Median bias reduction in cumulative link models

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ABSTRACT

This paper presents a novel estimation approach for cumulative link models, based on median bias reduction. The median bias reduced estimator is obtained as solution of an estimating equation based on an adjustment of the score. It allows to obtain higher-order median centering of maximum likelihood estimates without requiring their finiteness. The estimator is equivariant under componentwise monotone reparameterizations and the method is effective in preventing boundary estimates. Through simulation studies and an application, we compare the median bias reduced estimator with the two main competitors, the maximum likelihood and the mean bias reduced estimators. The method is seen to be highly successful in achieving median centering and shows remarkable properties under reparameterizations related to effect measure.

1. Introduction

Cumulative link models were proposed by McCullagh (1980), see also Agresti (2010), and are the most popular tool to handle ordinal outcomes, which are pervasive in many disciplines. One of the reasons for their popularity relies on the use of a single regression coefficient for each covariate for all response levels, making the effect simple to summarize. For these models, maximum likelihood (ML) is the most common estimation method. Despite this fact, it presents some problems and several proposals have been developed to solve them. One of the problems concerns the asymptotic approximation for the distribution of the ML estimator, which can be highly inaccurate with moderate sample information or sparse data. Another problem with ML estimation lies in boundary estimates, which can arise with positive probability in models for ordinal data and can cause several difficulties in the fitting process and inferential procedures.

The literature is rich in methods related to bias reduction of the ML estimator. Such methods can be distinguished (Kosmidis 2014a) into explicit methods, that focus on correcting the estimate, and implicit methods, based on correction of the estimating function. The main disadvantage of the former lies in the need for finiteness of ML estimates which is overcome by the latter, one of the reasons for their spread in applied statistics.

The estimation approaches based on an adjustment of the score allow, by introducing an asymptotically negligible bias in the score function, to obtain the mean bias reduced (mean BR) estimator, proposed by Firth (1993) and developed in Kosmidis and Firth (2009, 2010), and the median bias reduced (median BR) estimator, proposed by Kenne Pagui, Salvan, and Sartori (2017). A unified presentation for generalized linear models is given by Kosmidis, Kenne

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Supplemental data for this article is available online at https://doi.org/10.1080/03610918.2020.1869986.

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Pagui, and Sartori (2020) and for general models in Kenne Pagui, Salvan, and Sartori (2020). Such approaches do not require finiteness of the ML estimates. In addition, they are effective in preventing boundary estimates. The main difference between the two methods lies in the use of the mean and the median, respectively, as a centering index for the estimator. Mean BR achieves a first-order bias correction. The lack of equivariance under nonlinear reparameterizations is a disadvantage of this approach which is, however, overcome by practical advantages in applications. Median BR, proposed by Kenne Pagui, Salvan, and Sartori (2017) and further developed in Kenne Pagui, Salvan, and Sartori (2020), aims at median centering of the estimator, that is to obtain an estimator with the same probability of overestimating and underestimating each component of the true parameter value. This property is maintained under componentwise monotone reparameterizations. In the continuous case, the median BR estimator is componentwise third-order median unbiased.

Mean BR for cumulative link models is developed in Kosmidis (2014b), where finiteness and optimal frequentist properties are illustrated. However, the remarkable properties of mean BR are not preserved under nonlinear reparameterizations, such as the ordinal probability effect measure proposed by Agresti and Kateri (2017). On the other hand, median BR behaves equivariantly under such reparameterizations and may also turn out to be preferable to the transformed mean BR. Moreover, considering the ordinal probability effect measure proposed by Agresti and Kateri (2017), we exhibit the good performance achieved by the median BR estimator under componentwise monotone reparameterizations. Finally, we present an application where the median BR approach, like mean BR, is seen to be able to prevent boundary estimates.

