently for each simulated prior predictive dataset in the Monte Carlo approximation of the tail probability (3). Here our mixture approximations are obtained in quite a different way, and furthermore they are extremely fast to compute for every new dataset once the mixture approximation to the joint distribution of (θ, z) has been obtained. This is important in the application we discuss next, which is searching for weakly informative prior distributions, an application which was not considered in the work of [35].

3. WEAKLY INFORMATIVE PRIORS

3.1 Weakly informative priors from prior-data conflict checks

Weakly informative priors were first considered by [23], conceived as prior distributions which put some prior information into an analysis, but less than the analyst actually possesses. [17] gave a precise definition of a weakly informative prior with respect to a base prior used for an analysis in terms of prior-data conflict checks. We discuss this definition now.

Let $p_B(\theta)$ denote the elicited informative prior (called the baseline prior) used in the analysis. Let $p_W(\theta)$ denote some alternative prior. Suppose that M is a minimal sufficient statistic. Write $p_B(m)$ and $p_W(m)$ for the prior predictive densities for M for the priors $p_B(\theta)$ and $p_W(\theta)$ respectively. [18] consider using the prior predictive density ordinate for M as the statistic for a prior-data conflict check, and this is also used in the work of [17]. So if the prior $p_j(\theta)$ is used for the analysis, j = B, W then a tail probability for the prior-data conflict check is computed as

$$p_j = P(p_j(M) \le p_j(m_{\text{obs}})), \quad M \sim p_j(m),$$

where m_{obs} is the observed value for M, as this determines whether or not m_{obs} lies in a region with low probability with respect to $p_j(m)$. The definition of a weakly informative prior with respect to the base prior given in [17] is based on the idea that for data simulated under the base prior, there should be a reduction in the proportion of prior-data conflicts when the data are analyzed under the alternative prior rather than the base prior.

Suppose a conflict occurs if a *p*-value for a prior-data conflict check is less than α for some cutoff α . Let x_{α} be the α -quantile of the random variable $P_B(M')$, $M' \sim p_B(m)$, where

$$P_B(M') = P(p_B(M) \le p_B(M')) \quad M \sim p_B(m).$$

The distribution of $P_B(M')$ is that of the conflict *p*-value that is obtained when $p_B(\theta)$ is used in the analysis, and the data are simulated under the prior predictive for $p_B(\theta)$. If M is continuous then $P_B(M')$ will be uniform on [0, 1]. Next, consider the random variable $P_W(M')$, $M' \sim P_B(M)$, where

$$P_W(M') = P(p_W(M) \le p_W(M')) \quad M \sim p_W(m).$$

The distribution of $P_W(M')$ is that of a conflict *p*-value for data generated under the prior predictive for $p_B(\theta)$, when the analysis is done using $p_W(\theta)$.

We say the prior $p_W(\theta)$ is weakly informative with respect a similar way to Section 2.2, we can simulate data to $p_B(\theta)$ at level α if

$$P(P_W(M') \le x_\alpha) < \alpha,$$

which says that prior-data conflicts happen less often when the data are analyzed using $p_W(\theta)$ rather than $p_B(\theta)$, but the data are generated under $p_B(\theta)$. Instead of choosing a fixed level α one can also consider other stronger notions of uniform weak informativity - see [17] for details. [17] define the degree of weak informativity of $p_W(\theta)$ relative to $p_B(\theta)$ at level α to be

(9)
$$W_{\alpha} = 1 - \frac{P(P_W(M') \le x_{\alpha})}{x_{\alpha}},$$

which is the proportion of prior-data conflicts avoided by using $p_W(\theta)$ as the prior for the analysis, with data generated under $p_B(\theta)$. The degree of weak informativity of one prior with respect to another defined by (9) can be compared for different choices of the alternative prior, which do not need to belong to the same parametric family.

