

Bayesian model choice via mixture distributions with application to epidemics and population process models

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Abstract

We describe a new method for evaluating Bayes factors. The key idea is to introduce a hypermodel in which the competing models are components of a mixture distribution. Inference for the mixing probabilities then yields estimates of the Bayes factors. Our motivation is the setting where the observed data are a partially observed realisation of a stochastic population process, although the methods have far wider applicability. The methods allow for missing data and for parameters to be shared between models. Illustrative examples including epidemics, population processes and regression models are given, showing that the methods are competitive compared to existing approaches.

Keywords: Bayes factors; Data imputation; Epidemic models; Markov chain Monte Carlo methods; Model choice

1 Introduction

This paper describes a new method for evaluating Bayes factors. The method itself is quite general, and can be applied to data consisting of independent and identically distributed observations, or to data arising from more complex scenarios. Our motivation comes from the setting of partially observed population processes in which missing data imputation is typically required to facilitate inference. We start by describing the motivating problem before considering the general context.

Consider an observed sequence of event times, each event being of the same type, and suppose we wish to assess whether a homogeneous Poisson process or an alternative non-homogeneous Poisson process best fits the observations. Alternatively, suppose we have case-detection times in an outbreak of infectious disease, and wish to know which of two possible Susceptible-Infective-Removed disease transmission models is most plausible as a model for how the data were generated, assuming that removals correspond to case-detections. Both of these examples are special cases of a generic situation in which we wish to assess which of a number of proposed point-process models best fits the data to hand. In the first example there is one type of event, and all events are observed. In the second example there are two event types (infections and removals) but only the latter are observed. In both examples two models are compared, but in general we may have more models of interest.

In a Bayesian framework, questions of model choice can be addressed using Bayes factors, which quantify the relative likelihood of any two models given the data and within-model prior distributions. Bayes factors can suffer from two practical drawbacks, namely (i) they can be difficult to compute, and (ii) they can be highly sensitive to the choice of within-model prior distributions, and in particular apparently natural choices can give misleading results. Here our focus is towards addressing the first difficulty, but in respect of the second we briefly remark that alternative methods of Bayesian model assessment have their own difficulties in the setting we consider. For example, neither the Deviance Information Criterion nor Bayesian Information Criterion appear entirely natural for settings where the data are typically far from being independent observations, as is the case when the data are realisations of a stochastic process. For problems involving missing data, such as the epidemic example above, it is not even clear how suitable information criteria should best be defined (Celeux et al. (2006) give nine candidates, for instance). Finally, methods involving a comparison between the observed data and what the fitted model would predict typically involve a subjective judgement as to precisely what should be compared, and how.

In all but the simplest cases, Bayes factors must be evaluated numerically. In principle, this can be achieved via reversible jump Markov chain Monte Carlo methods (Green, 1995). To be precise, consider

two models M_1 and M_2 with parameters θ_1 and θ_2 , respectively, where $\theta_j \in \Theta_j$. Define $k \in \{1, 2\}$ to be a model indicator which specifies the model under consideration. Reversible jump methods proceed by defining a Markov chain with state space $\{1\} \times \Theta_1 \cup \{2\} \times \Theta_2$ such that the proportion of time for which $k = j$ converges to the posterior model probability $P(M_j|x)$, where x denotes the observed data. Given model prior probabilities $P(M_j)$, the Bayes factor in favour of model 1 is given by the expression $P(M_2)P(M_1|x)/P(M_1)P(M_2|x)$, which can be estimated from the Markov chain output. The main practical challenge in implementing reversible jump algorithms is constructing efficient between-model proposal distributions, i.e. defining how the Markov chain jumps between the different components of the union of model parameter spaces. Although there have been theoretical advances which address this issue (Brooks et al., 2003), for many problems it remains a case of trial and error.

In this paper we propose a new method for evaluating Bayes factors which goes some way to removing the implementation challenges of reversible jump methods. The key idea is to consider a hypermodel which is itself a mixture model whose components are the two or more competing models of interest. A Markov chain Monte Carlo algorithm can then be defined on the product space of all model parameters and mixture probabilities. Our key result, Lemma 1, shows that the Bayes factors for the models can be expressed in terms of the posterior means of the mixture probabilities, and thus estimated from the Markov chain output. Our methods allow the incorporation of missing data, and for model parameters to be shared between models.

Before proceeding to the details, we consider the general context. First, defining a Markov chain on a product (rather than union) of model-parameter spaces is the approach pioneered by Carlin and Chib (1995), and further developed to more general settings (Green and O’Hagan (1998), Dellaportas et al. (2002), Godsill (2001)). This approach, as for reversible jump methods, involves defining a probability distribution over the set of possible models, and introduces a parameter which indicates which model is chosen. In our setting the possible models are combined into one mixture model. The product-space approach also relies on defining so-called pseudo-priors for the within-model parameters, upon which algorithm efficiency is crucially dependent, and this can be difficult in practice. Our methods do not involve the need to introduce such pseudo-priors, although for some missing data problems we need to specify similar prior distributions for the missing data.

Second, computational methods for the Bayesian analysis of mixture models are well-established, both when the number of components in the mixture is known (Diebolt and Robert, 1994) and when it is not (Richardson and Green, 1997). The typical situation under consideration is one in which the data are assumed to comprise independent and identically distributed observations, each of which comes from the proposed mixture distribution(s). In contrast, for our methods we consider only one observation from the mixture model, but this single observation consists of all the observed data. In other words, rather than assuming each data point can individually come from any model in the mixture, we assume all data points come from one of the models in the mixture. This assumption is completely natural when the data are observations from a stochastic process and do not consist of independent points. However, our methods apply equally well to independent and identically distributed observations, as illustrated in the sequel.

The paper is structured as follows. Section 2 contains general theory which describes the inference framework in detail, and computational matters are described in Section 3. In Section 4 we present a number of examples to illustrate the methods. We conclude with discussion in Section 5.

2 General Theory

2.1 Preliminaries

In this section we introduce the underlying framework of interest. For ease of exposition we adopt the usual abuse of notation and terminology in which ‘a density $\pi(\theta)$ ’ can refer to both the density function π of a random variable θ , or the same function evaluated at a typical point θ .

2.2 Mixture model with no missing data

Suppose we observe data x , and wish to consider n competing models M_1, \dots, M_n . For $i = 1, \dots, n$ denote the probability density of x under model i by $\pi_i(x|\theta_i)$, where θ_i denotes the vector of within-model parameters, and set $\theta = (\theta_1, \dots, \theta_n)$. We assume that all the $\pi_i(x|\theta_i)$ are densities with respect to the same common reference measure. Define a mixture model by

$$\pi(x|\alpha, \theta) = \sum_{i=1}^n \alpha_i \pi_i(x|\theta_i), \quad (1)$$

where $\alpha = (\alpha_1, \dots, \alpha_n)$ satisfies $\sum_{i=1}^n \alpha_i = 1$ and $\alpha_i \geq 0$ for $i = 1, \dots, n$.

2.3 Mixture model with missing data

In our setting, the data x may be a partial observation of a stochastic process. In consequence, $\pi_i(x|\theta_i)$ in (1) may be intractable, meaning that it cannot be analytically or numerically evaluated in an efficient manner. We adopt data augmentation to overcome this problem, as follows. Let $y = (y_1, \dots, y_N)$ be a vector comprising different kinds of ‘missing data’, and for $i = 1, \dots, n$ let $\mathcal{I}(i) \subseteq \{1, \dots, N\}$ and define $y_{\mathcal{I}(i)}$ as the vector with components y_j , $j \in \mathcal{I}(i)$. Thus $y_{\mathcal{I}(i)}$ denotes the missing data for model i , in practice usually chosen to make the augmented probability density $\pi_i(x, y_{\mathcal{I}(i)}|\theta_i)$ tractable. If model i does not require missing data, then $y_{\mathcal{I}(i)}$ is null. Note that this formulation allows different models to share common elements of missing data. Conversely, if each model has its own missing data then we simply set $\mathcal{I}(i) = i$ for $i = 1, \dots, n$.

