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The use of mixture distributions in a Bayesian linear mixed effects model

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Preface

The following thesis work was conducted as part of the credits completion requirements of the MSc. Statistics programme at KU Leuven. The purpose of the thesis was to find out the efficacy of Bayesian model selection criteria, for choosing the right number of components in a mixture distribution of random effects, in a longitudinal model. When I began working on this project in August 2015, I had little idea that I would be able to go as far as I have been now. There were many significant obstacles on the way, such as derivations of the various definitions of Deviance information criteria and marginal likelihood, and choice of posterior predictive checks. While implementing them I realized that the simulation study for this thesis required much more computational power than I had. Although the pace of execution was slow, yet every time I had a result I was excited to see it. Looking backwards, I think it was perhaps the most interesting project I did in last 3 years. Through and through, I enjoyed every bit of this project. The entire work for this thesis has been done using R and JAGS (Just Another Gibbs Sampler). The source code, results of simulations and an electronic draft of this thesis can be downloaded from:
`https://github.com/anirudhtomer/MScThesis`

In chapter 1 an introduction to mixture distributions and their central role in the formulation of the problem statement for this thesis is presented. Since the project was done using Bayesian methods it became essential to give an introduction to the Bayesian paradigm in Chapter 2. Further in Chapter 3 the definition of a Bayesian heterogeneity model and issues related to parameter estimation are presented. Chapter 4 constitutes the analytical calculations I did for various classes of Deviance information criteria, marginal likelihood and posterior predictive checks. Chapter 5 includes the results of the simulation study that was performed to check the efficacy of the aforementioned Bayesian model selection methods. The results from Chapter 5 are used further in Chapter 6 to apply the right model selection criteria for modeling the Blood donor data set (Nasserinejad et al., 2015) using a Bayesian heterogeneity model.

I am grateful to my supervisor Professor Dr. Emmanuel Lesaffre for keeping faith in my capabilities and for guiding me in the right direction. I enjoyed the fact that he never spoon-fed me, yet was always approachable to discuss the statistical problems. He set very clear goals at the beginning of the year and continually monitored my progress thereafter. My interest in Bayesian statistics has grown by magnitudes under his supervision and I am looking forward to contribute more in this area. I would also like to extend my gratitude to Professor Geert Molenberghs and Professor Geert Verbeke for the captivating lectures on longitudinal data analysis, which empowered me with the tools required for performing the frequentist analysis of blood donor data set. I am thankful to Kazem Nasserinejad from ErasmusMC for resolving many of my queries regarding the blood donor data set, and to Igor Milhorança for providing the much needed inputs at crucial times. Lastly, I am grateful to my parents for the innumerable sacrifices they made to make sure I had as less obstacles as possible during my studies and I dedicate this work to them.

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Summary

In this master thesis we fitted a finite mixture distribution for the random effects in a Bayesian linear mixed model. A mixture distribution for random effects allows modeling the heterogeneity introduced by ignoring certain covariates in the mean structure of the model or to take into account the non normality of random effects. We generated multiple artificial data sets with different types of Gaussian mixture of random effects and used them for testing the effectiveness of Bayesian model selection criteria (DIC, Bayes Factor, PPC) for choosing the number of component densities in the mixture distribution of random effects. Since mixture models are missing data models, we implemented various definitions of DIC as given by Celeux et al., (2006) for such models. We found that conditional data DIC's which are usually reported by software such as JAGS are not reliable for selecting the number of mixture components. DIC 4 (section 4.8) which was based on complete data likelihood performed the best among all of the DIC's. The next best performing DIC was DIC 3(section 4.4) based on marginal data likelihood. We recommend using these DIC's along with posterior predictive checks (PPC) which also worked very well to detect overfitting. We found that if inverse gamma priors were used for variance components, and uniform distribution for correlation in the distribution of random effects, then PPC's based on such models give more extreme results in presence of overfitting the number of mixture components. We also calculated marginal likelihood for the various models using the approximation given by Chib, (1995) and found that it was not reliable for deciding the number of components required in the mixture of random effects.

While doing MCMC simulations we found some other interesting results as well, which although were not of primary interest, but are still worth mentioning here. We found that a Wishart prior for precision matrix(inverse of covariance matrix) of mixture components leads to posteriors which overestimate the precision when within subject variance is greater than between subject variance. Thus, it could be a good idea to decrease scale of the intercept and the covariate corresponding to random slope, so that the corresponding variances increase in magnitude. Further we also found that if mixture components are not well separated and the number of subjects are small, then using a Dirichlet prior with small values of hyperparameter (≤ 1) for the weight distribution of mixture components can lead to choosing underfitted models.

Contents

Chapter 1

Introduction

In this chapter we have introduced the concept of a mixture distribution and the challenges involved in estimation of parameters of a mixture distribution. We have also highlighted the benefits of using a Bayesian approach for parameter estimation. Lastly we have presented the goal of this master thesis, in which a mixture distribution plays the central role.

1.1 Mixture distribution

A mixture distribution is a probability distribution of a random variable formed from a group of other random variables. The formation of a mixture distribution can be seen as a two step process. In the first step a particular random variable is selected from a collection of random variables based on a certain probability of selection. In the second step a value is sampled for the selected random variable from its probability distribution. For e.g. the following random variable Y has a mixture density formed from 3 normally distributed random variables.

$$Y \sim \frac{1}{6}N(-10, 3) + \frac{1}{2}N(0, 1) + \frac{1}{3}N(4, 2)$$

Figure 1.1 shows the density function for Y. The density is trimodal with each mode corresponding to one of the components in the mixture. Mixtures such as Y which are formed from a finite sum of components are called finite mixtures. The components are also known as mixture components and their densities are called component densities. The constants multiplying the corresponding densities are called mixture weights. The mixture weights also represent the probability of selection of the component densities. Each mixture weight should be positive and the sum of all mixture weights should be equal to 1. While in our example all the mixture components belonged to the same parametric family i.e. Normal distribution, it is also possible to have mixture components from different parametric families. A mixture model where it is assumed that all data points are generated from a mixture of normally distributed component densities is called Gaussian mixture model (GMM). It is important to note that the idea of a mixture distribution is rather hypothetical, as it was shown in an example that a GMM of two components could be indistinguishable from a log-normal distribution, by Titterington, Smith, and Makov, (1986).

1.1.1 Formal definition for finite mixture distribution

Given a finite set of K probability density functions $p_1(y), p_2(y), \ldots, p_K(y)$ and weights $\eta_1, \eta_2, \ldots, \eta_K$, a random variable Y is said to have a finite mixture distribution if

$$p(y) = \sum_{k=1}^{K} \eta_k p_k(y)$$

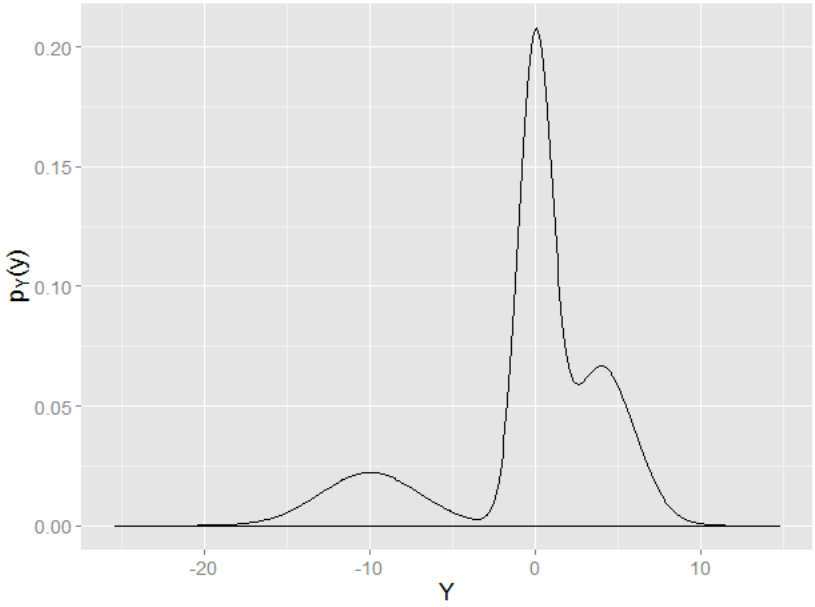


Figure 1.1: Mixture density of $Y \sim \frac{1}{6}N(-10,3) + \frac{1}{2}N(0,1) + \frac{1}{3}N(4,2)$

The vector of the weights $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots, \eta_K)^T$ is called the weight distribution. The k^{th} weight η_k corresponds to selection probability of the k^{th} component while sampling for Y. η_k can only take values from the K dimensional positive real coordinate space $\mathbb{R}^{+K}$ with an additional constraint, $\sum_{k=1}^{K} \eta_k = 1$.

1.1.2 Challenges

The primary challenge while modeling a mixture density for a random variable is that the number of mixture components (K), weight distribution ($\boldsymbol{\eta}$) and the corresponding parameters for component densities are rarely known in advance. Secondly, from a sample of N observations $y_1, y_2, \ldots, y_N$ sampled from the mixture density $p(y)$ one may not know which observation belongs to which component density. Formally, an allocation vector $\boldsymbol{S} = (S_1, S_2, \ldots, S_N)^T$ represents the allocation of observations to mixture components. i.e. $S_i = k$ represents that i^{th} observation belongs to k^{th} component density. Estimating the allocation vector is in fact solving the clustering problem, albeit using parametric methods in our case.

While Maximum Likelihood based methods such as the EM algorithm could be used to deal with the challenges mentioned above, there are certain downsides to them. Firstly it is well known that 95% confidence intervals of ML estimates are based on asymptotic normality of the estimators. Thus in case of small sample size, or small mixture weights the results will not be correct (Frühwirth-Schnatter, 2013, pg. 35). A Bayesian approach however is immune to these issues as the posterior distribution of parameters is allowed to be non-normal. Secondly, in case of univariate and multivariate GMM, the likelihood function

$$p(\boldsymbol{y}|\boldsymbol{\mu}, \boldsymbol{\sigma^2}, \boldsymbol{\eta}) = \prod_{i=1}^{N} \sum_{k=1}^{K} f_N(y_i; \mu_k, \sigma_k^2)\eta_k$$

is unbounded and has many spurious nodes near the boundary of the parameter space for variance(σ_k^2) of the components (Day, 1969; Kiefer and Wolfowitz, 1956). A Bayesian approach

however, handles this problem elegantly using priors for parameters of the component densities. For e.g. Frühwirth-Schnatter, (2013, pg. 176) combined the likelihood with the prior $p(\mu_k, \sigma_k^2) \propto p(\sigma_k^2), \sigma_k^2 \sim$ Inv-Gamma$(1, 4)$, and showed that it lead to a joint posterior density $p(\mu, \sigma^2|\boldsymbol{y})$ of parameters in which σ_k^2 was bounded away from 0. Thus all the spurious nodes near the boundary of the parameter space for σ_k^2 were cut out, whereas they were apparent for the surface of the likelihood function.

1.1.3 Applications of mixture distributions

Mixture models have found usage in a variety of domains. Some of the examples are:

- Spike sorting of neural data: Both GMM and mixture of multivariate t-distributions have been used.(Lewicki, 1994; Shoham, Fellows, and Normann, 2003).
- Speaker recognition as well as speech to text conversion algorithms have used mixture models (Povey et al., 2011; Simancas-Acevedo et al., 2001; Xiang and Berger, 2003).
- Image processing: GMM have been used to find features in an image, such as objects, boundaries etc. (Fu and Wang, 2012). For e.g. Yang, (1998) have used GMM to model the distribution of skin color pixels. Many authors have also proposed using GMM for face recognition. i.e. as a biometric identification mechanism.
- Finance: Brigo and Mercurio, (2002) proposed to use a log-normal mixture distribution for pricing of financial assets.
- Biology: Mixture models have found usage in genetics and cell biology.(Gianola et al., 2007; Sim et al., 2012)

The example applications we cited involved usage of mixture models to adjust for a hidden attribute in the data which could not be collected or to approximate a density which was not of a known form. However mixtures have also been used as supplementary method in various models, a list of which can be found in Frühwirth-Schnatter, (2013, pg. 238). One such usage in linear mixed models was proposed by Verbeke and Lesaffre, (1996) and it also formed the problem statement of this thesis.

1.2 Goal of master thesis

Verbeke and Lesaffre, (1996) proposed to use a finite mixture distribution of normally distributed components for the prior distribution of random effects in a linear mixed effects model (LMM). This particular LMM is also known as Heterogeneity model. In this thesis our focus was on the Bayesian version of the heterogeneity model, where all parameters involved are assigned a probability distribution. Needless to say, the issues described in section 1.1.2 are also applicable for the Bayesian heterogeneity model. The aim of this master thesis was to evaluate existing Bayesian approaches for model selection, namely Deviance Information Criterion (DIC), marginal likelihood and posterior predictive checks(PPC) for selecting the right number of mixture components for the distribution of random effects. Since we have worked within the Bayesian framework, we used MCMC methods instead of the frequentist point estimation methods. We also generated artificial data sets to check efficacy of each of the aforementioned model selection criteria and then used the most effective ones to decide the number of mixture components for the random effects distribution in Blood donor longitudinal data set (Nasserinejad et al., 2015).

Chapter 2

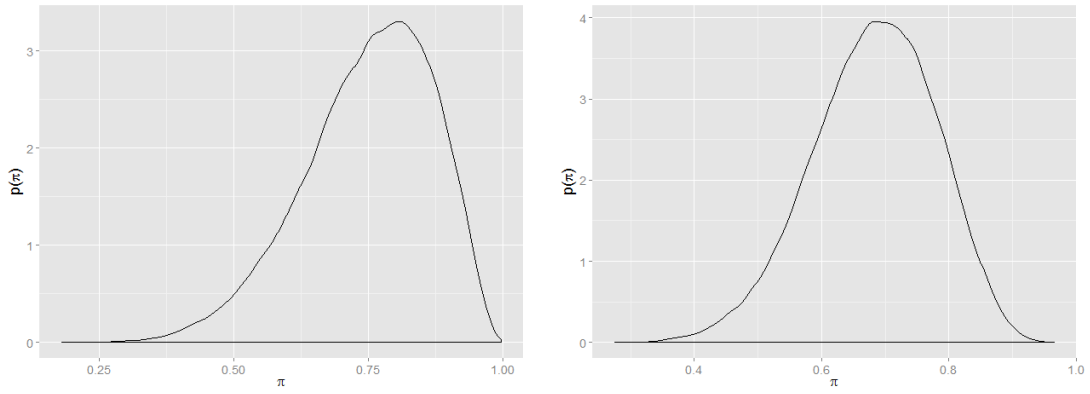
Bayesian paradigm

In this chapter we will give an introduction to the foundations of the Bayesian framework. i.e. Bayes rule and Bayesian summary measures.

2.1 The Bayesian motivation: A toy example

What primarily differentiates the Bayesian paradigm from frequentist paradigm is that the parameters are random variables rather than being a constant. The distribution of parameters based on the data at hand is called the posterior distribution, represented by $p(\theta|y)$. Whereas the initial distribution of parameters is called the prior distribution, represented by $p(\theta)$. We will now present an example to signify the ideological differences between the Bayesian paradigm and frequentist paradigm.

