Using history matching for prior choice

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Abstract

It can be important in Bayesian analyses of complex models to construct informative prior distributions which reflect knowledge external to the data at hand. Nevertheless, how much prior information an analyst can elicit from an expert will be limited due to constraints of time, cost and other factors. This paper develops effective numerical methods for exploring reasonable choices of a prior distribution from a parametric class, when prior information is specified in the form of some limited constraints on prior predictive distributions, and where these prior predictive distributions are analytically intractable. The methods developed may be thought of as a novel application of the ideas of history matching, a technique developed in the literature on assessment of computer models. We illustrate the approach in the context of logistic regression and sparse signal shrinkage prior distributions for high-dimensional linear models.

Keywords: Approximate Bayesian computation, Bayesian inference, History matching, Prior elicitation.

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1 Introduction

Elicitation of a prior distribution is an important part of Bayesian analysis. However, often a detailed representation of an expert’s beliefs is difficult to obtain, assuming it is reasonable to suppose that there are true probabilities representing an expert’s beliefs at all. Even if it were possible to perform comprehensive elicitations in complex multivariate situations, it might not be worth the cost involved in many cases. In complex models, how much prior information can be easily elicited from an expert will be limited due to constraints of time, cost and other factors. For an overview of modern prior elicitation methods including realistic goals of the process, ways of evaluating its success, and the cognitive biases that make it difficult see Garthwaite et al. (2005), O’Hagan et al. (2006), Daneshkhah and Oakley (2010), Martin et al. (2012), Simpson et al. (2015) and Morris et al. (2014), among others. For a recent discussion of model checking including criticism of the prior see Chapter 5 of Evans (2015).

Here we consider the problem of predictive elicitation, where prior information is given by certain limited constraints on prior predictive distributions which are not analytically tractable. By limited constraints we mean that the given prior information might rule out some distributions as unsuitable for the prior, but the prior information does not identify a unique suitable prior distribution. We will be concerned with developing effective numerical methods for finding a reasonable value or set of values for a prior hyperparameter so that the prior satisfies the constraints. It is not our intention in this manuscript to consider the best ways to elicit the predictive constraints from an expert - these are assumed to be given - and the numerical methods discussed here are a tool to be used as part of an iterative process of questioning and feedback in the elicitation context. A more comprehensive discussion of elicitation methods is given in the references above.

The method we propose can be thought of as a novel application of the method of
history matching (Craig et al. 1997) used in the literature on assessment of computer models. A recent application of history matching in the context of a complex infectious diseases model that describes the history matching approach is Andrianakis et al. (2015). We delay further discussion of the relevant literature to Section 3. Computer models, sometimes called “simulators”, are complex computer codes that take certain inputs or parameters and produce an output. The models can either be stochastic or deterministic. The goal of history matching is to eliminate regions of the computer model parameter space where predictions from the computer model are clearly inconsistent with observed data. This may result in the conclusion that there are no plausible values of the parameters given the level of model discrepancy considered to be reasonable, and the results of a history match can guide model development and make any subsequent calibration of the model more efficient.

To apply history matching to the problem of prior choice, we can view the prior hyperparameters as the computer model parameters, and use characteristics of the prior predictive densities as the computer model outputs. From these outputs an implausibility measure of the type used in history matching can be constructed. Similar to the computer models context, the approach can give an indication that there are no priors within the class considered satisfying the stated predictive constraints, as well as exploring the set of possible prior choices when the set of constraints allow for a number of suitable priors. The set of appropriate prior choices returned by the method can be used as a basis for making a unique prior choice less arbitrary, as a starting point for adding further information, or in a sensitivity analysis.

The method we discuss here, while focusing on computational problems, is in the tradition of predictive elicitation methods which elicit information about potentially observable data, rather than eliciting information about parameters directly. Examples of predictive elicitation methods in the literature for particular models include, for example, Kadane et al. (1980) and Garthwaite and Dickey (1988) for linear models, and Bedrick et al. (1996) for
generalized linear models, among many others. Another popular method for informative prior choice in this tradition is the “power prior” approach of Ibrahim and Chen (2000), where a tempered version of the likelihood for data from a past study is used as the basis for the prior; if no past study is available the data can also be imaginary data created by an expert. Extensions or modifications of the method include Neuenschwander et al. (2009) and the commensurate priors of Hobbs et al. (2011). However, as mentioned above, we do not focus here on best ways to elicit prior information for particular models, either predictively or on the parameters directly. Rather, we are concerned with algorithms for finding good priors satisfying stated prior predictive constraints already given and where the relevant prior predictive distributions are analytically intractable.

A simple expository example illustrates the main features of our approach. Suppose we are to observe a binomial random variable \( y \sim \text{Binomial}(n, p) \) and we are interested in inference about \( p \in (0, 1) \). We parametrize the model in terms of \( \beta = \log(p/(1-p)) \) and decide to choose a normal family for the prior on \( \beta \), \( N(0, \sigma_{\beta}^2) \), where \( \sigma_{\beta}^2 \) is to be chosen. We can think of the binomial model with this parametrization as a logistic regression with only an intercept. A less trivial logistic regression example is developed in Section 5.1. Naïvely it might be expected that setting \( \sigma_{\beta}^2 \) large would result in a non-informative prior. However, this is not the case as this would put most of the prior mass far away from 0 which correspond to values of \( p \) near 0 and 1. Setting \( \sigma_{\beta}^2 \) small, on the other hand, results in most of the prior mass for \( \beta \) near 0, which corresponds to \( p = 0.5 \). So both a large value of \( \sigma_{\beta}^2 \), as well as a small value, would usually not be suitable as a non-informative choice of the prior distribution – the choice of \( \sigma_{\beta}^2 \) requires thought and this example shows that a flat prior that ignores the parametrization of the model is unacceptable as a non-informative choice. It is also clear that when \( n \) is small, so that there is little information in the data, combining what is learned from the data with prior information may be very important, so that a non-informative prior choice would not be desirable from that point of view. Our logistic regression example in
Section 5.1 illustrates the difference that even some limited prior information can make to inference in a real example. While in the case of this example a uniform prior on \( p \) may result in inferences with good frequentist properties, things become much more complex in multiparameter problems. It is well appreciated in the objective Bayesian community that in multiparameter models the specification of a non-informative prior as a reference for an informative analysis is extremely subtle. The most successful approach to constructing non-informative priors in a general way is the reference prior approach (Berger et al. 2009). However, this approach requires the ability to analytically compute the Fisher information and in general different reference priors are required for different parameters of interest.

There is simply no such thing as a prior that can be considered non-informative for all functions of the parameter at once.

There are a variety of ways that prior information is formulated in the elicitation literature. In our expository example and in view of the observation that a too diffuse prior would lead to the prior for \( p \) concentrating on 0 or 1, we might consider the following requirement for the prior. First, let \( \hat{p} = y/n \) be the maximum likelihood estimator of \( p \), and define the summary statistic \( S = S(y) = \hat{p}(1 - \hat{p})/n \), which is an estimate of the variance of \( \hat{p} \). If \( p \) is close to 0 or 1, we would expect \( \hat{p} \) to be close to 0 or 1 and \( S \) to be small, so if the prior predictive for \( S \) concentrates on 0, this indicates the prior is putting most of its mass near values for \( p \) of 0 or 1. For some suitably chosen small value of \( S \), we might require that this value be implausible under the prior predictive distribution for \( S \) and so rule out such a prior. In this simple example it might be more natural to specify prior information on the parameter \( p \) directly, but in more complex examples prior information may be more easily expressed predictively in terms of observables as we have done here. The information we have specified in this case falls short of completely determining a prior, but the methods of this paper give ways of exploring prior hyperparameter choices compatible with such information that is easily specified and thought to be important. If the analyst feels that the accuracy of
any specified prior information is questionable, then, as in any Bayesian analysis, the prior
should be checked to see if it conflicts with the likelihood as a part of assessing sensitivity
of inferences to the prior.

