Empirical Best Prediction Under Unit-Level Logit Mixed Models

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The article applies unit-level logit mixed models to estimating small-area weighted sums of probabilities. The model parameters are estimated by the method of simulated moments (MSM). The empirical best predictor (EBP) of weighted sums of probabilities is calculated and compared with plug-in estimators. An approximation to the mean-squared error (MSE) of the EBP is derived and a bias-corrected MSE estimator is given and compared with parametric bootstrap alternatives. Some simulation experiments are carried out to study the empirical behavior of the model parameter MSM estimators, the EBP and plug-in estimators and the MSE estimators. An application to the estimation of poverty proportions in the counties of the region of Valencia, Spain, is given.

Key words: Poverty; method of moments; logit mixed models; empirical best predictor; mean-squared error; bootstrap.

1. Introduction

This article deals with the estimation of weighted sums of probabilities in domains where the sample size is not large enough to obtain reliable direct estimates. Small-area estimation (SAE) deals with this problem by introducing model-based or model-assisted estimators. See the monographs of [Rao \(2003\)](#) and [Rao and Molina \(2015\)](#), and the reviews of [Ghosh and Rao \(1994\)](#), [Rao \(1999\)](#), [Pfeffermann \(2002, 2013\)](#), and [Jiang and Lahiri \(2006\)](#) for an introduction to SAE.

The binomial-logit mixed models are generalized linear mixed models (GLMM) that take into account the between-domains variability that it is not explained through auxiliary variables by introducing random effects. The random effects are usually assumed to be normally distributed. Inferences based on GLMMs have some computational difficulties because the likelihood may involve high-dimensional integrals which cannot be evaluated analytically. This article uses the method of simulated moments (MSM), introduced by [Jiang \(1998\)](#), to fit the proposed model. This method approximates the method of moments (MM), is computationally attractive, and gives consistent estimators of model parameters.

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The article derives empirical best predictors (EBP) for estimating weighted sums of probabilities, where the weights are known quantities taken from administrative registers or census files. This is to say, the term “weighting” is distinct from sample survey weighting based on the survey design. The EBPs are sums of predicted values of probabilities (sometimes called soft estimates) rather than sums of target-variable predictions that must be 0 or 1 (hard estimates). The statistical methodology is taken and adapted from [Jiang and Lahiri \(2001\)](#) and [Jiang \(2003\)](#), where EBPs of functions of fixed effects and small-area-specific random effects were developed in the context of logistic mixed models and GLMM respectively. Furthermore, plug-in estimators are considered and empirically studied in simulation experiments.

The MSE is a standard accuracy measure for point estimators. [Jiang and Lahiri \(2001\)](#) and [Jiang \(2003\)](#) studied the approximation of the MSE of the EBP in the context of binary data and GLMM. Their approach is based on Taylor series expansions. They further gave a second-order bias-corrected estimator of the MSE. We adapt the MSE calculations given by these authors to the case of EBPs of weighted sums of probabilities. We give two analytical estimators of the MSE approximation, without and with a bias-correction term. As these MSE estimators are computationally expensive in practice, we consider the parametric bootstrap estimator introduced by [Gonzalez-Manteiga et al. \(2007\)](#) in the context of logistic mixed models. This approach was later extended by [Gonzalez-Manteiga et al. \(2008a,b\)](#) to nested error regression models and to multivariate area-level models respectively. As the simple parametric bootstrap method tends to underestimate the MSE when domain sizes are too small, we also give a double-bootstrap bias-corrected estimator by following [Hall and Maiti \(2006a,b\)](#).

[Jiang and Lahiri \(2001\)](#) and [Jiang \(2003\)](#) introduced the basic statistical methodology for EBPs of functions of fixed and random effects. They also studied the large sample properties of the EBPs and MSE estimators. However, they did not carry out simulation experiments to empirically investigate the behavior of the EBPs and MSE estimators in the standard small-area estimation setup, that is when the domain sample sizes are small. They also did not present applications to real data. This article in part covers this gap.

We carry out simulation experiments to investigate the behavior of the EBPs of weighted sums of probabilities and the corresponding MSE estimators. We investigate computational and numerical issues appearing in the implementation of the EBP methodology. The article also presents an application to 2012 data from the Spanish living conditions survey (SLCS2012) in the region of Valencia. The target of the application is the estimation of poverty proportions at county level.

Other SAE models for the estimation of poverty proportions are currently available. Without being exhaustive, we cite some basic references here. [Chambers et al. \(2012\)](#) introduce an M-quantile regression approach for binary data. [Farrell et al. \(1997\)](#) give bootstrap adjustments for empirical Bayes interval estimates of small-area proportions. [Malec et al. \(1997\)](#) gave some small-area inference methods for binary variables. By using unit-level linear mixed models, [Molina et al. \(2014\)](#) and [Molina and Rao \(2010\)](#) give several procedures for estimating poverty indicators. There is also [Elbers et al. \(2003\)](#) and its extensions, who use full unit record census data, rather than building a model-based census substitute from cross tabulations. Based on temporal and spatio-temporal area-level

models, [Esteban et al. \(2012a,b\)](#), [Marhuenda et al. \(2013\)](#), and [Morales et al. \(2015\)](#) give EBLUPs of poverty proportions.

The article is organized as follows. Section 2 introduces the unit-level binomial-logit mixed model and the employed fitting algorithm. Section 3 presents the EBPs (which in this article are synthetic because they assume random effects given small area are zero mean) and the plug-in estimators of weighted sums of probabilities. Section 4 gives an approximation to the MSE of the EBP and four estimators. The first two MSE estimators are plug-in derivations of the MSE approximation, without and with bias correction term. The third and fourth MSE estimators are based on parametric bootstrap. Section 5 presents three simulation experiments. The first simulation studies the behavior of the MSM fitting algorithm. The second simulation compares the performances of the EBPs and the plug-in estimators. The third simulation deals with the MSE estimators proposed in Section 4. All use relatively small populations in comparison with real-life applications. Section 6 applies the developed methodology to data from the SLCS2012 using model-based synthetic estimators with small-area level random effects only. The target is the estimation of poverty proportions at county level. Section 7 gives a discussion and some conclusions.

The article contains four appendixes. [Appendix A.1](#) gives the components of the updating equation of the MSM algorithm. [Appendix A.2](#) contains the proof of Proposition 4.1. [Appendix A.3](#) presents some routines for MSE calculation and [Appendix A.4](#) describes approximations of some derivatives needed for MSE calculation.

The article employs the notation $\mathbf{a} = \text{col}_{1 \leq i \leq I} (a_i)$ and $\mathbf{b} = \text{col}'_{1 \leq i \leq I} (b_i)$ for column and row vectors of size I respectively.

2. The Model

This section introduces a unit-level binomial-logit mixed model and its MSM fitting algorithm. Let D be the number of small areas or domains, with $d = 1, \dots, D$. Let $\{v_d : d = 1, \dots, D\}$ be a set of independent and identically distributed (i.i.d.) $N(0, 1)$ random effects, which is a reasonable assumption for sufficiently large domains. Note that in this model, random effects at finer levels are not considered. In matrix notation, we have $\mathbf{v} = (v_1, \dots, v_D)' \sim N_D(\mathbf{0}, \mathbf{I}_D)$, where $\mathbf{I}_D$ is the $D \times D$ unit matrix. The target variable y_{dj} represents the j th sample observation from domain d and its distribution, conditioned to the random effect v_d , is

$$y_{dj} | v_d \sim \text{Bin}(m_{dj}, p_{dj}), \quad d = 1, \dots, D, \quad j = 1, \dots, n_d, \quad (2.1)$$

where m_{dj} is a known size parameter. The binomial distribution is typically employed for counting numbers of successes. In official statistics, the sample units can be individuals, households, companies and so on. For individuals, we can investigate the presence of a characteristic of interest and the corresponding size parameter is one. For households and companies, we might be interested in counting the number of household members with lactose intolerance or the number of employees with a high salary. Then the size parameter is the number of household members or company workers, respectively. In all cases, we can assume that the size parameters are known quantities for the sampled elements. Note that in the model there is assumed to be no clustering at survey primary sampling unit level or at household level.

For the natural parameter, we assume

$$\eta_{dj} = \log \frac{p_{dj}}{1 - p_{dj}} = \mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d, \quad d = 1, \dots, D, \quad j = 1, \dots, n_d, \quad (2.2)$$

where $\phi > 0$ is a variance parameter, $\boldsymbol{\beta} = \text{col}_{1 \leq k \leq p}(\beta_k)$ is the column vector of regression parameters and $\mathbf{x}_{dj} = \text{col}'_{1 \leq k \leq p}(x_{djk})$ is a row vector of auxiliary variables. We also assume that the y_{dj} 's are independent conditioned to $\mathbf{v}$. It holds that

$$P(y_{dj}|\mathbf{v}) = P(y_{dj}|v_d) = \binom{m_{dj}}{y_{dj}} p_{dj}^{y_{dj}} (1 - p_{dj})^{m_{dj} - y_{dj}}, \quad (2.3)$$

$$p_{dj} = \frac{\exp\{\mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d\}}{1 + \exp\{\mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d\}}.$$

Let us define $\mathbf{y} = \text{col}_{1 \leq d \leq D}(\mathbf{y}_d)$, where $\mathbf{y}_d = \text{col}_{1 \leq j \leq n_d}(y_{dj})$. The marginal distribution of $\mathbf{y}$ is

$$P(\mathbf{y}) = \prod_{d=1}^D \int_R P(\mathbf{y}_d|v_d) f(v_d) dv_d,$$

where f is the standard normal probability density function and

$$P(\mathbf{y}_d|v_d) = \prod_{j=1}^{n_d} P(y_{dj}|v_d) = \prod_{j=1}^{n_d} \binom{m_{dj}}{y_{dj}} \frac{\exp\{y_{dj}(\mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d)\}}{[1 + \exp\{\mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d\}]^{m_{dj}}}$$

$$= \exp \left\{ \sum_{j=1}^{n_d} \log \binom{m_{dj}}{y_{dj}} + \sum_{j=1}^{n_d} y_{dj}(\mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d) - \sum_{j=1}^{n_d} m_{dj} \log[1 + \exp\{\mathbf{x}_{dj} \boldsymbol{\beta} + \phi v_d\}] \right\}.$$

Let $\boldsymbol{\theta} = (\boldsymbol{\beta}', \phi)'$ be the vector of model parameters. To fit the unit-level binomial-logit mixed model, we employ the MSM algorithm suggested by [Jiang \(1998\)](#). A natural set of equations for applying the method of moments is

$$0 = f_k(\boldsymbol{\theta}) = M_k(\boldsymbol{\theta}) - \hat{M}_k = \sum_{d=1}^D \sum_{j=1}^{n_d} E_{\boldsymbol{\theta}}[y_{dj}] x_{djk} - \sum_{d=1}^D \sum_{j=1}^{n_d} y_{dj} x_{djk}, \quad k = 1, \dots, p,$$

$$0 = f_{p+1}(\boldsymbol{\theta}) = M_{p+1}(\boldsymbol{\theta}) - \hat{M}_{p+1} = \sum_{d=1}^D E_{\boldsymbol{\theta}}[y_{d.}^2] - \sum_{d=1}^D y_{d.}^2,$$

where $y_{d.} = \sum_{j=1}^{n_d} y_{dj}$. For solving this system of nonlinear equations, which involve matching mean and sums of squares, the Newton-Raphson updating formula is

$$\boldsymbol{\theta}^{(r+1)} = \boldsymbol{\theta}^{(r)} - \mathbf{H}^{-1}(\boldsymbol{\theta}^{(r)}) \mathbf{f}(\boldsymbol{\theta}^{(r)}), \quad (2.4)$$

where $\theta_1 = \beta_1, \dots, \theta_p = \beta_p, \theta_{p+1} = \phi$ and

$$\boldsymbol{\theta} = \text{col}_{1 \leq k \leq p+1}(\theta_k), \quad \mathbf{f}(\boldsymbol{\theta}) = \text{col}_{1 \leq k \leq p+1}(f_k(\boldsymbol{\theta})), \quad \mathbf{H}(\boldsymbol{\theta}) = \left(\frac{\partial f_k(\boldsymbol{\theta})}{\partial \theta_\ell} \right)_{k, \ell=1, \dots, p+1}.$$

[Appendix A.1](#) gives the components of vector $\mathbf{f}$ and matrix $\mathbf{H}$ appearing in (2.4). As the expectations appearing in the components cannot be explicitly calculated, they are

approximated by Monte Carlo simulation. As the algorithm seed for β , we use $\beta^{(0)} = \tilde{\beta}$, where $\tilde{\beta}$ is the maximum-likelihood estimator under the model without random effects. In that model, the natural parameters are

$$\eta_{dj} = \mathbf{x}_{dj}\beta, \quad d = 1, \dots, D, \quad j = 1, \dots, n_d.$$

Concerning the variance parameter, we use

$$\phi^{(0)} = \left(\frac{1}{n} \sum_{d=1}^D \sum_{j=1}^{n_d} (\tilde{\eta}_{dj} - \hat{\eta}_{d.}^{dir})^2 \right)^{1/2}, \quad \hat{\eta}_{d.}^{dir} = \log \frac{\hat{p}_{d.}^{dir}}{1 - \hat{p}_{d.}^{dir}},$$

$$\hat{p}_{d.}^{dir} = \frac{1}{n_d} \sum_{j=1}^{n_d} \frac{y_{dj}}{m_{dj}}, \quad \tilde{\eta}_{dj} = \mathbf{x}_{dj}\tilde{\beta},$$

where $n = \sum_{d=1}^D n_d$ is the total sample size. A bootstrap algorithm to estimate $\text{var}(\hat{\theta})$ is

1. Fit the Model (2.1)–(2.2) to the sample and calculate $\hat{\theta}$.
2. Generate bootstrap samples $\{y_{dj}^{(b)} : d = 1, \dots, D, j = 1, \dots, n_d\}$, $b = 1, \dots, B$, from the fitted model. Fit the Model (2.1)–(2.2) to the bootstrap samples and calculate $\hat{\theta}^{(b)}$, $b = 1, \dots, B$, and $\bar{\theta} = \frac{1}{B} \sum_{b=1}^B \hat{\theta}^{(b)}$.
3. Output: $\widehat{\text{var}}_B(\hat{\theta}) = \frac{1}{B} \sum_{b=1}^B (\hat{\theta}^{(b)} - \bar{\theta})(\hat{\theta}^{(b)} - \bar{\theta})'$.

