Diagnostics for Variational Bayes approximations

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Abstract: Variational Bayes (VB) has shown itself to be a powerful approximation method in many application areas. This paper describes some diagnostics methods which can assess how well the VB approximates the true posterior, particularly with regards to its covariance structure. The methods proposed also allow us to generate simple corrections when the approximation error is large. It looks at joint, marginal and conditional aspects of the approximate posterior and shows how to apply these techniques in both simulated and real data examples.

Keywords and phrases: Variational Bayes, Diagnostics, Covariance matrix, Independent Metropolis-Hastings.

1. Introduction

This paper looks at diagnostics tests to evaluate the quality of variational Bayes (VB) solutions. As is typical with diagnostic testing in statistics - think of diagnostic testing in regression analysis for example - we look at necessary conditions for adequacy. A VB solution may be inadequate from a number of perspectives. Here we list some of the most important. Firstly, by definition the posterior covariance structure is distorted, so both posterior variances and correlations can be wrong. Secondly, VB convergence is only local, hence it might miss other ‘better’ solutions. In particular it might focus on a single mode of a multimodal solution. Thirdly, there may be errors in higher order posterior moments, such as skewness or kurtosis. A given diagnostic test is designed to detect a particular kind of error, and the key idea of this paper is to make available a number of computationally fast diagnostics, with a computation time of the order of the VB itself, which target particularly common forms of inadequacy, specifically the first on the list above.

The VB method provides a fast and analytical approximation to otherwise intractable posterior distributions. Early developments of the method can be found in applications to neural networks [15], [19], with further work in independent component analysis [17], [1], graphical models [29], [2], information
retrieval [4], and factor analysis [8]. Other applications of variational principle can be found in [10], [20], [5], [11], [28], while an excellent recent review can be found in [22].

The essence of the method relies on making simplifying assumptions about the posterior dependence of a problem. This results in a high dimension integral being decomposed into a set of low dimensional ones which may be expected to be more tractable. Various real-world applications have demonstrated that the VB method is very computationally efficient. For example, reversible jump MCMC [9] may require many millions of iterations to obtain posterior samples for a finite mixture of Normals, however, the VB approximations can need only a few hundred, even though each iteration of the VB method is very fast.

For the examples of this paper, and others, our studies show that VB can give good approximations to the posterior mean structure of a problem, and is good at finding overall structural features – such as the number of components in a mixture. However the posterior variance can be underestimated. This underestimation of the variance has also been reported by other researchers, for example, [3] and [26]. Moreover, by definition the general posterior dependence structure is distorted. This motivates the work in this paper to develop diagnostics to see how well the VB approximations represent the actual posterior covariance structures, and to some extent to provide corrections when these errors are large. We emphasize that these tests are only designed for these forms of error and may not detect errors of different kind.

We propose three diagnostics methods which only use the information obtained from VB approximations. The first method looks at the the joint posterior distribution and attempts to find an optimal affine transformation which links the VB and true posteriors. The second method is based on a marginal posterior density approximation technique proposed by Tierney, Kass, Kadane (1989) [27]. Here we work in specific low dimensional directions to estimate true posterior variances and correlations. The third method, based on a stepwise conditional approach, allows us to construct and solve a set of system of equations which lead to estimates of the true posterior variances and correlations.

This paper also proposes a novel method to calculate the variance of a marginal or conditional distributions of the posterior. This method uses an independent Metropolis-Hastings algorithm with the proposal kernel being configured by the VB approximations. Instead of using the sample moments, the variance of the target distribution is computed by reading the acceptance probability of the generated MCMC chain.

The paper is organized as follows. Section 2 presents the proposed methods in detail. Applications of the methods on the simulated data and real-world data are shown in Section 3. Conclusions and discussions are in Section 4.

2. The three diagnostic methods

Consider the posterior distribution of a $p-$dimensional vector parameter $\theta = (\theta_1, \cdots, \theta_p)$, with density function $p(\theta|x)$ where $x$ is an independent and identically distributed random sample. We denote the VB approximation by $q(\theta)$,
the true posterior mean by \( \mu = (\mu_1, \cdots, \mu_p) \), the covariance matrix by \( \Sigma \) with variance of \( \sigma_i^2, i = 1, \cdots, p \) and correlation coefficients \{\rho_{ij}\}.

### 2.1. Optimal affine transformations of joint distributions

We denote the random vector associated with a VB approximation by \( \eta \). We search for optimal affine transformations of \( \eta \) (denoted by \( A\eta + B \), over specified classes of \( p \times p \) matrices, \( A \) and \( p \times 1 \) vectors, \( B \)). The aim is to get close to \( \theta \), the random vector associated with the true posterior.

First, generate an independent random sample of size \( n \) from the VB distribution, denoted as \( \{\eta_i\}_{i=1}^n \). The values of \( A \) and \( B \) are obtained by maximizing a likelihood function, over the specified class, \( \text{Lik}(A, B) := \prod_{i=1}^n \left( \frac{p(\theta_i | y; A, B)}{\det(A)} \right) \), \( (2.1) \)

where \( \theta_i = A\eta_i + B \), and \( \det(A) \) is the determinant of \( A \) and the corresponding estimates are denoted by \( \hat{A} \) and \( \hat{B} \). Sampling from \( q(\eta) \) is typically straightforward since \( q(\eta) \) usually has a factorization form of \( q(\eta) = \prod_i q_i(\eta_i) \) and \( q_i(\eta_i) \) often have a well-known distributional form. The maximization of \( (2.1) \) with respect to \( A \) and \( B \) is possible because it does not require the unknown normalizing constant of the posterior, \( p(\theta | x) \).

For small or medium dimensional problems we only restrict the transformation matrix \( A \) to be general lower triangular, with the positive diagonal elements for identification reasons. For more complex problems sparser classes of matrices can be used, trading off the power of the test with speed.

### 2.2. Marginal approximations

This method considers a projection of the vector parameter \( \theta \) in a direction \( \alpha \), denoted by \( \alpha^T \theta \). The variance of \( \alpha^T \theta \) is given by \( \alpha^T \Sigma \alpha \), which is a function of \( \{\sigma_i^2\}_{i=1}^p \) and \( \{\rho_{ij}\} \). If we have the projections in different directions, we can obtain a system of equations which can be easily solved to obtain the values of \( \{\sigma_i^2\}_{i=1}^p \) and \( \{\rho_{ij}\} \).

The key computation of this method is to calculate the value of the marginal variance. In order to be computationally efficient and exploit the VB solution we propose the following new method.

Suppose \( p(\theta) \) is a target distribution and \( q(\theta) \) is a proposal distribution. The independent Metropolis-Hastings (IMH) algorithm will produce a transition from \( \theta^{(t)} \) to \( \theta^{(t+1)} \) as described in Algorithm 1. Theorem 2.1, proved in [23], establishes a connection between the expected acceptance rate (EAR) and the closeness of the target distribution \( p(\theta) \) and the proposal distribution \( q \) measured in Kullback-Leibler (KL) divergence.

**Theorem 2.1.** If there exists a constant \( M \) such that \( p(\theta) < Mq(\theta) \) for all \( \theta \), then \( KL(p|q) < \log(M) \) and the expected acceptance rate (EAR) is at least \( \frac{1}{M} \) when the chain is stationary.
Heuristically, Theorem 2.1 states the closer the target and the proposal, the higher the EAR. It is obvious that when \( p(\theta) \) and \( q(\theta) \) are identical, the optimal acceptance rate equals to one. This result is different from other types of Metropolis-Hastings algorithms. For examples, for random-walk Metropolis-Hastings algorithm the optimal acceptance rate is close to 0.234 \([24]\); for Metropolis adjusted Langevin algorithms an overall acceptance rate is close to 0.574 \([25]\).

Motivated by this general result, first consider a special case in which the target distribution is a univariate normal with mean of \( \mu \) and variance of \( \sigma^2_t \) and the proposal distribution is a normal with the same mean and variance \( \sigma^2_p \) (assume \( \sigma^2_p > \sigma^2_t \)). It can be shown that the EAR is monotone decreasing as the proposal variance of \( \sigma^2_p \) increases. Conversely, it says that given a fixed value of proposal variance of \( \sigma^2_p \), the value of the target variance \( \sigma^2_p \) is one-to-one correspondence to the value of EAR. This implies by monitoring the acceptance probability, we can obtain the value of the target variance. A table of expected acceptance rate versus the value of target variance is given in the Appendix.