In the next section we describe the basic way that we specify predictive information in
the later examples. We also review relevant concepts of Bayesian predictive model check-
ing, since the results of certain model checks for hypothetical data summaries are the way
that we formulate predictive constraints. Section 3 gives a brief introduction to the litera-
ture on history matching and regression ABC methods. Section 4 then discusses the new
approach using history matching and regression ABC for prior choice. Section 5 describes
some examples and Section 6 concludes.

2 Prior information and Bayesian model checks

Consider, for a parameter of interest $\theta$, a class of prior distributions $p(\theta|\lambda)$ indexed by a
hyperparameter $\lambda \in \Lambda$. The problem of prior choice is to choose $\lambda$. In predictive elicitation
the choice will be based on some characteristics of prior predictive distributions of data
or summaries of the data; see Kadane and Wolfson (1998, p. 4) for a discussion of the
distinction between predictive and structural elicitation. Here we will describe one useful
way of formulating predictive constraints for elicitation purposes, and certainly there may
be others. The idea is to use the results of model checks for specified hypothetical data as a
way of defining what it means for a prior elicitation to be good enough. In a sense, we treat
the problem of elicitation as one of model checking (for hypothetical data).

Suppose there are some summary statistics $S^j = S^j(y)$, $j = 1, \ldots, J$ of the hypothetical
data $y$, with density $p(y|\theta)$, and that for these summary statistics we are able to say for each
one whether certain values should be considered plausible or not under the prior if they were
to be observed. For $S^j$ we have a vector $h^j$ of hypothetical values supplied by an expert,
which we partition as \( h^j = (h^j_I, h^j_P) \), where \( h^j_I \) is a vector of values considered as implausible by the expert, and \( h^j_P \) is a vector of values considered to be plausible. We write \( B^j_I \) for the length of \( h^j_I \), \( B^j_P \) for the length of \( h^j_P \), \( B^j = B^j_I + B^j_P \), and \( B = \sum_{j=1}^J B^j \) for the total number of constraints.

In the expository example of the introduction, we considered a Binomial\((n,p)\) model parametrized through \( \beta = \log(p/(1-p)) \) with prior \( \beta \sim N(0,\sigma^2_\beta) \). Our suggested summary statistic for the elicitation was the estimated variance of the MLE, \( \hat{p}(1-\hat{p})/n \) where \( \hat{p} = y/n \), and a prior predictive distribution concentrated near zero would indicate an inappropriately large value for \( \sigma^2_\beta \) as this corresponds to most of the prior mass on \( p \) being near 0 or 1. A suitably small implausible value for the summary here could be obtained by determining a quantile of the summary statistic when the true \( p \) is close to 0 or 1, say 0.01 or 0.99.

We need to be precise about what plausible and implausible mean. Here the meaning of these terms arises from a prior predictive check (Box 1980). Let \( p(S^j|\lambda) \) be the prior predictive distribution for \( S^j \) under the prior \( p(\theta|\lambda) \), i.e.

\[
p(S^j|\lambda) = \int p(S^j|\theta)p(\theta|\lambda) \, d\theta.
\]

In the definition, the parameter \( \theta \) in the sampling distribution for \( S^j \) given \( \theta \) is integrated out according to the prior \( p(\theta|\lambda) \). The prior predictive \( p(S^j|\lambda) \) describes beliefs about \( S^j \) before any data are observed under the assumed prior \( p(\theta|\lambda) \), and is usually not available in closed form. Consider the \( p\)-values

\[
p^j_{I,b}(\lambda) = P(\log p(S^j|\lambda) \leq \log p(S^j = h^j_{I,b}|\lambda)), \tag{1}
\]

for \( S^j \sim p(S^j|\lambda) \) and \( j = 1, \ldots, J, b = 1, \ldots, B^j_I \) and

\[
p^j_{P,b}(\lambda) = P(\log p(S^j|\lambda) \leq \log p(S^j = h^j_{P,b}|\lambda)), \tag{2}
\]
where again \( S^j \sim p(S^j|\lambda) \) and \( j = 1, \ldots, J, \ b = 1, \ldots, B^j_p \). These \( p \)-values give a measure of how far out in the tails of \( p(S^j|\lambda) \) the various hypothetical summary values are, and hence how surprising they are. The \( p \)-values (1) and (2) are not easy to calculate, and simulation-based methods for approximating them are considered later. We define a “reasonable” prior \( p(\theta|\lambda) \) in light of the available prior information to be one for which given some appropriate cutoff value \( \alpha \), we have \( p^j_{I,b}(\lambda) < \alpha \) for \( j = 1, \ldots, J, \ b = 1, \ldots, B^j_I \) and \( p^j_{P,b}(\lambda) \geq \alpha \), \( j = 1, \ldots, J, \ b = 1, \ldots, B^j_P \) (i.e. the values \( S^j = h^j_{I,b} \) result in failing a prior predictive check at the cutoff \( \alpha \) for \( j = 1, \ldots, J, \ b = 1, \ldots, B^j_I \) and the values \( S^j = h^j_{P,b} \), \( j = 1, \ldots, J, \ b = 1, \ldots, B^j_P \) do not fail such a check). Here \( \alpha \) is chosen according to the degree of surprise that is considered relevant for the information we want to put into the prior. It is possible also to use a different cutoff \( \alpha \) for different checks (and in fact, when eliciting plausible and implausible summaries from an expert, values of \( \alpha \) would need to be given in order to explain to them what plausible and implausible means). The passing and failing of certain prior predictive checks for hypothetical data summaries represent constraints on what we consider a reasonable prior to be, and we wish to develop methods for searching the hyperparameter space to find corresponding priors satisfying our constraints. The summary statistics can either be univariate or multivariate. However, considering a vector valued \( S^j \) is more difficult computationally than considering univariate summaries due to the need to estimate the prior predictive density in (1) and (2). In our later examples we generally choose univariate \( S^j \). More comments on this, and a cautionary example, are given in Section 5.2. Generally we would want to choose the summary statistics \( S^j \) to be reflecting variation related to the parameter \( \theta \). This suggests making these summaries sufficient statistics, although non-trivial minimal sufficient statistics do not exist in many problems. Possible choices of the summaries include indicators for the data \( y \) belonging to some set (a suggestion made by an anonymous referee), or functions of a point estimator if these are available. Regarding the choice of the hypothetical values, if both plausible and implausible values are specified for
a given summary as a pair to convey information about the end point of a plausible range, then making these close together is more constraining. It is important, however, that the chosen values do not represent information more precise than an expert actually possesses.

The $p$-values (1) and (2) are examples of prior predictive $p$-values (Box 1980) and such $p$-values have in particular found use in the checking for prior-data conflicts when the summary statistic is a minimal sufficient statistic (Evans and Moshonov 2006) and for giving a precise formulation of the notion of a weakly informative prior (as in Evans and Jang (2011), inspired by earlier work of Gelman (2006)). When expressing prior information in terms of the results of model checks, the distinction between kinds of checks appropriate for different purposes is related to the choice of summary statistics. This is discussed further in Section 6. In the application here to problems of prior choice it is natural for us to focus on prior predictive checking. However, see also the discussion papers of Gelman et al. (1996) and Bayarri and Berger (2000) or Chapter 5 of Evans (2015) for a variety of perspectives on the broader problem of Bayesian model checking and different types of model checks. Now that we have outlined how we specify predictive constraints through prior predictive checks, we need effective methods to search the space of possible priors. Our approach adapts the technique of history matching for computer models for this task and this is described next.