3.2 Weakly informative priors based on conflict checks

In the formulation of weakly informative priors used in [17], the prior-data conflict check based on the prior predictive density ordinate for a minimal sufficient statistic can be replaced by some other prior-data conflict check. We consider this now for our prior-to-posterior divergence conflict checks. Let us consider a family of priors $p(\theta|\gamma)$ for searching for a weakly informative prior, where γ is an expansion parameter. We will assume the prior expansion will be chosen so that $p(\theta)$ corresponds to a prior within this family for some value $\gamma^{(0)}$ so that $p(\theta) = p(\theta|\gamma^{(0)})$ say, although this is not essential. Dealing with a baseline prior that does not belong to the family $p(\theta|\gamma)$ does not involve any alteration to the procedure we suggest below. In the case where the baseline prior is elicited, it seems natural that the family $p(\theta|\gamma)$ should be an expansion of the baseline prior, since we want to retain some of the information in the original prior. We can also consider choosing a weakly informative prior from a family that is a union of two different parametric families.

Write $\widetilde{G}(z,\gamma)$ for the statistic \widetilde{G} at (7) when the prior used for the analysis is $p(\theta|\gamma)$. We have previously discussed in Section 2.2 how to compute $\widetilde{G}(z, \gamma^{(0)})$ for abitrary observed summary statistics z by fitting a mixture model to simulated data $x_i = (\theta_i, z_i) \sim p(\theta|\gamma_0)p(z|\theta), i = 1, \dots, n.$ We now wish to approximate $\widetilde{G}(z,\gamma)$ for both arbitrary z and γ . We will accomplish this by expanding the original statistical model hierarchically to include γ as a parameter, giving the model $p(\gamma)p(\theta|\gamma)p(z|\gamma)$, where $p(\gamma)$ is a pseudoprior for γ . We call $p(\gamma)$ a pseudo-prior, since we employ it for purely computational reasons to enable us to approximate conditional posterior densities $p(\theta|z, \gamma)$. Proceeding in

$$x_i = (\gamma_i, \theta_i, z_i) \sim p(\gamma)p(\theta|\gamma)p(z|\theta),$$

 $i = 1, \ldots, n$, fit a Gaussian mixture model to these data, and then use the conditional distribution of θ given z, γ in the mixture as an estimated posterior distribution given z, γ and hence compute $G(z, \gamma)$.

The prior $p(\theta|\gamma)$ will be said to be weakly informative at level α relative to $p(\theta)$ for the approximate divergence check (8) if the random variable $P_{\gamma}(z'), z' \sim \int p(\theta) p(z|\theta) d\theta$, where

$$P_{\gamma}(z') = P(\widetilde{G}(z,\gamma) \ge \widetilde{G}(z',\gamma)), \quad z \sim \int p(\theta|\gamma)p(z|\theta) \, d\theta,$$

satisfies

$$P(P_{\gamma}(z') \le x_{\alpha}) < \alpha,$$

where x_{α} is the α -quantile of $P_{\gamma^{(0)}}$. To approximate the distribution of $P_{\gamma}(z')$, we need to simulate values for $z' \sim$ $\int p(\theta)p(z|\theta) d\theta$, and then for each of these simulations we must approximate the p-value (8) using Algorithm 1 to get a Monte Carlo empirical distribution approximating the distribution of $P_{\gamma}(z')$.

The degree of weak informativity of $p(\theta|\gamma)$ at level α with respect to $p(\theta) = p(\theta|\gamma^{(0)})$ for the approximate divergence check (8) is, similar to before, defined to be

$$W_{\alpha}(\gamma) = 1 - \frac{P(P_{\gamma}(z') \le x_{\alpha})}{x_{\alpha}}$$

It seems reasonable to try to choose a prior $p(\theta|\gamma)$ weakly informative compared to $p(\theta)$ by choosing γ such that

(10)
$$W_{\alpha}(\gamma) > \delta,$$

which would ensure that the proportion of conflicts is reduced by δ when data is simulated under the base prior and the analysis is done under the alternative prior. The constant δ needs to be chosen and choosing $\delta = 0.5$ would require reducing the proportion of conflicts by half, for example. If it is not possible to find any prior satisfying (10)we can look at maximizing $W_{\alpha}(\gamma)$. Later we consider checking the criterion (10) at a finite number of candidate values for γ chosen as a maximin latin hypercube design covering some rectangular search region.

