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Evaluating MCMC Convergence in a Bayesian Model of ST-Elevation Myocardial Infarction Female Patients in Malaysia

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ABSTRACT

The majority of research that looked at the Bayesian Markov Chain Monte Carlo (MCMC) approach for prognostic modelling of cardiovascular disease only focused on the use of the Bayesian approach in variable selection, model selection, and prior distribution selection. But very few of this research has looked at the Markov chains' convergence in the model. In this study, convergence diagnostics were carried out to evaluate the convergence of Markov chains using both visual inspection and additional diagnostics. The National Cardiovascular Disease Database-Acute Coronary Syndrome (NCVD-ACS) registry, which included 1248 female patients with ST-Elevation Myocardial Infarction (STEMI) between 2006 and 2013, was used for this study's analysis. The multivariate Bayesian model identified six significant variables: dyslipidaemia, myocardial infarction, smoking, renal disease, Killip class, and age group. The trace plots did not reveal any distinctive patterns based on these significant variables, and the model's MCMC mixing is typically good. While for the autocorrelation plots, mild autocorrelations for age group, Killip IV, as well as the intercept term in the model. Since there were only mild autocorrelations, no thinning is needed. Also, the Geweke diagnostic showed that the chain is divided into two windows containing a set fraction of the first and last iterations which produced standard Z-scores. The Geweke diagnostic did not provide evidence of non-convergence, as none of the Z-scores fell in the extreme tails of the N (0,1). In this study, a number of plots and additional diagnostic tools showed that the Markov chains have reached convergence, which is relevant to the general use of the MCMC approach.

Keywords:
Bayesian; Convergence; Diagnostic; Markov chain; ST-Elevation Myocardial Infarction

1. Introduction

Cardiovascular disease (CVD) is the main cause of death worldwide; an estimated 17.9 million people die from cardiovascular diseases (CVD) every year, and one-third of these deaths happen before the age of 70 [1–3]. In Malaysia alone, the leading cause of mortality is still CVD [4]. In comparison to the neighboring countries, Malaysians are developing CVD at a younger age, according to the National Cardiovascular Disease-Acute Coronary Syndrome Registry [5]. STEMI is the most

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lethal form of acute coronary syndrome; hence, it was chosen for this study [6]. Although STEMI is frequently assumed to affect men, it can also have an impact on women [7].

In comparison to male patients, female CVD patients, particularly STEMI, are understudied, poorly treated, and result in worse outcomes [7,8]. What's worse is that females have a lower survival rate following a STEMI than males do [9]. The pathophysiology, clinical presentation, and management outcomes are different for females, which is part of the reason for this, but there are other wider social and economic issues in society that have a significant impact on clinical outcomes [7,9,10].

Furthermore, there is inadequate representation of females in clinical trials, inadequate understanding of the mechanisms behind STEMI, and potentially significant sex-specific treatments. In addition, due to the index event bias, females with STEMI may have a poorer prognosis than males in the index episode, but they may appear to be "protected" in the event of a recurring episode [10]. For STEMI patients, it is essential to identify risk factors as soon as possible in order to commence treatment, counselling, and medication.

To identify the risk factor, a Bayesian approach is applied. This approach has grown in favor of a way to do a meta-analysis of medical data [11,12]. It is feasible to directly combine prior knowledge (prior) and current knowledge (current) about a particular variable in order to generate future predictions (posterior) using Bayes' Theorem [13,14]. This theorem provides a mathematical method to adjust the likelihood of a hypothesis based on new data or information, allowing a flexible and thorough framework for study.

Within the realm of medical research, this entails the incorporation of previous studies, expert viewpoints, and recently obtained data to enhance the accuracy and dependability of the conclusions. The Bayesian technique can enhance the evaluation of a novel treatment by incorporating previous clinical trials and expert consensus, in addition to fresh trial data, to improve the accuracy of estimations of treatment effectiveness [11]. This iterative procedure not only strengthens the reliability of the analysis but also enables ongoing updates when new data becomes available, rendering it especially valuable in the constantly evolving domain of medical research [13].