3 History matching and regression ABC methods: An overview

3.1 History matching

History matching (Craig et al. 1997) is a method used in the literature for assessing computer models. A computer model or simulator is a complex computer code that takes one or more inputs, which we denote as $\lambda$, and produces a set of outputs $\eta(\lambda) = (\eta_1(\lambda), \ldots, \eta_k(\lambda))^T$. We
are reusing our previous notation for prior hyperparameters deliberately here. In a history match there are some observed data \( y \), intended to correspond to the computer model outputs, and a so-called implausibility measure, which measures the degree of mismatch between the observations and the computer model output. The implausibility measure may be based on some implicit or explicit model allowing for measurement error, ensemble variability (the inherent variability of \( \eta(\lambda) \) when run multiple times at the same \( \lambda \) when the simulator is stochastic) and model discrepancy (a model term which represents beliefs about lack of fit of the simulator when run at its best input values). In the case of a computationally expensive model, we may also wish to use a flexible interpolator such as a Gaussian process (Rasmussen and Williams 2005) to interpolate or smooth the model outputs \( \eta(\lambda) \) based on simulator runs at a limited number of inputs to reduce computational demands. Such a model is called an emulator, and emulation uncertainty at inputs where the computer model has not been run can also be included within the implausibility measure.

History matching proceeds in waves, starting with a space-filling design covering the range of model inputs (\( \Lambda \)), and at each wave comes up with a current non-implausible region for the inputs, reducing the size of the non-implausible region at each stage. The phrase non-implausible rather than plausible is used since the non-implausible region consists only of the region of the space not ruled out yet as unsuitable. The iterative aspect of the process allows us to place more points adaptively in “promising” regions of the input space \( \Lambda \), something which is important when \( \lambda \) is high dimensional. If emulation is used for a computationally expensive model, performing more model evaluations in the interesting part of the space allows the quality of emulation to improve as more waves are considered. Thresholds on the implausibility measure determining the current implausible region may become more stringent as the waves proceed, and different observations may also be introduced sequentially in this process. The philosophy of history matching is not to find a “best input” for the model, but to explore the space of non-implausible values for the model parameters. The
non-implausible region at the end of the process may be empty if there are no parameters providing an adequate fit to the outputs. A history match can be instructive for guiding model development, and if a model is good enough to warrant the computational expense of calibration then the history match can be useful for developing efficient computational algorithms. History matching has been successfully used in petroleum reservoir modelling (Craig et al. 1997), galaxy formation models (Vernon et al. 2010, 2014), rainfall-runoff models (Goldstein et al. 2013), climate models (Williamson et al. 2013) and infectious diseases models (Andrianakis et al. 2015) among other applications. Relationships between history matching and approximate Bayesian computation (ABC) algorithms have been considered recently by Wilkinson (2014) and Holden et al. (2015).

Given an implausibility measure $I(\lambda)$, history matching proceeds in the following way.

1. Initialization. Set $w = 1$ and generate a collection of $r$ points $\lambda^{(1)}_1, \ldots, \lambda^{(1)}_r$ for $\lambda$ according to a space-filling design covering the range of the inputs, $\Lambda$.

2. Until some stopping rule is satisfied:
   
   (a) Calculate $I(\lambda^{(w)}_1), \ldots, I(\lambda^{(w)}_r)$.
   
   (b) Choose some subset of the collection of the current inputs, $\lambda^{(w)}_1, \ldots, \lambda^{(w)}_q$, as non-implausible based on thresholding the implausibility measure. This set of points is used to define a current non-implausible region $\Lambda^{(w)}$.
   
   (c) Generate points $\lambda^{(w+1)}_1, \ldots, \lambda^{(w+1)}_r$ according to a new space-filling design covering $\Lambda^{(w)}$ and set $w = w + 1$.

In Section 4 we describe how we implement the steps in the procedure above for our later applications. There are a variety of approaches in the existing history matching literature for the construction of the implausibility measure, the construction of space filling designs and other choices. In different applications the implausibility measure might change between
iterations or only a subset of observations might be considered in the early stages and the implausibility thresholds might change between iterations. In our later applications, at wave \( w \), the wave \( w + 1 \) samples are generated directly from the current ones without explicitly defining the set \( \mathbf{A}^{(w)} \), and so we don’t describe how this set is sometimes constructed in the history matching literature. A variety of approaches to this issue may be found in the above references. If an emulator is used in evaluation of the implausibility measure, additional model evaluations could be made at step 2 (b) for the current non-implausible points and the emulator updated appropriately. These additional model evaluations and updating of the emulator may be particularly important in the case of high-dimensional models, and the task of emulation becomes much simpler as the interesting region of the space shrinks over successive waves. See Algorithm 1 of Drovandi et al. (2017) for a typical implementation of history matching with sequential updating of an emulator.

3.2 Regression ABC methods

ABC methods are used in the Bayesian analysis of models where the likelihood is intractable (Tavaré et al. 1997; Pritchard et al. 1999; Beaumont et al. 2002). The basic idea of simple ABC methods is to conduct forward simulations from the model according to parameter values sampled from the prior and to then see whether the simulated data are similar to the observed data. If it is, then the parameter value that generated the simulated data is retained as one that might plausibly have generated the data. A recent review of these methods is given by Marin et al. (2011), but here we confine ourselves to describing only some regression based approaches used in the ABC literature which are relevant to the calculations done in the next section (Beaumont et al. 2002; Blum and François 2010).

Suppose that \( p(\mathbf{\theta}|\mathbf{\lambda}) \) is the prior, \( p(\mathbf{y}|\mathbf{\theta}) \) is the data model and \( \mathbf{y}_{\text{obs}} \) is the observed data. In ABC one simulates \( (\mathbf{\theta}_i, \mathbf{y}_i), i = 1, \ldots, I \) from the prior and then the simulated data are reduced to a summary statistic \( S_i = S(\mathbf{y}_i) \) with \( S_{\text{obs}} = S(\mathbf{y}_{\text{obs}}) \). The role of summary
statistics in an ABC analysis is to reduce the dimensionality of the data, and ideally the summary statistics should be nearly sufficient for $\theta$. The idea of regression based ABC methods is to use regression to obtain a conditional density estimate of $\theta$ given $S_{\text{obs}}$ (i.e. to approximate the posterior distribution $p(\theta|S_{\text{obs}})$). We assume that $S_{\text{obs}}$ contains most of the relevant information about $\theta$ in $y_{\text{obs}}$. Blum and François (2010), extending methods originally due to Beaumont et al. (2002), consider the regression model

$$\theta_i = \mu(S_i) + \sigma(S_i)\epsilon_i,$$

where $\mu(\cdot)$ and $\sigma(\cdot)$ are flexible mean and standard deviation functions (which they parametrize using neural networks) and the $\epsilon_i$ are zero mean variance one residuals. It is assumed above that $\theta$ is a scalar parameter, but extensions to the multivariate case are straightforward in which $\mu(S)$ and the $\epsilon_i$ are multivariate and $\sigma(S)$ is a matrix square root of the covariance matrix of $\theta$ given $S$. To obtain an approximate sample from $\theta|S_{\text{obs}}$, which we write as $\theta^a_i$, $i = 1, \ldots, I$ (i.e. an approximate sample from the posterior) we can consider fitting the regression model to obtain estimates $\hat{\mu}(\cdot)$ and $\hat{\sigma}(\cdot)$ of $\mu(\cdot)$ and $\sigma(\cdot)$ respectively, and then use empirical residuals in the fitted regression at $S = S_{\text{obs}}$:

$$\theta^a_i = \hat{\mu}(S_{\text{obs}}) + \hat{\sigma}(S_{\text{obs}})\hat{\epsilon}_i = \hat{\mu}(S_{\text{obs}}) + \hat{\sigma}(S_{\text{obs}})\hat{\sigma}(S_i)^{-1}(S_i - \hat{\mu}(S_i)),$$

$i = 1, \ldots, I$. In the discussion above it is also possible to localize the regression using a kernel function and attach weights to the adjusted sample values $\theta^a_i$ (Blum and François 2010).