3. Empirical Best Prediction

Let us assume that the unit-level binomial-logit mixed model (2.1)–(2.2), with random effects at domain level only, holds for all the units of a population U partitioned into D domains $U_1, \dots, U_D$ of sizes $N_1, \dots, N_D$. The best predictor (BP) of $p_{dj} = p_{dj}(\theta, v_d)$ and of the sum of probabilities $\mu_d = \mu_d(\theta, v_d) = \sum_{j=1}^{n_d} p_{dj}$ is

$$\hat{p}_{dj}(\theta) = E_{\theta}[p_{dj}|y_d] = \frac{\int_R \frac{\exp\{\mathbf{x}_{dj}\beta + \phi v_d\}}{1 + \exp\{\mathbf{x}_{dj}\beta + \phi v_d\}} P(y_d|v_d) f(v_d) dv_d}{\int_R P(y_d|v_d) f(v_d) dv_d} = \frac{A_{dj}}{C_d},$$

$$\hat{\mu}_d(\theta) = \sum_{j=1}^{n_d} \hat{p}_{dj}(\theta),$$

where f is the standard normal probability density function and

$$A_{dj} = \int_R \frac{\exp\{\mathbf{x}_{dj}\beta + \phi v_d\}}{1 + \exp\{\mathbf{x}_{dj}\beta + \phi v_d\}} \exp\left\{ \phi y_d v_d - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{\mathbf{x}_{di}\beta + \phi v_d\}] \right\} f(v_d) dv_d,$$

$$C_d = \int_R \exp\left\{ \phi y_d v_d - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{\mathbf{x}_{di}\beta + \phi v_d\}] \right\} f(v_d) dv_d. \quad (3.1)$$

The EBP of p_{dj} and μ_d are $\hat{p}_{dj}(\hat{\theta})$ and $\hat{\mu}_d(\hat{\theta})$ and they can be approximated by Monte Carlo simulation. If at least one of the auxiliary variables is continuous, the calculation of $\hat{\mu}_d(\hat{\theta})$ requires the availability of census files with the values of $\mathbf{x}_{dj}$ for all the units $j \in U_d$. Two data files (survey and census), with the same auxiliary variables, are then needed to

calculate the EBP of μ_d in this setup. In the real data case of Section 6, the x -values are only available for the sample units. The nonavailability of census data is the standard situation for the living conditions public statistics in most countries. This is why we study the special case where the covariates are categorical and take a finite number of values. For this last case, the EBPs can be calculated without having a full unit-record census file, with the caveats that using various cross-tabulations implies a specific, untested census structure, and excludes the use of continuous variables in the survey-based binomial-logit mixed model. However, the external-to-sample information can be obtained more easily from cross tabulations, as detailed unit-record data have limited availability.

Let us assume that $\mathbf{x}_{dj} \in \{\mathbf{z}_1, \dots, \mathbf{z}_K\}$ for all d and j . Define

$$\bar{\mu}_d = \frac{\mu_d}{N_d}, \quad \mu_d = \sum_{j=1}^{N_d} p_{dj} = \sum_{k=1}^K N_{dk} q_{dk}, \quad q_{dk} = \frac{\exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}}{1 + \exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}} \quad (3.2)$$

and $N_{dk} = \#\{j \in U_d : \mathbf{x}_{dj} = \mathbf{z}_k\}$ is the known size of the covariate class $\mathbf{z}_k$ at the domain d . The target of this section is the estimation of the parameters defined in (3.2).

The BP of the random effect, v_d , and of the weighted sums of probabilities, μ_d and $\bar{\mu}_d$, are

$$\hat{v}_d(\boldsymbol{\theta}) = E_{\boldsymbol{\theta}}[v_d | \mathbf{y}_d] = \frac{\int_R v_d P(\mathbf{y}_d | v_d) f(v_d) dv_d}{\int_R P(\mathbf{y}_d | v_d) f(v_d) dv_d} = \frac{A_d^v}{C_d}, \quad (3.3)$$

$$\hat{\mu}_d(\boldsymbol{\theta}) = E_{\boldsymbol{\theta}}[\mu_d | \mathbf{y}_d] = \sum_{k=1}^K N_{dk} E_{\boldsymbol{\theta}}[q_{dk} | \mathbf{y}_d] =: \psi_d(\mathbf{y}_d, \boldsymbol{\theta}), \quad \hat{\bar{\mu}}_d(\boldsymbol{\theta}) = \frac{\hat{\mu}_d(\boldsymbol{\theta})}{N_d}, \quad (3.4)$$

where the symbol $=:$ stands for notation,

$$E_{\boldsymbol{\theta}}[q_{dk} | \mathbf{y}_d] = \frac{\int_R \frac{\exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}}{1 + \exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}} P(\mathbf{y}_d | v_d) f(v_d) dv_d}{\int_R P(\mathbf{y}_d | v_d) f(v_d) dv_d} = \frac{A_{dk}^z}{C_d}$$

and

$$A_{dk}^z = \int_R \frac{\exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}}{1 + \exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}} \exp\left\{ \phi y_{d,v_d} - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{\mathbf{x}_{di} \boldsymbol{\beta} + \phi v_d\}] \right\} f(v_d) dv_d,$$

$$A_d^v = \int_R v_d \exp\left\{ \phi y_{d,v_d} - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{\mathbf{x}_{di} \boldsymbol{\beta} + \phi v_d\}] \right\} f(v_d) dv_d,$$

$$C_d = \int_R \exp\left\{ \phi y_{d,v_d} - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{\mathbf{x}_{di} \boldsymbol{\beta} + \phi v_d\}] \right\} f(v_d) dv_d. \quad (3.5)$$

The EBPs of v_d , μ_d and $\bar{\mu}_d$ are $\hat{v}_d = \hat{v}_d(\hat{\boldsymbol{\theta}})$, $\hat{\mu}_d(\hat{\boldsymbol{\theta}}) = \psi_d(\mathbf{y}_d, \hat{\boldsymbol{\theta}})$ and $\hat{\bar{\mu}}_d = \hat{\mu}_d(\hat{\boldsymbol{\theta}})/N_d$, respectively. They can be approximated by Monte Carlo simulation. For $\hat{v}_d(\hat{\boldsymbol{\theta}})$ and $\hat{\mu}_d(\hat{\boldsymbol{\theta}})$, the algorithm steps are

1. Estimate $\hat{\boldsymbol{\theta}} = (\hat{\boldsymbol{\beta}}', \hat{\phi})'$ and generate $v_d^{(s)}$ i.i.d. $N(0, 1)$, $v_d^{(S+s)} = -v_d^{(s)}$, $s = 1, \dots, S$, $d = 1, \dots, D$.
2. Calculate $\hat{v}_d = \hat{A}_d^v / \hat{C}_d$ and $\hat{\mu}_d(\hat{\boldsymbol{\theta}}) = \sum_{k=1}^K N_{dk} \hat{q}_{dk}$, where $\hat{q}_{dk} = \hat{A}_{dk}^z / \hat{C}_d$ and

$$\hat{A}_{dk}^z = \frac{1}{2S} \sum_{s=1}^{2S} \frac{\exp\{z_k \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}}{1 + \exp\{z_k \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}} \exp\left\{ \hat{\phi} y_{d.} v_d^{(s)} - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{x_{di} \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}] \right\},$$

$$\hat{A}_d^v = \frac{1}{2S} \sum_{s=1}^{2S} v_d^{(s)} \exp\left\{ \hat{\phi} y_{d.} v_d^{(s)} - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{x_{di} \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}] \right\},$$

$$\hat{C}_d = \frac{1}{2S} \sum_{s=1}^{2S} \exp\left\{ \hat{\phi} y_{d.} v_d^{(s)} - \sum_{i=1}^{n_d} m_{di} \log[1 + \exp\{x_{di} \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}] \right\}.$$

Note that the census unit-record data $\{x_{dj}\}$ is not needed to construct the EBPs (3.3) and (3.4), provided an implicit structure is assumed for the census data and no continuous variables are to be included in the survey-based model. Here we employ a set of marginal tables containing the population sizes N_{dk} . If there is no sample, that is $n_d = 0$ for a given domain d , then $\hat{v}_d(\hat{\boldsymbol{\theta}}) = 0$ and $\hat{\mu}_d(\hat{\boldsymbol{\theta}})$ can be approximated using a synthetic estimate based on the sampled domains. The method is as follows.

1. As above.
2. Calculate $\hat{\mu}_d(\hat{\boldsymbol{\theta}}) = \sum_{k=1}^K N_{dk} \hat{q}_{dk0}$, where

$$\hat{q}_{dk0} = \frac{1}{2S} \sum_{s=1}^{2S} \left\{ \frac{\exp\{z_k \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}}{1 + \exp\{z_k \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}} \right\}.$$

The plug-in and the synthetic plug-in estimators of p_{dj} , μ_d and $\bar{\mu}_d = \mu_d / N_d$ do not require running Monte Carlo simulation algorithms. They are

$$\hat{p}_{dj}^{in} = \frac{\exp\{x_{dj} \hat{\boldsymbol{\beta}} + \hat{v}_d\}}{1 + \exp\{x_{dj} \hat{\boldsymbol{\beta}} + \hat{v}_d\}}, \quad \hat{\mu}_d^{in} = \sum_{k=1}^K N_{dk} \frac{\exp\{z_k \hat{\boldsymbol{\beta}} + \hat{v}_d\}}{1 + \exp\{z_k \hat{\boldsymbol{\beta}} + \hat{v}_d\}}, \quad \hat{\bar{\mu}}_d^{in} = \frac{\hat{\mu}_d^{in}}{N_d}, \quad (3.6)$$

$$\hat{p}_{dj}^{syn} = \frac{\exp\{x_{dj} \hat{\boldsymbol{\beta}}\}}{1 + \exp\{x_{dj} \hat{\boldsymbol{\beta}}\}}, \quad \hat{\mu}_d^{syn} = \sum_{k=1}^K N_{dk} \frac{\exp\{z_k \hat{\boldsymbol{\beta}}\}}{1 + \exp\{z_k \hat{\boldsymbol{\beta}}\}}, \quad \hat{\bar{\mu}}_d^{syn} = \frac{\hat{\mu}_d^{syn}}{N_d}. \quad (3.7)$$

Remark 3.1. We can further define the population proportion $\bar{Y}_d = \frac{1}{N_d} \sum_{j=1}^{N_d} y_{dj}$. If $m_{dj} = 1$, $d = 1, \dots, D$, $j = 1, \dots, N_d$, it holds that

$$E[\bar{Y}_d | v_d] = \frac{1}{N_d} \sum_{j=1}^{N_d} p_{dj} = \sum_{k=1}^K w_{dk} q_{dk} = \bar{\mu}_d, \quad w_{dk} = \frac{N_{dk}}{N_d},$$

$$\text{var}[\bar{Y}_d | v_d] = \frac{1}{N_d^2} \sum_{j=1}^{N_d} p_{dj} (1 - p_{dj}) = \frac{1}{N_d} \sum_{k=1}^K w_{dk} q_{dk} (1 - q_{dk}) = \frac{\kappa_d}{N_d}, \quad 0 \leq \kappa_d \leq 1/4.$$

By applying the Tchebysheff's inequality, it holds that

$$P(|\bar{Y}_d - \bar{\mu}_d| < \varepsilon | v_d) \geq 1 - \frac{\text{var}[\bar{Y}_d | v_d]}{\varepsilon^2} = 1 - \frac{\kappa_d}{N_d \varepsilon^2}. \quad (3.8)$$

Equation (3.8) implies, for example, that $P(|\bar{Y}_d - \bar{\mu}_d| < \varepsilon | v_d) \geq 0.9$ if $\varepsilon = 10^{-2}$ and $N_d = \kappa_d 10^5$. Further, if $q_{dk} \approx 0.20$ for all k , then $\kappa_d \approx 0.16$ and $N_d \approx 16,000$ is smaller than the domain sizes appearing in the application to real data presented in Section 6. Thus, $\bar{\mu}_d$ can be assumed to be a good approximation of $\bar{Y}_d$.

