Approximating the marginal likelihood using copula

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Abstract

Model selection is an important activity in modern data analysis and the conventional Bayesian approach to this problem involves calculation of marginal likelihoods for different models, together with diagnostics which examine specific aspects of model fit. Calculating the marginal likelihood is a difficult computational problem. Our article proposes some extensions of the Laplace approximation for this task that are related to copula models and which are easy to apply. Variations which can be used both with and without simulation from the posterior distribution are considered, as well as use of the approximations with bridge sampling and in random effects models with a large number of latent variables. The use of a $t$-copula to obtain higher accuracy when multivariate dependence is not well captured by a Gaussian copula is also discussed.

Keywords: Bayesian model selection, bridge sampling, copula, Laplace approximation.

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1 Introduction

In Bayesian inference computation of marginal likelihoods is essential for calculating posterior model probabilities and Bayes factors, fundamental quantities for model comparison in the Bayesian framework. If $M_1$ and $M_2$ are two models to be compared with respective parameters $\theta_1$ and $\theta_2$, priors $p(\theta_1)$ and $p(\theta_2)$ and likelihoods $p(y|\theta_1)$ and $p(y|\theta_2)$ where $y = (y_1, ..., y_n)^T$ denotes the data then if $p(M_1)$ and $p(M_2)$ denote the prior probabilities for $M_1$ and $M_2$ then the ratio of their respective posterior probabilities is

$$\frac{p(M_1|y)}{p(M_2|y)} = \frac{p(M_1)}{p(M_2)} \times \frac{p(y|M_1)}{p(y|M_2)}$$

where $p(y|M_j) = \int p(\theta_j)p(y|\theta_j)d\theta_j$ is the marginal likelihood for model $M_j$ and the second term on the right side above is called the Bayes factor comparing $M_1$ to $M_2$.

There are many suggestions for how to calculate the marginal likelihood. One of the simplest methods is the Laplace approximation. We consider now a single model $M$ with parameter $\theta$ of dimension $p$, prior $p(\theta)$ and likelihood $p(y|\theta)$ with marginal likelihood

$$p(y) = \int p(\theta)p(y|\theta)d\theta. \quad (1)$$

Suppressing dependence on $y$, write $f(\theta) = p(\theta)p(y|\theta)$ and $g(\theta) = \log f(\theta)$. Let $\hat{\theta}$ be the mode of $g(\theta)$ and $H$ be the negative Hessian at the mode. The Laplace approximation approximates $g(\theta)$ by $g(\hat{\theta}) - 1/2(\theta - \hat{\theta})^T H(\theta - \hat{\theta})$. Substituting this into (1) and integrating gives

$$p(y) \approx (2\pi)^{p/2}|H|^{-1/2}f(\hat{\theta}) \quad (2)$$

where it can be shown that the error is of order $O(n^{-1})$. The right side of (2) is commonly
used for approximating the marginal likelihood in Bayesian inference but there has also been much interest in the use of the Laplace approximation for calculation of posterior moments in Bayesian applications (Tierney and Kadane, 1986). O’Hagan and Forster (2004), Chapter 9, is a good summary of these applications and associated theory.

There are many other suggested methods for computing the marginal likelihood which are simulation based. Raftery et al. (2007) and Newton and Raftery (1994) consider approaches based on using the so-called harmonic mean identity, an extension of which was discussed by Gelfand and Dey (1994). Such an approach can be unstable, although Raftery et al. (2007) suggest some possible solutions. Averaging the likelihood over parameters simulated from the prior is another possibility that directly uses the definition (1), but since the prior is overdispersed with respect to the likelihood this can be very inefficient requiring very large sample sizes. Several Markov chain Monte Carlo (MCMC) methods attempt to sample on the model and parameter space jointly. Carlin and Chib (1995) suggest an approach based on simulating on a product space. However this approach is hard to apply with a large number of models and requires choice of some tuning parameters that make the method unsuited to routine use. Green (1995) extends the Metropolis-Hastings algorithm to situations involving model uncertainty and his trans-dimensional MCMC method is the method of choice when there is a large number of models to be compared. However, devising MCMC moves to jump between different models in this framework is an art that requires problem specific insight. Several methods for calculating the marginal likelihood make use of the identity

\[ p(y) = \frac{p(\theta)p(y|\theta)}{p(\theta|y)} \]  

which holds for any value of \( \theta \) by a rearrangement of Bayes’ rule. To use this identity, simply observe that the numerator is easy to calculate at any \( \theta \) so that if we are able to estimate the posterior distribution \( p(\theta|y) \) at some point \( \hat{\theta} \) (usually some estimate of
the mode) then we immediately have an estimate of the marginal likelihood. The idea of estimating the marginal likelihood in this way is attributed to Julian Besag by Raftery (1996). Chib (1995) considered use of this identity in the case where a Gibbs’ sampling MCMC algorithm is employed, although when the Gibbs updates consist of many blocks several different runs are needed to get the required density estimate. Although there is a way of avoiding multiple runs, this may not work well in high dimensions (see Chib and Jeliazkov, 2001, for further discussion). Chib and Jeliazkov (2001) extended the method of Chib (1995) to the case of a general Metropolis-Hastings algorithm, although again if the Metropolis-Hastings scheme updates the parameters in many different blocks the method can be tedious to apply. Mira and Nicholls (2004) show that the method of Chib and Jeliazkov (2001) is a special case of the bridge estimator of Meng and Wong (1996) in the way that it estimates certain conditional densities and they also discuss optimality of the bridge sampling implementation. de Valpine (2008) also considers several further refinements of the approach. Gelman and Meng (1998) extend the bridge estimator of Meng and Wong (1986) to an approach they call path sampling – it is related in statistics to a method for high-dimensional integration discussed by Ogata (1989) and to previous work in statistical physics. Implementing path sampling can be quite computationally intensive, involving either several MCMC runs for different target distributions or an MCMC run over a joint distribution including an auxiliary variable. Friel and Pettitt (2008) provide one recent approach to the implementation of path sampling. Another recent novel approach to marginal likelihood calculation is given by Skilling (2006) although implementation of this approach involves possibly difficult simulations from constrained distributions. Han and Carlin (2000) give a survey of MCMC based methods for computing the marginal likelihood and suggest methods based on separate MCMC runs for different models such as those of Chib (1995) and Chib and Jeliazkov (2001) as being easiest to use when the number of models to be compared is small.
We restrict attention in what follows to methods which are easily employed given a simulated sample from the posterior distribution. However, we also consider an extension of the Laplace approximation which does not require simulation. Ways of combining simulation and the Laplace approximation for computing Bayes factors were considered in DiCiccio et al. (1997). They recommended for routine use a volume corrected version of the Laplace approximation, or for higher accuracy and where evaluations of the likelihood are inexpensive a Laplace approximation approach to attaining a near optimal implementation of bridge sampling. We discuss this last method later as the copula approximations we introduce here can be improved in much the same way.