In order to define a mixture model using missing data, it is necessary to introduce additional terms so that each component of the mixture is a probability density function on the possible values of x and y . To this end, we assume that there exist tractable probability densities $\pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta)$, where $y_{-\mathcal{I}(i)}$ denotes the vector with components y_j , $j \notin \mathcal{I}(i)$. If the latter set is empty then we set $\pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta) = 1$. We refer to the $\pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta)$ terms as *missing data prior densities*. In practice, they need not explicitly depend on any of x , $y_{\mathcal{I}(i)}$ or θ , depending on the application at hand.

Define an augmented mixture model by

$$\pi(x, y|\alpha, \theta) = \sum_{i=1}^n \alpha_i \pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta). \quad (2)$$

Here we assume that each $\pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta)$ term in the sum in (2) is a probability density with respect to a common reference measure, from which it follows that $\pi(x, y|\alpha, \theta)$ is also a probability density.

2.4 Bayes Factors

We now show how Bayes factors can be computed directly from certain summaries of the posterior distribution of α given the data x . We assume that α and θ are independent *a priori*, and that the prior density $\pi(\theta)$ has marginal densities $\pi_i(\theta_i)$, $i = 1, \dots, n$, which are equal to the desired within-model prior densities.

By Bayes’ Theorem,

$$\pi(\alpha|x) = \frac{\pi(x|\alpha)\pi(\alpha)}{\pi(x)} = \frac{\pi(\alpha) \sum_{i=1}^n \alpha_i m_i(x)}{\pi(x)},$$

where $\pi(\alpha)$ denotes the prior density of α and, for $i = 1, \dots, n$,

$$m_i(x) = \int \pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi(\theta) d\theta dy_{\mathcal{I}(i)} = \int \pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi_i(\theta_i) d\theta_i dy_{\mathcal{I}(i)},$$

integrating over all θ_j with $j \neq i$. Note also that

$$1 = \int \pi(\alpha|x) d\alpha = \pi(x)^{-1} \sum_{i=1}^n E[\alpha_i] m_i(x),$$

whence

$$\pi(x) = \sum_{i=1}^n E[\alpha_i] m_i(x). \quad (3)$$

Now for $i \neq j$, the Bayes factor in favour of M_i relative to M_j is defined to be $B_{ij} = B_{ij}(x) = m_i(x)/m_j(x)$. However,

$$\begin{aligned} E[\alpha_i|x] &= \int \alpha_i \pi(\alpha|x) d\alpha \\ &= \pi(x)^{-1} \int \alpha_i \left(\sum_{j=1}^n \alpha_j m_j(x) \right) \pi(\alpha) d\alpha \\ &= \pi(x)^{-1} \sum_{j=1}^n E[\alpha_i \alpha_j] m_j(x), \end{aligned}$$

which combined with (3) yields that

$$E[\alpha_i|x] = \frac{\sum_{j=1}^n E[\alpha_i \alpha_j] m_j(x)}{\sum_{j=1}^n E[\alpha_j] m_j(x)}, \quad i = 1, \dots, n. \quad (4)$$

Next, fix $k \in \{1, \dots, n\}$. Dividing the numerator and denominator of the fraction in (4) by $m_k(x)$ and rearranging we obtain

$$\sum_{j=1}^n (E[\alpha_j] E[\alpha_i|x] - E[\alpha_i \alpha_j]) B_{jk}(x) = 0, \quad i = 1, \dots, n. \quad (5)$$

It remains to solve equations (5) to find $B_{jk}(x)$, $j = 1, \dots, n$. Define A as the $n \times n$ matrix with elements

$$A_{ij} = E[\alpha_i|x] E[\alpha_j] - E[\alpha_i \alpha_j], \quad 1 \leq i, j \leq n.$$

Note that A depends on x , although we suppress this dependence in our notation. Define \tilde{A}_{-k} as the $(n-1) \times (n-1)$ matrix formed by removing the k th row and k th column of A . Similarly for $j \neq k$ define \tilde{A}_{-jk} as the $(n-1) \times (n-1)$ matrix formed from \tilde{A}_{-k} by replacing the elements A_{ij} with $-A_{ik}$, $i = 1, \dots, n, i \neq k$.

Lemma 1 (a) If $\det \tilde{A}_{-k} \neq 0$ then

$$B_{jk}(x) = \frac{\det \tilde{A}_{-jk}}{\det \tilde{A}_{-k}}. \quad (6)$$

(b) Suppose that $0 < m_i(x) < \infty$ for $i = 1, \dots, n$. Then if either (i) $n = 2$ and $0 < E[\alpha_1] < 1$, or (ii) α has a Dirichlet prior distribution, $\mathcal{D}(p_1, \dots, p_n)$, then

$$B_{jk}(x) = \frac{A_{jk}}{A_{kj}}.$$

The proof of Lemma 1 is in the Appendix. The result shows that the required Bayes factors can be expressed in terms of the prior distribution summaries $E[\alpha_i]$ and $E[\alpha_i \alpha_j]$ and the posterior means $E[\alpha_i|x]$, $i, j = 1, \dots, n$.

The condition on the determinant of \tilde{A}_{-k} in Lemma 1(a) is not vacuous in general, as illustrated by the somewhat pathological case where α_i has a point mass prior for all $i = 1, \dots, n$. Then for all $1 \leq i, j \leq n$, $E[\alpha_i|x] = E[\alpha_i]$ and $E[\alpha_i \alpha_j] = E[\alpha_i] E[\alpha_j]$, whence $A_{ij} = 0$ and (5) cannot be solved to find the Bayes factors.

At first sight the need for a Dirichlet prior on α to yield simple evaluation of the Bayes factors via Lemma 1 may appear restrictive. We make three remarks. First, the mixture construction is itself introduced solely as a tool for evaluation of Bayes factors, and so there is no particular need to assign an arbitrary prior distribution to α . Second, in practice a Dirichlet prior is both straightforward to use and flexible enough for computational purposes as described below. Third, it may well be that (6) holds for arbitrary prior distributions on α , subject to mild constraints which imply that $\det \tilde{A}_{-k} \neq 0$, but this does not appear straightforward to prove.

Finally, the simple form for the Bayes factor in Lemma 1 (b) is not true in general; an example for $n = 3$ can be found in the Appendix.

2.5 Two competing models

We give special attention to the case $n = 2$ since this is of practical importance. Here we have $\alpha = (\alpha_1, 1 - \alpha_1)$ and Lemma 1 yields that

$$B_{12} = \frac{E[\alpha_1] - E[\alpha_1^2] - E[\alpha_1|x](1 - E[\alpha_1])}{E[\alpha_1]E[\alpha_1|x] - E[\alpha_1^2]}.$$

It follows that

$$\frac{E[\alpha_1] - E[\alpha_1^2]}{1 - E[\alpha_1]} \leq E[\alpha_1|x] \leq \frac{E[\alpha_1^2]}{E[\alpha_1]},$$

with the upper and lower bounds corresponding to Bayes factors entirely in favour of models 1 and 2, respectively. A practical consequence is that any numerical estimate of $E[\alpha_1|x]$ lying outside these bounds must be incorrect.

Under the further assumption that $\pi(\alpha)$ is a uniform density, so that $\alpha_1 \sim U(0, 1)$, we obtain

$$B_{12} = \frac{3E[\alpha_1|x] - 1}{2 - 3E[\alpha_1|x]},$$

$$\pi(\alpha_1|x) \propto \alpha_1 m_1(x) + (1 - \alpha_1) m_2(x),$$

$$E[\alpha_1|x] = (2m_1(x) + m_2(x))/(3(m_1(x) + m_2(x))) \text{ and } 1/3 \leq E[\alpha_1|x] \leq 2/3.$$

Finally, if α is assigned a Dirichlet prior distribution, bounds for $E[\alpha_i|x]$ for any value of n can be obtained. Full details can be found in the proof of Lemma 1 in the Appendix.

3 Computation

3.1 Preliminaries

We now describe how to use the mixture framework in practice, specifically via Markov chain Monte Carlo methods. Our objective is to sample from the target density

$$\pi(\alpha, \theta, y|x) \propto \pi(x, y|\alpha, \theta) \pi(\alpha) \pi(\theta), \quad (7)$$

and the first issue is that of assigning any missing data prior density terms in $\pi(x, y|\alpha, \theta)$.