4. The MSE of the EBP

This section presents an approximation and gives four estimators of the MSE of the EBP of $\mu_d = \mu_d(\boldsymbol{\theta}, v_d)$. We assume that $m_{dj} = 1$, $d = 1, \dots, D$, $j = 1, \dots, n_d$, and that all the n_d s are bounded to be finite. This is the situation of the application to real data of Section 6. A consequence of the last assumption is that the total sample size n and the number of domains D are of the same order.

The MSE of the EBP can be decomposed into the following form

$$\begin{aligned} \text{MSE}(\hat{\mu}_d) &= E[(\hat{\mu}_d(\hat{\boldsymbol{\theta}}) - \mu_d(\boldsymbol{\theta}, v_d))^2] = E[(\{\hat{\mu}_d(\hat{\boldsymbol{\theta}}) - \hat{\mu}_d(\boldsymbol{\theta})\} + \{\hat{\mu}_d(\boldsymbol{\theta}) - \mu_d(\boldsymbol{\theta}, v_d)\})^2] \\ &= E[(\hat{\mu}_d(\hat{\boldsymbol{\theta}}) - \hat{\mu}_d(\boldsymbol{\theta}))^2] + E[(\hat{\mu}_d(\boldsymbol{\theta}) - \mu_d(\boldsymbol{\theta}, v_d))^2]. \end{aligned}$$

The second term of $\text{MSE}(\hat{\mu}_d)$ is

$$\begin{aligned} g_d(\boldsymbol{\theta}) &= E[(\hat{\mu}_d(\boldsymbol{\theta}) - \mu_d(\boldsymbol{\theta}, v_d))^2] = E[\hat{\mu}_d^2(\boldsymbol{\theta})] + E[\mu_d^2(\boldsymbol{\theta}, v_d)] - 2E[\hat{\mu}_d(\boldsymbol{\theta})E[\mu_d(\boldsymbol{\theta}, v_d) | \mathbf{y}_d]] \\ &= E[\mu_d^2(\boldsymbol{\theta}, v_d)] - E[\hat{\mu}_d^2(\boldsymbol{\theta})]. \end{aligned}$$

The first and second terms of $g_d(\boldsymbol{\theta})$ are

$$\begin{aligned} E[\mu_d^2(\boldsymbol{\theta}, v_d)] &= \int_R \left(\sum_{k=1}^K N_{dk} \frac{\exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}}{1 + \exp\{\mathbf{z}_k \boldsymbol{\beta} + \phi v_d\}} \right)^2 f(v_d) dv_d, \\ E[\hat{\mu}_d^2(\boldsymbol{\theta})] &= E[\psi_d^2(y_d, \boldsymbol{\theta})] = \sum_{j=0}^{n_d} \psi_d^2(j, \boldsymbol{\theta}) p_d(j, \boldsymbol{\theta}), \end{aligned}$$

where ψ_d was defined in (3.4),

$$\begin{aligned} p_d(j, \boldsymbol{\theta}) &= P(y_d = j) = \sum_{\mathbf{y}_d \in S_{n_d, j}} P(\mathbf{y}_d) = \sum_{\mathbf{y}_d \in S_{n_d, j}} \int_R P(\mathbf{y}_d | v_d) f(v_d) dv_d \\ &= \sum_{\mathbf{y}_d \in S_{n_d, j}} \left\{ \exp \left\{ \sum_{i=1}^{n_d} y_i \mathbf{x}_{di} \boldsymbol{\beta} \right\} \int_R \exp \left\{ j \phi v_d - \sum_{i=1}^{n_d} \log[1 + \exp\{\mathbf{x}_{di} \boldsymbol{\beta} + \phi v_d\}] \right\} f(v_d) dv_d \right\} \end{aligned} \quad (4.1)$$

and $S_{n_d, j} = \{\mathbf{y}_d = (y_1, \dots, y_{n_d}) \in \{0, 1\}^{n_d} : y_d = y_1 + \dots + y_{n_d} = j\}$.

Concerning the first term of $MSE(\hat{\mu}_d)$, we have

$$\begin{aligned}\hat{\mu}_d(\hat{\boldsymbol{\theta}}) - \hat{\mu}_d(\boldsymbol{\theta}) &= \psi_d(y_d, \hat{\boldsymbol{\theta}}) - \psi_d(y_d, \boldsymbol{\theta}) = \left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(y_d, \boldsymbol{\theta}) \right)' (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) \\ &\quad + \frac{1}{2} (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} \psi_d(y_d, \boldsymbol{\theta}) \right) (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) + o(\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2).\end{aligned}$$

Hereafter the symbols $o(\cdot)$, $O(\cdot)$ are understood in an appropriate sense, for example in probability. We assume that the $\mathbf{x}_{dj}$ s fulfill the regularity condition (23) of Jiang (2003). Then, we have $\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\| = O(D^{-1/2})$ and

$$E[(\hat{\mu}_d(\hat{\boldsymbol{\theta}}) - \hat{\mu}_d(\boldsymbol{\theta}))^2] = \frac{1}{D} E \left[\left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(y_d, \boldsymbol{\theta}) \right)' \sqrt{D}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) \right)^2 \right] + o(1/D).$$

Now consider $\hat{\boldsymbol{\theta}}_{d-}$, an estimator based on $\mathbf{y}_{d-} = (\mathbf{y}_{d'})_{d' \neq d}$, and write $\hat{\mu}_{d-} = \psi_d(y_d, \hat{\boldsymbol{\theta}}_{d-})$. By the independence of $\mathbf{y}_d$ and $\mathbf{y}_{d-}$, we have

$$\begin{aligned}a_d(\boldsymbol{\theta}) &= E \left[\left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(y_d, \boldsymbol{\theta}) \right)' \sqrt{D}(\hat{\boldsymbol{\theta}}_{d-} - \boldsymbol{\theta}) \right)^2 \right] \\ &= \sum_{j=1}^{n_d} E \left[\left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(y_d, \boldsymbol{\theta}) \right)' \sqrt{D}(\hat{\boldsymbol{\theta}}_{d-} - \boldsymbol{\theta}) \right)^2 \middle| y_d = j \right] p_d(j, \boldsymbol{\theta}) \\ &= \sum_{j=1}^{n_d} \left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(j, \boldsymbol{\theta}) \right)' \mathbf{V}_d(\boldsymbol{\theta}) \left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(j, \boldsymbol{\theta}) \right) p_d(j, \boldsymbol{\theta}),\end{aligned}$$

where $\mathbf{V}_d(\boldsymbol{\theta}) = DE[(\hat{\boldsymbol{\theta}}_{d-} - \boldsymbol{\theta})(\hat{\boldsymbol{\theta}}_{d-} - \boldsymbol{\theta})' | y_d = j] = DE[(\hat{\boldsymbol{\theta}}_{d-} - \boldsymbol{\theta})(\hat{\boldsymbol{\theta}}_{d-} - \boldsymbol{\theta})']$. Therefore,

$$MSE(\hat{\mu}_{d-}) = g_d(\boldsymbol{\theta}) + \frac{1}{D} a_d(\boldsymbol{\theta}) + o(1/D).$$

If the $\mathbf{x}_{dj}$ s also fulfill the regularity conditions (24) and (25) of Jiang (2003), then we may replace $\hat{\boldsymbol{\theta}}_{d-}$ by $\hat{\boldsymbol{\theta}}$, an estimator of $\boldsymbol{\theta}$ based on all data, and we obtain

$$MSE(\hat{\mu}_d) = g_d(\boldsymbol{\theta}) + \frac{1}{D} c_d(\boldsymbol{\theta}) + o(1/D), \quad (4.2)$$

where

$$c_d(\boldsymbol{\theta}) = \sum_{j=1}^{n_d} \left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(j, \boldsymbol{\theta}) \right)' \mathbf{V}(\boldsymbol{\theta}) \left(\frac{\partial}{\partial \boldsymbol{\theta}} \psi_d(j, \boldsymbol{\theta}) \right) p_d(j, \boldsymbol{\theta}), \quad \mathbf{V}(\boldsymbol{\theta}) = DE[(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})'].$$

A plug-in estimator of $MSE(\hat{\mu}_d)$ is

$$mse^P(\hat{\mu}_d) = g_d(\hat{\boldsymbol{\theta}}) + \frac{1}{D} c_d(\hat{\boldsymbol{\theta}}).$$

We have that $E[c_d(\hat{\boldsymbol{\theta}}) - c_d(\boldsymbol{\theta})] = o(1)$. However $E[g_d(\hat{\boldsymbol{\theta}}) - g_d(\boldsymbol{\theta})]$ is not of order $o(D^{-1})$.

Let $\hat{\boldsymbol{\theta}}$ be a truncated MM estimator. This is to say

$$\hat{\beta}_k = \begin{cases} -L_n & \text{if } \tilde{\beta}_k < -L_n, \\ \tilde{\beta}_k & \text{if } -L_n < \tilde{\beta}_k < L_n, \\ L_n & \text{if } \tilde{\beta}_k > L_n, \end{cases} \quad \hat{\phi} = \begin{cases} \tilde{\phi} & \text{if } \tilde{\phi} \leq L_n, \\ L_n & \text{if } \tilde{\phi} > L_n, \end{cases}$$

where $\tilde{\boldsymbol{\theta}} = (\tilde{\beta}_1, \dots, \tilde{\beta}_p, \tilde{\phi})'$ is an MM estimator. Under regularity conditions (23)–(25) of Jiang (2003) it can be proved that $E[\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}] = O(D^{-1})$ holds for the MM and for the truncated MM estimator (see Jiang 2003, 123). In what follows, we assume that $E[\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}] = O(D^{-1})$ holds. By the Taylor expansion, we have

$$g_d(\hat{\boldsymbol{\theta}}) = g_d(\boldsymbol{\theta}) + \left(\frac{\partial}{\partial \boldsymbol{\theta}} g_d(\boldsymbol{\theta}) \right)' (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2} (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} g_d(\boldsymbol{\theta}) \right) (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) + o(D^{-1}),$$

and hence

$$E[g_d(\hat{\boldsymbol{\theta}})] = g_d(\boldsymbol{\theta}) + \frac{1}{D} b_d(\boldsymbol{\theta}) + o(D^{-1}),$$

where

$$b_d(\boldsymbol{\theta}) = \left(\frac{\partial}{\partial \boldsymbol{\theta}} g_d(\boldsymbol{\theta}) \right)' DE[\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}] + \frac{1}{2} E \left[\sqrt{D}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} g_d(\boldsymbol{\theta}) \right) \sqrt{D}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) \right]. \quad (4.3)$$

Proposition 4.1 gives an approximation to the bias term b_d when $\hat{\boldsymbol{\theta}}$ is the truncated MM estimator. Appendix A.2 gives the proof.

