BIAS-CORRECTED AIC FOR SELECTING VARIABLES IN MULTINOMIAL LOGISTIC REGRESSION MODELS

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Abstract

In this paper, we consider the bias correction of Akaike’s information criterion (AIC) for selecting variables in multinomial logistic regression models. For simplifying a formula of the bias-corrected AIC, we calculate the bias of the AIC to a risk function through the expectations of partial derivatives of the minus log-likelihood function. As a result, we can express the bias correction term of the bias-corrected AIC with only three matrices consisting of the second, third, and fourth derivatives of the minus log-likelihood function. By conducting numerical studies, we verify that the proposed bias-corrected AIC performs better than the crude AIC.

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Key words: AIC, Bias correction, Multinomial logistic model, MLE, Partial differential operator, Variable selection.

1. INTRODUCTION

A multinomial logistic regression model is a regression model that generalizes a logistic regression by allowing more than two discrete outcomes. When categories are unordered, the multinomial logistic model is one strategy often used. The multinomial logistic regression model has been introduced in many textbooks for applied statistical analysis (see e.g., Hosmer & Lemeshow, 2000, Chapter 8.1), and even now it is widely used in biometrics, econometrics, psychometrics, sociometrics, and many other fields of applications for the prediction of probabilities of different possible outcomes of categorically distributed response variables by a set of explanatory variables (e.g., Briz & Ward, 2009; Choi

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In addition, the multinomial logistic regression model can be easily fitted to real data by using the “vglm” function in “R” (R Development Core Team, 2011). Since we would like to specify the factors affecting the probabilities of response variables in the regression analysis, searching for the optimal subset of explanatory variables is important.

Akaike’s information criterion (AIC) proposed by Akaike (1973, 1974) is widely used for selecting the best model among the candidate models (for details of statistical model selection, see e.g., Konishi, 1999; Burnham & Anderson, 2002; Konishi & Kitagawa, 2008). The model having the smallest AIC among the candidate models is regarded as the best model. In the multinomial logistic regression model, the subset of explanatory variables in the best model is the best subset. However, the AIC may perform poorly; that is, a model having too many parameters tends to be chosen as the best model when the sample size is small or the number of unknown parameters is large. Such a problem is often resolved by using a bias-corrected AIC (see e.g., Burnham & Anderson, 2002, Chapter 2.4). The AIC is an estimator of the risk function consisting of predictive Kullback-Leibler (K-L) information (Kullback & Leibler, 1951), which measures the discrepancy between the true model and the candidate model. The order of the bias of the AIC is $O(n^{-1})$ when the candidate model includes the true model, where $n$ is the sample size. Although the AIC is an asymptotic unbiased estimator of the risk function, it has a nonnegligible bias to the risk function when the sample size is small or the number of unknown parameters is large. A bias-corrected AIC called CAIC in this paper improves the bias of AIC to $O(n^{-2})$ under the assumption that the candidate model includes the true model.

The CAIC in the logistic regression models was obtained by Yanagihara, Sekiguchi and Fujikoshi (2003). But the CAIC in multinomial regression models has not been derived yet, although the multinomial logistic regression model is widely used in many application fields. The CAIC can be obtained by removing the bias of the AIC to the risk function from the AIC with the use of a consistent estimator of the bias. The bias of the AIC to the risk function is then evaluated by moments of the maximum likelihood estimator (MLE) of unknown parameters. Since such moments are represented by the moments of response variables, calculating the moments of response variables is essential for evaluating the bias of the AIC in the ordinary bias correction method, which is used in Yanagihara, Sekiguchi and Fujikoshi (2003) and Kamo, Yanagihara and Satoh (2012), etc. However, in the case of multiple response variables, calculations and expressions of the moments of the MLE mediated by the moments of response variables become complicated. Hence, without directly calculating the moments of response variables, we derive the moments of the MLE by using expectations of the partial derivatives of the minus log-likelihood function. This different approach from the ordinary bias correction method leads to a simple expression of the bias correction term of the CAIC. In fact, the bias correction term of our CAIC is represented by only three matrices consisting of the second, third, and fourth derivatives of the minus log-likelihood function.
The present paper is organized as follows. In Section 2, we give a stochastic expansion of the MLE. In Section 3, the CAIC in multinomial logistic regression models is proposed. In Section 4, we verify that the proposed CAIC has better performance than the AIC by conducting numerical experiments. In Section 5, we conclude our discussion. Technical details are provided in the Appendix.

2. STOCHASTIC EXPANSION OF MLE

Suppose that the data consists of a sequence \( \{ y_i, x_i \} \), where \( y_1, \ldots, y_m \) are \( r \)-dimensional independent unordered discrete random vectors, and \( x_1, \ldots, x_m \) are \( k \)-dimensional vectors of known constants. Let \( \beta = (\beta_1, \ldots, \beta_{kr})' \) be a \( kr \)-dimensional unknown regression coefficient vector that is partitioned as \( \beta = (\beta_1', \ldots, \beta_r')' \), where \( \beta_j \) is a \( k \)-dimensional vector denoted by \( \beta_j = (\beta_{j1} - 1 + 1, \ldots, \beta_{jk})' \).

In the multinomial logistic regression model, we assume that \( (y_{i0}, y_i')' = (y_{i0}, y_{i1}, \ldots, y_{ir})' \) is distributed according to the multinomial distribution with the number of events \( n_i = \sum_{j=0}^{r} y_{ij} \), \( n = \sum_{i=1}^{m} n_i \) and the cell probability vector \( p_i(\beta) = (p_{i0}(\beta), p_i(\beta)')' \), given by

\[
p_{i0}(\beta) = \frac{1}{1 + \sum_{j=1}^{r} \exp(x_i'\beta_j)}, \\
p_i(\beta) = (p_{i1}(\beta), \ldots, p_{ir}(\beta))' = \left( \frac{\exp(x_i'\beta_1)}{1 + \sum_{j=1}^{r} \exp(x_i'\beta_j)}, \ldots, \frac{\exp(x_i'\beta_r)}{1 + \sum_{j=1}^{r} \exp(x_i'\beta_j)} \right)'.
\]

The MLE of \( \beta \) is obtained by maximizing the log-likelihood function. By omitting the constant term, the log-likelihood function of the multinomial logistic regression model in (1) is expressed as

\[
\ell(\beta) = \sum_{i=1}^{m} \left\{ y_{i0} \otimes x_i)'\beta - n_i \log \left( 1 + \sum_{j=1}^{r} \exp(x_i'\beta_j) \right) \right\}.
\]

Hence, the MLE of \( \beta \) is given by

\[
\hat{\beta} = \arg \max_{\beta} \ell(\beta).
\]

To evaluate a bias of the AIC to the risk function, a stochastic expansion of \( \hat{\beta} \) is needed. The purpose of this section is to obtain the stochastic expansion \( \hat{\beta} \) up to the order \( n^{-3/2} \). Two cases serve as a framework for asymptotic approximations:

Case (i): \( n_j \)'s are fixed, and \( m \to \infty \),

Case (ii): \( m \) is fixed, \( n_j \to \infty \) and \( p_j^{-1} = n_j / n = O(1) \) for each \( j \).

