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Accepted Manuscript Version

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Publisher: Cogent OA

Journal: *Cogent Mathematics*

DOI: <http://doi.org/10.1080/23311835.2017.1421003>

Goodness of fit test for higher-order Binary Markov chain models

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Abstract

When the interest is in making statements about change based on repeated measurements of discrete data, one way to do so is by using Markov chain models. Goodness of fit is an important test for finding a good model that can be used for analyzing any underlying patterns and relationships in repeatedly measured data. To test for various associations in the models, the Likelihood Ratio and Wald tests were used. However, efficient score tests can also provide equally good tests and are easier alternatives. In this paper, we proposed an extension of Tsiatis' method for goodness of fit test on higher-order binary Markov chains. We applied Tsiatis' goodness of fit test in logistic regression models. The new method proposed in this paper was applied to real life data to examine the suitability of this technique.

1 Introduction

Markov chain models are used in various applied fields, such as time series analysis, longitudinal studies, life data, and environmental problems. The behavior of a Markov chain depends on the transition matrix, which contains transitional probabilities. In most practical studies, the transition matrix is unknown and needs to be estimated. Several methods are available for the estimation and test procedure of transition probabilities. However, most researchers have worked primarily on the estimation of parameters and only a few reports on test procedures. One of the most important tests on Markov chain models is the stationarity of transition probabilities and the goodness of fit of Markov chain models. This section presents a brief summary of the tests performed on Markov chain.

Anderson and Goodman (1957) obtained the maximum likelihood estimates and their asymptotic distribution for the transition probabilities in a Markov chain of arbitrary order with repeated observations of the chain. The likelihood ratio tests and chi-square tests used in contingency tables were obtained for testing these hypotheses. Billingsley (1961) used Whittle's formula, chi-square, and maximum likelihood methods to test for stationarity and order of the higher-order Markov chain. McQueen and Thorley (1991) used Markov chain to analyze annual stock returns. Albert (1994) proposed a class of Markov models for analyzing sequences of ordinal data from a relapsing-remitting disease, where the state space was expanded to include information about the ordinal severity score as well as the relapsing-remitting status. He proposed a parameterization that can reduce the number of parameters. It is noteworthy that most of these research works have been conducted for estimating parameters based on the first-order Markov chain. Recently, several new methods for higher-order Markov chains have been reported, where the estimation and test procedures became

quite complex due to the increased order of the models (Islam et al., 2006, 2008, 2012; Chowdhury et al., 2005; Rahman and Islam, 2007).

However, less effort is given towards studying the field of covariate-dependent Markov models (Muenz and Rubinstein, 1985; Yi et al., 2009). In this paper, a test procedure for the goodness of fit of a binary Markov chain model is proposed by extending Tsiatis' procedure (Tsiatis, 1980). The proposed test was extended for the second and higher-order of the Markov chain model. The efficient score test was used for testing null hypotheses, which only required the estimate of parameters under true null hypothesis. The proposed model and test procedures were thoroughly examined using a set of data for the elderly population and employing simulations.

Sirdari et al. (2012) proposed the goodness of fit test for higher-order binary Markov chain models based on marginal distribution. The problem with this proposal was that marginal distribution has limited assumptions because of the correlations between variables, which are not easy to estimate. Thus, the proposed model in this study was based on the conditional transition probabilities, which means that there is no correlation between variables.

2 A brief overview of the test proposed by Tsiatis (1980)

Tsiatis (1980) proposed a goodness of fit test for the logistic regression model. In terms of binary data analysis, this model relates the probability of a response to a set of covariates (χ_1, \dots, χ_p) according to Equation (2.1):

$$\log\{p_x/(1 - p_x)\} = \boldsymbol{\beta}'\boldsymbol{\chi}, \quad p_z = \frac{\exp(\boldsymbol{\beta}'\boldsymbol{\chi})}{\{1 + \exp(\boldsymbol{\beta}'\boldsymbol{\chi})\}} \quad (2.1)$$

where, $p_{\mathbf{x}}$ denotes the conditional probability of response given by the vector, $\mathbf{x} =$

(χ_1, \dots, χ_p) , $\chi_0 = 1$, and $\boldsymbol{\beta}' = (\beta_0, \dots, \beta_p)$ denotes the regression coefficients. The space of

covariates (χ_1, \dots, χ_p) is partitioned into k distinct region in p -dimensional space, denoted by

R_1, \dots, R_k . The indicator functions, $\mathbf{I}^{(j)}$ ($j = 1, \dots, k$), are defined by $\mathbf{I}^{(j)} = 1$ if $(\chi_1, \dots, \chi_p) \in R_j$ and $\mathbf{I}^{(j)} = 0$.

Tsiatis considered the following model in Equation (2.2):

$$\log\{p_{\mathbf{x}}/(1 - p_{\mathbf{x}})\} = \boldsymbol{\beta}'\mathbf{x} + \boldsymbol{\gamma}'\mathbf{I}, \quad (2.2)$$

where, $\mathbf{I}' = (I^{(1)}, \dots, I^{(k)})$ and $\boldsymbol{\gamma}' = (\gamma_1, \dots, \gamma_k)$. The goodness of fit test consists of testing the hypothesis $H_0: \gamma_1 = \dots = \gamma_k = 0$.

This test is based on the efficient score test, as represented by Equation 2.3:

$$T = \mathbf{Z}'\mathbf{V}^{-1}\mathbf{Z}, \quad (2.3)$$

where, \mathbf{Z}' is the k -dimensional vector $(\partial l/\partial \gamma_1, \dots, \partial l/\partial \gamma_k)$ and l denotes the log-likelihood.

The $k \times k$ matrix, \mathbf{V} is equal to:

$$\mathbf{V} = \mathbf{A} - \mathbf{BC}^{-1}\mathbf{B}',$$

where,

$$A_{jj'} = -\partial^2 l/\partial \gamma_j \partial \gamma_{j'} \quad (j, j' = 1, \dots, k),$$

$$B_{jj'} = -\partial^2 l/\partial \gamma_j \partial \beta_{j'} \quad (j = 1, \dots, k; j' = 0, \dots, p),$$

$$C_{jj'} = -\partial^2 l/\partial \beta_j \partial \beta_{j'} \quad (j, j' = 0, \dots, p)$$

All previous terms were evaluated at $\boldsymbol{\gamma} = 0$ and $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}$, where $\hat{\boldsymbol{\beta}}$ is the maximum likelihood estimate of the parameters when H_0 is true.