Nott et al. (2017) consider related methods for repeated conditional density estimation when we want to simulate from a data model for different values of a parameter and where that is expensive. For approximate simulation from the data model the roles of $S$ and $\theta$ are

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reversed in (3). Considering a univariate summary statistic,

\[ S_i = \mu(\theta_i) + \sigma(\theta_i)\epsilon_i, \] (4)

and then for a given \( \theta \) an approximate sample from \( S \) given \( \theta \) would be

\[ S_i^a = \hat{\mu}(\theta) + \hat{\sigma}(\theta)\hat{\sigma}(\theta_i)^{-1}(S_i - \hat{\mu}(\theta_i)), \]

for estimates \( \hat{\mu}(\theta) \) and \( \hat{\sigma}(\theta) \) of \( \mu(\theta) \) and \( \sigma(\theta) \). In the next section we use a model similar to (4) to simulate in a computationally thrifty way from a prior predictive distribution \( p(S|\lambda) \) for summary statistics \( S \) conditional on a prior hyperparameter \( \lambda \) with \( \theta \) integrated out according to the prior \( p(\theta|\lambda) \). Such approximate prior predictive samples are useful for estimating \( p(S_j|\lambda) \) (a quantity which appears in our prior predictive \( p \)-values (1) and (2)) and hence for choosing an appropriate value of \( \lambda \).

4 Proposed algorithm for prior choice

Our proposed algorithm applying history matching for prior choice will now be described. Let \( \lambda \) denote the prior hyperparameters in a problem of prior choice. Given \( \lambda \) we can compute certain features of prior predictive distributions as outputs of the Bayesian model. In the procedure of Section 2 we may consider the outputs to be the \( p \)-values in equations (1) and (2). From these an implausibility measure can be constructed based on desired constraints for the outputs. Later we use the implausibility measure

\[ I(\lambda) = \sum_{j=1}^{J} \sum_{b=1}^{B_j} \max(0, p_{l,b}^j(\lambda) - \alpha) + \sum_{j=1}^{J} \sum_{b=1}^{B_{P_j}} \max(0, \alpha - p_{P,b}^j(\lambda)) \] (5)
and we note that $I(\lambda)$ is 0 if the constraints considered in Section 2 are satisfied, i.e. $p_{l,b}^j(\lambda) < \alpha, j = 1, \ldots, J, b = 1, \ldots, B_l^j$ and $p_{p,b}^j(\lambda) \geq \alpha, j = 1, \ldots, J, b = 1, \ldots, B_P^j$, with $I(\lambda) > 0$ if one or more of these constraints are violated.

Consider once more the expository example of the introduction. There we considered for the binomial model Binomial($n, p$) parametrized by $\beta = \log(p / (1 - p))$ the summary statistic $\hat{p}(1 - \hat{p})/n$ with $\hat{p} = y/n$, and suggested defining some small value of this statistic as implausible as a way of constraining the prior to not place too much mass near values for $p$ of 0 or 1. In this example there is just a single $p$-value, corresponding to an implausible summary, and the above implausibility measure is given by this $p$-value minus $\alpha$ if the $p$-value is bigger than $\alpha$, and zero otherwise.

The search for prior hyperparameters satisfying the constraints can be performed using the methods of history matching with the implausibility measure (5). One might object that the threshold $\alpha$ used in our implausibility is somewhat artificial. However it should be kept in mind that this threshold is not used in a binary decision making context here, and that the purpose of $I(\lambda)$ is just to guide the search to a fruitful region of the hyperparameter space. Obtaining an exactly 0 value of $I(\lambda)$ may not be so important. The use of $p$-values in $I(\lambda)$ is convenient for the way that it puts information from the different summary statistics on the same scale, and we have found the choice (5) for the implausibility measure to be useful although there are certainly other ways that the implausibility could be defined.

Steps 2 b) and c) of the history matching algorithm given in Section 3.1 for wave $w$ are implemented in our later examples in the following way. First, choose some fraction $\gamma$ of $r$ in such a way that both $1/\gamma$ and $Q = \gamma r$ are integers. For instance, in the first example of Section 5 we use $\gamma = 0.1$ and $r = 100$. Next, choose the $Q$ values of $\lambda$ in the current wave for which $I(\lambda)$ is smallest. Write these values as $\lambda_{1}^{*(w)}, \ldots, \lambda_{Q}^{*(w)}$. Then for each of $q = 1, \ldots, Q$, generate $1/\gamma$ values from a normal distribution $N(\lambda_{k}^{*(w)}, \Sigma^{(w)})$ where $\Sigma^{(w)} = h^2 V_w, V_w$ is the sample covariance matrix of all the wave $w$ samples, and $h = \left(\frac{4}{(2d+1)Q}\right)^{1/(d+4)}$ where $d$
is the dimension of \( \lambda \). Note that this results in \( Q/\gamma = r \) samples that we take as the wave \( w + 1 \) samples. In our later examples we use the modified sampling approach in the \texttt{mvnorm} function in the R package \texttt{MASS} (Venables and Ripley 2002) with the option \texttt{empirical=TRUE} to obtain generated samples that have exactly the sample covariance matrix \( \Sigma^{(w)} \). The definition of \( \Sigma^{(w)} \) in the sample generation step is obtained by inflating an automatic choice of kernel bandwidth used in the multivariate kernel density estimation literature by a factor of 4 (Silverman 1986). There are other ways to generate a space-filling design for each wave; the idea above and that we implement later in examples is a simple one based on a similar suggestion in Andrianakis et al. (2015) based on perturbing values according to a normal kernel with enough variability to ensure that the new points are sufficiently different to the current one. The intuition behind our choice for \( h \) is that after pruning away the implausible samples in the current wave, we want to generate a set of points for the next wave that covers the distribution for the current set of non-implausible samples. The kernel estimate with bandwidth choice given above is just to make the next wave samples somewhat overdispersed compared to the distribution of current non-implausible samples. Note that if we were to simulate from the kernel density estimate fitted to the current non-implausible samples, that would correspond to choosing one of the non-implausible samples at random and then drawing from a normal density centered on that sample. Instead of choosing a point randomly in this process, if we ensure all the non-implausible samples are represented equally when drawing the next wave samples, we arrive at the procedure we have suggested above. Inflating the bandwidth choice of Silverman (1986) by 4 doubles the marginal standard deviations used in local perturbations of the current samples in the process of simulating the next wave samples. It is difficult to say anything about optimality of our suggested choice of \( h \). A larger value of \( h \) will ensure that the non-implausible region is not collapsed down too quickly, at the expense of additional computations. How quickly we should narrow down the non-implausible region also interacts with how many samples are used in the initial space-
filling design, and how smooth the implausibility measure is. The only remaining detail to specify in the algorithm is the stopping rule. A useful stopping rule is to stop when either a zero implausibility value has been found, or if there has been no further decrease in the minimum implausibility value found for a certain number of waves.

Computing the implausibility measures in the application of history matching to prior choice as discussed in Section 3 involves computation of the $p$-values in equations (1) and (2) for a large number of different values of $\lambda$ and this can be computationally burdensome. Our solution is to use the regression approximate Bayesian computation (ABC) methods introduced in Section 3.2 to approximate these $p$-values in a computationally thrifty way. The methods considered are based on those developed in Nott et al. (2017), and play a similar role in our later examples to the role of emulators in history matching for computationally expensive computer models.