In Section 2 we discuss generalizing the Laplace approximation by approximating the posterior distribution with a Gaussian copula. Density estimation using the Gaussian copula is sensible since in many cases we expect the posterior distribution to be close to normal, so that approximating the posterior with a flexible class of densities which contains the Gaussian as a special case is attractive. We also discuss generalizations where the Gaussian copula is replaced by a $t$-copula. Copula approximations to posterior distributions have not been used very much for Bayesian computation – a notable exception is Reichert et al. (2002) who considered their use in importance sampling schemes. In Section 3 we consider different ways to estimate the marginal distributions in the copula approximation, both with and without simulation output. Section 4 discusses the Laplace bridge estimator which uses an initial estimate of the marginal likelihood obtained by Laplace approximation in implementation of bridge sampling. A similar estimator using our copula framework is then considered. Section 5 considers performance of our methods in some simulated examples, Section 6 considers an example involving logistic regression, Section 7 considers a random effects heteroscedastic probit model for clustered binary data with a large number of latent variables and Section 8 concludes. The copula approximations we describe work well across the whole range of examples we consider, both real and simulated.
A copula Laplace approximation

A Gaussian copula distribution for a continuous random vector $\theta = (\theta_1, ..., \theta_p)^T$ is constructed from given marginal distributions $F_j(\theta_j)$ for $\theta_j$, $j = 1, ..., p$ and a correlation matrix for a latent Gaussian random vector. In particular, suppose $Z \sim N(0, \Lambda)$ where $\Lambda$ is a correlation matrix. Then if $\theta_j = F_j^{-1}(\Phi(Z_j))$ then $\theta_j$ has distribution $F_j$ since $\Phi(Z_j)$ is uniform and transforming a uniform random variable by the inverse of $F_j$ gives a random variable with distribution function $F_j$. Note that while the $\theta_j$ have given marginal distributions $F_j$, they are also correlated due to the correlation between the components of $Z$. For background on Gaussian copula and copula models more generally see Joe (1997). The density function of $\theta$ is (see, for example, Song, 2000)

$$q(\theta) = |\Lambda|^{-1/2} \exp \left( \frac{1}{2} \eta(\theta)^T (I - \Lambda^{-1}) \eta(\theta) \right) \prod_{j=1}^{p} f_j(\theta_j)$$ (4)

where $\eta = \eta(\theta) = (\eta_1, ..., \eta_p)^T$ with $\eta_j = \Phi^{-1}(F_j(\theta_j))$ and $f_j$ is the density function corresponding to $F_j$.

Now suppose we are able to obtain a copula approximation to a posterior distribution $p(\theta|y)$ for a parameter $\theta$, of the form (4). We discuss how to obtain such an approximation both with and without simulation later. Then given an estimate $\hat{\theta}$ of the mode of $p(\theta|y)$ we can employ the identity (3) and our copula density estimate at $\hat{\theta}$ to obtain the estimate

$$p(y) \approx p(\hat{\theta})p(y|\hat{\theta}) \frac{|\Lambda|^{1/2} \exp \left( -\frac{1}{2} \eta(\hat{\theta})^T (I - \Lambda^{-1}) \eta(\hat{\theta}) \right) \prod_{j=1}^{p} f_j(\hat{\theta}_j)}{\prod_{j=1}^{p} f_j(\hat{\theta}_j)}.$$ (5)

where $\Lambda$ is the correlation matrix and $f_j(\theta_j)$, $j = 1, ..., p$ are the marginal densities in our copula approximation. If $\hat{\theta}$ is the componentwise posterior median then $\eta(\hat{\theta}) = 0$ and we
obtain

\[ p(y) \approx \frac{p(\theta)p(y|\theta)|\Lambda|^{1/2}}{\prod_{j=1}^{p} f_j(\hat{\theta}_j)}. \] 

(6)

This estimate reduces to the ordinary Laplace approximation if we consider the special case where our Gaussian copula is a multivariate normal density estimate with mean the posterior mode and covariance matrix given by the inverse of the negative Hessian of the log posterior at the mode.

3 Estimating the marginals

To apply the approximation (6) we need a Gaussian copula approximation to the posterior distribution. We consider both analytic and simulation based methods for obtaining this, as well as an extension of the Gaussian copula approach which uses $t$-copula.

3.1 Analytic approach

Write, as in Section 1, $f(\theta) = p(\theta)p(y|\theta)$, $g(\theta) = \log f(\theta)$ and $H = -g''(\hat{\theta})$ for the matrix of negative second order partial derivatives of $g(\theta)$ evaluated at the mode $\hat{\theta}$. Decompose $H$ as $DCD^T$ where $C$ is a correlation matrix and $D = \text{diag}(d_j)$ and $H^{-1} = SAS^T$ where $A$ is a correlation matrix and $S = \text{diag}(s_j)$. Now consider a Gaussian copula density as an approximation to the posterior distribution, where the approximation to the marginal posterior distribution for $\theta_j$ is

\[ f_j(\theta_j) = \frac{f(\hat{\theta} + (\theta_j - \hat{\theta}_j)e_j)^{1/(d_j^2 s_j^2)}}{\int_{-\infty}^{\infty} f(\hat{\theta} + (\theta_j - \hat{\theta}_j)e_j)^{1/(d_j^2 s_j^2)} d\theta_j} \]