3 Goodness of fit test of first-order Markov chains

Consider the case of a single stationary process, (Y_1, \dots, Y_T) , generated by a binary Markov chain that uses values of 0 and 1. The transition matrix is defined by,

$$\mathbf{P} = \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} = \begin{bmatrix} 1 - p_{01} & p_{01} \\ 1 - p_{11} & p_{11} \end{bmatrix}$$

where $p_{jt} = \Pr(Y_t = 1 | Y_{t-1} = j); j = 0, 1, t = 1, \dots, T$.

The transition probabilities, p_{jt} , can be modeled using logistic regression, as shown by Model (3.1):

$$\text{logit}(p_{jt}) = \boldsymbol{\beta}_j' \boldsymbol{\chi}_t, \quad p_{jt} = \frac{\exp(\boldsymbol{\beta}_j' \boldsymbol{\chi}_t)}{1 + \exp(\boldsymbol{\beta}_j' \boldsymbol{\chi}_t)}. \quad (3.1)$$

Vector $\boldsymbol{\chi}_t$ contains covariates and it is equal to $\boldsymbol{\chi}_t = (1, \chi_{t1}, \dots, \chi_{tp})$. $\boldsymbol{\beta}_j$ is the vector of parameters, $\boldsymbol{\beta}_j = (\beta_{j0}, \beta_{j1}, \dots, \beta_{jp})$. The likelihood function that corresponds to Model (3.1) is:

$$L = \prod_t \prod_{j=0}^1 (1 - p_{jt})^{n_{j0t}} p_{jt}^{n_{j1t}}$$

where, n_{00t} , n_{01t} , n_{10t} , and n_{11t} are the number of transitions of each type observed at time t . The log-likelihood is as shown by Equation (3.2):

$$l = \sum_{t=1}^T \sum_{j=0}^1 \{n_{j1t} \boldsymbol{\beta}_j' \boldsymbol{\chi}_t - (n_{j0t} + n_{j1t}) \ln [1 + \exp(\boldsymbol{\beta}_j' \boldsymbol{\chi}_t)]\}. \quad (3.2)$$

The log-likelihood can be shown as, $l = \ln L = \ln L_0 + \ln L_1$, where,

$$\ln L_0 = \sum_{t=1}^T \{n_{01t} \boldsymbol{\beta}_0' \boldsymbol{\chi}_t - (n_{00t} + n_{01t}) \ln [1 + \exp(\boldsymbol{\beta}_0' \boldsymbol{\chi}_t)]\},$$

$$\ln L_1 = \sum_{t=1}^T \{n_{11t} \boldsymbol{\beta}_1' \boldsymbol{\chi}_t - (n_{10t} + n_{11t}) \ln [1 + \exp(\boldsymbol{\beta}_1' \boldsymbol{\chi}_t)]\}.$$

It was assumed that the space of covariate $(\chi_{t1}, \dots, \chi_{tp})$ was partitioned into G distinct regions in p -dimensional space, denoted by R_1, \dots, R_G . The indicator functions, $I_t^{(k)}$ ($k = 1, \dots, G$), are defined by $I_t^{(k)} = 1$ if $(\chi_{t1}, \dots, \chi_{tp}) \in R_k$ and $I_t^{(k)} = 0$.

Then, for a binary Markov chain, the following Model (3.3) was considered:

$$\text{logit}(p_{jt}) = \boldsymbol{\beta}_j' \boldsymbol{\chi}_t + \boldsymbol{\gamma}_j' \boldsymbol{I}_t, \quad (3.3)$$

where $\boldsymbol{I}_t = (I_t^{(1)}, \dots, I_t^{(G)})$ and $\boldsymbol{\gamma}_j = (\gamma_{j1}, \dots, \gamma_{jG})$ is an arbitrary covariate vector. This test was performed by testing the null hypothesis, $H_0: \gamma_{j1} = \dots = \gamma_{jG} = 0$. This hypothesis was proposed by partitioning the space of covariates into distinct regions and calculating a test statistic, which was a quadratic form of the observed counts, excluding the expected counts.

The efficient score test and the likelihood ratio test were also used. Both statistics have asymptotic chi-square distribution, with G degrees of freedom, as proven by Rao (1973). The current test used in this study was based on the efficient score test because it only requires an estimate of $\boldsymbol{\beta}_j$ under the null hypothesis, whereas the likelihood ratio statistics needs an estimate of $\boldsymbol{\gamma}_j$ under the alternative model. The test statistics is defined by Equation (3.4):

$$T = \boldsymbol{Z}' \boldsymbol{V}^{-1} \boldsymbol{Z}, \quad (3.4)$$

where, $\boldsymbol{Z}' = (\boldsymbol{Z}'_0 \quad \boldsymbol{Z}'_1)$ and $\boldsymbol{Z}'_j, j = 0, 1$ is the G -dimensional vector

$(\partial l / \partial \gamma_{j1}, \dots, \partial l / \partial \gamma_{jG})$. The matrix, \boldsymbol{V} , is equal to:

$$\boldsymbol{V} = \begin{pmatrix} \boldsymbol{V}_0 & 0 \\ 0 & \boldsymbol{V}_1 \end{pmatrix}$$

and the $G \times G$ matrix, $\boldsymbol{V}_j, j = 0, 1$

$$\boldsymbol{V}_j = \boldsymbol{A}_j - \boldsymbol{B}_j \boldsymbol{C}_j^{-1} \boldsymbol{B}_j'$$

where,

$$A_{jkk'} = -\partial^2 l / \partial \gamma_{jk} \partial \gamma_{jk'} \quad (k, k' = 1, \dots, G),$$

$$B_{jkk'} = -\partial^2 l / \partial \gamma_{jk} \partial \beta_{jk'} \quad (k = 1, \dots, G; k' = 0, \dots, p),$$

$$C_{jkk'} = -\partial^2 l / \partial \beta_{jk} \partial \beta_{jk'} \quad (k, k' = 0, \dots, p).$$

All previous terms were evaluated at $\boldsymbol{\gamma}_j = 0$ and $\boldsymbol{\beta}_j = \hat{\boldsymbol{\beta}}_j$, where $\hat{\boldsymbol{\beta}}_j$ is the maximum likelihood estimate of the parameters when H_0 is true. By using the standard likelihood theory, a test could be extracted in the quadratic form of observed counts minus expected counts, and whose large sample properties are easily established.