Although we only consider Case (i) in this paper, our formula can also be applied to Case (ii).

Suppose that \( x_1, \ldots, x_m \) are members of an admissible set \( \mathcal{F} \), i.e., \( x_1, \ldots, x_m \in \mathcal{F} \). To expand the MLE, we consider the following regularity assumptions (see e.g., Fahrmeir & Kaufmann, 1985):
C.1: \( \beta \in \mathcal{B} \), where \( \mathcal{B} \) is a convex and open set in \( \mathbb{R}^k \),

C.2: \((I_r \otimes x_i)\beta \in \Theta^0 \), \( i = 1, 2, \ldots \), for all \( \beta \in \mathcal{B} \), where \( \Theta^0 \) is the interior of the convex natural parameter space \( \Theta \subset \mathbb{R}^r \),

C.3: \( 3m_0 \) s.t. \( X'X \) has the full rank for \( m \geq m_0 \), where \( X = (x_1, \ldots, x_m)' \).

Condition C.1 guarantees the uniqueness of the MLE if it exists. Condition C.2 is necessary to obtain the multinomial logistic regression model for all \( \beta \). Condition C.3 ensures that \( \sum_{i=1}^{m} n_i \Sigma_i(\beta) \otimes x_i x_i' \) is positive definite for all \( \beta \in \mathcal{B}, m \geq m_0 \), where

\[
\Sigma_i(\beta) = \text{diag}(p_i(\beta)) - p_i(\beta)p_i(\beta)',
\]

Moreover, we prepare the following additional conditions to assure weak consistency and asymptotic normality of \( \hat{\beta} \), which can be derived by slightly modifying the results in Fahrmeir and Kaufmann (1985):

C.4: sequence \( \{x_i\} \) lies in \( \mathcal{F} \) with \((I_r \otimes x)'\beta \in \Theta^0, \beta \in \mathcal{B} \),

C.5: \( \lim \inf_{m \to \infty} \lambda(\sum_{i=1}^{m} n_i \Sigma_i(\beta) \otimes x_i x_i'/n) > 0 \), where \( \lambda(A) \) indicates the smallest eigenvalue of symmetric matrix \( A \).

According to Corollary 1 in Fahrmeir and Kaufmann (1985), \( \hat{\beta} \) has weak consistency and asymptotic normality under these conditions. Furthermore, from C.5, \( \sum_{i=1}^{m} n_i \Sigma_i(\beta) \otimes x_i x_i' = O(n) \) is satisfied.

Under the assumption that all conditions are satisfied, \( \hat{\beta} \) can be formally expanded as follows:

\[
\hat{\beta} = \beta + \frac{1}{\sqrt{n}} b_1 + \frac{1}{n} b_2 + \frac{1}{n \sqrt{n}} b_3 + O_p(n^{-2}),
\]

where \( b_1, b_2, \) and \( b_3 \) are \( kr \)-dimensional random vectors. The purpose of this section is achieved by specifying \( b_1, b_2, \) and \( b_3 \).

Since the log-likelihood function \( \ell(\beta) \) is a maximum at \( \beta = \hat{\beta} \), the first derivative of \( \ell(\beta) \) becomes \( 0_{kr} \) at \( \beta = \hat{\beta} \), i.e.,

\[
\left. \frac{\partial \ell(\beta)}{\partial \beta} \right|_{\beta = \hat{\beta}} = \sum_{i=1}^{m} \left\{ (y_i \otimes x_i) - n_i (p_i(\hat{\beta}) \otimes x_i) \right\} = 0_{kr},
\]

where \( 0_{kr} \) is a \( kr \)-dimensional vector of zeros. To expand equation (5), we prepare the following three matrices consisting of the second, third, and fourth derivatives of \( -\ell(\beta)/n \):

\[
G_2(\beta) = -\frac{1}{n} \frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta'}, \quad G_3(\beta) = -\frac{1}{n} \left( \frac{\partial}{\partial \beta'} \otimes \frac{\partial^2}{\partial \beta \partial \beta'} \right) \ell(\beta), \quad G_4(\beta) = -\frac{1}{n} \left( \frac{\partial^2}{\partial \beta \partial \beta'} \otimes \frac{\partial^2}{\partial \beta \partial \beta'} \right) \ell(\beta).
\]
The result of the first derivative of $-\ell(\beta)$ in (5) implies the following explicit forms of $G_2(\beta)$, $G_3(\beta)$, and $G_4(\beta)$ (details of the derivations are given in Appendix A.1):

\begin{align*}
G_2(\beta) &= \sum_{i=1}^{m} \rho_i \left\{ \frac{\partial p_i(\beta)}{\partial \beta'} \right\} \otimes x_i = \sum_{i=1}^{m} \rho_i \left( \Sigma_i(\beta) \otimes x_i x_i' \right), \\
G_3(\beta) &= \sum_{i=1}^{m} \rho_i \left\{ \left( \frac{\partial}{\partial \beta'} \otimes \frac{\partial}{\partial \beta'} \right) p_i(\beta) \right\} \otimes x_i = \sum_{i=1}^{m} \rho_i \left\{ \Delta_{3,i}(\beta) \otimes x_i x_i' \right\}, \\
G_4(\beta) &= \sum_{i=1}^{m} \rho_i \left\{ \left( \frac{\partial^2}{\partial \beta \partial \beta'} \otimes \frac{\partial}{\partial \beta'} \right) p_i(\beta) \right\} \otimes x_i = \sum_{i=1}^{m} \rho_i \left\{ \Delta_{4,i}(\beta) \otimes x_i x_i' \right\}, \quad (6, 7, 8)
\end{align*}

where $\Delta_{3,i}(\beta)$ and $\Delta_{4,i}(\beta)$ are $kr \times (kr)^2$ and $(kr)^2 \times (kr)^2$ matrices, respectively, which are defined by

