Bayesian MCMC Approach in Prognostic Modelling of Cardiovascular Disease in Malaysia: A Convergence Diagnostic

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Abstract. Most studies that considered the Bayesian Markov Chain Monte Carlo (MCMC) approach in prognostic modelling of cardiovascular disease were only focused on the application of the Bayesian approach in variable selection, model, and prior distribution choice. Yet rarely of these studies have explored the convergence of Markov chains in the model. In this study, convergence diagnostics were performed using both visual inspection and other diagnostic to assess the convergence of Markov chains. This study analysed 7180 male patients with ST-Elevation Myocardial Infarction (STEMI) from the National Cardiovascular Disease Database-Acute Coronary Syndrome (NCVD-ACS) registry from 2006 to 2013. Six significant variables were identified in the multivariate Bayesian model, namely diabetes mellitus, family history of cardiovascular disease, chronic lung disease, renal disease, Killip class and age group. Based on these significant variables, the trace plots showed no particular patterns, and the model's MCMC mixing is generally good. As for the Gelman plots, almost all the parameters stabilise around a value of 1.0 for chain segments containing the 100,000 iterations and the chains are converging near the end of the sampling period. Also, the Gelman-Rubin diagnostic showed model convergence where all variables with estimated potential scale reduction factors (PSRF) were equal to 1.0. Concerning generic use of the MCMC approach, the application of a variety of plots and other diagnostic tool in this study indicated that the Markov chains have reached convergence.

Keywords: Bayesian · Cardiovascular · Convergence · Diagnostic · Markov chain

1 Introduction

The body text starts with a standard first-level The most prevalent cause of death worldwide is cardiovascular disease (CVD) [1]. Low and middle-income countries, such as

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Malaysia, account for more than three-quarters of deaths due to CVD [1, 2]. Coronary heart disease, cerebrovascular disease, peripheral arterial disease, rheumatic heart disease, and congenital heart disease are all types of heart and blood vessel issues that are referred to as CVD [1]. By 2030, it is anticipated that 23.6 million individuals will die from CVD [3].

Men having a higher risk of CVD than women and at a younger age [4]. Even more dreadful, men with CVD are more prone to develop ST-Elevation Myocardial Infarction (STEMI) which is the deadliest type of CVD [5, 6]. Often, there are no symptoms associated with the underlying blood vessel disease. A heart attack or stroke may be the initial indication of underlying disease [7]. Additionally, men may have breathing difficulty or breathlessness, nausea or vomiting, dizziness, or a chilly sweat and turning pale [8]. It is critical to identify risk factors for cardiovascular disease as early as feasible in order to initiate care with counselling and medication.

A Bayesian approach is used to detect the risk factor. This approach has gained popularity as a method for meta-analytic review of clinical information [9, 10]. Using Bayes' Theorem, prior knowledge (prior) and current knowledge (current) about a variable of interest can be formally combined in order to make future predictions (posterior) [11, 12]. To our knowledge, Bayesian models based on the MCMC method have not been extensively applied in Malaysia for the analysis of CVD data. On top of that, most of the Bayesian studies in the literature did not perform the convergence diagnostic to assess the Markov chains convergence.

The stopping criteria of how long a Markov chain simulation should be run and monitoring of chain convergence are the issues and considerations that need to be addressed in prognostic Bayesian model to ensure that researchers are sampling from a chain that has converged after a desired burn-in period [13, 14]. Therefore, the major purpose of this study after the risk factors has been identified is to look at the convergence of Markov chains in a Bayesian model of male patients in Malaysia who have been diagnosed with CVD. In this study, Markov chains convergence was monitored through visual inspection and other diagnostic such as Gelman-Rubin diagnostic.

The study is organised as follows: Sect. 1 commences with a brief background of CVD, the Bayesian approach and convergence diagnostics, followed by Sect. 2 with materials and methods. The results of the Bayesian model and convergence diagnostics are presented in Sect. 3, followed by a discussion of the findings of the analysis in Sect. 4. Finally, Sect. 5 has the conclusion.