3.2 Missing data prior densities

Although the desired Bayes factors are invariant to the choice of any missing data prior densities, this choice is important in practice for computations. This is largely a problem-specific issue, but we make two general remarks. First, if all models share the same missing data (y_1 , say) then no missing data prior densities are required, and (7) becomes

$$\pi(\alpha, \theta, y|x) \propto \sum_{i=1}^n \alpha_i \pi_i(x, y_1|\theta_i) \pi(\alpha) \pi(\theta).$$

Second, it can be beneficial to assign missing data priors which mimic the marginal density of the $y_{-\mathcal{I}(i)}$ components in other models. As discussed below, the mixing properties of suitable Markov chain Monte Carlo algorithms are improved if the chains can easily move between different models, and such movement is hindered if the density of the missing data in one model is very different to the missing prior density assigned in another.

3.3 Markov chain Monte Carlo methods

Sampling from the target density defined at (7) will typically be possible via a range of standard Markov chain Monte Carlo methods, but here we offer some observations on practical aspects. The fact that the target density is a sum will usually make direct Gibbs sampling infeasible, but the approach of Diebolt and Robert (1994), which relies on the introduction of allocation variables which indicate the ‘true’ model as described in Dempster et al. (1977), can be adapted as follows.

Introduce $z = (z_1, \dots, z_n)$ such that $z_i \in \{0, 1\}$ and $\sum_{i=1}^n z_i = 1$. Thus z can take n possible values, each of which is a vector of zeroes other than a 1 at one position. Define the augmented likelihood

$$\pi(z, x, y|\alpha, \theta) = \prod_{i=1}^n (\alpha_i \pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta))^{z_i},$$

so that the augmented likelihood at (2) is recovered by summing over z . If the prior distribution on α is Dirichlet, $\mathcal{D}(p_1, \dots, p_n)$, it follows that α has full conditional distribution

$$\alpha|\dots \sim \mathcal{D}(p_1 + z_1, \dots, p_n + z_n).$$

The full conditional distribution of z is multinomial $\mathcal{M}(1; q_1, \dots, q_n)$, where the probabilities are given by

$$q_i \propto \alpha_i \pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta), \quad i = 1, \dots, n.$$

For $j = 1, \dots, n$, θ_j has full conditional distribution given by

$$\pi(\theta_j|\dots) \propto \pi(\theta) \pi_i(x, y_{\mathcal{I}(i)}|\theta_i) \pi_i(y_{-\mathcal{I}(i)}|x, y_{\mathcal{I}(i)}, \theta)$$

where i denotes the current model, i.e. $z_i = 1$. Simplification often occurs in practice: for instance, if $\theta_1, \dots, \theta_n$ are independent *a priori* and there are no missing data prior densities then we obtain

$$\pi(\theta_j | \dots) \propto \begin{cases} \pi_j(\theta_j) & z_j = 0, \\ \pi_j(x, y_{\mathcal{I}(j)} | \theta_j) \pi_j(\theta_j) & z_j = 1. \end{cases}$$

Finally, any missing data component y_j , $j = 1, \dots, N$, has full conditional distribution given by

$$\pi(y_j | \dots) \propto \begin{cases} \pi_i(x, y_{\mathcal{I}(i)} | \theta_i) & j \in \mathcal{I}(i), \\ \pi_i(y_{-\mathcal{I}(i)} | x, y_{\mathcal{I}(i)}, \theta_i) & j \notin \mathcal{I}(i), \end{cases}$$

where i denotes the current model.

The prior distribution for α can often be chosen to improve the mixing of the Markov chain. In particular this can be achieved by trying to make the multinomial distribution of z as close to uniform as possible. To illustrate this, consider the trivial example with two models in which $\pi_1(x)/\pi_2(x) = m_1(x)/m_2(x) = B_{12} = 50$. The full conditional distributions for z_1 and α_1 are, respectively, $Bern(50\alpha_1/(50\alpha_1 + (1 - \alpha_1)))$ and $Beta(z_1 + p_1, 1 - z_1 + p_2)$, where $Bern$ and $Beta$ respectively denote Bernoulli and Beta distributions. Setting $p_1 = p_2 = 1$ produced wildly different estimates for B_{12} (87.8, 40.9, 547.1) for three algorithm runs of 10^6 iterations, while repeating the exercise with $p_1 = 1$ and $p_2 = 50$ yielded estimates 50.3, 50.3 and 50.7.

It is of course not necessary to use allocation variables, and one can equally use any suitable Markov chain Monte Carlo scheme for the target density. However, the above illustrates the fact that the full conditional distributions of θ_i and any missing data will be of mixture form, which has implications for the design of efficient algorithms. Note that this also illustrates that the marginal densities $\pi(\theta_i | x)$ are mixtures, and in particular are not the same as those obtained from a single-model analysis, which are proportional to $\pi_i(x | \theta_i) \pi_i(\theta_i)$. The marginal densities can be either be explored via a standard single-model Markov chain Monte Carlo algorithm, or by using the allocation variables approach and conditioning the output on $z_i = 1$ to obtain within-model posterior density samples for θ_i .

3.4 Connections with other approaches

The framework we adopt is related to that described in Carlin and Chib (1995) and Godsill (2001), in which the target distribution of interest is defined over a product space of models and their parameters. In order to clarify the differences in our approach, consider the simplest possible setting in which we have two models defined by densities $\pi_1(x | \theta_1)$ and $\pi_2(x | \theta_2)$, and independent within-model prior densities $\pi_1(\theta_1)$ and $\pi_2(\theta_2)$. The framework of Carlin and Chib (1995) and Godsill (2001) introduces a model indicator $k \in \{1, 2\}$ to denote the ‘current’ model. The target density of interest is specified by

$$\pi(k, \theta_1, \theta_2 | x) \propto \pi_k(x | \theta_k) \pi_k(\theta_k | k) \pi(\theta_{3-k} | \theta_k, k) \pi(k),$$

where it is necessary to specify $\pi(\theta_{3-k} | \theta_k, k)$, i.e. the ‘prior’ for the non-current model parameter. Assuming θ_1 and θ_2 to be independent of each other and k gives that $\pi(\theta_{3-k} | \theta_k, k) = \pi_{3-k}(\theta_{3-k})$.

Conversely, our formulation has target density

$$\pi(\alpha, \theta_1, \theta_2 | x) \propto \pi(\alpha) \pi_1(\theta_1) \pi_2(\theta_2) [\alpha_1 \pi_1(x | \theta_1) + \alpha_2 \pi_2(x | \theta_2)].$$

If we adopt the allocation-variable approach, the target density becomes

$$\pi(z, \alpha, \theta_1, \theta_2 | x) \propto \pi(\alpha) \pi_1(\theta_1) \pi_2(\theta_2) [\alpha_1 \pi_1(x | \theta_1)]^{z_1} [\alpha_2 \pi_2(x | \theta_2)]^{z_2},$$

from which we see that it is the existence of the α parameter which distinguishes our formulation from that of Carlin and Chib (1995) and Godsill (2001). Since posterior estimation of α is what enables us to estimate Bayes factors, this difference is an important one.

The general formulation in Godsill (2001) also allows each model to potentially share parameters with other models. Specifically, the parameters of model k will be some subset of a set of parameters $\{\theta_1, \dots, \theta_N\}$. This is similar to the way we have dealt with missing data, although the two set-ups are not technically equivalent, and in particular one cannot simply treat our missing data as model parameters. The fundamental difference is that missing data may not always require a prior, whereas model parameters always do. For instance, if a density $\pi(x | \theta)$ is intractable, then our missing data approach uses Bayes’ Theorem in the form $\pi(\theta, y | x) \propto \pi(x, y | \theta) \pi(\theta)$ whereas augmenting with extra model parameter ψ gives $\pi(\theta, \psi | x) \propto \pi(x | \theta, \psi) \pi(\theta, \psi)$.

Finally, note that our approach also enables each model to potentially share parameters with other models, since we allow for arbitrary prior dependency between $\theta_1, \dots, \theta_n$. Example 2 below illustrates this idea.