4. EXAMPLES

4.1 Logistic regression example

We consider a logistic regression model as a first illustration of our methodology. Although the likelihood is tractable, we consider this example since weakly informative priors have been developed for this model in the literature, and it is interesting to compare the priors obtained using our approach with those in previous work. We develop a weakly



Figure 1. Degree of weak informativity for conflict check for logistic regression example with 14 mixture components (left) and 10 mixture components (right). The 14 component model was chosen by BIC.

informative prior in the context of a design from a real data set. [44] considered a bioassay experiment in which 5 animals at each of 4 dose levels were exposed to a toxin. For the purposes of considering weakly informative prior specification below we consider a hypothetical increase in the number of animals at each dose to 20. This is to make the continuity assumption involved in a joint modelling of data and parameters as a Gaussian mixture more reasonable. At each dose, the number of deaths was recorded. Writing y_i for the number of deaths at dose d_i , the model is $y_i \sim \text{Binomial}(20, p_i)$, $\text{logit}(p_i) = \theta_1 + \theta_2 d_i$, where the dose values have been log transformed, centred and scaled similar to [24].

Consider a prior distribution for $\theta = (\theta_1, \theta_2)^{\top}$ of the form $p(\theta|\gamma) = p(\theta_1|\gamma_1)p(\theta_2|\gamma_2)$ where $p(\theta_j|\gamma_j) = \phi(\theta_j; 0, \gamma_j^2)$, j = 1, 2 with $\phi(x; \mu, \sigma^2)$ denoting the normal density with mean μ and variance σ^2 . We use the base prior $\gamma^{(0)} = (1, 1)$. Next consider a uniform grid of 50 equally spaced values for γ_1 on the range [0.5, 10] and of 100 equally spaced values for γ_2 on the range [0.5, 20]. From these we can form a corresponding two-dimensional grid on $[0.5, 10] \times [0.5, 20]$. For each γ on the two-dimensional grid, we estimate the degree of weak informativity of $p(\theta|\gamma)$ with respect to the base prior at level 0.05.

Making the baseline variance parameters either larger or smaller can resolve a conflict in some instances. To get some intuition for this, consider the simple case of a logistic regression without covariates, $logit(p_i) = \theta_1$, with a normal prior $N(0, \gamma_1^2)$ on θ_1 . As $\gamma_1 \to \infty$, most prior mass is on large values of $|\theta_1|$, which corresponds to probabilities close to zero or one. On the other hand, choosing $\gamma_1 \to 0$ gives a prior on the probability concentrated around 0.5. So we can see that choosing γ_1 either very large or close to zero results in a highly informative prior, and so a choice of the prior variance parameter that avoids these extremes is necessary for a weakly informative choice. See [1] for some related discussion. For computing the approximate tail probabilities $\tilde{p}_{\rm KL}$ at (8), we used R = 1000 prior predictive simulations. The mixture approximation to the joint distribution was trained using the R package mclust [48] based on 100,000 simulations from the model, and a uniform distribution on $[0.5, 10] \times [0.5, 20]$ was assumed for a pseudo-prior distribution for γ in the mixture modelling. The number of clusters was chosen using the default method implemented by the mclustBIC function in mclust, searching up to a maximum of 15 clusters and considering 14 different possible choices for the mixture component covariance structure. In our later examples we use a similar approach to choosing the number of components. The final model chose by BIC contained 14 mixture components here.