Proposition 4.1. Let $\hat{\boldsymbol{\theta}}$ be the truncated MM estimator. Under regularity conditions (23)–(25) of Jiang (2003), it holds that $b_d(\boldsymbol{\theta}) = B_d(\boldsymbol{\theta}) + o(1)$, where

$$B_d(\boldsymbol{\theta}) = \frac{1}{2} \left\{ E[r_{D,d}] - \left(\frac{\partial}{\partial \boldsymbol{\theta}} g_d(\boldsymbol{\theta}) \right)' \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} E[\mathbf{q}_D] \right\},$$

$$r_{D,d} = \Delta_D' \mathbf{R}_d(\boldsymbol{\theta}) \Delta_D, \quad \mathbf{R}_d(\boldsymbol{\theta}) = \left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \right)' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} g_d(\boldsymbol{\theta}) \right) \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1},$$

$$\mathbf{q}_D = \text{col}_{1 \leq k \leq p+1} (q_{Dk}), \quad \mathbf{M}(\boldsymbol{\theta}) = \text{col}_{1 \leq k \leq p+1} (\mathbf{M}_k(\boldsymbol{\theta})), \quad \hat{\mathbf{M}} = \text{col}_{1 \leq k \leq p+1} (\hat{\mathbf{M}}_k),$$

$$q_{Dk} = \Delta_D' \mathbf{Q}_k(\boldsymbol{\theta}) \Delta_D, \quad \mathbf{Q}_k(\boldsymbol{\theta}) = \left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \right)' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} \mathbf{M}_k(\boldsymbol{\theta}) \right) \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1},$$

$$\Delta_D = \sqrt{D}(\hat{\mathbf{M}} - \mathbf{M}(\boldsymbol{\theta})), \quad \frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) = \left(\frac{\partial}{\partial \boldsymbol{\theta}_{k_2}} \mathbf{M}_{k_1}(\boldsymbol{\theta}) \right)_{k_1, k_2=1, \dots, p+1}.$$

Finally, an order $o(D^{-1})$ theoretical estimator of the MSE with bias correction is

$$\widehat{MSE}(\hat{\mu}_d) = g_d(\hat{\theta}) + \frac{1}{D} c_d(\hat{\theta}) - \frac{1}{D} B_d(\hat{\theta})$$

and the practical estimators, without and with bias correction, are

$$mse^0(\hat{\mu}_d) = \hat{g}_d(\hat{\theta}) + \frac{1}{D} \hat{c}_d(\hat{\theta}), \quad mse^1(\hat{\mu}_d) = mse^0(\hat{\mu}_d) - \frac{1}{D} \hat{B}_d(\hat{\theta}). \quad (4.4)$$

Appendix A.3 gives the Monte Carlo approximations $\hat{g}_d(\hat{\theta})$ and $\hat{c}_d(\hat{\theta})$ of $g_d(\hat{\theta})$ and $c_d(\hat{\theta})$ respectively, and the bootstrap estimator $\hat{B}_d(\hat{\theta})$ of $B_d(\hat{\theta})$. Appendix A.4 presents formulas of some derivatives needed to evaluate the abovementioned approximations.

Another approach to estimating the MSE is to use a parametric bootstrap. The following procedure calculates a bootstrap and a double-bootstrap bias-corrected estimator of $MSE(\hat{\mu}_d)$.

1. Fit the model to the sample and calculate $\hat{\theta} = (\hat{\beta}', \hat{\phi})'$.
2. Repeat B_1 times ($b_1 = 1, \dots, B_1$):
 - (a) For $d = 1, \dots, D, j = 1, \dots, n_d$, generate $v_d^{*(b_1)}$ i.i.d. $N(0,1)$ and calculate

$$p_{dj}^{*(b_1)} = \frac{\exp\{\mathbf{x}_{dj} \hat{\beta} + \hat{\phi} v_d^{*(b_1)}\}}{1 + \exp\{\mathbf{x}_{dj} \hat{\beta} + \hat{\phi} v_d^{*(b_1)}\}}, \quad y_{dj}^{*(b_1)} \sim \text{Bin}(m_{dj}, p_{dj}^{*(b_1)}),$$

$$\mu_d^{*(b_1)} = \mu_d(\hat{\theta}, v_d^{*(b_1)}) = \sum_{k=1}^K N_{dk} q_{dk}^{*(b_1)}, \quad q_{dk}^{*(b_1)} = \frac{\exp\{\mathbf{z}_k \hat{\beta} + \hat{\phi} v_d^{*(b_1)}\}}{1 + \exp\{\mathbf{z}_k \hat{\beta} + \hat{\phi} v_d^{*(b_1)}\}}.$$

- (b) For each bootstrap sample, calculate $\hat{\theta}^{*(b_1)}$ and the EBP $\hat{\mu}_d^{*(b_1)} = \hat{\mu}_d(\hat{\theta}^{*(b_1)})$.
- (c) Repeat B_2 times ($b_2 = 1, \dots, B_2$):
 - i. For $d = 1, \dots, D, j = 1, \dots, n_d$, generate $v_d^{*(b_1, b_2)}$ i.i.d. $N(0,1)$ and calculate

$$p_{dj}^{*(b_1, b_2)} = \frac{\exp\{\mathbf{x}_{dj} \hat{\beta}^{*(b_1)} + \hat{\phi}^{*(b_1)} v_d^{*(b_1, b_2)}\}}{1 + \exp\{\mathbf{x}_{dj} \hat{\beta}^{*(b_1)} + \hat{\phi}^{*(b_1)} v_d^{*(b_1, b_2)}\}},$$

$$y_{dj}^{*(b_1, b_2)} \sim \text{Bin}(m_{dj}, p_{dj}^{*(b_1, b_2)}),$$

$$\mu_d^{*(b_1, b_2)} = \mu_d(\hat{\theta}^{*(b_1)}, v_d^{*(b_1, b_2)}) = \sum_{k=1}^K N_{dk} q_{dk}^{*(b_1, b_2)},$$

$$q_{dk}^{*(b_1, b_2)} = \frac{\exp\{\mathbf{z}_k \hat{\beta}^{*(b_1)} + \hat{\phi}^{*(b_1)} v_d^{*(b_1, b_2)}\}}{1 + \exp\{\mathbf{z}_k \hat{\beta}^{*(b_1)} + \hat{\phi}^{*(b_1)} v_d^{*(b_1, b_2)}\}}.$$

- ii. For each bootstrap sample, calculate $\hat{\theta}^{*(b_1, b_2)}$ and the EBP

$$\hat{\mu}_d^{*(b_1, b_2)} = \hat{\mu}_d(\hat{\theta}^{*(b_1, b_2)}).$$

- iii. Output: $mse_d^{*(b_1)} = \frac{1}{B_2} \sum_{b_2=1}^{B_2} \left(\hat{\mu}_d^{*(b_1, b_2)} - \mu_d^{*(b_1, b_2)} \right)^2$.

3. Output:

$$mse^*(\hat{\mu}_d) = \frac{1}{B_1} \sum_{b_1=1}^{B_1} (\hat{\mu}_d^{*(b_1)} - \mu_d^{*(b_1)})^2, \quad mse^{**}(\hat{\mu}_d) = 2mse^*(\hat{\mu}_d) - \frac{1}{B_1} \sum_{b_1=1}^{B_1} mse_d^{*(b_1)}.$$

5. Simulation Experiments

In this section we present three simulation experiments. They are fully model-based and are linked to the case study of Section 6, but with much smaller sample and population sizes. All of them use the same simulation environment, which can be described in the following way. Take $N_d = 1,000$, $n_d = 5, 10, 20, 40$, $D = 30$. Note that, to enable computation, N_d is more than an order of magnitude smaller than specified in the approximation in probability used in (3.8). For $d = 1, \dots, D$, $j = 1, \dots, n_d$, generate regressors, x_{dj1} and x_{dj2} , classifying individuals into one of three possible classes (e.g., inactive, unemployed, and employed), so that they take on values $(x_{dj1}, x_{dj2}) \in \{(0, 0), (0, 1), (1, 0)\}$ with probabilities 0.3, 0.2, and 0.5, respectively. Generate $v_d \sim N(0, 1)$, $d = 1, \dots, D$. Take $\beta = (\beta_0, \beta_1, \beta_2) = (1/3, -3/2, 1/2)$ and $\phi = 1/2$. For $d = 1, \dots, D$, $j = 1, \dots, n_d$, generate the target variable

$$y_{dj} \sim \text{Bin}(m_{dj}, p_{dj}), \quad p_{dj} = \frac{\exp\{\beta_0 + x_{dj1}\beta_1 + x_{dj2}\beta_2 + \phi v_d\}}{1 + \exp\{\beta_0 + x_{dj1}\beta_1 + x_{dj2}\beta_2 + \phi v_d\}}, \quad m_{dj} = 1,$$

where $y_{dj} = 1$ ($= 0$) indicates that individual j of domain d is (not) below the poverty line and p_{dj} is the corresponding binomial probability. We choose $D = 30$ as a round figure close to the number $D = 34$ of domains in the real data.

As some of the theoretical results are asymptotic, we investigate cases with small to medium sample sizes. The selected scenario resembles the application to real data. For computational reasons, the population size $N = 30,000$ is much smaller than the population size $N = 4,990.277$ of the study case. Nevertheless, the simulations are illustrative and give useful information about how the methodology works in practice. Simulation 1 investigates the behavior of the model parameter estimators. Simulation 2 calculates the bias and the MSE of the EBP and the plug-in estimators under different scenarios. Simulation 3 compares the introduced MSE estimators.

5.1. Simulation 1

The target of Simulation 1 is to check the behavior of the fitting algorithm. The steps of Simulation 1 are

1. Repeat $K = 1,000$ times ($k = 1, \dots, K$).
 - 1.1. Generate a sample of size $n = \sum_{d=1}^D n_d$. Calculate $\hat{\beta}_0^{(k)}$, $\hat{\beta}_1^{(k)}$, $\hat{\beta}_2^{(k)}$ and $\hat{\phi}^{(k)}$.
2. Output: For $\theta \in \{\beta_0, \beta_1, \beta_2, \phi\}$, calculate the empirical bias and the root-MSE

$$BIAS = \frac{1}{K} \sum_{k=1}^K (\hat{\theta}^{(k)} - \theta), \quad RMSE = \left(\frac{1}{K} \sum_{k=1}^K (\hat{\theta}^{(k)} - \theta)^2 \right)^{1/2}.$$

Table 1. BIAS (left) and RMSE (right) for $D = 30$.

n	150	300	600	1,200	150	300	600	1,200
n_d	5	10	20	40	5	10	20	40
$\hat{\beta}_0$	0.004	-0.004	-0.003	-0.001	0.274	0.242	0.180	0.156
$\hat{\beta}_1$	-0.002	-0.005	0.006	0.004	0.346	0.301	0.223	0.158
$\hat{\beta}_2$	-0.012	0.010	0.010	0.007	0.474	0.372	0.261	0.187
$\hat{\phi}$	-0.103	-0.058	-0.042	-0.022	0.359	0.270	0.177	0.116

Table 1 presents the obtained results. This table shows that the empirical bias and root-MSE of the MSM estimators of the model parameters decrease as the sample size increases. This is coherent with the consistency property given by Theorem 1 of Jiang (1998).

5.2. Simulation 2

The target of Simulation 2 is to investigate the behavior of the EBP, the plug-in (IN) and synthetic plug-in estimators (SYN). The steps of Simulation 2 are

1. Repeat $K = 10,000$ times ($k = 1, \dots, K$)
 - 1.1. Generate the population in the same way as described at the beginning of this section and calculate

$$\mu_d^{(k)} = \frac{1}{N_d} \sum_{j=1}^{N_d} p_{dj}^{(k)}, \quad \bar{Y}_d^{(k)} = \frac{1}{N_d} \sum_{j=1}^{N_d} y_{dj}^{(k)}, \quad \nabla_d^{(k)} = \mu_d^{(k)} - \bar{Y}_d^{(k)}.$$

- 1.2. For $d = 1, \dots, D$, select a simple random sample s_d (without replacement) of size n_d and calculate $\hat{\theta}^{(k)} = (\hat{\beta}_0^{(k)}, \hat{\beta}_1^{(k)}, \hat{\beta}_2^{(k)}, \hat{\phi}^{(k)})$ and $\tilde{\theta}^{(k)} = (\tilde{\beta}_0^{(k)}, \tilde{\beta}_1^{(k)}, \tilde{\beta}_2^{(k)})$ under the logit model with and without random effects.

- 1.3. Calculate $\hat{\nu}_d^{(k)} = \hat{\nu}_d(\hat{\theta}^{(k)})$ and

$$\hat{\mu}_d^{ebp,k} = \frac{\hat{\mu}_d(\hat{\theta}^{(k)})}{N_d}, \quad \hat{\mu}_d^{in,k} = \frac{\hat{\mu}_d^{in}(\hat{\theta}^{(k)}, \hat{\nu}_d^{(k)})}{N_d}, \quad \hat{\mu}_d^{syn,k} = \frac{\hat{\mu}_d^{syn}(\tilde{\theta}^{(k)})}{N_d}, \quad d = 1, \dots, D.$$

2. For each $\hat{\mu}_d \in \{\hat{\mu}_d^{ebp}, \hat{\mu}_d^{in}, \hat{\mu}_d^{syn}\}$, calculate

$$B_d = \frac{1}{K} \sum_{k=1}^K \left(\hat{\mu}_d^k - \bar{\mu}_d^{(k)} \right), \quad E_d = \frac{1}{K} \sum_{k=1}^K \left(\hat{\mu}_d^k - \bar{\mu}_d^{(k)} \right)^2, \quad d = 1, \dots, D. \quad (5.1)$$

Figures 1, 2, and 3 present the boxplots of the empirical biases, B_{ds} , and mean-square errors, E_{ds} , of the EBP, the IN and the SYN defined in (3.4), (3.6), and (3.7) respectively. The SYN is based on the model without random effects and it is calculated from the corresponding parameter estimates $\tilde{\theta}$. Figures 1 and 3 show that the MSE of the EBP is lower than the MSE of the SYN, overall for domain samples sizes greater than ten. Furthermore, the EBP has slightly lower bias than the SYN. Further, the EBP has slightly lower bias and MSE than the IN.