After this motivation let us consider the method in practice. Consider two basics facts: firstly posteriors approach to normality when sample size is large, and secondly VB provides good mean structure approximations. Hence we propose a new method to compute the target variance. We call it a VB Adjusted Independent Metropolis-Hastings method (VBAIMH). The variance of the target distribution is obtained by checking the acceptance rate for a standard normal kernel centred at the VB mean, being used as the proposal. In fact, the idea of using acceptance rates to compute the target variances can be further extended to using acceptance rates as a key diagnostic to how close the VB distribution is to the true posterior. More discussion can be seen shortly.

The new approach above has several advantages. First it does not require any particular tuning tricks to run the IMH algorithm. We only need the posterior mean values produced by the VB approximation to configure the proposal kernel. This is a significant advantage over other MCMC methods, in which the implementation issues are the major concerns.

Secondly, this VB kernel allows the MCMC chain to locate the regions of high posterior probability more efficiently, since the proposal kernel is around the posterior mode, at least locally; then we only need a short chain to compute acceptance rates. This is another significant advantage over the other MCMC methods, where the computational cost can be a big concern. While the IMH algorithm is well known to perform poorly in high dimensions \([7]\), in this method we are sampling from a univariate distribution defined by the projections.

Third, when an acceptance rate is low, the generated sample may not represent the target distribution well, and the moments calculated upon these samples can be wrong. However, a low acceptance rate on its own reflects a significant discrepancy between the target and the proposal.

It is worth noting that when the projection is along the direction of a single parameter of \( \theta \); that is, for example, we set \( \alpha = (1, 0, \cdots, 0) \), the VBAIMH can provide a possible mechanism to calibrate the EAR as a diagnostic tool to measure inaccuracy in the marginal approximations of VB, by using \( q(\theta_i) \) directly as the proposal distribution. When the acceptance rate is low, it clearly
Algorithm 1 Independent Metropolis-Hastings (IMH) algorithm

Given $\theta^{(t)}$

**Step 1** propose $\eta^t \sim q$.

**Step 2** Accept $\theta^{(t+1)} = \begin{cases} 
\eta^t & \text{with prob. } \min\left\{ \frac{\pi(\eta^t)p(\eta^t)}{\pi(\theta^{(t)})q(\eta^t)} , 1 \right\}; \\
\theta^{(t)} & \text{otherwise.} \end{cases}$

indicates the approximation will be inaccurate. Thus it gives us two uses: firstly a diagnostics tool in the general case and secondly it is possible to give a correction to the VB approximation. More discussion can be found in Section 4.

The above idea can be further extended to more general situations, where the diagnostics are targeted to more specific errors. For example, if only a subset of parameters is of immediate concern, which is of particular usefulness in the high dimensional problems.

To run an IMH algorithm we also need to know the density function of $\alpha^T \theta$, at least up to scaling by a normalizing constant. Tierney, Kass, and Kadane (1989)[27] proposed an elegant marginal approximation of this posterior distribution.

Suppose the parameter of interest is $\omega = g(\theta)$, where $g$ is a continuous real-valued function on $\mathbb{R}^p$. The posterior distribution of $p(\omega|x)$ can be approximated as follows

$$p(\omega|x) \propto \frac{\hat{p}(\omega|x)}{|R_\omega|^{1/2}(b_\omega^2 R_\omega^{-1} b_\omega)^{1/2}}, \quad (2.2)$$

where

$$\hat{p}(\omega|x) = \sup_{\theta: g(\theta) = \omega} p(\theta|x), b_\omega = \left. \frac{\partial g(\theta)}{\partial \theta} \right|_{\theta = \theta_\omega}, R_\omega = \left. \frac{\partial^2 \log p(\theta|x)}{\partial \theta \partial \theta^T} \right|_{\theta = \theta_\omega},$$

and $\theta_\omega$ conditionally maximizes $p(\theta|x)$ with respect to $\theta$ for each given $\omega$.

### 2.3. The conditional stepwise method

The unknown quantities in a true posterior covariance matrix $\Sigma$ are $\{\sigma_i^2\}_{i=1}^P$ and $\{\rho_{ij}\}$ and the difference between these and the VB versions which we are using as our diagnostics. The stepwise method looks at conditional distributions constructed from the true posterior and compares them to ones based on the VB solution. Algorithm 2 gives a description on the proposed method. The three steps can be explained as follows.

Step 1 uses a linear transformation of $Y = Q\theta$ to scale the variances of $\{\sigma_i^2\}_{i=1}^P$ to be the ratios of $\{\sigma_i^2\}_{i=1}^P$ over their variational estimations, and uses a linear transformation of $Z = MY$ to further scale these ratios to be one, which only leaves $\{\rho_{ij}\}$ in $\Sigma$ to be found.
Step 2 finds a series of conditional bivariate random vector \( U_{ij} \), to which the eigenvalues of their covariance matrix can be computed numerically after a rotation.

Step 3 constructs a system of equations of \( f_k(\{\rho_{ij}\}) \) by linking the analytical expression of the correlation coefficient for the conditional bivariate \( U_{ij} \), obtained based on the posterior normality (when sample size is large), to their numerical values of \( r_k \), obtained by using the relationship between eigenvalues, and variances and correlation coefficients in a bivariate covariance matrix. The values of \( \{\sigma^2_i\}_i=1^p \) can be obtained by reversing Step 1.

**Algorithm 2** The stepwise method

**Step 1**

- Define \( Y = Q\theta \) and \( \mu = Q\mu = (\mu^1, \cdots, \mu^p) \), where \( Q = \left( \frac{1}{\text{var}_y(\theta_j)} \right) \) is a diagonal matrix. Denote \( Y_{1|Y_{-1}} \) as the conditional \( Y_1 \) conditioning on \( Y_j = \mu^j, j \neq i \).
- Denote \( m^2_i = \text{var}(Y_{1|Y_{-1}}) \). Obtain \( m^2_i, i = 1, \cdots, p \), numerically.
- Define \( Z = MY \), and \( \mu_{zj} = MU = (\mu^1, \cdots, \mu^p) \), where \( M = \left( \frac{1}{\text{var}_z} \right) \) is a diagonal matrix.

**Step 2**

- Denote \( U_{ij} = Z_{ij}|Z_{-ij}, i \neq j \) as the conditional bivariate \( (Z_i, Z_j) \) conditioning on \( Z_t = \mu^t, t \neq i, j \).
- Let \( R = \left( \begin{array}{cc} \cos(\frac{\pi}{2}) & -\sin(\frac{\pi}{2}) \\ \sin(\frac{\pi}{2}) & \cos(\frac{\pi}{2}) \end{array} \right) \). Define \( V_k = (V_{k,1}, V_{k,2}) = RU_{ij} \), where \( k = 1, \cdots, \frac{p(p-1)}{2} \) for all the pair of \( i \neq j \). Denote \( \lambda^2_{k,1} = \text{var}(V_{k,1}) \) and \( \lambda^2_{k,2} = \text{var}(V_{k,2}) \).
- Obtain \( \lambda^2_{k,1} \) and \( \lambda^2_{k,2}, k = 1, \cdots, \frac{p(p-1)}{2} \), numerically.

**Step 3**

- Based on the posterior normality assumption, compute the correlation coefficient for the conditional bivariate \( U_{ij} \), and denote it as \( f_k(\{\rho_{ij}\}) \), where \( k = 1, \cdots, \frac{p(p-1)}{2} \), for all the pair of \( i \neq j \).
- Compute \( r_k = \frac{(\lambda^2_{k,1} - 1)}{(\lambda^2_{k,2} + 1)} \), \( k = 1, \cdots, \frac{p(p-1)}{2} \). Solve the system of equations of \( f_k(\{\rho_{ij}\}) = r_k \) to obtain the value of \( \{\rho_{ij}\} \).
- Based on the posterior normality assumption, compute the conditional variances of \( var(Y_{1|Y_{-1}}) \), and denote it as \( g_i(\sigma^2_i) \), where \( i = 1, \cdots, p \). Solve the equation \( g_i(\sigma^2_i) = m^2_i \) to obtain the value of \( \sigma^2_i \).