Suppose we wish to approximate $I(\lambda)$ for a possibly large set of different $\lambda$ values, $\lambda^n$, $n = 1, \ldots, N$. These values might be a grid over the region of interest for $\lambda$ if $\lambda$ is low-dimensional, or in the history matching procedure they might be the hyperparameter values generated in the current wave. Let $p(\lambda)$ be a pseudo-prior for $\lambda$ which covers the range of the values of $\lambda$ of interest. This pseudo-prior is not to be used for inference but is used in generation of samples of the summaries $S^j$. We simulate values $(\lambda_i, \theta_i, y_i)$ from $p(\lambda)p(\theta|\lambda)p(y|\theta)$, $i = 1, \ldots, I$ independently. From the $y_i$ we obtain simulated summaries $S^j_i = S^j(y_i)$, $i = 1, \ldots, I$, $j = 1, \ldots, J$. We can obtain an approximate sample from $p(S^j|\lambda)$ for any given value of $\lambda$ by considering the regression adjustment methods of Section 3 applied to the regression model

$$S^j_i = \mu^j(\lambda_i) + \sigma^j(\lambda_i)\epsilon_i,$$

where the $\epsilon_i$ are independent and identically distributed errors with mean zero and variance
one and $\mu^j(\lambda)$ and $\sigma^j(\lambda)$ are flexible mean and standard deviation functions. This is similar to the regression adjustment approach considered for equation (4) in Section 3 applied to the marginalized model for the summaries where $\theta$ has been integrated out according to $p(\theta|\lambda)$. Extension to the case where $S^j_i$ is multivariate can also be considered but in our later examples the $S^j_i$ are each univariate summaries. Fitting the regression model locally, based on a certain number of nearest neighbours of $\lambda$, is often useful. This is something we consider later in the examples with a nearest neighbour distance following the default choice in the R package abc (Csilléry et al. 2012). Although we do not describe in detail the implementation of regression adjustment in the abc package, for the method of Blum and François (2010) $\mu^j(\cdot)$ and $\sigma^j(\cdot)$ are parametrized by neural network models, and these functions are estimated in a two step procedure. In the first step, the mean function is estimated assuming the variance is constant. Then the logarithm of the variance function is estimated by fitting a second neural network model to the logarithm of the squared residuals from the first stage fit. The fitting can be localized, in the sense that only a certain number of nearest neighbour points closest to the target covariate value are used (where closest is in the sense of a scaled Euclidean distance, with the scaling for each covariate based on the mean absolute deviation of values for the covariate). The abc package also implements linear regression (Beaumont et al. 2002) and other regression adjustments. In general, there can be a trade-off between the flexibility of the regression model used for the adjustment, and the size of the neighbourhood required with less flexible regression models requiring smaller neighbourhoods. As mentioned above we use the default tuning parameter values implemented in the abc package and refer the reader to Csilléry et al. (2012) for further details.

An approximate sample from $p(S^j_i|\lambda^n)$ is

$$\hat{S}^j_{i,n} = \hat{\mu}^j(\lambda^n) + \hat{\sigma}^j(\lambda^n)\hat{\sigma}(\lambda_i)^{-1}(S^j_i - \hat{\mu}^j(\lambda_i)), \quad i = 1, \ldots, I, \quad j = 1, \ldots, J$$

(6)
and then we can construct a kernel density estimate of \( p(S^j|\lambda^l) \), written \( \hat{p}(S^j|\lambda^l) \), from these approximate samples. The kernel density estimate is constructed independently for each summary statistic. How close this kernel density estimate is to the predictive density it approximates depends on how well the regression adjusted samples approximate a draw from the predictive density, as well as other factors such as the kernel, sample size and bandwidth choice. The quality of the regression adjusted samples for approximating a sample from the true prior predictive can be very good if the regression fitting is done in a small neighbourhood and that neighbourhood contains a large number of samples. If the predictive density varies smoothly with \( \lambda \) then the predictive density changes very little throughout a small neighbourhood of the targeted \( \lambda \) value. When fitting locally with sufficient samples the regression adjustment has little effect and the regression adjusted sample is indistinguishable from a sample from the true prior predictive as the neighbourhood shrinks. Of course, achieving a very small neighbourhood size containing a large number of samples in local fitting involves simulating a large number of summary statistic values and a heavy computational burden.

The computation of the estimated \( p \)-values \( \hat{p}^j_{I,b}(\lambda^n), j = 1, \ldots, J, b = 1, \ldots, B^j_I \) and \( \hat{p}^j_{P,b}(\lambda^n), j = 1, \ldots, J, b = 1, \ldots, B^j_P \), can be performed using the following algorithm.

1. Given the input hyperparameter \( \lambda^n \), obtain approximate samples \( \hat{S}^{j,n}_i, i = 1, \ldots, I \) from \( p(S^j|\lambda^n), j = 1, \ldots, J \), according to (6).

2. For each statistic \( S^j, j = 1, \ldots, J \), calculate a kernel estimate of \( p(S^j|\lambda^n) \) at \( \hat{S}^{j,n}_i \),

\[
\hat{p}(\hat{S}^{j,n}_i|\lambda^n), i = 1, \ldots, I, h^j_{I,b}, b = 1, \ldots, B^j_I \text{ and } h^j_{P,b}, b = 1, \ldots, B^j_P.
\]

3. Calculate

\[
\hat{p}^j_{I,b}(\lambda^n) = \frac{1}{I} \sum_{i=1}^I I(\log \hat{p}(S^j = \hat{S}^{j,n}_i|\lambda^n) \leq \log \hat{p}(S^j = h^j_{I,b}|\lambda^n)), \ j = 1, \ldots, J, \ b = 1, \ldots, B^j_I,
\]
and

\[ \hat{p}_{P,b}^j(\lambda^n) = \frac{1}{I} \sum_{i=1}^{I} I(\log \hat{p}(S^j = \hat{S}^j_i | \lambda^n) \leq \log \hat{p}(S^j = h_{P,b}^j | \lambda^n)), \quad j = 1, \ldots, J, \quad b = 1, \ldots, B_P. \]

Given the estimated \(p\)-values for a certain \(\lambda^n\) we can check whether it is acceptable according to our criteria by checking if \(\hat{p}_{L,b}^j(\lambda^n) < \alpha, \quad j = 1, \ldots, J, \quad b = 1, \ldots, B_L\) and \(\hat{p}_{P,b}^j(\lambda^n) \geq \alpha, \quad j = 1, \ldots, J, \quad b = 1, \ldots, B_P\). An approximate implausibility value \(I(\lambda^n)\) can also be computed from the \(p\)-values. Note that the regression ABC computations are being used in a screening process to remove highly implausible values of the hyperparameters and high precision is not needed. Once a hyperparameter value is chosen based on the regression calculations as giving a prior satisfying the desired constraints we can check its suitability. We can do this by generating a large number of values of \(S^j, \quad j = 1, \ldots, J\) from the prior predictive distribution for the chosen \(\lambda\), and from these approximate the \(p\)-values accurately, to check that the regression approximations were good enough. Such a procedure would not be feasible for a large number of different candidate values of \(\lambda\), which is why the regression approximations are used within the history matching algorithm. However, after the history matching is completed and we have identified one or a small number of suitable \(\lambda\), it is quite feasible to generate a large sample from the prior predictive distribution for these, without using the regression methods, in order to confirm their suitability.

The approach we have described of approximating prior predictive samples based on local regression adjustments can fail when the prior predictive density changes rapidly as a function of \(\lambda\), and it may also be difficult to apply in high dimensions. It is also assumed above that summary statistics are generated once at the beginning of the history match according to values for \(\lambda\) simulated under the pseudo-prior \(p(\lambda)\). It was mentioned in Section 3 that a powerful aspect of history matching is the way that additional model evaluations (or summary statistic simulations in the present case) can be made as the waves of the history
matching proceed. That is, we can generate additional summary statistic simulations at each of the current non-implausible $\lambda$ values in the history matching waves to improve the quality of the regression adjustment approach for approximating the prior predictive distribution in the interesting parts of the hyperparameter space. This is most interesting when the number of hyperparameters is large, and for our highest dimensional example later (with four hyperparameters) we consider such an approach. Emulation methods are thoroughly developed in the existing literature for deterministic computer models. However, where stochastic models are considered, and the task is to emulate the distribution of an output as a function of inputs, simple methods such as just emulating means and variances are often considered. This may be sufficient, depending on what is required for the chosen implausibility measure. In our application, capturing more complex features of the prior predictive density becomes important. The regression ABC approach outlined here is not the only one that could be considered. However, a comparison of different conditional density estimation methods in this application is beyond the scope of the present work.

