Catalogue no. 12-001-X
ISSN 1492-0921

Survey Methodology

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Release date: December 15, 2020

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Survey Methodology, December 2020
Vol. 46, No. 2, pp. 145-180
Statistics Canada, Catalogue No. 12-001-X

Estimation and inference of domain means subject to qualitative constraints

Cristian Oliva-Aviles, Mary C. Meyer and Jean D. Opsomer[1]

Abstract

In many large-scale surveys, estimates are produced for numerous small domains defined by cross-classifications of demographic, geographic and other variables. Even though the overall sample size of such surveys might be very large, samples sizes for domains are sometimes too small for reliable estimation. We propose an improved estimation approach that is applicable when "natural" or qualitative relationships (such as orderings or other inequality constraints) can be formulated for the domain means at the population level. We stay within a design-based inferential framework but impose constraints representing these relationships on the sample-based estimates. The resulting constrained domain estimator is shown to be design consistent and asymptotically normally distributed as long as the constraints are asymptotically satisfied at the population level. The estimator and its associated variance estimator are readily implemented in practice. The applicability of the method is illustrated on data from the 2015 U.S. National Survey of College Graduates.

Key Words: Design-based estimation; Monotone estimation; National Survey of College Graduates.

1 Introduction

For many large-scale surveys, a goal is to produce estimates for a large number of domains, many of which might have small sample size. These domains are typically created by cross-classifying categorical variables such as demographic, geographic or other similar characteristics of interest. For instance, the U.S. Current Population Survey releases estimates for domains defined by sex, age, race and/or educational attainment. Similarly, the U.S. American Community Survey produces detailed estimates by sex, age, race/ethnicity for different levels of geography (depending on the release). In another example we will discuss further below, the U.S. National Survey of College Graduates is interested in estimates defined by crossing level and field of degree, occupation and gender. Depending on the survey program, such "granular" estimates are often as important as the higher-level or population estimates.

However, although the overall sample size of such surveys might be very large, samples sizes for numerous domains are often too small for reliable estimates. One possible approach to avoid this problem could be to aggregate small domains into bigger scales so that more reliable direct estimators can be produced for those scales, leading to the generation of more aggregated information than the actual desired scale. An alternative to producing small domain estimates could be changing from a design-based to a model-based estimation methodology such as small area models. While that is certainly a statistically valid approach for creating precise estimates at small scales, it is labor-intensive and sensitive to potential model misspecification. It also replaces the sampling error by model error, so that the mode of inference changes. For those reasons, statistical agencies prefer to stay within the design-based approach, which offers robustness and also allows to stay with the standard mode of inference for surveys.

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In this paper, we present an estimation approach that is applicable when "natural" or qualitative relationships are expected to hold among the domain means at the population level. These relationships can be used to stabilize the sample domain estimates, while staying within the design-based mode of estimation and inference. The type of relationships we are considering here lead to inequalities among population domain means. For instance, certain job types might be expected to receive better salaries than others, or individuals with graduate degrees in a given discipline are expected to have higher salaries than those without graduate degrees in that discipline. However, given that small domains tend to produce estimates with high variability, such expected population-level relationships are often violated at the sample level. While such violations should be expected by data users due to statistical variability, they might lead them to question the overall reliability of the survey, by producing "absurd" estimates.

There is a large literature in survey statistics related to calibrating survey estimates, see e.g. Särndal, Swensson and Wretman (1992) for an overview. While these estimators also rely on constraints, there are important differences, including the fact that the constraints are equality constraints and that they are applied to the survey weights, not the estimates themselves. While we do not explore this here, it would be possible to combine calibration and constrained estimation, since the latter could use calibrated domain estimates as the starting point for constructing constrained domain estimates. In the model-based setting, Rueda and Lombardía (2012) adapted methods in small area estimation for the case of monotonically ordered domain means.

Recently, Wu, Meyer and Opsomer (2016) proposed a domain mean estimation methodology that relies on the assumption of monotone population domain means along a single domain-defining categorical variable (e.g., age classes). By combining the monotonicity information of domain means and design-based estimators in the estimation stage, they proposed a *constrained* estimator that respects the monotone assumption. Such an estimator was shown to improve precision and variability of domain mean estimates in comparison with direct estimators, given that the assumption of monotonicity is reasonable.

We generalize this work here by allowing a much larger class of constraints between domain means, applicable to the multi-dimensional setting. Many other types of constraints beyond monotonicity may be expected to hold between population domain means in real surveys, especially in the presence of domains defined by the cross-classifications of many categorical variables. In general, any set of linear inequality constraints can be represented through a *constraint matrix*, where each row defines a constraint and each column a domain mean. For illustration of a constraint matrix, suppose the variable of interest is the annual average salary of faculty in land-grant universities of a certain size. Further, consider domains generated from the cross-classification of the variables job position (x_1; 1 = Untenured and 2 = Tenured) and three specific departments (x_2; 1 = Anthropology, 2 = English and 3 = Engineering). Under the assumptions that, on average within a discipline, tenured faculty have higher salaries than untenured faculty; and that, within tenured and untenured, Engineering faculty members are expected to have higher salaries than those in either the Anthropology or English departments, then we can express the corresponding restrictions as,

$$\mathbf{A}\boldsymbol{\mu} \geq \mathbf{0}, \quad \text{where} \quad \mathbf{A} = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \\ -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}, \tag{1.1}$$

$\boldsymbol{\mu} = (\mu_{11}, \mu_{21}, \mu_{12}, \mu_{22}, \mu_{13}, \mu_{23})^{\top}$, with μ_{ij} representing the mean of the domain that corresponds to $x_1 = i$ and $x_2 = j$; $\mathbf{0}$ being the zero vector, and the inequality being element-wise. This paper describes a new constrained estimator for population domain means that respect constraints that can be expressed with matrix inequalities of the form given in (1.1). By combining design-based domain mean estimators with these shape constraints, we propose a broadly applicable estimator that improves precision and variability of the most common direct estimators.

The remainder of the paper is organized as follows. In Section 2 we formally introduce the constrained estimator and propose a linearization-based method for variance estimation. This section also contains some scenarios of interest where shape constraints can naturally arise for survey data. Section 3 states the main theoretical properties of the constrained estimator. The necessary assumptions used in these theoretical derivations are also stated in this section. Proofs of main theorems and auxiliary lemmas are provided in the Appendix. Section 4 shows through simulations that the constrained estimator improves domain mean estimation and variability in comparison with the unconstrained estimator, even when the assumed shape holds only approximately at the population level. Section 5 demonstrates the advantages of the proposed methodology on real survey data through an application to the 2015 National Survey of College Graduates. A few concluding remarks are provided in Section 6.

2 Constrained estimation and inference for domain means

2.1 Notation and preliminaries

Let U_N be the set of elements in a population of size N. Consider a sample s_N of size n_N that is drawn from U_N using a probability sampling design $p_N(\cdot)$. Denote $\pi_{k,N} = \Pr(k \in s_N)$ and $\pi_{kl,N} = \Pr(k \in s_N,\ l \in s_N)$ as the first and second order inclusion probabilities, respectively. Assume that $\pi_{k,N} > 0$, $\pi_{kl,N} > 0$ for $k, l \in U_N$. To simplify notation, we will adopt the usual convention of suppressing the subscript N unless it is needed for clarity. Denote $\{U_d\}_{d=1}^{D}$ as a domain partition of U, where D is the number of domains and each U_d is of size N_d. Also, let s_d be the subset of size n_d of s that belongs to U_d.

For any study variable y, $\bar{\mathbf{y}}_U = \left(\bar{y}_{U_1}, \ldots, \bar{y}_{U_D}\right)^\top$ denotes the vector of population domain means, where

$$\bar{y}_{U_D} = \frac{\sum_{k \in U_d} y_k}{N_d}. \tag{2.1}$$

We will focus on the Hájek estimator of $\bar{y}_{U_D}$, given by

$$\tilde{y}_{s_d} = \frac{\sum_{k \in s_d} y_k / \pi_k}{\hat{N}_d} \tag{2.2}$$

with $\hat{N}_d = \sum_{k \in s_d} 1/\pi_k$, and let $\tilde{\mathbf{y}}_s$ to be the vector of estimators. The results will also hold for the Horvitz-Thompson estimator with minor modifications, but it will not be explicitly addressed in what follows.

2.2 Proposed estimator

Assume there is information available regarding relationships between the population domain means that can be expressed with m constraints through a $m \times D$ *irreducible* constraint matrix $\mathbf{A}$. A matrix $\mathbf{A}$ is irreducible if none of its rows is a positive linear combination of other rows, and if the origin is also not a positive linear combination of its rows (Meyer, 1999). In practical terms, this means that there are no redundant constraints in $\mathbf{A}$. To take advantage of $\tilde{\mathbf{y}}_s$ to obtain an estimator that respects these shape constraints, we propose the constrained estimator $\tilde{\boldsymbol{\theta}}_s = \left(\tilde{\theta}_{s_1}, \ldots, \tilde{\theta}_{s_D}\right)^\top$ to be the unique vector that solves the following constrained weighted least squares problem,

$$\min_{\boldsymbol{\theta}} (\tilde{\mathbf{y}}_s - \boldsymbol{\theta})^\top \mathbf{W}_s (\tilde{\mathbf{y}}_s - \boldsymbol{\theta}) \quad \text{subject to} \quad \mathbf{A}\boldsymbol{\theta} \geq \mathbf{0}; \tag{2.3}$$

where $\mathbf{W}_s$ is the diagonal matrix with elements $\hat{N}_1/\hat{N}$, $\hat{N}_2/\hat{N}$, …, $\hat{N}_D/\hat{N}$, and $\hat{N} = \sum_{d=1}^{D} \hat{N}_d$. The constrained problem in equation (2.3) can be alternatively written as finding the unique vector $\tilde{\boldsymbol{\phi}}_s$ that solves

$$\min_{\boldsymbol{\phi}} \| \tilde{\mathbf{z}}_s - \boldsymbol{\phi} \|^2 \quad \text{subject to} \quad \mathbf{A}_s\boldsymbol{\phi} \geq \mathbf{0}, \tag{2.4}$$

where $\tilde{\mathbf{z}}_s = \mathbf{W}_s^{1/2} \tilde{\mathbf{y}}_s$, $\boldsymbol{\phi} = \mathbf{W}_s^{1/2} \boldsymbol{\theta}$, and $\mathbf{A}_s = \mathbf{A}\mathbf{W}_s^{-1/2}$. The transformed constrained matrix $\mathbf{A}_s$ is also irreducible if $\mathbf{A}$ is, and it depends on the sample although $\mathbf{A}$ does not. The solution $\tilde{\boldsymbol{\phi}}_s$ is the *projection* of $\tilde{\mathbf{z}}_s$ onto the set of vectors $\boldsymbol{\phi}$ that satisfy the condition $\mathbf{A}_s\boldsymbol{\phi} \geq \mathbf{0}$. This set is a polyhedral convex cone, called the *constraint cone* Ω_s defined by $\mathbf{A}_s$; specifically,

$$\Omega_s = \{\boldsymbol{\phi} \in \mathbb{R}^D : \mathbf{A}_s\boldsymbol{\phi} \geq \mathbf{0}\}. \tag{2.5}$$

We use the notation $\tilde{\boldsymbol{\phi}}_s = \Pi(\tilde{\mathbf{z}}_s \mid \Omega_s)$, where $\Pi(\mathbf{u} \mid \mathcal{S})$ stands for the projection of $\mathbf{u}$ onto the set $\mathcal{S}$, i.e., the closest vector in $\mathcal{S}$ to $\mathbf{u}$.

Projections onto such cones are well understood; see Rockafellar (1970) or Meyer (1999) for details. In terms of this work, the main results from cone projection theory are summarized here. The cone can be characterized by a set of *edges* generating the cone; that is, a vector is in the cone if and only if it is a linear combination of the edges with non-negative coefficients. (Picture a pyramid with vertex at the origin, extending out indefinitely.) Subsets of the edges define the *faces* of the cone, and the projection of $\tilde{\mathbf{z}}_s$ onto the cone lands on one of the faces. Once the edges defining this face are determined, the projection can be characterized as an ordinary least-squares projection onto the linear space spanned by this subset of edges. This property is crucial for both the algorithm for projection and for inference, because the projection onto the cone can be characterized as a linear projection.