Table 1: Pines data set: Comparison of Bayes factors from different methods.

| Method | Bias | Standard Error |
|-----------------------------------|------|----------------|
| RJMCMC | 67 | 2678 |
| RJ corrected | 9 | 124 |
| Power posterior (serial MCMC) | 10 | 132 |
| Power posterior (population MCMC) | 22 | 154 |
| Mixture method | 10 | 39 |

4 Examples

In this section we illustrate the theory with two examples of classical data sets comprising independent observations, and three examples featuring population processes or epidemics.

Example 1: Non-nested regression models for Pines data We consider the well-known model choice problem of assigning non-nested linear regression models to the pines data set in Williams (1959). These data have been analyzed by several authors (see, for example, Han and Carlin, 2001; Carlin and Chib, 1995; Friel and Pettitt, 2008) in order to compare methods for estimating Bayes factors. The data describe the maximum compression strength parallel to the grain y_i , the density x_i , and the resin-adjusted density z_i for 42 specimens of radiata pine. The two competing models we consider are

$$\begin{aligned} M_1 : \quad y_i &= \alpha + \beta(x_i - \bar{x}) + \epsilon_i, & \epsilon_i &\sim N(0, \sigma^2); \\ M_2 : \quad y_i &= \gamma + \delta(z_i - \bar{z}) + \eta_i, & \eta_i &\sim N(0, \tau^2), \end{aligned}$$

which in vector notation we write as $Y = X(\alpha, \beta)^T + \epsilon$ and $Y = Z(\gamma, \delta)^T + \eta$. We assigned identical prior distributions to the papers cited above, i.e. $N(\mu_0, v_0) \equiv N((3000, 185)^T, \text{diag}(10^6, 10^4))$ prior distributions for $(\alpha, \beta)^T$ and $(\gamma, \delta)^T$, and $IG(a_0, b_0) \equiv IG(3, (2 \times 300^2)^{-1})$ prior distributions for σ^2 and τ^2 , where $IG(a, b)$ denotes an inverse gamma distribution with probability density function

$$f(x) = \frac{1}{\exp(1/bx)\Gamma(a)b^a x^{a+1}}.$$

We assigned a Beta(100, 1) prior distribution for α_1 . Using the allocation variables approach, parameter updates for a Gibbs sampling algorithm are as follows, where $\theta_1 = (\alpha, \beta, \sigma^2)$ and $\theta_2 = (\gamma, \delta, \tau^2)$:

$$\begin{aligned} \alpha_1 | \dots &\sim \text{Beta}(100 + z_1, 2 - z_1), \\ z_1 | \dots &\sim \text{Bern}\left(\frac{\alpha_1 \pi_1(x|\theta_1)}{\alpha_1 \pi_1(x|\theta_1) + (1 - \alpha_1) \pi_2(x|\theta_2)}\right), \\ \theta_i | \dots &\sim \begin{cases} (N(\mu_0, v_0), IG(a_0, b_0)) & z_i = 0, \\ (N(\mu_i, v_i), IG(a_i, b_i)) & z_i = 1, \end{cases} \end{aligned}$$

where $v_1 = (v_0^{-1} + \sigma^{-2} X^T X)^{-1}$, $v_2 = (v_0^{-1} + \tau^{-2} Z^T Z)^{-1}$, $\mu_1 = v_1(v_0^{-1} \mu_0 + \sigma^{-2} X^T Y)$, $\mu_2 = v_2(v_0^{-1} \mu_0 + \tau^{-2} Z^T Y)$, $a_1 = a_2 = (n/2) + a_0$, $b_1 = [b_0 + (1/2)(Y - X(\alpha, \beta)^T)^T(Y - X(\alpha, \beta)^T)]^{-1}$ and $b_2 = [b_0 + (1/2)(Y - Z(\gamma, \delta)^T)^T(Y - Z(\gamma, \delta)^T)]^{-1}$.

We carried out 100 runs of our method, this being the same as the number of runs used for the methods described in Friel and Pettitt (2008). Friel and Pettitt (2008) also compared conventional reversible jump methods (with each model *a priori* equally likely), ‘corrected’ Reversible jump methods (model priors chosen to improve mixing) and two power posterior methods (Serial and Population Markov chain Monte Carlo). Full details can be found in Friel and Pettitt (2008), and for convenience we simply quote the results obtained in Table 1, along with our result. The bias is calculated by comparison with the estimate of 4862 obtained by numerical integration in Green and O’Hagan (1998). It can be seen that our method is certainly competitive.

Example 2: Three logistic regression models for Pima Indians data The well-known Pima Indians data set consists of diabetes incidence for $n = 532$ Pima Indian women along with data on seven covariates, and can be naturally modelled using logistic regression. In Friel and Wyse (2012), two specific models are considered. These models (M_2 and M_3 , here) have four explanatory variables in common (number of pregnancies, plasma glucose concentration, body mass index and diabetes pedigree function) while M_2 has one additional variable (age). The corresponding Bayes factor B_{23} is calculated using various different methods

in Friel and Wyse (2012), yielding values in the range 12.83 to 13.96, the latter value coming from a lengthy reversible jump MCMC run which could plausibly be regarded as the most reliable estimate.

To illustrate our method for three models we also consider an additional model M_1 , which has the same explanatory variables as M_2 other than diabetes pedigree function. Defining the vector of binary response data $x = (x_1, \dots, x_n)$, for $i = 1, 2, 3$ model i has likelihood

$$\pi_i(x|\theta_i) = \prod_{j=1}^n p_{i,j}^{x_j} (1 - p_{i,j})^{1-x_j}$$

where $p_{i,j}$ is the probability of incidence for individual j under model i , itself defined in terms of the model i covariates for individual j , $z_{ij} = (1, z_{ij}^{(1)}, \dots, z_{ij}^{(d_i)})$, and the model i parameter vector $\theta_i = (\theta_{i0}, \theta_{i1}, \dots, \theta_{id_i})^T$ via the relation

$$\log \left(\frac{p_{i,j}}{1 - p_{i,j}} \right) = \theta_i^T z_{ij},$$

where d_i is the number of explanatory variables in model i , so that $d_1 = 3$, $d_2 = 4$ and $d_3 = 5$. Thus the parameters of the three models under consideration are all of different dimension. The elements θ_{ij} of θ_i are each assigned independent Gaussian prior distributions with mean zero and variance 100.

We estimated Bayes factors as follows. First, we assume *a priori* that $\theta_{1j} = \theta_{2j} = \theta_{3j}$ for $j = 0, \dots, 3$, so that in fact we only have six parameters (namely $\theta_{30}, \dots, \theta_{35}$) in the mixture model formulation. Although this assumption is not necessary, it was found to help the mixing of the MCMC algorithm. Thus the target density is

$$\pi(\alpha, \theta_1, \theta_2, \theta_3|x) \propto (\alpha_1 \pi_1(x|\theta_1) + \alpha_2 \pi_2(x|\theta_2) + \alpha_3 \pi(x|\theta_3)) \pi(\alpha) \pi(\theta_1, \theta_2, \theta_3)$$

where $\alpha_3 = 1 - \alpha_1 - \alpha_2$, $\theta_1 = (\theta_{30}, \dots, \theta_{33})^T$, $\theta_2 = (\theta_{30}, \dots, \theta_{34})^T$, $\theta_3 = (\theta_{30}, \dots, \theta_{35})^T$ and $\pi(\theta_1, \theta_2, \theta_3) = \pi(\theta_{30}, \dots, \theta_{35})$ is a product of six Gaussian density functions. We set $\alpha \sim \mathcal{D}(1, 1, 1)$ *a priori*.

We implemented our method using an allocation variable approach with Metropolis-Hastings updates for the θ_{3j} parameters. From 10^7 iterations of the resulting Markov chain we obtained estimates $B_{12} = 0.048$ and $B_{23} = 13.94$. The latter is in line with the values reported in Friel and Wyse (2012), especially the reversible jump MCMC estimate of 13.96, while the former is close to an estimate of 0.042 which we obtained using the Laplace approximation method (Tierney and Kadane, 1986) described in Friel and Wyse (2012).