\begin{align*}
\Delta_{3,i}(\beta) &= \sum_{a=1}^{r} p_{ia}(\beta)e_a' \otimes x_i' \otimes (e_a - p_i(\beta))(e_a - p_i(\beta))' - p_i(\beta)' \otimes x_i' \otimes \Sigma_i(\beta), \\
\Delta_{4,i}(\beta) &= \sum_{a=1}^{r} p_{ia}(\beta)(e_a - p_i(\beta))(e_a - p_i(\beta))' \otimes x_i x_i' \otimes (e_a e_a' - e_a p_i(\beta)' - p_i(\beta)e_a') \\
&\quad - \Sigma_i(\beta) \otimes x_i x_i' \otimes (\Sigma_i(\beta) - p_i(\beta)p_i(\beta)') \\
&\quad - \sum_{a,b}^{r} p_{ia}p_{ib}(\beta)(e_a - p_i(\beta))(e_b - p_i(\beta))' \otimes x_i x_i' \otimes (e_a e_a' + e_b e_b'). \quad (9)
\end{align*}

Here, $e_j$ is an $r$-dimensional $j$th coordinate unit vector whose $j$th element is 1 and others are 0, and the notation $\sum_{a_1, \ldots, a_r}$ means $\sum_{a_1=1}^{r} \cdots \sum_{a_r=1}^{r}$.

Applying a Taylor expansion around $\hat{\beta} = \beta$ to equation (5) yields

\begin{align*}
\frac{1}{n} \sum_{i=1}^{m} \left\{ (y_i - n_i p_i(\beta)) \otimes x_i \right\} &= G_2(\beta)(\hat{\beta} - \beta) + \frac{1}{2} G_3(\beta) \left\{ (\hat{\beta} - \beta) \otimes (\hat{\beta} - \beta) \right\} \\
&\quad + \frac{1}{6} \left\{ I_{kr} \otimes (\hat{\beta} - \beta)' \right\} G_4(\beta) \left\{ (\hat{\beta} - \beta) \otimes (\hat{\beta} - \beta) \right\} + O_p(n^{-2}). \quad (10)
\end{align*}

Notice that the order of the left-hand side of equation (10) is $O_p(n^{-1/2})$. By comparing the $O_p(n^{-1/2})$, $O_p(n^{-1})$, and $O_p(n^{-3/2})$ terms after substituting (4) into (10), $b_1$, $b_2$, and $b_3$ in (4) are specified as

\begin{align*}
b_1 &= \frac{1}{\sqrt{n}} G_2(\beta)^{-1} \sum_{i=1}^{m} \left\{ (y_i - n_i p_i(\beta)) \otimes x_i \right\}, \\
b_2 &= -\frac{1}{2} G_2(\beta)^{-1} G_3(\beta)(b_1 \otimes b_1), \\
b_3 &= -\frac{1}{2} G_2(\beta)^{-1} \left\{ G_3(\beta)(b_1 \otimes b_2 + b_2 \otimes b_1) + \frac{1}{3} (I_{kr} \otimes b_1') G_4(\beta)(b_1 \otimes b_1) \right\}. \quad (11)
\end{align*}

We use the stochastic expansion of $\hat{\beta}$ with $b_1$, $b_2$, and $b_3$ to evaluate the bias of the AIC to the risk function.
3. MAIN RESULT

Let $L(β)$ be a loss function defined by

$$L(β) = E[-2\ell(β)] = -2\sum_{i=1}^{m} n_i \left\{ (p_i^* \otimes x_i)\beta - \log \left( 1 + \sum_{j=1}^{r} \exp(x'_jβ_j) \right) \right\},$$

where $p_i^*$ is the cell probability vector of the true model. Then, the risk function consisting of the predictive K-L information is given by

$$R = E[L(\hat{β})].$$

In this section, we propose a CAIC that improves the bias of the AIC to $O(n^{-2})$ under the assumption that the candidate model includes the true model. Notice that the crude AIC is defined by

$$AIC = -2\ell(\hat{β}) + 2kr.$$  

Thus, it is sufficient to derive the bias of $-2\ell(\hat{β})$ to $R$ for evaluating the bias of the AIC. Also notice that $p_i^* = p(x_i)$ holds when the candidate model includes the true model. Then, the bias of $-2\ell(\hat{β})$ to $R$ under the assumption that the candidate model includes the true model is expanded as

$$B = R - E[-2\ell(\hat{β})]$$

$$= 2\sum_{i=1}^{m} E \left\{ ((y_i - n_i p_i(β)) \otimes x_i)\hat{β} \right\}$$

$$= 2\sqrt{n} E \left[ b'_1 G_2(β)\hat{β} \right]$$

$$= 2 \left\{ \sqrt{n} E[b'_1 G_2(β)β] + E[b'_1 G_2(β)b_1] + \frac{1}{\sqrt{n}} E[b'_1 G_2(β)b_2] + \frac{1}{n} E[b'_1 G_2(β)b_3] \right\} + O(n^{-2}),$$

where matrices $G_2(β), G_3(β), \text{ and } G_4(β)$ are given by (6), (7), and (8), respectively, and $kr$-dimensional random vectors $b_1, b_2, \text{ and } b_3$ are given by (11). In many cases of practical interest, a moment of statistic can be expanded as a power series in $n^{-1}$ (see e.g., Hall, 1992, p. 46). Hence, the order of the remainder term of (15) is shown by $O(n^{-2})$, not $O(n^{-3/2})$. Indeed, an $n^{-3/2}$ term of the stochastic expansion of $\sum_{i=1}^{m} \{(y_i - n_i p_i(β)) \otimes x_i\}'\hat{β}$ in the bias can be expressed as a fifth-order polynomial of elements of $b_1$. Since $b_1$ has an asymptotic normality, the expectation of an odd-order polynomial of elements of $b_1$ becomes $O(n^{-1/2})$. Given this fact, the order of the remainder term of the expansion in (15) is $O(n^{-2})$.