It is evident that the log-likelihood for Model (3.3) can be achieved by inserting Equation (3.2), as follows:

$$\begin{aligned} l &= \sum_{t=1}^T \sum_{j=0}^1 [n_{j1t} (\boldsymbol{\beta}'_j \boldsymbol{\chi}_t + \boldsymbol{\gamma}'_j \boldsymbol{I}_t) - (n_{j0t} + n_{j1t}) \ln \{1 + \exp(\boldsymbol{\beta}'_j \boldsymbol{\chi}_t + \boldsymbol{\gamma}'_j \boldsymbol{I}_t)\}] \\ &= \ln L_0 + \ln L_1 = l_0 + l_1. \end{aligned}$$

The k th element of vector $\boldsymbol{\chi}_t$ used in the computation of Equation (3.4) is the partial derivative of $l_j, j = 0, 1$, with respect to γ_{jk} at $\boldsymbol{\gamma}_j = 0$ and $\boldsymbol{\beta}_j = \hat{\boldsymbol{\beta}}_j$,

$$\sum_{t=1}^T n_{j1t} I_t^{(k)} - \sum_{t=1}^T (n_{j0t} + n_{j1t}) I_t^{(k)} \left[\frac{\exp(\boldsymbol{\beta}'_j \boldsymbol{\chi}_t)}{1 + \exp(\boldsymbol{\beta}'_j \boldsymbol{\chi}_t)} \right] = O_{jk} - E_{jk},$$

where, O_{jk} and E_{jk} are the observed and expected numbers of responses in the k th region. Therefore, Equation (3.4) is the quadratic form of the vector of observed counts minus expected counts.

Quantities necessary for computing the covariance matrix, $\boldsymbol{V}_j, j = 0, 1$ are as follows:

$$A_{jkk'} = \begin{cases} \sum_{\xi_k} (n_{j0t} + n_{j1t}) \hat{p}_{jt} (1 - \hat{p}_{jt}) & k = k' \\ 0 & k \neq k'; k, k' = 1, \dots, G \end{cases}$$

$$B_{jkk'} = \sum_{\xi_k} (n_{j0t} + n_{j1t}) \chi_{tk'} \hat{p}_{jt} (1 - \hat{p}_{jt}) \quad (k = 1, \dots, G; k' = 0, \dots, p),$$

$$C_{jkk'} = \sum_{t=1}^T (n_{j0t} + n_{j1t}) \chi_{tk} \chi_{tk'} \hat{p}_{jt} (1 - \hat{p}_{jt}) \quad (k, k' = 0, \dots, p),$$

where, ξ_k denotes the set of indices t , such that

$$(\chi_{t1}, \dots, \chi_{tp}) \in R_k, \quad \hat{p}_{jt} = \exp(\hat{\beta}'_j \chi_t) / \{1 + \exp(\hat{\beta}'_j \chi_t)\}.$$

4 Extension of the model for higher-order Markov chains

Consider the n th-order Markov model for times, $t - n, t - (n - 1), \dots, t - 1$, and t , with transition matrix, \mathbf{P} , and its components:

$$p_{r \dots s j t} = \Pr(Y_t = 1 \mid Y_{t-n} = r, \dots, Y_{t-2} = s, Y_{t-1} = j); j, s, r = 0, 1, t = 1, \dots, T.$$

The logistic regression model for $p_{r \dots s j t}$ is:

$$\text{logit}(p_{r \dots s j t}) = \beta_{r \dots s j} \chi_t, \quad p_{r \dots s j t} = \frac{\exp(\beta_{r \dots s j} \chi_t)}{1 + \exp(\beta_{r \dots s j} \chi_t)},$$

where vector, $\chi_t = (1, x_{t1}, \dots, x_{tp})$, contains covariates and $\beta_{l \dots s j} =$

$(\beta_{r \dots s j 0}, \beta_{r \dots s j 1}, \dots, \beta_{r \dots s j p})$ is the vector of parameters.

The likelihood function corresponding to this model is as follows:

$$L = \prod_{t=1}^T \prod_{j=0}^1 \prod_{s=0}^1 \dots \prod_{r=0}^1 (1 - p_{r \dots s j t})^{n_{r \dots s j 0t}} p_{r \dots s j t}^{n_{r \dots s j 1t}}$$

The log-likelihood is:

$$l = \sum_{t=1}^T \sum_{j=0}^1 \sum_{s=0}^1 \dots \sum_{r=0}^1 \{n_{r \dots s j 1t} \beta_{r \dots s j} \chi_t - (n_{r \dots s j 0t} + n_{r \dots s j 1t}) \ln [1 + \exp(\beta_{r \dots s j} \chi_t)]\}$$

$$= \sum_{r,s,j=0}^1 \ln L_{r\dots sj},$$

where for $r,s,j = 0, 1$,

$$\ln L_{r\dots sj} = \sum_{t=1}^T \left\{ n_{r\dots sj1t} \boldsymbol{\beta}_{r\dots sj}' \boldsymbol{\chi}_t - (n_{r\dots sj0t} + n_{r\dots sj1t}) \ln [1 + \exp(\boldsymbol{\beta}_{r\dots sj}' \boldsymbol{\chi}_t)] \right\}.$$

Then, Model (3.3) can be extended for order n , which can be written as shown by Equation (4.1):

$$\log it(p_{r\dots sjt}) = \boldsymbol{\beta}_{r\dots sj}' \boldsymbol{\chi}_t + \boldsymbol{\gamma}_{r\dots sj}' \boldsymbol{I}_t; \quad r, s, j = 0, 1. \quad (4.1)$$

The related null hypothesis is $H_0: \gamma_{r\dots sj1} = \dots = \gamma_{r\dots sjG} = 0$, and the test statistic is shown by Equation (4.2):

$$T = \boldsymbol{Z}' \boldsymbol{V}^{-1} \boldsymbol{Z}, \quad (4.2)$$

where, \boldsymbol{Z} is a 2^n -dimensional vector with elements of:

$$\boldsymbol{z}_{r\dots sj}' = \left(\frac{\partial l}{\partial \gamma_{r\dots sj1}}, \dots, \frac{\partial l}{\partial \gamma_{r\dots sjG}} \right), \quad r, s, j = 0, 1.$$