2. Cumulative link models

Let $Y_i$ be the ordinal outcome, with $c$ categories, for subject $i$, $i = 1, ..., n$. Let $p_{ij} = \Pr(Y_i = j)$ be the probability to observe category $j$, $j = 1, ..., c - 1$, for subject $i$, and $\Pr(Y_i \leq j) = \sum_{k=1}^{j} p_{ik}$ the cumulative probability. With $x_{i}$, $i = 1, ..., n$, a $p$-dimensional row vector of covariates, the cumulative link model (McCullagh 1980) links the cumulative probabilities to a linear predictor, $\eta_{ij} = \alpha_{j} + x_{i}'\beta, j = 1, ..., c - 1$, via the relationship

$$g(\Pr(Y_i \leq j|x_{i})) = \eta_{ij},$$

(1)

where $g(\cdot)$ is a given link function and $\beta^\top = (\beta_1, ..., \beta_p)$ is the regression parameter vector. This class of models assumes that the effects of $x_{i}$, expressed through $\beta$, are the same for each $j = 1, ..., c - 1$. The intercept parameters $\alpha_{j}, j = 1, ..., c - 1$, satisfy $-\infty = \alpha_0 \leq \alpha_1 \leq ... \leq \alpha_{c-1} \leq \alpha_c = +\infty$, since $\Pr(Y_i \leq j)$ is increasing in $j$ for each fixed $x_{i}$. Model (1) has an interpretation in terms of an underlying latent variable (see e.g., Agresti 2010, Section 3.3.2), that is the ordinal outcome $Y_i$ can be seen as the discretization of a latent continuous random variable $Y_i^\ast$, satisfying a regression model $Y_i^\ast = -x_{i}'\beta + \varepsilon_{i}, i = 1, ..., n$. The random variables $\varepsilon_{i}$ are independent and identically distributed with $E(\varepsilon_i) = 0$ and cumulative distribution function $G(\cdot)$. By assigning threshold values $\alpha_{j}, j = 1, ..., c$, such that we observe $Y_i = j$ if $\alpha_{j-1} \leq Y_i^\ast < \alpha_{j}$, with $-\infty = \alpha_0 \leq \alpha_1 \leq ... \leq \alpha_{c-1} \leq \alpha_c = +\infty$, the equivalent formulation of model (1) is obtained

$$\Pr(Y_i \leq j|x_{i}) = \Pr(Y_i^\ast \leq \alpha_{j}|x_{i}) = \Pr(\varepsilon_{i} < \alpha_{j} + x_{i}'\beta) = G(\eta_{ij}),$$

with $j = 1, ..., c - 1$. Common choices for $G(\cdot)$ are the logistic, standard normal or extreme value distribution. The cumulative logit model, also known as proportional odds model (McCullagh
1980, Section 2), is obtained assuming $G(\eta_{ij}) = \exp(\eta_{ij})/\{1 + \exp(\eta_{ij})\}$, the cumulative probit model is recovered with $G(\eta_{ij}) = \Phi(\eta_{ij})$, and the cumulative complementary log-log link model, also known as proportional hazards model (McCullagh 1980, Section 3), setting $G(\eta_{ij}) = 1 - \exp\{-\exp(\eta_{ij})\}$.

The popularity of model (1) is linked to its parsimony since it uses a single parameter for each predictor, in addition to the latent variable interpretation. The cumulative link model can be inadequate because of misspecification of the linear predictor or due to departure from the assumption that the covariate effect is the same for each $j, j = 1, \ldots, c - 1$. Several models have been proposed that relax the latter assumption (for a detailed description see Fullerton and Xu 2016). Instances are the partial cumulative link model, which first appeared in the literature as partial proportional odds model (Peterson and Harrell 1990), or the nonparallel cumulative link model. Both include the cumulative link model as a special case. However, despite their flexibility, they may present some difficulties either from a computational or from the interpretation point of view, especially with data sets with several predictors.

### 2.1. Maximum likelihood, bias reduction and boundary estimates

As the sample size increases, the probability of unique ML estimates tends to one (McCullagh 1980, Section 6.3). However, for finite sample sizes, the ML estimator has a positive probability of being on the boundary of the parameter space. In cumulative link models (1), boundary estimates are estimates of the regression parameters with infinite components, and/or consecutive intercept estimates having the same value. Pratt (1981) showed that zero counts for a middle category $j, j = 2, \ldots, c - 1$, produce consecutive equal intercept estimates, that is $\hat{\beta}_{j-1} = \hat{\beta}_j$, and if the first or the last category have zero observed counts, then the estimates for $\beta_1$ or $\beta_{c-1}$ are infinite. Agresti (2010, Section 3.4.5) describes some settings where infinite ML estimates occur for the regression parameters.