From elementary linear algebra and the definition of $b_2$ in (11), $b'_1 G_3(β)b_2$ in (15) is expressed by the function of $b_1$ as

$$b'_1 G_2(β)b_2 = -\frac{1}{2} b'_1 G_3(β)(b_1 \otimes b_1) = -\frac{1}{2} \text{tr}\{ G_3(β)(b_1 \otimes b_1) \}. \quad (16)$$
Since the derivative is invariant to changes in the order of differentiation, we have

\[ b'_1 G_3(\beta)(b_1 \otimes b_2) = b'_1 G_3(\beta)(b_2 \otimes b_1) = b'_2 G_3(\beta)(b_1 \otimes b_1) = (b_1 \otimes b_1)' G_3(\beta)' b_2. \]

It follows from the above equations that

\[ b'_1 G_3(\beta)(b_1 \otimes b_2 + b_2 \otimes b_1) = 2(b_1 \otimes b_1)' G_3(\beta)' b_2 \]

\[ = -(b_1 \otimes b_1)' G_3(\beta)' G_2(\beta)^{-1} G_3(\beta)(b_1 \otimes b_1) \]

\[ = -\text{tr} \left\{ G_3(\beta)' G_2(\beta)^{-1} G_3(\beta)(b_1 b'_1 \otimes b_1 b'_1) \right\}. \]

Thus, from the above result and the definition of \( b_n \) in (11), \( b'_1 G_4(\beta) b_3 \) in (15) is expressed by the function of \( b_1 \) as

\[ b'_1 G_2 b_3 = -\frac{1}{2} b'_1 G_3(\beta)(b_1 \otimes b_2 + b_2 \otimes b_1) - \frac{1}{6} b'_1 (I_{kr} \otimes b'_1) G_4(\beta)(b_1 \otimes b_1) \]

\[ = \frac{1}{2} \text{tr} \left\{ G_3(\beta)' G_2(\beta)^{-1} G_3(\beta)(b_1 b'_1 \otimes b_1 b'_1) \right\} - \frac{1}{6} \text{tr} \left\{ G_4(\beta)(b_1 b'_1 \otimes b_1 b'_1) \right\}. \]  

(17)

Hence, equations (16) and (17) indicate that the expansion of \( B \) in (15) can be calculated until the fourth moment of \( b_1 \).

Since \( b_1 \) consists of a centralized \( y_i \), we can directly calculate the expectations in (15) by centralized moments of \( y_1, \ldots, y_m \). Then, all combinations of multivariate moments of \( y_i - n_i p_i(\beta) \) are needed until the fourth-order. However, it is troublesome to calculate the third- and fourth-order multivariate moments of \( y_i - n_i p_i(\beta) \), because we have to consider all combinations of the multivariate moments. For simplicity, the relations between the moments of \( b_1 \) and the expectations of the derivatives of \( -\ell(\beta) \) with respect to \( \beta \) are used instead of calculating the multivariate moments of \( y_i - n_i p_i(\beta) \). It is easy to obtain \( E[b_1] = 0_{kr} \) because \( E[y_i] = n_i p_i(\beta) \). From the result of the first derivative of \( \ell(\beta) \) in (5) and the definition of \( b_1 \) in (11), we can see that

\[ -\frac{\partial}{\partial \beta} \ell(\beta) = -\sqrt{n} G_2(\beta) b_1. \]

Notice that \( G_2(\beta) \), \( G_3(\beta) \), and \( G_4(\beta) \) are constant matrices and \( -E[\partial \ell(\beta)/\partial \beta] = 0_{kr} \). By applying general formulas of expectations (A.7) in Appendix A.2 to the case of the multinomial logistic regression model, the following equations are obtained:

\[ n G_2(\beta) = n G_2(\beta) E[b_1 b'_1] G_2(\beta), \]

\[ n G_3(\beta) = n \sqrt{n} G_2(\beta) E[b_1 b'_1] (G_2(\beta) \otimes G_2(\beta)), \]

\[ n G_4(\beta) = \frac{n^2}{2} (G_2(\beta) \otimes G_2(\beta)) E[b_1 b'_1 b_1 b'_1] (G_2(\beta) \otimes G_2(\beta)) \]

\[ - n^2 \left\{ \text{vec}(K_{kr}) (G_2(\beta) \otimes G_2(\beta)) + \text{vec}(G_2(\beta)) \text{vec}(G_2(\beta))' \right\}, \]

where \( \text{vec}(A) \) is an operator to transform a matrix to a vector by stacking the first to the last column of \( A \), i.e., \( \text{vec}(A) = (a_1', \ldots, a_m')' \) when \( A = (a_1, \ldots, a_m) \) (see e.g., Harville, 1997, Chapter 16.2).
and $K_m$ is the $m^2 \times m^2$ vec-permutation matrix such that vec($B$) = $K_m$vec($B'$) when $B$ is an $m \times m$ matrix (see e.g., Harville, 1997, Chapter 16.3). These results lead us to the simple expression of moments of $b_1$ as

$$E[b_1b'_1] = G_2(\beta)^{-1},$$

$$E[b'_1 \otimes b_1b'_1] = \frac{1}{n} G_2(\beta)^{-1}G_3(\beta)(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1}),$$

$$E[b_1b'_1 \otimes b_1b'_1] = (I_{k_2, r} + K_{kr})(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1}) + \text{vec}(G_2(\beta)^{-1})\text{vec}(G_2(\beta)^{-1})' + O(n^{-1}).$$

The result in (18) implies that

$$E[b'_1G_2(\beta)b_1] = E[\{G_2(\beta)b_1b'_1\}] = \text{tr}\{G_2(\beta)G_2(\beta)^{-1}\} = kr. \tag{21}$$

Similarly, from (19) and (16), we have

$$E[b'_1G_2(\beta)b_2] = -\frac{1}{2}E[\text{tr}\{G_3(\beta)'(b'_1 \otimes b_1b'_1)\}]$$

$$= -\frac{1}{2\sqrt{n}} \text{tr}\left\{G_3(\beta)'G_2(\beta)^{-1}G_3(\beta)'G_2(\beta)^{-1} \otimes G_2(\beta)^{-1}\right\}. \tag{22}$$

Notice that $G_3(\beta)K_{kr} = G_3(\beta)$ holds because the derivative is invariant to changes in the order of differentiation. By using this fact and equation (20), the expectation of the first part in (17) is given by

$$E\left[\text{tr}\left\{G_3(\beta)'G_2(\beta)^{-1}G_3(\beta)(b_1b'_1 \otimes b_1b'_1)\right\}\right]$$

$$= \text{tr}\left\{G_3(\beta)'G_2(\beta)^{-1}G_3(\beta)'(I_{k_2, r} + K_{kr})(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1})\right\}$$

$$+ \text{vec}((G_2(\beta)^{-1}))'G_3(\beta)'G_2(\beta)^{-1}G_3(\beta)\text{vec}(G_2(\beta)^{-1}) + O(n^{-1})$$

$$= 2\text{tr}\left\{G_3(\beta)'G_2(\beta)^{-1}G_3(\beta)'(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1})\right\}$$

$$+ \text{vec}((G_2(\beta)^{-1}))'G_3(\beta)'G_2(\beta)^{-1}G_3(\beta)\text{vec}(G_2(\beta)^{-1}) + O(n^{-1}). \tag{23}$$