Suppose there are three people A, B and C of whom A and B each are captains of a sports team and C is the referee who tosses the coin. Let us assume that based on experiences of an old friend, captain B gets to know that the referee purposefully attempts at getting a heads on the toss. However given the nature of this problem, it is hard to quantify this belief in a single real number. Instead a belief that there is a 70 to 90% chance that the result will be a heads is more likely than a belief that there is exactly an 80% chance for the same. One might also have a slightly vague belief that there is more than 50% chance that the toss will result into a heads. Secondly, given the fact that not all coins are alike it is impossible for the probability of getting a heads to be constant, even if the referee tosses identically on each trial.



(a) Prior $p(\pi)$: $\beta(9, 3)$ (b) Posterior $p(\pi|\boldsymbol{y})$: $\beta(15, 7)$

Figure 2.1: Prior and posterior PDF for π; the probability of getting heads.

While subjective, the beliefs of captain B represent the prior probability distribution of a random variable in Bayesian paradigm. In our example the random variable is probability (π) of getting a heads. In figure 2.1a we can see one such prior distribution corresponding to the belief that the chance of getting a heads on the toss is more than getting tails and it is more likely to be somewhere between 70 to 90%.

2.2 Bayes rule

We will now present the Bayes rule which is central to the Bayesian parameter estimation process. The Bayes rule for the estimating the continuous parameter π is given by

$$p(\pi|\boldsymbol{y}) = \frac{L(\pi|\boldsymbol{y})p(\pi)}{p(\boldsymbol{y})} = \frac{L(\pi|\boldsymbol{y})p(\pi)}{\int_0^1 L(\pi|\boldsymbol{y})p(\pi)\,\mathrm{d}\pi} \tag{2.1}$$

The result $p(\pi|\boldsymbol{y})$ is called the posterior distribution of the parameter. The posterior $p(\pi|\boldsymbol{y})$ can be used to make statistical inference about the parameter π. An intuitive way to get the motivation behind the Bayes rule is that, one can imagine the denominator as marginal probability of $\boldsymbol{y}$ calculated using the law of total probability. This is more evident in the categorical case though.

We can apply Bayes rule to estimate parameters in context of the current example. Suppose after 10 matches captain B observed that 6 times out 10 the toss resulted in a heads. Assuming that the tosses were independent, then given the likelihood function $L(\pi|\boldsymbol{y})$, the MLE of π will be $\hat{\pi} = 0.6$. Whereas Bayes rule gives us the entire posterior distribution of parameter π as shown in figure 2.1b. The mean value $E(p(\pi|\boldsymbol{y}))$ of the posterior distribution is 0.7, which if we compare with the MLE $\hat{\pi}$=0.6 we can see that Bayesian posterior mean is influenced by the prior as well.

2.3 The role of prior distribution

We can see in equation 2.1 that the computation of posterior involves solving the integral in the denominator. One can avoid solving the integral by choosing a prior such that the resulting posterior is from the same parametric family as the prior and thus available in closed form. Such priors are termed as conjugate priors. However it is not always feasible to choose a conjugate prior; For e.g. if the prior belief $p(\pi)$ in our example is that it is trimodal then we will have to use numerical approximation for calculation of the posterior. The most widely used algorithms for posterior approximation are Markov chain Monte Carlo (MCMC) techniques such as Gibbs sampling, Metropolis hastings algorithm, Hamiltonian Monte Carlo and their variants etc. The priors can also be classified as informative or non-informative/vague/diffuse. The prior we chose in our example was informative, whereas a diffuse prior could have been the uniform distribution $U(0, 1)$. In absence of prior knowledge a non informative prior is advised. A more detailed overview of the priors can be found in Lesaffre and Lawson, (2012).

2.4 Bayesian inference

Given the posterior distribution of a parameter $p(\theta|y)$ one can use the point estimates such as median, mean $E_\theta(\theta|y)$, or MAP (maximum a posteriori) $\arg\max_\theta p(\theta|y)$ for inference. It is however the interval estimates where the Bayesian paradigm contrasts more with frequentist approach. Bayesian 95% interval estimates are called credible intervals. While the frequentist 95% confidence intervals is interpreted as the interval in which 95 out of 100 times one can find the population parameter θ, the Bayesian 95% credible interval is interpreted as the interval from which parameter θ takes a value 95 out of 100 times. The credible interval can be equal

tailed or a highest posterior density interval (HPDI). The Bayesian paradigm also allows one to make inference on future values of the data by taking the current data into account. This is done using the posterior predictive distribution (PPD)

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta)p(\theta|y)\,\mathrm{d}\theta$$

The point and interval summary measures for PPD are similar to the ones for posterior distribution of parameters $p(\theta|y)$. We will also discuss Bayesian model selection in the forthcoming chapters.

2.5 Bayesian software

Various Bayesian software tools such as BUGS, STAN, PROC MCMC in SAS etc. are used for running the MCMC procedures mentioned above. For the purpose of this thesis we stuck to JAGS which is from the BUGS (Bayesian inference Using Gibbs Sampling) family. We also used the R package R2jags to execute JAGS code via R.

Chapter 3

Bayesian linear mixed effects model

3.1 Introduction to linear mixed model

A linear mixed effects model, also known as linear mixed model(LMM) is a statistical model for data which is hierarchical in structure. For e.g. one such hierarchy could be, repeated observations taken from multiple patients and patients grouped under multiple hospitals. The specialty of these models is that apart from the fixed effects, they also model the correlation between the observations falling in the same group at a certain level in the hierarchy. The correlation is modeled using the random effects and the response is modeled as a linear function of both fixed and random effects.

There are many synonymous terminologies for data sets which are hierarchical in nature albeit with subtle nuances differentiating them. In this thesis our focus will be on longitudinal data sets. A longitudinal data set is the one where multiple observations are collected from subjects at different points in time. For e.g. measurement of hemoglobin of 20 patients with observations taken every month for a period of 24 months. The observations collected from a subject will be correlated, and given the fact that a linear model imposes homoscedasticity, it is not suitable for use in such scenarios.

3.1.1 LMM definition

Following the notations from Lesaffre and Lawson, (2012), the LMM for the observations of the i^{th} subject among the n subjects is given by

$$\boldsymbol{y}_i = \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_i + \boldsymbol{\varepsilon}_i \tag{3.1}$$

where $1 \leq i \leq n$,
$\boldsymbol{y}_i = (y_{i1}, y_{i2}, \ldots, y_{im_i})^T$ is a vector of observations for the i^{th} subject taken at m_i time points,
$\boldsymbol{X}_i = (\boldsymbol{x}_{i1}^T, \boldsymbol{x}_{i2}^T, \ldots, \boldsymbol{x}_{im_i}^T)^T$ is the $m_i \times (d+1)$ design matrix for the i^{th} subject,
$\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_d)^T$ is a $(d+1) \times 1$ vector of fixed effects with β_0 being the intercept,
$\boldsymbol{Z}_i = (\boldsymbol{z}_{i1}^T, \boldsymbol{z}_{i2}^T, \ldots, \boldsymbol{z}_{im_i}^T)^T$ is the $m_i \times q$ design matrix of covariates multiplying the random effects,
$\boldsymbol{b}_i = (b_{0i}, b_{1i}, \ldots, b_{(q-1)i})^T$ is a $q \times 1$ vector of random effects with b_{0i} being the random intercept. The random effects $\boldsymbol{b}_i \sim N_q(\boldsymbol{0}, G)$ with G being the $q \times q$ covariance matrix,
$\boldsymbol{\varepsilon}_i = (\varepsilon_{i1}, \varepsilon_{i2}, \ldots, \varepsilon_{im_i})^T$ is a $m_i \times 1$ vector of measurement errors. The errors $\boldsymbol{\varepsilon}_i \sim N_{m_i}(\boldsymbol{0}, R_i)$ with R_i being the $(m_i \times m_i)$ covariance matrix of errors,

The errors $\boldsymbol{\varepsilon}_i$ and the random effects $\boldsymbol{b}_i$ are assumed to be independent. R_i is usually a diagonal matrix of the form $\sigma^2 I_{m_i}$. While one might only model the correlation between the observations of a subject using random effects, it is also possible to model the serial correlation component.

3.2 Motivation for Bayesian linear mixed model

One of issues with the frequentist LMM is that while the parameters in matrices G and R_i are estimated using ML/REML, only a point estimate is further used in estimation of fixed effects(see Verbeke and Molenberghs, 2009, chap. 5). Hence the uncertainty in estimation of random effects is ignored. Although frequentist inference approaches try to mitigate this issue by modifying the distributional assumptions of the test statistic for fixed effects (Verbeke and Molenberghs, 2009, pg. 56), a Bayesian approach considers the variability in parameter estimates in the first place. A similar problem occurs in the estimation of $\boldsymbol{b}_i$. The frequentist strategy is to use Empirical Bayes estimates, where the the posterior distribution of random effects uses point estimates of parameters G and R_i. Thus the uncertainty in estimation is ignored again. On the other hand the Bayesian approach averages over the entire posterior distribution of the hyperparameters to obtain the posterior $p(\boldsymbol{b}_i|\boldsymbol{y})$. In light of these reasons, in this thesis we will model our data using Bayesian linear mixed models.

The Bayesian linear mixed model or BLMM can be obtained by assigning a distribution to all the parameters involved in a LMM. This means that the model presented in section 3.1.1 can be extended by giving a prior distribution for the following:

- $\sigma^2 \sim p(\sigma^2)$
- $\boldsymbol{\beta} \sim p(\boldsymbol{\beta})$
- $G \sim p(G)$

3.3 Motivation for mixture of random effects

As we saw above, the random effects are assumed to be multivariate normally distributed. It could be too strong an assumption though in certain cases. A classical example are the longitudinal studies where at any time point we would like to categorize subjects in groups. For e.g. group with a high risk of having a certain disease in future vs. group with a low risk. While in retrospective studies this task is easier as we know exactly which patients were diagnosed with the disease and which were not, however in a study where we would like to categorize patients into different groups well before diagnosis this could be difficult. Here is a toy example for it. Imagine that in a longitudinal study we are measuring a response Y which is an indicator of a disease. Assume that from a previous study it is known that patients which are in high risk group for the disease tend to have a higher response Y during all times. Also assume that the trend of Y over time remains the same for both groups otherwise. Figure 3.1 shows individual profiles of such subjects from a simulated dataset. Looking at this plot we can say that a random intercept component will be enough to model individual profiles. Since we will not be knowing which patient belongs to which group, this heterogeneity can be appropriately modeled by considering that the random intercept is a mixture of two normal components. Another reason for using a mixture distribution is that the random effects distribution may not be of a known form and the mixture distribution may very well approximate it.

In a LMM is quite common to use histogram of Empirical Bayes estimates of random effects to detect groups of individuals. However Verbeke and Lesaffre, (1996) have shown that if the prior is misspecified(for e.g. if in our example we use a univariate normal distribution), then the histogram of estimates of random effects will be shrunk towards the prior distribution. Thus it would be impossible to classify the subjects into different categories based on Empirical Bayes estimates of random effects as they are incorrect. A solution to this problem is using a mixture

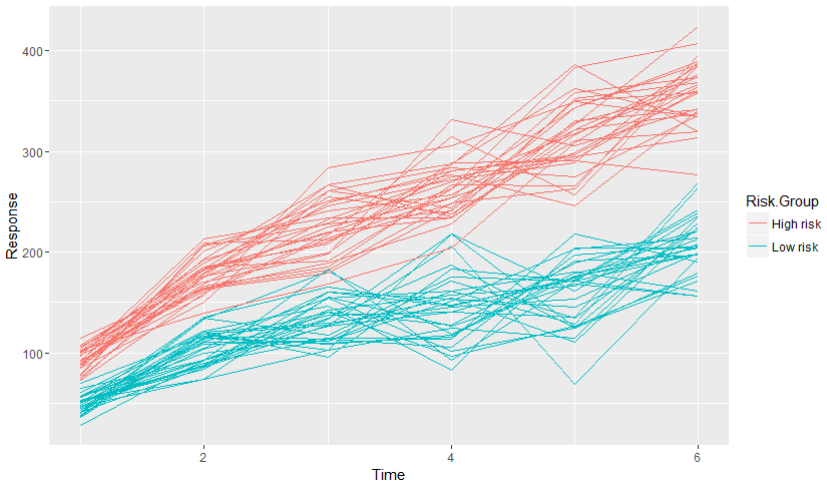


Figure 3.1: Individual profiles of 30 subjects from each group.

of Gaussian components for random effects distribution. Such a linear mixed model is termed as a Heterogeneity model.

3.3.1 Bayesian heterogeneity model

The formal definition of a Bayesian heterogeneity model can be given by extending the Bayesian linear mixed model definition given in section 3.2. Since, now the random effects have a Gaussian mixture distribution we will use the following notation to express the distribution mathematically.

$$\boldsymbol{b}_i \sim \sum_{k=1}^{K} \eta_k N_q(\boldsymbol{b}_k^C, G_k)$$

where $\boldsymbol{b}_k^C$ and G_k are the mean vector and covariance matrices for the k^{th} component in the mixture distribution respectively. The vector $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots, \eta_K)^T$ is the weight distribution for the component densities. The vector $\boldsymbol{S} = (S_1, S_2, ..., S_n)^T$ represents the allocation vector for the n subjects. Since we are following the Bayesian paradigm, in addition to prior distribution for β and σ^2 we also have prior for $\boldsymbol{\nu} = (\boldsymbol{b}_1^C, \boldsymbol{b}_2^C, \ldots, \boldsymbol{b}_K^C, G_1, G_2, \ldots, G_K, \boldsymbol{\eta})$.

3.4 Estimation of parameters in the Bayesian heterogeneity model

In this section we will discuss some of the challenges in Bayesian estimation of parameters in the Bayesian heterogeneity model. We will also discuss the approaches we used to deal with them in this thesis.

3.4.1 Marginal vs. Hierarchical model

Suppose that in the heterogeneity model we know the allocations S_i as well as the random effect $\boldsymbol{b}_i$ for every subject. Then conditional on knowing $S_i = k$ the following LMM equation has a hierarchical interpretation.

$$\begin{aligned} \boldsymbol{y}_i | \boldsymbol{b}_i, S_i &\sim N(\boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_i, \boldsymbol{\varepsilon}_i) \\ \boldsymbol{\varepsilon}_i &\sim N_{m_i}(\boldsymbol{0}, R_i) \end{aligned} \tag{3.2}$$

It is important to note that the distribution of $\boldsymbol{y}_i$ does not directly depend on allocation S_i due to hierarchical independence. i.e. It is $\boldsymbol{b}_i$ which depends on S_i because $\boldsymbol{b}_i|S_i \sim N(\boldsymbol{b}_{S_i}^C, G_{S_i})$, however if one knows the random effect then knowing the allocation is not necessary in the hierarchical model. i.e. $p(\boldsymbol{y}_i|\boldsymbol{b}_i, S_i) = p(\boldsymbol{y}_i|\boldsymbol{b}_i)$. One can however integrate out the random effects $\boldsymbol{b}_i$ and obtain the corresponding marginal Bayesian heterogeneity model,

$$\begin{aligned} \boldsymbol{y}_i|S_i &\sim N(\boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_{S_i}^C, \boldsymbol{\varepsilon}_i^*) \\ \boldsymbol{\varepsilon}_i^* &\sim N_{m_i}(\boldsymbol{0}, \boldsymbol{Z}_i G_{S_i} \boldsymbol{Z}_i^T + R_i) \end{aligned} \tag{3.3}$$

The marginal model is recommended by Frühwirth-Schnatter, Tüchler, and Otter, (2004) for good mixing of chains, and while doing the simulation study(presented in chapter 5) we found that claim to be true. However, the marginal model took quite a long time for each iteration. It also did not give posterior estimates of the random effects $\boldsymbol{b}_i$ which were required for calculation of certain definitions of DIC (discussed in chapter 4). Besides we found that a model with hierarchical centering took less time for each iteration and had as much autocorrelation in the posterior density samples as with the use of the marginal model.