and $e_j$ is a $p$-vector of zeros but with a one in the $j$th position and the copula correlation matrix is $A$. 
The intuition behind this density estimate is as follows. We estimate the marginal for \( \theta_j \) by considering a slice through the function \( f(\theta) \) with values of \( \theta_i, \ i \neq j \), fixed at their modal values (this is the function \( f(\hat{\theta} + (\theta_j - \hat{\theta}_j)e_j) \) and then overdisperse by raising this function to a power and normalizing. Note that if \( f(\theta) \) is proportional to a multivariate Gaussian, then \( f(\hat{\theta} + (\theta_j - \hat{\theta}_j)e_j) \) is proportional to the conditional density of \( \theta_j \) given that the other components are fixed at their modal values. This conditional distribution has as its mean the unconditional mean of \( \theta_j \), and the variance \( 1/s^2_j \). Then raising this function to the power of \( 1/(d_j^2 s^2_j) \) and normalizing maintains the mean while changing the variance from \( 1/s^2_j \) to \( d^2_j \), which is the unconditional variance for \( \theta_j \) (in the multivariate Gaussian case). So this operation gives the correct marginal distribution when \( f(\theta) \) is proportional to a multivariate Gaussian. The approximation to the marginal is also exact in the case of independence (where \( d^2_j s^2_j = 1 \) and \( A = I \)). Choice of the copula correlation matrix as \( A \) is also made to ensure that the approximation to the joint posterior is exact in the case of \( p(\theta|y) \) being multivariate normal. The copula approximation is of interest in itself apart from the application to computing marginal likelihoods. In particular, for a Gaussian copula expectations for low-dimensional marginal distributions are easily calculated. For instance, suppose that we want to approximate for the \( j \)th component \( \theta_j \) of \( \theta \) the posterior expectation \( E(h(\theta_j)|y) \). Then this is easily obtained from our copula approximation as

\[
\int h(\theta_j)g_j(\theta_j)d\theta_j
\]

where \( g_j(\theta_j) \) is the marginal for \( \theta_j \). This expression is easily evaluated with one-dimensional numerical integration. The approximation is exact both in the Gaussian case and in the case where components of the posterior are independent and it seems preferable to the simple normal approximation.
3.2 Simulation based approach

An alternative and more accurate approach to approximating the posterior distribution by a Gaussian copula involves using a simulation based method. Suppose that we have a sample $\theta^{(1)}, ..., \theta^{(s)}$ from the posterior distribution $p(\theta | y)$ obtained by some method such as MCMC. Consider the estimate $\hat{\theta}$ where $\hat{\theta}$ consists of the componentwise median. We estimate the quantities $f_j(\hat{\theta}_j)$ using kernel density estimates based on the simulation output. We note that Hsiao et al. (2004) have considered multivariate kernel density estimation in conjunction with the formula (3) for estimating the marginal likelihood but clearly this approach is limited to fairly low dimensional situations. It only remains to specify how we obtain the correlation matrix $\Lambda$ in our copula approximation to the posterior.

Let $r_{jk}$ be the rank of $\theta_{k}^{(j)}$ among the values $\theta_{k}^{(i)}$, $i = 1, ..., s$. Define the $p$-vector $Z^{(j)}$ to have $k$th component $Z_k^{(j)} = \Phi^{-1}((r_{jk} - 0.5)/s)$ where $\Phi$ denotes the standard normal distribution function. We obtain $\Lambda$ as the estimated correlation matrix of $Z^{(1)}, ..., Z^{(s)}$, which we obtain by the robust method of Rosseuw and Van Zomeren (1990) rather than using the sample correlation matrix, similar to Di Ciccio et al. (1997) in their implementation of a simulation based Laplace approximation. Roughly speaking, the above construction estimates the marginal distribution for a copula with the empirical distribution function and then transforms to the latent Gaussian variables assumed in the copula construction to obtain an estimate of the copula correlation.

We can extend our Gaussian copula approximation to a $t$-copula. Laplace-type approximations using the multivariate $t$-distribution have been considered previously (Leonard, Hsu and Ritter, 1994). A $t$-copula distribution with $\nu$ degrees of freedom for a continuous random vector $\theta = (\theta_1, ..., \theta_p)^T$ with marginals $F_1(\theta_1), ..., F_p(\theta_p)$ has density

$$q(\theta) = \frac{f_p(\eta(\theta); 0, \Lambda, \nu)}{\prod_{j=1}^{p} f_1(\eta_j(\theta_j); 0, 1, \nu)} \prod_{j=1}^{p} f_j(\theta_j)$$
where $f_k(\eta; 0, \Lambda, \nu)$ is the $k$-dimensional multivariate $t$-density with mean 0, scale $\Lambda$ and degrees of freedom $\nu$, $\eta(\theta) = (\eta_1, ..., \eta_p)^T$ with $\eta_j = \eta_j(\theta_j) = F_j^{-1}(F_j(\theta_j); 0, 1, \nu)$ where $F_k(\eta; 0, \Lambda, \nu)$ is the distribution function for $f_k(\eta; 0, \Lambda, \nu)$, and $f_j(\theta_j)$ is the density for $F_j(\theta_j)$. If we have an approximation to the posterior distribution of this form we can again obtain an estimate of the marginal likelihood based on the estimated posterior density at some value $\hat{\theta}$. Taking again $\hat{\theta}$ as the componentwise median, we obtain

$$p(y) \approx \frac{p(\hat{\theta})p(y|\hat{\theta})}{\prod_{j=1}^p f_j(\hat{\theta}_j)} \frac{\Gamma \left( \frac{\nu+p}{2} \right)^p}{\Gamma \left( \frac{\nu+1}{2} \right) \Gamma \left( \frac{p}{2} \right) \Gamma \left( \frac{\nu}{2} \right)^{p-1}}.$$ 

Of course, as $\nu \to \infty$ this reduces to our former approximation based on the Gaussian copula.