As far as we have noticed, Malaysia has not utilized Bayesian models based on the Markov Chain Monte Carlo (MCMC) approach widely for the analysis of CVD data. Additionally, the majority of Bayesian studies in the literature didn't employ convergence diagnostic to assess the Markov chains' convergence. In order to ensure that researchers are sampling from a chain that has converged after a desired burn-in period, prognostic Bayesian models must take into account stopping criteria for how long a Markov chain simulation should be run as well as monitoring of chain convergence [15,16]. Thus, the main objective of this study is to examine the convergence of Markov chains in a Bayesian model of female patients in Malaysia who has been diagnosed with CVD after the risk factors have been discovered. In this study, the convergence of the Markov chains was monitored using visual inspection and additional diagnostics such as the Geweke diagnostic.

2. Methodology

2.1 Source of Data

The National Cardiovascular Disease Database-Acute Coronary Syndrome (NCVD-ACS) registry was used to identify 1248 female patients with ST-Elevation Myocardial Infarction (STEMI) between 2006 and 2013. Data were gathered from the time a female STEMI patient was admitted to the hospital until 30 days following discharge. Variables related to demographics, risk factors, comorbidities, clinical presentations, and treatments were categorized. The Killip classification,

based on clinical presentation, forecasts a patient's likelihood of surviving within 30 days, with Killip class IV patients having a higher risk of dying [17].

2.2 Statistical Methods

The data has been divided into training and test datasets in a 70:30 proportion. The test dataset was used to validate the model after it had been built using the training dataset. Univariate logit models were built for the Bayesian analysis to determine significant variables individually. A multivariate model was then used to obtain the estimated posterior means for the parameters. With "1" denoting death and "0" denoting alive or otherwise, a logistic regression model was implemented to estimate the likelihood of the outcome variable. Non-informative priors were used in this study as the regression parameters' descriptions were insufficient. The posterior distribution is generated by Bayesian model development by multiplying the prior distribution by a likelihood function and dividing the result by the data distribution. This posterior distribution is then used to develop all Bayesian inferences. Eq. (1) demonstrates how Bayes' theorem is used to derive the posterior distribution 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.

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

The MCMC approach is then used to estimate the posterior distribution. MCMC refers to algorithms for estimating and inferring model parameters that combine the Monte Carlo method and a mathematical random process known as Markov chains [18].

For all simulation work in this study, multiple parallel chains with different starting points were implemented using the Bayesian MCMC approach to monitor chain convergence. At the univariate level, numerous chains were run for 10,000 iterations each [19,20] with a burn-in of 1000 [6,19] to mitigate some of the effects of the parameter's initial values. The multivariate simulation runs were set to 100,000 iterations, with the first 10,000 burn-in samples excluded from the study [6,21].

By using MCMC, samples from the posterior distribution are produced, and one of the objectives is to determine whether these samples are sufficiently close to the posterior to be used for inference. The estimated Monte Carlo (MC) error for the posterior means can be used to monitor the convergence of the model's Markov chains [22,23]. The variability of each estimate generated by a Markov chain simulation is measured by the MC error [24]. When lower values of MC errors obtain, the parameter estimates are more accurate [15,25]. As the number of iterations increases, the MC error value decreases and ought to be small [26]. The MC error must be smaller than 5% of the posterior standard deviation to ensure model convergence [23,27]. Therefore, a very much smaller value of MC error is obtained.

Furthermore, there are two other main methods for determining convergence: visual inspection and additional diagnostics. There are trace and autocorrelation plots for visual inspection. Additional diagnostics such as the Geweke diagnostic are also carried out in this study.

2.2.1 Visual Inspection

The most basic approach to evaluate convergence is to simply plot and look at the traces of the observed MCMC sample. A trace plot is a plot of the iteration number against the value of the draw of the parameter at each iteration. Viewing the trace plots of the individual parameters is an excellent

concept. The plot has a tendency to develop poor mixing if there is a strong association in the parameter space [15,28].