The key computations in Algorithm 2 involve computing the values of a univariate conditionally or marginal variances, that is \( m^2_i, i = 1, \cdots, p \) in Step 1 and \( \lambda^2_{k,1} \) and \( \lambda^2_{k,2}, k = 1, \cdots, \frac{p(p-1)}{2} \) in Step 2. Again, these values can be computed by the VBAIMH method. The definition of \( r_k \) in Step 3 derives from the following fact. For a bivariate distribution, suppose the variances are \( \sigma^2_1 \) and \( \sigma^2_2 \) and correlation is \( \rho \). The eigenvalues of covariance matrix are given as

\[
\lambda = \frac{(\sigma^2_1 + \sigma^2_2) \pm \sqrt{(\sigma^2_1 - \sigma^2_2)^2 + 4\rho^2\sigma^2_1\sigma^2_2}}{2}.
\]

When \( \sigma^2_1 = \sigma^2_2 \), the eigenvalues are given by
\[ \lambda_1 = (1 + \rho)\sigma^2, \quad \text{and} \quad \lambda_2 = (1 - \rho)\sigma^2. \]

Then it is easy to show that
\[ \rho = \frac{\left(\frac{\lambda_1}{\lambda_2} - 1\right)}{\left(\frac{\lambda_1}{\lambda_2} + 1\right)}. \] (2.3)

To illustrate the method, we provide a three-dimension example which can be found in the Appendix.

3. Numerical studies

In this section, we will work through four models with simulated or real datasets to demonstrate the proposed methods. For each model we compute its variational approximation, obtained by minimizing the the Kullback-Leibler (KL) divergence [16]. The distributional families of these approximations range widely; for example in the cases considered here they are Normal, \(t\), Beta, Inverse Gamma, and Dirichlet.

We start with a very basic illustrative example: a large sample multivariate normal case with simulated data. The second example looks at a Normal random sample with unknown mean and variance with a real data set. In this case posterior normality is not assumed, showing that normality is not needed for the methods to have power. We thirdly consider a two-component mixture of Normals model and finally a regime-switching lognormal model. This last model can be considered a high-dimensional case with six interest parameters, and 528 latent nuisance parameters. These models present a wide range of complex dependence structures, and MCMC methods have been intensively studied with them; these models will provide good testimony for the proposed methods. For the regime-switching lognormal model, we used the real data set of the TSX monthly total return index in the period from January 1956 to December 1999, which contains 528 observations in total, see for discussion [12], [13], and [14].

3.1. Multivariate normal distributions

We consider a 3-dimension vector parameter \( \theta = (\theta_1, \theta_2, \theta_3) \), and the posterior distribution of \( \theta \) and its VB approximation are all assumed to be a multivariate Normal distribution, and these two normal distributions have the same mean values. For the illustration purposes we will arbitrarily choose the values of the covariance matrices for the true posterior and the VB approximation. The following is an example; the actual variances are chosen to be 0.1\(^2\), 1.3\(^2\), and 4\(^2\) with correlation 0.51 between \( \theta_1 \) and \( \theta_2 \), 0.37 between \( \theta_1 \) and \( \theta_3 \), and \(-0.3\). In the VB approximation, the variances are assumed to be \( \frac{0.1^2}{2.2} \), \( \frac{1.3^2}{5.1} \), and \( \frac{4^2}{6.9} \), and all correlation are assumed 0.

Our goal is that given the covariance of VB approximations and the density function of the posterior distribution up to a normalizing constant we will compute the true covariance structure, more precisely, to find the values of correlation coefficients of 0.51, 0.37, and \(-0.3\) and the ratios of the posterior variances versus the VB variances, 2.2, 5.1, and 6.9.
We first apply the affine transformation method. A sample of size of 600 is generated from the VB distribution. We restrict the transformation matrix $A$ to be a lower triangular matrix with positive diagonal elements. There is no constraints on the three parameters in the translation vector $B$. Maximizing the posterior probability over these 9 parameters can be done with the Newton’s method or standard search methods. The resulted $\hat{A}$ and $\hat{B}$ are given by

$$
\hat{A} = \begin{pmatrix}
1.527 & 0.000 & 0.000 \\
10.498 & 2.007 & 0.000 \\
23.601 & -3.627 & 1.918
\end{pmatrix}; \quad 
\hat{B} = \begin{pmatrix}
-0.004 \\
-1.1089 \\
1.758
\end{pmatrix}
$$

Given $\hat{A}$ and $\hat{B}$, the estimated $\hat{\Sigma}_p$ can be computed by $\hat{A} \Sigma_v \hat{A}^T$. The second column in Table 1 gives the estimated variance ratios and correlation coefficients from $\hat{\Sigma}_p$. We see these estimates are close to the actual values, which is given in the first column.

| direction | Acceptance rate | EAR reading: $l_i$ |
|-----------|-----------------|--------------------|
| $(1, 1, 1)$ | 0.790 | 1.94 |
| $(1, -1, 1)$ | 0.805 | 1.86 |
| $(1, 1, -1)$ | 0.764 | 2.12 |
| $(1, -1, -1)$ | 0.764 | 0.47 |
| $(1, 0.5, 1)$ | 0.865 | 1.52 |
| $(0.5, 1.5, 1)$ | 0.791 | 1.94 |

Second, we use the method using marginal approximations. It requires 6 projections. We denote a projection direction as $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, and the marginal variance along the projection direction as $l$. Thus, we can obtain a polynomial equation involving $\sigma_i^2$ and $\rho_{ij}$ given by

$$
a_1^2 \sigma_1^2 + a_2^2 \sigma_2^2 + a_3^2 \sigma_3^2 + 2 a_1 \alpha_2 \rho_{12} \sigma_1 \sigma_2^2 + 2 a_1 \alpha_3 \rho_{13} \sigma_1 \sigma_3^2 + 2 a_2 \alpha_3 \rho_{23} \sigma_2 \sigma_3^2 = l
$$

For each direction we simulate a sample of size 6000 and use the last 50% sample points to calculate the acceptance rate. The values of $l$ (Table 2) are obtained from EAR table readings. Solving the 6 polynomial equations, we obtained the following values: $\sigma_1 = 1.59, \sigma_2 = 2.19, \sigma_3 = 2.65, \rho_{12} = 0.56, \rho_{13} = 0.32, \rho_{23} = -0.30$. The variance ratios are given in the third column in Table 1. We can see these estimates are consistent with those above and the true ones.
Finally, we work through the conditional stepwise method. The notation used here follow that given in Algorithm 2. For Step 1 and 2, we simulate a sample of size 5000 and use the last 50% sample points to calculate the acceptance rate, and the conditional variance is obtained from EAR readings. All numerical results are given in Table 3. Solving the polynomial equations obtains the values for $\rho_{12} = 0.50$, $\rho_{13} = 0.40$ and $\rho_{23} = -0.28$ and the variance ratios, that are given in the fourth column in Table 1.