Once more we need some simple way to estimate $\Lambda$ and in this case $\nu$ from simulation output to apply this formula. Let $r_{jk}$ be the rank of $\theta_k^{(j)}$ among the values $\theta_k^{(i)}$, $i = 1, ..., s$. For fixed degrees of freedom $\nu$ let $T_k^{(j)} = F^{-1}_1((r_{jk} - 0.5)/s; 0, 1, \nu)$, $T^{(j)} = (T_1^{(j)}, ..., T_p^{(j)})^T$ and let $\Lambda(\nu)$ be obtained as the maximum likelihood estimator of the correlation matrix assuming the $T^{(j)}$ are independent and identically distributed from a multivariate $t$-distribution with mean 0, scale $\Lambda$ and degrees of freedom $\nu$. On the copula scale one can consider the data $R^{(j)}$ with $R_k^{(j)} = (r_{jk} - 0.5)/s$ and assuming the $R^{(j)}$ are independent and identically distributed from the density

$$\frac{f_p(F_1^{-1}(r_1; 0, 1, \nu), ..., F_p^{-1}(r_p; 0, 1, \nu); 0, \Lambda(\nu), \nu)}{\prod_{j=1}^p f_1(F_j^{-1}(r_j; 0, 1, \nu); 0, 1, \nu)}$$

obtain a maximum likelihood estimator for $\nu$ numerically by a grid search.

4 Laplace bridge estimator

DiCiccio et al. (1997) find that combining Laplace approximation and the bridge estimator of Meng and Wong (1996) is very effective in improving accuracy. In its most general form the bridge estimator can estimate a ratio of marginal likelihoods but here we just consider
a special case where interest centres on calculation of a single marginal likelihood. We want to calculate the normalizing constant (marginal likelihood) \( p(y) \) in \( p(\theta|y) \propto p(\theta)p(y|\theta) \).

Suppose we have some density \( r(\theta) \) (where in this discussion there is no unknown normalizing constant for \( r \)) and let \( t(\theta) \) be any function of \( \theta \) such that

\[
0 < \left| \int t(\theta) r(\theta) p(\theta)p(y|\theta)d\theta \right| < \infty.
\]

Then it is easily shown that

\[
p(y) = \frac{\int p(\theta)p(y|\theta)t(\theta)r(\theta)d\theta}{\int r(\theta)t(\theta)p(\theta)p(y|\theta)d\theta}.
\]

If we have a sample \( \theta^{(1)}, ..., \theta^{(s)} \) from \( p(\theta|y) \) and a sample \( \tilde{\theta}^{(1)}, ..., \tilde{\theta}^{(s)} \) from \( r(\theta) \), then we have

\[
p(y) \approx \frac{1}{s} \sum_{i=1}^{s} t(\tilde{\theta}^{(i)}) p(\tilde{\theta}^{(i)}) p(y|\tilde{\theta}^{(i)}) \frac{1}{s} \sum_{i=1}^{s} t(\theta^{(i)}) r(\theta^{(i)})
\]

Meng and Wong (1996) show that the optimal choice of the function \( t(\theta) \) is

\[
\left\{ \frac{s p(\theta)p(y|\theta)}{p(y)} + Sr(\theta) \right\}^{-1}.
\]

Actually, (7) is the optimal choice when the generated samples from both \( p(\theta|y) \) and \( r(\theta) \) are independent. For the samples from \( p(\theta|y) \) which are usually generated via MCMC this is usually not the case and an adjustment could be made to account for the typically positive correlation, although we have not done this here. Note also that (7) involves \( p(y) \), which is unknown. It is possible to implement an iterative version of bridge sampling where \( p(y) \) is successively refined in (7) (Meng and Wong, 1996). The Laplace bridge estimator simply uses the Laplace approximation to estimate \( p(y) \) in (7) for the purpose of determining a \( t(\theta) \) for implementation of bridge sampling, and uses the usual normal approximation for \( r(\theta) \).
We can similarly suggest estimating \( p(y) \) with our Gaussian copula approach, and using our Gaussian copula approximation to the posterior for \( r(\theta) \) with kernel density estimates based on the simulation output for the marginals. Note that simulating directly from a Gaussian copula is straightforward.

5 Simulation studies

To evaluate the accuracy of our methods we consider their use for calculating the normalizing constant for some known density functions. Of course, the normalizing constant is known to be one here so accuracy of the approximations is easily assessed. We consider the multivariate skew \( t \) distribution of Branco and Dey (2001). This is a convenient distribution to use since it can accommodate both skewness and heavy tails, it is easy to simulate from non-iteratively and its density function is easy to calculate. Branco and Dey (2001), p. 105, consider a generalized multivariate skew \( t \) distribution but here we just consider the special case of their multivariate skew \( t \). For \( Y = (Y_1, ..., Y_k)^T \) the density is

\[
f_Y(y) = 2 f_k(y; \mu, \Lambda, \nu) F_1 \left( \frac{\delta^T \Lambda^{-1} (y - \mu)}{\sqrt{1 - \delta^T \Lambda^{-1} \delta}} \frac{\nu + k}{\nu + (y - \mu)^T \Lambda^{-1} (y - \mu)}; 0, 1, \nu + k \right)
\] (8)

where as before \( f_k(y; \mu, \Lambda, \nu) \) is the \( k \)-dimensional multivariate \( t \) distribution with mean \( \mu \), scale matrix \( \Lambda \) and \( \nu \) degrees of freedom, \( F_k(y; \mu, \Lambda, \nu) \) is the corresponding density function, and \( \delta = (\delta_1, ..., \delta_k)^T \) is a vector of skewness parameters. Obviously with \( \delta = 0 \) we obtain the ordinary multivariate \( t \) distribution. For our simulations we choose \( \mu = 0, \Lambda = I \) and \( \delta \) of the form \((\delta_1, 0, ..., 0)^T\). Choosing \( \Lambda \) and \( \delta \) in this way means that only the first component of \( Y \) is skewed, with \( \delta_1 \) controlling skewness, \( \delta_1 > 0 \) giving positive skewness and \( \delta_1 < 0 \) giving negative skewness. The random vector \( Y \) with density (8) may be constructed in the following way. Let \( Z = [X_0 X]^T \) be a \((k + 1)\)-dimensional multivariate \( t \) distributed
random vector with $X_0$ a scalar and $X$ a $k$-vector,

$$\mu^* = (0, \mu^T)^T \quad \Lambda^* = \begin{bmatrix} 1 & \delta^T \\ \delta & \Lambda \end{bmatrix}$$

where $\mu^*$ and $\Lambda^*$ are partitioned in the same way as $Z$. Then $Y$ has the distribution of $X|X_0 > 0$. Note that this construction gives a simple non-iterative way of simulating from this distribution.