For this work, we will project $\tilde{\mathbf{z}}_s$ onto the *polar cone* Ω_s^0 (Rockafellar, 1970, page 121), defined as

$$\Omega_s^0 = \{\boldsymbol{\rho} \in \mathbb{R}^D: \langle \boldsymbol{\rho}, \boldsymbol{\phi} \rangle \leq 0, \ \forall \boldsymbol{\phi} \in \Omega_s\}, \tag{2.6}$$

where $\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^\top \mathbf{v}$. That is, the polar cone is the set of vectors that form obtuse angles with all vectors in Ω_s. The polar cone is analogous to the orthogonal space in linear least-squares projections, in that the projection of a vector onto the polar cone is the residual of its projection onto the constraint cone, and vice-versa. Meyer (1999) showed that the negative rows of an irreducible matrix are the *edges* (generators) of the polar cone, leading to the following characterization of the polar cone in (2.6):

$$\Omega_s^0 = \left\{\boldsymbol{\rho} \in \mathbb{R}^D: \boldsymbol{\rho} = \sum_{j=1}^{m} a_j \boldsymbol{\gamma}_{s_j}, \ a_j \geq 0, \ j = 1, 2, \ldots, m\right\}, \tag{2.7}$$

where $\boldsymbol{\gamma}_{s_1}, \boldsymbol{\gamma}_{s_2}, \ldots, \boldsymbol{\gamma}_{s_m}$ are the rows of $-\mathbf{A}_s$. Robertson, Wright and Dykstra (1988, page 17) established necessary and sufficient conditions for a vector $\tilde{\boldsymbol{\phi}}_s$ to be the projection of $\tilde{\mathbf{z}}_s$ onto Ω_s. That is, $\tilde{\boldsymbol{\phi}}_s \in \Omega_s$ solves the constrained problem in (2.4) if and only if

$$\langle \tilde{\mathbf{z}}_s - \tilde{\boldsymbol{\phi}}_s, \tilde{\boldsymbol{\phi}}_s \rangle = 0, \quad \text{and} \quad \langle \tilde{\mathbf{z}}_s - \tilde{\boldsymbol{\phi}}_s, \boldsymbol{\phi} \rangle \leq 0, \ \forall \boldsymbol{\phi} \in \Omega_s.$$

Moreover, the above conditions can be adapted to the polar cone as follows: the vector $\tilde{\boldsymbol{\rho}}_s \in \Omega_s^0$ minimizes $\|\tilde{\mathbf{z}}_s - \boldsymbol{\rho}\|^2$ over Ω_s^0 if and only if

$$\langle \tilde{\mathbf{z}}_s - \tilde{\boldsymbol{\rho}}_s, \tilde{\boldsymbol{\rho}}_s \rangle = 0, \quad \text{and} \quad \langle \tilde{\mathbf{z}}_s - \tilde{\boldsymbol{\rho}}_s, \boldsymbol{\gamma}_{s_j} \rangle \leq 0 \quad \text{for} \quad j = 1, 2, \ldots, m. \tag{2.8}$$

The conditions in (2.8) can be used to show that the projection of $\tilde{\mathbf{z}}_s$ onto the polar cone Ω_s^0 coincides with the projection onto the linear space generated by the edges $\boldsymbol{\gamma}_{s_j}$ such that $\langle \tilde{\mathbf{z}}_s - \tilde{\boldsymbol{\rho}}_s, \boldsymbol{\gamma}_{s_j} \rangle = 0$. This set of edges could be empty, meaning that the projection onto Ω_s^0 is equal to the projection onto the zero vector. In that case, the unconstrained minimum satisfies all the constraints. Alternatively, this set of edges might not be unique. To formalize these ideas, denote $V_{s,J} = \{\boldsymbol{\gamma}_{s_j}: j \in J\}$ for any $J \subseteq \{1, 2, \ldots, m\}$. Define the set $\bar{\mathcal{F}}_{s,J}$ as,

$$\bar{\mathcal{F}}_{s,J} = \left\{ \boldsymbol{\rho} \in \mathbb{R}^D: \ \boldsymbol{\rho} = \sum_{j \in J} a_j \boldsymbol{\gamma}_{s_j}, \ \ a_j \geq 0, \ \ j \in J \right\}, \tag{2.9}$$

where $\bar{\mathcal{F}}_{s,\varnothing} = \mathbf{0}$ by convention. (Technically, this set is the closure of a face of the cone.) That is, $\bar{\mathcal{F}}_{s,J}$ is a closed polyhedral sub-cone of Ω_s^0 that starts at the origin and is defined by the edges in $V_{s,J}$. Further, let $\mathcal{L}(V_{s,J})$ be the linear space generated by the vectors in $V_{s,J}$. It is shown in Meyer (1999) that projecting onto Ω_s^0 is equivalent to projecting onto $\mathcal{L}(V_{s,J})$, for an appropriate set J. If the rows of the constraint matrix $\mathbf{A}$ are linearly independent, then the minimal set J is unique; otherwise there may be more than one J that defines the linear space. In the latter case, however, the projection is still unique (see Theorem 1 of the next section).

Wu et al. (2016) considered the solution to (2.3), in the special case of a monotone relationship between domains defined along a single categorical variable. In that case, the solution is equivalent to that of the Pooled Adjacent Violator Algorithm (PAVA), which has an explicit expression in terms of a pooling of neighboring domains. The theoretical results in Wu et al. (2016) were obtained using that explicit expression, and hence do not apply to the more general setting considered here. Nevertheless, as was the case with the simple 6-domain example in Section 1 and in many situations of practical interest, the specific matrix $\mathbf{A}$ will often correspond to a multivariate *partial ordering* of the domain means. Under partial ordering, the solution to the constrained minimization in (2.3) is again equivalent to a pooling of neighboring domains in such a way that the partial order constraints are respected. See for instance Robertson et al. (1988, page 23) for an explicit expression of this pooled domain expression under partial ordering, including the definition of the pooling. However, unlike PAVA in the univariate case, this does not lead to a practical general computational algorithm. In the current paper, we will allow for arbitrary irreducible constraint matrix $\mathbf{A}$, which will include partial ordering and univariate monotonicity as special cases.

One possible general approach to computing $\tilde{\boldsymbol{\phi}}_s$ is based on the edges of the constraint cone Ω_s. However, the number of edges can be considerably larger than the number of constraints for large values of D, especially for the case when there are more constraints than domains (see Meyer, 1999). Moreover, given the lack of a general closed form solution for the edges of Ω_s (when $m > D$), the edges need to be computed numerically in that case. This task is computationally demanding, which makes this approach an inefficient way to compute $\tilde{\boldsymbol{\phi}}_s$. A more efficient algorithm based on computing the projection onto the polar cone has been developed: the Cone Projection Algorithm (CPA) (Meyer, 2013). This alternative approach takes advantage of the easy-to-find edges $\boldsymbol{\gamma}_{s_j}$ of the polar cone, the conditions in (2.8), and the fact that $\Pi(\tilde{\mathbf{z}}_s \,|\, \Omega_s) = \tilde{\mathbf{z}}_s - \Pi(\tilde{\mathbf{z}}_s \,|\, \Omega_s^0)$. The latter fact is a key component on the proofs of the main theoretical results shown in this paper. CPA has been implemented in the software R into the `coneproj` package. See Liao and Meyer (2014) for further details.

For the situations in which the constraints correspond to complete or partial ordering, the CPA solution once again corresponds to domain pooling. After this, the domain mean estimates can be explicitly

computed as sample-based domain means for the CPA-determined pooled domains. This greatly facilitates incorporating this methodology into survey estimation practice, because the pooled domain definitions can be readily communicated as part of the instructions accompanying a survey dataset release, and the estimates can be calculated without requiring access to specialized software.

2.3 Variance estimation of $\tilde{\theta}_{s_d}$

Estimating appropriately the variance of $\tilde{\theta}_{s_d}$ is a complicated task, derived from the fact that the projection of $\tilde{\mathbf{z}}_s$ onto Ω_s^0 (or onto Ω_s) might not always land on the same linear space $\mathcal{L}(V_{s,J})$ for different samples s. To better understand that, we define $\mathcal{G}_s$ as the set of all subsets $J \subseteq \{1, 2, \ldots, m\}$ such that $\Pi(\tilde{\mathbf{z}}_s \mid \Omega_s^0) = \Pi(\tilde{\mathbf{z}}_s \mid \mathcal{L}(V_{s,J})) \in \bar{\mathcal{F}}_{s,J}$, as defined in (2.9). As noted earlier, there could be different sets J_1 and J_2 such that the projection onto the polar cone Ω_s^0 is equal to projecting onto either $\mathcal{L}(V_{s,J_1})$ or $\mathcal{L}(V_{s,J_2})$. However, independently of which set is chosen, the projection $\tilde{\boldsymbol{\rho}}_s$ is unique.

To illustrate the above point, consider the following restrictions when there are only 3 domains: the first domain mean is expected to be at the most equal to the second domain mean, and the third domain mean is expected to be at least equal to the average of the first two domain means. Hence, the constraint matrix $\mathbf{A}$ can be expressed as

$$\mathbf{A} = \begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 2 \end{pmatrix}.$$

Suppose it is observed that $\tilde{y}_{s_1} = \tilde{y}_{s_2} < \tilde{y}_{s_3}$. The transformed vector $\tilde{\mathbf{z}}_s$ has elements of the form

$$\tilde{z}_{s_1} = \sqrt{\frac{\hat{N}_1}{\hat{N}}}\,\tilde{y}_{s_1}, \quad \tilde{z}_{s_2} = \sqrt{\frac{\hat{N}_2}{\hat{N}}}\,\tilde{y}_{s_2}, \quad \tilde{z}_{s_3} = \sqrt{\frac{\hat{N}_3}{\hat{N}}}\,\tilde{y}_{s_3}.$$

In this setting, it is straightforward to see that $\Pi(\tilde{\mathbf{z}}_s \mid \Omega_s^0) = \mathbf{0}$. In the process of computing it using the general algorithm, we project $\tilde{\mathbf{z}}_s$ onto each of the $2^2 = 4$ linear spaces generated by the polar cone edges

$$\boldsymbol{\gamma}_{s_1} = \left(\sqrt{\frac{\hat{N}}{\hat{N}_1}}, -\sqrt{\frac{\hat{N}}{\hat{N}_2}}, 0\right)^{\mathsf{T}}, \quad \boldsymbol{\gamma}_{s_2} = \left(\sqrt{\frac{\hat{N}}{\hat{N}_1}}, \sqrt{\frac{\hat{N}}{\hat{N}_2}}, -2\sqrt{\frac{\hat{N}}{\hat{N}_3}}\right)^{\mathsf{T}}.$$

Hence, it can be seen that the conditions $\Pi(\tilde{\mathbf{z}}_s \mid \Omega_s^0) = \mathbf{0} = \Pi(\tilde{\mathbf{z}}_s \mid \mathcal{L}(V_{s,J})) \in \bar{\mathcal{F}}_{s,J}$ are satisfied only for $J = \varnothing$ and $J = \{1\}$, which implies that $\mathcal{G}_s = \{\varnothing, \{1\}\}$. Moreover, note that $V_{s,\varnothing}$ and $V_{s,\{1\}}$ do not span the same linear spaces, which is what complicates the variance estimation of $\tilde{\theta}_{s_d}$. In the model-based case with continuous variables, the set of sample vectors where these scenarios occur has measure zero. However, they cannot be excluded in the design-based setting.

We propose a variance estimator for $\tilde{\theta}_{s_d}$ that relies on the sets in $\mathcal{G}_s$ and is based on linearization methods. Consider any fixed set $J \in \mathcal{G}_s$, and let $\mathbf{P}_{s,J}$ be the projection matrix corresponding to the linear space $\mathcal{L}(V_{s,J})$, where $\mathbf{P}_{s,\varnothing}$ is the matrix of zeros by convention. By the selection of J, then $\tilde{\boldsymbol{\rho}}_s$

can be expressed as $\mathbf{P}_{s,J}\tilde{\mathbf{z}}_s$, which implies that $\tilde{\boldsymbol{\theta}}_s$ can be written as $\tilde{\boldsymbol{\theta}}_{s,J} = \tilde{\mathbf{y}}_s - \mathbf{W}_s^{-1/2}\mathbf{P}_{s,J}\mathbf{W}_s^{1/2}\tilde{\mathbf{y}}_s$, where we add the subscript J in $\tilde{\boldsymbol{\theta}}_s$ to be aware that the expression depends on the chosen J.