3.4.2 Hierarchical centering

The random effects $\boldsymbol{b}_i$ in a mixed model can be seen as random deviations from the fixed effects $(\boldsymbol{\beta})$ with a mean $\boldsymbol{0}$. For a longitudinal data set, it means that the overall effect of a covariate such as the intercept for a subject should be the sum of both fixed and random effects. In this case matrices $\boldsymbol{X}$ and $\boldsymbol{Z}$ both share columns corresponding to the variable intercept. To enforce the mean $\boldsymbol{0}$ on the random effects in a mixture distribution of random effects, the following condition should be satisfied.

$$E(\boldsymbol{b}_i|\boldsymbol{\nu}) = \sum_{k=1}^{K} \eta_k N_q(\boldsymbol{b}_k^C, G_k) = 0 \tag{3.4}$$

where $\boldsymbol{\nu}$ is defined in section 3.3.1. This further means that $E(\boldsymbol{y}_i|\boldsymbol{\nu}) = \boldsymbol{X}_i\boldsymbol{\beta}$. This parametrization, which was also used in the original paper on Heterogeneity model (Verbeke and Lesaffre, 1996) is called the non-centralized parametrization. The centralized parametrization assumes that the random effects are not deviations from the fixed effects and are centered around a non zero mean.

The choice of parametrization has an effect on the rate of convergence of the chains in MCMC process. While doing the simulation study we observed that imposing the constraint in equation 3.4 drastically slowed the convergence as well increased the autocorrelation in parameter estimates. Thus, in this thesis we have only used hierarchically centered parametrization.

3.4.3 Starting values

The choice of starting values is important in mixtures especially when the components are not well separated. In the R package bayesmix (Gruen and Plummer, 2015) the authors used $\frac{1}{k+1}, \frac{2}{k+1}, ..., \frac{2}{k+1}$ quantiles of the sample data for the starting values of the means $\mu_1, \mu_2, ..., \mu_K$ of the K components. In the Bayesian heterogeneity model we first extract the random component from the data as described in section 5.1.1 and then calculate the sample quantiles. We found out that it resulted into chains with an improved convergence. We also calculated starting values for the fixed effects β using OLS because OLS parameter estimates are unbiased and consistent [pg. 50](Verbeke and Molenberghs, 2009).

3.4.4 Choice of priors

Since we are following the Bayesian paradigm, parameters in the Bayesian heterogeneity model are random variables and thus require a prior distribution. For the k^{th} component in the mixture of random effects, both the mean b_k^C and covariance matrix G_k are unknown. To obtain the joint posterior of these parameters as a known density one can use the conditionally conjugate prior $b_k^C|G_k \sim N(\boldsymbol{\mu}_0, \frac{G_K}{g_0})$ and $G_k^{-1} \sim \mathcal{W}(n_0, \Psi)$. Here $\boldsymbol{\mu}_0, g_0, n_0, \Psi$ are the hyperparameters for the corresponding prior distributions. During our simulations we found that choosing $g_0 = 1$ yielded very high values for variance components whereas for g_0 > 1 JAGS was unable to find a sampler. We thus stuck to widespread alternative practice of specifying independent priors for the mean (b_k^C) and covariance matrix (G_k) (Gelman and Hill, 2006, chap. 17). For e.g. a common non informative prior for b_k^C (say, having only random intercept and slope) is $N(\mathbf{0}, \begin{bmatrix} 10^5 & 0 \\ 0 & 10^5 \end{bmatrix})$. This prior is equivalent of specifying independent diffuse univariate normal priors for the mean of random intercept and random slope respectively.

Choice of prior for covariance matrix

The choice of prior for the covariance matrix (G_k) is an interesting problem. Lesaffre and Lawson, (2012, pg. 260) suggest using an inverse Wishart prior with small diagonal elements for the scale hyperparameter and degrees of freedom hyperparameter equal to the dimension of G_k. For e.g $IW(\begin{bmatrix} 0.01 & 0 \\ 0 & 0.01 \end{bmatrix}, 2)$ could be one such prior. The corresponding prior for precision matrix G_k^{-1} will be the Wishart prior $W(\begin{bmatrix} 10 & 0 \\ 0 & 10 \end{bmatrix}, 2)$. i.e. the scale of Wishart prior is inverse of the scale hyperparameter for inverse Wishart distribution. As we found later in our simulations, a big value for diagonal elements of scale matrix of Wishart distribution influenced the posterior more than the likelihood did.

Lesaffre and Lawson, (2012, pg. 260) also suggest using independent gamma priors for random intercept and random slope and uniform prior $U(-1, 1)$ for the correlation between the two. The upside of this approach is that it gives almost the same estimates as one can get from frequentist analysis, but the downside is that MCMC iterations are slower because the posterior is not available as a known density. Another benefit of this approach, as we later found out during simulations is that when the mixture distribution is overfitted, then the extra components tend to have very high variance estimates for random intercept and random slope. This property can be used to make decisive posterior predictive checks.

Choice of priors for β and σ^2

We assume that the parameters β and σ^2 are independent from $\boldsymbol{b}_1^C, \boldsymbol{b}_2^C, ..., \boldsymbol{b}_K^C, G_1, G_2, ..., G_K, \boldsymbol{\eta}$. The problem of choosing a conjugate prior for β and σ^2 is similar to what we discussed in the section above. The solution thus is alike, i.e. using independent univariate normal priors such as $N(0, 10000)$ for each of the β_d and a Gamma$(0.0001, 0.0001)$ prior for $\tau = \frac{1}{\sigma^2}$ (Gelman and Hill, 2006, chap. 17).

Choice of prior for η

The conjugate prior for the weight distribution $\boldsymbol{\eta}$ is the Dirichlet prior Dir$(a_0, a_1, ..., a_K)$. Frühwirth-Schnatter, (2013, pg. 105) suggest choosing values of hyperparameters $a_0, a_1, ..., a_K$ to be

greater than 1 in cases where one of the components is nearly empty. If one chooses the hyper-parameters to be equal to 1 then label switching is observed whenever one of the components is nearly empty or whenever the components are fused (section 5.1.3). We found out during the simulation study that choosing larger values for the hyperparameter indeed mitigated the issue of label switching, however in case of severe overfitting it also became almost as much informative as the likelihood.

3.4.5 Label Switching

We use a mixture distribution for random effects in the Bayesian heterogeneity model. However we do not know the allocation vector $\boldsymbol{S}$ in advance. In this case the mixture likelihood for the response $\boldsymbol{y}$ is given by the equation 4.1. The mixture likelihood function is symmetrical and has $K!$ modes (Frühwirth-Schnatter, 2013, pg. 44). This creates a problem called label switching while doing the MCMC procedure.

The label switching problem can be explained with the following example. Suppose we have a mixture distribution $0.5N(5,1) + 0.5N(7,1)$ of two components C_1 and C_2 and we have few observations sampled from the mixture. Using the MCMC procedure we can one estimate the parameters of the two components. The MCMC procedure for missing data models like mixture models uses a technique called data augmentation. The idea of data augmentation is similar to the frequentist EM algorithm. i.e. we begin with some random allocation vector $\boldsymbol{S}_{\text{initial}}$ and estimate parameters using the complete data likelihood. An example expression of a complete data likelihood for Bayesian heterogeneity model is expression 4.6. For the MCMC sampler, labels μ_1 and μ_2 exist for the two means, however either one can correspond to μ_{C1} or μ_{C2}. i.e. labels are not associated with actual components from the beginning. Assume that the allocation vector $\boldsymbol{S}_{\text{initial}}$ is such that it assigns all observations from component C_1 under label 1 and all observations from component C_2 under label 2. Under such a scheme a posterior sample $(\mu_1, \mu_2) = (5, 7)$ is likely. However if we take a conjugate of this allocation vector then $(\mu_1, \mu_2) = (7, 5)$ is also likely to be sampled. This can be attributed to the fact that we have a mixture likelihood function which is bimodal. In cases where the components are not well separated, because of a certain scheme of allocations $\boldsymbol{S}$, the sampler might sample μ_1 from both modal regions of the likelihood resulting into a posterior which is bimodal as well. However it can also lead to partially explored posteriors, which may not be useful for making any inference.

Dealing with label switching

One of the techniques used for dealing with label switching is imposing a formal identifiability constraint such as $\mu_1 < \mu_2$. However Frühwirth-Schnatter, Tüchler, and Otter, (2004) suggest that arbitrary identifiability constraints should not be applied as they are often ineffective. Instead in an example they chose an identifiability constraint based on pre-analysis of the various modal regions. In the case of Bayesian heterogeneity model the mean is a vector comprising of random intercept and random slope means. We applied identifiability constraints on the mean vector based on graphical exploration of the mixture density as shown in section 5.1.1. It is important to note that if more components than needed are chosen, then label switching is unavoidable, and should also be seen as an indicator for overfitting (Frühwirth-Schnatter, 2013, pg. 104).

One of the other interesting techniques to deal with label switching is post-processing of MCMC chains by relabeling the output(Richardson and Green, 1997; Stephens, 2000). We too employed this technique in the approximation of marginal likelihood (section 4.2), as that procedure also involves running further MCMC chains (expression 4.16). As we later figured out in our simulations, without careful relabeling of output one may obtain a Bayes factor $\to 0$ and thus reject the model outright.

Chapter 4

Model selection criteria

In most cases we do not know the right number of components in a mixture distribution in advance. As part of this thesis we will compare 3 of the existing Bayesian methods for finding the right number of mixture components.

4.1 Deviance information criteria

The Deviance information criteria or DIC was first proposed by Spiegelhalter et al., (2002) for Bayesian model selection. The motivation for DIC is similar to frequentist AIC/BIC criteria in the sense that DIC also penalizes more elaborate models using a penalty component. If $p(\boldsymbol{\theta}_p) = p(\boldsymbol{\theta}|\boldsymbol{y})$ corresponds to the posterior distribution of parameters $\boldsymbol{\theta}$, then the definition for DIC is given by

$$\mathsf{DIC} = -2\log p(\boldsymbol{y}|\bar{\boldsymbol{\theta}}_p) + 2\mathsf{p_D}$$

where $\bar{\boldsymbol{\theta}}_p = \mathsf{E}(\boldsymbol{\theta}_p)$ is the posterior mean of the parameters. The penalty for model complexity is given by $\mathsf{p_D} = -2\mathsf{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p)) + \log p(\boldsymbol{y}|\bar{\boldsymbol{\theta}}_p))$. It can also be written as,

$$\mathsf{p_D} = \overline{D(\boldsymbol{\theta})} - D(\bar{\boldsymbol{\theta}})$$

where $\overline{D(\boldsymbol{\theta})}$ is the posterior mean of Bayesian deviance $D(\boldsymbol{\theta})$, and $D(\bar{\boldsymbol{\theta}})$ is the Bayesian deviance evaluated at the posterior mean of the parameters. Bayesian deviance is defined as $D(\boldsymbol{\theta}) = -2\log p(\boldsymbol{y}|\boldsymbol{\theta}) + 2\log f(\boldsymbol{y})$. We do not discuss the term $f(\boldsymbol{y})$ because it cancels out in the expression for $\mathsf{p_D}$. For consistency of notation, here onwards we will use $\overline{D(\boldsymbol{\theta}_p)}$ and $D(\bar{\boldsymbol{\theta}}_{\boldsymbol{p}})$ in the expression for $\mathsf{p_D}$.

4.1.1 DIC for missing data models

Mixture models and mixed models are both a member of the class of models called missing data models. The allocation vector $\boldsymbol{S}$ in a mixture model, and the matrix of random effects $\boldsymbol{b} = (\boldsymbol{b}_1^T, \boldsymbol{b}_1^T, ..., \boldsymbol{b}_n^T)^T$ in a LMM, are not observed directly. Thus one could have various incompatible definitions of DIC based on observed data likelihood, complete data likelihood and conditional data likelihood, as shown by Delorio and Robert in a discussion on the paper of Spiegelhalter et al., (2002). Further, Celeux et al., (2006) proposed multiple definitions of DIC under each of the aforementioned likelihood classes and showed that each has a different value and thus a different impact on model selection. In this thesis we took some of those definitions and applied them on the Bayesian heterogeneity model.

Observed DIC

Let us denote the set of all the unknown parameters in the Bayesian heterogeneity model as $\boldsymbol{\theta}$. i.e. $\boldsymbol{\theta} = (\beta, \sigma^2, \boldsymbol{\nu})$, where $\boldsymbol{\nu}$ is as defined in section 3.3.1. The first category of DIC is associated with observed data likelihood $f(\boldsymbol{y}|\boldsymbol{\theta})$ which can be obtained by marginalizing over the allocation S_i and random effects $\boldsymbol{b}_i$ for the subjects. The following expression gives the observed data likelihood for the Bayesian heterogeneity model.

$$f(\boldsymbol{y}|\boldsymbol{\theta}) = \prod_{i=1}^{n} \sum_{k=1}^{K} f_N(\boldsymbol{y}_i; \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_k^C, \boldsymbol{Z}_i G_k \boldsymbol{Z}_i^T + R_i)\eta_k \tag{4.1}$$

Based on equation 4.1 we will now extend the definition of the various definitions of DIC proposed by Celeux et al., (2006). The first one is the classical definition for DIC, as shown below.

$$\text{DIC}_1 = -4\text{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p)) + 2\log p(\boldsymbol{y}|\bar{\boldsymbol{\theta}}_p)) \tag{4.2}$$

where $\boldsymbol{\theta}_p$ and $\bar{\boldsymbol{\theta}}_p$ are as defined in section 4.1. One of the problems with DIC_1 is that in case of label switching, one may obtain a negative p_D. In our simulation study we encountered this problem as well (section 5.1.3). The reason is that when label switching happens, mean of the posteriors may take a value which lies somewhere in between the various modes. On the other hand, in such a scenario a posterior mode is going to take a value from only one of the modal regions. Thus the next definition of DIC is formed by replacing posterior mean with posterior mode in the calculation of $D(\bar{\boldsymbol{\theta}}_p)$.

$$\text{DIC}_2 = -4\text{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p)) + 2\log p(\boldsymbol{y}|\hat{\boldsymbol{\theta}}_p)) \tag{4.3}$$

where $\hat{\boldsymbol{\theta}}_{\boldsymbol{p}} = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\boldsymbol{y})$. Celeux et al., (2006) further suggest that for models where non identifiability of parameters is endemic, as in the case of mixtures usually, one should use the following estimator for the approximation of the density $p(\boldsymbol{y}|\boldsymbol{\theta})$,

$$\hat{f}_{\boldsymbol{\theta}}(\boldsymbol{y}) = \prod_{i=1}^{n} \hat{f}_{\boldsymbol{\theta}}(\boldsymbol{y}_i) = \prod_{i=1}^{n} \frac{1}{m} \sum_{l=1}^{m} \sum_{k=1}^{K} f_N(\boldsymbol{y}_i; \boldsymbol{X}_i\boldsymbol{\beta}^{(l)} + \boldsymbol{Z}_i\boldsymbol{b}_k^{C(l)}, \boldsymbol{Z}_i G_k^{(l)} \boldsymbol{Z}_i^T + R_i^{(l)})\eta_k^{(l)}$$

where $\boldsymbol{\beta}^{(l)}, \boldsymbol{b}_k^{C(l)}, G_k^{(l)}, R_i^{(l)}, \eta_k^{(l)}$ are the samples from the l^{th} MCMC iteration of a chain of length m. The estimator is also called the MCMC predictive density estimator, and gives us the next definition of DIC.