Kosmidis (2014b) demonstrates that meanBR is a general effective strategy to prevent boundary estimates. The same advantage will be seen to hold for median BR in Secs. 4 and 5. With particular regard to boundary estimates of the intercept parameters, Kosmidis (2014b, Section 8.3, Remark 1) showed that the ML estimate of the regression parameters is invariant with respect to grouping of unobserved categories with the adjacent ones. So, likelihood inference on the regression parameters is possible if one or more categories are unobserved. The same appears to hold for mean BR and will be seen to hold in all examples considered for median BR. The only difference with respect to ML estimates is that if the first or the last category has zero counts, then the mean and median BR estimates are typically finite.

### 2.2. An ordinal probability effect measure

A useful monotone transformation of regression parameters related to binary covariates was proposed by Agresti and Kateri (2017) to overcome the difficulty for practitioners to interpret nonlinear measures, such as probits and odds ratios. This reparameterization allows an interpretation in terms of “ordinal superiority”, that is the probability that an observation from one group falls above an independent observation from the other group, adjusting for other covariates. For a vector of covariates $x = (x_1, \ldots, x_p)$, let $x_r$ a binary variable which is a group indicator for an observation. Let $Y_{i0}, Y_{i1}$ be the independent outcomes from the groups $x_{ir} = 0$ and $x_{ir} = 1$, respectively. For ordinal responses, the ordinal superiority measure, $\gamma \in [0, 1]$, is defined as

$$
\gamma = \Pr(Y_{i0} > Y_{i1}|x_i \setminus \{x_{ir}\}) + \frac{1}{2} \Pr(Y_{i0} = Y_{i1}|x_i \setminus \{x_{ir}\}).
$$

Based on model (1), Agresti and Kateri (2017) show that the exact ($=$) or approximate ($\approx$) expressions of $\gamma$ for the parameter related to the binary covariate, $\beta_r$, are $\gamma(\beta_r) \approx$
exp \left( -\beta_r / \sqrt{2} \right) / \{1 + \exp \left( -\beta_r / \sqrt{2} \right) \} \), considering the logit link function, \( \gamma(\beta) = \Phi(-\beta / \sqrt{2}) \) for the probit link, and \( \gamma(\beta) = \exp (-\beta_r / \sqrt{2}) \{1 + \exp (-\beta_r) \} \) for the complementary log-log link.

3. Median bias reduction

For a regular parametric model with \( p \)-dimensional parameter \( \theta = (\theta_1, \ldots, \theta_p^\top) \), let \( \ell(\theta) \) be the log-likelihood based on a sample of size \( n \) and \( U_r(\theta) = \partial \ell(\theta) / \partial \theta_r, r = 1, \ldots, p \), the \( r \)-th component of the score \( U(\theta) \). Moreover, let \( j(\theta) = -\partial^2 \ell(\theta) / \partial \theta \partial \theta^\top \) be the observed information matrix and \( i(\theta) = E_\theta \{ j(\theta) \} \) the expected information matrix, which we assume to be of order \( O(n) \). We denote with \( [i(\theta)^{-1}]_r \) the \( r \)-th column of \( i(\theta)^{-1} \) and with \( i''(\theta) \) the \( (r, r) \) element of \( i(\theta)^{-1} \).

The median BR estimator, \( \hat{\theta} \), is obtained as solution of the estimating equation \( \tilde{U}(\theta) = 0 \), where
\[
\tilde{U}(\theta) = U(\theta) + \tilde{A}(\theta),
\]
with
\[
\tilde{A}(\theta) = A^*(\theta) - i(\theta)F(\theta).
\]
The vector \( A^*(\theta) \) has components
\[
A^*_r = \frac{1}{2} \text{tr}\{i(\theta)^{-1}(P_r + Q_r)\},
\]
with \( P_r = E_\theta \{ U(\theta)U(\theta)^\top U_r \} \) and \( Q_r = -E_\theta \{ j(\theta)U_r \}, r = 1, \ldots, p \). The vector \( F(\theta) \) has components \( F_r = [i(\theta)^{-1}]_r F_r \), where \( F_r \) has elements
\[
F_{r,t} = \text{tr}\{h_r\{(1/3)P_t + (1/2)Q_t\}\}, \quad r, t = 1, \ldots, p,
\]
with the matrix \( h_r \) given by
\[
h_r = \frac{[i(\theta)^{-1}]_r [i(\theta)^{-1}]_r^\top}{i''(\theta)} , \quad r = 1, \ldots, p.
\]
We refer to Kenne Pagui, Salvan, and Sartori (2020) for further details about the computation of \( \tilde{A}(\theta) \) and for the relation with the mean BR estimator (Firth 1993), \( \hat{\theta}^* \). The latter is seen to be based on an adjusted score of the form (2) with \( \tilde{A}(\theta) = A^*(\theta) \).