While the autocorrelation plot shows the first several lag-autocorrelations for each parameter in each chain and the degree of association between MCMC samples with various lags between them. The level of correlation between each MCMC sample and itself, for instance, is represented by a lag of 0. The iterative samples are regarded as independent and the Markov chains as convergent if the autocorrelation levels among them fall to zero after some finite lags [29].

2.2.2 Geweke Diagnostic

The Geweke diagnostic examines the first and last non-overlapping parts of the Markov chain and compares their means, using a difference of means test to determine whether the two parts of the chain are drawn from the same distribution. The test statistic is a standard *Z*-score with autocorrelation-adjusted standard errors. According to Geweke (1992), the Geweke diagnostic did not provide indications of non-convergence if none of the *Z*-scores fall in the extreme tails *N* (0,1) [30]. The statistic which this diagnostic is based is given by

$$Z = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{\hat{S}_1(0)/n_1 + \hat{S}_2(0)/n_2}} \quad (2)$$

where $\overline{x}_1$ is the sample mean in an early segment of the chain, $\overline{x}_2$ is the sample mean in a later segment and the variance estimate $\widehat{S}(0)$ is calculated as the spectral density at frequency zero to account for serial correlation in the sampler output.

3. Results

Descriptive statistics for the training dataset, which comprised 1248 STEMI female patients, revealed that female patients of ethnic Malay made up more than 50% of all patients (55.9%), even though they were not displayed. The majority (56.6%) of female patients were under the age of 65. The most frequent risk factor for STEMI in female patients was hypertension (74.5%) [31], followed by diabetes mellitus (55.6%) and dyslipidemia (35.8%), respectively. The most prevalent comorbidity was myocardial infarction (MI), which was followed by renal disease and cerebrovascular disease. Killip I (59.6%) and Killip II (25.1%) were the most common diagnoses in female patients at the time of presentation. Treatment-wise, cardiac catheterization (34.4%) was the most often performed procedure which similar with the results from the previous study [32,33], followed by percutaneous coronary intervention (PCI) (28%).

Table 1 shows the results of univariate analysis of the Bayesian model for female patients. If the *p*-value for the likelihood ratio test is less than 0.25 and the 75% credible interval of the posterior mean does not contain zero, a variable is deemed significant at the univariate level [6,21]. Seven of the fifteen variables were significant namely dyslipidemia, family history of CVD, MI history, smoking status, renal illness, Killip class, and age group of the patients, according to the Bayesian univariate analysis in Table 1.

Table 1
Results of univariate analysis of the Bayesian model

Variable	Characteristic	Posterior mean (75% Credible Interval)	Odds ratio (OR)	*p*-value
Ethnicity	Chinese	0.216 (-0.060, 0.495)	1.241	
	Indian	-0.244 (-0.539, 0.087)	0.783	0.389
	Others	-0.679 (-1.226, 0.181)	0.507	
Age group	Age (≥65)	1.039 (0.791, 1.273)	2.826	<0.001
Diabetes Mellitus	Yes	0.166 (-0.068, 0.400)	1.181	0.400
Hypertension	Yes	0.252 (-0.037, 0.516)	1.287	0.258
Smoking status	Yes	-0.672 (-1.410, -0.057)	0.511	0.132
Dyslipidemia	Yes	-0.482 (-0.728, -0.215)	0.618	0.02
Family history of CVD	Yes	-0.779 (-1.206, -0.202)	0.459	0.082
MI history	Yes	0.642 (0.329, 0.974)	1.900	0.018
Chronic lung disease	Yes	0.580 (-0.240, 1.263)	1.786	0.424
Cerebrovascular disease	Yes	-0.168 (-0.687, 0.565)	0.845	0.890
Peripheral vascular disease	Yes	-0.947 (-1.103, -0.105)	0.391	0.458
Renal disease	Yes	1.147 (0.757, 1.560)	3.165	<0.001
Killip class	Killip class II	0.881 (0.584, 1.191)	2.413	
	Killip class III	1.474 (1.042, 1.958)	4.367	<0.001
	Killip class IV	2.646 (2.321, 2.953)	14.100	
PCI	Yes	-0.069 (-0.321, 0.197)	0.933	0.792
Cardiac catheterization	Yes	-0.123 (-0.363, 0.129)	0.884	0.530