### Table 3

| Marginal variance | Acceptance rate | EAR table readings | Eigenvalue ratio |
|-------------------|----------------|--------------------|------------------|
| $m_1^2$           | 0.989          | 0.97               | -                |
| $m_2^2$           | 0.730          | 2.42               | -                |
| $m_3^2$           | 0.620          | 3.6                | -                |
| $\lambda_{1,1}^2, \lambda_{1,2}^2$ | 0.832, 0.651 | 0.588, 3.220       | -                |
| $\lambda_{2,1}^2, \lambda_{2,2}^2$ | 0.848, 0.681 | 0.602, 2.800       | -                |
| $\lambda_{3,1}^2, \lambda_{3,2}^2$ | 0.718, 0.852 | 2.520, 0.625       | -                |
| $r_1$             | -              | -                  | 0.691            |
| $r_2$             | -              | -                  | 0.646            |
| $r_3$             | -              | -                  | -0.603           |

### 3.2. Normal random sample

In this example, we consider a real dataset which contains 1033 records of weights for some Major League Baseball (MLB) Players [21]. Plots suggests that it may be reasonable to model the data by a normal distribution with the mean $\mu$ and variance $\sigma^2$. We are interested in making inferences on $\mu$ and $\sigma^2$. In a Bayesian setting, we consider the priors as $\mu \sim N(\gamma, \eta^2)$ and $\sigma^2 \sim IG(\alpha, \beta)$, where IG denotes the inverse Gamma distribution. This setting is referred as a semi-conjugate prior [6]. The joint posterior distribution for $\mu$ and $\sigma^2$ is given by

$$p(\mu, \sigma^2 | y) \sim \left( \frac{1}{\sigma^2} \right)^{-(\frac{\alpha}{2}+\alpha+1)} \exp \left( -\frac{1}{\sigma^2} \left( \frac{S^2}{2} + \beta + \frac{n(\mu - \bar{y})}{2} \right) - \frac{\mu - \gamma}{2\eta^2} \right),$$

where $\bar{y}$ is the sample mean and $S^2$ is the total sum of squares of $y$. The values of hyper-parameters are chosen to be $\alpha = 2$, $\beta = 440.64$, $\gamma = 221.86$, and $\eta^2 = 1$, where the values for $\beta$ and $\gamma$ derives from the mean and variance of the dataset respectively.

Despite the apparent simplicity of this model, the actual marginal posteriors for $\mu$ and $\sigma^2$ have no closed analytic forms. We consider the VB approximation, having a form of $q(\mu, \sigma^2) = q(\mu)q(\sigma^2)$. VB converges after 14 iterations. The distributions for $q(\mu)$ and $q(\sigma^2)$ are given as follows;

As a standard comparison, we run a Gibbs sampler, and simulate a sample of size $10^5$ from the posterior distribution. Table 5 gives a comparison of posterior mean and posterior covariance estimated by the VB approximation and the MCMC sample moments. The third row in Table 5 gives the ratios of posterior
Table 4

The marginal distributions of VB approximations

| Parameter | Distribution (VB) |
|-----------|-------------------|
| $\mu$     | $N(208.09, 0.32)$ |
| $\sigma^2$| $IG(518.50, 249154.70)$ |

Table 5

Posterior mean and covariance

| Method      | Posterior mean: $(\mu, \sigma^2)$ | Posterior covariance: $(\mu, \sigma^2)$ |
|-------------|-----------------------------------|----------------------------------------|
| Gibbs samples | $(208.10, 481.79)$ | $0.60^2 \times 0.34^2 \times 0.60 \times 22.64^2$ |
| VB approx.   | $(208.09, 481.46)$ | $0.56^2 \times 0.60 \times 21.18^2$ |
| Ratios      | $(1, 1)$               | $(1.13, 1.14)$                         |

mean and the ratios of posterior variance. We can see that the means estimated by both methods are almost identical. However the variances approximated by VB are slightly underestimated, (as expected from our discussion above) and it is obvious VB distorts the posterior dependence structure.

We applied the three proposed methods to this problem. All the setting and routines used here are very similar to the those used in the previous example. The numerical results produced by each method are given in the Appendix. The final results for three methods are given in Table 6. We see that all of the methods perform well.

Table 6

MLB Players weights: 3 methods

| Method      | Variance ratios | Correlation coeff. |
|-------------|-----------------|--------------------|
| Gibbs       | 1.13            | 1.14               | 0.34                |
| Affine      | 1.09            | 1.13               | 0.30                |
| Marginal    | 1.08            | 1.20               | 0.35                |
| Stepwise    | 1.13            | 1.14               | 0.35                |

3.3. Finite mixture models

In this example, we considers a two-component mixture of normals. The density function is given by $f(x_i|\Psi) = \pi \phi(x_i|\mu_1, \sigma_1^2) + (1-\pi) \phi(x_i|\mu_2, \sigma_2^2)$, where $0 < \pi < 1$, $\phi$ is the normal density function, $\Psi = (\pi, \mu_1, \sigma_1, \mu_2, \sigma_2)$ are the model parameters. Based on the conjugacy consideration, We choose the following prior distributions,

$$p(\pi) = \text{Beta} \left( \frac{a_0}{2}, \frac{a_0}{2} \right), \ a_0 > 0;$$

$$p(\mu_j, \sigma_j^2) = N(\mu_j|\sigma_j^2, c_j, \frac{\sigma_j^2}{\sigma_j^2} IG(\sigma_j^2; e_j, f_j), j = 1, 2.$$
where \( a_0, c_j, d^2_j, e_j, f_j \) are hyper-parameters. Given a dataset \( x = \{x_i\}_{i=1}^n \), the posterior distribution is given by

\[
p(\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2 | x) \propto \prod_{i=1}^{n} f(x_i | \Psi)p(\pi)p(\mu_1, \sigma_1^2)p(\mu_2, \sigma_2^2).
\]

We consider such a VB approximation having a factorization as

\[
q(\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2) = q(\pi)q(\mu_1 | \sigma_1^2)q(\sigma_1^2)q(\mu_2 | \sigma_2^2)q(\sigma_2^2).
\]

For illustration, we consider a special model

\[
f(x) = 0.4\phi(x; 1, 1) + 0.6\phi(x; 3.5, 0.5).
\]

A sample dataset of size 400 was generated from this model. Figure 1 shows the histogram of the dataset. The VB method for this dataset converges after 122 iterations. The approximation distributions are given in Table 7.

| Parameter          | Distribution (VB)                        |
|--------------------|------------------------------------------|
| \( \pi \)         | Beta(167.35, 232.67)                      |
| \( \mu_1 | \sigma_1^2 \)  | N(1.13, \sigma_1^2/168.34)               |
| \( \sigma_1^2 \)  | IG(85.66, 76.56)                           |
| \( \mu_2 | \sigma_2^2 \)  | N(3.57, \sigma_2^2/233.66)               |
| \( \sigma_2^2 \)  | IG(118.33, 50.31)                         |

**Table 7**

The marginal distributions of VB approximations

Alternatively, we run a Gibbs sampler, and simulate a sample of size \( 2 \times 10^6 \) from the posterior distribution. The posterior mean and covariance estimated by the VB approximations and by the MCMC sample moments are given in Table 8 and 9. The ratios of posterior means and the ratios of posterior variances are given in the last row in Table 8 and 9. These ratios indicate that the means estimated by both methods are almost identical. However VB underestimated the
actual posterior variances, and again strongly distorts the correlation structure.

The proposed methods are applied to this mixture problem. For the VBAIMH method, we generate 4000 samples to compute acceptance rates. The sample size is much smaller than is used in the Gibbs sampler, to which we use a large sample size to ensure the chain has in fact converged.

In addition, we note that in this example we have targeted the most general form of linear transformation to correct any inadequacy in posterior mean and variance. In fact a diagnostic test can be designed to be targeted at more special concerns. For example the matrix $A$ in the transformation might be restricted to be of a particular class such as diagonal or banded. This would be particularly useful in high dimensional problems where the dimension of the space of $A$ could become problematic.

All numerical results associated with each method are given in the Appendix. The final results are given in Table 10. We see all the estimates are close to the values computed by using MCMC samples (the first column).

### 3.4. The regime-switching model

Our final example considers the high-dimensional regime-switching lognormal model (RSLN), proposed by [12], which is used to model the switching processes between different states or regimes in many time series. For this example we consider a real dataset of the TSX monthly total return index in the period from January 1956 to December 1999 (528 observations in total). This dataset is studied in [12], [13], and [14] in the context of maximum likelihood and MCMC methods. We offer an VB solution for this model in [30].