Moreover, since the derivative is invariant to changes in the order of differentiation, we can see that $G_4(\beta)K_{kr} = G_4(\beta)$ and

$$\text{tr}\left\{G_4(\beta)(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1})\right\} = \text{vec}(G_2(\beta)^{-1})'G_4(\beta)\text{vec}(G_2(\beta)^{-1}).$$

By using the above relations and equation (20), the expectation of the second part in (17) is given by

$$E\left[\text{tr}\{G_4(\beta)(b_1b'_1 \otimes b_1b'_1)\}\right]$$

$$= \text{tr}\left\{G_4(\beta)'(I_{k_2, r} + K_{kr})(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1})\right\}$$

$$+ \text{vec}(G_2(\beta)^{-1})G_4(\beta)\text{vec}(G_2(\beta)^{-1}) + O(n^{-1})$$

$$= 3\text{tr}\{G_4(\beta)(G_2(\beta)^{-1} \otimes G_2(\beta)^{-1})\} + O(n^{-1}). \tag{24}$$
Hence, from equations (17), (23), and (24), we can see that
\[
E \left[ \mathbf{b}' \mathbf{G}_2 \mathbf{b}_3 \right] = \text{tr} \left\{ \mathbf{G}_3'(\beta)' \mathbf{G}_2(\beta)^{-1} \mathbf{G}_3(\beta)(\mathbf{G}_2(\beta)^{-1} \otimes \mathbf{G}_2(\beta)^{-1}) \right\}
\]
\[
+ \frac{1}{2} \text{vec}((\mathbf{G}_2(\beta)^{-1}))'(\mathbf{G}_3(\beta)' \mathbf{G}_2(\beta)^{-1} \mathbf{G}_3(\beta) \text{vec}((\mathbf{G}_2(\beta)^{-1}))
\]
\[- \frac{1}{2} \text{tr} \left\{ \mathbf{G}_4(\beta)(\mathbf{G}_2(\beta)^{-1} \otimes \mathbf{G}_2(\beta)^{-1}) \right\} + O(n^{-1}).
\]

(25)

Consequently, by substituting \( E \left[ \mathbf{b}' \mathbf{G}_2(\beta) \beta \right] = 0 \), and equations (21), (22), and (25) into (15), the bias of \(-2\ell(\hat{\beta})\) to \( R \) is expanded as
\[
\mathcal{B} = 2kr + \frac{1}{n} \left\{ \alpha_1(\beta) + \alpha_2(\beta) - \alpha_3(\beta) \right\} + O(n^{-2}),
\]
where coefficients \( \alpha_1(\beta) \), \( \alpha_2(\beta) \), and \( \alpha_3(\beta) \) are given by
\[
\alpha_1(\beta) = \text{tr} \left\{ \mathbf{G}_3(\beta)' \mathbf{G}_2(\beta)^{-1} \mathbf{G}_3(\beta)(\mathbf{G}_2(\beta)^{-1} \otimes \mathbf{G}_2(\beta)^{-1}) \right\},
\]
\[
\alpha_2(\beta) = \text{vec}((\mathbf{G}_2(\beta)^{-1}))'(\mathbf{G}_3(\beta)' \mathbf{G}_2(\beta)^{-1} \mathbf{G}_3(\beta) \text{vec}((\mathbf{G}_2(\beta)^{-1})),
\]
\[
\alpha_3(\beta) = \text{tr} \left\{ \mathbf{G}_4(\beta)(\mathbf{G}_2(\beta)^{-1} \otimes \mathbf{G}_2(\beta)^{-1}) \right\}.
\]

(26)

The CAIC can then be defined by adding an estimated \( B \) to \(-2\ell(\hat{\beta})\), i.e.,
\[
\text{CAIC} = -2\ell(\hat{\beta}) + 2kr + \frac{1}{n} \left\{ \alpha_1(\hat{\beta}) + \alpha_2(\hat{\beta}) - \alpha_3(\hat{\beta}) \right\}.
\]

(27)

For an actual data analysis, an R-script for calculating the CAIC in (27) is provided in Appendix A.3. The CAIC improves the bias of the AIC to \( O(n^{-2}) \), although the order of the bias of the AIC is \( O(n^{-1}) \), i.e., the following equations are satisfied:
\[
R - E[AIC] = O(n^{-1}), \quad R - E[CAIC] = O(n^{-2}),
\]
where \( R \) is the risk function given by (13).

4. NUMERICAL STUDIES

In this section, we conduct numerical studies to show that the CAIC in (27) works better than the crude AIC in (14). To compare the performances of the AIC and the CAIC, the following two properties are considered:

(I) the selection probability: the frequency of the model chosen by minimizing the information criterion.

(II) the prediction error of the best model (\( PE_B \)): the risk function of the best model chosen by the information criterion, which is defined by
\[
PE_B = E[\mathcal{L}(\hat{\beta}_B)],
\]
where \( \mathcal{L}(\beta) \) is the loss function given by (12) and \( \hat{\beta}_B \) is the MLE of \( \beta \) under the best model.
Table 1: Selection probability of the model and the prediction error of the best model

<table>
<thead>
<tr>
<th>Case</th>
<th>m</th>
<th>Criterion</th>
<th>Selection Probability</th>
<th>PE_B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>AIC</td>
<td>M_1</td>
<td>M_2</td>
</tr>
<tr>
<td>1</td>
<td>20</td>
<td>AIC</td>
<td>1.81</td>
<td>0.29</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CAIC</td>
<td>3.19</td>
<td>0.66</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>AIC</td>
<td>0.01</td>
<td>0.00</td>
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<tr>
<td></td>
<td></td>
<td>CAIC</td>
<td>0.01</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>AIC</td>
<td>77.22</td>
<td>10.92</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CAIC</td>
<td>82.63</td>
<td>10.06</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>AIC</td>
<td>79.21</td>
<td>10.89</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CAIC</td>
<td>80.99</td>
<td>10.58</td>
</tr>
</tbody>
</table>

Note: The selection probability of the true model is marked in bold.

These two properties were evaluated by a Monte Carlo simulation with 10,000 iterations. The information criterion with the higher selection probability of the true model and the smaller prediction error of the best model is regarded as a high-performance model selector. In the basic concept of the AIC, a good model selection method is one that chooses the best model so that the prediction is improved. Hence, PE_B is a more important property than is the selection probability.