Figure 1 plots $W_{0.05}(\gamma)$, for the mixture model chosen by BIC as well as a mixture model with 10 components to explore sensitivity of estimates of weak informativity to the number of mixture components used. Little sensitivity is observed, particularly in the region where the degree of weak informativity is large, if a sufficiently large number of mixture components is chosen. Figures 2 and 4 in [34] and [17] respectively are qualitatively similar to Figure 1, although the definition of a weakly informative prior depends on the prior-data conflict check used, and our check is different to that used by these authors. From Figure 1 we see that making the variance parameters γ_1 and γ_2 somewhat larger than their baseline values leads to a weakly informative prior. However, if these parameters are made too large this does not lead to a weakly informative prior, consistent with the intuition obtained from the case discussed above of a logistic regression with an intercept only. In situations where γ is higher-dimensional, it is not possible to evaluate the degree of weak informativity on a grid. In these cases

we generate a certain number of values according to a minimax latin hypercube or some other space-filling design [47] to cover the search space for γ , and evaluate the degree of weak informativity on the design points. Generating 100 minimax latin hypercube design points in this example on $[0.5, 10] \times [0.5, 10]$ and choosing the value for γ maximizing the degree of weak informativity with respect to γ_1 and γ_2 gave a value $\gamma = (2.6, 2.5)$.

4.2 Multivariate *g*-and-*k* example

The g-and-k distribution [45] is defined through its quantile function,

$$Q(p; A, B, g, k) = A + B\left(1 + c\frac{1 - \exp(-gz(p))}{1 + \exp(-gz(p))}\right)(1 + z(p)^2)^k z(p),$$

$$p \in (0, 1)$$

where $z(p) = \Phi^{-1}(p)$ with $\Phi(\cdot)$ the standard normal distributon function, and A, B, g and k are location, scale, skewness and kurtosis parameters, with B > 0. The constant c is conventionally fixed at 0.8, which results in the constraint k > -0.5. The closed form quantile function makes simulation from the distribution easy using the inversion method by computing Q(U; A, B, g, k) for $U \sim U[0, 1]$. This makes likelihood-free inference methods attractive [3]. Although it is possible to calculate the density function numerically with sufficient computational effort [39], an additional motivation for using likelihood-free methods in this example is to robustify a Bayesian analysis to outliers. The octile-based summary statistics described below allow a robust Bayesian analysis where inference is insensitive to extreme outliers, and the summary statistic likelihood is intractable, leading to an interest in likelihood-free inference methods.

We consider here the multivariate g-and-k model described in [14]. Their model uses a univarviate g-and-k distribution for each marginal, and a Gaussian copula with a correlation matrix C for the dependence structure. Precisely, let y_i , i = 1, ..., n, be the data, where $y_i = (y_{i1}, ..., y_{iJ})^{\top}$. The values y_{ij} , i = 1, ..., n, are iid and follow a univariate g-and-k distribution with parameters $\theta_j = (A_j, B_j, g_j, k_j)$. We write the density of y_{ij} as $f(y_{ij}; \theta_j)$, with corresponding distribution function $F(y_{ij}; \theta_j)$. Define $\theta = (\theta_1^{\top}, ..., \theta_J^{\top}, C)$, and then the joint density of y_i is

$$f(y_i;\theta) = |C|^{-1/2} \exp\left(-\frac{1}{2}\eta_i^\top (I - C^{-1})\eta_i\right) \prod_{j=1}^J f(y_{ij};\theta_j),$$

where $\eta_i = (\eta_{i1}, \ldots, \eta_{iJ})^{\top}$, with $\eta_{ij} = \Phi^{-1}(F(y_{ij}; \theta_j))$. If $Z = (Z_1, \ldots, Z_J) \sim N(0, C)$, and we compute $(F^{-1}(\Phi(Z_1); \theta_1), \ldots, F^{-1}(\Phi(Z_J); \theta_J)^{\top}$, then this produces a simulation from the model.