2 Materials and Methods

2.1 Source of Data

Between 2006 and 2013, 7180 male patients diagnosed with ST-Elevation Myocardial Infarction (STEMI) were identified using the National Cardiovascular Disease Database-Acute Coronary Syndrome (NCVD-ACS) registry. From the moment a male STEMI patient was hospitalised to the hospital until 30 days after release, data were collected. Demographic, risk factor, comorbidity, clinical presentation, and treatment variables were classified. In terms of clinical presentation, the Killip classification predicts a

patient's chance of survival within 30 days, with Killip class IV patients having a greater chance of death [15].

2.2 Ethical Approval

The Medical Review & Ethics Committee (MREC) of Malaysia's Ministry of Health (MOH) approved this NCVD registry study. (Approval Code: NMRR-07-20-250). MREC waived informed consent for NCVD.

2.3 Statistical Methods

The data was split into training and test datasets in a 70:30 proportion. The training dataset was utilised to construct the model, while the test dataset was utilised to verify the model. Univariate logit models were designed for the Bayesian analysis to identify significant variables individually. The parameters' estimated posterior means were then obtained through the use of a multivariate model. A logistic regression model was applied to determine the likelihood of the outcome variable, with "1" reflecting death and "0" reflecting alive or otherwise. Due to the lack of details on the regression parameters, non-informative priors were used in this study. Bayesian model development generates the posterior distribution by multiplying the prior distribution by a likelihood function and then dividing it by the data distribution. This posterior distribution is used to construct all Bayesian inferences. As shown in Eq. (1), the posterior distribution is derived using Bayes' theorem.

$$p(\theta|y) = \frac{p(\theta)p(y|\theta)}{p(y)} \tag{1}$$

where y is the data point, θ some model parameter, $p(\theta)$ is the prior probability before knowing any information about y, $p(y|\theta)$ is the likelihood function that indicates the probability of observing y conditioned on θ, and $p(\theta|y)$ is the posterior probability after observing y. The posterior distribution is then estimated using the Markov chain Monte Carlo (MCMC) approach, which refers to algorithms for estimating and inferring model parameters that combine the Monte Carlo method and a mathematical random process known as Markov chains [16].

In this study, multiple parallel chains with distinct starting points were implemented using the Bayesian MCMC approach for all simulation work to monitor chains convergence. Model was developed at the univariate level by running the numerous chains for 10,000 iterations each [17–20] with a 1000 burn-in [17, 19, 20] to remove some of the effects of the parameter's starting values [21]. Simulator runs were set to 100,000 iterations at the multivariate level, with the first 10,000 burn-in samples excluded from the study [19, 20].

Samples from the posterior distribution are generated by MCMC, and to tell whether these samples are adequately near to the posterior to be applied for inference is part of the objectives. Model's Markov chains convergence can be monitored through estimated Monte Carlo (MC) error for the posterior means [22, 23]. MC error measures the variableness of each estimate produced by Markov chain simulation [13, 24]. Better accuracy

in parameter estimates when small values of MC errors are obtained [13, 25]. MC error value decreases as the number of iterations increase and should naturally be small [26]. In order to achieve model convergence MC error should be less than 5% of the posterior standard deviation [23, 27]. Thus, a very much smaller value of MC error is obtained.

Additionally, there are other two main ways to check for convergence, first is by using visual inspection and second is by performing other diagnostics. As for visual inspection there are trace and Gelman plots. In this study, other diagnostic such as the Gelman-Rubin diagnostic is performed.

Gelman-Rubin Diagnostic

Gelman-Rubin is a statistical test that determines whether there is a substantial variation in variance within and between several chains by referring to the potential scale reduction factors (PSRF) values [28]. In order to obtain the PSRF, the following steps are followed:

i) Using a variety of randomly generated starting values, chains, each of length are generated.
ii) The first n draws in each chain are discarded.
iii) The variance within and between chains are determined.
iv) The estimated variance of the parameter as a weighted sum of the within-chain and between-chain variance is calculated.
v) The PSRF or known as $\hat{R}$ is calculated.