Now, observe that $\tilde{\boldsymbol{\theta}}_{s,J}$ is a smooth non-linear function of the $\hat{t}_d$'s and the $\hat{N}_d$'s, where $\hat{t}_d$ is the Horvitz-Thompson estimator of $t_d = \sum_{k\in U_d} y_k$. Therefore, treating J as fixed, we obtain the asymptotic variance of $\tilde{\theta}_{s_d,J}$ via Taylor linearization (Särndal et al., 1992, page 175) as

$$\mathrm{AV}\left(\tilde{\theta}_{s_d,J}\right) = \sum_{k\in U}\sum_{l\in U}\Delta_{kl}\frac{u_k}{\pi_k}\frac{u_l}{\pi_l}, \tag{2.10}$$

where $\Delta_{kl} = \pi_{kl} - \pi_k\pi_l$, and

$$u_k = \sum_{i=1}^{D}\alpha_i\, y_k 1_{k\in U_i} + \sum_{i=1}^{D}\beta_i 1_{k\in U_i} \quad \text{for} \quad k = 1,\ 2,\ \ldots,\ N,$$

with 1_A being the indicator variable for the event A, and

$$\alpha_i = \left.\frac{\partial\tilde{\theta}_{s_d,J}}{\partial\hat{t}_i}\right|_{(\hat{t}_1,\ldots,\hat{t}_D,\hat{N}_1,\ldots,\hat{N}_D)=(t_1,\ldots,t_D,N_1,\ldots,N_D)}; \quad \beta_i = \left.\frac{\partial\tilde{\theta}_{s_d,J}}{\partial\hat{N}_i}\right|_{(\hat{t}_1,\ldots,\hat{t}_D,\hat{N}_1,\ldots,\hat{N}_D)=(t_1,\ldots,t_D,N_1,\ldots,N_D)}.$$

In addition, a consistent estimator of the asymptotic variance in (2.10) is given by

$$\hat{V}\left(\tilde{\theta}_{s_d,J}\right) = \sum_{k\in s}\sum_{l\in s}\frac{\Delta_{kl}}{\pi_{kl}}\frac{\hat{u}_k}{\pi_k}\frac{\hat{u}_l}{\pi_l}, \tag{2.11}$$

where

$$\hat{u}_k = \sum_{i=1}^{D}\hat{\alpha}_i\, y_k 1_{k\in s_i} + \sum_{i=1}^{D}\hat{\beta}_i 1_{k\in s_i} \quad \text{for} \quad k = 1,\ 2,\ \ldots,\ N,$$

with $\hat{\alpha}_i$, $\hat{\beta}_i$ obtained from α_i, β_i by substituting the appropriate Horvitz-Thompson estimators for each population total. We propose the estimator in (2.11), computed at the J obtained in the sample, as a variance estimator of $\tilde{\theta}_{s_d}$.

To provide a clear example of the proposed variance estimator for $\tilde{\theta}_{s_d}$, consider the setting presented at the beginning of this subsection. Since $\mathcal{G}_s = \{\varnothing, \{1\}\}$, it might be of interest to compute the estimated variance of $\tilde{\theta}_{s_d,J}$ for $J = \{1\}$ and certain d. The matrix $\mathbf{P}_{s,\{1\}}$ is the projection matrix corresponding to the linear space generated by $\boldsymbol{\gamma}_{s_1}$, given by

$$\mathbf{P}_{s,\{1\}} = \left(\hat{N}_1+\hat{N}_2\right)^{-1}\begin{pmatrix} \hat{N}_2 & -\sqrt{\hat{N}_1\hat{N}_2} & 0 \\ -\sqrt{\hat{N}_1\hat{N}_2} & \hat{N}_1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Note that $\mathbf{P}_{s,\{1\}}$ is a function of $(\hat{N}_1,\ \hat{N}_2,\ \hat{N}_3)$ because $\boldsymbol{\gamma}_{s_1}$ is. Using the above equation, $\tilde{\boldsymbol{\theta}}_{s,\{1\}}$ can be simplified to the following expression,

$$\tilde{\boldsymbol{\theta}}_{s,\{1\}} = \left(\tilde{\theta}_{s_1,\{1\}},\ \tilde{\theta}_{s_2,\{1\}},\ \tilde{\theta}_{s_3,\{1\}}\right)^{\mathsf{T}} = \left(\frac{\hat{N}_1\tilde{y}_{s_1} + \hat{N}_2\tilde{y}_{s_2}}{\hat{N}_1 + \hat{N}_2},\ \frac{\hat{N}_1\tilde{y}_{s_1} + \hat{N}_2\tilde{y}_{s_2}}{\hat{N}_1 + \hat{N}_2},\ \tilde{y}_{s_3}\right)^{\mathsf{T}}$$
$$= \left(\frac{\hat{t}_1 + \hat{t}_2}{\hat{N}_1 + \hat{N}_2},\ \frac{\hat{t}_1 + \hat{t}_2}{\hat{N}_1 + \hat{N}_2},\ \frac{\hat{t}_3}{\hat{N}_3}\right)^{\mathsf{T}}.$$

Therefore, given a domain d, the α's and β's can be derived by taking the partial derivatives of $\tilde{\theta}_{s_d,\{1\}}$ with respect to the $\hat{t}$'s and $\hat{N}$'s, and evaluating such derivatives at the t's and N's. For $d = 2$, that is,

$$\alpha_1 = \alpha_2 = \frac{1}{N_1 + N_2}, \qquad \alpha_3 = 0,$$
$$\beta_1 = \beta_2 = -\frac{t_1 + t_2}{(N_1 + N_2)^2},\ \beta_3 = 0.$$

The $\hat{\alpha}$'s and $\hat{\beta}$'s are computed by substituting Horvitz-Thompson estimators in the above equations, which are then used to evaluate $\hat{u}_k$ for each k in the sample s. Finally, the proposed variance estimator in (2.11) can be computed.

3 Properties of the constrained estimator

3.1 Assumptions

To derive our theoretical results, we make assumptions on the asymptotic behavior of the population U_N and the sampling design p_N:

A1. The number of domains D is fixed.

A2. $\limsup_{N\to\infty} N^{-1}\sum_{k\in U}|y_k|^r < \infty$, for $r = 1,\ 2$.

A3. For $d = 1, \ldots, D$, there exist constants μ_d and $r_d > 0$ such that $\bar{y}_{U_d,N} - \mu_d = O(N^{-1/2})$ and $N_{d,N}/N - r_d = O(N^{-1/2})$, for all d.

A4. The sample size n_N is non-random and satisfies $0 < \lim_{N\to\infty} n_N/N < 1$. In addition, there exists ε, $0 < \varepsilon < 1$, such that $n_{d,N} \geq \varepsilon n_N/D$ for all d and all N.

A5. For all N, $\min_{k\in U_N}\pi_k \geq \lambda > 0$, $\min_{k,l\in U_N}\pi_{kl} \geq \lambda^* > 0$, and

$$\limsup_{N\to\infty} n_N \max_{k,l\in U_N:\ k\neq l}|\Delta_{kl}| < \infty.$$

A6. The Horvitz-Thompson estimator $\hat{\mathbf{x}}_{s_N}$ of the $2D$-dimensional vector of population means $\bar{\mathbf{x}}_{U_N} = N^{-1}(t_1, \ldots, t_D, N_1, \ldots, N_D)^\top$ satisfies

$$\mathrm{var}_{p_N}(\hat{\mathbf{x}}_{s_N})^{-1/2}(\hat{\mathbf{x}}_{s_N} - \bar{\mathbf{x}}_{U_N}) \xrightarrow{d} \mathcal{N}(\mathbf{0}, \mathbf{I}_{2D}),$$

and

$$\hat{\mathrm{var}}(\hat{\mathbf{x}}_{s_N}) - \mathrm{var}_{p_N}(\hat{\mathbf{x}}_{s_N}) = o_p(n_N^{-1});$$

where $\mathbf{I}_q$ denotes the identity matrix of dimension q, the design variance-covariance matrix $\mathrm{var}_{p_N}(\hat{\mathbf{x}}_{s_N})$ is positive definite, and $\hat{\mathrm{var}}(\hat{\mathbf{x}}_{s_N})$ is the Horvitz-Thompson estimator of var_{p_N}.

Assumption A1 establishes that the number of domains remains constant as the population size changes. The condition in Assumption A2 is made to ensure design consistency of Horvitz-Thompson estimators at the population and domain levels. In particular, note that this condition is satisfied when the variable y is bounded, which can be naturally assumed for many types of survey variables. Assumption A3 guarantees that the population domain means and sizes converge to the limiting values μ_d and r_d, respectively. Alternatively, the μ values can be thought as superpopulation expectations for a distribution that generates the population elements y_k as independent draws. In fact, our theoretical results depend on whether the assumed constraints hold for these superpopulation expectations and not for the population domain means. Although this might seem to be inappropriate given our interest on using constraints at the population level, Assumption A3 ensures that the shape of the domain means would be reasonably close to the shape of the superpopulation means. Assumption A4 states that the sample size in each domain cannot be smaller than a fraction of the ratio n/D, which would be obtained by dividing equally the sample size over all domains. This assumption aims to ensure that the moments of smooth functions of the $N^{-1}\hat{t}_d$ and the $N^{-1}\hat{N}_d$ are bounded. Also, it assumes that the sample size is non-random. This can be adapted to a random sample size by imposing certain conditions on the expected sample size $\mathbb{E}_p(n)$. Assumption A5 establishes non-zero lower bounds for both first and second order inclusion probabilities, and states that the design covariances Δ_{kl} must converge to zero at least as fast as n^{-1}. Assumption A6 ensures asymptotic normality for $\hat{\mathbf{x}}_{s_N}$, which is needed to maintain normality properties on non-linear estimators that are expressed as smooth functions of $\hat{\mathbf{x}}_{s_N}$. It is also used to establish consistency conditions on the variance-covariance estimator. For specific designs, asymptotic normality results are available in the literature, including the classical result by Hájek (1960) for Poisson sampling and simple random sampling without replacement. Additional central limit theorems for stratified sampling include Krewski and Rao (1981), who considered stratified unequal probability samples with replacement, Bickel and Freedman (1984), who considered stratified simple random sampling without replacement, and Breidt, Opsomer and Sanchez-Borrego (2016), who considered general unequal probability designs, with or without replacement.

3.2 Main results

We derive the theoretical properties of the constrained estimator by focusing on the projection onto Ω_s^0 instead of Ω_s. Recall that the edges of the polar cone Ω_s^0 are simply the m rows of $-\mathbf{A}_s$, denoted by $\boldsymbol{\gamma}_{s_j}$; and that $\tilde{\boldsymbol{\rho}}_s$, the projection onto Ω_s^0, can be described by the sets $J \in \mathcal{G}_s$. Being able to characterize the property that $J \in \mathcal{G}_s$ in terms of the vectors in $V_{s,J}$ allow us to obtain theoretical convergence rates, which are used to develop inference properties of the constrained estimator. When the set $J \in \mathcal{G}_s$ produces a set of linear independent vectors $V_{s,J}$, then it is straightforward that $\tilde{\boldsymbol{\rho}}_s$ can be written as $\mathbf{P}_{s,J}\,\tilde{\mathbf{z}}_s = \mathbf{A}_{s,J}^{\top}\left(\mathbf{A}_{s,J}\mathbf{A}_{s,J}^{\top}\right)^{-1}\mathbf{A}_{s,J}\,\tilde{\mathbf{z}}_s$, where $\mathbf{A}_{s,J}$ denotes the matrix formed by the rows of $\mathbf{A}_s$ in positions J. Hence, based on the conditions in (2.8), $J \in \mathcal{G}_s$ if and only if

$$\left\langle \tilde{\mathbf{z}}_s - \mathbf{P}_{s,J}\,\tilde{\mathbf{z}}_s,\ \boldsymbol{\gamma}_{s_j} \right\rangle \le 0 \quad \text{for} \quad j \notin J, \quad \text{and} \quad \left(\mathbf{A}_{s,J}\,\mathbf{A}_{s,J}^{\top}\right)^{-1}\mathbf{A}_{s,J}\,\tilde{\mathbf{z}}_s \ge \mathbf{0} \tag{3.1}$$

in this case, where the latter condition assures that $\Pi\left(\tilde{\mathbf{z}}_s \,|\, \mathcal{L}\left(V_{s,J}\right)\right) \in \bar{\mathcal{F}}_{s,J}$. However, it is possible that the set $J \in \mathcal{G}_s$ produces a set of linearly dependent vectors $V_{s,J}$. In that case, Theorem 1 below guarantees that it is always possible to find a subset $J^* \subset J$ such that V_{s,J^*} is a linearly independent set that spans the same linear space as $V_{s,J}$ and that satisfies $J^* \in \mathcal{G}_s$. Thus, analogous conditions as in (3.1) can be established using J^* instead of J.