To identify prognostic indicators, the seven significant variables were once again incorporated into a Bayesian multivariate analysis. The Bayesian model's multivariate analysis generates the results shown in Table 2. After a burn-in period of 10,000, the posterior means were determined with a Monte Carlo error of less than 5%. Only six of the seven initial variables, namely dyslipidemia, MI, smoking, renal illness, Killip class, and age group of the patients, were shown to be statistically significant in the multivariate analysis.

Female patients with dyslipidemia had a lower mortality risk (OR = 0.53). While female patients with a history of MI were 1.88 times more likely to die than those without. Unexpectedly, patients who smoked had a lower mortality rate than non-smokers (OR = 0.40). Renal disease increased the risk of death by 2.29 times compared to those without it. Patients in Killip class IV had a 16.54 times higher mortality rate than those in Killip class I, as was expected. Additionally, the risk of death was three times higher for female patients from the age group ≥ 65 than those from the age group < 65. The stationarity of the MCMC algorithm needs to be validated when the model's results are generated. The Markov chain convergence was demonstrated using both visual inspection and additional diagnostics.

Table 2
Results of multivariate analysis of the Bayesian model

Variable	Posterior mean	SE	MC error	OR (95% Credible Interval)
Dyslipidaemia	-0.638	0.044	0.00077	0.528 (0.312, 0.861)
MI history	0.631	0.048	0.00043	1.879 (1.024, 2.984)
Smoking	-0.911	0.081	0.00054	0.402 (0.124, 0.972)
Renal disease	0.829	0.072	0.00057	2.291 (1.051, 3.923)
Killip class II	0.860	0.049	0.00070	2.363 (1.369, 2.975)
Killip class III	1.141	0.077	0.00072	3.130 (1.254, 7.283)
Killip class IV	2.806	0.050	0.00069	16.544 (12.247, 20.992)
Age (≥ 65)	1.101	0.040	0.00044	3.007 (1.862, 4.688)