Example 3: Poisson process vs. linear birth process Our first population process example is analytically tractable and illustrates that our methods produce results in agreement with the known true values. Consider data given by the vector of event times $x = (x_1, \dots, x_n)$ observed during a time interval $[0, T]$, where $0 \leq x_1 \leq x_2 \leq \dots \leq x_n \leq T$. We will compare two models, namely a homogeneous Poisson process of rate λ (M_1) and a linear birth process $\{X(t) : t \in [0, T]\}$ with per-capita birth rate μ and $X(0) = 1$ (M_2). Suppose further that λ and μ are assigned independent exponential prior distributions with mean θ^{-1} . The model likelihoods, which we write as densities with respect to the reference measure induced by a unit rate Poisson process on $[0, T]$, are

$$\pi_1(x|\lambda) = \lambda^n \exp\{-(\lambda - 1)T\}, \quad \pi_2(x|\mu) = n! \mu^n \exp\{-\mu[(n+1)T - S(x)] + T\},$$

where $S(x) = \sum_{j=1}^n x_j$. In this setting no missing data are required so we use the model defined at (1). The Bayes factor in favour of M_1 relative to M_2 is

$$\begin{aligned} B_{12} &= \frac{\int \pi_1(x|\lambda) \pi(\lambda) d\lambda}{\int \pi_2(x|\mu) \pi(\mu) d\mu} = \frac{\int_0^\infty \theta \lambda^n \exp\{-\lambda(T + \theta)\} d\lambda}{\int_0^\infty \theta n! \mu^n \exp\{-\mu[(n+1)T - S(x) + \theta]\} d\mu} \\ &= \frac{[(n+1)T - S(x) + \theta]^{n+1}}{(T + \theta)^{n+1} n!}. \end{aligned}$$

Assuming that $\alpha_1 \sim U(0, 1)$ *a priori*, a simple Gibbs sampler for the target density consists of parameter

Table 2: Example 3: Bayes factors from algorithm output (\hat{B}_{12}) compared to true values (B_{12}).

| n | T | $S(x)$ | θ | \hat{B}_{12} | B_{12} |
|-----|-----|--------|----------|----------------|----------|
| 5 | 10 | 36 | 1 | 1.15 | 1.148 |
| 5 | 10 | 36 | 0.01 | 1.58 | 1.587 |
| 5 | 10 | 25 | 1 | 10.25 | 10.239 |
| 10 | 20 | 150 | 1 | 0.18 | 0.181 |

updates as follows:

$$\begin{aligned}
\alpha_1 | \dots &\sim \text{Beta}(z_1 + 1, 2 - z_1), \\
z_1 | \dots &\sim \text{Bern} \left(\frac{\alpha_1 \pi_1(x|\lambda)}{\alpha_1 \pi_1(x|\lambda) + (1 - \alpha_1) \pi_2(x|\mu)} \right), \\
\lambda | \dots &\sim \begin{cases} \Gamma(1, \theta) & z_1 = 0, \\ \Gamma(n + 1, T + \theta) & z_1 = 1, \end{cases} \\
\mu | \dots &\sim \begin{cases} \Gamma(n + 1, (n + 1)T - S(x) + \theta) & z_1 = 0, \\ \Gamma(1, \theta) & z_1 = 1, \end{cases}
\end{aligned}$$

where $\Gamma(m, \xi)$ denotes a Gamma distribution with density $f(x) \propto x^{m-1} \exp(-\xi x)$.

Typical results from algorithm runs are given in Table 2, illustrating that the Gibbs sampler recovers the true known values. We found that the algorithm mixing was good in all cases.

Finally, we comment on the relationship between the above algorithm and standard reversible jump methods. The latter requires a way of proposing a value of μ given λ for jumps from M_1 to M_2 , and vice versa. In practice it is not immediately obvious how best to do this, but an approach suggested in Green (2003) is to propose μ independently of λ , ideally according to the within-model density $\pi(\mu|x)$. This is similar to what we obtain above.

Example 4: Epidemic model with two different infection periods Recall the standard Susceptible-Infective-Removed epidemic model (see e.g. Andersson and Britton (2000), Chapter 2), defined as follows. A closed population contains $N + a$ individuals of whom N are initially susceptible and a initially infective. Each infective remains so for a period of time distributed according to a specified random variable T_I , known as the infectious period, after which it becomes removed and plays no further part in the epidemic. During its infectious period an infective makes contact with each other member of the population at times given by a homogeneous Poisson process of rate β/N , and any contact occurring with a susceptible individual results in that individual immediately becoming infective. The infectious periods of different individuals and the Poisson processes between different pairs of individuals are assumed to be mutually independent. The epidemic ends when there are no infectives left in the population.

A distinguishing characteristic of infectious disease data is that the infection process itself is rarely observed, and so we suppose that the data r consist of n observed removal times $r_1 \leq \dots \leq r_n$. We consider two competing models, namely that $T_I \sim \Gamma(1, \gamma)$ (M_1) and $T_I \sim \Gamma(m, \lambda)$ (M_2), where the shape parameter m will be assumed known. Both model likelihoods $\pi_1(r|\gamma)$ and $\pi_2(r|\lambda)$ are intractable in practice since their evaluation relies on integrating over all possible realisations of the infection process, and so we introduce missing data as follows.

For $j = 1, \dots, n$ define i_j as the infection time of the individual removed at time r_j . We assume that there is $a = 1$ initial infective, denoted by p , so that $i_p \leq i_j$ for all $j \neq p$. For simplicity we assume *a priori* that p is equally likely to be any of the n infected individuals and that i_p has an improper uniform prior density on $(-\infty, r_1)$. Finally, define $i = \{i_j : i \neq p\}$ to be the $n - 1$ non-initial infection times. For $k = 1, 2$ the augmented model likelihoods, which we write here with respect to Lebesgue measure on \mathbb{R}^{2n-1} , are

$$\pi_k(i, r|p, i_p, \beta_k, \eta_k) = \left(\prod_{j=1; j \neq p}^n (\beta_k/N) I(i_j -) \right) \exp \left\{ -(\beta_k/N) \int_{i_p}^{r_n} S(t) I(t) dt \right\} \left(\prod_{j=1}^n f_k(r_j - i_j | \eta_k) \right),$$

where $S(t)$ and $I(t)$ denote respectively the numbers of susceptibles and infectives at time t , $I(t-) = \lim_{s \uparrow t} I(s)$, β_k denotes the parameter β under M_k , f_k denotes the infectious period density under M_k , $\eta_1 = \gamma$ and $\eta_2 = \lambda$ (see e.g. O'Neill and Roberts (1999), Streftaris and Gibson (2004), Höhle and O'Neill (2005)).

Note that in this formulation, the missing data i , p and i_p are assumed common to both models, although these quantities could also be model-specific.

The target density of interest is

$$\pi(\alpha_1, \beta_1, \beta_2, \gamma, \lambda | r) \propto [\alpha_1 \pi_1(i, r | p, i_p, \beta_1, \gamma) + (1 - \alpha_1) \pi_2(i, r | p, i_p, \beta_2, \lambda)] \pi(\beta_1) \pi(\beta_2) \pi(\gamma) \pi(\lambda).$$

Note that here we need no missing data priors densities because the the missing data appear in both model likelihoods. Prior distributions for β_1, β_2, γ and λ were all set as $\Gamma(1, 1)$, and $\alpha_1 \sim \text{Beta}(p_1, p_2)$.