Theorem 1. *Let $\mathbf{A}$ be a $m \times D$ irreducible matrix with rows $-\boldsymbol{\gamma}_j$. Let Ω^0 be its corresponding polar cone. For any set $J \subseteq \{1, 2, \ldots, m\}$, define $V_J = \{\boldsymbol{\gamma}_j;\ j \in J\}$. Further, denote $\bar{\mathcal{F}}_J$ to be the subcone of Ω^0 generated by the edges given by the set J. For a vector $\mathbf{z}$, define its set $\mathcal{G}$ to be formed by all sets $J \subseteq \{1, 2, \ldots, m\}$ such that $\Pi(\mathbf{z}\,|\,\Omega^0) = \Pi(\mathbf{z}\,|\,\mathcal{L}(V_J)) \in \bar{\mathcal{F}}_J$. Suppose J is a non-empty set such that V_J is a linearly dependent set and $J \in \mathcal{G}$. Then, there exists $J^* \subset J$ such that V_{J^*} is a linearly independent set, $\mathcal{L}(V_{J^*}) = \mathcal{L}(V_J)$, and $J^* \in \mathcal{G}$.*

All above concepts that have been defined at the sample level can be analogously defined at the superpopulation level. In particular, let $\mathcal{G}_\mu$ be the set of all subsets $J \subseteq \{1, \ldots, m\}$ such that $\Pi\left(\mathbf{z}_\mu \,|\, \Omega_\mu^0\right) = \Pi\left(\mathbf{z}_\mu \,|\, \mathcal{L}\left(V_{\mu,J}\right)\right) \in \bar{\mathcal{F}}_{\mu,J}$, where $\mathbf{z}_\mu$, Ω_μ^0, $V_{\mu,J}$ and $\bar{\mathcal{F}}_{\mu,J}$ are the analogous versions of $\tilde{\mathbf{z}}_s$, Ω_s^0, $V_{s,J}$ and $\bar{\mathcal{F}}_{s,J}$ obtained by substituting $\tilde{\mathbf{y}}_s$ and $\mathbf{W}_s$ by $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_D)$ and $\mathbf{W}_\mu = \operatorname{diag}(r_1, r_2, \ldots, r_D)$. Necessary and sufficient conditions as in (2.8) can be analogously established to characterize the vector $\boldsymbol{\rho}_\mu$ to be the projection onto Ω_μ^0.

Recall the set $\mathcal{G}_s$ could vary for different samples. Also, note that highly variable small samples are likely to choose sets $J \in \mathcal{G}_s$ that are not chosen in the "asymptotically correct" $\mathcal{G}_\mu$. However, as the sample size increases, these incorrect choices are less likely to occur since the sample domain means get closer to the limiting population domain means. This idea is made more precise in Theorem 2, which states that sets that are not in $\mathcal{G}_\mu$ have an asymptotically negligible probability of being chosen in the sample.

Theorem 2. *Consider any set $J \subseteq \{1, 2, \ldots, m\}$ such that $J \notin \mathcal{G}_\mu$. Then, $P(J \in \mathcal{G}_s) = O(n^{-1})$.*

Theorem 3 below shows the asymptotic normality of the constrained estimator and justifies the use of the linearization-based variance estimator for the observed projection (or pooling, in the case of partial ordering) for asymptotic inference for the finite population domain mean. This generalizes Theorem 2 of Wu et al. (2016), where only monotone restrictions were considered. Note the presence of a bias term B in the mean of the asymptotic distribution. This undesirable situation occurs when there is more than one set $J \in \mathcal{G}_\mu$ such that their corresponding edges in $V_{\mu,J}$ span different linear spaces, or equivalently, that the projection onto the polar cone Ω_μ^0 belongs to the intersection of those different linear spaces. However, when the constraints hold strictly, i.e., $\mathbf{A}\boldsymbol{\mu} > \mathbf{0}$, the vector $\mathbf{z}_\mu$ is strictly inside the constraint cone Ω_μ, and in this case there is no set $J \neq \varnothing$ such that $\Pi(\mathbf{z}_\mu \,|\, \mathcal{L}(V_{\mu,J})) = \mathbf{0}$. Thus, in this case, the bias term vanishes.

Theorem 3. *Suppose that* $\boldsymbol{\mu}$ *satisfies* $\mathbf{A}\boldsymbol{\mu} \geq \mathbf{0}$. *Consider any set* J *such that* $J \in \mathcal{G}_s$. *Then*

$$\hat{V}\left(\tilde{\theta}_{s_d,J}\right)^{-1/2}\left(\tilde{\theta}_{s_d} - \bar{y}_{U_d}\right) \xrightarrow{\mathcal{L}} \mathcal{N}(B,\ 1),$$

for any $d = 1,\ 2,\ \ldots,\ D$, *where* $B = O\left(\sqrt{\frac{n}{N}}\right)$ *is a bias term that vanishes when* $\mathbf{A}\boldsymbol{\mu} > \mathbf{0}$.

Theorem 3 relies on the fact that the assumed shape constraints hold for the vector of limiting domain means $\boldsymbol{\mu}$ instead of for the vector of population domain means $\bar{\mathbf{y}}_U$. In the next section, we show through simulations that the constrained estimator improves both estimation and variability when the population domains are approximately close to the assumed shape, in comparison with unconstrained estimators.

4 Performance of constrained estimator

4.1 Simulations

We run simulation experiments to measure the performance of the proposed methodology to carry out estimation and inference of population domain means. Given a pair of natural numbers D_1 and D_2, we generate the limiting domain means μ_d from the monotone bivariate function $\mu(x_1,\ x_2)$ given by

$$\mu(x_1,\ x_2) = \sqrt{1 + 4x_1/D_1} + \frac{4\exp(0.5 + 2x_2/D_2)}{1+\exp(0.5 + 2x_2/D_2)}.$$

The μ_d are created by evaluating $\mu(x_1,\ x_2)$ at every combination of $x_1 = 1,\ 2,\ \ldots,\ D_1$ and $x_2 = 1,\ 2,\ \ldots,\ D_2$, producing a total number of domains equal to $D = D_1 D_2$. We set $D_1 = 6$ and $D_2 = 4$. Note that although the function $\mu(x_1,\ x_2)$ produces a matrix rather than a vector of domain means, it can be vectorized in order to represent the limiting domain means as the vector $\boldsymbol{\mu}$. For each domain d, we generate its $N_d = N/D = 400$ elements by adding independent and normally distributed noise with mean 0 and variance σ^2 to the μ_d. Once the elements of the population have been simulated, then the

population domain means $\bar{\mathbf{y}}_U$ are computed. The population domain means used for simulations when $\sigma = 1$ are displayed in Figure 4.1. Observe that these domain means are reasonably (not strictly) monotone with respect to x_1 and x_2.

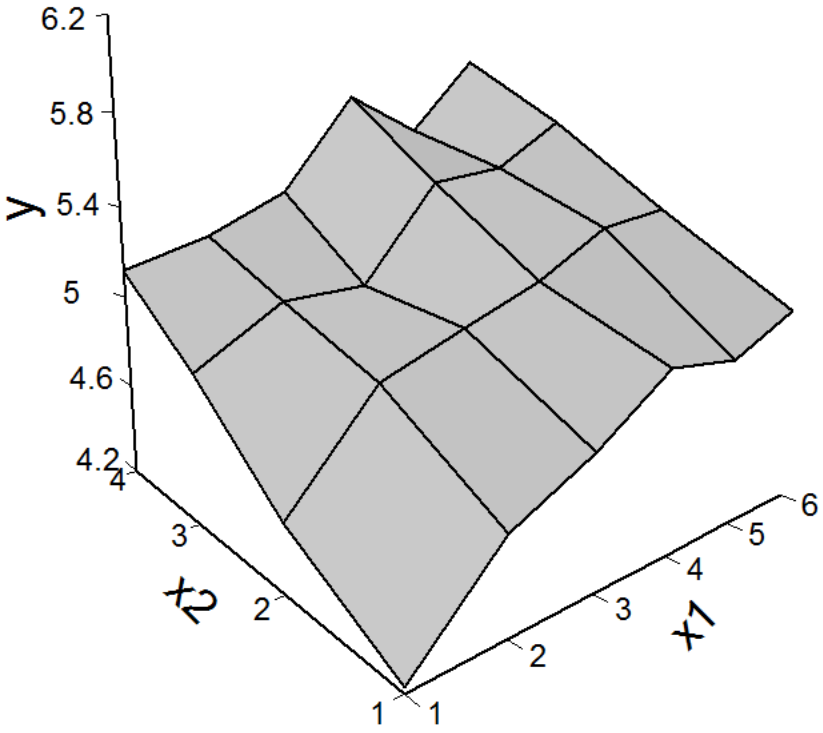


Figure 4.1 Population domain means for simulations when $\sigma = 1$.

Samples are drawn from a stratified sampling design without replacement, with 4 strata that cut across the D domains. Strata are constructed using an auxiliary variable ν that is correlated with the variable of interest y. The vector ν is created by adding independent standard normally distributed noise to $\sigma d/D$, for each element in domain d. Then, stratum membership is assigned by sorting the vector ν and creating 4 blocks of $N/4 = 2{,}400$ elements each based on the sorted ν. To make the design informative, we sample $n = 480$ elements divided across strata in (60, 120, 120, 180). This probability sampling design is similar to the one described in Wu et al. (2016).

We consider 4 different scenarios obtained from the combination of two possible types of shape constraints and $\sigma = 1$ or 2. The first type of constraints assumes the population domain means are monotone increasing with respect to both x_1 and x_2 (double monotone), while the second type of constraints assumes monotonicity only with respect to x_1 (only x_1 monotone). For a fixed σ, the exact

same population is considered for the two possible types of constraints. For each scenario, the unconstrained $\tilde{\mathbf{y}}_s$ and constrained $\tilde{\boldsymbol{\theta}}_s$ estimates are computed along with their linearization-based variance estimates (see (2.11)). Constrained estimates are computed using the CPA, and their variance estimates are computed by relying on the sample-selected set $J \in \mathcal{G}_s$. In addition, 95% Wald confidence intervals based on the normal distribution are constructed for both estimators.

To measure the precision of $\tilde{\mathbf{y}}_s$ and $\tilde{\boldsymbol{\theta}}_s$ as estimators of the population domain means $\bar{\mathbf{y}}_U$, we consider the Weighted Mean Squared Error (WMSE) given by

$$\text{WMSE}(\tilde{\boldsymbol{\varphi}}_s) = \text{E}\left[(\tilde{\boldsymbol{\varphi}}_s - \bar{y}_U)^\top \mathbf{W}_U (\tilde{\boldsymbol{\varphi}}_s - \bar{y}_U)\right],$$

where $\tilde{\boldsymbol{\varphi}}_s$ could be either the unconstrained or constrained estimator and $\mathbf{W}_U$ is the diagonal matrix with elements N_d / N, $d = 1, \ldots, D$. The WMSE values are approximated by simulations as

$$\frac{1}{B}\sum_{b=1}^{B}(\tilde{\boldsymbol{\varphi}}_s^{(b)} - \bar{\mathbf{y}}_U)^\top \mathbf{W}_U (\tilde{\boldsymbol{\varphi}}_s^{(b)} - \bar{\mathbf{y}}_U),$$

where B is the number of simulations, and $\tilde{\boldsymbol{\varphi}}_s^{(b)}$ is the estimator for the b^{th} sample.

Simulation results are summarized in Figures 4.2 - 4.5, and are based on $R = 10{,}000$ replications. These display the 24 domains divided in groups of 6, where each group is assumed to be monotone. For the double monotone scenario, similar plots with groups of 4 monotone domains each can be also pictured. As illustrated in the fits of a single sample in these figures, it can be seen that the constrained estimates can be exactly equal to the unconstrained estimates for some domains. In those cases, their variance estimates are also equal. Overall, confidence intervals for the constrained estimator tend to be tighter in comparison with those for the unconstrained estimator. On average, the constrained estimator behaves slightly differently than the population domain means, due to the latter's non-strict monotonicity. As an advantage, the percentiles for the constrained estimator are narrower, demonstrating that the distribution of the proposed estimator is tighter than the distribution of the unconstrained estimator. For small values of σ, the unconstrained estimates are more likely to satisfy the assumed restrictions, which leads to small improvements on the constrained estimator over the unconstrained. In contrast, shape assumptions tend to be more severely violated in unconstrained estimates for larger values of σ, allowing the proposed estimator to gain much more efficiency on these cases. This latter property can be noted by observing that the constrained estimator percentile band gets farther away from the unconstrained estimator band as σ increases.