$$\text{DIC}_3 = -4\text{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p)) + 2\log \hat{f}_{\boldsymbol{\theta}}(\boldsymbol{y}) \tag{4.4}$$

The benefit of using DIC_3 is that p_D always takes a positive value. While doing the simulation study we found that not only was this claim true, but p_D also never took extreme values; even when models were severely overfitted leading to label switching. Lastly, in each of the equations 4.2, 4.3, 4.4, $\text{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p))$ can be calculated by using the following approximation.

$$\text{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p)) = \frac{1}{m} \sum_{l=1}^{m} \log p(\boldsymbol{y}|\boldsymbol{\theta}_p^{(l)}) \tag{4.5}$$

Complete DIC

The second class of the DIC is based on the complete data likelihood. The complete data for the i^{th} subject in a Bayesian heterogeneity model consists of $(\boldsymbol{y}_i, S_i, \boldsymbol{b}_i)$. For the i^{th} subject we will denote the complete data by $\boldsymbol{y}_i^F$ and for the entire data set we will denote it by $\boldsymbol{y}^F$. The following equation shows the complete data likelihood for the Bayesian heterogeneity model.

$$
\begin{aligned}
f(\boldsymbol{y}^F|\boldsymbol{\theta}) &= \prod_{i=1}^{n} f(\boldsymbol{y}_i|\boldsymbol{b}_i, S_i) f(\boldsymbol{b}_i|S_i) f(S_i) \\
&= \prod_{i=1}^{n} f_N(\boldsymbol{y}_i; \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_i, R_i) f_N(\boldsymbol{b}_i; \boldsymbol{b}^C_{S_i}, G_{S_i}) f(S_i; \boldsymbol{\eta})
\end{aligned} \tag{4.6}
$$

Based on the complete data $\boldsymbol{y}^F$, the complete data DIC is given by following expression,

$$
\text{DIC} = -4\text{E}_{\boldsymbol{\theta}_p}(\log p(\boldsymbol{y}^F|\boldsymbol{\theta}_p)) + 2\log p(\boldsymbol{y}^F|\bar{\boldsymbol{\theta}}_p)) \tag{4.7}
$$

where $\boldsymbol{\theta}_p$ is same as $\boldsymbol{\theta}|\boldsymbol{y}^F$. Since part of the complete data are not observed, Celeux et al., (2006) propose integrating the expression in 4.7 with respect to the missing data $\boldsymbol{y}^M = (\boldsymbol{b}, \boldsymbol{S})$ to obtain the following definition of DIC.

$$
\text{DIC}_4 = -4\text{E}_{\boldsymbol{\theta},\boldsymbol{y}^M|\boldsymbol{y}}(\log p(\boldsymbol{y}^F|\boldsymbol{\theta}_p)) + 2\text{E}_{\boldsymbol{y}^M|\boldsymbol{y}}(\log p(\boldsymbol{y}^F|\bar{\boldsymbol{\theta}}_p)) \tag{4.8}
$$

The first part of the formula for DIC_4 is not available in closed form for Bayesian heterogeneity model, however it can still be approximated using the output of Gibbs sampler in the same way as in 4.5; though one has to also use the simulated $\boldsymbol{y}^M$ from the MCMC iterations. The motivation for this approximation is that during each iteration of the Gibbs sampler, parameter values are sampled from the conditional distribution of the parameters. i.e. in our case conditional on the other parameters and unobserved data both. We further verified the approximation by comparing the results of DIC_4 calculation done using the closed form solution for a mixture distribution, with the aforementioned approximation, both suggested by Celeux et al., (2006). We found both of the results to be differing only in the decimal places.

The second part of DIC_4, i.e. $\text{E}_{\boldsymbol{y}^M|\boldsymbol{y}}(\log p(\boldsymbol{y}^F|\bar{\boldsymbol{\theta}}_p))$, is also not straightforward to compute. While the expectation over unobserved data $\boldsymbol{y}^M$ can be approximated in the same way as in 4.5, however for calculating $\bar{\boldsymbol{\theta}}_p$ Celeux et al., (2006) suggested using the posterior estimates $(\boldsymbol{y}^M|\boldsymbol{y})$ of the unobserved data. We will now give the formula for the expected values of parameters of interest during the l^{th} iteration, i.e. $\bar{\boldsymbol{\beta}}^{(l)}$, $\bar{\sigma^2}^{(l)}$ and $\bar{\boldsymbol{\nu}}^{(l)}$.

$$
\bar{\boldsymbol{\beta}}^{(l)} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{Z}\boldsymbol{b}^{(\boldsymbol{l})})
$$

$$
\bar{\sigma^2}^{(l)} = \frac{(\boldsymbol{y} - \boldsymbol{Z}\boldsymbol{b}^{(\boldsymbol{l})} - \boldsymbol{X}\bar{\boldsymbol{\beta}}^{(l)})^T(\boldsymbol{y} - \boldsymbol{Z}\boldsymbol{b}^{(\boldsymbol{l})} - \boldsymbol{X}\bar{\boldsymbol{\beta}}^{(l)})}{(\sum_{i=1}^{n} m_i - p - 1) - 2}
$$

$$
\bar{\boldsymbol{b}_k^C}^{(l)} = \frac{\sum_{i=1}^{n} I(S_i^{(l)} = k)\boldsymbol{b}_{\boldsymbol{i}}^{(\boldsymbol{l})}}{n_k^{(l)}}
$$

$$
\bar{G_k^{(l)}} = \frac{\sum_{i=1}^{n} I(S_i^{(l)} = k)(\boldsymbol{b}_{\boldsymbol{i}}^{(l)} - \bar{\boldsymbol{b}_k^C}^{(l)})(\boldsymbol{b}_{\boldsymbol{i}}^{(l)} - \bar{\boldsymbol{b}_k^C}^{(l)})^T}{(n_k^{(l)} - 1) - \text{rank}(\bar{\boldsymbol{b}_k^C}^{(l)}) - 1}
$$

$$
\bar{\eta_k^{(l)}} = \frac{a_k + n_k^{(l)}}{\sum_{u=1}^{K} a_u + n}
$$

The next definition of DIC under the class of complete data DIC is motivated by the fact that the at times $\text{E}(\boldsymbol{y}^M|\boldsymbol{y})$ takes values outside the support of the joint distribution of $\boldsymbol{b}, \boldsymbol{S}$ (Celeux et al., 2006). Thus using MAP(maximum a posteriori) as the estimate instead (expression 4.3), the following definition of DIC is proposed.

$$
\text{DIC}_5 = -4\text{E}_{\boldsymbol{\theta},\boldsymbol{y}^M|\boldsymbol{y}}(\log p(\boldsymbol{y}^F|\boldsymbol{\theta}_p)) + 2\log p(\boldsymbol{y}, \hat{\boldsymbol{y}}^M|\hat{\boldsymbol{\theta}}) \tag{4.9}
$$

Conditional DIC

The third class of the DIC is based on the assumption that $\boldsymbol{y}^M$ can be seen as an additional parameter rather than as missing data. We will represent the new posterior parameter space as $\boldsymbol{\theta}^{\text{cond}} = (\boldsymbol{\theta}, \boldsymbol{y}^M)$. Correspondingly the posterior density of the parameter $\boldsymbol{\theta}^{\text{cond}}$ is denoted as $p(\boldsymbol{\theta}_p^{\text{cond}})$. The following equation shows the conditional data likelihood,

$$f(\boldsymbol{y}|\boldsymbol{\theta}^{\text{cond}}) = \prod_{i=1}^{n} f_N(\boldsymbol{y}_i; \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_i, R_i) \tag{4.10}$$

Based on this conditional likelihood, Celeux et al., (2006) proposed the following DIC definition.

$$\text{DIC}_6 = -4\text{E}_{\boldsymbol{\theta}_p^{\text{cond}}}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p^{\text{cond}})) + 2\log p(\boldsymbol{y}|\hat{\boldsymbol{\theta}}_p^{\text{cond}})) \tag{4.11}$$

where $\hat{\boldsymbol{\theta}}_p^{\text{cond}} = \arg\max_{\boldsymbol{\theta}^{\text{cond}}} p(\boldsymbol{\theta}^{\text{cond}}|\boldsymbol{y})$, and $\text{E}_{\boldsymbol{\theta}_p^{\text{cond}}}(\log p(\boldsymbol{y}|\boldsymbol{\theta}_p))$ can be approximated as done in equation 4.5.

4.2 Marginal Likelihood

The marginal likelihood of the data represents the probability of data given the model. This can be calculated by marginalizing the likelihood over the model parameters $\boldsymbol{\theta}$.

$$p(\boldsymbol{y}|M) = \int p(\boldsymbol{y}|\boldsymbol{\theta}, M)p(\boldsymbol{\theta}|M)\,\mathrm{d}\boldsymbol{\theta} \tag{4.12}$$

Given two competing models for the data, M_1 and M_2, one can further use 4.12 to calculate the odds of model M_1 against the model M_2 given the data. These odds are called the Posterior odds and can be written as,

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

where $\frac{p(M_1)}{p(M_2)}$ is called prior odds, and $\frac{p(\boldsymbol{y}|M_1)}{p(\boldsymbol{y}|M_2)}$ is called the Bayes Factor. Since we have the same prior belief in each of these models, prior odds is equal to 1. Marginal likelihood is a relative measure of model fit and unless prior odds are not equal to 1, marginal likelihood will be equal to Bayes Factor. To calculate the Bayes Factor we will use the method proposed by Chib, (1995). Chib's idea is that one can rewrite the Bayes rule in equation 2.1 to get the marginal likelihood formula as

$$m(\boldsymbol{y}) = p(\boldsymbol{y}|M) = \frac{L(\boldsymbol{\theta}|\boldsymbol{y}, M)p(\boldsymbol{\theta}|M)}{p(\boldsymbol{\theta}|\boldsymbol{y}, M)} \tag{4.13}$$

Equation 4.13 is valid for all $\boldsymbol{\theta}$, though Chib recommends using posterior mode $\arg\max_\theta p(\boldsymbol{\theta}|\boldsymbol{y})$ of parameters or the maximum likelihood estimate $\arg\max_\theta L(\boldsymbol{\theta}|\boldsymbol{y})$. We decided to choose the latter of the two. Further, in context of the Bayesian heterogeneity model, we will denote the selected parameter value as $\boldsymbol{\theta}^* = (\boldsymbol{\beta}^*, \sigma^{2^*}, \boldsymbol{\nu}^*)$. Thus Chib's approximation for marginal likelihood on log scale is given by,

$$\log \hat{m}(\boldsymbol{y}) = \log L(\boldsymbol{\theta}^*|\boldsymbol{y}) + \log p(\boldsymbol{\theta}^*) - \log p(\boldsymbol{\theta}^*|\boldsymbol{y}) \tag{4.14}$$

Note that we have dropped the model indicator M from equation 4.14 for readability. We will now show calculations for determining the marginal likelihood value using Chib's approximation.

Firstly $\log L(\boldsymbol{\theta}^*|\boldsymbol{y}) = f(\boldsymbol{y}|\boldsymbol{\theta}^*)$ can be easily determined using the formula given in equation 4.1. The calculation of $\log p(\boldsymbol{\theta}^*)$ is also straightforward because we take independent priors for the

parameters in our model, the details of which are given in section 3.4.4. Assuming that the parameters of component densities of the mixture distribution of random effects are independent, one can use the following to calculate $\log p(\boldsymbol{\theta}^*|\boldsymbol{y})$.

$$\log p(\boldsymbol{\theta}^*|\boldsymbol{y}) = \sum_{k=1}^{K} \log p(G_k^*|\boldsymbol{y}) + \sum_{k=1}^{K} \log p(\boldsymbol{b}_k^{C^*}|G_k^*, \boldsymbol{y}) + \log p(\sigma^{2^*}|G_k^*, \boldsymbol{b}_k^{C^*}, \boldsymbol{y}) + \log p(\boldsymbol{\beta}^*|G_k^*, \boldsymbol{b}_k^{C^*}, \sigma^{2^*}, \boldsymbol{y}) + \log p(\boldsymbol{\eta}^*|G_k^*, \boldsymbol{b}_k^{C^*}, \sigma^{2^*}, \boldsymbol{\beta}^*, \boldsymbol{y}) \quad (4.15)$$

An interesting problem one faces in such an expansion is that the posteriors may not be available as a well known density. For e.g. one can choose independent inverse gamma priors for variance parameters of random effects and a uniform prior for correlation. However the posterior density of parameters in such a case will not be well known. While one may try to approximate it with a known density, however Chib's approximation procedure requires doing it multiple times, making it practically infeasible. An obvious alternative is to choose conjugate priors in such a situation. However as we mentioned in section 3.4.4 the joint conjugate prior in the case of unknown mean and covariance matrix is a Normal-inverse-Wishart prior and the joint posterior is a Normal-inverse-Wishart posterior. Although it is common to use independent priors for mean and covariance matrix in practice while using BUGS family of software, the problem of posterior being from an unknown family remains the same. Chib, (1995) suggested using the Rao-Blackwellization method to solve this problem. For e.g. the Rao-Blackwellized estimate of $p(G_k^*|\boldsymbol{y})$ is given by,

$$\begin{aligned}
\prod_{k=1}^{K} p(G_k^*|\boldsymbol{y}) &= \int \prod_{k=1}^{K} p(G_k^*|\boldsymbol{y}, \boldsymbol{b}, \boldsymbol{S}, \boldsymbol{b}_k^C) p(\boldsymbol{b}_1^C, \boldsymbol{b}_2^C, ..., \boldsymbol{b}_K^C, \boldsymbol{b}, \boldsymbol{S}|\boldsymbol{y}) \, \mathrm{d}\boldsymbol{b}_1^C \, \mathrm{d}\boldsymbol{b}_2^C ... \, \mathrm{d}\boldsymbol{b}_K^C \, \mathrm{d}\boldsymbol{b} \, \mathrm{d}\boldsymbol{S} \\
&\approx \frac{1}{m} \sum_{l=1}^{m} \prod_{k=1}^{K} p(G_k^*|\boldsymbol{y}, \boldsymbol{b}^{(l)}, \boldsymbol{S}^{(l)}, \boldsymbol{b}_k^{C^{(l)}}) \qquad (4.16) \\
&\approx \frac{1}{m} \sum_{l=1}^{m} \prod_{k=1}^{K} f_{\mathcal{W}^{-1}}(G_k^*; n_k^{(l)} + n_0, \Psi + \sum_{i=1}^{n_k^{(l)}} (\boldsymbol{b}_{\boldsymbol{i}}^{(l)} - \boldsymbol{b}_k^{C^{(l)}})(\boldsymbol{b}_{\boldsymbol{i}}^{(l)} - \boldsymbol{b}_k^{C^{(l)}})^T)
\end{aligned}$$

where, $n_k^{(l)}$ are number of subjects classified under component k in iteration l and (n_0, Ψ) are the parameters for the inverse Wishart distribution specified as prior for the variance covariance matrix of the component densities. In 4.16 one approximates the integral with the samples obtained from the MCMC iterations. As we can see the benefit of this approach is that $p(G_k^*|\boldsymbol{y}, \boldsymbol{b}^{(l)}, \boldsymbol{S}^{(l)}, \boldsymbol{b}_k^{C^{(l)}})$ is the well known inverse Wishart density. However for the choice of independent inverse gamma priors for variance parameters of random effects and a uniform prior for correlation, one will have to manually approximate the posterior densities with a well known density as many times as the length of the MCMC chain. The use kernel density estimation procedures can also be dismissed because the posteriors may require approximation using different parametric families. It is because of these reasons we avoided calculation of Bayes factor in the case where we took independent inverse gamma priors for variance of random effects and uniform prior for correlation.