5 Examples

We illustrate our methodology in three examples. In the first two examples there are just two hyperparameters to be chosen and we can plot the way that the predictive $p$-values in our checks vary with the hyperparameters over a grid; such plots are useful for checking the results of the history match. Both the $p$-values at the grid points in these plots, as well as the $p$-values used to approximate the implausibility measure for the history matching samples, are obtained using regression ABC approximations to the prior predictive densities of the summaries. In the third example there are four hyperparameters to be chosen, and consideration of a grid of hyperparameter values is no longer feasible.
5.1 Logistic regression example

We consider a logistic regression for an experiment described in Racine et al. (1986) where 5 animals at each of 4 dose levels were exposed to a toxin. We write the dose levels as $x_1 < x_2 < x_3 < x_4$ and assume that these values have been transformed to a log scale, centered and scaled as in Gelman et al. (2008). If $y_i$ is the number of animals killed at dose level $x_i$, the data model is $y_i \sim \text{Binomial}(5, p_i)$ with $\log(p_i/(1-p_i)) = \beta_0 + \beta_1 x_i$. Gelman et al. (2008) consider a prior on $\beta$ where $\beta_0$ and $\beta_1$ follow independent Cauchy distributions centered on zero with scale $\lambda_1 = 10$ and $\lambda_2 = 2.5$ respectively. Here we consider $\lambda = (\lambda_1, \lambda_2)$ as hyperparameters to be chosen, with $\lambda \in [0.5, 10] \times [0.5, 10]$.

Our elicitation method requires us to specify some hypothetical data to be plausible or implausible under the prior. Write $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1)$ for the posterior mode of $\beta$ based on independent normal $N(0, 100)$ priors on $\beta_0, \beta_1$. Note that the normal prior here is used only in the computation of $\hat{\beta}$: the parametric prior family being used in the elicitation is the Cauchy family described above. Note that $\hat{\beta}$ is similar to the MLE in non-degenerate settings but will exist even when the MLE does not. For each dose $x_i$, let $\hat{p}_i = 1/(1+\exp(-\hat{\beta}_0 - \hat{\beta}_1 x_i))$ be the corresponding fitted probability of death at dose $x_i$ under the fitted model. Let us consider the summary statistic $S^1 = \sum_{i=1}^4 5\hat{p}_i(1-\hat{p}_i)$ which is the sum of the variances of the responses when $\beta = \hat{\beta}$. The statistic $S^1$ will tend to be small if all the responses are close to either zero or the maximum value of 5 resulting in fitted probabilities at the different dose levels all close to zero or one. If all $\hat{p}_i$ are equal to either 0.01 or 0.99, then the value of $S^1$ would be 0.198 and we might wish the prior to express the information that this is an implausible value for $S^1$. The summary $S^1$ is the natural extension to the logistic regression case of the summary statistic used in the expository example of the introduction.

In this example we might also expect that it would not be surprising if the fitted probability of death goes from a value near zero at the lowest dose to a value near 1 at the highest dose, in a fairly smooth way. If $\hat{p}_1 = 0.01, \hat{p}_2 = 0.25, \hat{p}_3 = 0.75$ and $\hat{p}_4 = 0.99$, then the cor-
responding value of $S^1$ would be 1.974. We consider a prior within our framework in which $S^1 = 0.198$ is considered to be implausible, and $S^1 = 1.974$ is considered to be plausible. This is weak prior information, but enough to constrain hyperparameter choice in a useful way. Although it is discrete, $S^1$ is treated as a continuous quantity in our calculations. This is a reasonable approximation when the number of different possible values is large, as here.

For the hypothetical data summary $S^1 = 0.198$, we compute the predictive $p$-value for the summary statistics chosen using the method of Section 4 and using a grid of 10,000 $\lambda$ values in our target range $\lambda \in [0.5, 10] \times [0.5, 10]$ with the grid formed from 100 equally spaced values in each dimension. The regression adjustment calculations for computation of the $p$-values are done using the default implementation of the abc function in the abc R package (Csilléry et al. 2012). We used 400,000 simulated values of the summary statistic $S^1$, local linear regression adjustment and 1,000 nearest neighbours in the localized regression ABC procedure. This means that in (6) the mean and log standard deviation functions $\mu^j(\lambda)$ and $\log \sigma^j(\lambda)$ are assumed to be linear functions of $\lambda$, and the regression is fitted based on the nearest 1000 neighbours to the target $\lambda$ values. Nearest means in the sense of scaled Euclidean distance, where each component of $\lambda$ is being scaled by the mean absolute deviation. This is the default local linear regression adjustment implemented in the abc R package (Csilléry et al. 2012). A plot of how the $p$-value changes as a function of $\lambda$ is shown in the left panel of Figure 1. Note the two blue regions in the graph where the $p$-value is small; the region on the left occurs for hyperparameter values where 0.198 is an implausibly small value, whereas the region on the right occurs for hyperparameter values for which 0.198 is implausibly large. A similar plot of the $p$-value as a function of $\lambda$ for the check with $S^1 = 1.974$ is shown in the right panel. An acceptable value for $\lambda$ is a value in the dark grey region in the left panel (small $p$-value indicating a prior-data conflict) and avoiding the dark grey region in the right panel (a $p$-value which is not small indicating the absence of a conflict). The points overlaid on the graphs are obtained from using the
Figure 1: Prior predictive p-value as a function of $\lambda$ for logistic regression example. p-value for check for $S^1 = 0.198$ (left) and for $S^1 = 1.974$ (right). In both graphs the overlaid points are from the fourth wave of the history match and the minimum implausibility obtained is zero.

history matching method of Section 3. In the history match the algorithm is initialized with a maximin latin hypercube design of $r = 100$ points, $\gamma = 0.1$ and the points shown in the graph are the retained values after 4 waves. The $p$-values in the implausibility measure are again computed using the method of Section 4. The minimum implausibility obtained is 0, i.e. we are successful at finding hyperparameter values satisfying the constraints. As mentioned above, in considering this example Gelman et al. (2008) considered a default prior with $\lambda_1 = 10$ and $\lambda_2 = 2.5$. This is a weakly informative choice for the prior, and it can be seen from Figure 1 that to match the information we have suggested putting into our analysis a smaller value of $\lambda_1$ is needed. Also shown in Figure 2 are the marginal posterior distributions of $\beta_0$ and $\beta_1$ for the default prior with $\lambda_1 = 10$ and $\lambda_2 = 2.5$, as well as for two hyperparameter values obtained from the history match. The posterior distributions are computed for the observed data of $(y_1, y_2, y_3, y_4) = (0, 1, 3, 5)$. In this example it is seen that the prior information we have put in makes some difference to the resulting inference, particularly for the intercept.
5.2 Sparse signal shrinkage prior

Next we consider prior choice for a linear model with a sparse signal shrinkage prior on the coefficients. The shrinkage prior we consider is the horseshoe+ prior of Bhadra et al. (2015). The need in modern data analysis to consider increasingly complex models with respect to both the number of parameters and hierarchical structure has resulted in a very large literature on sophisticated shrinkage priors in a range of applications. We consider only the horseshoe+ prior for a high-dimensional linear model in this example, but the kind of analysis we do here could be done for other shrinkage priors, of which there are many. Bhadra et al. (2015) give a survey of the current state of the art in the area. We describe a general version of our model first which also incorporates observation specific mean shift terms that can account for outliers in the model, using similar ideas to those considered in She and Owen (2011). A simplified version of the model with two hyperparameters will be considered in this subsection, and the more general form of the model with four hyperparameters will be
considered in the next subsection.