Introducing the allocation variable z_1 yields the full conditional distributions below, each of which yields a simple Gibbs update for the parameter in question.

$$\begin{aligned} \alpha_1 | \dots &\sim \text{Beta}(z_1 + p_1, 1 - z_1 + p_2), \\ z_1 | \dots &\sim \text{Bern} \left(\frac{\alpha_1 \pi_1(i, r | p, i_p, \beta_1, \gamma)}{\alpha_1 \pi_1(i, r | p, i_p, \beta_1, \gamma) + (1 - \alpha_1) \pi_2(i, r | p, i_p, \beta_2, \lambda)} \right), \\ \beta_1 | \dots &\sim \begin{cases} \Gamma(n, N^{-1} \int_{i_p}^{r_n} S(t) I(t) dt + 1) & z_1 = 0, \\ \Gamma(1, 10^{-3}) & z_1 = 1, \end{cases} \\ \beta_2 | \dots &\sim \begin{cases} \Gamma(1, 1) & z_1 = 0, \\ \Gamma(n, N^{-1} \int_{i_p}^{r_n} S(t) I(t) dt + 1) & z_1 = 1, \end{cases} \\ \gamma | \dots &\sim \begin{cases} \Gamma(n + 1, \sum_{j=1}^n (r_j - i_j) + 1) & z_1 = 0, \\ \Gamma(1, 1) & z_1 = 1, \end{cases} \\ \lambda | \dots &\sim \begin{cases} \Gamma(1, 1) & z_1 = 0, \\ \Gamma(nm + 1, \sum_{j=1}^n (r_j - i_j) + 1) & z_1 = 1, \end{cases} \end{aligned}$$

Finally, the infection time parameters i , i_p and p are updated using a Metropolis-Hastings step as follows. One of the n infected individuals, j say, is chosen uniformly at random. A proposed new infection time for j is defined as $i_j^* = r_j - x$, where x is sampled from a $\Gamma(1, \delta)$ distribution. Note that this may also result in proposed new values for p and i_p ; either way, proposed values are denoted i^* , i_p^* and p^* and accepted with probability

$$1 \wedge \frac{\pi_k(i^*, r | p^*, i_p^*, \beta_k, \eta_k)}{\pi_k(i, r | p, i_p, \beta_k, \eta_k)} \exp(\delta(i_j - i_j^*)),$$

where $k = 2 - z_1$ denotes the current model.

To illustrate the algorithm, we considered the Susceptible-Infective-Removed model with $N = 50$, $a = 1$, various β values and $\Gamma(\tilde{m}, \tilde{\lambda})$ infectious periods with three different choices for $(\tilde{m}, \tilde{\lambda})$. For each scenario we simulated 100 data sets, and evaluated the Bayes factor using the above algorithm for each data set. For two of the $(\tilde{m}, \tilde{\lambda})$ pairs we set the shape parameter m in M_2 equal to \tilde{m} , and for one we did not. In practice, one is rarely interested in data from epidemics with few cases, so we also evaluated the Bayes factors using a subset of each of the 100 simulations in which the epidemic had clearly ‘taken off’, evaluated by eye, which we refer to as major epidemics. The numbers of major epidemics were 63, 56 and 65 for scenarios A, B and C, respectively.

Table 3 contains a summary of the Bayes factors estimated from the simulated data sets. In scenarios A, B and C the true models are M_2 , both M_1 and M_2 , and M_1 respectively. The estimated Bayes factors behave as we might expect, giving clear evidence in favour of models M_2 and M_1 for scenarios A and C respectively, whilst for scenario B the mean of B_{12} is close to the true value of 1. In scenario A there is a marked difference in the Bayes factors when using all simulations compared to using only major epidemics. A possible explanation is that major epidemics contain more data, and so any difference between the models becomes easier to detect. There is a less pronounced difference in Bayes factors in scenario C, although the large posterior standard deviations suggest there is no compelling evidence for a clear difference in this case.

Example 5: Epidemic model vs. Poisson process Our final example is motivated by the situation in which we wish to decide whether observed cases of disease are the result of an epidemic (with transmission between individuals) or simply sporadic events. Specifically, suppose we observe n events at times $0 < r_1 < \dots < r_n < T$, and let $r = (r_1, \dots, r_n)$. Under model M_1 , r is a vector of event times of a homogeneous Poisson process of rate λ observed during the time interval $[0, T]$. Under model M_2 , r is a vector of removal times in a Susceptible-Infective-Removed epidemic model with exponentially distributed infectious periods, again observed during $[0, T]$.

Table 3: Example 4: Bayes factors from algorithm output.

| Scenario | True model | β | M_2 | $E[B_{12}](st.dev.)$ (all simulations) | $E[B_{12}](st.dev.)$ (major epidemics) |
|----------|-------------------|---------|----------------------|---|---|
| A | $\Gamma(5, 5)$ | 2 | $\Gamma(5, \lambda)$ | 0.06 (0.06) | 0.008 (0.006) |
| B | $\Gamma(1, 0.75)$ | 1 | $\Gamma(1, \lambda)$ | 1.03 (0.17) | 1.05 (0.22) |
| C | $\Gamma(1, 1)$ | 3 | $\Gamma(2, \lambda)$ | 3022 (3969) | 2291 (3428) |

As for the previous example, we proceed by adding unobserved infection times in order to obtain a tractable likelihood for M_2 . For simplicity we assume that there is one initial infective at time zero, and furthermore that there is a population of N individuals in total, where $N \geq n$. Unlike the previous example, in which we unobserved infection times with observed removal times, we here define $i = (i_2, \dots, i_m)$ to be a vector of m ordered infection times, so that $0 = i_1 < i_2 < \dots < i_m$, where $n \leq m \leq N$. The reason for this approach is that it appears to be easier when it comes to assigning missing data prior densities, as described below. Note also that under M_2 we allow the possibility that the epidemic is still in progress at time T .

The likelihood for M_1 and augmented likelihood for M_2 are respectively given by

$$\begin{aligned}\pi_1(r|\lambda) &= \lambda^n \exp\{-\lambda T\}, \\ \pi_2(i, r|\beta, \gamma) &= \left(\prod_{j=2}^m \beta S(i_j -) I(i_j -) \right) \left(\prod_{j=1}^n \gamma I(r_j -) \right) \exp\left\{ - \int_0^T \beta S(t) I(t) + \gamma I(t) dt \right\}.\end{aligned}$$

To proceed we require a missing data prior density $\pi_1(i|r, \lambda, \beta, \gamma)$. Now for a given ordered vector of event times r , $\pi_2(i, r|\beta, \gamma) > 0$ if and only if $i \in \mathcal{F}(r)$, where

$$\mathcal{F}(r) = \{i : i_1 < i_2 < \dots < i_m < T; i_k < r_{k-1}, k = 1, \dots, n+1; i_k < T, k = n+2, \dots, m\}.$$

One way to define $\pi_1(i|r, \lambda, \beta, \gamma)$ is via the following construction, which simulates an element of $\mathcal{F}(r)$. First, select m according to some probability mass function f on $\{n, n+1, \dots, N\}$. Next, sequentially set $i_2 \sim \text{TrExp}(\mu; i_1, r_1)$, $i_3 \sim \text{TrExp}(\mu; i_2, r_2)$, \dots , $i_{n+1} \sim \text{TrExp}(\mu; i_n, r_n)$, $i_{n+2} \sim \text{TrExp}(\mu; i_{n+1}, T)$, \dots , $i_m \sim \text{TrExp}(\mu; i_{m-1}, T)$, where $\text{TrExp}(\mu; a, b)$ denotes an exponential random variable with rate μ , truncated to the interval (a, b) . This in turn induces a probability distribution with density

$$\pi_1(i|r) = f(m) \prod_{j=1}^{m-1} \frac{\mu \exp(-\mu i_j)}{\exp(-\mu i_{j-1}) - \exp(-\mu s_{j-1})}, \quad i \in \mathcal{F}(r),$$

where $s_j = r_j$ for $j = 1, \dots, n$ and $s_j = T$ for $n < j \leq m$, and we set $\pi_1(i|r, \lambda, \beta, \gamma) = \pi_1(i|r)$.

We remark that it is not necessary to define the missing data prior density in this manner. For instance, one could proceed by choosing m as before and then assigning a uniform density to the set $\{i : i_2 < i_3 < \dots < i_m\}$. The practical drawback with this is that, if using allocation variables, the Markov chain can never leave model M_1 if i is such that $\pi_2(i, r|\beta, \gamma) = 0$.

Prior distributions were assigned as $\beta \sim \Gamma(\nu_\beta, \mu_\beta)$, $\gamma \sim \Gamma(\nu_\gamma, \mu_\gamma)$, $\lambda \sim \Gamma(\nu_\lambda, \mu_\lambda)$ and $\alpha_1 \sim \text{Beta}(p_1, p_2)$.