The regime-switching lognormal model with a fixed finite number, K, of regimes can be described as a bivariate discrete time process with the ob-
Table 10
Two-component mixtures of Normals: 3 methods

|        | Gibbs | Affine | Marginal | Stepwise |
|--------|-------|--------|----------|----------|
| \( \pi \) | 3.42  | 3.64   | 5.56     | 3.06     |
| \( \mu_1 \) | 3.54  | 4.51   | 4.73     | 4.12     |
| \( \mu_2 \) | 1.90  | 3.53   | 2.37     | 2.70     |
| \( \sigma^2_1 \) | 3.78  | 3.35   | 4.15     | 3.21     |
| \( \rho_{12} \) | 0.83  | 0.76   | 0.63     | 0.71     |
| \( \rho_{13} \) | 0.81  | 0.68   | 0.59     | 0.63     |
| \( \rho_{23} \) | 0.94  | 0.71   | 0.87     | 0.65     |
| \( \rho_{14} \) | 0.69  | 0.66   | 0.47     | 0.64     |
| \( \rho_{24} \) | 0.84  | 0.73   | 0.82     | 0.70     |
| \( \rho_{34} \) | 0.73  | 0.59   | 0.76     | 0.53     |
| \( \rho_{15} \) | -0.60 | -0.61  | -0.46    | -0.58    |
| \( \rho_{25} \) | -0.66 | -0.61  | -0.66    | -0.58    |
| \( \rho_{35} \) | -0.76 | -0.63  | -0.71    | -0.60    |
| \( \rho_{45} \) | -0.50 | -0.50  | -0.54    | -0.47    |

served data sequence \( w_{1:T} = \{w_t\}_{t=1}^T \) and the unobserved regime sequence \( S_{1:T} = \{S_t\}_{t=1}^T \), where \( S_t \in \{1, \ldots, K\} \) and \( T \) is the number of observations. This unobserved sequence forms the high dimensional latent structure for this problem. The logarithm of \( w_t \), denoted by \( y_t = \log w_t \), is assumed normally distributed having mean \( \mu_i \) and variance \( \sigma^2_i \) both dependent on the hidden regime \( S_t \). The sequence of \( S_{1:T} \) is assumed to follow a first order Markov chain having transition probabilities \( A = (a_{ij}) \) with the probabilities \( \pi = (\pi_i)_{i=1}^K \) to start the first regime.

In the Bayesian framework, we use a symmetric Dirichlet prior for \( \pi \), that is

\[
p(\pi) = \text{Dir}(\pi; \frac{C^\pi}{K}, \ldots, \frac{C^\pi}{K}), \text{ for } C^\pi > 0.
\]

Let \( a_i \) denote the \( i^{th} \) row vector of \( A \). The prior for \( A \) is chosen as

\[
p(A) = \prod_{i=1}^K p(a_i) = \prod_{i=1}^K \text{Dir}(a_i; \frac{C^A}{K}, \ldots, \frac{C^A}{K}), \text{ for } C^A > 0.
\]

The prior distribution for \( \{ (\mu_i, \sigma^2_i) \}_{i=1}^K \) is chosen normal-inverse gamma,

\[
p(\{ (\mu_i, \sigma^2_i) \}_{i=1}^K) = \prod_{i=1}^K \text{N}(\mu_i|\sigma^2_i; \gamma, \frac{\sigma^2_i}{\eta^2})\text{IG}(\sigma^2_i; \alpha, \beta).
\]

In the above setting, \( C^\pi, C^A, \gamma, \eta^2, \alpha, \text{ and } \beta \) are hyper-parameters. Thus, the joint posterior distribution of \( \pi, A, \{ \mu_i, \sigma^2_i \}_{i=1}^K, \text{ and } S_{1:T} \) can be obtained as,

\[
P(\pi, A, \{ \mu_i, \sigma^2_i \}_{i=1}^K, S_{1:T} | y_{1:T}) \propto p(S_1 | \pi) \prod_{i=1}^{T-1} p(S_{i+1} | S_i; A) \prod_{t=1}^T p(y_t | S_t; \{ \mu_i, \sigma^2_i \}_{i=1}^K) \]

\[
p(\pi)p(A)p(\{ \mu_i, \sigma^2_i \}_{i=1}^K).
\]

(3.1)
we choose the variational approximation which is factorized as follows

\[ q(\pi, A, \{\mu_i, \sigma^2_i\}_{i=1}^K, S_{1:T}) = q(\pi) \prod_{i=1}^K q(a_i) \prod_{i=1}^K q(\mu_i|\sigma^2_i)q(\sigma^2_i)q(S_{1:T}). \]

In [30], we show that VB suggests a two-regime RSLN model for the monthly TSX total return data. The VB approximations are given as follows:

| Parameter | Distribution (VB) |
|-----------|-------------------|
| \(\mu_1\) | \(t_{454.61}(0.0123, 37078.19)\) |
| \(\sigma_1^2\) | IG(227.30, 0.28) |
| \(\mu_2\) | \(t_{80.39}(-0.0161, 12987.55)\) |
| \(\sigma_2^2\) | IG(40.20, 0.24) |
| \(a_{1,2}\) | Dirichlet(15.21, 434.78) |
| \(a_{2,1}\) | Dirichlet(15.00, 61.21) |

The marginal distributions of VB approximations

The posterior mean and covariance estimated by the VB approximations and by the MCMC sample moments (cited from [13]) are given in Table 12 and 13. The ratios of posterior means is given in the last column in Table 12, and the ratios of posterior variances in the last row in Table 13. These ratios indicate that the means estimated by both methods are almost identical. However VB underestimated the actual posterior variances, and again strongly distorts the correlation structure.

| Post. mean: the regime-switching lognormal model | Gibbs | VB | Ratios |
|-------------------------------------------------|-------|----|--------|
| \(\mu_1\) | 0.0122 | 0.0123 | 0.991 |
| \(\sigma_1\) | 0.0351 | 0.0349 | 1.006 |
| \(a_{1,2}\) | 0.0334 | 0.0338 | 0.988 |
| \(\mu_2\) | -0.0164 | -0.0161 | 1.0198 |
| \(\sigma_2\) | 0.0804 | 0.0777 | 1.035 |
| \(a_{2,1}\) | 0.2058 | 0.1969 | 1.045 |

| Post. cov.: the regime-switching lognormal model | Gibbs | VB | Ratios |
|-------------------------------------------------|-------|----|--------|
| s.d.: 0.002, 0.002, 0.012, 0.010, 0.009, 0.065 |        |    |        |
| correlation coeff.: -0.16, 0.17, -0.34, -0.10, -0.11, 0.08, -0.17, 0.22, -0.25, -0.15, 0.06, -0.04, 0.34, -0.14, 0.12 |        |    |        |
| s.d.: 0.0017, 0.00008, 0.0085, 0.0089, 0.0010, 0.045 |        |    |        |
| correlation coeff.: | 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 |        |    |        |

The proposed methods are applied to this RSLN model. Again, we use 4000
samples to compute the acceptance rates in VBAIMH, which significantly shorten the computational time, compared with other MCMC methods.

In this example, we work through a complete cycle of the stepwise method to obtain the exact estimations on variances and correlation coefficients, which provide a quantitative correction on VB approximations. In fact, each step of the stepwise method can provide a qualitative diagnostics. Table 21 gives all numerical results in the stepwise method. The values of $m_i$ in Step 1 are all greater than 1, which indicates that the VB variances are smaller than the true ones, since a conditional variance always penalizes the marginal variance. In Step 2, the values of the pair of $\lambda_{k,1}$ and $\lambda_{k,2}$ provide possible information about the sign of the correlation. The final results are given in Table 14.

**Table 14**

| The regime-switching lognormal model: 3 methods |
|------------------|------------------|------------------|------------------|
|                | Gibbs            | Affine           | Marginal         | Stepwise         |
| $\mu_1$        | 2.12             | 1.44             | 1.97             | 1.22             |
| $\sigma^2_1$   | 24.46            | 1.60             | 1.76             | 1.63             |
| $\sigma^2_{1,2}$ | 1.47             | 2.81             | 1.41             | 2.21             |
| $\mu_2$        | 1.19             | 1.20             | 1.82             | 1.33             |
| $\sigma^2_2$   | 8.21             | 1.57             | 2.00             | 1.49             |
| $\sigma^2_{2,2}$ | 1.46             | 2.34             | 2.15             | 1.96             |
| $\rho_{12}$    | -0.1630          | -0.1217          | -0.1175          | -0.1266          |
| $\rho_{13}$    | 0.1681           | 0.2228           | 0.1220           | 0.1367           |
| $\rho_{23}$    | -0.3438          | -0.2970          | -0.3831          | -0.3388          |
| $\rho_{14}$    | -0.1043          | -0.1294          | -0.1874          | -0.1275          |
| $\rho_{24}$    | -0.1094          | -0.0903          | -0.0649          | -0.0865          |
| $\rho_{34}$    | 0.0796           | 0.0221           | 0.0856           | 0.0507           |
| $\rho_{15}$    | -0.1678          | -0.1856          | -0.1061          | -0.1328          |
| $\rho_{25}$    | 0.2235           | 0.1793           | 0.1008           | 0.1390           |
| $\rho_{35}$    | -0.2517          | -0.1604          | -0.2890          | -0.2160          |
| $\rho_{45}$    | -0.1476          | -0.0747          | -0.0116          | -0.0231          |
| $\rho_{16}$    | 0.0552           | 0.0528           | 0.0942           | 0.0640           |
| $\rho_{26}$    | -0.0374          | -0.0690          | 0.0461           | -0.0772          |
| $\rho_{36}$    | 0.3385           | 0.3985           | 0.5947           | 0.3518           |
| $\rho_{46}$    | -0.1433          | -0.1154          | -0.1664          | -0.0989          |
| $\rho_{56}$    | 0.1238           | 0.1291           | 0.1434           | 0.1023           |