The within chain variance, W is obtained by:

$$W = \frac{1}{m}\sum_{j=1}^{m} s_j^2 \tag{2}$$

where s_j^2 is the variance of the jth chain,
n is the number of iterations,
m is the number of chains,
θ_{ij} is the model parameter i in jth chain,
$\overline{\theta}_j$ is the sample posterior mean.
While the between chain variance, B is given by:

$$B = \frac{n}{m-1}\sum_{j=1}^{m} (\overline{\theta}_j - \overline{\theta})^2 \tag{3}$$

where $\overline{\theta} = \frac{1}{m}\sum_{j=1}^{m}\overline{\theta}_j$.
The estimated variance is given by the weighted average of W and B:

$$\hat{Var}(\theta) = \left(1 - \frac{1}{n}\right)W + \frac{1}{n}B \tag{4}$$

Finally, the PSRF is obtained by:

$$\text{PSRF} = \sqrt{\frac{\hat{Var}(\theta)}{W}} \tag{5}$$

3 Results

Although not displayed, the results of descriptive statistics for the training dataset, which included 5026 male patients, suggested that male patients of ethnic Malay accounted for more than 50% of all patients (59.3%). Male patients were overwhelmingly under the age of 65 (81.2%). With almost 75% of male patients, smoking was the most prominent risk factor. Myocardial infarction (MI) was the most frequently reported comorbidity (13.6%). On presentation, Killip I (66.9%) and Killip II (22.2%) were the most common diagnoses in male patients. Regarding treatment, the most often performed procedure was cardiac catheterisation (38.6%).

A variable is considered significant at the univariate level if the P-value for the likelihood ratio test is less than 0.25 and the 75% credible interval does not contain zero [19, 20]. The Bayesian univariate analysis revealed that nine out of the fifteen variables were significant. The nine significant variables were again integrated in a Bayesian multivariate analysis to determine prognostic factors. Table 1 showed the result of multivariate analysis of the Bayesian model. The posterior means were obtained after a burn-in period of 10,000 with Monte Carlo error less than 5% [23, 27]. Out of nine variables earlier, only diabetes mellitus, family history of CVD, chronic lung disease, renal disease, Killip class, and age group were discovered to be significant in the multivariate analysis.

Diabetic male patients had 1.61 times the chance of dying as non-diabetic male patients. Surprisingly, an odds ratio (OR) of 0.56 for family history of CVD revealed that patients with a family history of CVD had a 56% lower chance of dying than those who did not. With an odds ratio of 1.60, patients with chronic lung disease had a greater chance of dying. Meanwhile, patients in Killip class IV had an odds ratio of 18.0, which meant they had a greater chance of dying than those in Killip class I. Furthermore, patients with renal illness had a considerably greater mortality rate with OR 2.49 than those without it. Mortality risk was 2.42 times greater for male patients aged 65 and older than for those aged 65 and younger. When the model's findings are computed, the stationarity of the MCMC algorithm must be verified.

Both visual inspection and other diagnostic were displayed to illustrate the Markov chain convergence.

3.1 Visual Inspections

The visual inspections of Markov chains convergence for Bayesian model of male patients were performed using trace plot and Gelman plot. Figure 1 shows the trace plots of significant variables from the Bayesian multivariate analysis. The trace plots showed no particular patterns, and the MCMC mixing is generally good for Bayesian model of male patients. In Fig. 2, the median and 97.5% quantiles of the shrink factor sampling distribution are displayed versus the maximum iteration number using Gelman plots. To confirm that the chain has converged, both the median and 97.5% quantile must converge to a stable value. The plots shown that both the median and 97.5% quantile for almost all the parameters stabilize around a value of 1.0 for chain segments containing the 100,000 iterations and the chains are converging near the end of the sampling period.

Table 1. Results of Bayesian multivariate analysis of model for male patients.