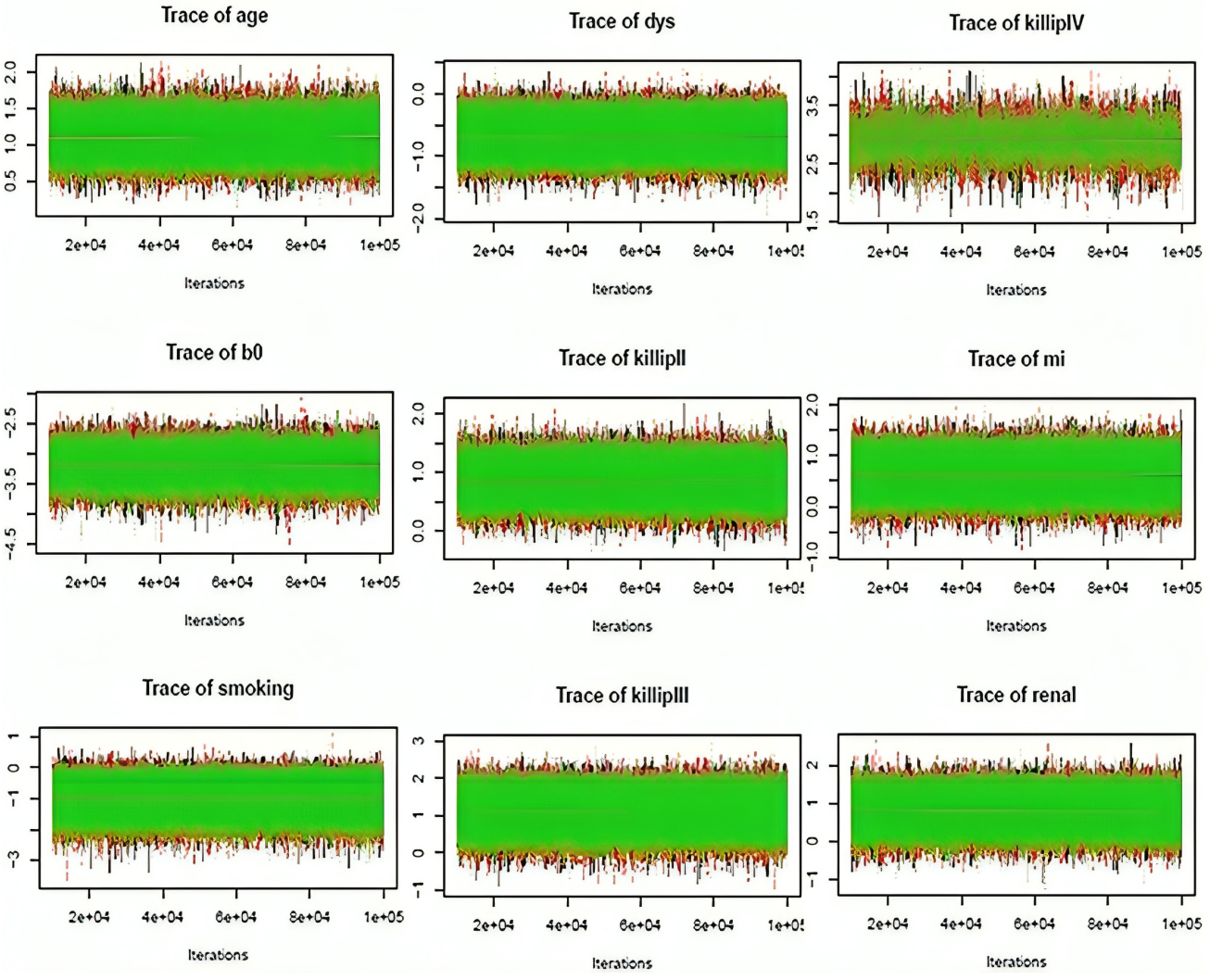

Fig. 1. Trace plots of the Bayesian model

3.1 Visual Inspections

The visual inspections of Markov chains convergence for the Bayesian model of female patients were performed using trace plots and autocorrelation plots. Figure 1 shows the trace plots of significant variables from the Bayesian multivariate analysis. The trace plots show no specific trends, and the mixing of MCMC tends to be good for the Bayesian model of female patients. Figure 2 showed that the autocorrelation levels among variables fall to zero after some finite lags which indicates the convergence of the Markov chains. Moreover, Figure 2 suggests mild autocorrelations for the age group, Killip IV as well as the intercept term in the Bayesian model for female patients. Since there were only mild autocorrelations, no thinning is needed.