4. Discussion

The variational method essentially provides posterior marginal approximations, which can be inaccurate in a number of ways. The present paper aims to provide fast and easy-to-use diagnostics, which mainly target on inadequacy in the covariance structure. From the above numerical studies we can see all three methods can provide both diagnostics showing the quality of the VB approximation and also, in these examples, good estimates on the actual posterior variances and correlations. These methods are easy to use. They are free of any sophisticated tuning techniques or special expertise and are highly computational efficient compared with the traditional sampling based methods.

This paper introduces a novel way to use acceptance rates. The idea is that the acceptance rate can act as a key diagnostic to how close the VB distribution
is to the true posterior. As discussed in Section 2.2, EAR could be calibrated as a diagnostics tool to measure the inadequacy in marginal approximations by using VB approximations directly as the proposal distributions in VBAIMH. For the situation when posteriors depart from normality, a low acceptance rate still indicate an inaccurate approximation. However, to quantify a particular form of inaccuracy, a single value of EAR may be diluted by the confounding of many factors; inadequate variance, inadequate skewness, inadequate tail behaviour. In the further research, separating these confounding factors would be a necessary step toward measuring a special form of inadequacy.

For high dimensional problems, the three proposed methods can be designed to target more specific situations. For example, the covariance matrix might be sparse; a subset of the parameters might be of immediate concern. As discussed in Section 2.2, Section 3.3, and Section 3.4, the three methods can offer different strategies to address the special form of diagnostics. In the affine method, the transformation matrix $A$ might be restricted to be a particular class. In the marginal method, the projections might be set to particular directions. In the stepwise method, the steps might be applied to a subset of the parameters, conditioning on other parameters.

For each individual method, we have some further comments. The affine transformation based method relies on using approximate linear relationship between the VB approximation and the actual posterior as a diagnostics and potentially a correction. In cases where, for example, strong skewness is present in the posterior the correction will of course not be exact, but it will still be a useful diagnostics tool.

As Leonard, Hsu and Tsui (1989)[18] point out, the marginal approximation of Tierney, Kass, and Kadane (1989), primarily justified by asymptotically $n \to \infty$, might be insufficient for finite $n$; they also show a number of examples in which the method of Tierney, Kass, and Kadane introduces excessive skewness in the marginal approximations. We also find the inadequacy in the method of Tierney, Kass, and Kadane in our numerical studies. For example: Table 15 gives the values of 15 marginal variances along 15 directions in the mixture problem. The first row is the analytical results calculated from the covariance matrix obtained from a Gibbs samples. The second row is based on the posterior marginal approximation. We can see some discrepancy between this two sets of numbers. Even though, the method based on the marginal approximation still works well. Leonard, Hsu and Tsui (1989)[18] proposed a refinement on the method of Tierney, Kass, and Kadane (1989), that could be considered in future work.

### Table 15

| l1 | l2 | l3 | l4 | l5 | l6 | l7 | l8 |
|----|----|----|----|----|----|----|----|
| Gibbs | 3.415 | 0.590 | 1.312 | 0.801 | 6.630 | 0.916 | 0.672 | 0.659 |
| Aprx. | 3.703 | 0.999 | 1.854 | 1.31 | 4.818 | 1.394 | 1.052 | 0.912 |

| l9 | l10 | l11 | l12 | l13 | l14 | l15 |
|----|----|----|----|----|----|----|
| Gibbs | 0.495 | 2.510 | 0.650 | 0.712 | 1.976 | 0.436 | 2.987 |
| Aprx. | 0.792 | 3.376 | 0.915 | 1.133 | 2.477 | 0.634 | 2.96 |
Another potential concern when using the marginal approximation method is that we need to perform a constrained maximization at each sampling step. The maximization can often be completed in straightforward fashion such as the standard Newton’s method or search methods. However a optimization at each sampling step may affect the computational efficiency.

The VBAIMH provides a fast means to calculate the variance of the target distribution. When using this approach two particular issues arise. First, as discussed previously when the target variance of \( \sigma^2 \) is greater than the proposal variance of \( \sigma_p^2 \), the EAR is also monotone decreasing as \( \sigma_p^2 \) increases. Similarly, when \( \sigma_t^2 < \sigma_p^2 \) the EAR is also monotone decreasing as \( \sigma_t^2 \) decreases. This means that we need to determine if \( \sigma_t^2 < \sigma_p^2 \) or not, before determining the value of \( \sigma_t^2 \). In practice, we can assume \( \sigma_t^2 > \sigma_p^2 \) and pick a value of \( \sigma_t^2 \) from the EAR table, and then use this new value as the proposal variance and run the IMH again. If the new acceptance rate is close to one or increases, this means \( \sigma_t^2 > \sigma_p^2 \) otherwise \( \sigma_t^2 < \sigma_p^2 \). If \( \sigma_t^2 < \sigma_p^2 \) is the case, the true value of \( \sigma_t^2 \) is the reciprocal of the value read from the EAR table.

Second, if the approximate normality of posterior distributions does not hold well, for example in the cases where strong skewness is present, the variance read from the EAR table will confound these non-normality effects and will deviate from the true value. As discussed above, when we pick a value of \( \sigma_t^2 \) from the EAR table and use this new value as the proposal variance to run another IMH algorithm, if the new acceptance rate is not close to one, this implies that the normality does not hold well and usually it is skewness presents. When this happens, we need to adjust the value read from the EAR table. We usually scale the readings as \( c\sigma_t^2 \). Based on our various numerical studies, a reasonable choice on the scale \( c \) is 0.85.

5. Appendix

5.1. Stepwise method: a 3-dimension example

All the notations used here are defined in Algorithm 2. We consider a vector parameter \( \theta = (\theta_1, \theta_2, \theta_3) \), and denote its posterior variance and correlation as \( \sigma_1^2, \sigma_2^2, \sigma_3^2 \), and \( \rho_1, \rho_2, \rho_3 \).

Step 1. Define \( s_i^2 = \sigma_i^2/var_{\theta_i}(\theta_i), i = 1, 2, 3. \) Then, by the linear transformation of \( Y = Q\theta \), the variances of \( Y \) are given by \( s_1^2, s_2^2, \) and \( s_3^2 \) respectively, with the correlation coefficients of \( \rho_1, \rho_2 \) and \( \rho_3 \) unchanged. Based on the posterior normality conditions, the conditional variance of \( var(Y_1|Y_2, Y_3) \), \( var(Y_2|Y_1, Y_3) \), and \( var(Y_3|Y_2, Y_1) \) are given respectively

\[
\begin{align*}
var(Y_1|Y_2, Y_3) &= \left(1 - \frac{\rho_1^2 + \rho_2^2 - 2\rho_1\rho_2\rho_3}{1 - \rho_3^2}\right)s_1^2 = m_1^2 \quad (5.1) \\
var(Y_2|Y_1, Y_3) &= \left(1 - \frac{\rho_1^2 + \rho_3^2 - 2\rho_1\rho_2\rho_3}{1 - \rho_2^2}\right)s_2^2 = m_2^2 \quad (5.2) \\
var(Y_3|Y_2, Y_1) &= \left(1 - \frac{\rho_2^2 + \rho_3^2 - 2\rho_2\rho_1\rho_3}{1 - \rho_1^2}\right)s_3^2 = m_3^2 \quad (5.3)
\end{align*}
\]

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The value of \( m_1^2, m_2^2 \), and \( m_3^2 \) can be obtained numerically by using the VBAIMH algorithm. After linear transformation of \( Z = MY \), the variance of \( Z_1, Z_2, \) and \( Z_3 \) are given respectively by

\[
\begin{align*}
\text{var}(Z_1) &= \frac{1 - \rho_3^2}{1 - (\rho_1^2 + \rho_2^2 + \rho_3^2) - 2\rho_1\rho_2\rho_3}, \\
\text{var}(Z_2) &= \frac{1 - \rho_2^2}{1 - (\rho_1^2 + \rho_2^2 + \rho_3^2) - 2\rho_1\rho_2\rho_3}, \\
\text{var}(Z_3) &= \frac{1 - \rho_1^2}{1 - (\rho_1^2 + \rho_2^2 + \rho_3^2) - 2\rho_1\rho_2\rho_3},
\end{align*}
\]

where only \( \rho_1^2, \rho_2^2, \) and \( \rho_3^2 \) are involved.