Fig. 1. Boxplots of B_d (left) and E_d (right) defined in (5.1) for EBP and $n_d \in \{5, 10, 20, 40\}$.

Let us illustrate the difference between domain parameters $\hat{\mu}_d^{(k)}$ and $\bar{Y}_d^{(k)}$ in the simulations. As the calculated differences do not depend on d in the simulated scenario, Table 2 presents the quantiles of $\nabla_d^{(k)}$ for $N_d = 1,000$ and $d = 1$. In the interquartile range, the absolute difference is lower than 10^{-2} .

5.3. Simulation 3

The target of Simulation 3 is to investigate the behavior of the four MSE estimators, the analytic estimator $mse^0(\hat{\mu}_d)$, the analytic estimator with bias correction $mse^1(\hat{\mu}_d)$, the bootstrap estimator $mse^*(\hat{\mu}_d)$ and the double-bootstrap bias-corrected estimator $mse^{**}(\hat{\mu}_d)$ of the EBP. The number of first-stage bootstrap resamples is $B_1 = 100$. By following Erciulescu and Fuller (2014), the number of second-stage bootstrap resamples is $B_2 = 1$. The steps of Simulation 3 are

1. Repeat $K = 1,000$ times ($k = 1, \dots, K$)
 - 1.1. Generate the population in the same way as described at the beginning of this section.
 - 1.2. For $d = 1, \dots, D$, select a simple random sample s_d (without replacement) of size n_d . Calculate $mse_d^{0(k)} = mse^0(\hat{\mu}_d)/N_d^2$, $mse_d^{1(k)} = mse^1(\hat{\mu}_d)/N_d^2$, $mse_d^{*(k)} = mse^*(\hat{\mu}_d)/N_d^2$ and $mse_d^{**(k)} = mse^{**}(\hat{\mu}_d)/N_d^2$, $d = 1, \dots, D$.

Fig. 2. Boxplots of B_d (left) and E_d (right) defined in (5.1) for IN and $n_d \in \{5, 10, 20, 40\}$.

Fig. 3. Boxplots of B_d (left) and E_d (right) defined in (5.1) for SYN and $n_d \in \{5, 10, 20, 40\}$.

2. For every $mse \in \{mse^0, mse^1, mse^*, mse^{**}\}$, calculate

$$mse_d = \frac{1}{K} \sum_{k=1}^K mse_d^{(k)}, \quad e_d = \frac{1}{K} \sum_{k=1}^K \left(mse_d^{(k)} - E_d^{ebp} \right)^2, \quad d = 1, \dots, D,$$

where E_d^{ebp} , $d = 1, \dots, D$, is taken from the output of Simulation 2.

Figure 4 presents the plots of the four MSE estimators. This figure shows that the bias correction used in mse_d^1 as well as in mse_d^{**} does not work for domain sample sizes around $n_d = 10$. It starts to be effective if $n_d \geq 20$, when both mse_d^1 and mse_d^{**} seem to estimate the real value of the simulated mean-squared error E_d^{ebp} quite well.

Figure 5 contains the boxplots of the empirical MSEs, e_d^0 , e_d^1 , e_d^* and e_d^{**} , of the MSE estimators mse_d^0 , mse_d^1 , mse_d^* and mse_d^{**} . The analytic estimators, mse_d^0 and mse_d^1 , perform better than the parametric bootstrap estimators mse_d^* , mse_d^{**} . Further, the bias-corrected estimator, mse_d^1 , has the lowest MSEs. It can be also seen that in the case of the double-bootstrap estimator mse_d^{**} the gained bias correction comes at the cost of increased variability of this estimator.

Remark 5.1. The approximation of terms g_d , c_d and B_d used correspondingly in the mse_d^0 and mse_d^1 estimators entails some implementational and computational difficulties. First of all, to be able to calculate the B_d term one has to implement all formulas for the needed derivatives, which are partly presented in Appendix A.4. A greater difficulty is that the calculation of the probabilities (4.1) and their derivatives appearing in the g_d , c_d and B_d terms is computationally expensive if $n_d \geq 40$, because calculating the sum in (4.1) requires an iterative enumeration of all the elements of the subset $S_{n_d,j} \subset \{0, 1\}^{n_d}$ and the size of $S_{n_d,j}$ is $\binom{n_d}{j}$, which increases exponentially with n_d when j is around $n_d/2$, for

Table 2. Quantiles of $\nabla_d^{(k)}$ for $N_d = 1,000$, $d = 1$.

∇_1	min	Q_1	Q_2	Q_3	max
Quantiles	−0.0549	−0.0098	−0.0003	0.0093	0.0559

Fig. 4. Plots of E_d^{ebp} , mse_d^0 , mse_d^1 and mse_d^* for $n_d = 10$ (left) and $n_d = 20$ (right).

example if $n_d = 40$ the sum over the set $S_{40,20}$ has around $1.4 \cdot 10^{11}$ summands which must be evaluated and counted up for each domain d . This difficulty can be solved in some manner in a simulation experiment when the sizes n_d are small and the same for all d so that the set of all possible $y_d \in S_{n_d,j}$ can be stored once in memory or on a disc. But in practical application when the sizes n_d are different and some of them are large, there are complications with implementation and computation time.

The parametric bootstrap MSE estimators, mse_d^* , mse_d^{**} , avoid the computational problems of their analytic counterparts, mse_d^0 and mse_d^1 , and present quite good behavior. To illustrate the performance of the bootstrap estimator mse_d^* for higher values of n_d , in Figure 6 we present results of this estimator for $n_d = 40$. We can observe that for this sample size, the estimator mse_d^* is practically unbiased and the double bootstrap is not needed.

6. Application to SLCS Data

Alleviating poverty is one of the main social tasks in the European Union (EU). Following the instructions of EUROSTAT, European countries implement a Living Conditions

Fig. 5. Plots of e_d^0 , e_d^1 and e_d^* for $n_d = 10$ (left) and $n_d = 20$ (right).

Fig. 6. Plot of E_d^{ebp} and mse_d^* for $n_d = 40$.

Survey to estimate poverty indicators. We use the SLCS2012 data from the Autonomous Community of Valencia (East of Spain). This region has three provinces, Alicante, Castellón and Valencia, encoded as 3, 12, and 46 by the Spanish Statistical Office. The provinces are partitioned into 9, 8, and 17 comarcas (counties) respectively, but only 8, 4, and 14 appear in the SLCS2012. The target domains are the counties, there are thus $D = 34$ domains, but not all of them appear in the sample. The SLCS2012 sample size is $n = 2,678$. The SCLCS2012 is a two-stage area sampling design with census section as the primary units and main family addresses as the ultimate sampling units. The sampling frame is the Population Census updated from the Municipal Register.

The SLCS2012 gives information about the equivalent personal incomes, which are obtained by dividing the total household income by the equivalent total of household members. This total is calculated as a weighted sum assigning weights 1 to the first adult, 0.5 to remaining adults and 0.3 to children under 14 years of age. The weighting for obtaining the equivalent household size and income in the SLCS2012 file is done by following the instructions of EUROSTAT. The weights are based on socioeconomic theory and are not sampling weights.

The Spanish Statistical Office builds the data files of the SLCS2012 and assigns the same household equivalent income to all the household members. Because of this fact, individual-level models are not as explanatory as they hypothetically could be. One could think of fitting models at the household level. However, we cannot follow such approach because the domain-level aggregated auxiliary variables, which are used to construct a model-based census, are only available for individuals and not for households.

EUROSTAT defines the poverty line as the 60% of the median of the equivalent personal incomes in the whole country. A person is classified as poor if their equivalent personal income (denoted as E_{dj} for individual j of domain d) is lower than the poverty line. The poverty proportion is the proportion of people below the poverty line. The 2012 poverty line is $z = 6,840$ (in euros per annum per person) for the region of Valencia.

The poverty proportions at the domain levels are

$$\bar{Y}_d = \frac{1}{N_d} \sum_{j=1}^{N_d} y_{dj}, \text{ where } y_{dj} = I(E_{dj} < z), \quad d = 1, \dots, D, \quad j = 1, \dots, N_d. \quad (6.1)$$

This article estimates domain poverty proportions by using the EBPs of the corresponding weighted sums of probabilities based on unit-level logit mixed models, with random effects at domain level only. This approach requires unit-level survey data for fitting the models, and cross-classified domain level census data for constructing the EBPs. At the unit level, data is taken from the SLCS2012 and the target variable indicates whether individuals are below the poverty line (or not). As the target variable is dichotomic, we employ logit regression models.

In addition to the SLCS2012 data, we take auxiliary aggregated data from the 2012 Labour Force Survey (SLFS2012) file, which contains survey data about the labor market. The sizes of domains crossed by labor status (employed, unemployed, inactive and below 15 years old) are taken from this file. Note that by summing up in the labor categories we obtain the estimated domain sizes. We have taken the estimated domain sizes from SLFS2012 in the estimation of the EBPs. The 2012 population size for the region of Valencia, estimated from SLFS2012, is $N = 4,990,277$.

We remark that we have estimated the population sizes N_{dk} using SLFS2012 data and we have ignored their variability. As we have not got good covariates at the county level from Spanish administrative registers, we have instead employed SLFS2012 data and have taken the selected covariates as true aggregated values. This is a drawback of this application to real data, as it leads to underestimates of the MSE. Nevertheless, the sample size of the SLFS2012 is much higher than the one of the SLCS2012. This is why we have followed this practical approach.

For $d = 1, \dots, D$, $j = 1, \dots, N_d$, we assume that $y_{dj}|v_d \sim \text{Bin}(1, p_{dj})$, where $v_1, \dots, v_D$ are i.i.d. $N(0, 1)$ and

$$\text{logit}(p_{dj}) = \beta_0 + \beta_1 \text{employed}_{dj} + \beta_2 \text{unemployed}_{dj} + \beta_3 \text{inactive}_{dj} + \phi v_d. \quad (6.2)$$

Table 3 presents the estimates of the model parameters and the corresponding p -values. We observe that the more people are employed and inactive, the smaller is the probability of being below the poverty line, and the more people are unemployed, the bigger is this probability.

Pearson residuals are calculated for each domain and covariate class. Conditionally on v_d , the sum of y_{dj} over the domain d and the covariate class k is binomially distributed with parameters (N_{dk}, p_{dk}) , where N_{dk} is the number of observations in the area d and the covariate class k and p_{dk} is the corresponding model probability.

Figure 7 (left) presents a dispersion graph of residuals. The residuals are mainly located in the interval $(-2, 2)$ and they do not present any visible nonrandom pattern. Figure 7 (right) presents a boxplot of the residuals. The marked residual 7 is an outlier under the standard normal distribution. We have also fitted Model (6.2) to the data without the observations belonging to the subset (domain crossed by covariate class) marked by 7. The obtained parameter estimates do not differ significantly from the one appearing in Table 3. Therefore, we calculate the EBPs with the parameter estimates given by this table.

Table 3. Estimates of model parameters.

	estimate	standard error	p-value
β_0	-1.1773	0.1473	1.33E-15
β_1	-0.8354	0.1522	4.02E-08
β_2	0.5379	0.1559	0.000558
β_3	-0.4040	0.1445	0.005177
ϕ	0.3986		

In order to check the assumption that the random effects at domain level have the standard normal distribution, we calculated the EBP $\hat{v}_d$ of the random effects v_d and we present their Q-Q plot in Figure 8. We can observe quite good agreement and moreover, the Kolmogorov-Smirnov test does not reject the hypothesis $H_0 : F_{\hat{v}_d} = F_{N(0,1)}$ with p -value equal to 0.9653. Because random effects at finer levels are not incorporated into the model, these cannot be tested.

Table 4 presents the direct (dir) and EBP (ebp) estimates of the domain poverty proportions, the corresponding variance (var) and bootstrap MSE (mse) estimates and the relative root mean-squared errors in % (rrmse). We have employed the simple parametric bootstrap with $B = 500$ resamples. The columns labeled n and $\hat{N}$ contain the SLCS2012 sample sizes and the SLFS2012-based estimated population sizes (number of individuals), respectively. The columns labeled prov and com indicate the provinces and the counties, respectively.