Variable	Posterior Mean	SE	MC Error	OR (95% Credible Interval)
Diabetes Mellitus	0.477	0.011	0.00022	1.612 (1.254, 2.078)
Family history of CVD	−0.588	0.020	0.00038	0.555 (0.356, 0.845)
Chronic lung disease	0.471	0.029	0.0061	1.602 (1.239, 2.040)
Renal disease	0.910	0.021	0.00043	2.485 (1.538, 3.938)
Killip class II	0.779	0.013	0.00028	2.179 (1.556, 3.037)
Killip class III	2.134	0.019	0.00038	8.449 (5.456, 13.039)
Killip class IV	2.890	0.012	0.00027	17.993 (12.480, 24.661)
Age (≥65)	0.885	0.011	0.00023	(1.840, 3.189)

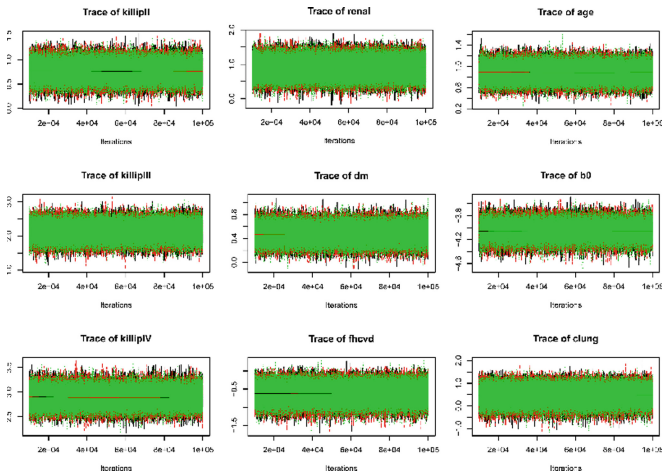

Fig. 1. Trace plots of Bayesian model for male patients.

3.2 Other Diagnostics

The Gelman-Rubin diagnostic in Table 2 showed models convergence for male where all variables with estimated PSRF were equal to 1.0. Multivariate PSRF that was proposed by Brooks and Gelman was also obtained with the value of 1.0 [29]. The changes of PSRF through the iterations can be seen using the previous Gelman plots in Fig. 2. These values suggest that the models have converged to the target posterior distribution as the PSRF is close to or equals to 1.

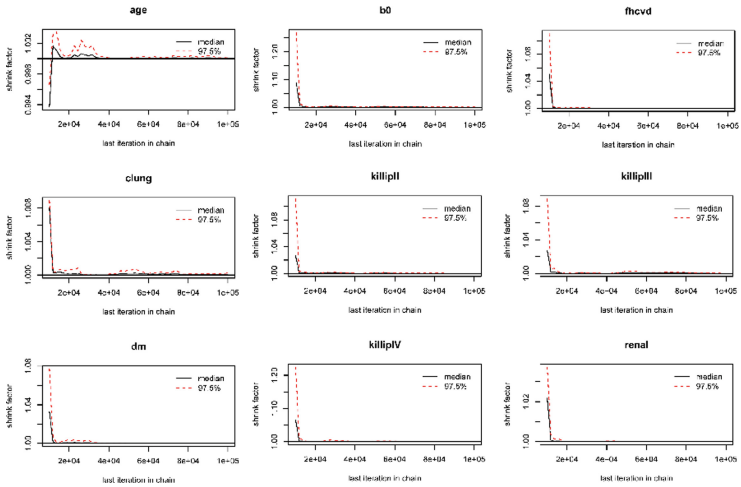

Fig. 2. Gelman plots of Bayesian model for male patients.

4 Discussion

In the development of prognostic Bayesian model, other than model building strategies and selection of prior [30, 31], the stopping criteria in terms of how long a Markov chain simulation should be run and chain convergence have also become important issues to be focused on [13, 14]. This study has demonstrated how both of the latter issues been assessed using CVD data of male patients in Malaysia. Six significant variables were found in the multivariate Bayesian model of male patients. Based on these significant variables, convergence was assessed.