Step 2. There are three bivariate random vectors in total in \( Z: U_{12} = (Z_1, Z_2|Z_3), U_{13} = (Z_1, Z_3|Z_2), \) and \( U_{23} = (Z_2, Z_3|Z_1) \). The two random variables in \( U_{12} \) have equal variances, similar for \( U_{13}, \) and \( U_{23} \). By the eigen-decomposition, the covariance matrix of \( U_{12} \) can be expressed as \( \text{var}(U_{12}) = R^T \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} R \), where \( R \) is the rotation matrix defined in Algorithm 2, and \( \lambda_1 \) and \( \lambda_2 \) are the eigenvalues of \( \text{var}(U_{12}) \). Thus, the covariance matrix of \( V_1 \) is diagonal with \( \lambda_1 \) and \( \lambda_2 \) as the entries. The values of \( \lambda_1 \) and \( \lambda_2 \) can be computed numerically, by running the VBAIMH algorithm.

Step 3. Based on the posterior normality conditions, the correlation coefficient \( r_1 \) of \( U_{12}, r_2 \) of \( U_{13}, \) and \( r_3 \) of \( U_{23} \) are given respectively by

\[
\begin{align*}
r_1 &= \frac{(\rho_1 - \rho_2\rho_3)}{\sqrt{(1 - \rho_3^2)(1 - \rho_1^2)}} \quad (5.4) \\
r_2 &= \frac{(\rho_2 - \rho_1\rho_3)}{\sqrt{(1 - \rho_3^2)(1 - \rho_1^2)}} \quad (5.5) \\
r_3 &= \frac{(\rho_3 - \rho_1\rho_2)}{\sqrt{(1 - \rho_1^2)(1 - \rho_1^2)}} \quad (5.6)
\end{align*}
\]

Given the values of \( \lambda_1 \) and \( \lambda_2 \) in Step 2, we can obtain the value of \( r_1 \) by computing \( r_1 = (\frac{\lambda_1^2}{\lambda_2^2} - 1) / (\frac{\lambda_1^2}{\lambda_2^2} + 1) \); similar to compute \( r_2 \) and \( r_3 \). Thus, we can obtain and solve a system of three polynomial equations given in \( 5.4, 5.5, \) and \( 5.6 \) to obtain the values of \( \rho_1, \rho_2, \) and \( \rho_3 \); further, the value of \( s_1^2, s_2^2, \) and \( s_3^2 \) can be obtained by solving \( 5.1, 5.2, \) and \( 5.3 \), and then the value of \( \sigma_1^2, \sigma_2^2, \) and \( \sigma_3^2 \).

5.2. Numerical results for the example of Normal random sample

For the affine transformation method, the resulted \( \hat{A} \) and \( \hat{B} \) is given by,

\[
\hat{A} = \begin{pmatrix} 1.049 & 0.000 \\ 11.824 & 1.018 \end{pmatrix} ; \hat{B} = \begin{pmatrix} -10.119 \\ -2469.079 \end{pmatrix}.
\]
For the marginal approximation method, the directional vectors with the corresponding acceptance rates and EAR table readings are given in Table 16.

| direction | Acceptance rate | EAR reading: $l_1$ |
|-----------|----------------|------------------|
| $l_{1/2}^1 (1, 1)$ | 0.861 | 1.55 |
| $l_{1/2}^1 (1, -1)$ | 0.901 | 0.74 |
| $l_{1/2}^1 (1, 0.5)$ | 0.966 | 0.893 |

The numerical results for the stepwise method for each step are given in Table 17.

| Variance | Acceptance rate | EAR readings | Ratio |
|----------|----------------|--------------|-------|
| 1 $m_1^2$ | 0.991 | 1.03 | - |
| 1 $m_2^1$ | 0.906 | 1.13 | - |
| 2 $l_{1/2}^1, l_{1/2}^2$ | 0.881, 0.889 | 0.694, 1.44 | - |
| 3 $r_1$ | - | - | 2.075 |

5.3. Numerical results for mixture of Normals model

For the affine transformation method, the estimated $\hat{A}$ and $\hat{B}$ is given by,

$$\hat{A} = \begin{pmatrix} 1.907 & 0.000 & 0.000 & 0.000 & 0.000 \\ 4.822 & 1.372 & 0.000 & 0.000 & 0.000 \\ 2.227 & 0.329 & 1.255 & 0.000 & 0.000 \\ 4.867 & 0.862 & 0.235 & 1.210 & 0.000 \\ -1.593 & -0.190 & -0.342 & -0.011 & 1.177 \end{pmatrix} ; \hat{B} = \begin{pmatrix} -0.368 \\ -2.399 \\ -2.199 \\ -4.003 \\ 2.026 \end{pmatrix}.$$ 

For the marginal approximation method, it requires 15 projections. The directional vectors with the corresponding acceptance rates and EAR table readings are given in Table 18.

For the stepwise method. The numerical results for Step 1 and 2 are given in Table 19.
5.4. Numerical results for the regime-switching lognormal model

For the affine transformation method, the estimated $\hat{A}$ and $\hat{B}$ is given by,

$$\hat{A} = \begin{pmatrix} 1.200 \\ -0.008 & 1.257 \\ 1.864 & -45.563 & 1.570 \\ -0.722 & -11.953 & 0.026 & 1.076 \\ -0.156 & 2.657 & -0.342 & -0.014 & -0.013 & 1.208 \\ 2.195 & -52.512 & 3.292 & -1.028 & 11.013 & 1.361 \end{pmatrix} ; \hat{B} = \begin{pmatrix} -0.002 \\ 0.000 \\ 0.017 \\ 0.024 \\ -0.002 \\ -0.220 \end{pmatrix}.$$

For the marginal approximation method, it requires 21 projections. The directional vectors with the corresponding acceptance rates and EAR table readings are given in Table 20.

For the stepwise method. The numerical results for Step 1 and 2 are given in Table 21.