Our simulations investigated the effects of heavy tails (through $\nu$), skewness (through $\delta_1$) and dimensionality on the accuracy of the method we have discussed. In particular, for each of our methods we considered every combination of $\nu = 3, 10$, $\delta_1 = 0, 0.5, 0.99$ and $k = 2, 5, 10$ dimensions. The methods we compare are the ordinary Laplace approximation (L1), a Laplace approximation where we use the componentwise posterior median and minimum volume ellipsoid covariance estimation method of Rosseuw and Van Zomeren (1990) from simulation output rather than the mode and negative inverse Hessian (L2), our copula Laplace approximation without simulation (CL1), our copula approximation with simulation (CL2), the $t$-copula approximation (TC), the Laplace bridge estimator (LB) and the copula bridge estimator (CLB). For the methods based on simulation, we used 10,000 replications. For method L2, the use of the componentwise median and minimum volume ellipsoid methods for estimating the mean and covariance were discussed in DiCiccio et al. (1997) and found to work well in high dimensions. For the two variants of bridge estimation we also used 10,000 simulations from $r(\theta)$, and for the copula bridge estimator we estimated the marginals using a kernel density estimator (we used the default implementation of the density function in the stats package of R, R core development team, 2005). For the simulation based methods we report average values obtained over 50 simulation replicates, with the standard deviation over replicates in brackets. Of course there are ways to approximate standard errors based on a single replicate (de Valpine, 2008, for example) but we
have chosen not to do this here for the purposes of our simulation studies. In practice such methods are of course very important. In our tables we have reported the estimated value of the log of the normalizing constant (true value 0) rather than the normalizing constant itself. The results are shown in Tables 1-3. The main conclusions which emerge are that the copula approximations improve over the respective Laplace approximations for the variants both with and without simulation. Generally performance of all methods deteriorates with higher dimension and heavier tails, as might be expected. Perhaps not intuitively for some of the methods performance improves with increasing skewness. Both variants of bridge estimation work well, but the copula bridge method seems to improve over the Laplace bridge method in the 10-dimensional case with skewness, with a smaller standard deviation over replicates. The $t$-copula works extremely well, but perhaps this is not surprising given that the test function is constructed from a generalization of the multivariate $t$-distribution. In the $t$-copula, the estimate of the degrees of freedom was chosen from a grid including integer values 1 to 10, 15, 20 and 50. In our later real examples the $t$-copula approximation fares less well than in these simulations.

6 Low birthweight example

For a real example we consider calculation of marginal likelihoods for model comparison in a regression with binary response. In particular, we consider the low birth weight data reported by Hosmer and Lemeshow (1989) which are concerned with 189 births at a US hospital in a study where it was desired to found out which predictors of low birthweight were important in the hospital where the study was carried out. The binary response is an indicator for birthweight being less than 2.5 kg. After transforming the predictors as described in Venables and Ripley (2002) there are ten covariates, two continuous and eight binary predictors. These covariates are shown in Table 4. For our analysis of the data, we
consider generalized linear models with logit and robit links (with three degrees of freedom for the robit link), using the default prior for logistic regression given by Gelman et al. (2008) on coefficients for both the choices of link function. See Gelman and Hill (2007) pp. 124-125 for a brief introduction to robit regression. Venables and Ripley (2002) consider model selection for this example and the logit link using a stepwise approach. They also consider the inclusion of second order interaction terms. The final model they choose includes all the predictors in Table 4 as main effects except for the indicators for race, as well as interaction terms age*ftv1, age*ftv2+ and smoke*ui. Here we consider a direct comparison of the model including all the original predictors as main effects with the final model of Venables and Ripley (2002) for both the logit and robit links. Note that the comparisons between links here are non-nested and not easily done via traditional hypothesis testing approaches. Venables and Ripley (2002) also consider examining the adequacy of their linear model with second order interactions by expanding to a generalized additive model with smooth terms for the covariates age, age*ftv1, age*ftv2+ and lwt. We consider a similar model here, but we simply use second order polynomials for representing the additive smooth terms which should be adequate for the purposes of model checking. For these three different models and the two different choices of link function we calculated the log marginal likelihood using the same methods considered in our simulation study. We also considered the same comparisons for a random sample from the original data set of size \( n = 50 \) to show how the accuracy of the approximations is affected by sample size. For generating MCMC iterates we used a Metropolis-Hastings scheme with normal random walk proposal with the covariance based on the Hessian of the log posterior at the mode. The results of these comparisons are shown in Tables 5 and 6. Also shown in the table is a “gold standard” value (GS) for each case obtained by Laplace bridge with \( s = S = 100,000 \). Using this value for comparison, we obtain a similar picture of the performance of the respective methods to that obtained from the simulation study. All methods are remarkably accurate for the full data set. In the small
sample setting of the randomly chosen subset, the copula approximations improve over their simpler Laplace approximation variants, and bridge sampling works well with the copula approach showing less variability than the Laplace bridge for the highest-dimensional case. For the $t$-copula, we estimated the degrees of freedom choosing from a grid of integer values where the maximum value is 50 – generally the largest value of 50 was chosen in nearly every case, so that performance is generally similar but slightly inferior to the Gaussian copula approximation.