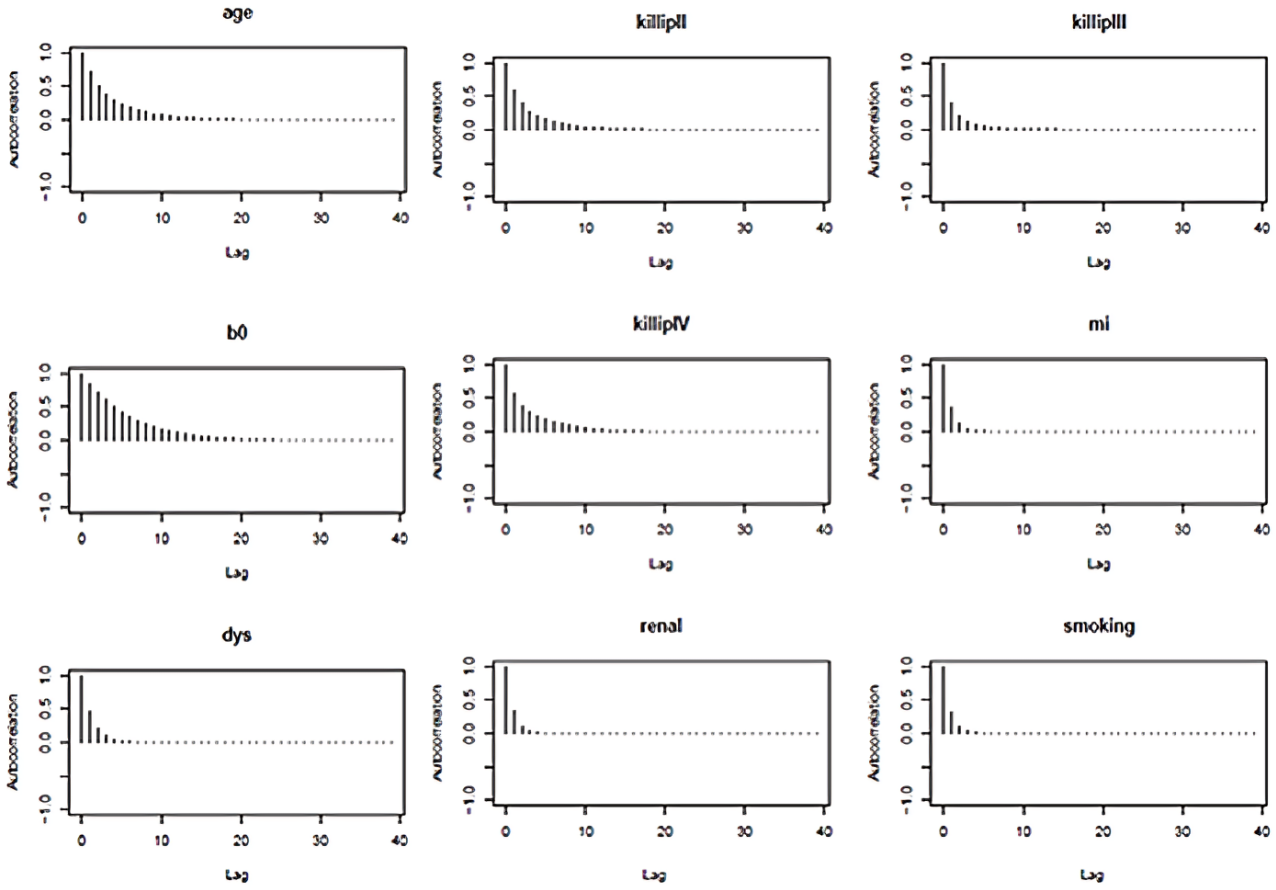

Fig. 2. Autocorrelation plots of the Bayesian model

3.2 Additional Diagnostics

The Geweke diagnostic test from Table 3 showed that the chain is divided into two windows containing a set fraction of the first and last iterations, which produced standard Z-scores. Since the statistic is only applicable to a single chain, the test was applied separately to each of the three chains. The Geweke diagnostic did not provide evidence of non-convergence, as none of the Z-scores fell in the extreme tails of the N (0,1).

Table 3
Geweke diagnostic of the Bayesian model

Variable	*Z*-scores		
	Chain 1	**Chain 2**	**Chain 3**
Intercept	-0.1115	0.8412	-0.5679
Dyslipidaemia	1.1277	-0.4595	-0.2875
MI history	-0.9045	-0.2918	-0.1747
Smoking	-0.5304	-1.346	-1.1230
Renal disease	2.4484	0.2209	1.6134
Killip class II	0.1099	-0.5830	-0.2436
Killip class III	1.2203	-0.4922	-0.2293
Killip class IV	-0.8977	-0.2538	0.5114
Age (≥ 65)	0.5981	-0.9824	1.8316

Fraction in 1st window = 0.1 Fraction in 2nd window = 0.5

4. Discussion

In addition to model-building methods and prior selection [34,35], additional important aspects in the development of prognostic Bayesian models include stopping criteria for Markov chain simulations and chain convergence [15,16]. This study has shown how the latter two aspects were evaluated using CVD data from Malaysian female patients. The multivariate Bayesian model of female patients revealed six significant variables. Convergence was then assessed based on these significant variables. The maximum number of iterations for an MCMC simulation should be used to achieve model convergence [36]. Since computing technology has evolved, iterations up to millions of runs are no longer seen as impossible. While other research suggested that at least 1000 and up to a million iterations should be used for estimation, in this study, 100,000 iterations with a burn-in of 10,000 were adequate to achieve convergence [20].