We prepared eight candidate models M_1, ..., M_8, with m = 20 and 50, n_i = 5 (i = 1, ..., m) and r = 2. An m x 8 matrix of explanatory variables X = (x_1, ..., x_m) was constructed as follows. The first column of X is 1_m, where 1_m is an m-dimensional vector of ones, and the remaining seven columns of X were generated randomly from the binomial distribution B(1, 0.5). Simulation data were generated from the multinomial distribution with the true cell probability consisting of \( \beta^\ast = (\beta_1^\ast, \beta_2^\ast)' \). In this simulation study, we prepared two \( \beta^\ast \), as follows:

Case 1 :  \( \beta_1^\ast = (0, 0.2, -1.0, 0, 0, 0, 0, 0)' \),  \( \beta_2^\ast = (-0.1, -0.4, 1.2, 0, 0, 0, 0, 0)' \),

Case 2 :  \( \beta_1^\ast = (-0.5, 0, 0, 0, 0, 0, 0, 0)' \),  \( \beta_2^\ast = (0.7, 0, 0, 0, 0, 0, 0, 0)' \).

The matrix of explanatory variables in M_j consists of the first j columns of X (j = 1, ..., 8). Thus, the true model in Case 1 is M_3, and the true model in Case 2 is M_1.

Table 1 shows the two properties (I) and (II). In the table, the selection probability of the true model is marked in bold. From this table, we can see that the selection probabilities and the prediction errors of the CAIC were improved in comparison with those of the AIC in all situations. We simulated several other models and obtained similar results.

5. CONCLUSION AND DISCUSSION

In this paper, we proposed the CAIC for selecting variables in the multinomial logistic regression model. The proposed CAIC improves the bias of the AIC to \( O(n^{-2}) \), although the order of the bias of the AIC is \( O(n^{-1}) \). By using relations between the moments of \( b_1 \) and expectations of the
derivatives of \(-\ell(\beta)\) instead of directly calculating the moments of \(y_i\) to evaluate the moments of \(b_1\), a simple expression of the CAIC is developed. Indeed, the bias correction term of the proposed CAIC is represented by only three matrices \(G_2(\hat{\beta}), G_3(\hat{\beta}),\) and \(G_4(\hat{\beta})\), which consist of the second, third, and fourth derivatives of \(-\ell(\beta)\). Even though expressions of \(G_2(\hat{\beta}), G_3(\hat{\beta}),\) and \(G_4(\hat{\beta})\) are not simple, we can derive the bias correction term of the CAIC from linear functions of \(G_2(\hat{\beta})^{-1}, G_3(\hat{\beta}),\) and \(G_4(\hat{\beta})\). This is a desirable character of the CAIC.

In all situations of the simulation study, the CAIC improved the crude AIC in the sense of making a high selection probability of the true model and a small prediction error of the best model chosen by the information criterion. However, the improvements were smaller when the sample size was large. This is natural because the CAIC is proposed so that the bias of the AIC is corrected when the sample size is small. Needless to say, the AIC and the CAIC are asymptotical equivalents. Hence, the difference between two criteria becomes small when the sample size is increased. The sample sizes of our simulation were 100 and 250. Nevertheless, a clear difference exists in the performances of the CAIC and the AIC. This difference indicates that the CAIC is valuable even when the sample size is not so small. Consequently, we recommend using the CAIC instead of the AIC for selecting multinomial logistic regression models.

The simple expression of the proposed CAIC is based on the property that the second derivatives of \(-\ell(\beta)\) do not depend on response variables. A generalized linear model (GLM) with a natural link and a known dispersion parameter, e.g., a logistic regression model or a Poisson regression model, will have this property. Then, we can simply express the bias-corrected AIC just like the proposed CAIC in (27) in the same way presented in Section 3. Namely, the bias-corrected AIC with constant second derivatives of the minus log-likelihood function may be stated by

$$\text{CAIC} = \text{AIC} + \gamma_1(\hat{\theta}) + \gamma_2(\hat{\theta}) - \gamma_3(\hat{\theta}),$$

where \(\hat{\theta}\) is the MLE of unknown parameter \(\theta\), and coefficients \(\gamma_1(\theta), \gamma_2(\theta),\) and \(\gamma_3(\theta)\) are given by

$$\gamma_1(\theta) = \text{tr}\left\{C(\theta)'H(\theta)^{-1}C(\theta)(H(\theta)^{-1} \otimes H(\theta)^{-1})\right\},$$

$$\gamma_2(\theta) = \text{vec}((H(\theta)^{-1}))'C(\theta)'H(\theta)^{-1}C(\theta)\text{vec}((H(\theta)^{-1})),$$

$$\gamma_3(\theta) = \text{tr}\left\{Q(\theta)(H(\theta)^{-1} \otimes H(\theta)^{-1})\right\}.$$

Here, \(H(\theta), C(\theta),\) and \(Q(\theta)\) are matrices consisting of the second, third, and fourth derivatives, respectively, of the minus log-likelihood function and are defined by (A.5) in Appendix A.2.

APPENDIX

A.1. EXPLICIT FORMS OF \(G_2(\beta), G_3(\beta),\) AND \(G_4(\beta)\)

In this subsection, for simplicity, we write \(\Sigma_i(\beta), p_i(\beta),\) and \(p_{ij}(\beta)\) as \(\Sigma_i, p_i,\) and \(p_{ij},\) respectively.
Notice that

\[
\frac{\partial p_i}{\partial \beta_j} = p_{ij} (e_j - p_i) x'_i, \quad (j = 1, \ldots, r),
\]

where \(e_j\) is the \(j\)th coordinate unit vector, which is used in equation (9). This result and equation (3) imply that

\[
\frac{\partial p_i}{\partial \beta'} = (p_{i1} (e_1 - p_i) x'_1, \ldots, p_{ir} (e_r - p_i) x'_r) = \Sigma_i \otimes x'_i.
\]

Substituting the above result into the definition of \(G_3(\beta)\) yields equation (6). Furthermore, from the definitions of \(G_3(\beta)\) and \(G_4(\beta)\), we can see that \(\Delta_{3,i}(\beta)\) and \(\Delta_{4,i}(\beta)\) in (7) and (8), respectively, satisfy

\[
\Delta_{3,i}(\beta) = \frac{\partial}{\partial \beta'} \otimes \Sigma_i, \quad \Delta_{4,i}(\beta) = \frac{\partial^2}{\partial \beta \partial \beta'} \otimes \Sigma_i.
\]