In terms of variability, the constrained estimator has the smaller variance of the two estimators. Interestingly, it gets overestimated by its corresponding linearization-based variance estimate. In contrast, the variance estimate of the unconstrained estimator underestimates the true variance, which is a known and often observed drawback of linearization variances. Despite this difference, confidence intervals for both estimators demonstrate a similar good coverage rate when $\sigma = 1$, meanwhile such coverage gets slightly improved by the constrained estimator when $\sigma = 2$.

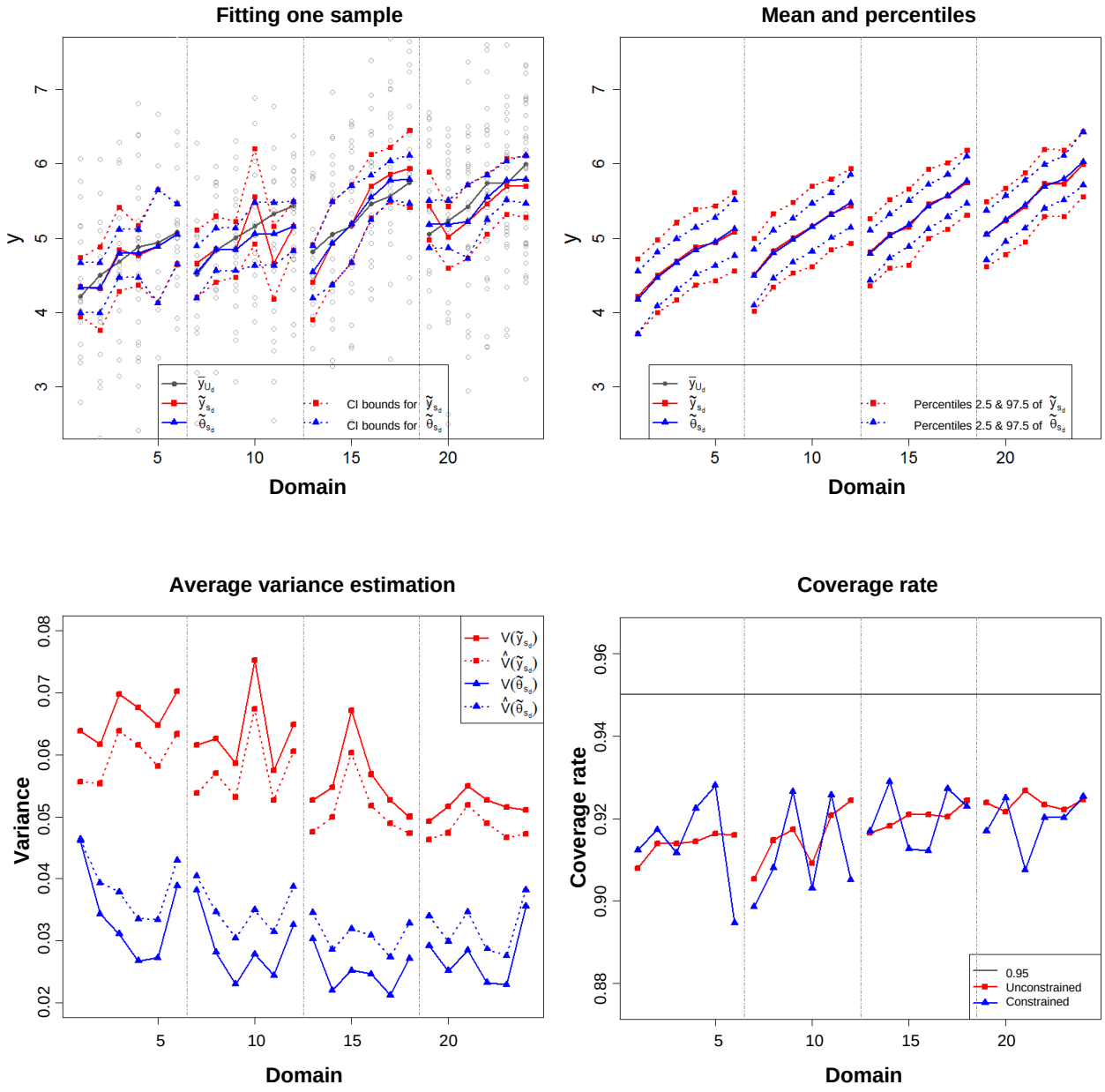


Figure 4.2 Plots of simulation results for the unconstrained and constrained estimators under the double monotone scenario with $\sigma = 1$. In the "Mean and percentiles" plot, $\bar{y}_{U_d}$ is hidden by $\tilde{y}_{s_d}$.

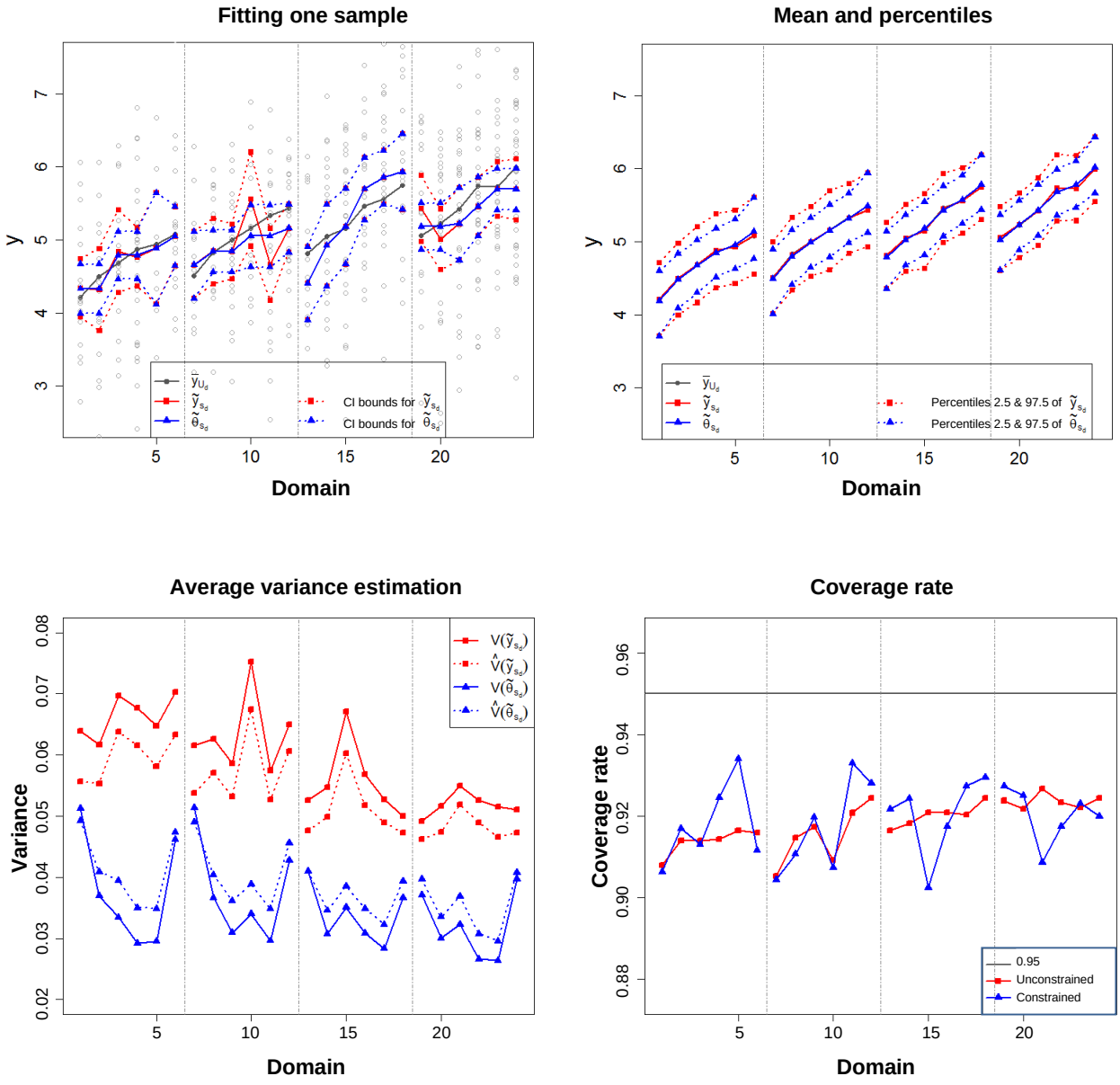


Figure 4.3 Plots of simulation results for the unconstrained and constrained estimators under the only x_1 monotone scenario with $\sigma = 1$. In the "Mean and percentiles" plot, $\bar{y}_{U_d}$ is hidden by $\tilde{y}_{s_d}$.

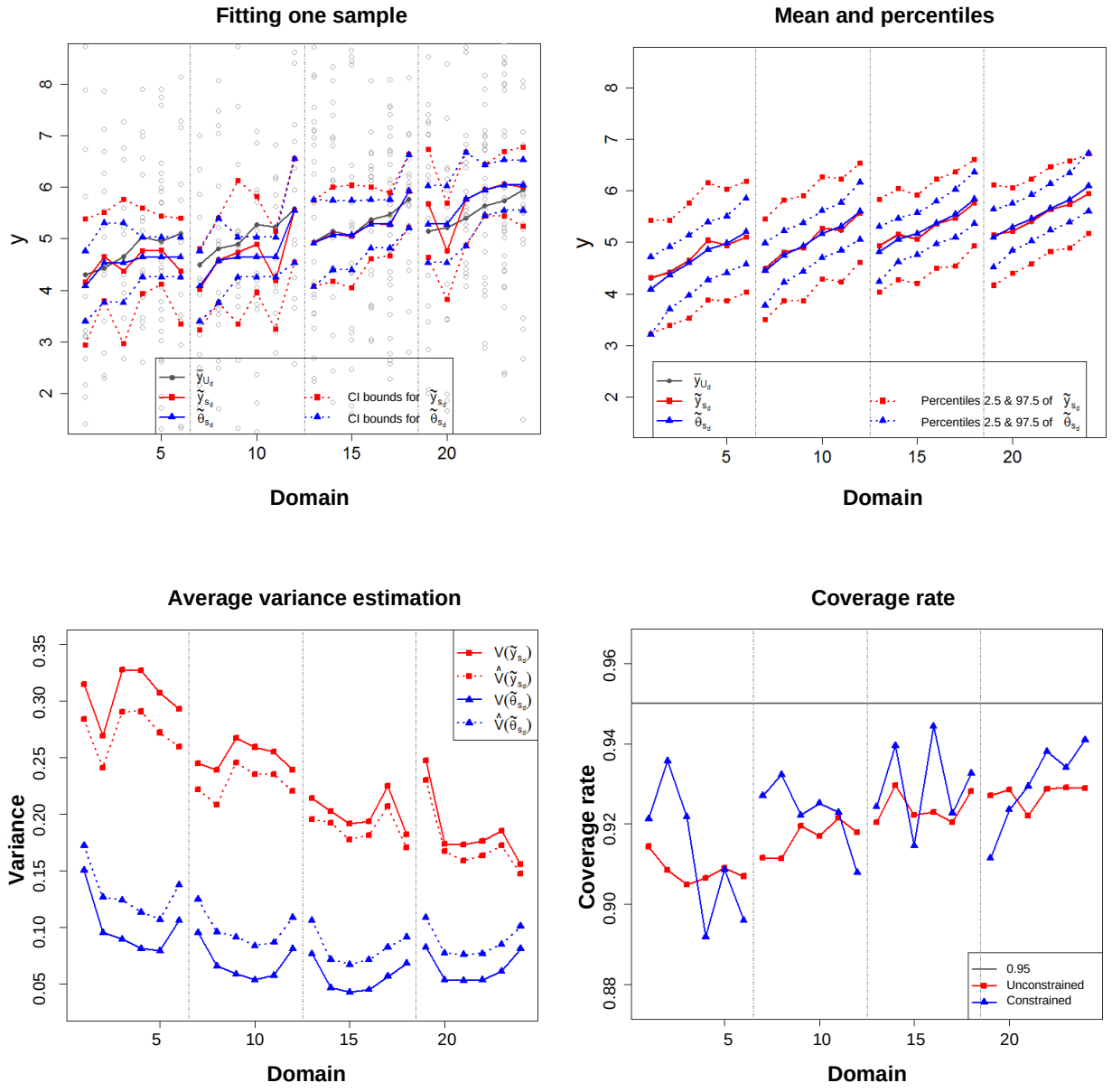


Figure 4.4 Plots of simulation results for the unconstrained and constrained estimators under the double monotone scenario with $\sigma = 2$. In the "Mean and percentiles" plot, $\bar{y}_{U_d}$ is hidden by $\tilde{y}_{s_d}$.