In order to achieve model convergence, the number of iterations for an MCMC simulation should be as large as possible [32]. With the advancements in computing technology, iterations up to millions of runs are no longer considered impossible. In this study, 100,000 iterations with a burn-in of 10,000 were sufficient to achieve convergence, whereas other studies indicated that at least 1000 and up to a million iterations should be employed for estimation [17, 18].

Additionally, the number of chains must be considered. Geweke advocated for the use of a very long run on a single chain in order to discover novel posterior modes [33]. As in this study, multiple chains were used in the motivation of other study where multiple chains enable comparison of the chains' convergence, which is monitored using analysis of variance between and within the chains [28].

As stated earlier, in this study, Markov chains convergence was monitored through both visual inspection and other diagnostic such as Gelman-Rubin diagnostic. More than one convergence diagnostics were needed as there is no one complete test which gives the whole perspective of model convergence [14]. Additionally, each diagnostic looking at different perspective for example trace plot is used to look at the mixing of the Markov chain, while the Gelman plot illustrates the Gelman and Rubin's shrink factor evolution with increasing iterations [28].

Table 2. Gelman-Rubin diagnostic of Bayesian model for male patients

Variable	Potential scale reduction factors	
	Point est.	Upper CI
Diabetes Mellitus	1	1
Family history of CVD	1	1
Chronic lung disease	1	1
Renal disease	1	1
Killip class II	1	1
Killip class III	1	1
Killip class IV	1	1
Age (≥65)	1	1
Deviance	1	1
Multivariate PSRF: 1		

Moreover, by performing only visual inspection cannot strongly guarantee convergence. A primary reason that visual inspection alone cannot strongly ensure convergence is a phenomenon called metastability, in which the chain may abruptly migrate to another area of the parameter space after some period of stability around this value [34]. Thus, other diagnostic such as Gelman-Rubin diagnostic was needed in order to obtain robust conclusion on model convergence.

Convergence is most easily assessed by plotting and inspecting MCMC sample traces. A trace plot plots the number of iterations versus the value of the parameter's draw at each iteration. It is good to look at the trace-plots of the individual parameters. As in this study, all the six parameters including the intercept (*b0*) in Fig. 1 showed no particular patterns, and the MCMC mixing is generally good. If there is a strong correlation in parameter space, then the plot tends to get bad mixing [35].

While the Gelman plots in Fig. 2 showed the progression of Gelman and Rubin's shrink factor as the iterations number increases. The Markov chain is divided into bins. The Gelman-Rubin shrink factor is then computed on a repeated basis. By computing the shrink factor at numerous points in time, Gelman plots demonstrated whether the shrink factor has truly converged or is still fluctuating [29].

While in Table 2, the PSRF denoted an estimate of the factor that determines the magnitude of the current distribution relative to the target distribution, which could be reduced if the simulations were continued indefinitely. As the number of iterations approaches infinity, each PSRF decreases to 1. When there is approximate convergence, the PSRF is close to 1 [29]. In this study, a PSRF of 1 indicates that the variance between chains and within chains are equal. Otherwise, PSRF values greater than 1 indicate non-convergence [36]. A general goal is to achieve PSRF less than 1.10 [37].

5 Conclusion

In this study, the Markov chains convergence of a prognostic Bayesian model was monitored through both visual inspections, namely trace and Gelman plots, and other diagnostic such as the Gelman-Rubin diagnostic. Diabetes mellitus, family history of cardiovascular disease, chronic lung disease, renal disease, Killip class, and age group were identified as important variables in this prognostic Bayesian model of CVD male patients. The findings of the convergence diagnostics in this study illustrated that for the trace plots there were no specific patterns based on these significant variables, and the MCMC mixing seems to be favourable for the model. In terms of the Gelman plots, practically all of the parameters for chain segments containing 100,000 iterations settle around 1.0, and the chains are converging near the end of the sampling period. In addition, when all variables with an estimated PSRF were equal to 1.0, the Gelman-Rubin diagnostic confirmed model convergence. Thus, the convergence diagnostics are required to ensure that researchers are sampling from a chain that has converged after a desired burn-in period.

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