5.5. The EAR table

The EAR table, shown in Table 22, is composed as follows: the label for rows contains the first two digits of the target variance; the label for columns contains the decimal of the target variance; the values within the table are expected acceptance rates. For example: if one obtains an acceptance rate of 0.5555, then one would look for the rows to find 4 and the columns to 0.6 which yields the target variance is 4.6.
Table 19
The stepwise method: mixtures of Normals

| Variance | Acceptance rate | EAR readings | Ratio |
|----------|-----------------|--------------|-------|
| $m_1^2$  | 0.933           | 1.230        | -     |
| $m_2^2$  | 0.885           | 1.428        | -     |
| $m_3^2$  | 0.923           | 1.286        | -     |
| $m_4^2$  | 0.817           | 1.512        | -     |
| $m_5^2$  | 0.933           | 1.425        | -     |

| $\lambda_{1,1}^2, \lambda_{1,2}^2$ | 0.917, 0.879 | 0.776, 1.462 | -     |
| $\lambda_{2,1}^2, \lambda_{2,2}^2$ | 0.935, 0.919 | 0.816, 1.282 | -     |
| $\lambda_{3,1}^2, \lambda_{3,2}^2$ | 0.888, 0.848 | 0.803, 1.303 | -     |
| $\lambda_{4,1}^2, \lambda_{4,2}^2$ | 0.885, 0.906 | 1.221, 0.827 | -     |

| $\lambda_{5,1}^2, \lambda_{5,2}^2$ | 0.900, 0.911 | 0.802, 1.331 | -     |
| $\lambda_{6,1}^2, \lambda_{6,2}^2$ | 0.857, 0.795 | 0.701, 1.660 | -     |
| $\lambda_{7,1}^2, \lambda_{7,2}^2$ | 0.885, 0.921 | 1.174, 0.858 | -     |
| $\lambda_{8,1}^2, \lambda_{8,2}^2$ | 0.906, 0.880 | 0.887, 1.090 | -     |
| $\lambda_{9,1}^2, \lambda_{9,2}^2$ | 0.857, 0.890 | 1.356, 0.754 | -     |
| $\lambda_{10,1}^2, \lambda_{10,2}^2$ | 0.978, 0.822 | 0.984, 0.934 | -     |

| $r_1$ | - | - | -0.097 |
| $r_2$ | - | - | -0.222 |
| $r_3$ | - | - | -0.238 |
| $r_4$ | - | - | -0.192 |
| $r_5$ | - | - | -0.248 |
| $r_6$ | - | - | -0.406 |
| $r_7$ | - | - | -0.155 |
| $r_8$ | - | - | -0.103 |
| $r_9$ | - | - | -0.285 |
| $r_{10}$ | - | - | -0.026 |

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### Table 21

**The stepwise method: the regime-switching lognormal model**

| Variance | Acceptance rate | EAR readings | Ratio |
|----------|----------------|--------------|-------|
| $m_1^2$  | 0.951          | 1.15         | -     |
| $m_2^2$  | 0.862          | 1.42         | -     |
| $m_3^2$  | 0.817          | 1.61         | -     |
| $m_4^2$  | 0.928          | 1.28         | -     |
| $m_5^2$  | 0.807          | 1.35         | -     |

| $\lambda_{1,1}^2, \lambda_{1,2}^2$ | 0.929, 0.936 | 1.29, 0.91 | -     |
| $\lambda_{2,1}^2, \lambda_{2,2}^2$ | 0.949, 0.931 | 0.97, 1.30 | -     |
| $\lambda_{3,1}^2, \lambda_{3,2}^2$ | 0.950, 0.960 | 1.18, 0.89 | -     |
| $\lambda_{4,1}^2, \lambda_{4,2}^2$ | 0.844, 0.875 | 1.61, 0.90 | -     |

| $\lambda_{5,1}^2, \lambda_{5,2}^2$ | 0.966, 0.962 | 0.98, 1.14 | -     |
| $\lambda_{6,1}^2, \lambda_{6,2}^2$ | 0.871, 0.873 | 1.51, 0.77 | -     |
| $\lambda_{7,1}^2, \lambda_{7,2}^2$ | 0.921, 0.943 | 1.27, 0.91 | -     |
| $\lambda_{8,1}^2, \lambda_{8,2}^2$ | 0.921, 0.774 | 0.88, 2.09 | -     |
| $\lambda_{9,1}^2, \lambda_{9,2}^2$ | 0.952, 0.907 | 0.99, 1.04 | -     |
| $\lambda_{10,1}^2, \lambda_{10,2}^2$ | 0.926, 0.930 | 0.94, 1.29 | -     |
| $\lambda_{11,1}^2, \lambda_{11,2}^2$ | 0.858, 0.819 | 1.53, 0.77 | -     |
| $\lambda_{12,1}^2, \lambda_{12,2}^2$ | 0.917, 0.783 | 0.76, 2.00 | -     |
| $\lambda_{13,1}^2, \lambda_{13,2}^2$ | 0.866, 0.884 | 0.96, 0.96 | -     |
| $\lambda_{14,1}^2, \lambda_{14,2}^2$ | 0.930, 0.961 | 1.19, 0.94 | -     |
| $\lambda_{15,1}^2, \lambda_{15,2}^2$ | 0.889, 0.810 | 0.82, 1.22 | -     |

| $r_1$   | -          | -          | -0.127 |
| $r_2$   | -          | -          | 0.137  |
| $r_3$   | -          | -          | -0.338 |
| $r_4$   | -          | -          | -0.128 |
| $r_5$   | -          | -          | -0.087 |
| $r_6$   | -          | -          | 0.057  |
| $r_7$   | -          | -          | -0.133 |
| $r_8$   | -          | -          | 0.139  |
| $r_9$   | -          | -          | -0.216 |
| $r_{10}$| -          | -          | -0.023 |
| $r_{11}$| -          | -          | 0.064  |
| $r_{12}$| -          | -          | -0.077 |
| $r_{13}$| -          | -          | 0.352  |
| $r_{14}$| -          | -          | -0.099 |
| $r_{15}$| -          | -          | 0.102  |
### Table 22

**EAR table: variance versus expected acceptance rate**

|     | 0     | 0.1   | 0.2   | 0.3   | 0.4   | 0.5   | 0.6   | 0.7   | 0.8   | 0.9   |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1   | 1.0000| 0.9697| 0.9422| 0.9165| 0.8936| 0.8720| 0.8517| 0.8330| 0.8157| 0.7990|
| 2   | 0.7833| 0.7690| 0.7553| 0.7423| 0.7299| 0.7182| 0.7067| 0.6960| 0.6860| 0.6761|
| 3   | 0.6671| 0.6577| 0.6492| 0.6406| 0.6325| 0.6249| 0.6175| 0.6104| 0.6034| 0.5969|
| 4   | 0.5903| 0.5842| 0.5782| 0.5719| 0.5664| 0.5609| 0.5555| 0.5502| 0.5450| 0.5405|
| 5   | 0.5354| 0.5306| 0.5261| 0.5221| 0.5174| 0.5131| 0.5089| 0.5049| 0.5011| 0.4971|
| 6   | 0.4937| 0.4897| 0.4861| 0.4827| 0.4791| 0.4758| 0.4725| 0.4693| 0.4660| 0.4634|
| 7   | 0.4602| 0.4571| 0.4542| 0.4513| 0.4485| 0.4460| 0.4431| 0.4404| 0.4376| 0.4355|
| 8   | 0.4325| 0.4304| 0.4279| 0.4251| 0.4232| 0.4207| 0.4184| 0.4162| 0.4139| 0.4118|
| 9   | 0.4098| 0.4077| 0.4056| 0.4034| 0.4013| 0.3998| 0.3975| 0.3956| 0.3936| 0.3916|
| 10  | 0.3900| 0.3883| 0.3864| 0.3849| 0.3829| 0.3809| 0.3794| 0.3776| 0.3759| 0.3744|
| 11  | 0.3728| 0.3713| 0.3698| 0.3682| 0.3664| 0.3651| 0.3638| 0.3620| 0.3608| 0.3592|
| 12  | 0.3581| 0.3563| 0.3550| 0.3538| 0.3520| 0.3509| 0.3497| 0.3486| 0.3474| 0.3458|
| 13  | 0.3444| 0.3432| 0.3419| 0.3408| 0.3396| 0.3384| 0.3370| 0.3361| 0.3346| 0.3337|
| 14  | 0.3325| 0.3311| 0.3302| 0.3292| 0.3277| 0.3271| 0.3257| 0.3250| 0.3235| 0.3226|
| 15  | 0.3217| 0.3209| 0.3206| 0.3215| 0.3165| 0.3157| 0.3148| 0.3137| 0.3127| 0.3117|
| 16  | 0.3121| 0.3108| 0.3100| 0.3090| 0.3082| 0.3074| 0.3064| 0.3054| 0.3047| 0.3039|
| 17  | 0.3030| 0.3023| 0.3013| 0.3005| 0.2993| 0.2989| 0.2979| 0.2970| 0.2964| 0.2954|
| 18  | 0.2947| 0.2940| 0.2930| 0.2924| 0.2915| 0.2909| 0.2901| 0.2894| 0.2886| 0.2877|
| 19  | 0.2870| 0.2861| 0.2854| 0.2852| 0.2844| 0.2834| 0.2827| 0.2822| 0.2814| 0.2808|