For some \((M \times p)\) design matrix \(X\) consider the model

\[
y = \beta_0 1_M + X\beta + \delta + \epsilon, \tag{7}
\]

where \(y = (y_1, \ldots, y_M)^T\) is an \(M\)-vector of responses, \(\beta_0\) is an intercept term, \(1_M\) denotes an \(n\)-vector of ones, \(\beta\) is a \(E \times 1\) vector of regression coefficients, \(\delta = (\delta_1, \ldots, \delta_M)^T\) is an \(M\)-vector of mean shift parameters intended to be sparse and which allows for outliers in a small number of observations, and \(\epsilon \sim N(0, \sigma^2 I)\). The model is not identifiable unless sparsity assumptions are made for \(\delta\), and in the case where \(E > M\), which is the case we consider here, we also need to make some assumptions of sparsity for \(\beta\).

We consider a Bayesian analysis with priors \(\beta_0 \sim N(0, \sigma_0^2)\) and \(\sigma \sim HC(0, A_\sigma)\) (where \(HC(0, A_\sigma)\) denotes the half Cauchy distribution with scale parameter \(A_\sigma\)). The elements of \(\beta\) are independent in their prior, \(\beta_e \sim N(0, \sigma_e^2)\), with \(\sigma_e \sim HC(0, A_\beta \gamma_e)\), \(\gamma_e \sim HC(0, 1)\), \(e = 1, \ldots, E\), and \(A_\beta\) is a scale parameter to be chosen. Similarly in the prior for \(\delta\) the elements of \(\delta\) are independent in the prior with \(\delta_m \sim N(0, \tau_m^2)\), \(\tau_m^2 \sim HC(0, A_\delta \zeta_m)\), \(\zeta_m \sim HC(0, 1)\) for \(m = 1, \ldots, M\), where \(A_\delta\) is a hyperparameter to be chosen. The prior specification is complete once the hyperparameters \(\sigma_0^2, A_\sigma, A_\beta\) and \(A_\delta\) are fixed. In the current section we consider the model where \(\delta = 0\) and hence there is no need to set \(A_\delta\) and where \(\sigma_0^2\) is fixed at 100. The full model is considered further in the next subsection.

We consider choice of \((A_\sigma, A_\beta)\) in the context of the sugar data set considered in Brown et al. (1998). In this dataset there are \(E = 700\) predictors in the training sample, 3 response variables and 125 observations in the training set, so that we are considering a case where \(E > M\). We consider the response variable glucose and center and scale all columns of the design matrix. Now consider applying our method. For summary statistics, we define \(S^1\) to
be the log of the marginal variance of \( y \) averaging over the predictors, i.e. \( S^1 = \log s^2 \) where

\[
s^2 = \frac{1}{n-1} \sum_{j=1}^{M} (y_j - \bar{y})^2,
\]

where \( \bar{y} \) is the sample mean of \( y \). We take the log in defining \( S^1 \) since \( s^2 \) can have quite a heavy tailed prior predictive distribution due to the half-Cauchy prior on \( \sigma \). Some idea of the range of the responses marginally is very likely to be available in applications and so it may be easy to specify what would be plausible or implausible values for \( S^1 \). We consider \( S^1 = \log 16 \) to be plausible and \( S^1 = \log 50 \) to be implausible (the marginal variance for the observed data is about 16 here).

We also consider another summary statistic \( S^2 = S^2(y) \) defined as follows. This summary statistic is an adjusted \( R^2 \) type measure of how much variation is explained by the predictors, but one that is appropriate to the situation of more covariates than observations and which is based on a simple version of the refitted cross-validation method of Fan et al. (2012). Details of computation of this adjusted \( R^2 \) measure are given in the Appendix. We want to require that both \( S^2 = 0.05 \) as well as \( S^2 = 0.95 \) are plausible, so that the model allows both a small or large amount of variation in the response variable to be explainable through the regression \( a \ priori \).

Figure 3 shows plots of the \( p \)-values for the tests based on the four summary statistics as \((A_\sigma, A_\beta) \) vary. The plots are for \( 100 \times 100 \) grids equally spaced in each dimension for \((A_\sigma, \log A_\beta) \) covering the range \([0, 2] \times [-\log 100p, -\log p] \). The regression adjustment calculations for computation of the \( p \)-values are done using 100,000 evaluations of the summary statistics with local linear regression adjustments and 1,000 nearest neighbours. Similar to the last example overlaid on the graphs are the retained points from the third wave of a history match implemented in the same way as the previous example with \( r = 100 \) and \( \gamma = 0.1 \). The history match succeeds in finding prior hyperparameter values corresponding
Figure 3: Prior predictive $p$-value as a function of $(A_\sigma, A_\beta)$ for sparse signal shrinkage example. $p$-value for check for $S^1 = \log 16$ (top left), $S^1 = \log 50$ (top right), $S^2 = 0.05$ (bottom left) and $S^2 = 0.95$ (bottom right). In both graphs the overlaid points are from the third wave of the history match and the minimum implausibility obtained is zero. In the panels in the top row the contour line is at the level 0.05.
to priors which satisfy the constraints. In the top right plot we want to be in the darkest
grey region (i.e. the corresponding summary is implausible), and in the other plots we want
to avoid the darkest grey region (i.e. the corresponding summaries are plausible). In the
top two panels in Figure 3 the contour line is at the level 0.05, showing we have succeeded
in finding points satisfying the constraint.

It is interesting to see what happens in this example when we change the prior on $\beta$ to
$\beta_j \sim N(0, A_\beta)$, so that now $A_\beta$ is a scale parameter to be chosen in a normal prior, but
where our predictive constraints remain the same. We continue to use the notation $A_\beta$ for
the scale parameter in the prior on $\beta$ even though this is of course a different parameter
in the two priors. State of the art sparsity inducing priors like the horseshoe+ have good
frequentist performance in a number of senses as described in Bhadra et al. (2015). Here we
illustrate a more Bayesian way in which this prior is good in this example. Before we did
a history match in this example we expected that the normal prior would work poorly in
the sense of not being able to capture the information that either a large or small amount
of the variation in the response should be explainable through the covariates \textit{a priori}. Our
intuition was incorrect, and it was in fact possible to satisfy our constraints. The results of
wave 5 of our history match for the normal prior are shown in Figure 4.

However, now consider the following. If $S^1 = \log 16$ and $S^2 = 0.95$ should both be plau-
sible, perhaps we should also require that $(S^1, S^2) = (\log 16, 0.95)$ should be plausible in the
joint prior predictive for $(S^1, S^2)$. Figure 5 shows kernel estimates of the joint prior predictive
density for $(S^1, S^2)$ for the horseshoe+ and normal priors for two particular hyperparameter
values achieving zero implausibility, based on 1000 prior predictive samples. We can see
that $(S^1, S^2) = (\log 16, 0.95)$ is plausible for the horseshoe+ prior, but not for the normal
prior. The explanation for this is that it is only when the noise variance is small that the
regression can explain a lot of the variation in the case of the normal prior. The behaviour
of the horseshoe+ prior, however, is more acceptable. This example illustrates perhaps some
Figure 4: Prior predictive $p$-value as a function of $(A_\sigma, A_\beta)$ for normal prior example. $p$-value for check for $S^1 = \log 16$ (top left), $S^1 = \log 50$ (top right), $S^2 = 0.05$ (bottom left) and $S^2 = 0.95$ (bottom right). In both graphs the overlaid points are from the third wave of the history match and the minimum implausibility obtained is 0.
of the pitfalls of considering plausible and implausible values for one-dimensional summary statistics separately. While this is a useful strategy for defining constraints, and it makes computations more convenient, once a reasonable candidate hyperparameter value is found it may be useful to consider the behaviour of the joint prior predictive for several summaries simultaneously.