Proceeding further with the Rao-Blackwellization procedure one can obtain the following approximations for the remaining parameters.

$$\prod_{k=1}^{K} p(\boldsymbol{b}_k^{C^*}|G_k^*, \boldsymbol{y}) \approx \frac{1}{m} \sum_{l=1}^{m} \prod_{k=1}^{K} f_N(\boldsymbol{b}_k^{C^*}; (G_0^{-1} + n_k^{(l)} G_k^{*-1})^{-1} (G_0^{-1} \boldsymbol{\mu}_0 + n_k^{(l)} G_k^{*-1} \bar{\boldsymbol{b}_{ik}^{(l)}}), (G_0^{-1} + n_k G_k^{*-1})^{-1}) \quad (4.17)$$

$$p(\sigma^{2^*}|G_k^*, \boldsymbol{b}_k^{C^*}, \boldsymbol{y}) \approx \frac{1}{m}\sum_{l=1}^{m} f_{Inv-Gamma}(\sigma^{2^*}; \alpha_0 + \frac{\sum_{i=1}^{n} m_i}{2}, \beta_0 + \frac{\sum_{i=1}^{n}\sum_{j=1}^{m_i}(y_{ij} - \boldsymbol{x_{ij}}\boldsymbol{\beta}^{(l)} - \boldsymbol{z_{ij}}\boldsymbol{b_i^{(l)}})}{2}) \tag{4.18}$$

$$p(\boldsymbol{\beta}^*|G_k^*, \boldsymbol{b}_k^{C^*}, \sigma^{2^*}, \boldsymbol{y}) \approx \frac{1}{m}\sum_{l=1}^{m} f_N(\boldsymbol{\beta}^*; (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{Z}\boldsymbol{b}^{(l)}), \sigma^{2^*}(\boldsymbol{X}^T\boldsymbol{X})^{-1}) \tag{4.19}$$

$$p(\boldsymbol{\eta}^*|G_k^*, \boldsymbol{b}_k^{C^*}, \sigma^{2^*}, \boldsymbol{\beta}^*, \boldsymbol{y}) \approx \frac{1}{m}\sum_{l=1}^{m} f_{Dir}(\boldsymbol{\eta}^*; a_{01} + n_1^{(l)}, a_{02} + n_2^{(l)}, ..., a_{0K} + n_K^{(l)}) \tag{4.20}$$

where, $(\boldsymbol{\mu}_0, G_0)$ are the parameters for the multivariate normal prior for the mean $\boldsymbol{b}_k^C$ of the k^{th} component density,
$\bar{\boldsymbol{b}}_{ik}^{(l)} = \frac{\sum_{i=1}^{n} I(S_i^{(l)}=k)\boldsymbol{b_i^{(l)}}}{n_k^{(l)}}$ is the mean of the estimated random effects corresponding to the n_k subjects classified under the k^{th} component in the l^{th} MCMC iteration,
(α_0, β_0) are the parameters of the inverse gamma density specified as the prior for the within subject variance σ^2,
$a_{01}, a_{02}, ..., a_{0K}$ are the parameters of the Dirichlet density specified as the prior for component weight vector $\boldsymbol{\eta}$.

Using these values an estimate of $\log p(\boldsymbol{\theta}^*|\boldsymbol{y})$ can be obtained and can be further substituted in equation 4.14 to obtain $\log \hat{m}(\boldsymbol{y})$. In models where marginal likelihood is known to work well as a model selection criteria, models with higher value of $\log \hat{m}(\boldsymbol{y})$ should be preferred.

4.3 Posterior predictive checks

The motivation behind a posterior predictive check is to evaluate the model fit using simulations from the posterior predictive distribution(PPD) $p(\tilde{\boldsymbol{y}}|\boldsymbol{y})$. For a simple model such as $y_i = \mu + \varepsilon_i, \varepsilon_i \sim N(0, \sigma^2)$, one can perform an informal check by sampling 1000(say) values from the PPD 20(say) times and compare the histogram of the original sample with the histogram of the data sampled from PPD. If the histograms do not match then one can say that the model does not fit the data well.

In context of mixture distributions Frühwirth-Schnatter, (2013) suggest that one should first sample allocation vector $\tilde{\boldsymbol{S}}$ based on the posterior density of the weight distribution $p(\boldsymbol{\eta}|\boldsymbol{y})$ and then generate samples from $p(\tilde{\boldsymbol{y}}|\tilde{\boldsymbol{S}}, \boldsymbol{\theta}_p)$. A similar approach can be followed in hierarchical models by first generating new random effects $\tilde{\boldsymbol{b}}$. This was termed as the Mixed predictive approach by Marshall and Spiegelhalter, (2003). Although they suggested a cross validation method where $\tilde{\boldsymbol{b}}|\boldsymbol{y}_{(i)}$ were used, we did not follow this approach as it required a significant amount of computational resources. As an alternative of mixed predictive approach, one can use the posterior allocations $\boldsymbol{b}|\boldsymbol{y}$ instead of $\tilde{\boldsymbol{b}}$. However the problem with this approach is that it leads to a more conservative posterior predictive check (Congdon, 2010).

4.3.1 PPC for the Bayesian heterogeneity model

Detecting overfitting the number of components

When more than the required number of components are fitted to the mixture distribution of random effects then during the MCMC procedure some of the components may remain empty.

i.e. no observation gets allocated to some of the components. In such a case, the posterior of variance covariance matrix G_k as well as of mean $\boldsymbol{b}_k^C$ is sampled from the prior distribution. Since the prior we considered were non informative, the posterior samples of parameters are arbitrarily large or small values. Thus the random effects $\tilde{\boldsymbol{b}}$ sampled from the posterior distribution of the empty components, and the posterior predictive sample $\tilde{\boldsymbol{y}}|\tilde{\boldsymbol{b}}$ will also be arbitrarily small or large. This property can be employed to form a posterior predictive check. However this approach is only possible with mixed predictive checking. The reason is that, in our simulation study we found that the posterior samples $\boldsymbol{b}_i|\boldsymbol{y}$ do not show any anomaly even if the mixture distribution of random effects is overfitted/underfitted. Thus following the classical PPC one may not be able to detect over/under fitting based on the posterior samples $\boldsymbol{b}_i|\boldsymbol{y}$.

We will now discuss two of the issues with the above approach and their solutions. Firstly, the weights η_k of empty components are sampled from the Dirichlet posterior which gets information from all other components as well. Thus iterations in which the components remain empty, the weights also remain small. This problem can be obviated by sampling a large number of observations from the posterior predictive distribution. The second problem is that if one uses a Wishart prior for the variance covariance matrix of component densities then although it is non-informative for the correlation, it imposes certain restrictions on the variances. One can instead choose independent gamma priors for variances and uniform prior for correlation in such a scenario, albeit under the restriction that the sample variance covariance matrix is invertible.

The first step in the mixed predictive check approach for Bayesian heterogeneity model is to sample the new allocations $\tilde{\boldsymbol{S}}$. The second step is to sample the random effects $\tilde{\boldsymbol{b}}_i|\tilde{S}_i$ for the subjects. We propose the following test statistic based on these sampled random effects.

$$T(\boldsymbol{r}) = \frac{1}{\sum_{i=1}^{n} m_i} \sum_{i=1}^{n} \sum_{j=1}^{m_i} (r_{ij} - \bar{r}_{i.})^2 \tag{4.21}$$

where, $r_{ij} = \boldsymbol{z}_{ij}\tilde{\boldsymbol{b}}_i + \varepsilon_{ij}$ for the mixed predictive distribution of the random effects and $\bar{r}_{i.} = \frac{1}{m_i}\sum_{j=1}^{m_i} r_{ij}$. For the observed data set, r_{ij} can be calculated as $r_{ij} = y_{ij} - \boldsymbol{x}_{ij}\boldsymbol{\beta}_p$, where $p(\boldsymbol{\beta}_p) = p(\boldsymbol{\beta}|\boldsymbol{y})$. When the number of components in the mixture distribution of random effects are more than required, then during some of the iterations the test statistic for the mixed predictive data will have arbitrarily large values.

Underfitting the number of components

The Bayesian heterogeneity model poses a unique problem for detecting underfitting via PPC. We found in our simulation study that it is not possible to distinguish the distribution of the test statistic $T(\boldsymbol{r})$ with underfitted mixture of random effects from the distribution of the test statistic with rightly fitted mixture of random effects. The reason for it is that the full Bayesian estimates for random effects $\boldsymbol{b}_i$ can be almost the same for underfitted as well as rightly and overfitted models. This further results into an almost equal estimate of within subject variance σ^2 for the various models. The mean structure parameter estimates are also almost the same and thus eventually with these minor differences it is impossible to differentiate between the models using PPC. One way to circumvent this issue is to fit as many components as possible till overfitting is detected, and then the choice among the underfitted models could be done on the basis of interpretation of the clusters and the size of the clusters.

4.3.2 Posterior predictive p-values

The motivation of Posterior predictive p-values(PPP) is similar to frequentist p-values. The PPP are however averaged over the entire posterior distribution of the test statistic. Given a

test statistic $T(\boldsymbol{y})$, the frequentist p-value is equal to the probability $P(T(\tilde{\boldsymbol{y}}) > T(\boldsymbol{y}))$, where $p(\tilde{\boldsymbol{y}}) = p(\boldsymbol{y}|\hat{\boldsymbol{\theta}})$. In the Bayesian paradigm the parameter $\boldsymbol{\theta}$ has a posterior distribution. Thus, although the same probability for the test statistic is calculate as before, but it is averaged over the entire posterior distribution $p(\theta|\boldsymbol{y})$. A small PPP value indicates bad model fit. In context of the Bayesian heterogeneity model PPP values may not be as desirable for testing over/under fitted for the reasons mentioned in the previous subsection. However they can still be used to detect a poor fit to the data itself.

Chapter 5

Simulation study

In this chapter we share results from the simulation study we performed to check the efficacy of the model selection criteria described in Chapter 4. We implemented the Bayesian heterogeneity model using the R package R2jags (Su and Yajima, 2015) and analyzed the MCMC chains using the R package ggmcmc (Marín, 2016). For the calculation of marginal likelihood we required the density function of Wishart distribution, which was available in two packages, namely MCMCpack and mixAK. There were inconsistencies in the results from the two implementations and we eventually used mixAK (Komárek, 2015) as the MCMCpack package produced density function value to be ∞ in some cases.

5.1 Data sets for simulation study

The data sets we simulated were motivated by the study on predicting Zebu cow's weights in sub Saharan Africa (Lesosky et al., 2012). We assumed our response to be the weight of the Zebu cows. The predictors we considered were hypothetical, namely gender of a cattle (Male/Female), birth year of the cattle (1996/1997), age of the cattle at the first measurement and the time at which measurement was taken. The measurements of the cows were done at 10 different equally spaced time intervals. We further added subject specific random intercept and random slope effect to each response so that the repeated measurements for a given cow were correlated. Simultaneously we made sure that these cow specific random effects were mixture distributed. We will refer to the cows as subjects here forth.

5.1.1 Description of each data set

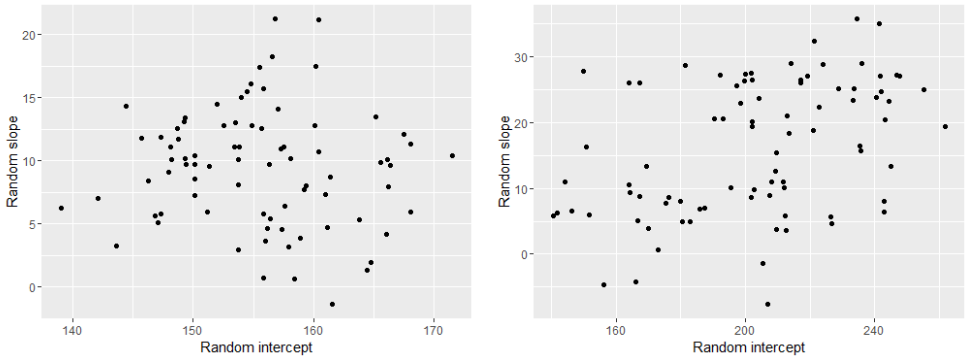
Our aim was to create data sets differing in number of mixture components for random effects, number of subjects, statistical power to detect the fixed effects, separation of mixture components and number of subjects per component. To analyze the efficacy of model selection criteria under these different scenarios we created multiple data sets. To get a rough idea about the random effects in each of these data sets, we first did a graphical analysis. For this purpose we first regressed the response $\boldsymbol{y}$ on the 3 predictors: age, gender and birth year of cattle using OLS(section 3.4.3). It is also possible to use linear mixed model for estimating the fixed effects. We then regressed the residuals $y_{ij} - \boldsymbol{x}_{ij}\beta$ on the intercept and time of measurement for every subject separately to obtain a rough estimate $\tilde{\boldsymbol{b}}_i$ of the random effect of subjects. This estimator however overestimates the actual size of the random effects as within subject variance is also included. It is not possible to use Empirical Bayes estimates of the random effects because they may fail to reflect the heterogeneity in the random effects population (Verbeke and Lesaffre, 1996). Lastly, it is important to note that fitting an incorrect mean structure can lead to a incorrect representation of the random effects distribution as shown in figure 5.1b.

Data set 1: No mixture distribution of random effects

The first data set we created was without a mixture of random effects. i.e. $\boldsymbol{b}_i \sim N(0, G)$. In total we generated data of 80 subjects, each having 10 repetitions. Based on the approach mentioned above, a plot of the random effect values for this data set is shown in figure 5.1a.

Data set 2: 3 well separated components for the mixture of random effects

The next data set we created had 3 well separated components forming the mixture distribution of random effects. In total we generated data of 180 subjects, each having 10 repetitions. A plot of the rough estimates of random effect values for this data set is shown in figure 5.2a.



(a) Data set 1 (b) Data set 2: Missing covariate age

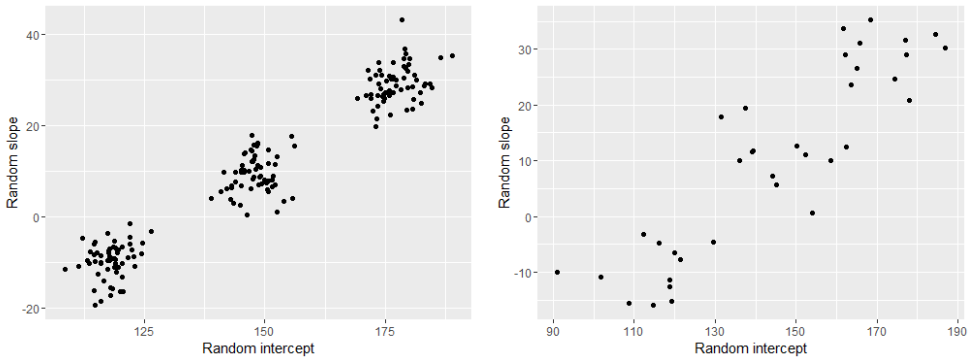
Figure 5.1: Rough estimate $\tilde{\boldsymbol{b}_i}$ for random effects

Data set 3: 3 well separated components but less subjects

This data is similar to Data set 2 in all regards except for the number of subjects. We generated only 36 subjects in total in this data set. A plot of the rough estimates of random effect values for this data set is shown in figure 5.2b.