A Markov chain Monte Carlo algorithm is easily developed in a similar manner to the previous example. Specifically we have the following full conditional distributions:

$$\begin{aligned}\alpha_1 | \dots &\sim \text{Beta}(z_1 + p_1, 1 - z_1 + p_2), \\ z_1 | \dots &\sim \text{Bern}\left(\frac{\alpha_1 \pi_1(r|\lambda) \pi_1(i|r)}{\alpha_1 \pi_1(r|\lambda) \pi_1(i|r) + (1 - \alpha_1) \pi_2(i, r|\beta, \gamma)}\right), \\ \lambda | \dots &\sim \begin{cases} \Gamma(\nu_\lambda, \mu_\lambda) & z_1 = 0, \\ \Gamma(n + \nu_\lambda, T + \mu_\lambda) & z_1 = 1, \end{cases} \\ \beta | \dots &\sim \begin{cases} \Gamma(m - 1 + \nu_\beta, \int_0^T S(t) I(t) dt + \mu_\beta) & z_1 = 0, \\ \Gamma(\nu_\beta, \mu_\beta) & z_1 = 1, \end{cases} \\ \gamma | \dots &\sim \begin{cases} \Gamma(n + \nu_\gamma, \int_0^T I(t) dt + \mu_\gamma) & z_1 = 0, \\ \Gamma(\nu_\gamma, \mu_\gamma) & z_1 = 1. \end{cases}\end{aligned}$$

Updates for i are achieved as follows. If $z_1 = 1$ then i has full conditional density $\pi_1(i|r)$ which can be sampled as described above. If $z_1 = 0$ then i can be updated by moving, adding or deleting infection times as described in O'Neill and Roberts (1999).

To illustrate this algorithm we considered a data set taken from an outbreak of Gastroenteritis described in Britton and O'Neill (2002) which take the form of 28 case detection times among a population of 89 individuals. The daily numbers of cases on days 0 to 7 are given respectively by

$$1, 0, 4, 2, 3, 3, 10, 5.$$

Strictly speaking, such data should be analysed by allowing the unknown time of the initial infection, i_1 , to be estimated (see e.g. O'Neill and Roberts (1999)). Since our main objective here is to illustrate our methodology, we instead make the simplifying assumption that day 0 actually corresponded to the start of the outbreak, and then consider the remaining 27 case detection times.

For the missing data prior density $\pi_1(i|r)$ we set

$$f(m) = \frac{(1 - \theta)^{m-n}\theta}{1 - (1 - \theta)^{N-n+1}}, \quad m = n, \dots, N,$$

so that m has a truncated Geometric distribution with parameter θ , and set $\mu = 4$ in the truncated exponential distribution.

We ran the algorithm with two choices of T , the time of observation, with β , γ and μ all given $Exp(1)$ prior distributions. First, with $T = 10$ we estimated the Bayes factor in favour of the Poisson model to be 0.003, here using $p_1 = 400, p_2 = 1$ to obtain reasonable mixing in the algorithm. So in this case there appears to be overwhelming evidence to suggest that the case detection times are better described by an epidemic model than a Poisson process. Second, we set $T = 3.5$ and used only the case observation times up until day 3. We estimated the Bayes factor in favour of the Poisson model to be 21.1. In comparison to the $T = 10$ case we would certainly expect a value closer to 1, since there are less data, and equally it is intuitively reasonable that there are insufficient data to provide evidence in favour of an epidemic.

5 Discussion

We have presented a new method for evaluating Bayes factors. Although motivated by epidemic models and population processes, our approach is clearly applicable in more general settings, as illustrated by the pines data set and Pima Indians data set examples in Section 4. The methods permit data imputation as necessary, and can cater for models which share common parameters.

The methods we propose are not without drawbacks. First, in common with the product-space methods it seems likely that they are best suited to situations in which there are only a small number of competing models, although we have not investigated this issue in this paper. Second, constructing missing data prior densities, when required, seems likely to require problem-specific insights in order to obtain reasonably efficient algorithms. Intuitively we expect that it is best to choose missing data prior distributions to mimic the true distribution of missing data in competing models. These aspects, as well as the method in general, appear worthy of more detailed exploration.

Acknowledgement

We thank Christian Robert and Andy Wood for helpful discussions about this work. We acknowledge funding from UK Engineering and Physical Sciences Research Council.

Appendix

Proof of Lemma 1 (a) Define

$$\mathbf{b} = [B_{1k}(x) \cdots B_{nk}(x)]^T,$$

so that (5) can be written as the matrix equation $A\mathbf{b} = \mathbf{0}$. Since $B_{kk}(x) = 1$, we can rewrite (5) as

$$\sum_{j \neq k} A_{ij} B_{jk}(x) = -A_{ik}, \quad i = 1, \dots, n. \quad (8)$$

Now, for $1 \leq l, j \leq n$,

$$\begin{aligned}
A_{lj} &= E[\alpha_l | x] E[\alpha_j] - E[\alpha_l \alpha_j] \\
&= E[\alpha_j] \left(1 - \sum_{i \neq l} E[\alpha_i | x] \right) - E \left[\left(1 - \sum_{i \neq l} \alpha_i \right) \alpha_j \right] \\
&= - \sum_{i \neq l} (E[\alpha_j] E[\alpha_i | x] - E[\alpha_i \alpha_j]) \\
&= - \sum_{i \neq l} A_{ij}.
\end{aligned} \tag{9}$$

Summing (8) over $i \neq k$ and using (9) now yields

$$\begin{aligned}
\sum_{i \neq k} \sum_{j \neq k} A_{ij} B_{jk}(x) &= - \sum_{i \neq k} A_{ik} \\
\text{so } \sum_{j \neq k} \left(\sum_{i \neq k} A_{ij} \right) B_{jk}(x) &= - \sum_{i \neq k} A_{ik} \\
\text{so } \sum_{j \neq k} A_{kj} B_{jk}(x) &= -A_{kk},
\end{aligned}$$

which is the equation obtained from (8) when $i = k$. In other words, at least the k th equation in (8) is redundant. It is therefore sufficient to consider the system of equations defined by

$$\tilde{A}_{-k} \tilde{\mathbf{b}} = \tilde{\mathbf{c}}, \tag{10}$$

where $\tilde{\mathbf{b}}$ is the $(n-1) \times 1$ column vector formed by removing $B_{kk}(x) = 1$ from \mathbf{b} , and $\tilde{\mathbf{c}}$ is the $(n-1) \times 1$ column vector with components $-A_{ik}$ for $i = 1, \dots, n, i \neq k$. Application of Cramer's rule to solve (10) now yields part (a).

(b) For the second part, we require some preliminary results. Write $E[\alpha_i | x] = f(m_i(x))$, say. From (4) we have

$$\begin{aligned}
f(m_i(x)) &= \frac{\sum_{j=1}^n E[\alpha_i \alpha_j] m_j(x)}{\sum_{j=1}^n E[\alpha_j] m_j(x)} \\
&= \frac{\sum_{j \neq i} E[\alpha_i \alpha_j] m_j(x) + E[\alpha_i^2] m_i(x)}{\sum_{j \neq i} E[\alpha_j] m_j(x) + E[\alpha_i] m_i(x)}.
\end{aligned}$$

Differentiation yields that $f'(m_i(x)) \geq 0$ if and only if $C \geq 0$, where

$$C = \sum_{j \neq i} (E[\alpha_i^2] E[\alpha_j] - E[\alpha_i] E[\alpha_i \alpha_j]) m_j(x).$$

Thus if $C \geq 0$ we obtain the bounds

$$\frac{\sum_{j \neq i} E[\alpha_i \alpha_j] m_j(x)}{\sum_{j \neq i} E[\alpha_j] m_j(x)} \leq E[\alpha_i | x] \leq \frac{E[\alpha_i^2]}{E[\alpha_i]}, \tag{11}$$

and moreover the lower and upper bounds are attained when $m_i(x) = 0$ and $m_i(x) \rightarrow \infty$, respectively. In particular, for $C > 0$ and $0 < m_i(x) < \infty$ then both inequalities are strict. If $C \leq 0$ then the inequalities in (11) are simply reversed. From now on we assume that $0 < m_i(x) < \infty$ for all $i = 1, \dots, n$.