Kenne Pagui, Salvan, and Sartori (2017) show that in the continuous case, each component of \( \tilde{\theta}, \hat{\theta}, r = 1, \ldots, p \), is median unbiased with an error of order \( O(n^{-3/2}) \), i.e., \( \text{Pr}_\theta(\tilde{\theta}_r \leq \theta_r) = \frac{1}{2} + O(n^{-3/2}) \), compared to the ML estimator, which is median unbiased with an error of order \( O(n^{-1/2}) \). Moreover, the asymptotic distribution of \( \tilde{\theta} \) is the same as that of the ML estimator, \( \hat{\theta} \), and of the mean BR estimator, \( \hat{\theta}^* \), that is \( N_p(\theta, i(\theta)^{-1}) \).

The quantities needed for computing (2) in cumulative link models (1) have been obtained using the simplified algebraic form developed in Kenne Pagui, Salvan, and Sartori (2020). Details are provided in the Supplementary Material. R code for implementation is available at https://homes.stat.unipd.it/eulogecloviskennepagui/content/links.

The equation \( \tilde{U}(\theta) = 0 \) is usually solved numerically, although a finite solution is not always guaranteed. The numerical solutions of \( \tilde{U}(\theta) = 0 \) can be obtained by a Fisher scoring-type algorithm, whose \((k+1)\)-th iteration is
\[
\theta^{(k+1)} = \theta^{(k)} + i(\theta^{(k)})^{-1}U(\theta^{(k)}) + i(\theta^{(k)})^{-1}\tilde{A}(\theta^{(k)}),
\]
which differs from the analogue for the ML estimates only by the addition of the term \( i(\theta^{(k)})^{-1}\tilde{A}(\theta^{(k)}) \). We adopt, as a stopping criterion for the algorithm, the condition \( |\tilde{U}(\theta^{(k)})| < q \), for every \( r = 1, \ldots, p \), and we set, as default, \( q = 10^{-10} \).
The algorithm needs a starting value, \( \theta^{(0)} \), whose determination is not trivial and can result in nonconvergence of (3). When available, the ML estimate, \( \hat{\theta} \), or the mean BR estimate, \( \hat{\theta}^* \), are suitable starting values, which are also able to speed up the convergence. We set the starting values following a strategy similar to that used in Christensen (2019) for cumulative link models (1). The starting value for the regression coefficients, \( \beta \), is set to zero. The intercept parameters, \( \alpha_j, j = 1, \ldots, c - 1 \), are initialized to \( \alpha_j^{(0)} = G^{-1}(j/c) \), where \( G(\cdot) \) is the cumulative distribution function of the error terms, according to the latent variable interpretation discussed in Sec. 2.

In order to recognize boundary estimates, we adapt the diagnostics in Lesaffre and Albert (1989), identifying infinite estimates if their absolute value and the corresponding standard error are greater than some thresholds. Categories with zero observed counts are grouped, except when it happens at the extreme categories.

4. Simulation study

We conducted a simulation study to assess the performance of the median BR estimator, \( \hat{\theta} \), in cumulative link models (1) with \( \theta = (x^\top \beta)^\top \). We compare it with the ML, \( \hat{\theta} \), and mean BR, \( \hat{\theta}^* \), estimators in terms of empirical probability of underestimation (PU%), estimated relative (mean) bias (RB%), and empirical coverage of the 95% Wald-type confidence interval (WALD%).