Data set 4: 3 fused components for the mixture of random effects

In this data set we simulated the random effects from a mixture distribution which had 3 fused components. For e.g. if one sees the plot of the rough estimates of random effect values for this data set (figure 5.3a) then it is not clear if there are more than 2 components.



(a) Data set 2 (b) Data set 3

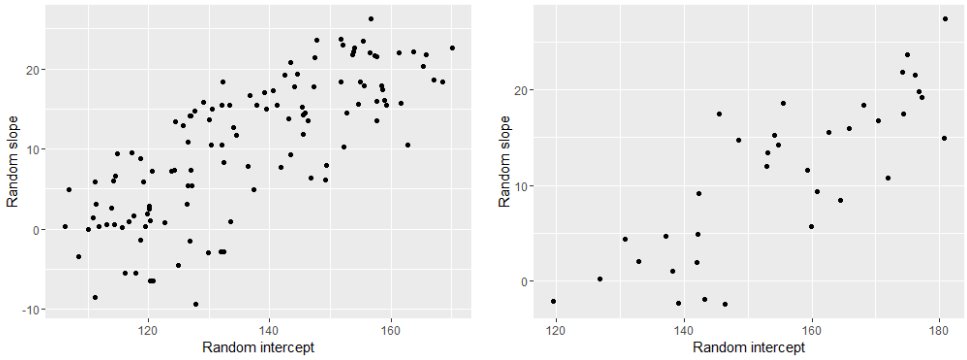
Figure 5.2: Rough estimate $\tilde{\boldsymbol{b}_i}$ for random effects

Data set 5: 3 fused components but less subjects

This data is similar to Data set 4 in all regards except for the number of subjects. We generated only 36 subjects in total in this data set. A plot of the rough estimates of random effect values for this data set is shown in figure 5.3b.

Data set 6: 5 well separated components

In this data set we simulated the random effects from a mixture distribution which had 5 well separated components. However this time we generated unequal number of subjects for every component. The plot of the rough estimates of random effect values for this data set is shown in figure 5.4a.

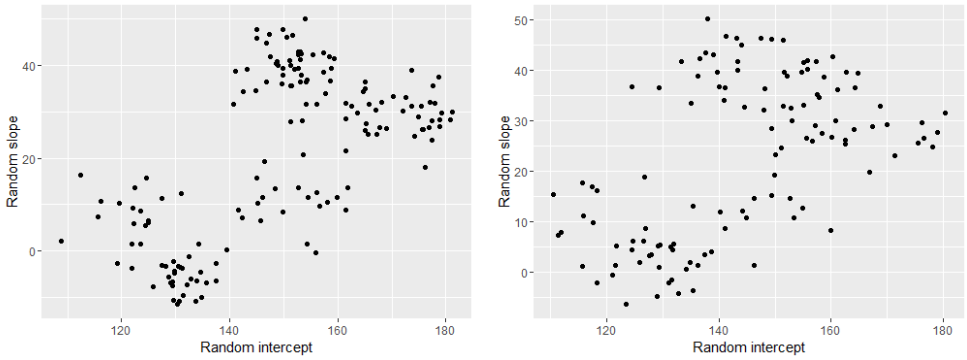


(a) Data set 4 (b) Data set 5

Figure 5.3: Rough estimate $\tilde{b_i}$ for random effects

Data set 7: 5 fused components

This data is similar to Data set 6 in all regards except that the number of subjects per component are less, and the components are not so well separated. The plot of the rough estimates of random effect values for this data set is shown in figure 5.4b.



(a) Data set 6 (b) Data set 7

Figure 5.4: Rough estimate $\tilde{b_i}$ for random effects.

5.1.2 Running MCMC simulations

We will first discuss some of the issues we while doing the MCMC simulations. The first one was label switching across the chains while calculating Bayes factor using Chib's approximation; i.e.

label 1 corresponding to component 1 in one chain and corresponding to some other component in another chain. This gave inconsistent and incorrect estimates for the various calculations we did. Although we dealt with it using the mechanisms given in section 3.4.5, mechanisms such as applying an identifiability constraint decreased the speed of simulations drastically. The second issue was high autocorrelation in the chains. We tried various strategies for it. For e.g. using a marginal model which provides implicit blocking was helpful and so was hierarchical centering. However despite these measures we had to employ a thinning of 1 per 100 iterations and in some cases 1 per 200 iterations to make sure the resulting chains were not autocorrelated. Since we lacked computational resources required to run long chains we had to be content with chains of length 1300 (after thinning). Lastly, we observed that in models where mixture of random effects was fitted with more components than needed, there was very high autocorrelation in the chain which could not be reduced despite longer chains. The convergence tests for such chains showed that the chains did not converge for some of the parameters of the component densities. The parameters corresponding to fixed effects converged in such chains though. Given that some of the component density parameters were not converged, it makes little sense to compare DIC, Marginal likelihood and PPC based on such models with models for which the chains converged. Despite that when we tried to check the aforementioned model selection criteria for such models we found some interesting patterns which we will discuss in the next section.

5.1.3 Deviance information criteria

The Deviance information criteria like all other results are based on a single chain and have been rounded to the nearest integer. Table 5.1 shows the values of the various deviance information criteria (section 4.1) applied to data set 1. Since the data set 1 had no mixture of random effects, models with 2 or more components are overfitting the data. As we mentioned above the chains did not converge for some of the parameters in the models with more components than needed, we can see that indeed calculating DIC_1 on such models gives misleading and unrealistic results such as DIC being 9 for model with 4 components. We also obtained a negative value (-602) for p_{D_1} when we fitted 3 components. Celeux et al., (2006) noted that this may happen when posterior mean borrows from several modal regions of the posterior density and ends up with a value that is located between modes. As a remedial measure Celeux et al., (2006) suggested using DIC_3 instead of the other two observed data DIC measures.

Table 5.1: DIC and p_D for data set 1. True number of components = 1

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	4143	4144	4143	5160	4402	3483
2	4146	4147	4145	5161	4403	3480
3	3536	4148	4147	5163	4388	3465
4	9	4151	4149	5166	4407	3485

# Comp Fitted	p_{D_1}	p_{D_2}	p_{D_3}	p_{D_4}	p_{D_5}	p_{D_6}
1	9	9	9	903	145	125
2	9	10	9	903	145	122
3	-602	9	8	901	126	107
4	9	11	9	903	145	127

Table 5.2 shows the values of various DIC we obtained for data set 2. One of the patterns we observe in these results is that the DIC_4 value decreased continuously till the right number

of components were fitted, whereas for the overfitted models it either decreased by a bit or remained more or less the same. A similar pattern is observed for DIC_5 and DIC_3. However it seems that they are not as discerning as DIC_4. DIC_1 and DIC_6 do not seem to have any clear pattern. It is important to note that while we did observe some patterns, we only consider DIC calculations valid for up to models with 3 components as the rest did not converge.

Table 5.2: DIC and p_D for data set 2. True number of components = 3

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	9966	9959	9965	12921	10531	7855
2	9865	9849	9864	12498	10458	7860
3	9664	9665	9663	11847	10244	7870
4	9516	9654	9664	11834	10266	7888
5	7370	9729	9666	11812	10277	7870
6	9498	9661	9668	11833	10242	7857

# Comp Fitted	p_{D1}	p_{D2}	p_{D3}	p_{D4}	p_{D5}	p_{D6}
1	9	2	8	2670	279	269
2	15	-1	14	2344	304	272
3	21	21	20	1933	331	282
4	-125	13	23	1913	345	298
5	-2270	89	26	1889	355	280
6	-147	16	23	1912	321	269

Table 5.3 shows the values of the various DIC applied to the data set 3. Firstly we can see that DIC_6 prefers model with 2 components over a model with 3 components, which is an incorrect choice of the number of the components in mixture. DIC_5 exhibits the same problem. DIC_1 and DIC_2 both have lowest DIC for the model with 3 components among the converged models however unlike DIC_3 and DIC_4 they do not exhibit the pattern of DIC remaining almost the same for overfitted models. This presence of this pattern is important because overfitted models do not converge and DIC_1 and DIC_2 exhibit no pattern to detect the boundary point beyond which all models are overfitted. This makes them unusable in a practical scenario. The magnitudes of all of the the DIC have decreased in comparison to DIC for data set 2 because the sample size for this data set is only 36 subjects compared to 180 subjects in the former.

Table 5.4 shows the results of applying various DIC to data set 4. So far we have observed that DIC_1 to DIC_4 can be used to detect the right number of components. Since the components in this data set are fused, with the large number of subjects the following results are interesting to analyze. We can see that DIC_1 to DIC_4 can still be used to select the right number of components among the converged models. However only DIC_4 still follows the pattern that we have discussed so far. To further validate the pattern, we decided to decrease the number of subjects to 36.

From the table 5.5, which shows the results of DIC for data set 5, it seems that the pattern we saw so far for DIC_4 doesn't exist anymore. The peculiarity of this data set was that the number of subjects were less and the components were fused. Thus we observed that some of the components remained empty even when we fitted the right number of components. As we discussed in section 3.4.4 one can use a Dirichlet prior with slightly bigger hyperparameters to avoid empty components, although at the risk of becoming too informative. We changed the prior for weight distribution from $\text{Dir}(1, 1, ..., 1)$ to $\text{Dir}(3, 3, ..., 3)$ and fitted models with 2, 3

Table 5.3: DIC and p_D for data set 3. True number of components = 3

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	2013	2012	2012	2611	2118	1570
2	1989	1949	1987	2497	2013	1562
3	1942	1942	1940	2339	2039	1571
4	1943	1944	1942	2342	2034	1559
5	1936	1940	1944	2344	2049	1580
6	1695	1948	1945	2344	2053	1579

# Comp Fitted	p_{D1}	p_{D2}	p_{D3}	p_{D4}	p_{D5}	p_{D6}
1	8	7	7	545	52	45
2	14	-26	12	465	-20	35
3	17	17	15	370	70	46
4	16	17	15	370	62	34
5	8	11	15	370	75	56
6	-235	17	15	368	77	53

Table 5.4: DIC and p_D for data set 4. True number of components = 3

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	6568	6566	6566	8454	6899	5197
2	6531	6523	6530	8263	6946	5253
3	6497	6492	6497	8017	6898	5263
4	6347	6480	6488	7955	6898	5253
5	6321	6463	6485	7932	6743	5259
6	6382	6329	6489	7948	6611	5259

# Comp Fitted	p_{D1}	p_{D2}	p_{D3}	p_{D4}	p_{D5}	p_{D6}
1	9	8	8	1694	139	127
2	14	7	13	1527	210	182
3	20	14	19	1341	222	187
4	-115	17	26	1287	230	181
5	-138	4	26	1265	76	187
6	-81	-134	26	1275	-62	185

and 4 components for the mixture. With 2 components we found $DIC_4 = 2441 (p_{D4} = 461)$ and $DIC_3 = 1937 (p_{D3} = 14)$. For 3 components we obtained DIC_4 = 2352 whereas for 4 components we obtained $DIC_4 = 2346$ and $DIC_3 = 1925$. In light of these results one can still justify the pattern we have observed for DIC_4 so far. However it seems that the pattern is not equally clear for DIC_3. An interesting result from this exercise was that the choice of $Dir(1, 1, ..., 1)$ prior is prone to underfitting when the components are fused and observations are less. Lastly, we also modeled the data using smaller values for Dirichlet prior hyperparameters; for e.g. $Dir(0.1, 0.1, ..., 0.1)$ prior. However it performed as worse as the $Dir(1, 1, ..., 1)$ prior for the current data set.

Table 5.6 shows the results of applying DIC to the various models fitted for data set 6. The pattern of DIC_4 remaining stable for overfitted models is visible here as well. Interestingly it also exhibited by DIC_3, which can be attributed to the fact that the components are well separated. DIC_5 and DIC_6 select underfitted models whereas DIC_1 and DIC_2 still select the right model

Table 5.5: DIC and p_D for data set 5. True number of components = 3

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	1944	1943	1943	2500	1879	1364
2	1936	1941	1945	2487	1919	1408
3	1886	-3353	1944	2453	$-\infty$	1525
4	1892	1904	1944	2439	1851	1389
5	1902	1840	1942	2418	704	336
6	1883	1919	1933	2371	2023	1538

# Comp Fitted	p_{D1}	p_{D2}	p_{D3}	p_{D4}	p_{D5}	p_{D6}
1	9	7	7	510	-110	-119
2	2	7	11	500	-68	-73
3	-42	-5281	16	470	$-\infty$	41
4	-34	-22	18	459	-130	-93
5	-21	-83	19	442	-1272	-1146
6	-31	5	19	407	59	55

among the models which have converged chains.

Table 5.6: DIC and p_D for data set 6. True number of components = 5

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	8982	8981	8980	11847	9251	6655
2	8829	8827	8827	11327	9293	6838
3	8745	8742	8744	11036	9251	6895
4	8669	8672	8677	10737	9208	6925
5	8649	8643	8648	10601	9165	6909
6	8096	8697	8650	10594	9183	6923
7	7770	8364	8651	10593	7613	6919
8	8196	8640	8653	10597	9143	6927

# Comp Fitted	p_{D1}	p_{D2}	p_{D3}	p_{D4}	p_{D5}	p_{D6}
1	9	9	7	2591	-5	-14
2	14	13	12	2224	190	169
3	20	16	19	2035	250	223
4	19	23	27	1824	296	251
5	31	26	30	1725	289	232
6	-520	81	33	1711	300	246
7	-848	-254	34	1706	-1274	244
8	-424	19	33	1711	257	248

Table 5.7 shows the results of applying DIC to the various models fitted for data set 7. Based on figure 5.4b it is difficult to identify more than 3 components in this mixture. However once again DIC_4 seem to be identifying the right number of components correctly. DIC_3 does not seem to work well in this case, which as we saw earlier happens when the components are fused. Interestingly DIC_1 selects the right model only by virtue of a difference of DIC value of 1 between model with 4 components and 5 components.

Table 5.7: DIC and p_D for data set 7. True number of components = 5

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1	6708	6707	6706	8819	6977	5071
2	6606	6605	6604	8443	6946	5135
3	6539	6538	6537	8178	6944	5204
4	6506	6514	6521	8078	6915	5196
5	6505	6500	6508	7984	6896	5202
6	6465	6501	6510	7988	6895	5196
7	6200	6500	6512	7989	6883	5190
8	6448	6498	6516	7995	6901	5196

# Comp Fitted	p_{D1}	p_{D2}	p_{D3}	p_{D4}	p_{D5}	p_{D6}
1	9	8	7	1903	61	53
2	15	14	13	1636	139	120
3	21	20	19	1456	221	185
4	12	20	26	1381	218	176
5	26	22	29	1308	220	182
6	-14	21	30	1307	214	176
7	-282	18	30	1305	198	168
8	-36	14	32	1307	213	175

Given the results of DIC_1 for data set 7, it is important to note that when components were fused, then even with a very large number of MCMC iterations we observed the DIC to be varying by a margin of 10 to 20 across chains. Thus if the classical rule of thumb (DIC difference of 5 to 10) is used to select the models based on the DIC value then it is highly plausible to refute a single model across multiple chains.