The matrix, \boldsymbol{V} is the $2^n \times 2^n$ diagonal matrix, with components of $G \times G$ matrix. $\boldsymbol{V}_{r\dots sj}$; $r, s, j = 0, 1$;

$$\boldsymbol{V}_{r\dots sj} = \boldsymbol{A}_{r\dots sj} - \boldsymbol{B}_{r\dots sj} \boldsymbol{C}_{r\dots sj}^{-1} \boldsymbol{B}_{r\dots sj}'$$

where,

$$\boldsymbol{A}_{r\dots sjkk'} = -\frac{\partial^2 l}{\partial \gamma_{r\dots sjk} \partial \gamma_{r\dots sjk'}} \quad (k, k' = 1, \dots, G),$$

$$\boldsymbol{B}_{r\dots sjkk'} = -\frac{\partial^2 l}{\partial \gamma_{r\dots sjk} \partial \beta_{r\dots sjk'}} \quad (k = 1, \dots, G; k' = 0, \dots, p),$$

$$\boldsymbol{C}_{r\dots sjkk'} = -\frac{\partial^2 l}{\partial \beta_{r\dots sjk} \partial \beta_{r\dots sjk'}} \quad (k, k' = 0, \dots, p), \quad (r, s, j = 0, 1).$$

The log-likelihood based on Model (4.1) is as follows:

$$\begin{aligned}
l &= \sum_{t=1}^T \sum_{j=0}^1 \sum_{s=0}^1 \cdots \sum_{r=0}^1 \{n_{r\dots sj1t}(\boldsymbol{\beta}_{r\dots sj}\boldsymbol{\chi}_t + \boldsymbol{\gamma}_{r\dots sj}\mathbf{I}_t) - (n_{r\dots sj0t} + n_{r\dots sj1t})\ln[1 + \exp(\boldsymbol{\beta}_{r\dots sj}\boldsymbol{\chi}_t + \boldsymbol{\gamma}_{r\dots sj}\mathbf{I}_t)]\} \\
&= \sum_{r,s,j=0}^1 \ln L_{r\dots sj} = \sum_{r,s,j=0}^1 l_{r\dots sj}
\end{aligned}$$

The partial derivative of $l_{r\dots sj}$, $l, s, j = 0, 1$ with respect to $\gamma_{r\dots sjk}$, $r, s, j = 0, 1$ at

$$\boldsymbol{\gamma}_{r\dots sj} = \mathbf{0} \text{ and } \boldsymbol{\beta}_{r\dots sj} = \hat{\boldsymbol{\beta}}_{r\dots sj},$$

$$\sum_{i=1}^n n_{r\dots sj1t} I_t^{(k)} - \sum_{i=1}^n (n_{r\dots sj0t} + n_{r\dots sj1t}) I_t^{(k)} \left[\frac{\exp(\boldsymbol{\beta}_{r\dots sj}\boldsymbol{\chi}_t)}{\{1 + \exp(\boldsymbol{\beta}_{r\dots sj}\boldsymbol{\chi}_t)\}} \right] = O_{r\dots sjk} - E_{r\dots sjk}.$$

5 Application

We applied the proposed test on the Health and Retirement Study (HRS) data to demonstrate its application. This is a longitudinal household survey dataset for the study of retirement and health among the elderly in the United States. The RAND Centre collected these data to study aging, with funding and support from the National Institute on Aging (NIA) and the Social Security Administration (SSA). These data were collected from 1992 to 2006 in 8 waves for 30,405 people. We considered individuals who attended the program in 1992 and then, followed up until 2006. The study was about depression among individuals (0 for no depression and 1 for depression), and age (yearly), gender (0 for male and 1 for female), body mass index (BMI), and drinking (0 for not drinking and 1 for drinking), which were considered as covariates. The space of covariate $(\chi_{t1}, \dots, \chi_{tp})$ was partitioned into four distinct regions: (male and not drinking); (male and drinking); (female and not drinking); and

(female and drinking). Some of these variables may contain missing values because the referenced person did not respond to the waves. Thus, we had to drop the ID of individuals from all waves if there were missing values for these covariates. There were 668 missing values in the covariates, which included 353 IDs, i.e., these individuals responded for the outcome variable, but not for the covariates. Thus, 353 IDs were dropped from the data in this work. Additionally, S-Plus functions modified by Chowdhury et al. (2005) were developed and used to estimate the parameters of the model. The Newton-Raphson method was used in this program for parameter estimation.

Table 1 shows the different types of transition counts for the first- and second-order transitions. Meanwhile, Table 2 shows the estimated values for the covariate-dependent Markov models for different types of transitions. The results are for the first- and second-order Markov models.

Billingsley's chi-square statistics were computed by using $\sum_{ij} (f_{ij} - f_i p_{ij})^2 / (f_i p_{ij})$, and Tsiatis' statistics were estimated using Equations (3.4) and (4.2). The results showed that the data satisfied the models for the first- and second-order Markov chains. Both Billingsley's and Tsiatis' statistics showed similar results. However, Billingsley's test statistics does not depend on covariates. Thus, it was used in this study to compare the results with results of the extended test based on Tsiatis' statistics.

Table 1: Transition counts of Markov chain of depression data for the first- and second-order

| Transition time | | | t | |
|-----------------|---------|---------|------|------|
| First order | $t - 1$ | | 0 | 1 |
| | 0 | | 3951 | 1455 |
| | 1 | | 1930 | 257 |
| Second order | $t - 2$ | $t - 1$ | t | |
| | 0 | 0 | 3473 | 1396 |
| | 1 | 0 | 680 | 221 |
| | 0 | 1 | 269 | 29 |
| | 1 | 1 | 568 | 151 |

Estimates of the parameters for the first-order transitions demonstrated negative association between the transitions from no depression to depression with age and drinking, while positive associations were obtained with BMI and sex (females have higher risks). Those who did not change their status from depression were found to be associated negatively with age and positively with drinking. Both the Billingsley and the proposed tests showed that the first-order models can be accepted. Similarly, the second-order models indicated that age and drinking were negatively associated, while sex was positively associated for the 0-0-1 type of transition. Sex and BMI were positively associated and drinking was negatively associated for the 1-0-1 transition type, while age was negatively associated, but drinking was positively associated for the 1-1-1 transition type. Interestingly, the second-order models also appeared to have good fit in favor of the null hypothesis. These results demonstrated that both the first- and second-order models could be employed for the given set of data.