Notice that the \((a, b)\)th element of \(\Sigma_i\) is \(p_{ia} \delta_{ab} - p_{ia} p_{ib}\), where \(\delta_{ab}\) is the Kronecker delta, i.e., \(\delta_{aa} = 1\) and \(\delta_{ab} = 0\) for \(a \neq b\). This equation leads us to other expressions of \(\Delta_{3,i}(\beta)\) and \(\Delta_{4,i}(\beta)\), as follows:

\[
\Delta_{3,i}(\beta) = \sum_{a,b} \frac{\partial}{\partial \beta'} (p_{ia} \delta_{ab} - p_{ia} p_{ib}) \otimes e_a e'_b, \quad \Delta_{4,i}(\beta) = \sum_{a,b} \frac{\partial^2}{\partial \beta \partial \beta'} (p_{ia} \delta_{ab} - p_{ia} p_{ib}) \otimes e_a e'_b. \quad (A.1)
\]

Derivatives of \(p_{ia}\) are calculated as

\[
\frac{\partial p_{ia}}{\partial \beta} = p_{ia} (e_a - p_i) \otimes x_i,
\]

\[
\frac{\partial^2 p_{ia}}{\partial \beta \partial \beta'} = p_{ia} (e_a - p_i) (e_a - p_i)' \otimes x_i x'_i - p_{ia} \Sigma_i \otimes x_i x'_i
\]

\[
= p_{ia} \{ (e_a - p_i) (e_a - p_i)' - \Sigma_i \} \otimes x_i x'_i,
\]

\[
\frac{\partial^2 p_{ia} p_{ib}}{\partial \beta \partial \beta'} = p_{ib} \frac{\partial^2 p_{ia}}{\partial \beta \partial \beta'} + \frac{\partial p_{ia}}{\partial \beta} \frac{\partial p_{ib}}{\partial \beta'} + \frac{\partial p_{ia}}{\partial \beta} \frac{\partial p_{ib}}{\partial \beta'} + p_{ia} \frac{\partial^2 p_{ib}}{\partial \beta \partial \beta'}
\]

\[
= p_{ia} p_{ib} \{ (e_a + e_i - 2p_i) (e_a + e_i - 2p_i)' - 2\Sigma_i \} \otimes x_i x'_i.
\]

By substituting the above derivatives into (A.1), we have

\[
\Delta_{3,i}(\beta) = \sum_{a,b} \{ \delta_{ab} p_{ia} (e_a - p_i)' - p_{ia} p_{ib} (e_a - p_i)' \} \otimes x'_i \otimes e_a e'_b
\]

\[
= \sum_{a,b} \{ (\delta_{ab} - p_{ib}) (e_a - p_i)' - p_{ib} (e_a - p_i)' \} \otimes x'_i \otimes e_a e'_b
\]

\[
= \sum_{a=1}^r p_{ia} (e_a \otimes x_i)' \otimes \{ (e_a - p_i) (e_a - p_i)' \} - (p_i \otimes x_i)' \otimes \Sigma_i,
\]

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and

\[ \Delta_{i,j}(\beta) = \sum_{a,b} p_{ia} \left( \delta_{ab} \{(e_a - p_i)(e_a - p_i)' - \Sigma_i \} - p_{ib} \{(e_a + e_b - 2p_i)(e_a + e_b - 2p_i)' - 2\Sigma_i \} \right) \otimes x_i x_i' \otimes e_a e_b' \]

\[ = \sum_{a=1}^r p_{ia}(e_a - p_i)(e_a - p_i)' \otimes x_i x_i' \otimes (e_a e_a' - e_a p_i - p_i e_a') \]

\[ - \Sigma_i \otimes x_i x_i' \otimes (\Sigma_i - p_i p_i') \]

The above two equations indicate that explicit forms of \( G_3(\beta) \) and \( G_4(\beta) \) are given in (7) and (8), respectively.

### A.2. Expectations of derivatives of the minus log-likelihood function

In this subsection, we derive general formulas of the expectations of derivatives of the minus log-likelihood function. Let \( f(u|\theta) \) be a joint probability density function of \( u \) specified by \( q \)-dimensional parameter vector \( \theta \), and \( L(\theta) \) be a minus log-likelihood function defined by \( L(\theta) = -\log f(u|\theta) \). Suppose that

\[ \frac{\partial f}{\partial \theta_a} = \frac{\partial}{\partial \theta_a} f(u|\theta) \]

By carrying out tedious calculations, we have

\[ L_a = -\frac{f_a}{f} \]

\[ L_{ab} = L_a L_b - \frac{f_{ab}}{f} \]

\[ L_{abc} = \sum_{[3]} L_{[abc]} = L_{ab} L_{cd} + \sum_{[3]} L_{[abc]} \]

\[ L_{abcd} = \sum_{[4]} L_{[abcd]} = L_{ab} L_{cd} + \sum_{[3]} L_{[abcd]} \]

where \( \sum_{[j]} \) is the summation of a total of \( j \) terms of different combinations, e.g., \( \sum_{[3]} L_{ab} L_{cd} = L_{ab} L_{cd} + L_{ac} L_{bd} + L_{ad} L_{bc} \). It follows from \( \int f d\mathbf{u} = 1 \) that

\[ E \left[ \frac{f_{a_1 \cdots a_j}}{f} \right] = \int \frac{f_{a_1 \cdots a_j}}{f} f d\mathbf{u} = \int \frac{\partial^j}{\partial \theta_{a_1} \cdots \partial \theta_{a_j}} f d\mathbf{u} = \frac{\partial^j}{\partial \theta_{a_1} \cdots \partial \theta_{a_j}} \int f d\mathbf{u} = 0. \]  

The above equation can be satisfied when \( u \) is continuous. Even when \( u \) is discrete, we can obtain the same result by replacing the integration with a summation. Equations (A.2) and (A.3) imply that

\[ E[L_a] = 0, \quad E[\dot{L}_{ab}] = E[\dot{L}_a \dot{L}_b], \quad E[\dot{L}_{abc}] = -E[\dot{L}_a \dot{L}_b \dot{L}_c] + \sum_{[3]} E[\dot{L}_a \dot{L}_b \dot{L}_c], \]

\[ E[\dot{L}_{abcd}] = E[\dot{L}_a \dot{L}_b \dot{L}_c \dot{L}_d] - \sum_{[6]} E[\dot{L}_a \dot{L}_b \dot{L}_c \dot{L}_d] + \sum_{[3]} E[\dot{L}_a \dot{L}_b \dot{L}_c \dot{L}_d] + \sum_{[4]} E[\dot{L}_a \dot{L}_b \dot{L}_c \dot{L}_d]. \]  