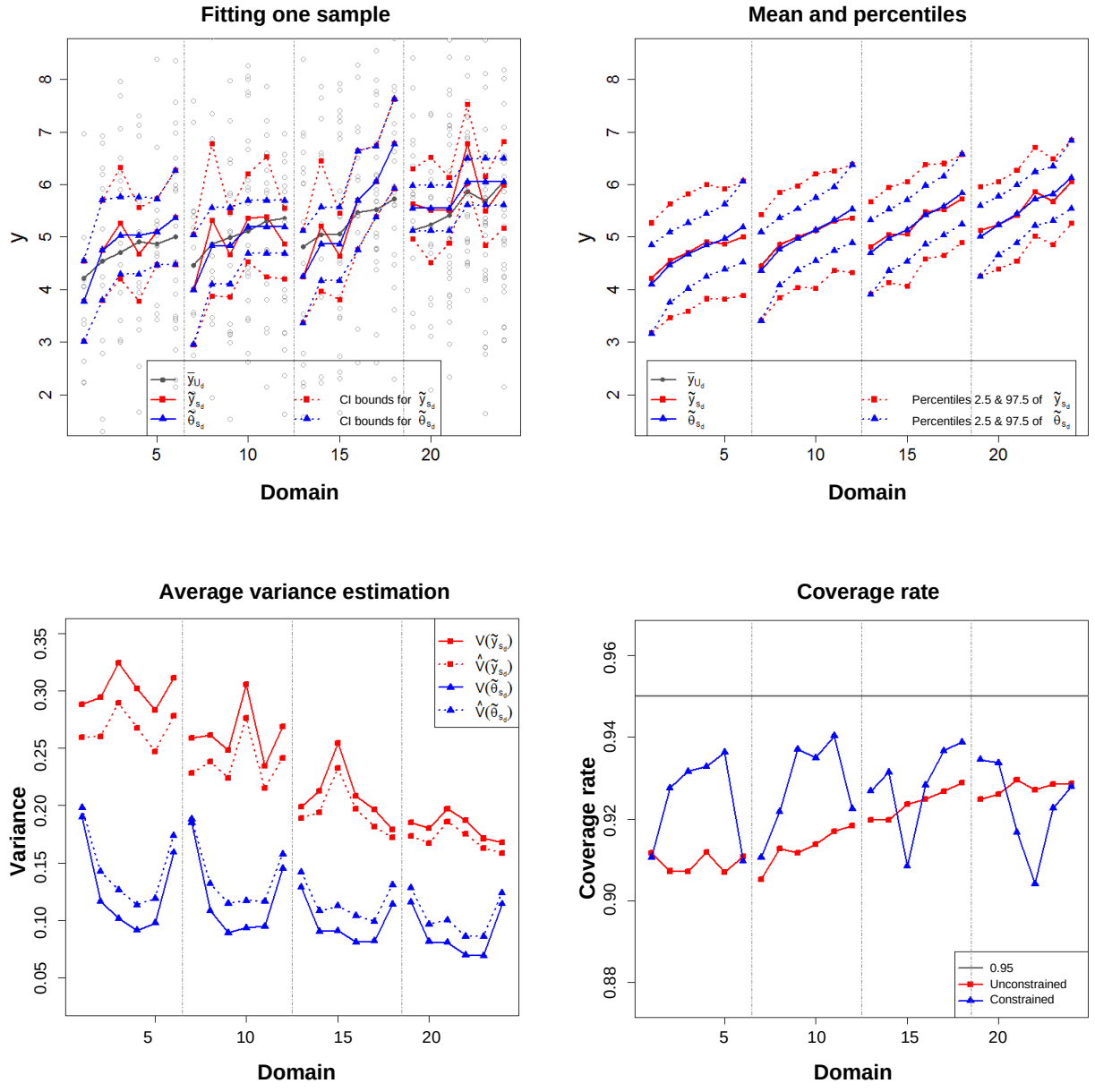


Figure 4.5 Plots of simulation results for the unconstrained and constrained estimators under the only x_1 monotone scenario with $\sigma = 2$. In the "Mean and percentiles" plot, $\bar{y}_{U_d}$ is hidden by $\tilde{y}_{s_d}$.

Table 4.1 shows that the constrained estimator is more precise on average than the unconstrained estimator. The precision of the constrained estimator improves when the monotonicity with respect to the two variables is assumed, instead of only with respect to x_1. This is expected here, because the underlying surface is indeed doubly monotone, so that the estimator benefits from imposing the stronger constraint.

Table 4.1
Empirical WMSE values

	Unconstrained	Only x_1 monotone	Double monotone
$\sigma = 1$	0.0593	0.0362	0.0298
$\sigma = 2$	0.2384	0.1175	0.0832

4.2 Replication methods for variance estimation

In practice, it is common for large-scale surveys to use replication-based methods for variance estimation. Examples of such surveys are the last editions of the NHANES and the National Survey of College Graduates (NSCG). To study the performance of replication-based variance estimators under the proposed constrained methodology, we carry out simulation studies based on the delete-a-group Jackknife (DAGJK) variance estimator proposed by Kott (2001).

We perform replication-based simulation experiments using the setting described in Section 4.1. To compute the DAGJK variance estimator, we first randomly create G equal-sized groups within each of the 4 strata. Then, for each replicate $g = 1, \ldots, G$, we delete the g^{th} group in each of the strata, adjust the remaining weights by $w_k^{(g)} = \left(\frac{G}{G-1}\right) w_k$, where $w_k = \pi_k^{-1}$; and compute the replicate constrained estimate $\tilde{\boldsymbol{\theta}}_s^{(g)}$ using the adjusted weights. The DAGJK variance estimate of $\tilde{\theta}_{s_d}$, $\hat{V}_{\text{JK}}\left(\tilde{\theta}_{s_d}\right)$, is obtained by calculating

$$\hat{V}_{\text{JK}}\left(\tilde{\theta}_{s_d}\right) = \frac{G-1}{G}\sum_{g=1}^{G}\left(\tilde{\theta}_{s_d}^{(g)} - \tilde{\theta}_{s_d}\right)^2.$$

A replication-based variance estimator of $\tilde{y}_{s_d}$ is obtained by substituting $\tilde{\boldsymbol{\theta}}_s$ by $\tilde{\mathbf{y}}_s$.

Our simulations consider only the double monotone scenario, with $\sigma = 1$ or 2, and $G = 10$, 20 or 30. The sample size is set to either $n = 480$ or $n = 960$, where the latter case is obtained by doubling the original sample size in each strata. Figures 4.6 - 4.9 contain simulation results based on 10,000 replications. In contrast to the behavior of the linearization-based variance estimates, it can be seen that the DAGJK estimates tend to overestimate the variance of the unconstrained estimator, as is often observed in practice. Both replication-based and linearization-based variance estimates of the constrained estimator overestimate the true variance, so that the results are more consistent across variance estimation methods. As the number of groups G increases, DAGJK estimates tend to be greater, especially for small values of σ. Such increments on DAGJK estimates have the direct consequence of increasing the coverage rate as G gets larger. In addition, the coverage rate for both estimators is improved (closer to

0.95) when the sample size is increased. Overall, it appears that replication variance estimation is a practical alternative to linearization.

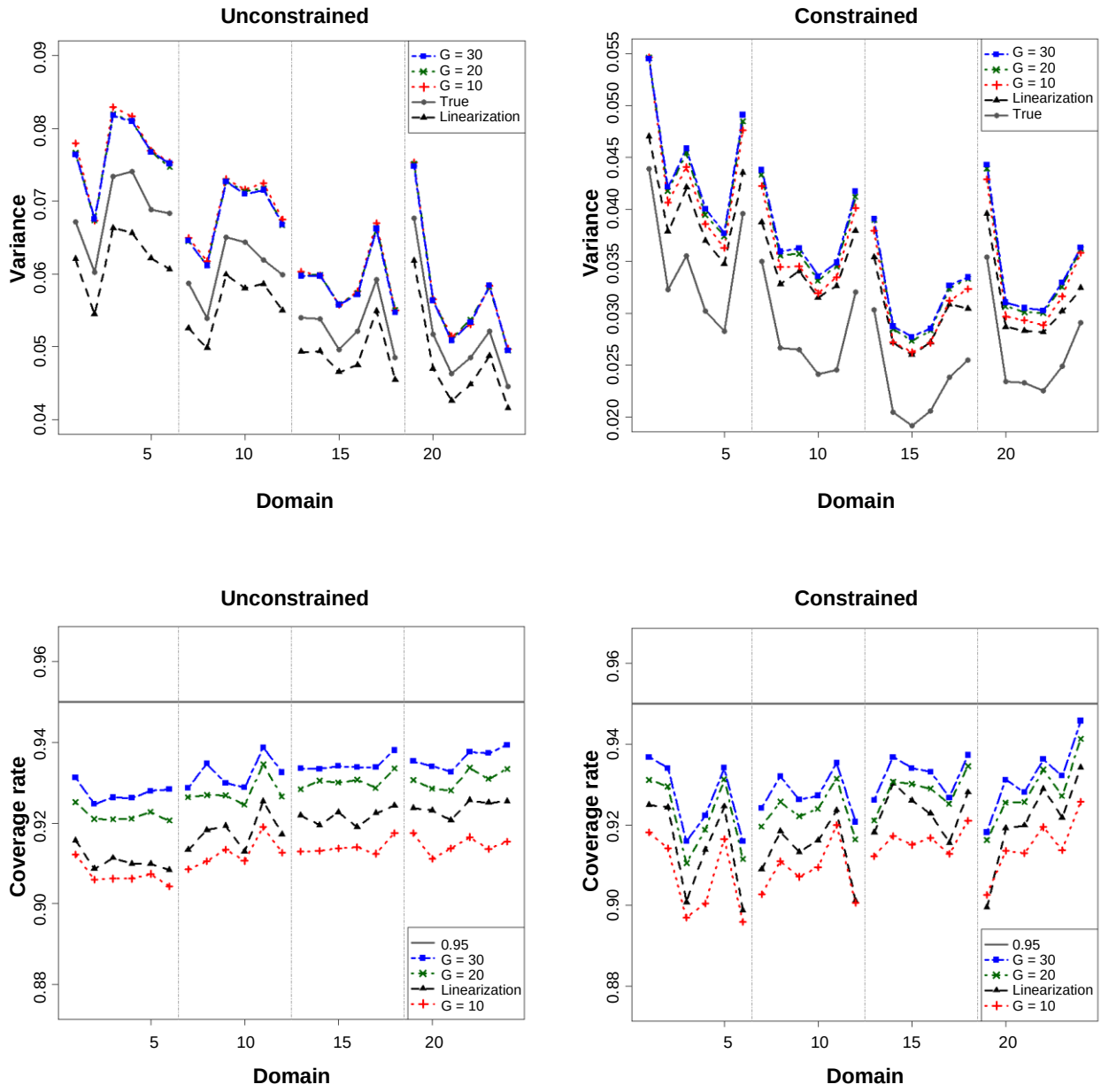


Figure 4.6 Variance estimation (top) and coverage rate (bottom) simulation results based on linearization and DAGJK methods for the unconstrained (left) and constrained (right) estimators, under the double monotone scenario with $n_N = 480$ and $\sigma = 1$.