7 A high-dimensional example

Our last example concerns a complex random effects model for a dataset concerned with stated preferences of Australian women on whether or not to have a papsmear test (Fiebig and Hall, 2005). There are 79 women in the study and each is presented with 32 different scenarios. The response is an indicator for whether the women would undertake a papsmear test so there are 32 repeated binary observations on each of the 79 women. We consider the following random effects heteroscedastic probit model which was considered in Gu et al. (2008) and analyzed using a Bayesian approach. Following the notation of Gu et al. (2008) and letting $i = 1, ..., 79$ index the different women or clusters, and $j = 1, ..., 32$ index observations within clusters, the binary observation $y_{ij}$ is considered to arise from a continuous latent variable $y_{ij}^*$ by

$$y_{ij} = \begin{cases} 
1 & \text{if } y_{ij}^* > 0 \\
0 & \text{otherwise.}
\end{cases}$$
Similar latent variable formulations are often used in Bayesian analyses of simple probit models (Albert and Chib, 1993). The $y^*_{ij}$ follow the model

$$y^*_{ij} = x_{ij}\beta + \mu_i + \nu_{ij}$$

where $\mu_i$ is a subject or cluster specific random effect, $x_{ij}$ is a vector of covariates, $\beta$ is an unknown vector of regression coefficients and $\nu_{ij} \sim N(0, \sigma^2_{ij})$ with $\sigma^2_{ij} = \exp(w_{ij}\delta)$ where $w_{ij}$ is a vector of covariates (often $x_{ij} = w_{ij}$) and $\delta$ is a vector of unknown coefficients. For identifiability an intercept should not be included in $w_{ij}$. The covariates used to define $x_{ij}$ and $w_{ij}$ in this example are shown in Table 1. Gu et al. (2008) use the following priors for $\beta$, $\delta$ and $\sigma^2_{\mu}$. First,

$$\beta | \delta \sim N(0, c_\beta (\tilde{X}^T \tilde{X})^{-1})$$

where $c_\beta$ is set to the total number of observations ($32 \times 79$ here) and $\tilde{X} = D(\delta)^{-1}X$ where $X = (x_{11}^T, ..., x_{1,32}^T, ..., x_{79,32}^T)^T$ and

$$D(\delta) = \text{diag} \left( \exp \left( \frac{w_{11}\delta}{2} \right), ..., \exp \left( \frac{w_{1,32}\delta}{2} \right), ..., \exp \left( \frac{w_{79,32}\delta}{2} \right) \right)^T.$$  

Then $\delta \sim N(0, c_\delta I)$ and $\sigma^2_\delta, c_\delta \sim \text{IG}(a, b)$ independently where $a = 1 + 10^{-10}$, $b = 1 + 10^{-5}$ and IG denotes the inverse gamma distribution. An efficient MCMC sampling scheme can be developed with $\beta$ and $\mu = (\mu_1, ..., \mu_{79})^T$ updated as a single block with a Gibbs sampling step, $\delta$ updated using a Metropolis-Hastings step and $\sigma^2_\delta$ and $c_\delta$ updated with Gibbs sampling steps. See Gu et al. (2008) for details. If we set $\delta = 0$ in this model, this results in a homoscedastic random effects probit model and it is of some interest to compare this model with the full model. See Gu et al. (2008) for references and discussion.

This is a challenging example because of the presence of the latent variables $y^*_{ij}$ and $\mu$. Our approach effectively integrates out the latent variables which is important since
otherwise we obtain a very high-dimensional problem. We will apply the formula (3) for estimating the marginal likelihood with \( \theta = (\delta^T, \beta^T, \sigma^2_{\mu}, c_\delta)^T \). Note that it is difficult to apply bridge sampling with \( \mu \) integrated out as this requires evaluating \( p(y|\theta) \) for a large number of different values of \( \theta \). To apply our approach we need to be able to estimate \( p(y|\theta) \) at a single value \( \theta^* \). As before, assume that we have an MCMC sample from \( p(\theta, y^*, \mu|y) \).

We can use for \( \theta^* = (\delta^*T, \beta^*T, \sigma^2_{\mu}, c_\delta^*)^T \) the componentwise posterior median, say. Then to estimate \( p(y|\theta^*) \) we can simulate values \( \mu^{(1)}, ..., \mu^{(s)} \) from \( p(\mu|\sigma^2_{\mu}) \) and compute

\[
\frac{1}{s} \sum_{i=1}^{s} p(y|\theta^*, \mu^{(i)}).
\]

To use (3) to estimate \( p(y) \), it only remains to estimate \( p(\theta^*|y) \). With our copula approach, we can do this directly by fitting a Gaussian copula model to the simulation output. We also consider a simple normal density estimate, which is similar to the Laplace-Metropolis estimator of Lewis and Raftery (1997). For comparison, we implement the computationally intensive but also more accurate method of Chib and Jeliazkov (2001) which can be applied with latent variable models such as the one considered here. Write

\[
p(\theta^*|y) = p(\delta^*|y)p(\beta^*|\delta^*, y)p(\sigma^2_{\mu}|\beta^*, \delta^*, y)p(c_\delta^*|\beta^*, \delta^*, \sigma^2_{\mu}, y).
\]

(9)

In the present context, we use the approach of Chib and Jeliazkov (2001) to estimate each of the terms on the right hand side of (9). This requires separate runs for the different blocks of parameters in the decomposition (see Chib and Jeliazkov, 2001, for further discussion). The terms for \( \beta, \sigma^2_{\mu} \) and \( c_\delta \) are relatively easily handled as full conditionals are available for these parameters, but \( \delta \) is updated by a Metropolis-Hastings step. It is of interest to see whether the rather tedious but accurate multiple runs approach of Chib and Jeliazkov (2001) results in very similar results to an approximation which requires less coding effort.
and computation time. Table 8 shows the results for the approach of Chib and Jeliazkov (CJ), copula approximation (CL) and normal approximation (L). The log marginal likelihood is estimated for both heteroscedastic and homoscedastic models.

The copula approximations work well for much less computational effort. The additional computational effort for the copula approximation is essentially negligible once the MCMC run for the full model is obtained whereas CJ requires 2 additional reduced MCMC runs where first $\delta^*$ and then $\beta^*$ and $\delta^*$ are held fixed. In the table as before we report a mean and standard deviation (bracketed) across 50 simulation replicates for each of the methods. We also tried the $t$-copula approximation but this was similar but slightly inferior to the Gaussian copula approximation.