Table 2: Estimates of parameters of covariate-dependent first- and second-order Markov models and testing the goodness of fit.

| First-order | | | | |
|--------------------------|------------|-----------------|-------------------|---------|
| Transition type | Covariates | Estimated value | s.e. | p-value |
| 0→1 | Constant | 4.631 | 0.349 | 0.000 |
| | Age | -0.096 | 0.005 | 0.000 |
| | Sex | 0.129 | 0.066 | 0.051 |
| | BMI | 0.011 | 0.006 | 0.078 |
| | Drinking | -0.215 | 0.066 | 0.0011 |
| 1→1 | Constant | 8.378 | 0.825 | 0.000 |
| | Age | -0.118 | 0.012 | 0.000 |
| | Sex | 0.019 | 0.148 | 0.896 |
| | BMI | 0.007 | 0.012 | 0.577 |
| | Drinking | 0.552 | 0.148 | 0.0002 |
| Billingsley's chi-square | | 3.94E-13 | (p-value=0.999) | |
| Proposed test statistics | | 1.207 | (p-value=0.997) | |
| Second-order | | | | |
| Transition type | Covariate | Estimated value | s.e. | p-value |
| 0→0→1 | Constant | 4.360 | 0.385 | 0.000 |
| | Age | -0.090 | 0.005 | 0.000 |
| | Sex | 0.224 | 0.068 | 0.0011 |
| | BMI | 0.009 | 0.006 | 0.153 |
| | Drinking | -0.282 | 0.067 | 0.0003 |
| 1→0→1 | Constant | -2.996 | 0.999 | 0.003 |
| | Age | 0.020 | 0.015 | 0.178 |
| | Sex | 0.335 | 0.174 | 0.053 |
| | BMI | 0.026 | 0.016 | 0.104 |
| | Drinking | -0.278 | 0.160 | 0.082 |
| 0→1→1 | Constant | 2.261 | 2.250 | 0.315 |
| | Age | 0.006 | 0.034 | 0.870 |
| | Sex | 0.195 | 0.423 | 0.646 |
| | BMI | -0.015 | 0.036 | 0.682 |
| | Drinking | -0.101 | 0.410 | 0.805 |
| 1→1→1 | Constant | 9.295 | 1.217 | 0.000 |
| | Age | -0.142 | 0.019 | 0.000 |
| | Sex | 0.026 | 0.220 | 0.907 |
| | BMI | 0.007 | 0.015 | 0.670 |
| | Drinking | 0.513 | 0.222 | 0.021 |
| Billingsley's chi-square | | 2.13E-08 | (p-value=0.999) | |
| Proposed test statistics | | 2.057 | (p-value=0.999) | |

6 Simulation

Data generated by the techniques provided by Ghosh and Mukerjee (2001), and Leisch et al. (1998), were used to examine the suitability of the proposed models. In these techniques, bindata package in R were employed for generating correlated binary data. First, data were generated from the multivariate normal random variables, and then, they were transformed into binary data. In this study, two variables were generated as the outcome variables at time t and $t - 1$ for the first-order Markov model, with various combinations of probabilities of occurring 1 and 0 to obtain different correlations. These results were used to compare the models under independent and selected values of measure of association. For models 1, 2, and 3, the data were generated based on correlation of 0.4 between the outcome variables at time $t - 1$ and t for the first-order, and at time $t - 2$, $t - 1$, and t for the second-order. Similarly, models 4, 5, and 6 were generated with correlation of 0, while models 7, 8, and 9 considered correlation of -0.4. For each model, four covariates were also generated, corresponding to the correlated response variables by considering different correlations with the outcome variables. These estimates and tests were repeated 500 times for all models, and for sample sizes of 250, 500, and 1,000 for different correlations between outcome variables. The models that were used for this simulation study were different applications of the conditional model verified in Model (3.3). The extended Tsatis' test for the first-order Markov model, as shown by Equation (4.2), had involved covariate patterns. Nonetheless, Billingsley's test, which was represented by $\sum_{ij} (f_{ij} - f_i p_{ij})^2 / (f_i p_{ij})$, was used to compare the obtained results, with and without covariates. In other words, the Markov models were estimated using covariates and were employed in this test.

Table 3 shows the simulation results for the first-order model, which included frequencies by transition type, correlation between outcome variables in the bivariate

Bernoulli population, average estimates of the parameters, and the number of rejected hypotheses in 500 times of simulation for these models using Billingsley's test and the proposed test as an extension of Tsiatis' test. Acceptance of the null hypothesis, $H_0: \gamma_{j1} = \dots = \gamma_{jG} = 0$, would indicate a good fit of Model (4.1) to the data. The percentage of rejection for Billingsley's test was 0 because the test procedure did not consider any covariate. However, in the proposed extension, models with covariate dependence were used. Hence, it can be concluded that the proposed test statistics depended on the covariate-dependent transition probabilities, where the selection of appropriate variables in the model may influence the goodness of fit, to a large extent. This observation implied that the proposed test may display deviations for a good fit in some instances. In other words, the goodness of fit test proposed by this study, as an extension of the Tsiatis' test, depended on the model's specifications in terms of the explanatory power of the selected variables. Based on the estimated covariates for the first-order transition from 0 to 1, we observed a positive association with variable 1, and a transition from 1 to 1, which has negative association with variable 1 for all models, except with model 4 (sample size of 250, with correlation of 0). The rejection percentage had varied for the first-order model, mainly in the range of 4.8% to 6.6%. This result showed that the proposed test method was satisfactory for different sizes of samples, with different correlation of outcome variables based on the first-order Markov chain model.

The simulation results for the second-order model are given in Table 4. The table shows the number of transition types, correlation between outcome variables, average estimates of the parameters, and the number of rejected hypotheses, $H_0: \gamma_{r\dots sj1} = \dots = \gamma_{r\dots sjG} = 0$, in 500 times of simulations for the models. Results for the second-order models showed that there was no association between covariates and outcome variables, which was expected because

of the higher order of the underlying Markov chain. Only two models, 3 and 6, with sample size of 1,000 and correlations of 0 and 0.4, have negative associations with variable 2 in different types of transitions. The range of rejection percentage of the null hypothesis for the extended Tsiatis' test was 3.6% to 6.2% for models 1 to 9 in the second-order. Thus, these models were acceptable for different sizes of samples and different correlations between outcome variables. Results from Billingsley's test were compared with results from the proposed extension of Tsiatis' test; the number of rejected null hypothesis was zero for Billingsley's test because it does not depend on covariates. The number of rejected null hypothesis for model 3 was the lowest.