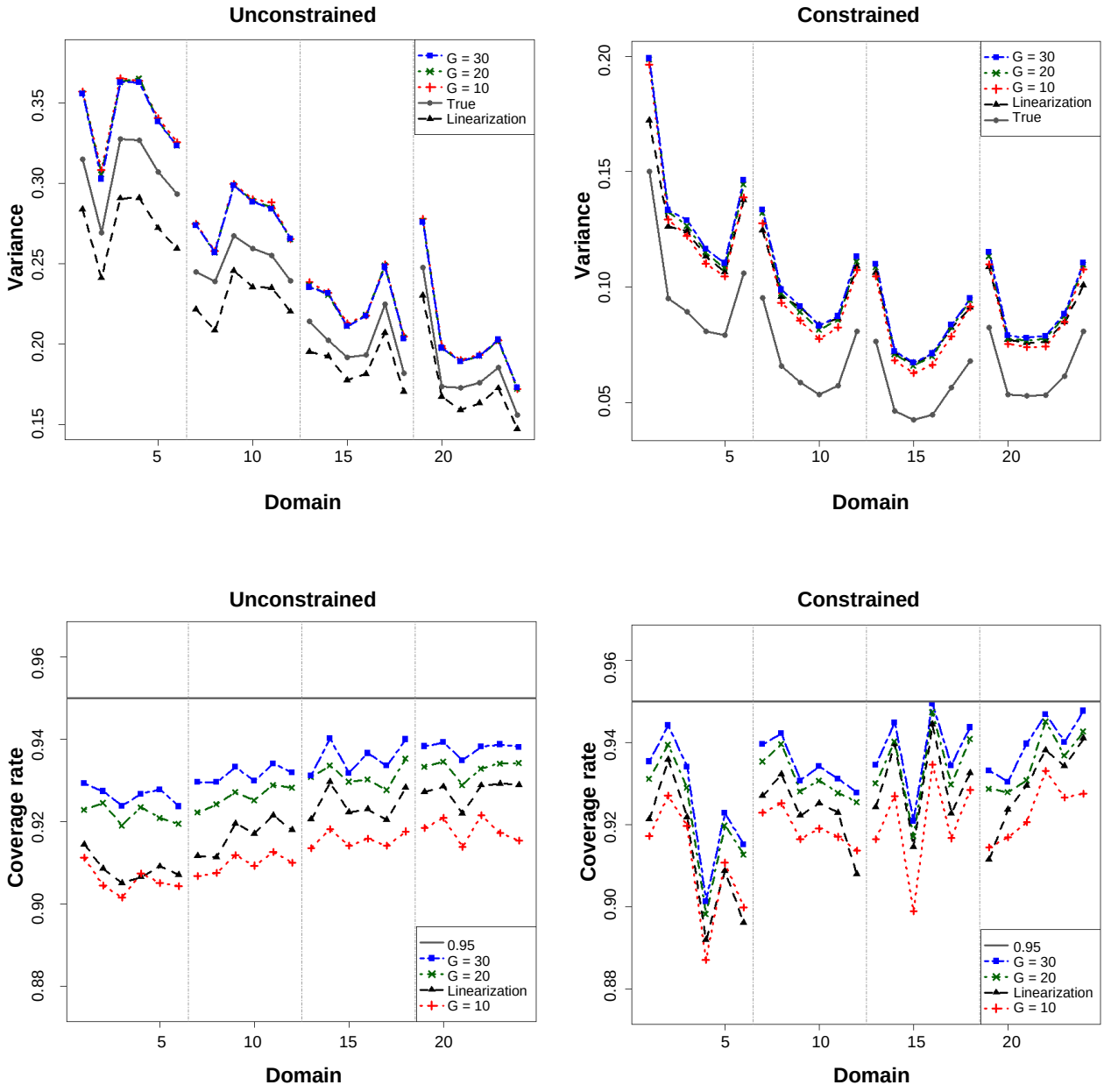


Figure 4.7 Variance estimation (top) and coverage rate (bottom) simulation results based on linearization and DAGJK methods for the unconstrained (left) and constrained (right) estimators, under the double monotone scenario with $n_N = 480$ and $\sigma = 2$.

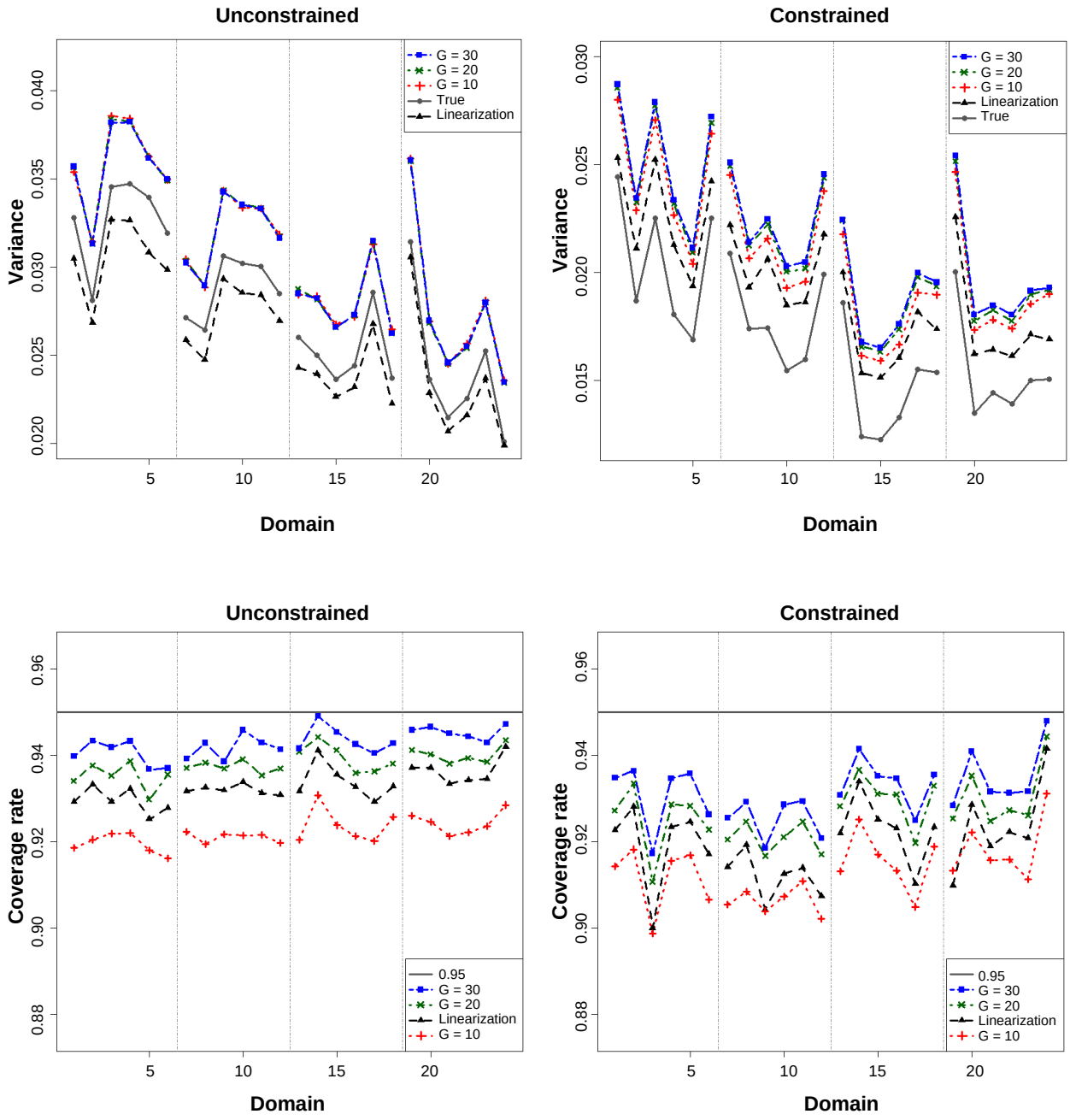


Figure 4.8 Variance estimation (top) and coverage rate (bottom) simulation results based on linearization and DAGJK methods for the unconstrained (left) and constrained (right) estimators, under the double monotone scenario with $n_N = 960$ and $\sigma = 1$.

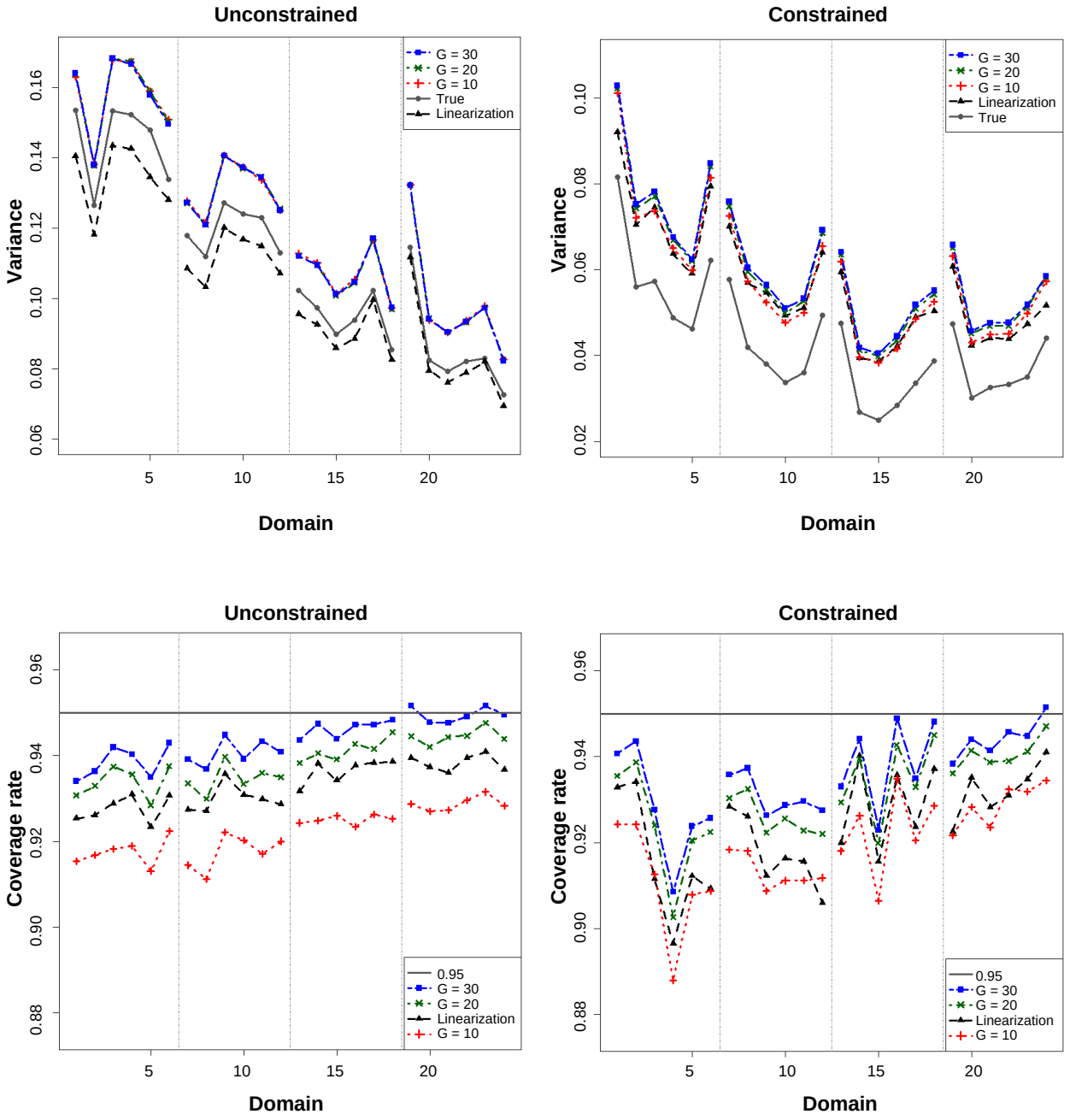


Figure 4.9 Variance estimation (top) and coverage rate (bottom) simulation results based on linearization and DAGJK methods for the unconstrained (left) and constrained (right) estimators, under the double monotone scenario with $n_N = 960$ and $\sigma = 2$.

5 Application of constrained estimator to NSCG

To demonstrate the utility of the proposed constrained methodology in real survey data, we consider the 2015 National Survey of College Graduates (NSCG), which is sponsored by the National Center for Science and Engineering Statistics (NCSES) within the National Science Foundation, and is conducted by the U.S. Census Bureau. The 2015 NSCG data and documentation are available on the NSF website (www.nsf.gov/statistics/srvygrads). The purpose of the NSCG is to provide data on the characteristics of U.S. college graduates, with particular focus on those in the science and engineering workforce.