Table 4 shows that the EBPs have lower MSEs conditional on the model being correct than the direct estimates in areas with small sample sizes ($n_d < 90$) and comparable or slightly higher MSEs in the rest of domains.

Table 5 presents the EBPs (ebp) of the domain poverty proportions, the corresponding MSE estimates (mse) and the relative root mean-squared errors in % (rrmse) for counties with zero sample size in SLCS2012. For these counties, the direct estimators are not calculable, as there is no sample.

Fig. 7. Dispersion graph (left) and boxplot (right) of the residuals.

Fig. 8. Q - Q plot of $\hat{v}_d$ with respect to $N(0, I)$ distribution.

Figure 9 (left) plots EBP and direct poverty-incidence estimates and Figure 9 (right) plots the estimated MSEs of poverty-incidence estimates. These figures show that the EBPs have a lower estimated MSE than the direct estimates.

7. Discussion and Conclusions

Binomial-logit regression models are a flexible class of modelling dichotomic and count variables. This work estimates poverty proportions in counties of the region of Valencia, Spain, by using a model-based unit-level logit mixed model with a domain-level random error (but without reference to survey clustering or survey weighting), and using predictors of weighted sums of probabilities. We fit the model by the method of simulated moments. We consider the EBP and two plug-in estimators and we compare them in a simulation study, based (due to computational complexity) on a small sample and a very small census.

The assumed binomial-logit model with normally distributed domain random effects is widely used in small-area estimation when the parameter of interest is a proportion or a sum of probabilities. The model can be extended from $v_d \sim \text{Normal}$ to $v_d \sim F$, where F is a cumulative distribution function with support on the real line. The extension to heteroscedasticity can also be formulated. If we do this however, we would have to study which of the properties of the binomial logit-normal models still hold in the new model, or how they are modified. Working with a well-studied model has the advantage of having mathematical (e.g., asymptotic) results on the model parameter estimators. In particular, some properties established by Jiang (1998, 2003) and Jiang and Lahiri (2001) are employed in the article to derive the approximation to the model-based MSE of the EBP, conditional on a specified model and without random effects at levels finer than domain.

For the EBP, we derive a model-based MSE and introduce four estimators. The first two are analytic estimators without and with bias correction of the second order. The third and

Table 4. Direct and EBP poverty-proportions estimates.

prov	com	n	$\hat{N}$	dir	var	rrmse	ebp	mse	rrmse
46	17	12	35415	0.3085	0.0164	41.52	0.1957	0.0035	30.23
12	7	17	28715	0.3010	0.0113	35.32	0.2231	0.0031	25.11
46	12	18	88625	0.0000	0.0076		0.1384	0.0032	40.94
46	22	18	30672	0.5010	0.0101	20.04	0.2405	0.0030	22.76
3	31	37	151846	0.0133	0.0051	536.71	0.1149	0.0029	46.60
46	18	37	55440	0.1103	0.0049	63.65	0.1582	0.0027	32.76
46	23	45	75157	0.2490	0.0051	28.65	0.1982	0.0026	25.87
46	21	47	53869	0.2454	0.0036	24.53	0.2528	0.0028	21.06
12	3	56	86580	0.2993	0.0034	19.56	0.2796	0.0026	18.34
3	34	66	282076	0.1216	0.0032	46.40	0.1659	0.0025	29.90
46	24	66	86138	0.1251	0.0025	39.82	0.1615	0.0025	31.14
46	25	75	177618	0.1711	0.0031	32.49	0.2009	0.0021	23.04
3	28	82	76849	0.3962	0.0027	13.05	0.1817	0.0021	25.31
3	29	85	228083	0.0868	0.0025	57.58	0.1270	0.0020	35.56
12	6	88	182172	0.1823	0.0020	24.69	0.1855	0.0024	26.42
3	27	92	125445	0.2995	0.0019	14.39	0.2688	0.0022	17.33
46	16	109	139697	0.2995	0.0022	15.58	0.2617	0.0021	17.44
46	11	109	179960	0.1984	0.0016	20.37	0.1543	0.0022	30.71
12	5	117	251429	0.3141	0.0029	17.19	0.1812	0.0021	25.05
46	20	124	260449	0.0223	0.0012	158.11	0.0747	0.0019	58.38
46	13	125	184704	0.1265	0.0014	29.11	0.1456	0.0019	30.25
3	30	147	239247	0.1774	0.0016	22.31	0.2021	0.0016	19.60
3	33	154	266020	0.2967	0.0011	11.20	0.2898	0.0017	14.25
46	14	213	373164	0.2527	0.0010	12.52	0.2509	0.0012	13.76
3	32	298	467602	0.1830	0.0006	13.24	0.1568	0.0011	21.00
46	15	441	781222	0.2134	0.0005	10.08	0.1926	0.0013	18.41

fourth estimators are based on a parametric bootstrap. We analyze the behavior of the proposed estimators in a small simulation study. Estimating the bias correction term is computationally intensive and the results of the analytic estimators without and with bias correction are quite similar for very small domain sample sizes, although this conclusion may require modification if cluster and household level random effects are included or survey weighting used. The MSE analytical estimators are consistent, but they are not practical for medium- and large-domain sample sizes, because the calculation of the term

Table 5. EBP poverty-proportions estimates for counties without sample ($n_d = 0$).

prov	com	$\hat{N}$	ebp	mse	rrmse
3	26	22310	0.1943	0.0034	30.13
12	1	7819	0.1680	0.0024	29.36
12	2	6868	0.1712	0.0029	31.70
12	4	16109	0.1780	0.0022	26.23
12	8	5529	0.1781	0.0035	33.11
46	9	1826	0.1879	0.0029	28.52
46	10	14400	0.1964	0.0036	30.69
46	19	7222	0.1920	0.0029	28.28

Fig. 9. EBP and direct poverty-proportions estimates (left) and estimated MSEs (right).

g_d involves iteratively finding the $\binom{n_d}{j}$ subsets of size j of a set of size n_d . This problem requires a high-speed computer with large RAM memory for $n_d \geq 40$, so would be difficult to implement for most real-world applications where samples in each surveyed domain are almost always much larger.

Our simulations are computationally intensive in two senses. First, they are carried out at the unit level as we deal with unit-level models and not at the area level. Second and more importantly, all the considered methodology is computationally expensive. The fitting method (MSM) proposed by Jiang (1998) has nice asymptotic properties and allows approximating the MSE of the EBP. However, it requires solving a nonlinear system of equations by using a Newton-Raphson algorithm, where the components of the updating formula have to be approximated by Monte Carlo simulation in each algorithm step. Therefore, it is not a high-speed procedure. The calculation of the EBPs for $d = 1, \dots, D$, requires evaluating integrals by Monte Carlo simulation. This is again time consuming. The calculation of the MSE estimators (analytic and bootstrap) are even more time consuming than the calculation of the EBPs.

The computational burden is not a major problem for the application of the model to real data (with only one sample) provided domain sizes are kept small, but it is a major problem for the 1,000 samples in the simulation (which is why sample and population sizes have been kept very small there). For example, we parallelized Simulation 3 in several computers and they ran for two weeks before obtaining the results. This is why we have simplified the simulation scenario and have implemented a reduced-in-size version. The small sample and population sizes necessary for the simulation do however reduce general applicability of the results.

Jiang and Lahiri (2001) did not present any application to data. This article shows that the EBP methodology may with further development be applicable to real small-area estimation problems. One exception is Jiang and Lahiri's MSE estimator, which would instead need an alternative computationally feasible approach. As a good alternative, we suggest the introduced parametric bootstrap procedure, which does not have the same computational drawbacks, is easy to implement, and has generally good behavior.

In the application to poverty data from the SLCS2012, we use the EBPs to estimate poverty proportions. We take the model-based MSE for a synthetic estimator estimated via the parametric bootstrap as a performance measure. The units are taken to be individuals,

not households, and the model is fitted without adjustment for the complex structure of the survey design. From the point of view of modelling the survey data, it would be better to work with households as sampling units (instead of individuals), because some survey variables (like income) are household variables. The problem appears when calculating the EBPs. In the Spanish case, we do not have a full unit-record census file and we instead need to rely on categorical covariates only, taken from census cross tabulations. Consequently, the population sizes available in covariates classes crossed by domains are individual based. The corresponding information is not available for households. This is the reason we have treated individuals as sampling units.

The introduced model has only one random effect for domains. In future, we might consider hierarchical models with random effects on the different levels of the hierarchy. This would allow more accurate modelling, including household effects. The model proposed in this article is however purely model-based, without reference to the structure of the complex survey design, so does not include stratification, clustering or survey-based weighting. Therefore, model assumptions need to be comprehensively checked to the extent possible by using diagnostic tools, like graphical methods, testing procedures and residual analysis. For a simple random sample, at unit level the $\{y_{dj}\}$ are independent, conditional on the model and the domain-level random effects. The same is true if we consider stratified random sampling with domains nested within strata. For more complex designs (like a design clustered within domains) this assumption will not hold.

Another issue that remains to be studied is how survey weighting could be included in the analysis. For example, how best to introduce the survey weights in the model-based methodology to reduce the design bias of predictors? The difficult problems linked with survey-design issues for small-area predictors based on binomial-logit mixed models will require further research.

Appendix

A.1. Components of MM Newton-Raphson Algorithm

The MM Newton-Raphson algorithm is specified if we calculate the expectations appearing in $f(\theta)$ and its partial derivatives. The expectation of y_{dj} is

$$E_{\theta}[y_{dj}] = E_v[E_{\theta}[y_{dj}|\mathbf{v}]] = E_v[m_{dj}p_{dj}]$$

and the corresponding derivatives are

$$\frac{\partial E_{\theta}[y_{dj}]}{\partial \beta_k} = E_v[m_{dj}p_{dj}(1 - p_{dj})x_{dj k}], \quad \frac{\partial E_{\theta}[y_{dj}]}{\partial \phi} = E_v[m_{dj}p_{dj}(1 - p_{dj})v_d].$$

The expectation of y_d^2 is $E_{\theta}[y_d^2] = E_v[E_{\theta}[y_d^2|\mathbf{v}]]$, where

$$y_d^2 = \sum_{j=1}^{n_d} y_{dj}^2 + \sum_{j_1 \neq j_2}^{n_d} y_{dj_1} y_{dj_2},$$

$$E_{\theta}[y_{dj}^2|\mathbf{v}] = \text{var}_{\theta}[y_{dj}|\mathbf{v}] + E_{\theta}^2[y_{dj}|\mathbf{v}] = m_{dj}p_{dj}(1 - p_{dj}) + m_{dj}^2p_{dj}^2.$$

Therefore, we have

$$E_{\theta}[y_d^2] = E_v \left[\sum_{j=1}^{n_d} m_{dj} p_{dj} (1 - p_{dj}) + \left(\sum_{j=1}^{n_d} m_{dj} p_{dj} \right)^2 \right].$$

Let us define $\xi_d = \sum_{j=1}^{n_d} m_{dj} p_{dj}$. The derivatives of $E_{\theta}[y_d^2]$ are

$$\frac{\partial E_{\theta}[y_d^2]}{\partial \beta_k} = \sum_{j=1}^{n_d} E_v[m_{dj} p_{dj} (1 - p_{dj}) \{1 - 2(p_{dj} - \xi_d)\} x_{dj k}],$$

$$\frac{\partial E_{\theta}[y_d^2]}{\partial \phi} = \sum_{j=1}^{n_d} E_v[m_{dj} p_{dj} (1 - p_{dj}) \{1 - 2(p_{dj} - \xi_d)\} v_d].$$

The elements of the matrix of first partial derivatives are

$$H_{k\ell} = \frac{\partial f_k(\theta)}{\partial \theta_{\ell}} = \sum_{d=1}^D \sum_{j=1}^{n_d} \frac{\partial E_{\theta}[y_{dj}]}{\partial \theta_{\ell}} x_{dj k}, \quad k = 1, \dots, p, \quad \ell = 1, \dots, p+1,$$

$$H_{p+1\ell} = \frac{\partial f_{p+1}(\theta)}{\partial \theta_{\ell}} = \sum_{d=1}^D \frac{\partial E_{\theta}[y_d^2]}{\partial \theta_{\ell}}, \quad \ell = 1, \dots, p+1,$$

where $\theta_1 = \beta_1, \dots, \theta_p = \beta_p, \theta_{p+1} = \phi$. The expectations appearing in $f(\theta)$ and $H(\theta)$ can be approximated by Monte Carlo simulation.