For a multivariate dataset of exchange rate returns discussed in [14], [31] consider prior densities for the θ_i that

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are independent for $j = 1, \ldots, J$, with θ_j uniform on $[-0.1, 0.1] \times [0, 0.05] \times [-1, 1] \times [-0.2, 0.5]$. For the copula correlation matrix C, we follow [37] and consider a normal prior on a spherical parametrization of the elements of C [38] to make the parameters unconstrained. This is explained further below. We will consider a multivariate model with J = 3 components, and the unconstrained parameters for this model will be denoted by $w = (w_1, w_2, w_3)$. In a spherical parametrization the parameters w determine the correlation matrix C through its lower-triangular Cholesky factor $L, C = LL^{\top}$, by

$$L = \begin{bmatrix} 1 & 0 & 0\\ \cos \gamma_1 & \sin \gamma_1 & 0\\ \cos \gamma_2 & \sin \gamma_2 \cos \gamma_3 & \sin \gamma_2 \sin \gamma_3 \end{bmatrix},$$

where $\gamma_j = \pi/(1 + \exp(-w_j))$, j = 1, 2, 3. [37] considered a prior on w which is multivariate normal, $N(0, (1.75)^2 I_3)$, where I_q denotes the identity matrix of dimension q. Although a uniform prior on the correlation matrix could be considered, when J is large it is preferable in many applications to use a prior that shrinks towards independence.

The transformation to make the parametrization of the correlation matrix unconstrained makes valid prior specification easy in the mathematical sense. However, the transformed parameters are not easy to relate to prior knowledge we would typically have, regarding the correlation parameters directly. This increases the possibility of specifying a prior distribution that is informative in ways that are not intended. For a base prior in this example we will consider a multivariate normal distribution $N(0, (0.5)^2 I_3)$, which is more informative than the prior used in [37], and then search for a weakly informative prior relative to this base prior. In searching for a weakly informative prior, we consider prior distributions of the form $N(0, \gamma^2 I_3)$, where the parameter γ lies in the range [0.5, 5]. For summary statistics, we use the same summary statistics as in [37]. These are robust estimates of location, scale, skewness and kurtosis based on octiles considered in [14] for each marginal (4 summary statistics for each component), and rank correlations for all pairs of components (3 summary statistics). There are 15 summary statistics in total. Since we are interested in weakly informative priors for the correlation parameters, we consider conflict checks based on the prior-to-posterior divergence for w, and we assume that all the information in the summary statistics about w is contained in the 3 rank correlation summary statistics summarizing the dependence structure. For approximating our Kullback-Leibler divergence statistics it is then only necessary to consider approximating the joint distribution of $(\gamma, w, S(w))$, where we assume a pseudo-prior for γ that is uniform on [0.5, 5] and S(w) denotes the three-dimensional vector of the pairwise rank correlations. We use 100,000 simulations of γ , w and S(w) from the model to train the mixture model, and for approximating tail probabilities $\tilde{p}_{\rm KL}$ at (8), we used R = 1000prior predictive simulations.



Figure 2. Degree of weak informativity for conflict check for multivariate g-and-k example.

Figure 2 plots the degree of weak informativity of the prior for different γ with respect to the base prior with $\gamma = 0.5$. Values of γ in the range 1 to 2 here are maximally weakly informative with respect to the base prior. For the base prior and a weakly informative prior with $\gamma = 1$, we simulated 1000 draws, and transformed these draws to the corresponding correlations C_{12} , C_{13} and C_{23} . The result is shown in Figure 3. For the weakly informative prior, the implied marginal priors on the correlations are closer to uniform. However, it is clear that the marginal prior distribution on the correlations depends on the ordering of the components, due to the way that the unconstrained parameters are defined using a Cholesky decomposition.

4.3 Simple recruitment, boom and bust model

[20] discusses the motivation for likelihood-free inference methods as an alternative to state space methods for likelihood estimation in time series models with complex nonlinear dynamics and chaotic behaviour, with likelihood-free methods sometimes being preferable when there is low process noise or model misspecification. Our next example considers an ecological time series model representing the fluctuation of the population size of a certain group over time, considered in [21] and [4], who both find that more flexible methods than the synthetic likelihood method of [50] and able to deal with non-Gaussian distributions of summary statistics are needed. Let N_t , $t = 0, 1, \ldots$ represent population sizes at discrete integer times t. Given N_t and the parameters $\theta = (r, \kappa, \alpha, \beta)$, the conditional distribution of N_{t+1} is

$$N_{t+1} \sim \begin{cases} \text{Poisson}(N_t(1+r)) + \epsilon_t & \text{if } N_t \leq \kappa \\ \text{Binom}(N_t, \alpha) + \epsilon_t & \text{if } N_t > \kappa \end{cases}$$

where $\epsilon_t \sim \text{Poisson}(\beta)$. In this model r is a growth parameter, κ is a threshold where exceedance of the threshold leads to a crash, α is a survival probability controlling the speed of the crash and β is the mean for a recruitment process. We consider a time series of length 250, and in simulating from the model we use 50 burn-in values after initializing the process at the integer part of the threshold κ .