We can envisage a role for our copula approximations in conjunction with the CJ approach and similar approaches in high-dimensional situations. One could use a copula approximation for some blocks of parameters in estimating the conditional distribution in (9). When it is natural to use a large number of small blocks in the MCMC scheme the method of CJ may be very tedious to apply so grouping some small blocks together and applying a copula approximation while dealing with the remaining blocks using the CJ approach (for instance for blocks where the full conditional is available) is potentially attractive. The greater accuracy of the copula approximation compared to the normal approximation would allow the consideration of a larger number of smaller blocks.

8 Discussion and Conclusions

With large datasets becoming increasingly common in statistical applications there has been recent renewed interest in fast deterministic approximations like the Laplace approximation as an alternative to Monte Carlo methods or to improve the implementation of Monte Carlo methods in certain problems. Among the methods we have considered, the copula
approximations are the ones that work well across the whole range of real and simulated examples that we have discussed, and the copula methods usually improve on their simpler Laplace type variants both with and without simulation. We believe our methods have great potential to be used both by themselves, in combination with other methods, and even in conjunction with MCMC algorithms where there is a need for better proposal distributions. Investigation of these applications is continuing.

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Table 1: Methods L1, L2, CL1, CL2, TC, LB and CLB applied to integrate multivariate skew t densities in 2 dimensions with 3 and 10 degrees of freedom and zero, moderate and extreme skewness. The estimated log of the integral of the density (true value 0) is reported.

| Degrees of freedom | Method | Skewness |
|--------------------|--------|----------|
|                    |        | $\delta_1 = 0$ | $\delta_1 = 0.5$ | $\delta_1 = 0.99$ |
| 3                  | L1     | -0.51    | -0.51    | -0.60    |
|                    | L2     | 0.09 (0.02) | 0.07 (0.02) | -0.30 (0.02) |
|                    | CL1    | -0.16    | -0.17    | -0.17    |
|                    | CL2    | 0.20 (0.02) | 0.18 (0.03) | 0.09 (0.03) |
|                    | TC     | 0.04 (0.03) | 0.03 (0.02) | -0.01 (0.02) |
|                    | LB     | 0.00 (0.01) | 0.00 (0.01) | 0.00 (0.01) |
|                    | CLB    | 0.00 (0.00) | 0.00 (0.00) | 0.00 (0.01) |
| 10                 | L1     | -0.18    | -0.18    | -0.34    |
|                    | L2     | -0.03 (0.01) | -0.04 (0.02) | -0.27 (0.02) |
|                    | CL1    | -0.05    | -0.05    | -0.05    |
|                    | CL2    | 0.07 (0.03) | 0.07 (0.03) | 0.04 (0.03) |
|                    | TC     | 0.02 (0.03) | 0.02 (0.03) | 0.01 (0.03) |
|                    | LB     | 0.00 (0.00) | 0.00 (0.00) | 0.00 (0.01) |
|                    | CLB    | 0.00 (0.00) | 0.00 (0.00) | 0.00 (0.00) |
Table 2: Methods L1, L2, CL1, CL2, TC, LB and CLB applied to integrate multivariate skew t densities in 5 dimensions with 3 and 10 degrees of freedom and zero, moderate and extreme skewness. The estimated log of the integral of the density (true value 0) is reported.

| Degrees of freedom | Method | Skewness          |
|-------------------|--------|-------------------|
|                   |        | $\delta_1 = 0$   | $\delta_1 = 0.5$ | $\delta_1 = 0.99$ |
| 3                 | L1     | -1.55             | -1.55             | -1.69             |
|                   | L2     | 1.08 (0.03)       | 1.02 (0.03)       | 0.50 (0.04)       |
|                   | CL1    | -1.04             | -1.05             | -1.06             |
|                   | CL2    | 0.66 (0.04)       | 0.60 (0.05)       | 0.32 (0.06)       |
|                   | TC     | 0.08 (0.05)       | 0.04 (0.05)       | -0.01 (0.06)      |
|                   | LB     | 0.00 (0.01)       | 0.00 (0.01)       | 0.00 (0.02)       |
|                   | CLB    | 0.00 (0.00)       | 0.00 (0.00)       | 0.00 (0.00)       |
| 10                | L1     | -0.68             | -0.68             | -0.85             |
|                   | L2     | -0.31 (0.03)      | 0.30 (0.03)       | 0.08 (0.04)       |
|                   | CL1    | -0.42             | -0.42             | -0.42             |
|                   | CL2    | 0.18 (0.05)       | 0.16 (0.04)       | 0.08 (0.05)       |
|                   | TC     | 0.06 (0.04)       | 0.05 (0.05)       | -0.04 (0.07)      |
|                   | LB     | 0.00 (0.01)       | 0.00 (0.01)       | 0.00 (0.01)       |
|                   | CLB    | 0.00 (0.00)       | 0.00 (0.00)       | 0.00 (0.00)       |
Table 3: Methods L1, L2, CL1, CL2, TC, LB and CLB applied to integrate multivariate skew t densities in 10 dimensions with 3 and 10 degrees of freedom and zero, moderate and extreme skewness. The estimated log of the integral of the density (true value 0) is reported.