Table 3: 500 Simulations for Obtaining the Estimates of Associations Based on the Proposed First-order Models

| | | Model 1 - size 250 | | Model 2 - size 500 | | Model 3 - size 1000 | | Model 4 - size 250 | | Model 5 - size 500 | |
|-----------------------------------|----------|--------------------|---------|--------------------|---------|---------------------|---------|--------------------|---------|--------------------|---------|
| Transition type | | | | | | | | | | | |
| 00 | | 61 | | 121 | | 243 | | 50 | | 100 | |
| 01 | | 65 | | 129 | | 257 | | 50 | | 100 | |
| 10 | | 14 | | 29 | | 58 | | 75 | | 150 | |
| 11 | | 110 | | 221 | | 442 | | 75 | | 150 | |
| Correlation of response variables | | 0.4 | | 0.4 | | 0.4 | | 0 | | 0 | |
| Estimates of Parameters | | estimate | p-value | estimate | p-value | estimate | p-value | estimate | p-value | estimate | p-value |
| 0 to 1 | Constant | -0.868 | 0.115 | -0.843 | 0.025 | -0.830 | 0.002 | -0.916 | 0.130 | -0.877 | 0.040 |
| | V1 | 1.422 | 0.011 | 1.386 | 0.000 | 1.360 | 0.000 | 0.972 | 0.143 | 0.942 | 0.043 |
| | V2 | 0.301 | 0.438 | 0.290 | 0.383 | 0.287 | 0.304 | 0.341 | 0.396 | 0.357 | 0.313 |
| | V3 | 0.093 | 0.482 | 0.109 | 0.469 | 0.101 | 0.464 | 0.517 | 0.321 | 0.469 | 0.237 |
| | V4 | 0.305 | 0.423 | 0.262 | 0.380 | 0.259 | 0.293 | 0.759 | 0.263 | 0.751 | 0.126 |
| 1 to 1 | Constant | - | 0.19 | - | 0.08 | - | 0.01 | 1.233 | 0.04 | 1.200 | 0.00 |

| | | | | | | | | | | | |
|--|----------------------------------|--------|-------|--------|-------|--------|-------|----------|-------|----------|-------|
| | nt | 1.181 | 5 | 1.114 | 4 | 1.044 | 9 | | 5 | | 5 |
| | V1 | -1.776 | 0.059 | -1.696 | 0.005 | -1.685 | 0.000 | -0.914 | 0.072 | -0.907 | 0.012 |
| | V2 | -0.365 | 0.444 | -0.257 | 0.453 | -0.250 | 0.418 | -0.364 | 0.352 | -0.350 | 0.273 |
| | V3 | -0.013 | 0.483 | -0.037 | 0.483 | -0.061 | 0.468 | -0.496 | 0.292 | -0.491 | 0.161 |
| | V4 | -0.252 | 0.452 | -0.253 | 0.448 | -0.285 | 0.376 | -0.693 | 0.157 | -0.665 | 0.058 |
| | Billingsley | 0.008 | 0.951 | 0.010 | 0.938 | 0.019 | 0.907 | 2.50E-05 | 0.999 | 1.06E-05 | 0.999 |
| | No. of tests accepting H_0 | 500 | | 500 | | 500 | | 500 | | 500 | |
| | Proposed test | 8.646 | 0.462 | 8.267 | 0.481 | 8.172 | 0.481 | 8.159 | 0.486 | 8.403 | 0.470 |
| | No. of tests accepting H_0 | 460 | | 467 | | 476 | | 474 | | 470 | |
| | Proportion of rejection of H_0 | 40/500 | | 33/500 | | 24/500 | | 26/500 | | 30/500 | |

Table 3: Continued

| | | Model 6 - size 1000 | | Model 7 - size 250 | | Model 8 - size 500 | | Model 9 - size 1000 | |
|-----------------------------------|----------|---------------------|---------|--------------------|---------|--------------------|---------|---------------------|---------|
| Transition | | | | | | | | | |
| 00 | | 201 | | 26 | | 51 | | 102 | |
| 01 | | 200 | | 99 | | 200 | | 399 | |
| 10 | | 300 | | 75 | | 148 | | 298 | |
| 11 | | 300 | | 50 | | 101 | | 201 | |
| Correlation of response variables | | 0 | | -0.4 | | -0.4 | | -0.4 | |
| Estimates of Parameters | | estimate | p-value | estimate | p-value | estimate | p-value | estimate | p-value |
| 0 to 1 | Constant | -0.875 | 0.003 | 0.485 | 0.314 | 0.489 | 0.202 | 0.492 | 0.081 |
| | V1 | 0.926 | 0.004 | 1.797 | 0.028 | 1.707 | 0.002 | 1.688 | 0.000 |
| | V2 | 0.351 | 0.215 | 2.183 | 0.036 | 1.961 | 0.002 | 1.931 | 0.000 |
| | V3 | 0.470 | 0.112 | 0.709 | 0.274 | 0.666 | 0.172 | 0.635 | 0.066 |
| | V4 | 0.743 | 0.028 | -0.715 | 0.269 | -0.666 | 0.166 | -0.653 | 0.063 |
| 1 to 1 | Constant | 1.190 | 0.000 | 2.463 | 0.003 | 2.315 | 0.000 | 2.291 | 0.000 |
| | V1 | -0.885 | 0.000 | -1.731 | 0.013 | -1.635 | 0.001 | -1.613 | 0.000 |
| | V2 | -0.342 | 0.154 | -1.621 | 0.011 | -1.546 | 0.000 | -1.529 | 0.000 |
| | V3 | -0.491 | 0.060 | -0.645 | 0.242 | -0.605 | 0.153 | -0.611 | 0.042 |
| | V4 | -0.664 | 0.007 | 0.666 | 0.247 | 0.642 | 0.116 | 0.657 | 0.024 |
| Billingsley | | 4.79E-06 | 0.999 | 0.011 | 0.935 | 0.011 | 0.934 | 0.011 | 0.923 |
| No. of tests accepting H_0 | | 500 | | 500 | | 500 | | 500 | |
| Proposed test | | 8.167 | 0.489 | 8.383 | 0.467 | 8.439 | 0.468 | 8.448 | 0.463 |
| No. of tests accepting H_0 | | 472 | | 471 | | 475 | | 473 | |
| Proportion of rejection of H_0 | | 28/500 | | 29/500 | | 25/500 | | 27/500 | |