5.1.4 Marginal likelihood

We implemented Chib's approximation mentioned in section 4.2. Table 5.8 shows the results of $\log \hat{m}(\boldsymbol{y})$ for the various models we fitted to data set 1 to data set 7. One can see that even among the well converged models there is no obvious pattern visible in these results to conclude the efficacy of Bayes factor in selection of a model. For e.g. in case of data set 6 we had 5 well separated components in the mixture distribution of random effects. When we fitted 1,2,3,4 and 5 components to this data set we had MCMC chains with good convergence and no multi-modality was observed for the posteriors. However we can see that marginal likelihood preferred fitting 1 component over higher number of components. For data set 3 where we had 3 well separated components but only 36 subjects in total, we can observe that marginal likelihood wrongly prefers model with 2 components and not model with 3 components. Thus Marginal likelihood does not seem to be an effective method to choose the right number of components in the mixture of random effects.

5.1.5 Posterior predictive check (PPC)

We implemented the PPC outlined in section 4.3. Since the PPC we used were designed to detect non identifiability due to empty components, it worked irrespective of the size of the data set or how well separated the components were. Thus we found the results of PPC to be consistent across the various data sets. Because of this reason, we will only discuss the results of fitting various number of components in data set 6. It is important to note that, like DIC we also applied

Table 5.8: $\log \hat{m}(\boldsymbol{y})$ for data set 1

Fitted	1 Comp	2 Comp	3 Comp	4 Comp	5 Comp	6 Comp	7 Comp	8 Comp
Data set 1	-2120	-2128	-2139	-2142				
Data set 2	-5019	-4989	-4937	-4925	-4938	∞		
Data set 3	-1038	-1044	-1042	-645	-1003	∞		
Data set 4	-3317	-3318	-3322	-3332	-3348	∞		
Data set 5	-1001	-1016	-1032	-1041	-1058	∞		
Data set 6	-4545	-4492	-4477	-4467	-4473	∞	-4498	-3985
Data set 7	-3397	-3379	-3373	-3380	-2749	∞	∞	-3416

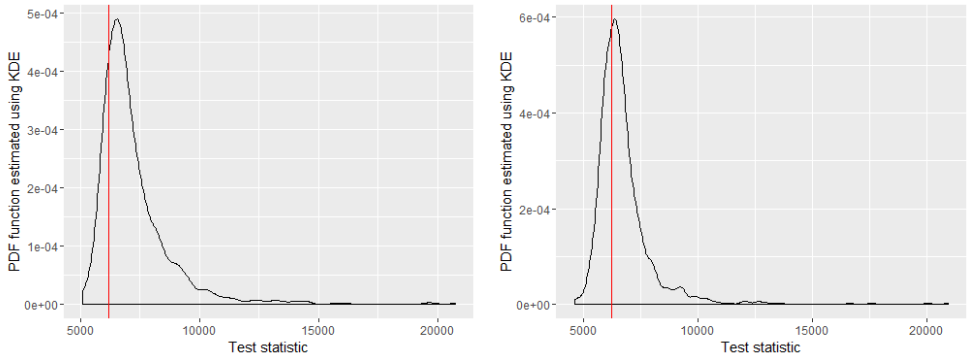
PPC to models which overfitted the mixture of random effects and also did not converge. Figure 5.5a to 5.5h show the distribution of the test statistic 4.21 for the various models we fitted to data set 6. It can be seen that the distribution is positively skewed whenever overfitting is present. On the other hand the distribution of the test statistic is more or less the same in cases of underfitting.

Table 5.9: PPP values for the various models fitted to data set 6.

# Components fitted	1	2	3	4	5	6	7	8
PPP Value	0.500	0.500	0.492	0.500	0.500	0.581	0.674	0.775

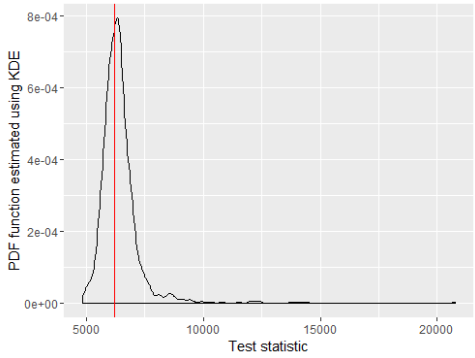
We also calculated posterior predictive p-values for the various number of components we fitted to data set 6. They are shown in Table 5.9. As one can see the PPP values are equal (0.5) for all the underfitted models. Based on the graphical PPC and these PPP values the choice between the underfitted models cannot be made. On the other hand for models with overfitted components, the PPP values increase as overfitting increases. It is important to note that while we looked for larger PPP-values to detect overfitting, it is also possible to obtain a small PPP-value indicating that the model is badly fitting in general.

We observed a more severe impact of overfitting when we used independent inverse gamma priors for the variance components of G_k and uniform prior $U(-1, 1)$ for correlation. To show the resulting distribution of the test statistic, we had to log transform it because otherwise the values were too large to be plotted in a single graph. For data set 2 we overfitted the mixture of random effects by using 4 components in the mixture. As shown in Figure 5.6a the test statistic is inflated by a large margin, which was also discussed in section 4.3. Interestingly when we fitted the right number of components the test statistic was not inflated, but as shown in Figure 5.6b the model is not fitting well to the data. The PPP-value we observed was 1. To diagnose this problem we checked the posteriors for variance covariance matrices and found them to be underestimating the sample data's variance covariance of the random effects. This indicated that the test statistic could be used to detect bad fitting models, however differentiating among models with less number of components might not be possible.

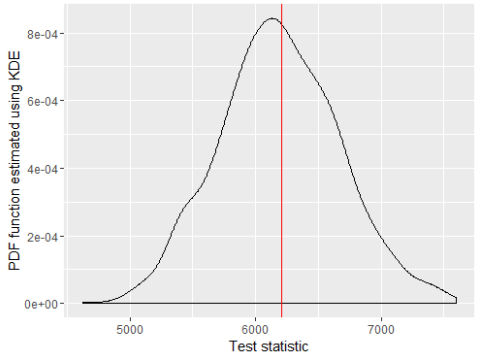


(a) # components fitted = 8

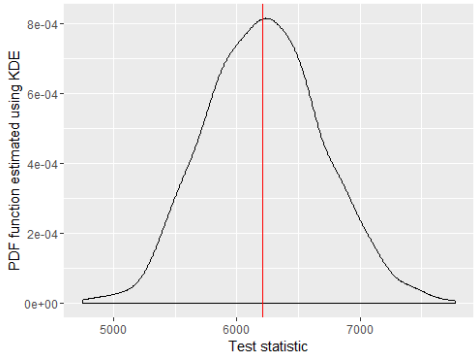
(b) # components fitted = 7



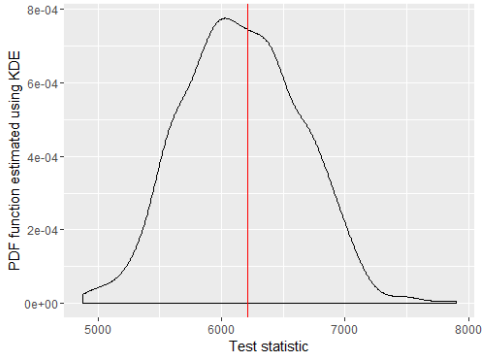
(c) # components fitted = 6



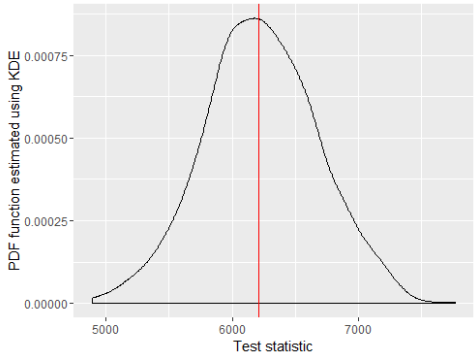
(d) # components fitted = 5



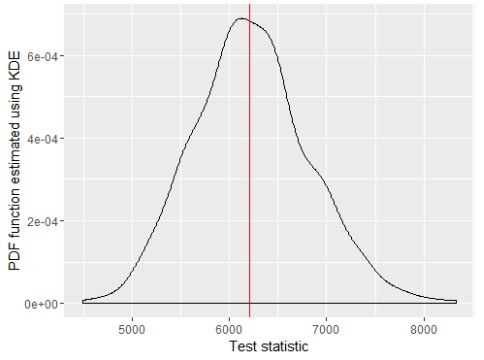
(e) # components fitted = 4



(f) # components fitted = 3

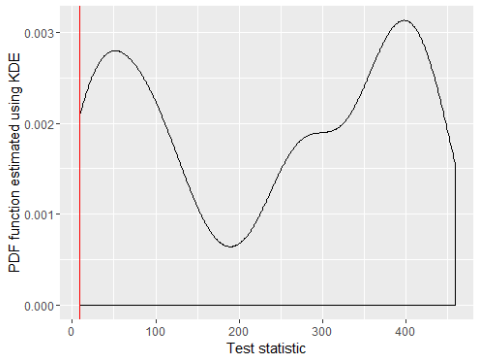


(g) # components fitted = 2

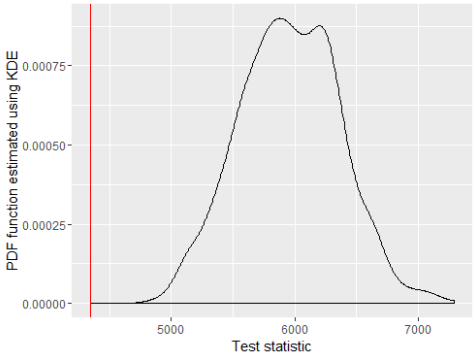


(h) # components fitted = 1

Figure 5.5: PDF function of $T(\tilde{\boldsymbol{r}})$ estimated using KDE. The red line shows the value of the test statistic $T(\boldsymbol{r})$ based on the observed data.



(a) 4 components fitted for data set 2. log scale is used.



(b) 3 components fitted for data set 2

Figure 5.6: PDF function of $T(\tilde{\boldsymbol{r}})$ estimated using KDE. The red line shows the value of the test statistic $T(\boldsymbol{r})$ based on the observed data. Independent gamma priors for precision and uniform prior for correlation is used.

Chapter 6

Analysis of blood donor data set

In this chapter we are presenting the analysis of the blood donor data set (Nasserinejad et al., 2015) using the Bayesian heterogeneity model. The data set consists of 1595 male blood donors who donated blood multiple times over a period of many years. On each occasion when they visited the donation center, the following information was noted: Season in which blood was donated (Cold/Hot), Volume of blood donated (ml), age at the time of donation (years), a binary indicator Donate (yes/no) specifying if the donor was allowed to donate the blood, Hemoglobin (Hb) of the patient at the time of donation, and the date of visit. Nasserinejad et al., (2013, 2015, 2016) have analyzed this data set extensively using transition models, mixed models, growth mixture models and latent class mixed effects transition models. The analysis was used to predict the Hb level of donors so that they are invited for donation at an optimal time, i.e. when their Hb levels are not too low because of the previous donations and other factors.

For the purpose of this thesis we did not use the entire data set of 1595 patients as Bayesian computation for heterogeneity model using the entire data set required large amount of computational resources. Instead we used a simple random sample of the data consisting of 250 subjects.

6.1 Motivation for analysis with Bayesian heterogeneity model

In the analysis using growth mixture models Nasserinejad et al., (2015) found 4 different underlying subpopulations in the data set. Firstly, those which had a relatively stable Hb level over donations. Secondly, those which had a higher Hb level than those in category 1 and showed a slow decline of Hb level over donations. Thirdly, those which showed a moderately sharp decline in Hb level over donations, and lastly those which showed a steep decline in Hb levels despite beginning at high initial Hb levels. Because of the presence of different subpopulations, a single methodology to decide the time of next blood donation for subjects from all subpopulations may not be effective. The aim of applying the Bayesian heterogeneity model to this dataset is to provide an alternative modeling framework for such data sets.

6.2 Frequentist analysis

We began with a frequentist analysis of the blood donor data set to select the right mean structure for our models ahead. This was necessary because omitting a required covariate in the mean structure can lead to incorrect estimates of the covariance matrix. Secondly, a frequentist analysis provided us good starting values for the various parameters in our model. Thirdly we could check if the Bayesian analysis results are consistent with the frequentist analysis results. For the random effects structure we considered a model with both random intercept and random

slope. For the choice of random slope we selected the number of donations in last 2 years as that was deemed as a suitable variable for random slope by Nasserinejad et al., (2015). For selecting the mean structure we did F-tests and likelihood ratio tests based on ML. We found the following mean structure to be suitable.

$$\begin{aligned} \boldsymbol{y}_{ij} = \beta_0 + \beta_1 * \text{Age}_{ij} + \beta_2 * \text{Season}_{ij} + \beta_3 * \text{Donate}_{ij} + \beta_4 * \text{TSPD}_{ij} \\ +\beta_4 * \#\text{donationLast2Years}_{ij} + \beta_5 * \#\text{donationLast2Years}_{ij} * \text{TSPD}_{ij} \\ +\beta_6 * \#\text{donationLast2Years}_{ij} * \text{Donate}_{ij} + \beta_7 * \#\text{donationLast2Years}_{ij}^2 \\ +b_0 + b_1 * \#\text{donationLast2Years}_{ij} + \varepsilon_{ij} \end{aligned} \tag{6.1}$$

where, Age and TSPD have been standardized to have mean 0 and variance 1, #donationLast2Years$_{ij}$ have been downscaled by a factor of 100 so that the random slope variance scale is upscaled. Similarly the intercept we used was 0.1, thus upscaling the random intercept variance. We will now present the fixed effect and random effect variance estimates of equation above. It is important to note that this model assumes a single multivariate normal distribution for the distribution of random effects.

Table 6.1: Table of frequentist fixed effects estimates for model 6.1

Effect (β)	Estimate	Standard Error
intercept	94.121	0.429
Age	-0.086	0.026
#donationLast2Years	-7.265	1.555
TSPD	-0.036	0.015
Season (Hot)	-0.080	0.016
Donate (TRUE)	0.155	0.037
#donationLast2Years * TSPD	0.020	0.006
#donationLast2Years * Donate	4.689	0.995
#donationLast2Years^2	-52.796	15.237

Cov Parm	Estimate
$G[1,1]$	19.971
$G[1,2]$	-14.266
$G[2,2]$	40.183
σ^2	0.201

6.3 Bayesian analysis

We next fitted the same model with Bayesian approach, although we also fitted mixtures with more number of components in the random effects. We first began with the approach in 5.1.1 to get a rough idea of the number of components. Figure 6.1 shows that there could be perhaps 1 component, or if there are more they have small number of subjects. Besides as we know these values overestimate the exact random effects thus if there are more than 1 component, we will have to use a slightly higher value for the hyperparameter of the Dirichlet prior in such case. We used Dir$(2, 2, ...2)$. Firstly in a mixture of only 1 component, i.e. no mixture case had the same mean value for fixed effect and random effect posterior distributions.