[4] considered a prior uniform on $[0,1] \times [10,80] \times [0,1] \times [0,1]$. We change the U[0,1] prior for r to a Beta(5,5) prior to obtain the base prior for constructing a weakly informative alternative. The summary statistics z are constructed following [4]. For a time series x of length T, define differences and ratios $d_x = \{x_i - x_{i-1}; i = 2, \ldots, T\}$ and $r_x = \{x_i/x_{i-1}; i = 2, \ldots, T\}$, respectively. We use the sample mean, variance, skewness and kurtosis of x, d_x and r_x as the summary statistics, so that z is 12-dimensional. To search for a weakly informative prior, consider prior distributions for r of the form $r \sim \text{Beta}(\gamma, \gamma)$, so that the mean is fixed at 0.5 but the variance changes with γ .

We use 100,000 simulations from the joint distribution of γ, r and z to train the mixture model, where a pseudo-prior uniform on [0.2, 9] was considered for γ . For approximating tail probabilities we used R = 1000 prior predictive simulations. Figure 4 plots the degree of weak informativity of the prior for different γ with respect to the base prior with $\gamma = 5$.

We choose here a value of $\gamma = 0.2$ as a weakly informative choice. To show that using a weakly informative prior can make a difference for Bayesian inference, Figure 5 shows, for a simulated time series, the estimated univariate posterior densities for the two prior distributions, while Figure 6 shows estimated bivariate posterior densities. The simulated time series is of length 250 with true parameter values $r = 0.4, \kappa = 50, \alpha = 0.09$ and $\beta = 0.05$ and the posterior density estimation was done using an ABC method. The ABC analysis was based on 500,000 samples from the prior and a neural network regression adjustment using the abc function in the abc R package [13] with a tolerance of 0.05 and other algorithmic settings at default values. Given the complex interactions between the parameters, changing the marginal prior on r affects posterior inference not just for r but also for the other parameters, particularly κ and α .



Figure 3. Prior distribution on correlations for original ($\gamma = 0.5$, blue) and weakly informative prior ($\gamma = 1$, red) for multivariate g-and-k example.



Figure 4. Degree of weak informativity for conflict check for boom and bust example.

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Figure 5. Estimated univariate posterior marginal densities for boom and bust example.



Figure 6. Estimated bivariate posterior marginal densities for boom and bust example. The top and bottom rows shows estimates for the baseline and weakly informative priors respectively.

5. DISCUSSION

Informative priors are often needed in typical applications of likelihood-free inference. The complex models for which likelihood-free inference methods are useful often contain weakly identified parameters where the regularization provided by an informative prior is valuable. Some likelihoodfree algorithms require a proper prior, and the computational efficiency of such algorithms may depend on how informative the prior is, which creates the temptation to specify priors for computational convenience. It seems important then to develop new tools for assessing the sensitivity of Bayesian inferences to the prior in the likelihood-free setting. We have developed here methods for checking for prior-data conflict, as well as methods for specifying weakly informative priors relative to the prior used in the analysis which are useful for sensitivity analyses and for revealing possible deficiencies in prior elicitation and model understanding.

Our approach to making the computations tractable in our conflict checks and in searching for weakly informative priors uses Gaussian mixture approximations to posterior distributions and this may be rather crude, particularly with high-dimenisonal parameters or summary statistics. While rough calculations may be good enough for diagnostics and exploring alternative prior specifications, an interesting direction for future work is to investigate better approaches to the likelihood-free inference while still allowing the repeated calculation of posterior densities for different data that is necessary here.

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