5.3 An example with higher-dimensional hyperparameter

Continuing the last example, consider the full model (7) described in Section 5.2 where now we allow \( \delta \) to be nonzero. We also consider the situation where \( \sigma_0^2 \) is not fixed in the prior for \( \beta_0 \). Now we have four hyperparameters to be chosen, \((\sigma_0, A_\sigma, A_\beta, A_\delta)\). Unlike the previous two examples with only two hyperparameters, it is not feasible to use a grid-based approach to produce plots of how the prior predictive p-values vary over the hyperparameters for
comparison with the results of the history match. We retain the summary statistics and constraints of Section 5.2, with the difference that $s^2$ is replaced by a robust measure of scale (the median absolute deviation estimator), and in the linear regression fits for the refitted cross-validation procedure we use the robust \texttt{lmrob} function in \texttt{R} (Rousseeuw et al. 2015) to obtain the adjusted $R^2$ estimate. We also add to the constraints of Section 5.2 three additional constraints. We choose a summary statistic $S^3$ to be the log of the absolute value of the median of the responses, and specify $S^3 = \log 15$ to be plausible, and $S^3 = \log 20$ to be implausible. As an additional summary statistic we use the following procedure. We consider the log sample kurtosis of the residuals obtained from the \texttt{lmrob} function averaged over 10 split samples using the same refitted cross-validation procedure as for the adjusted $R^2$ measure. This is intended to be some sample measure of the “tailedness” of the distribution. Writing $S^4$ for this statistic, we consider $S^4 = \log 50$ to be implausible. The value of $\log 50$ was obtained as the log of the approximate median of sample kurtosis values from a Cauchy distribution sample of size 125. Note that we use sample kurtosis here as a summary of the data without worrying about whether any corresponding population quantity exists. The information in this last summary statistic is intended to state the requirement that we should not have a very large proportion of very extreme outliers. Figure 6 shows pairwise scatter plots of the hyperparameter values on a log scale in wave 1 through wave 5 of a history match with $r = 1000$ and $\gamma = 0.1$ and the first wave initialized with a maximin latin hypercube design covering the range $[\exp(-3), \exp(2)] \times [\exp(-5), \exp(1)] \times [10^{-6}, 0.5] \times [10^{-6}, 0.5]$ for the hyperparameters. The history match succeeds in finding prior hyperparameter values corresponding to priors which satisfy the constraints.

In Section 4 it was mentioned that it may be helpful to adaptively generate new summary statistic simulations as the waves of the history match proceed. The results of Figure 6 were obtained without doing this, using 100,000 simulations at the beginning of the procedure. Figure 7 shows 8 waves of a history match where the initial number of summary statistic
Figure 6: Pairwise scatterplots of hyperparameters on log scale of wave 1 to wave 5 of the history match. The minimum implausibility value obtained in wave 5 is 0.
simulations was reduced to 10,000, with 1,000 additional simulations added at each wave (100 further simulations at each of the 10 non-implausible values retained at each wave). The results are similar to before, but now the total number of model simulations has been reduced to 18,000 rather than 100,000. Although this is not a very high-dimensional example, this illustrates the point that this adaptive approach to the model simulations to improve the quality of the regression ABC adjustment can be very important as the number of hyperparameters increases. Effectively the additional model simulations allow us to use smaller neighbourhoods in this local nonparametric procedure. Any approach to flexible conditional density estimation could be used instead of the regression ABC approach for approximating the prior predictive densities as a function of the hyperparameters, but any such alternative method will also benefit from additional model simulations in the important region of the space. Figure 8 shows estimated prior predictive densities of the summary statistics used in the history match obtained from one of the hyperparameter values with implausibility zero in Figure 6, \((\sigma_0, A_\sigma, A_\beta, A_\gamma) = (3.91, 0.016, 0.000013, 0.000045)\). The graphs presented are histograms and kernel density estimates based on 1000 prior predictive samples.

6 Discussion

We have considered a novel application of the ideas of history matching used in the assessment of computer models to the problem of prior choice. By defining the implausibility measure in the history match through some prior predictive constraints, we are able to implement predictive elicitation even for complex models. Regression adjustment ABC methods are also used to ease the computational burden in application of the method. We believe the analyses presented in some of the examples are insightful, and in some cases led to some new understanding of the effects of the parameter prior on the prior predictive densities.
Figure 7: Pairwise scatterplots of hyperparameters on log scale of wave 1 to wave 8 of the history match with additional model simulations at each wave. The minimum implausibility value obtained in wave 8 is 0.
Figure 8: Prior predictive densities of $S_1$, $S_2$, $S_3$, $S_4$ for hyperparameter value achieving zero implausibility. The red and blue numbers are the plausible (blue) and implausible (red) hypothetical values for the summaries used in the history match.
Further investigation is needed to see how well the methods we have developed scale to problems where the number of hyperparameters is much larger. Also, it is not clear whether the specific form for the implausibility measure that was chosen was the best one. Although, as we have stressed throughout the manuscript, we are focusing mostly on computational questions in this paper it is also worth considering how the methods and algorithms developed are best integrated within an elicitation procedure in complex applied problems.

As noted in the introduction, while in this work we specify constraints in the form of passing or failing model checks for hypothetical data, the constraints could also be specified in some other way in our procedure, such as through inequalities on quantiles of predictive distributions. The numerical search procedures developed later can also be used with constraints in these other forms. Our method can also apply in situations where prior information is expressed directly on the parameter itself rather than predictively. It is not uncommon for prior distributions to be specified conditionally through a hierarchy, and for marginal prior distributions for functions of the parameter to be unavailable analytically. We can consider tail probabilities for such marginal priors or inequalities on quantiles for such priors in the same basic framework as our predictive methods. Again, indicator functions for certain sets such as expressing order constraints on certain parameters might be one useful way of adding information. The ABC computations in our method are similar to those used in Nott et al. (2017) for finding weakly informative priors and many of the elicitation calculations can be reused for finding such a weakly informative prior in the event that there is a prior-data conflict. Also worthy of further investigation is whether greater use can be made of the full set of prior distributions returned by the history match. Here we have simply focused on choice of a single “adequate” prior but there is a richer source of information that can be used in the results of the history matching procedure.
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References


Appendix

We outline here the calculation of the adjusted $R^2$ type measure used as a summary in the example of Section 5.2. A refitted cross-validation approach (Fan et al. 2012) is used based on 10 random splits. The algorithm is as follows.

1. For $j = 1, \ldots, 10$,

   (a) Split the data $y$ into two halves, $y = (y^{(1)}^T, y^{(2)}^T)$. Split $X$ similarly as $X = [X^{(1)}^T \ X^{(2)}^T]^T$.

   (b) Compute the absolute value of the Pearson correlation of $y^{(1)}$ with column $i$ of $X^{(1)}$. Write this as $R^{i,j,1}$, $i = 1, \ldots, p$. Similarly compute the absolute value of the Pearson correlation of $y^{(2)}$ with column $i$ of $X^{(2)}$ and write this as $R^{i,j,2}$, $i = 1, \ldots, p$.

   (c) Let $S^*(k)$ denote the indices $i$ of the predictors with the $M/4$ largest values of $R^{i,j,k}$, $k = 1, 2$.

   (d) Write $X_{S^*(1)}^{(1)}$ for the submatrix of $X^{(1)}$ which retains only columns $i \in S^*(2)$, and similarly $X_{S^*(2)}^{(2)}$ is the submatrix of $X^{(2)}$ which retains only columns $i \in S^*(1)$.

   Fit a linear regression model of $y^{(1)}$ on $X_{S^*(1)}^{(1)}$ and write the adjusted $R^2$ for this regression as $R^{(j,1)}$. Similarly fit a linear regression model of $y^{(2)}$ on $X_{S^*(2)}^{(2)}$ and write the adjusted $R^2$ for this regression as $R^{(j,2)}$. Write $R^{(j)} = 0.5 \times (R^{(j,1)} + R^{(j,2)})$.

2. $S^2(y) = \frac{1}{10} \sum_{j=1}^{10} R^{(j)}$