Table 4: 500 Simulations for Obtaining the Estimates of Associations Based on the Proposed Second-order Models

| | Model 1 - size 250 | Model 2 - size 500 | Model 3 -size 1000 |
|------------|--------------------|--------------------|--------------------|
| Transition | | | |
| 000 | 67 | 132 | 262 |
| 001 | 15 | 31 | 61 |
| 100 | 22 | 44 | 88 |
| 101 | 22 | 43 | 88 |
| 010 | 22 | 43 | 87 |
| 011 | 22 | 44 | 88 |
| 110 | 15 | 31 | 62 |
| 111 | 65 | 132 | 264 |

| Correlation of response variables | | 0.4 | | 0.4 | | 0.4 | |
|-----------------------------------|----------|----------|---------|----------|---------|----------|---------|
| Estimates of parameters | | Estimate | p-value | estimate | p-value | estimate | p-value |
| 0→0→1 | Constant | -0.816 | 0.244 | -0.724 | 0.136 | -0.701 | 0.036 |
| | V1 | 0.670 | 0.313 | 0.585 | 0.258 | 0.559 | 0.133 |
| | V2 | 0.938 | 0.273 | 0.835 | 0.168 | 0.831 | 0.059 |
| | V3 | 0.449 | 0.386 | 0.401 | 0.347 | 0.397 | 0.247 |
| | V4 | 0.347 | 0.446 | 0.312 | 0.435 | 0.337 | 0.339 |
| 1→0→1 | Constant | -1.025 | 0.232 | -0.989 | 0.101 | -0.951 | 0.031 |
| | V1 | 0.605 | 0.334 | 0.601 | 0.242 | 0.582 | 0.116 |
| | V2 | 0.861 | 0.272 | 0.855 | 0.117 | 0.796 | 0.036 |
| | V3 | 0.425 | 0.404 | 0.397 | 0.369 | 0.419 | 0.235 |
| | V4 | 0.335 | 0.438 | 0.295 | 0.411 | 0.268 | 0.353 |
| 0→1→1 | Constant | 1.035 | 0.235 | 0.990 | 0.101 | 0.938 | 0.031 |
| | V1 | -0.610 | 0.353 | -0.595 | 0.240 | -0.566 | 0.132 |
| | V2 | -0.902 | 0.262 | -0.840 | 0.151 | -0.806 | 0.049 |
| | V3 | -0.467 | 0.413 | -0.432 | 0.341 | -0.391 | 0.272 |
| | V4 | -0.348 | 0.446 | -0.302 | 0.417 | -0.304 | 0.364 |
| 1→1→1 | Constant | 1.333 | 0.244 | 1.255 | 0.116 | 1.235 | 0.027 |
| | V1 | -0.621 | 0.374 | -0.613 | 0.255 | -0.601 | 0.131 |
| | V2 | -0.814 | 0.263 | -0.813 | 0.129 | -0.781 | 0.032 |
| | V3 | -0.483 | 0.398 | -0.418 | 0.356 | -0.421 | 0.269 |
| | V4 | -0.341 | 0.437 | -0.291 | 0.417 | -0.293 | 0.353 |
| Billingsley | | 2.86E-04 | 1.000 | 5.01E-05 | 1.000 | 1.66E-05 | 1.000 |
| No. of tests accepting H_0 | | 500 | | 500 | | 500 | |
| Proposed test | | 16.913 | 0.445 | 16.650 | 0.459 | 15.804 | 0.503 |
| No. of tests accepting H_0 | | 475 | | 472 | | 482 | |
| Proportion of rejection of H_0 | | 25/500 | | 28/500 | | 18/500 | |

Table 4: Continued

| | Model 4 - size 250 | Model 5 - size 500 | Model 6 -size 1000 |
|------------|--------------------|--------------------|--------------------|
| Transition | | | |
| 000 | 31 | 63 | 126 |
| 001 | 31 | 62 | 125 |
| 100 | 32 | 63 | 124 |
| 101 | 31 | 62 | 125 |
| 010 | 31 | 63 | 125 |
| 011 | 31 | 62 | 125 |
| 110 | 31 | 63 | 125 |
| 111 | 32 | 62 | 125 |

| Correlation of response variables | | 0 | | 0 | | 0 | |
|-----------------------------------|----------|----------|---------|----------|---------|----------|---------|
| Estimates of parameters | | Estimate | p-value | estimate | p-value | estimate | p-value |
| 0→0→1 | Constant | -0.771 | 0.266 | -0.704 | 0.144 | -0.724 | 0.034 |
| | V1 | 0.615 | 0.343 | 0.577 | 0.260 | 0.581 | 0.125 |
| | V2 | 0.912 | 0.288 | 0.847 | 0.163 | 0.838 | 0.053 |
| | V3 | 0.412 | 0.400 | 0.378 | 0.362 | 0.406 | 0.240 |
| | V4 | 0.381 | 0.441 | 0.320 | 0.422 | 0.317 | 0.373 |
| 1→0→1 | Constant | -1.083 | 0.229 | -0.976 | 0.111 | -0.964 | 0.029 |
| | V1 | 0.644 | 0.353 | 0.547 | 0.266 | 0.572 | 0.123 |
| | V2 | 0.879 | 0.259 | 0.806 | 0.144 | 0.788 | 0.045 |
| | V3 | 0.474 | 0.409 | 0.436 | 0.327 | 0.429 | 0.228 |
| | V4 | 0.326 | 0.448 | 0.321 | 0.389 | 0.296 | 0.337 |
| 0→1→1 | Constant | 1.013 | 0.239 | 1.004 | 0.112 | 0.931 | 0.033 |
| | V1 | -0.580 | 0.359 | -0.639 | 0.222 | -0.557 | 0.133 |
| | V2 | -0.942 | 0.251 | -0.795 | 0.177 | -0.794 | 0.049 |
| | V3 | -0.434 | 0.409 | -0.427 | 0.339 | -0.401 | 0.251 |
| | V4 | -0.310 | 0.454 | -0.306 | 0.419 | -0.278 | 0.370 |
| 1→1→1 | Constant | 1.291 | 0.254 | 1.270 | 0.101 | 1.241 | 0.025 |
| | V1 | -0.611 | 0.377 | -0.605 | 0.264 | -0.597 | 0.146 |
| | V2 | -0.849 | 0.253 | -0.789 | 0.130 | -0.778 | 0.038 |
| | V3 | -0.450 | 0.434 | -0.440 | 0.360 | -0.429 | 0.261 |
| | V4 | -0.330 | 0.437 | -0.300 | 0.421 | -0.301 | 0.337 |
| Billingsley | | 3.38E-04 | 1.000 | 7.01E-05 | 1.000 | 2.14E-05 | 1.000 |
| No. of tests accepting H_0 | | 500 | | 500 | | 500 | |
| Proposed test | | 17.477 | 0.425 | 16.562 | 0.464 | 16.517 | 0.473 |
| No. of tests accepting H_0 | | 559 | | 476 | | 473 | |
| Proportion of rejection of H_0 | | 41/500 | | 24/500 | | 27/500 | |