We consider sample sizes, \( n = 50, 100, 200 \), and different link functions \( g(\cdot) \), namely the logit, probit and complementary log-log (cloglog) link functions. We generate the covariate \( x_1 \) from a standard Normal, \( x_2 \) and \( x_3 \) from Bernoulli distributions with probabilities 0.5 and 0.8 respectively, and \( x_4 \) from a Poisson with mean 2.5. Assuming that the response has three categories, we fit the model

\[
g\{\Pr(Y_i \leq j|x_i)\} = \alpha_j + x_{i1}\beta_1 + x_{i2}\beta_2 + x_{i3}\beta_3 + x_{i4}\beta_4, \quad j = 1, 2; \quad i = 1, \ldots, n,
\]

considering 10,000 replications, with covariates fixed at the observed value and true parameter \( \theta_0 \). Setting \( \theta_0 = (-1, 2, 1, -1, 1, -1) \) for the logit link function, approximate relations with parameters for different link functions are obtained through a first order Taylor expansion of \( g(\cdot) \) around 0.5. In particular, probit and complementary log-log parameters are approximately equal to logit parameters times 0.6 and 0.7, respectively, with the addition of \(-0.4\) for complementary log-log intercept parameters. This leads to \( \theta_0 = (-0.6, 1.2, 0.6, -0.6, 0.6, -0.6) \) for the probit link function, and \( \theta_0 = (-1.1, 1, 0.7, -0.7, 0.7, -0.7) \) for the complementary log-log link function.

Table 1 contains the numerical results for all link functions considered. Boundary estimates occurred using ML with percentage frequencies 2.82%, 2.75% and 2.44%, with \( n = 50 \), and 0.08%, 0.1% and 0.04%, with \( n = 100 \), for the logit, probit and complementary log-log link functions, respectively. Instead, mean and median BR estimates are always finite. It appears that the new method proves to be remarkably accurate in achieving median centering and shows a lower estimated relative bias than ML and comparable with that of the mean BR estimator, as well as a good empirical coverage of the 95% Wald-type confidence intervals. The differences between the three estimators are appreciable in lower sample size settings and become much less pronounced as the sample size increases.

Table 2 shows the estimated relative bias under monotone reparameterizations of the parameters related to the binary covariates, considering the ordinal probability effect measure presented in Sec. 2.2. In the new parameterization, it appears that the median BR estimator has the best performance in terms of estimated relative bias, if compared with ML and mean BR, which is not equivariant under this type of reparameterization.
and crashing the grapes, \( x_1 \), and contact between juice and skin, \( x_2 \). Each factor has two levels, “cold” and “warm” for temperature and “yes” and “no” for contact. For each of the four treatment

| Link  | \( \beta_1 \) | \( \beta_2 \) | \( \beta_3 \) | \( \beta_4 \) |
|-------|--------------|--------------|--------------|--------------|
| logit | 40.94        | 14.50        | 94.97        |              |
|       | 55.34        | 14.90        | 94.76        |              |
|       | 44.63        | 13.50        | 96.48        |              |
|       | 62.99        | 16.50        | 95.19        |              |
|       | 54.14        | -0.50        | 95.94        |              |
|       | 48.38        | 0.90         | 96.35        |              |
|       | 53.01        | -0.30        | 96.96        |              |
|       | 45.71        | 0.40         | 94.46        |              |
| probit| 50.83        | 2.90         | 95.92        |              |
|       | 50.12        | 4.20         | 95.89        |              |
|       | 50.12        | 8.70         | 97.03        |              |
|       | 50.22        | 4.30         | 95.54        |              |
| cloglog| 40.31       | 14.50        | 94.12        |              |
|       | 55.40        | 14.67        | 94.26        |              |
|       | 45.35        | 12.67        | 96.35        |              |
|       | 63.26        | 15.83        | 94.16        |              |
|       | 53.79        | -0.83        | 95.56        |              |
|       | 48.67        | 0.67         | 96.06        |              |
|       | 52.93        | -1.33        | 97.13        |              |
|       | 44.93        | -0.33        | 94.87        |              |
|       | 50.81        | 2.33         | 95.54        |              |
|       | 50.46        | 3.50         | 95.71        |              |
|       | 50.24        | 6.00         | 96.89        |              |
|       | 49.67        | 3.33         | 95.36        |              |
|       | 39.59        | 15.29        | 94.07        |              |
|       | 55.42        | 13.86        | 94.25        |              |
|       | 46.72        | 15.57        | 95.46        |              |
|       | 62.53        | 16.00        | 94.23        |              |
|       | 55.26        | -1.14        | 95.36        |              |
|       | 48.95        | 0.57         | 96.09        |              |
|       | 54.39        | -0.86        | 95.83        |              |
|       | 44.90        | 0.29         | 94.73        |              |
|       | 51.31        | 2.57         | 95.40        |              |
|       | 50.55        | 3.43         | 95.72        |              |
|       | 50.77        | 12.14        | 96.04        |              |
|       | 49.95        | 4.14         | 95.29        |              |