Now if $n = 2$ then (11) yields that for $i \neq j$,

$$\frac{E[\alpha_1 \alpha_2]}{E[\alpha_j]} \neq E[\alpha_i | x],$$

from which it follows that $A_{ij} = E[\alpha_i | x] E[\alpha_j] - E[\alpha_1 \alpha_2] \neq 0$. The result for $n = 2$ now follows directly from part (a).

For the final part, in which α has a Dirichlet prior distribution, we first show that $\det \tilde{A}_{-k} \neq 0$, so that (10) has a unique solution. Secondly we show that this solution is given by $B_{jk}(x) = A_{jk}/A_{kj}$.

We start with conditions under which $C > 0$. Specifically, if $\text{Cov}(\alpha_i, \alpha_j) < 0$ for all $i \neq j$ and $\text{Var}(\alpha_i) > 0$ then

$$\begin{aligned} E[\alpha_i]E[\alpha_j] &> E[\alpha_i\alpha_j] \\ \text{so } E[\alpha_i^2]E[\alpha_i]E[\alpha_j] &> E[\alpha_i]^2E[\alpha_i\alpha_j], \end{aligned}$$

from which it follows that $C > 0$.

Next, suppose that $\alpha \sim \mathcal{D}(p_1, \dots, p_n)$ and set $p_0 = \sum_{i=1}^n p_i$. Thus for $i \neq j$, $E[\alpha_i\alpha_j] = p_i p_j / (p_0(p_0 + 1))$, $E[\alpha_i] = p_i / p_0$, $E[\alpha_i^2] = p_i(p_i + 1) / p_0(p_0 + 1)$, $\text{Cov}(\alpha_i, \alpha_j) < 0$ and $\text{Var}(\alpha_i) > 0$. It follows that $C > 0$ and that (11) simplifies to

$$\frac{p_i}{p_0 + 1} < E[\alpha_i|x] < \frac{p_i + 1}{p_0 + 1}. \quad (12)$$

Next, note that for $i \neq j$ we have

$$\begin{aligned} A_{ij} &= E[\alpha_j]E[\alpha_i|x] - E[\alpha_i\alpha_j] \\ &= \frac{p_j}{p_0} \left(E[\alpha_i|x] - \frac{p_i}{p_0 + 1} \right) \\ &= b_j a_i(x), \end{aligned}$$

say, where $b_j = p_j / p_0$. It follows from (12) that $A_{ij} > 0$. Similarly

$$\begin{aligned} A_{ii} &= \frac{p_i}{p_0} \left(E[\alpha_i|x] - \frac{p_i + 1}{p_0 + 1} \right) \\ &= b_i \tilde{a}_i(x), \end{aligned}$$

say. Recall that \tilde{A}_{-k} is the matrix A with the k th row and column deleted. It now follows that

$$\det(\tilde{A}_{-k}) = \left(\prod_{i \neq k} b_i \right) \det(D + E),$$

where D is an $(n-1) \times (n-1)$ diagonal matrix with entries $\tilde{a}_i(x) - a_i(x) = -1/(p_0 + 1)$, $i \neq k$, and E is an $(n-1) \times (n-1)$ matrix consisting of $(n-1)$ identical columns, each of which contains the $(n-1)$ entries a_i , $i \neq k$. Moreover we can write E as the product uv^T , where u is an $(n-1) \times 1$ column vector with entries a_i , $i \neq k$, and v is the $(n-1) \times 1$ column vector of 1's. In particular, $\det \tilde{A}_{-k} \neq 0$ if and only if $\det(D + E) = \det(D + uv^T) \neq 0$.

Now from the matrix determinant lemma,

$$\det(D + uv^T) = (1 + v^T D^{-1} u) \det(D),$$

and since $\det(D) = (-1/(p_0 + 1))^{n-1} \neq 0$, we focus on $1 + v^T D^{-1} u$. Now

$$\begin{aligned} 1 + v^T D^{-1} u &= 1 - \sum_{i \neq k} (p_0 + 1) a_i(x) \\ &= 1 - \sum_{i \neq k} [(p_0 + 1) E[\alpha_i|x] - p_i] \\ &= 1 - (p_0 + 1)(1 - E[\alpha_k|x]) + (p_0 - p_k) \\ &= E[\alpha_k|x](p_0 + 1) - p_k > 0, \end{aligned}$$

where the last inequality follows from (12). Hence $\det \tilde{A}_{-k} \neq 0$ as required.

Finally, we show that for $i \neq k$, (8) is satisfied by $B_{jk}(x) = A_{jk}/A_{kj}$. First, it is straightforward to show that for $i \neq k$,

$$\tilde{a}_i(x) + \sum_{j \neq k; j \neq i} a_j(x) = -a_k(x). \quad (13)$$

Now,

$$\begin{aligned}
\sum_{j \neq k} A_{ij} \frac{A_{jk}}{A_{kj}} &= b_i \tilde{a}_i(x) \frac{b_k a_i(x)}{b_i a_k(x)} + \sum_{j \neq k; j \neq i} b_j a_i(x) \frac{b_k a_j(x)}{b_j a_k(x)} \\
&= \frac{a_i(x) b_k}{a_k(x)} \left(\tilde{a}_i(x) + \sum_{j \neq k; j \neq i} a_j(x) \right) \\
&= \frac{a_i(x) b_k}{a_k(x)} (-a_k(x)) \\
&= -A_{ik},
\end{aligned}$$

using (13). Hence for $i \neq k$, (8) is satisfied by $B_{jk}(x) = A_{jk}/A_{kj}$ as required.

Example A1 To illustrate the calculations in part (a), consider the case $n = 3$, $k = 1$. The equation $\mathbf{A}\mathbf{b} = \mathbf{0}$ is

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} 1 \\ B_{21} \\ B_{31} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix},$$

and so

$$\tilde{A}_{-1} = \begin{bmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{bmatrix}, \quad \tilde{\mathbf{b}} = \begin{bmatrix} B_{21} \\ B_{31} \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} -A_{21} \\ -A_{31} \end{bmatrix}.$$

Applying Lemma 1 yields

$$B_{21} = \frac{\det \tilde{A}_{-21}}{\det \tilde{A}_{-1}} = \frac{\det \begin{bmatrix} -A_{21} & A_{23} \\ -A_{31} & A_{33} \end{bmatrix}}{\det \tilde{A}_{-1}}, \quad B_{31} = \frac{\det \tilde{A}_{-31}}{\det \tilde{A}_{-1}} = \frac{\det \begin{bmatrix} A_{22} & -A_{21} \\ A_{32} & -A_{31} \end{bmatrix}}{\det \tilde{A}_{-1}}.$$

Example A2 To show that $B_{jk}(x)$ does not equal A_{jk}/A_{kj} in general, suppose that $n = 3$, that $m_i(x) = i$ for $i = 1, 2, 3$, and that α has a mixed Dirichlet prior distribution given by

$$\alpha \sim (0.5)\mathcal{D}(1, 1, 1) + (0.5)\mathcal{D}(1, 2, 1).$$

Direct calculation then yields that $E[\alpha_1] = E[\alpha_3] = 7/24$, $E[\alpha_2] = 10/24$ and

$$\begin{bmatrix} E[\alpha_1^2] & E[\alpha_1 \alpha_2] & E[\alpha_1 \alpha_3] \\ E[\alpha_2 \alpha_1] & E[\alpha_2^2] & E[\alpha_2 \alpha_3] \\ E[\alpha_3 \alpha_1] & E[\alpha_3 \alpha_2] & E[\alpha_3^2] \end{bmatrix} = \frac{1}{20} \begin{bmatrix} 2 & 2 & 1 \\ 2 & 6 & 2 \\ 1 & 2 & 2 \end{bmatrix},$$

whence $E[\alpha_1|x] = 31/120$, $E[\alpha_2|x] = 50/120$ and $E[\alpha_3|x] = 39/120$. Thus $A_{21}/A_{12} = 86/46$ while $B_{21} = m_2(x)/m_1(x) = 2$.

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