To do the Bayesian analysis we ran 150000 iterations with a thinning of 100 and burn-in of 25000 iterations. For chains with higher number of components we used 200000 iterations

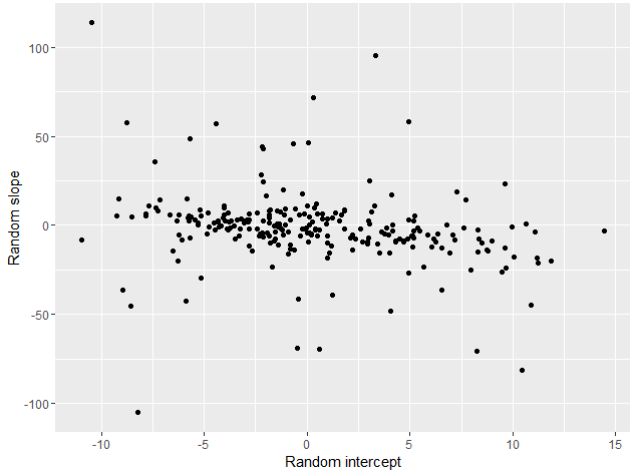


Figure 6.1: Rough estimate $\tilde{b_i}$ for random effects

with a thinning of 150. For each of the resulting MCMC chains we calculated the various definitions of definitions given in section 4.1, the results of which are presented in Table 6.2. In the simulation study we observed that DIC_4 was the most reliable of the DIC's and so we will discuss it first. It seems that there are not more than 2-3 components. The difference between DIC of mixture of 1 component and of 2 components is much larger than that between 2 and 3 components. To further verify this we used posterior predictive checks. However instead of randomly generating number of donations in last 2 years we sampled them from the subjects which were not considered for analysis due to computational restrictions. As shown in Figure 6.2c to 6.2e, it is clear that 3 or more components are an overfit. Secondly we can see that the posterior predictive distribution of the test statistic overlaps the distribution of test statistic with the sample data. Thus we will stick to the choice of 2 components.

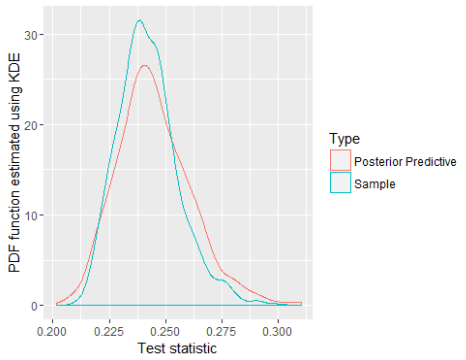
Table 6.2: DIC for blood donor data set

# Comp Fitted	DIC_1	DIC_2	DIC_3	DIC_4	DIC_5	DIC_6
1 comp	4817	4816	4818	7077	7532	4353
2 comp	4810	4804	4814	7040	7492	4339
3 comp	4744	4777	4814	7032	7458	4344
4 comp	4608	4723	4814	7031	7360	4332
5 comp	4461	4459	4818	7031	7108	4327

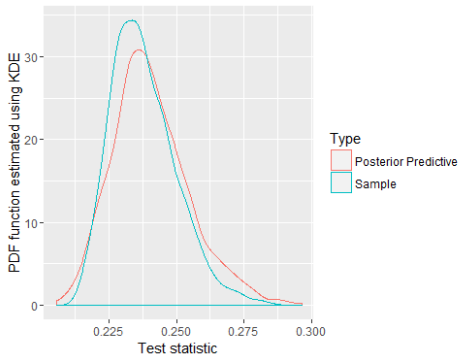
# Comp Fitted	p_{D_1}	p_{D_2}	p_{D_3}	p_{D_4}	p_{D_5}	p_{D_6}
1 comp	13	12	15	13	468	302
2 comp	17	11	21	19	471	281
3 comp	-48	-15	22	25	451	284
4 comp	-183	-67	23	30	360	272
5 comp	-334	-336	23	28	104	269

6.3.1 Parameter estimates

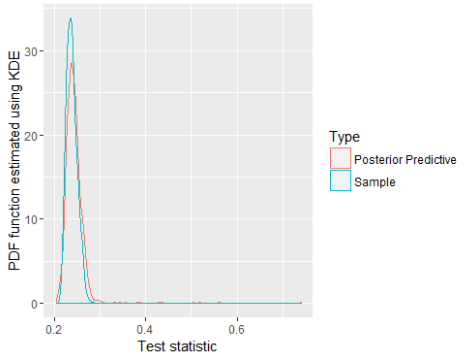
For the 2 components we will now present the summary of the parameter estimates. Firstly in Figure 6.3 we can see that the two components are equal in weight distribution. However



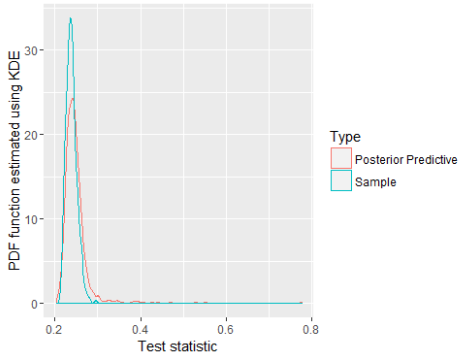
(a) 1 components fitted for blood donor data set



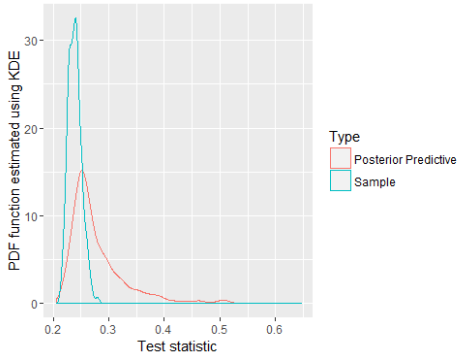
(b) 2 components fitted for blood donor data set



(c) 3 components fitted for blood donor data set



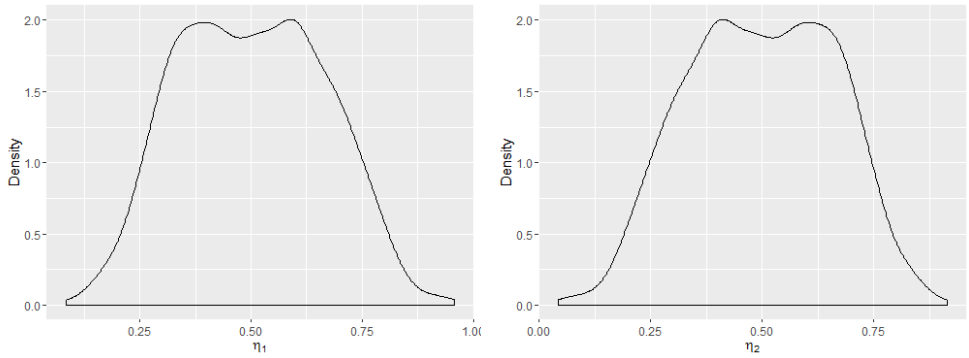
(d) 4 components fitted for blood donor data set



(e) 5 components fitted

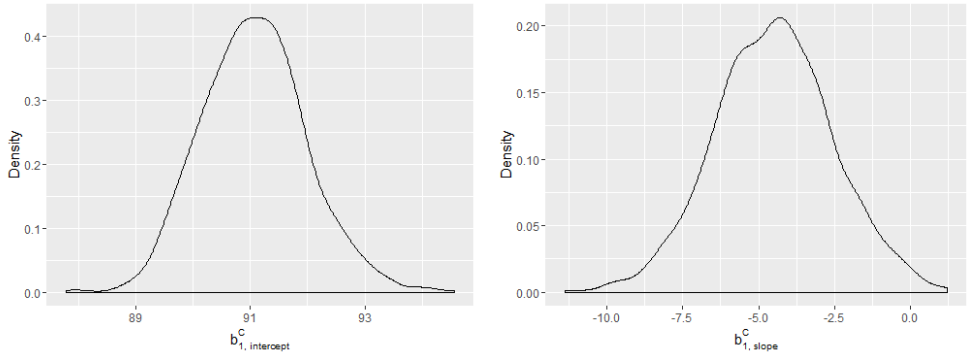
Figure 6.2: PDF function of $T(\tilde{\boldsymbol{r}})$ estimated using KDE for blood donor data set. The red line shows the value of the test statistic $T(\boldsymbol{r})$ based on the observed data.

the posterior of the weights is bimodal for both of them. Although this is usually a sign of label switching....hmm but my means don't seem to be having label switching. need to check this.

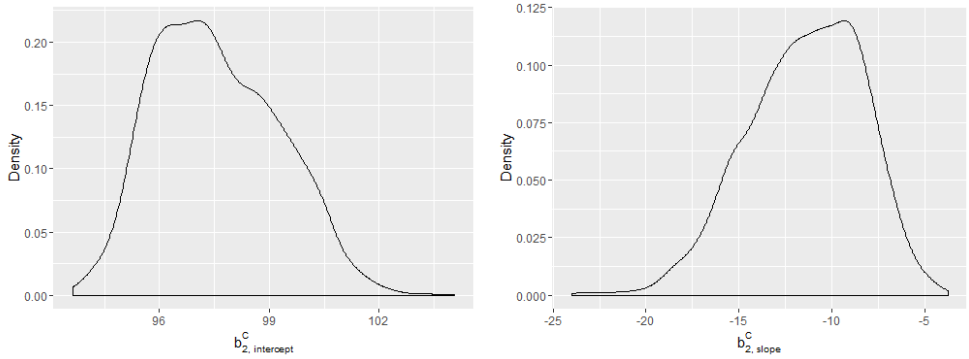


(a) Weight for the first component η_1 (b) Weight for the second component η_2

Figure 6.3: Weight distribution for the components of the mixture of random effects.

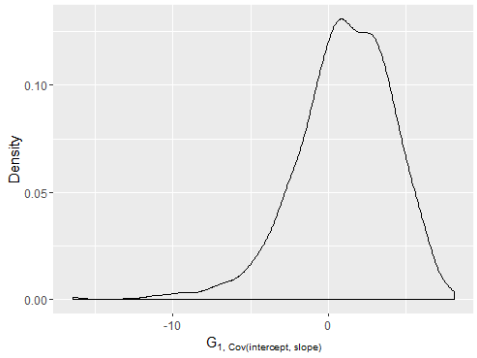


(a) Intercept location for the first component $b_{1,\text{intecept}}$ (b) Slope location for the first component $b_{1,\text{slope}}$

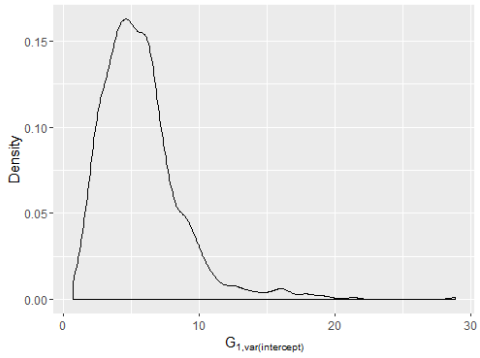


(c) Intercept location for the second component $b_{2,\text{intecept}}$ (d) Slope location for the second component $b_{2,\text{slope}}$

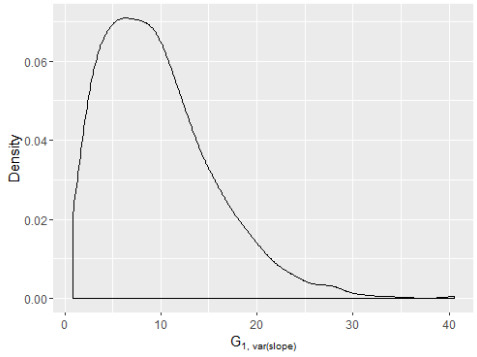
Figure 6.4: The location parameters for the components of the mixture of random effects.



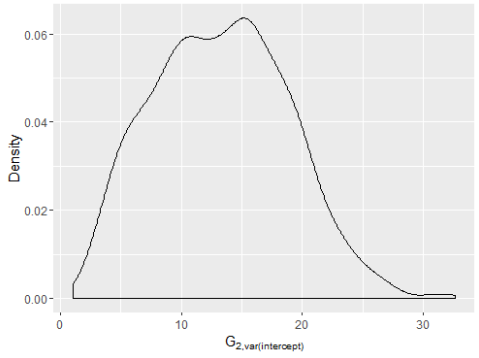
(a) Intercept variance for the first component



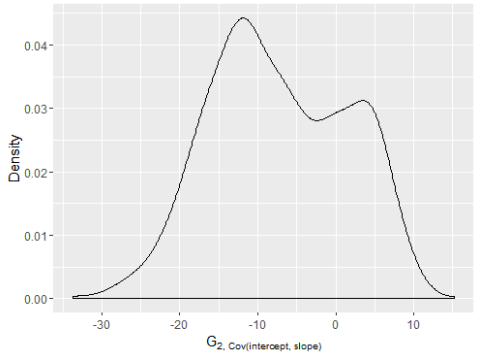
(b) Covariance between intercept and slope for the first component



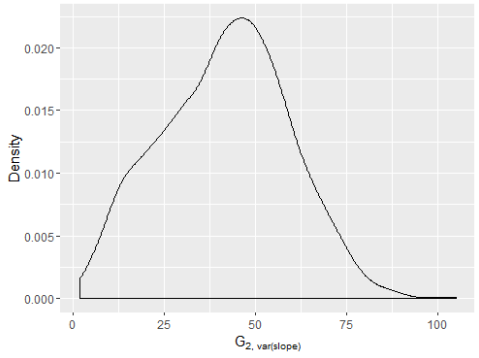
(c) Slope variance for the first component



(d) Intercept variance for the second component



(e) Covariance between intercept and slope for the second component



(f) Slope variance for the second component

Figure 6.5: The variance covariance parameters for the components of the mixture of random effects.

Chapter 7

Conclusion

As part of this thesis we evaluated the efficacy of DIC, Marginal likelihood and Posterior predictive checks for selecting the right number of components in the mixture distribution of random effects for a Bayesian heterogeneity model. We first gave the various definitions of DIC based on observed data likelihood, complete data likelihood and conditional data likelihood. We found that DIC_4 is the most reliable among the various definitions of the DIC's, which matches the findings of Celeux et al., (2006). The pattern we observed was that DIC_4 decreases by a large margin till the right number of components are fitted and then remains almost the same for overfitted models. However if the components are fused, or if the number of subjects are less one will see difference in DIC till right number of components is moderately large. DIC_3 performs similarly only when the components are well separated. Celeux et al., (2006) had also found DIC_3 to be the second most reliable DIC criteria. Lastly, we confirmed the suggestion of Frühwirth-Schnatter, (2013) that that in cases where components were not well separated and subjects were less, one may have to use a dirichlet prior with slightly large values for the hyperparameter to avoid non identifiability due to empy components. Applying DIC otherwise can lead to choosing less components than there are in reality.

Secondly, we found that Bayes Factor via Chib's approximation was not a reliable method to detect the number of components. It however still showed signs of rightly choosing the model with only 1 component in the mixture. We also found that one has to put constraints on the ordering of the components in the MCMC simulations, otherwise while doing chib's approximation one may get further MCMC chains with a different ordering of components. This can result into very large Bayes factor estimates.

Lastly, for posterior predictive checks we found that overfitting can be detected easily by exploiting non identifiability due to empty components. Empty components have posterior estimates sampled from the priors, thus giving estimates which do not support the data. However because these components have very small weights, a test statistic using information from all other components also supports the data at hand to some extent. One can still see a heavy tailed skewed distribution for test statistic though. If one doesn't follow the mixed predictive approach by Marshall and Spiegelhalter, (2003) then it can be difficult to detect overfitting/underfitting as full bayes estimates of the random effects are support the data well even when underfitting/overfitting is present. Even with the mixed predictive approach it is difficult to detect underfitting as all models give more or less the same fit to the data. Having said that in case the number of components are fitted correctly, but the posterior estimates are poor then the poor model fit can still be detected via PPC as we saw in the case of using uniform prior for correlation and indepdent gamma priors for precision of precision matrix of components.

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