A.2. Proof of Proposition 4.1

A first-order multivariate Taylor expansion of $M(\hat{\theta})$ around θ yields

$$M(\hat{\theta}) = M(\theta) + \left(\frac{\partial}{\partial \theta} M(\theta) \right) (\hat{\theta} - \theta) + o(\|\hat{\theta} - \theta\|).$$

Therefore

$$\hat{\theta} - \theta = \left(\frac{\partial}{\partial \theta} M(\theta) \right)^{-1} (M(\hat{\theta}) - M(\theta)) + o(\|\hat{\theta} - \theta\|). \quad (\text{A.1})$$

Let us consider a univariate second order Taylor expansion of $M_k(\hat{\theta})$ around θ and substitute (A.1) in the quadratic term, that is

$$\begin{aligned} M_k(\hat{\theta}) &= M_k(\theta) + \left(\frac{\partial}{\partial \theta} M_k(\theta) \right)' (\hat{\theta} - \theta) + \frac{1}{2} (\hat{\theta} - \theta)' \left(\frac{\partial^2}{\partial \theta^2} M_k(\theta) \right) \\ &\quad (\hat{\theta} - \theta) + o(\|\hat{\theta} - \theta\|^2) \\ &= M_k(\theta) + \left(\frac{\partial}{\partial \theta} M_k(\theta) \right)' (\hat{\theta} - \theta) + \frac{1}{2} (M(\hat{\theta}) - M(\theta))' \left(\left(\frac{\partial}{\partial \theta} M(\theta) \right)^{-1} \right)' \\ &\quad \cdot \left(\frac{\partial^2}{\partial \theta^2} M_k(\theta) \right) \left(\frac{\partial}{\partial \theta} M(\theta) \right)^{-1} (M(\hat{\theta}) - M(\theta)) + o(\|\hat{\theta} - \theta\|^2). \end{aligned}$$

The corresponding multivariate Taylor expansion of $\mathbf{M}(\hat{\boldsymbol{\theta}})$ around $\boldsymbol{\theta}$ is

$$\begin{aligned}\mathbf{M}(\hat{\boldsymbol{\theta}}) &= \mathbf{M}(\boldsymbol{\theta}) + \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right) (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2} \underset{1 \leq k \leq p+1}{\text{col}} \left((\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta}))' \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \right)' \\ &\quad \cdot \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} \mathbf{M}_k(\boldsymbol{\theta}) \right) \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} (\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta})) + o(\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2) \\ &= \mathbf{M}(\boldsymbol{\theta}) + \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right) (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2D} \mathbf{q}_D + o(\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2).\end{aligned}$$

Therefore

$$\hat{\boldsymbol{\theta}} - \boldsymbol{\theta} = \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \left[(\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta})) - \frac{1}{2D} \mathbf{q}_D \right] + o(\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2). \quad (\text{A.2})$$

By substituting (A.2) in (4.3), we obtain

$$\begin{aligned}b_d(\boldsymbol{\theta}) &= \left(\frac{\partial}{\partial \boldsymbol{\theta}} g_d(\boldsymbol{\theta}) \right)' D \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \{E[\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta})] - \frac{1}{2D} E[\mathbf{q}_D]\} \\ &\quad + \frac{1}{2} E \left[\sqrt{D} \left[(\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta}))' - \frac{1}{2D} \mathbf{q}'_D \right] \left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \right)' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} g_d(\boldsymbol{\theta}) \right) \right. \\ &\quad \cdot \left. \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \sqrt{D} \left[(\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta})) - \frac{1}{2D} \mathbf{q}_D \right] \right] + Do(\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2).\end{aligned}$$

On the one hand, we substitute $\mathbf{M}(\hat{\boldsymbol{\theta}})$ by $\hat{\mathbf{M}}$, so that $E[\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta})] = E[\hat{\mathbf{M}} - \mathbf{M}(\boldsymbol{\theta})] = 0$. All the quadratic forms in the second summand containing $\mathbf{q}_D$ are $o(1)$. Therefore

$$\begin{aligned}b_d(\boldsymbol{\theta}) &= -\frac{1}{2} \left(\frac{\partial}{\partial \boldsymbol{\theta}} g_d(\boldsymbol{\theta}) \right)' \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} E[\mathbf{q}_D] \\ &\quad + \frac{1}{2} E \left[\sqrt{D} (\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta}))' \left(\left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \right)' \left(\frac{\partial^2}{\partial \boldsymbol{\theta}^2} g_d(\boldsymbol{\theta}) \right) \right. \\ &\quad \cdot \left. \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} \sqrt{D} (\mathbf{M}(\hat{\boldsymbol{\theta}}) - \mathbf{M}(\boldsymbol{\theta})) \right] + o(1) \\ &= \frac{1}{2} \left\{ E[r_{D,d}] - \left(\frac{\partial}{\partial \boldsymbol{\theta}} g_d(\boldsymbol{\theta}) \right)' \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\boldsymbol{\theta}) \right)^{-1} E[\mathbf{q}_D] \right\} + o(1) = B_d(\boldsymbol{\theta}) + o(1).\end{aligned}$$

A.3. MSE Components

The MSE estimators $mse^0(\hat{\mu}_d)$ and $mse^1(\hat{\mu}_d)$ given by (4.4) have the components g_d , c_d and B_d . This appendix gives algorithms for approximating them.

The term $g_d(\hat{\boldsymbol{\theta}})$ can be approximated by $\hat{g}_d(\hat{\boldsymbol{\theta}}) = \hat{E}[\hat{\mu}_d^2(\hat{\boldsymbol{\theta}})] - \hat{E}[\hat{\mu}_d^2(\hat{\boldsymbol{\theta}})]$, where the expectations are calculated by Monte Carlo simulation. This is to say, generate $v_d^{(s)}$ to be i.i.d. $N(0, 1)$ random variables and $v_d^{(S+s)} = -v_d^{(s)}$, $s = 1, \dots, S$, and calculate

$$\begin{aligned}\hat{E}[\hat{\mu}_d^2(\hat{\boldsymbol{\theta}})] &= \frac{1}{2S} \sum_{s=1}^{2S} \left(\sum_{k=1}^K N_{dk} \frac{\exp\{z_k \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}}{1 + \exp\{z_k \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}} \right)^2, \\ \hat{E}[\hat{\mu}_d^2(\hat{\boldsymbol{\theta}})] &= \sum_{j=0}^{n_d} \hat{\psi}_d^2(j, \hat{\boldsymbol{\theta}}) \hat{p}_d(j, \hat{\boldsymbol{\theta}}),\end{aligned}$$

where $\hat{\psi}_d(y_d, \hat{\boldsymbol{\theta}}) = \sum_{k=1}^K N_{dk} \frac{\hat{A}_{dk}^z}{\hat{C}_d}$ and

$$\hat{p}_d(j, \hat{\boldsymbol{\theta}}) = \sum_{y \in S_{n_d, j}} \left\{ \exp \left\{ \sum_{i=1}^{n_d} y_i \mathbf{x}_{di} \hat{\boldsymbol{\beta}} \right\} \frac{1}{2S} \sum_{s=1}^{2S} \exp \left\{ j \hat{\phi} v_d^{(s)} - \sum_{i=1}^{n_d} \log [1 + \exp\{\mathbf{x}_{di} \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}] \right\} \right\}.$$

The term $c_d(\hat{\boldsymbol{\theta}})$ can be approximated by

$$\hat{c}_d(\hat{\boldsymbol{\theta}}) = \sum_{j=1}^{n_d} \left(\frac{\partial}{\partial \boldsymbol{\theta}} \hat{\psi}_d(j, \hat{\boldsymbol{\theta}}) \right)' \hat{\mathbf{V}}(\hat{\boldsymbol{\theta}}) \left(\frac{\partial}{\partial \boldsymbol{\theta}} \hat{\psi}_d(j, \hat{\boldsymbol{\theta}}) \right) \hat{p}_d(j, \hat{\boldsymbol{\theta}}),$$

where $\hat{\mathbf{V}}(\hat{\boldsymbol{\theta}}) = D \widehat{\text{var}}_B(\hat{\boldsymbol{\theta}})$.

The bias correction term $B_d(\boldsymbol{\theta})$ can be approximated by parametric bootstrap, that is

1. Fit the model to the sample and calculate $\hat{\boldsymbol{\theta}}, \mathbf{R}_d(\hat{\boldsymbol{\theta}}), \mathbf{M}(\hat{\boldsymbol{\theta}})$ and $\mathbf{Q}_k(\hat{\boldsymbol{\theta}})$.
2. Generate bootstrap samples $\{y_{dj}^{(b)} : d = 1, \dots, D, j = 1, \dots, n_d\}$, $b = 1, \dots, B$, from the fitted model.
3. For each bootstrap sample, calculate $\Delta_D^{(b)} = \sqrt{D}(\hat{\mathbf{M}}^{(b)} - \mathbf{M}(\hat{\boldsymbol{\theta}}))$, where $\hat{\mathbf{M}}^{(b)} = \text{col}_{1 \leq k \leq p+1}(\hat{M}_k^{(b)})$, $\hat{M}_k^{(b)} = \sum_{d=1}^D \sum_{j=1}^{n_d} y_{dj}^{(b)} x_{djk}$, $k = 1, \dots, p$, $\hat{M}_{p+1}^{(b)} = \sum_{d=1}^D (y_d^{(b)})^2$, and calculate

$$r_{D,d}^{(b)} = \Delta_D^{(b)'} \mathbf{R}_d(\hat{\boldsymbol{\theta}}) \Delta_D^{(b)}, \quad q_{Dk}^{(b)} = \Delta_D^{(b)'} \mathbf{Q}_k(\hat{\boldsymbol{\theta}}) \Delta_D^{(b)}, \quad q_D^{(b)} = \text{col}_{1 \leq k \leq p+1}(q_{Dk}^{(b)}).$$

4. Calculate $\hat{E}_B[r_{D,d}] = \frac{1}{B} \sum_{b=1}^B r_{D,d}^{(b)}$, $\hat{E}_B[q_D] = \frac{1}{B} \sum_{b=1}^B q_D^{(b)}$.
5. Output: $\hat{B}_d(\hat{\boldsymbol{\theta}}) = \frac{1}{2} \left\{ \hat{E}_B[r_{D,d}] - \left(\frac{\partial}{\partial \boldsymbol{\theta}} \hat{g}_d(\hat{\boldsymbol{\theta}}) \right)' \left(\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{M}(\hat{\boldsymbol{\theta}}) \right)^{-1} \hat{E}_B[q_D] \right\}$.

A.4. Derivatives Needed to Calculate MSE Components

To calculate the approximation of the terms c_d and particularly B_d we need to evaluate first and second order derivatives of $g_d(\boldsymbol{\theta})$ and $M_k(\boldsymbol{\theta})$ (cf. Proposition 4.1.). In this appendix we present formulas for derivatives of these and other necessary terms with respect to parameters β_r , $r = 1, \dots, p$, in the case of first order and with respect to $\beta_s \beta_r$, $r, s = 1, \dots, p$, in the case of second order. The derivatives with respect to ϕ , $\beta_r \phi$ and ϕ^2 can be obtained in a similar form and they are omitted here.

A.4.1. Derivatives of $\mathbf{M}(\boldsymbol{\theta})$

We recall that $\mathbf{M}(\boldsymbol{\theta}) = \text{col}_{1 \leq k \leq p+1} (M_k(\boldsymbol{\theta}))$, where

$$M_k(\boldsymbol{\theta}) = \sum_{d=1}^D \sum_{j=1}^{n_d} E_{\boldsymbol{\theta}}[y_{dj}] x_{dj k} = \sum_{d=1}^D \sum_{j=1}^{n_d} x_{dj k} E_v[p_{dj}],$$

$$M_{p+1}(\boldsymbol{\theta}) = \sum_{d=1}^D E_{\boldsymbol{\theta}}[y_{d.}^2] = \sum_{d=1}^D E_v \left[\sum_{j=1}^{n_d} p_{dj}(1 - p_{dj}) + \left(\sum_{j=1}^{n_d} p_{dj} \right)^2 \right].$$

Let us define $\xi_d = \sum_{j=1}^{n_d} p_{dj}$ for p_{dj} given in (2.3) and note that

$$\frac{\partial p_{dj}}{\partial \beta_r} = x_{dj r} p_{dj} (1 - p_{dj}), \quad \frac{\partial p_{dj}(1 - p_{dj})}{\partial \beta_r} = x_{dj r} p_{dj} (1 - p_{dj}) (1 - 2p_{dj})$$

and

$$\frac{\partial (p_{dj} - \xi_d)}{\partial \beta_s} = x_{djs} p_{dj} (1 - p_{dj}) - \sum_{i=1}^{n_d} p_{di} (1 - p_{di}) x_{dis}.$$