Table 4: Continued

| | | Model 7 - size 250 | | Model 8 - size 500 | | Model 9 -size 1000 | |
|-----------------------------------|----------|--------------------|---------|--------------------|---------|--------------------|---------|
| Transition | | | | | | | |
| 000 | | 16 | | 31 | | 62 | |
| 001 | | 59 | | 119 | | 237 | |
| 100 | | 28 | | 56 | | 112 | |
| 101 | | 22 | | 44 | | 88 | |
| 010 | | 22 | | 44 | | 88 | |
| 011 | | 28 | | 56 | | 112 | |
| 110 | | 59 | | 118 | | 238 | |
| 111 | | 16 | | 32 | | 63 | |
| Correlation of response variables | | -0.4 | | -0.4 | | -0.4 | |
| Estimates of parameters | | Estimate | p-value | estimate | p-value | estimate | p-value |
| 0→0→1 | Constant | -0.068 | 0.479 | -0.060 | 0.498 | -0.063 | 0.468 |
| | V1 | -0.051 | 0.487 | -0.053 | 0.485 | -0.066 | 0.454 |
| | V2 | -0.053 | 0.466 | -0.072 | 0.500 | -0.061 | 0.472 |
| | V3 | -0.024 | 0.500 | -0.046 | 0.479 | -0.012 | 0.501 |
| | V4 | -0.091 | 0.498 | -0.085 | 0.474 | -0.092 | 0.479 |
| 1→0→1 | Constant | -0.164 | 0.479 | -0.173 | 0.456 | -0.179 | 0.367 |
| | V1 | -0.090 | 0.473 | -0.045 | 0.505 | -0.042 | 0.489 |
| | V2 | -0.078 | 0.503 | -0.061 | 0.494 | -0.060 | 0.502 |
| | V3 | -0.056 | 0.493 | 0.034 | 0.514 | -0.011 | 0.494 |
| | V4 | -0.096 | 0.477 | -0.102 | 0.488 | -0.085 | 0.481 |
| 0→1→1 | Constant | 0.041 | 0.489 | 0.082 | 0.492 | 0.092 | 0.501 |
| | V1 | 0.090 | 0.455 | 0.032 | 0.489 | 0.052 | 0.495 |
| | V2 | 0.139 | 0.489 | 0.096 | 0.476 | 0.053 | 0.511 |
| | V3 | 0.351 | 0.409 | 0.152 | 0.465 | 0.014 | 0.491 |
| | V4 | 0.418 | 0.459 | 0.219 | 0.489 | 0.133 | 0.496 |
| 1→1→1 | Constant | 0.326 | 0.484 | 0.183 | 0.504 | 0.185 | 0.460 |
| | V1 | -0.004 | 0.403 | 0.346 | 0.449 | 0.179 | 0.500 |
| | V2 | 0.133 | 0.456 | 0.027 | 0.474 | 0.059 | 0.485 |
| | V3 | -0.005 | 0.240 | 0.114 | 0.361 | 0.249 | 0.450 |
| | V4 | 0.289 | 0.361 | 0.212 | 0.452 | 0.272 | 0.477 |
| Billingsley | | 9.51E-03 | 1.000 | 3.86E-03 | 1.000 | 1.12E-03 | 1.000 |
| No. of tests accepting H_0 | | 500 | | 500 | | 500 | |
| Proposed test | | 15.810 | 0.508 | 17.039 | 0.442 | 16.388 | 0.478 |
| No. of tests accepting H_0 | | 479 | | 469 | | 473 | |
| Proportion of rejection of H_0 | | 21/500 | | 31/500 | | 27/500 | |

7 Conclusion

An extension of Tsiatis' test procedure was proposed in this study for first- and higher-order binary Markov models by considering repeated measures. Most of the test procedures for stationarity and order of Markov chains were based on the likelihood ratio test and the usual chi-square test. We have shown a goodness of fit for the Markov chain by considering the efficient score test, which only requires estimated parameters under the null hypothesis. The utility of the proposed test has been examined, with an example for real life data. The results indicated the suitability of these techniques. Additionally, simulation results demonstrated a Type I error for the proposed test. In addition, the proposed test procedure was extended for higher-order models and can be extended to test the order of binary Markov chains.

Acknowledgments

We are grateful to the HEQEP in project 3293, from the Department of Applied Statistics, East West University, and for the sponsorships by the UGC, Bangladesh and the World Bank. We are also thankful to Dr. Rafiqul Islam Chowdhury for giving us permission to use the "kernopt markov.gen" program for parameter estimates. We would also like to thank the Health and Retirement Study (HRS) center for giving us permission to use RAND data in the application of the model.

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ACCEPTED MANUSCRIPT

In this paper, an important test procedure arising from repeated measurements of discrete data has been introduced. In real life situations the change in the status of a disease or other outcome variables need to be examined. These changes need to be studied to understand the underlying factors influencing transitions in the status during specified time intervals. We can employ Markov models in order to find the relationships between the risk factors and outcome variables. The models can be of first or higher orders. One formidable challenge in employing these models is to confirm goodness of the model for first or higher order. This paper provides a simple test that can be used to test goodness of fit of higher order Markov models with covariate dependence for binary data. The proposed test procedure appears to be very useful technique in providing the goodness of fit of higher order binary Markov chains.

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