The number of chains must also be taken into account. In order to find novel posterior modes, Geweke suggested using a very long run on a single chain [30]. Similar to other studies, this study also used numerous chains to compare the chains' convergence, which was monitored using analysis of variance both within and between the chains [37]. As previously mentioned, the convergence of the Markov chains was monitored in this study using both visual inspection and additional diagnostics like the Geweke diagnostic. As there is no single comprehensive test that provides the full perspective of model convergence, a number of convergence diagnostics were required [16]. Furthermore, each diagnostic assesses the convergence from a different perspective. For instance, the trace plot examines the mixing of the Markov chain, whereas the autocorrelation plot shows the first several lag-autocorrelations for each parameter in each chain [34].

Furthermore, convergence cannot be firmly verified by completing a visual inspection alone. A phenomenon known as metastability, in which the chain may unexpectedly migrate to another part of the parameter space after some period of stability around this value, is a major reason why visual inspection alone cannot firmly verify convergence [35]. Therefore, additional diagnostics, such as the Geweke diagnostic, were required to reach a reliable convergence conclusion. Plotting and examining MCMC sample traces make it the easiest to determine convergence. An iteration count versus the value of the parameter's draw at each iteration is plotted on a trace plot. Viewing the trace plots of the individual parameters is an appealing concept. All six parameters, including the intercept (b0) in Figure 1, did not show any distinctive patterns in this study, and the MCMC mixing was typically good.

The plot has a tendency to have poor mixing if there is a strong correlation in the parameter space [35]. Similarly, the autocorrelation plots showed mild autocorrelations for certain variables in the model.

Table 3 compares the means of the first 10% of the chain and the latter 50% of the chain using the Geweke diagnostic. Stationary time series are particular types of MCMC procedures. Geweke (1992) therefore proposed a spectral density convergence diagnostic based on the spectral density for time series. According to the Geweke diagnostic, two subsequences' measurements in a convergent chain should be equal [38]. Geweke diagnostic does not require the sampler output to be assumed to be normally distributed [30]. Regardless of the underlying distribution, the limiting distribution of the test statistic is standard normal. When Z is large ($|Z| > 1.96$) the null hypothesis of equal location that predicts convergence is rejected [38]. The algorithm demonstrates that Geweke diagnostic places more emphasis on testing stationary than mixing. The notion that the two subsequences are asymptotically independent is one that underlies Geweke diagnostic. The first 10% and the last 50% were therefore recommended [30].

5. Conclusion

In this study, visual inspections, such as trace and autocorrelation plots, and additional diagnostics, including the Geweke diagnostic, were used to access the Markov chains convergence of a prognostic Bayesian model. In this prognostic Bayesian model of STEMI female patients, dyslipidemia, myocardial infarction, smoking, renal disease, Killip class, and age group were found to be significant variables. The results of the convergence diagnostics in this study showed that the model's MCMC mixing is normally good and that the trace plots did not show any distinctive patterns based on these significant variables. Mild autocorrelations for age group, Killip IV, and the intercept term in the model are shown in the autocorrelation plots. No thinning is required since there were only mild autocorrelations. The Geweke diagnostic also revealed that the chain is split into two windows that each contain a particular proportion of the first and last iterations, which resulted in standard Z-scores. Since none of the Z-scores fell in the extreme tails of the N (0,1), the Geweke diagnostic did not reveal signs of non-convergence. Plots and additional diagnostic tools used in this study demonstrated that the Markov chains have reached convergence, which is relevant to the general use of the MCMC approach.

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