The first and second order partial derivatives of $M_k(\boldsymbol{\theta})$ are for $k, r, s = 1, \dots, p$

$$\frac{\partial M_k}{\partial \beta_r} = \sum_{d=1}^D \sum_{j=1}^{n_d} x_{dj k} x_{dj r} E_v[p_{dj}(1 - p_{dj})],$$

$$\frac{\partial M_{p+1}}{\partial \beta_r} = \sum_{d=1}^D \sum_{j=1}^{n_d} x_{dj r} E_v[p_{dj}(1 - p_{dj}) \{1 - 2(p_{dj} - \xi_d)\}],$$

$$\frac{\partial^2 M_k}{\partial \beta_s \partial \beta_r} = \sum_{d=1}^D \sum_{j=1}^{n_d} x_{dj k} x_{dj r} x_{djs} E_v[p_{dj}(1 - p_{dj})(1 - 2p_{dj})],$$

$$\frac{\partial^2 M_{p+1}}{\partial \beta_s \partial \beta_r} = \sum_{d=1}^D \sum_{j=1}^{n_d} x_{dj r} E_v[x_{djs} p_{dj}(1 - p_{dj})(1 - 2p_{dj}) \{1 - 2(p_{dj} - \xi_d)\}$$

$$- 2p_{dj}^2(1 - p_{dj})^2 x_{djs} + 2p_{dj}(1 - p_{dj}) \sum_{i=1}^{n_d} p_{di}(1 - p_{di}) x_{dis}].$$

A.4.2. Derivatives of $C_d(j, \boldsymbol{\theta})$ and $A_{dk}^z(j, \boldsymbol{\theta})$

Let us denote

$$R_d(\boldsymbol{\theta}, j, v_d) = R_d(j) = \exp \left\{ j \phi v_d - \sum_{i=1}^{n_d} \log[1 + \exp\{\mathbf{x}_{di} \boldsymbol{\beta} + \phi v_d\}] \right\}.$$

Then C_d , defined in (3.1), can be written for $y_d. = j$ in the form

$$C_d(j, \boldsymbol{\theta}) = C_d(j) = \int_R R_d(\boldsymbol{\theta}, j, v_d) f(v_d) dv_d \quad (\text{A.3})$$

and its first and second order partial derivatives are

$$\begin{aligned}\frac{\partial C_d(j)}{\partial \beta_r} &= - \int_R R_d(j) \left(\sum_{i=1}^{n_d} p_{di} x_{dir} \right) f(v_d) dv_d, \\ \frac{\partial^2 C_d(j)}{\partial \beta_s \partial \beta_r} &= \int_R R_d(j) \left\{ \left(\sum_{i=1}^{n_d} p_{di} x_{dir} \right) \left(\sum_{i=1}^{n_d} p_{di} x_{dis} \right) \right. \\ &\quad \left. - \sum_{i=1}^{n_d} p_{di} (1 - p_{di}) x_{dir} x_{dis} \right\} f(v_d) dv_d.\end{aligned}$$

The term A_{dk}^z , defined in (3.5), can be expressed for $y_d = j$ and q_{dk} , given in (3.2), as

$$A_{dk}^z(j, \boldsymbol{\theta}) = A_{dk}^z(j) = \int_R q_{dk} R_d(\boldsymbol{\theta}, j, v_d) f(v_d) dv_d$$

and its first and second order partial derivatives are

$$\begin{aligned}\frac{\partial A_{dk}^z(j)}{\partial \beta_r} &= \int_R q_{dk} R_d(j) \left\{ (1 - q_{dk}) z_{kr} - \sum_{i=1}^{n_d} p_{di} x_{dir} \right\} f(v_d) dv_d, \\ \frac{\partial^2 A_{dk}^z(j)}{\partial \beta_s \partial \beta_r} &= \int_R q_{dk} (1 - q_{dk}) z_{ks} R_d(j) \left\{ (1 - q_{dk}) z_{kr} - \sum_{i=1}^{n_d} p_{di} x_{dir} \right\} f(v_d) dv_d \\ &\quad - \int_R q_{dk} R_d(j) \left(\sum_{i=1}^{n_d} p_{di} x_{dis} \right) \left\{ (1 - q_{dk}) z_{kr} - \sum_{i=1}^{n_d} p_{di} x_{dir} \right\} f(v_d) dv_d \\ &\quad + \int_R q_{dk} R_d(j) \left\{ -q_{dk} (1 - q_{dk}) z_{kr} z_{ks} - \sum_{i=1}^{n_d} p_{di} (1 - p_{di}) x_{dir} x_{dis} \right\} f(v_d) dv_d.\end{aligned}$$

A.4.3. Derivatives of $p_d(j, \boldsymbol{\theta})$

From the definitions of $p_d(j, \boldsymbol{\theta}) = p_d(j)$ in (4.1) and of $C_d(j, \boldsymbol{\theta}) = C_d(j)$ in (A.3), it follows that

$$p_d(j, \boldsymbol{\theta}) = \sum_{\mathbf{y} \in \mathcal{S}_{n_d, j}} \left[\exp \left\{ \sum_{i=1}^{n_d} y_i \mathbf{x}_{di} \boldsymbol{\beta} \right\} C_d(j, \boldsymbol{\theta}) \right].$$

So that the first- and second-order partial derivatives of $p_d(j)$ are

$$\frac{\partial p_d(j)}{\partial \beta_r} = \sum_{\mathbf{y} \in \mathcal{S}_{n_d, j}} \exp \left\{ \sum_{i=1}^{n_d} y_i \mathbf{x}_{di} \boldsymbol{\beta} \right\} \left[\left(\sum_{i=1}^{n_d} y_i x_{dir} \right) C_d(j) + \frac{\partial C_d(j)}{\partial \beta_r} \right],$$

$$\begin{aligned} \frac{\partial^2 p_d(j)}{\partial \beta_s \partial \beta_r} = & \sum_{y \in S_{n_d j}} \exp \left\{ \sum_{i=1}^{n_d} y_i x_{di} \boldsymbol{\beta} \right\} \left[\left(\sum_{i=1}^{n_d} y_i x_{dir} \right) \left(\sum_{i=1}^{n_d} y_i x_{dis} \right) C_d(j) \right. \\ & \left. + \left(\sum_{i=1}^{n_d} y_i x_{dir} \right) \frac{\partial C_d(j)}{\partial \beta_s} + \left(\sum_{i=1}^{n_d} y_i x_{dis} \right) \frac{\partial C_d(j)}{\partial \beta_r} + \frac{\partial^2 C_d(j)}{\partial \beta_s \partial \beta_r} \right]. \end{aligned}$$

A.4.4. Derivatives of $\psi_d(y_d, \boldsymbol{\theta})$

The first- and second-order partial derivatives of

$$\psi_d(j, \boldsymbol{\theta}) = \psi_d(j) = \sum_{k=1}^K N_{dk} \frac{A_{dk}^z(j)}{C_d(j)},$$

defined in (3.4), are

$$\begin{aligned} \frac{\partial \psi_d(j, \boldsymbol{\theta})}{\partial \theta_r} = & \sum_{k=1}^K N_{dk} \left\{ \frac{\frac{\partial A_{dk}^z(j)}{\partial \theta_r}}{C_d(j)} - \frac{A_{dk}^z(j) \frac{\partial C_d(j)}{\partial \theta_r}}{C_d^2(j)} \right\}, \\ \frac{\partial^2 \psi_d(j, \boldsymbol{\theta})}{\partial \theta_s \partial \theta_r} = & \sum_{k=1}^K N_{dk} \left\{ \frac{\frac{\partial^2 A_{dk}^z(j)}{\partial \theta_s \partial \theta_r}}{C_d(j)} - \frac{\frac{\partial A_{dk}^z(j)}{\partial \theta_r} \frac{\partial C_d(j)}{\partial \theta_s} + \frac{\partial A_{dk}^z(j)}{\partial \theta_s} \frac{\partial C_d(j)}{\partial \theta_r} + A_{dk}^z(j) \frac{\partial^2 C_d(j)}{\partial \theta_s \partial \theta_r}}{C_d^2(j)} \right. \\ & \left. + \frac{2A_{dk}^z(j) \frac{\partial C_d(j)}{\partial \theta_s} \frac{\partial C_d(j)}{\partial \theta_r}}{C_d^3(j)} \right\}. \end{aligned}$$

A.4.5. Derivatives of $g_d(\boldsymbol{\theta})$

We recall that

$$g_d(\boldsymbol{\theta}) = \int_R \left(\sum_{k=1}^K N_{dk} q_{dk}(\boldsymbol{\theta}, v_d) \right)^2 f(v_d) dv_d - \sum_{j=0}^{n_d} \psi_d^2(j, \boldsymbol{\theta}) p_d(j, \boldsymbol{\theta}).$$

The first order partial derivatives of $g_d(\boldsymbol{\theta})$ are

$$\begin{aligned} \frac{\partial g_d(\boldsymbol{\theta})}{\partial \beta_r} = & 2 \int_R \left(\sum_{k=1}^K N_{dk} q_{dk} \right) \left(\sum_{k=1}^K N_{dk} q_{dk} (1 - q_{dk}) z_{kr} \right) f(v_d) dv_d \\ & - 2 \sum_{j=0}^{n_d} \psi_d(j) \frac{\partial \psi_d(j)}{\partial \beta_r} p_d(j) - \sum_{j=0}^{n_d} \psi_d^2(j) \frac{\partial p_d(j)}{\partial \beta_r}. \end{aligned}$$

The second order partial derivatives of $g_d(\boldsymbol{\theta})$ are

$$\begin{aligned} \frac{\partial^2 g_d(\boldsymbol{\theta})}{\partial \beta_s \partial \beta_r} &= 2 \int_R \left(\sum_{k=1}^K N_{dk} q_{dk} (1 - q_{dk}) z_{ks} \right) \left(\sum_{k=1}^K N_{dk} q_{dk} (1 - q_{dk}) z_{kr} \right) f(v_d) dv_d \\ &\quad + 2 \int_R \left(\sum_{k=1}^K N_{dk} q_{dk} \right) \left(\sum_{k=1}^K N_{dk} q_{dk} (1 - q_{dk}) (1 - 2q_{dk}) z_{kr} z_{ks} \right) f(v_d) dv_d \\ &\quad - 2 \sum_{j=0}^{n_d} \frac{\partial \psi_d(j)}{\partial \beta_s} \frac{\partial \psi_d(j)}{\partial \beta_r} p_d(j) - 2 \sum_{j=0}^{n_d} \psi_d(j) \frac{\partial^2 \psi_d(j)}{\partial \beta_s \partial \beta_r} p_d(j) - 2 \sum_{j=0}^{n_d} \psi_d(j) \frac{\partial \psi_d(j)}{\partial \beta_r} \frac{\partial p_d(j)}{\partial \beta_s} \\ &\quad - 2 \sum_{j=0}^{n_d} \psi_d(j) \frac{\partial \psi_d(j)}{\partial \beta_s} \frac{\partial p_d(j)}{\partial \beta_r} - \sum_{j=0}^{n_d} \psi_d^2(j) \frac{\partial^2 p_d(j)}{\partial \beta_s \partial \beta_r}. \end{aligned}$$

A.4.6. Approximations of the Derivatives

The integrals appearing in the described derivatives can be approximated by Monte Carlo simulation. To illustrate the procedure, we present the corresponding formulas used to approximate the derivatives of the term $C_d(j)$ derived in Section A.4.2. The approximations of the derivatives of the remaining terms can be done in a similar way.

For $s = 1, \dots, S$, let $v_d^{(s)}$ be i.i.d. $N(0, 1)$ random variables and $v_d^{(S+s)} = -v_d^{(s)}$. The partial derivatives of $C_d(j)$ can be approximated as follows:

$$\begin{aligned} \frac{\partial \hat{C}_d(j)}{\partial \beta_r} &= -\frac{1}{2S} \sum_{s=1}^{2S} \hat{R}_d^{(s)}(j) \left(\sum_{i=1}^{n_d} \hat{p}_{di}^{(s)} x_{dir} \right), \\ \frac{\partial^2 \hat{C}_d(j)}{\partial \beta_s \partial \beta_r} &= \frac{1}{2S} \sum_{s=1}^{2S} \hat{R}_d^{(s)}(j) \left\{ \left(\sum_{i=1}^{n_d} \hat{p}_{di}^{(s)} x_{dir} \right) \left(\sum_{i=1}^{n_d} \hat{p}_{di}^{(s)} x_{dis} \right) \right. \\ &\quad \left. - \sum_{i=1}^{n_d} \hat{p}_{di}^{(s)} (1 - \hat{p}_{di}^{(s)}) x_{dir} x_{dis} \right\}, \end{aligned}$$

where

$$\hat{R}_d^{(s)}(j) = R(\hat{\boldsymbol{\theta}}, j, v_d^{(s)}) \quad \text{and} \quad \hat{p}_{di}^{(s)} = \frac{\exp\{\mathbf{x}_{di} \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}}{1 + \exp\{\mathbf{x}_{di} \hat{\boldsymbol{\beta}} + \hat{\phi} v_d^{(s)}\}}.$$

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