Table 2. Estimated relative bias (RB%) for \( \gamma(\beta_2) \) and \( \gamma(\beta_3) \). For ML, RB% is conditional upon finiteness of the estimates.

| Link  | \( \gamma(\beta_2) \) | \( \gamma(\beta_3) \) |
|-------|------------------------|------------------------|
| logit | -1.05                  | -1.30                  |
|       | -0.42                  | -1.30                  |
|       | -0.18                  | -1.70                  |
|       | -0.18                  | -0.09                  |
|       | -0.14                  | -0.10                  |
|       | -0.10                  | -0.14                  |
|       | -0.11                  | -0.18                  |
|       | -0.05                  | -0.18                  |
|       | -0.61                  | -0.33                  |
|       | -0.16                  | -1.36                  |

5. Application

We consider the data analyzed in Randall (1989), related to a factorial experiment for investigating the factors that affect the bitterness of wine. There are two factors, temperature at the time of crashing the grapes, \( x_1 \), and contact between juice and skin, \( x_2 \). Each factor has two levels, “cold” and “warm” for temperature and “yes” and “no” for contact. For each of the four treatment
conditions, two bottles were assessed by a panel of nine judges, giving \( n = 72 \) observations. As in Christensen (2019, Section 4.8), we consider the outcomes obtained by combining the three central categories and we fit the model

\[
\text{logit}\left\{ \Pr(Y_i \leq j | x_i) \right\} = \alpha_j + x_{i1}\beta_1 + x_{i2}\beta_2, \quad j = 1, 2; \quad i = 1, \ldots, 72.
\]

Table 3 shows the coefficient estimates obtained with ML, mean BR and median BR. Both mean and median BR approaches are able to solve the boundary estimates problem.

Table 4 shows the simulation results for the regression parameters considering 10,000 replications, with covariates fixed at the observed value and true parameter \( \theta_0 = (−1, 4, −2, −1) \). We found 979 samples out of 10,000 with ML boundary estimates. Instead, mean and median BR estimates are always finite. Therefore, results in Table 4 for percentage relative bias and coverage of ML are conditional upon finiteness and comparisons should be made with caution. In particular, an explanation of the high relative bias of median BR estimator of \( \beta_1 \) is that, although finite, the estimator could be quite large because of the smaller shrinkage performed by median BR in comparison with mean BR. On the other hand, median BR is again highly accurate in achieving median centering and shows a good empirical coverage of the 95% Wald-type confidence intervals.

Under the monotone reparameterization of the coefficients related to the binary covariates, proposed by Agresti and Kateri (2017) and presented in Sec. 2.2, the estimated percentage relative bias is \(-0.81\% , -1.79\% \) and \(-0.15\% \) for \( \gamma(\beta_1) \), and \( 0.69\% , -0.94\% \) and \(-0.13\% \) for \( \gamma(\beta_2) \), with ML, mean BR and median BR, respectively. For ML, it should be recalled that the estimated relative bias is conditional upon finiteness of the estimates. It is noteworthy that the median BR estimator has lower estimated relative mean bias that the ML and the transformed mean BR estimators.

### 6. Discussion

This paper proposes to use the adjusted score function for median bias reduction in cumulative link models. The resulting median BR estimator has probability 1/2 of underestimating each component of the true parameter value with high accuracy. Despite the fact that ML is the estimation method of choice for cumulative link models, the approaches based on an adjustment of the score aiming at mean and median BR have proven to be a notable improvement with respect to ML with moderate sample sizes. In this context, simulation studies confirm that median BR succeeds in achieving componentwise median centering, showing a smaller median bias than ML and mean BR estimators. Moreover, median BR exhibits a noteworthy smaller bias than the ML, as
well as a good empirical coverage of the Wald-type confidence intervals. In addition, median BR, as mean BR, is seen to be able to prevent ML boundary estimates, which can arise in models for ordinal data. Simulation results have also shown that median BR is preferable to ML and mean BR under some monotone reparameterizations of regression parameters related to binary covariates.

**Funding**

Alessandra Salvan was supported by the University of Padova under grant BIRD185955.

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