| Degrees of freedom | Method | Skewness          |
|--------------------|--------|-------------------|
| 3                  |        | \( \delta_1 = 0 \) | \( \delta_1 = 0.5 \) | \( \delta_1 = 0.99 \) |
|                    | L1     | -3.58             | -3.58             | -3.74             |
|                    | L2     | 3.89 (0.07)       | 3.72 (0.08)       | 2.89 (0.06)       |
|                    | CL1    | -2.97             | -2.97             | -2.98             |
|                    | CL2    | 2.91 (0.08)       | 2.76 (0.08)       | 2.15 (0.08)       |
|                    | TC     | 0.16 (0.07)       | 0.03 (0.08)       | -0.48 (0.34)      |
|                    | LB     | 0.00 (0.03)       | 0.00 (0.03)       | 0.00 (0.04)       |
|                    | CLB    | 0.00 (0.01)       | 0.00 (0.02)       | 0.01 (0.01)       |
| 10                 | L1     | -1.89             | -1.89             | -2.07             |
|                    | L2     | 1.51 (0.04)       | 1.48 (0.04)       | 1.19 (0.04)       |
|                    | CL1    | -1.50             | -1.50             | -1.50             |
|                    | CL2    | 1.18 (0.09)       | 1.13 (0.08)       | 0.97 (0.06)       |
|                    | TC     | 0.10 (0.07)       | 0.08 (0.06)       | -0.12 (0.05)      |
|                    | LB     | 0.00 (0.01)       | 0.00 (0.01)       | 0.00 (0.02)       |
|                    | CLB    | 0.00 (0.00)       | 0.00 (0.00)       | 0.00 (0.00)       |

Table 4: Predictors for low birth weights data set

| Predictor | Description |
|-----------|-------------|
| age       | age of mother in years |
| lwt       | weight of mother (lbs) at least menstrual period |
| raceblack | indicator for race=black (0/1) |
| raceother | indicator for race other than white or black (0/1) |
| smoke     | smoking status during pregnancy (0/1) |
| ptd       | previous premature labors (0/1) |
| ht        | history of hypertension (0/1) |
| ui        | has uterine irritability (0/1) |
| ftv1      | indicator for one physician visit in first trimester (0/1) |
| ftv2+     | indicator for two or more physician visits in first trimester (0/1) |
Table 5: Approximations to log marginal likelihoods for models $M_0$ (linear model with all original predictors and no interactions), $M_1$ (interaction model of Venables and Ripley) and $M_2$ (model with additive terms for continuous covariates) for low birthweight example.

| Link function | Method | $M_0$   | $M_1$   | $M_2$   |
|---------------|--------|---------|---------|---------|
|               |        |         |         |         |
| Logistic      | L1     | -124.3  | -120.0  | -122.4  |
|               | L2     | -124.4 (0.2) | -120.1 (0.3) | -122.5 (0.3) |
|               | CL1    | -124.2  | -119.8  | -122.1  |
|               | CL2    | -124.3 (0.3) | -120.0 (0.5) | -122.4 (0.5) |
|               | TC     | -124.6 (0.4) | -120.4 (0.4) | -123.1 (0.5) |
|               | LB     | -124.1 (0.0) | -119.7 (0.0) | -122.0 (0.1) |
|               | CLB    | -124.3 (0.0) | -120.0 (0.0) | -122.5 (0.1) |
|               | GS     | -124.1  | -119.7  | -122.0  |
| Robit         | L1     | -132.9  | -128.1  | -131.4  |
|               | L2     | -132.2 (0.2) | -127.2 (0.2) | -129.9 (0.3) |
|               | CL1    | -132.7  | -127.8  | -129.6  |
|               | CL2    | -132.6 (0.3) | -127.8 (0.5) | -130.7 (0.5) |
|               | TC     | -132.9 (0.4) | -127.9 (0.3) | -131.1 (0.5) |
|               | LB     | -132.4 (0.0) | -127.4 (0.1) | -130.3 (0.1) |
|               | CLB    | -132.7 (0.0) | -127.7 (0.0) | -130.8 (0.1) |
|               | GS     | -132.5  | -127.5  | -130.3  |
Table 6: Approximations to log marginal likelihoods for models $M_0$ (linear model with all original predictors and no interactions), $M_1$ (interaction model of Venables and Ripley) and $M_2$ (model with additive terms for continuous covariates) for randomly chosen subset of size 50 for low birthweight example.

| Link function | Method | $M_0$ | $M_1$ | $M_2$ |
|---------------|--------|-------|-------|-------|
| Logistic      | L1     | -37.9 | -38.1 | -38.6 |
|               | L2     | -35.7 (0.4) | -34.8 (1.0) | -33.2 (0.6) |
|               | CL1    | -36.9 | -36.7 | -35.7 |
|               | CL2    | -36.8 (0.3) | -36.5 (0.7) | -35.9 (0.4) |
|               | TC     | -36.9 (0.3) | -36.6 (0.3) | -36.5 (0.9) |
|               | LB     | -36.6 (0.2) | -36.0 (0.4) | -35.2 (0.6) |
|               | CLB    | -36.9 (0.2) | -36.5 (0.1) | -36.0 (0.3) |
|               | GS     | -36.6 | -36.1 | -35.4 |
| Robit         | L1     | -43.2 | -43.1 | -43.1 |
|               | L2     | -39.3 (0.4) | -38.3 (0.9) | -36.8 (0.9) |
|               | CL1    | -39.9 | -38.5 | -37.0 |
|               | CL2    | -41.1 (0.3) | -40.6 (0.6) | -39.8 (0.6) |
|               | TC     | -41.5 (0.5) | -40.8 (0.8) | -40.1 (0.7) |
|               | LB     | -40.8 (0.3) | -40.1 (0.7) | -39.0 (0.9) |
|               | CLB    | -41.2 (0.4) | -40.6 (0.2) | -39.9 (0.4) |
|               | GS     | -40.7 | -40.3 | -39.5 |

Table 7: Predictors for papsmear data set

| Predictor | Description                                      |
|-----------|--------------------------------------------------|
| knowgp    | 1 if the GP is known to the patient; 0 otherwise |
| sexgp     | 1 if the GP is male; 0 otherwise                 |
| testdue   | 1 if the patient is due or overdue for a paptest; 0 otherwise |
| drec      | 1 if the GP recommends that the patient has a paptest; 0 otherwise |
| papcost   | cost of test in Australian dollars                |
Table 8: Approximations to log marginal likelihoods for heteroscedastic and homoscedastic models for the papsmear data.

| Method | Model            | Heteroscedastic | Homoscedastic |
|--------|------------------|-----------------|---------------|
| L      | -1101.8 (0.5)    | -1119.1 (0.2)   |
| CL     | -1101.4 (0.5)    | -1118.9 (0.2)   |
| CJ     | -1101.5 (0.5)    | -1118.9 (0.2)   |