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Let us consider a vector of the first derivatives, and matrices of the second, third, and fourth derivatives, which are defined as

$$
g(\theta) = -\frac{\partial}{\partial \theta} \ell(\theta), \quad H(\theta) = -\frac{\partial^2}{\partial \theta \partial \theta^T} \ell(\theta),$$

$$C(\theta) = -\left(\frac{\partial}{\partial \theta^T} \otimes \frac{\partial^2}{\partial \theta \partial \theta^T}\right) \ell(\theta), \quad Q(\theta) = -\left(\frac{\partial^2}{\partial \theta \partial \theta^T} \otimes \frac{\partial^2}{\partial \theta \partial \theta^T}\right) \ell(\theta).$$

(A.5)

From the expectations in (A.4), we obtain

$$E[H(\theta)] = E[g(\theta)g(\theta)^T],$$

$$E[C(\theta)] = -E[g(\theta)^T \otimes g(\theta)g(\theta)^T] + E[H(\theta) \otimes g(\theta)^T] + E[g(\theta)\text{vec}(H(\theta))^T],$$

$$E[Q(\theta)] = E[g(\theta)^T g(\theta)g(\theta)^T]$$

$$- (I_q^2 + K_q) E[g(\theta)^T g(\theta)^T \otimes H(\theta)] (I_q^2 + K_q) - E[\text{vec}(g(\theta)^T) \text{vec}(H(\theta))^T] - E[\text{vec}(H(\theta))^T \text{vec}(g(\theta)^T) \text{vec}(H(\theta))^T]$$

$$+ (I_q^2 + K_q) E[\{H(\theta) \otimes H(\theta)\}] + E[\text{vec}(H(\theta))^T \text{vec}(g(\theta)^T) \text{vec}(H(\theta))^T]$$

$$+ E[\{g(\theta) \otimes C(\theta)\}] (I_q^2 + K_q) + (I_q^2 + K_q) E[\{g(\theta)^T \otimes C(\theta)^T\}].$$

Recall that $E[g(\theta)] = 0_q$ holds. Furthermore, we note that $C(\theta)$ and $Q(\theta)$ are constant when $H(\theta)$ is constant. Hence, when $H(\theta)$ is constant, $H(\theta), C(\theta),$ and $Q(\theta)$ become simpler, as follows:

$$H(\theta) = E[g(\theta)g(\theta)^T],$$

$$C(\theta) = -E[g(\theta)^T \otimes g(\theta)g(\theta)^T],$$

$$Q(\theta) = E[g(\theta)^T g(\theta)g(\theta)^T] - (I_q^2 + K_q) \{H(\theta) \otimes H(\theta)\} - \text{vec}(H(\theta))^T \text{vec}(H(\theta))^T.$$

(A.7)

A.3. R-SCRIPT FOR CALCULATING THE CAIC

In this subsection, we provide the R-script for calculating the CAIC in (27). In the script, a variable $Y$ corresponds to the $m \times (r + 1)$ matrix whose $(a, b + 1)$th element is $y_{ab}$, and a variable $X$ corresponds to the $m \times k$ matrix $X$ whose first column is $1_m$. When we fit the multinomial logistic regression model to the data, it is only necessary to carry out the command `vglm(Y ~ X, family=multinomial).

```r
library(VGAM)

# X: Explanatory variables
# Y: Response variables
CAIC.MLRM.f <- function(X, Y){
    vec.func <- function(A){
        x <- dim(A)[1]
    }
}
```

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y <- dim(A)[2]
Res <- NULL
for (i in 1:y){
    temp <- t(t(A[,i]))
    Res <- rbind(Res,temp)}
}

ei.vec <- function(p,i){
e <- matrix(c(rep(0,p)),ncol=1)
e[i] <- 1
}

n <- sum(Y)
k <- dim(X)[2]
rho <- apply(Y,1,sum)/n

if(dim(X)[2]==1){est <- vglm(Y~1,family=multinomial)}
if(dim(X)[2]>1){est <- vglm(Y~X[-1],family=multinomial)}

AIC <- AIC(est)
P <- fitted(est)

G_2 <- matrix(0,(k*r),(k*r))
G_3 <- matrix(0,k*r,(k*r)^2)
G_4 <- matrix(0,(k*r)^2,(k*r)^2)
for (i in 1:m){
x_i <- X[i,]
xx_i <- x_i%*%t(x_i)
p_i <- P[i,-1]
pp_i <- p_i%*%t(p_i)
S_i <- diag(p_i)-pp_i
G_2 <- G_2+rho[i]*(S_i%x%xx_i)
D3 <- (-1)*(t(p_i%x%x_i)%x%S_i)
D4 <- (-1)*(S_i%x%xx_i%x%(S_i-pp_i))
for (j in 1:r){
e_j <- ei.vec(r,j)
\( e_{jj} <- e_j \times t(e_j) \)
\( r_j <- e_j - p_i \)
\( r_{jj} <- r_j \times t(r_j) \)
\( pe_j <- p_i \times t(e_j) \)
\( ep_j <- t(pe_j) \)
\( D3 <- D3 + p_i[j] \times (t(e_j) \times x_i) \times t(r_{jj}) \)
\( D4 <- D4 + p_i[j] \times (r_{jj} \times x_i) \times (e_{jj} - ep_j - pe_j) \)
for (s in 1:r)
\{
  e_s <- ei.vec(r, s)
  e_js <- e_j \times t(e_s)
  e_sj <- t(e_js)
  r_s <- e_s - p_i
  r_js <- r_j \times t(r_s)
  D4 <- D4 - p_i[j] \times p_i[s] \times (r_js \times x_i) \times (e_js + e_sj)
} \}
\( G_3 <- G_3 + \rho[i] \times D3 \times x_i \)
\( G_4 <- G_4 + \rho[i] \times D4 \times x_i \}
invG_2 <- solve(G_2)
vinvG_2 <- vec.func(invG_2)
a1 <- sum(diag(G_3 \times invG_2 \times t(G_3) \times invG_2))
a2 <- t(vinvG_2) \times t(G_3) \times invG_2 \times invG_2 \times G_3 \times invG_2
a3 <- sum(diag(G_4 \times invG_2 \times invG_2))
CAIC <- AIC + (1/n) \times (a1 + a2 - a3)
CAIC

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