We consider the total earned income before deductions in previous year (2014) to be the variable of interest (denoted by EARN). To avoid the high skewness of this variable, a log transformation is performed. Moreover, we take into account only those who reported a positive earning amount. A total of 76,389 observations was considered in our analysis. In addition, 252 domains are considered. These are determined by the cross-classification of four predictor variables. These variables and their assumed constraints are as follows:

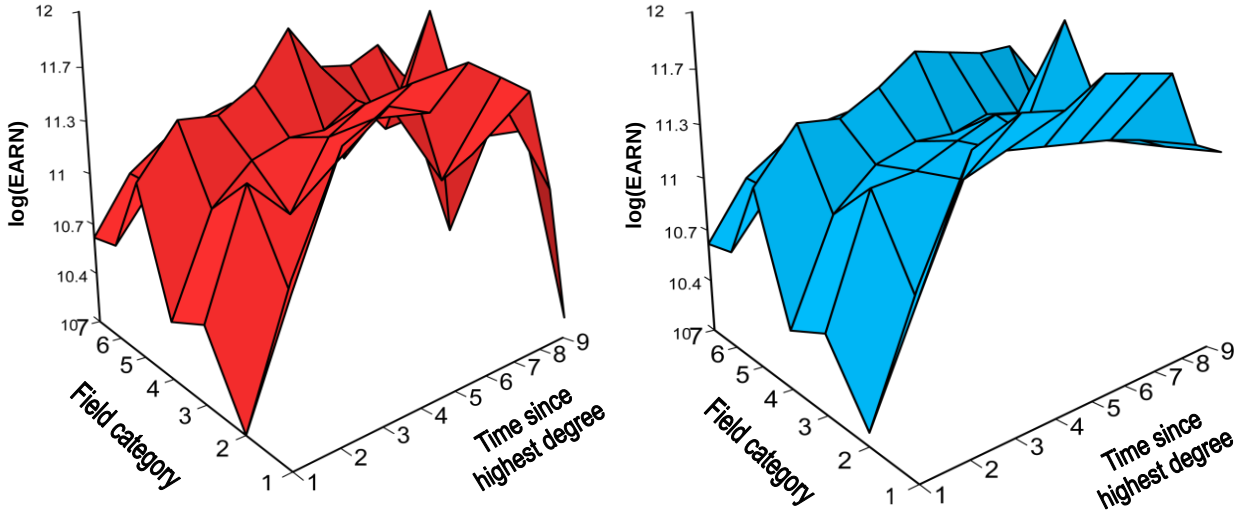
- *Time since highest degree*. This variable defines the year of award of highest degree. The period from 2015 to 1959 is divided into 9 categories, where the first 8 categories (denoted by 1-8) are of 6 years each, and the last category (denoted by 9) is of 9 years. *Constraint:* given the other predictors, the average total earned income increases with respect to the time since highest degree from year category 1 to 7. No assumption is made with respect to categories 8 and 9, as those people are likely to be retired (at least 42 years since their highest degree).
- *Field of study*. This nominal variable defines the field of study for highest degree, based on a major group categorization provided within the 2015 NSCG. The 7 categories for this variable are:

  1: Computer and mathematical sciences,
  2: Biological, agricultural and environmental life sciences,
  3: Physical and related sciences,
  4: Social and related sciences,
  5: Engineering,
  6: S&E-related fields,
  7: Non-S&E fields.

  Constraint: given the other predictors, the average total earned income for each of the fields 2 and 4 is less than for the fields 1, 3 and 5. No assumption is made with respect to categories 6 and 7, as they cover many fields for which a reasonable order restriction might be complicated to impose.
- *Postgrad.* This binary variable defines whether the highest degree is at the postgraduate level (YES) or at the Bachelor's level (NO). *Constraint:* given the other predictors, the average total earned income is higher for those with postgraduate studies.

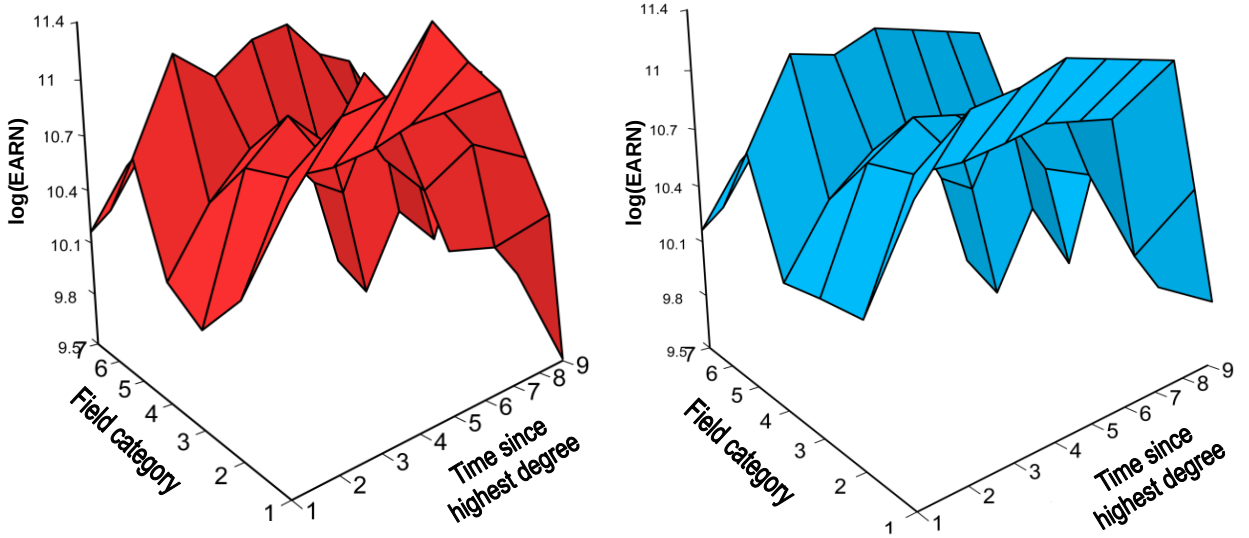
- *Supervise.* This binary variable defines whether supervising others is a responsibility in the principal job (YES) or not (NO). *Constraint:* given the other predictors, the average total earned income is higher for those who supervise others in their principal job.

Figures 5.1 and 5.2 show the unconstrained and constrained estimates for each of the four groups obtained from the cross-classification of the Postgrad and Supervise binary variables. Note that since the assumed constraints constitute a partial ordering, then the constrained estimates are obtained by pooling domains. These figures show that the constrained estimator has a smoother behavior than the unconstrained. Moreover, it tends to correct for the some of the "spikes" produced by the unconstrained estimator, which are usually a consequence of a very small sample size.



(a) Supervise = YES (unconstrained).

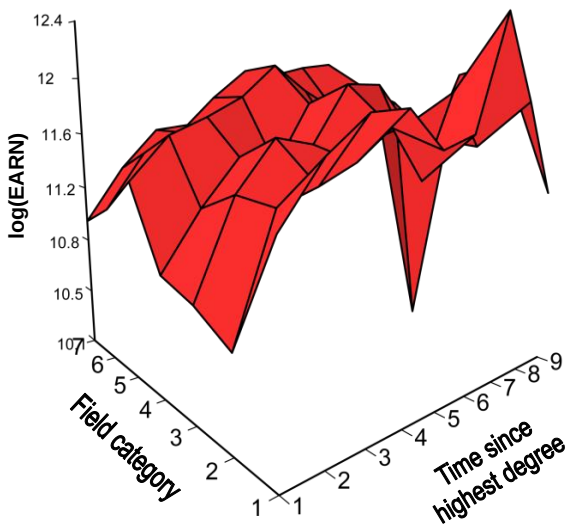
(b) Supervise = YES (constrained).



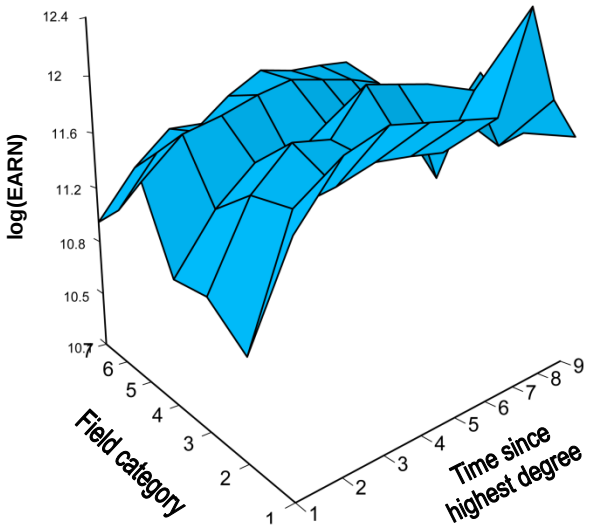
(c) Supervise = NO (unconstrained).

(d) Supervise = NO (constrained).

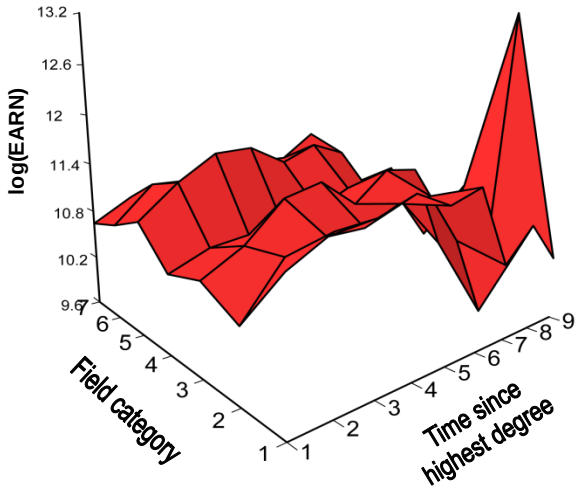
Figure 5.1 Unconstrained (left) and constrained (right) domain mean estimates for the 2015 NSCG data, given that Postgrad = NO is fixed.



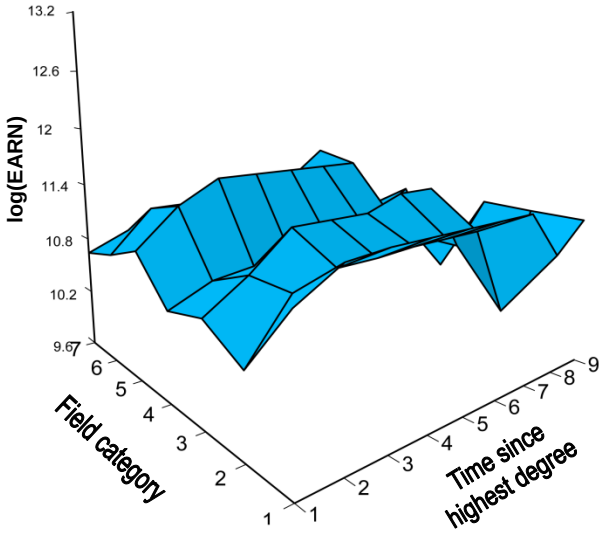
(a) Supervise = YES (unconstrained).



(b) Supervise = YES (constrained).



(c) Supervise = NO (unconstrained).



(d) Supervise = NO (constrained).

Figure 5.2 Unconstrained (left) and constrained (right) domain mean estimates for the 2015 NSCG data, given that Postgrad = YES is fixed.

Standard errors for both unconstrained and constrained estimates are computed using the 2015 NSCG replicate weights, which are based on successive difference replication method (Opsomer, Breidt, White and Li, 2016). The replicate weights and adjustment factors were provided by the Program Director of the Human Resources Statistics Program from the NCSES and are available upon request.

Figure 5.3 displays the ratio of these estimates for each of the 252 domains. In the vast majority of cases, the standard error estimates of the proposed estimator are lower than those for the unconstrained estimator, with improvements of as much as 7 times smaller. However, there are some cases where the opposite behavior occurs. These are investigated in Figure 5.4, which shows plots of two different domain

"slices": one with respect to the Time since highest degree variable and other with respect to Field category. These plots include unconstrained and constrained estimates, Wald confidence intervals and sample sizes. Each of these two slices contain one of the two domains that can be easily identified in Figure 5.3 to have the smallest ratios.

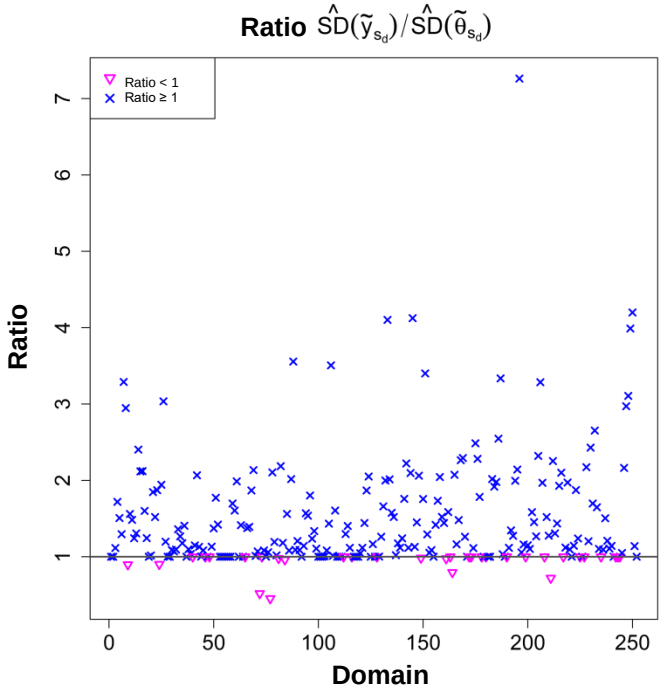
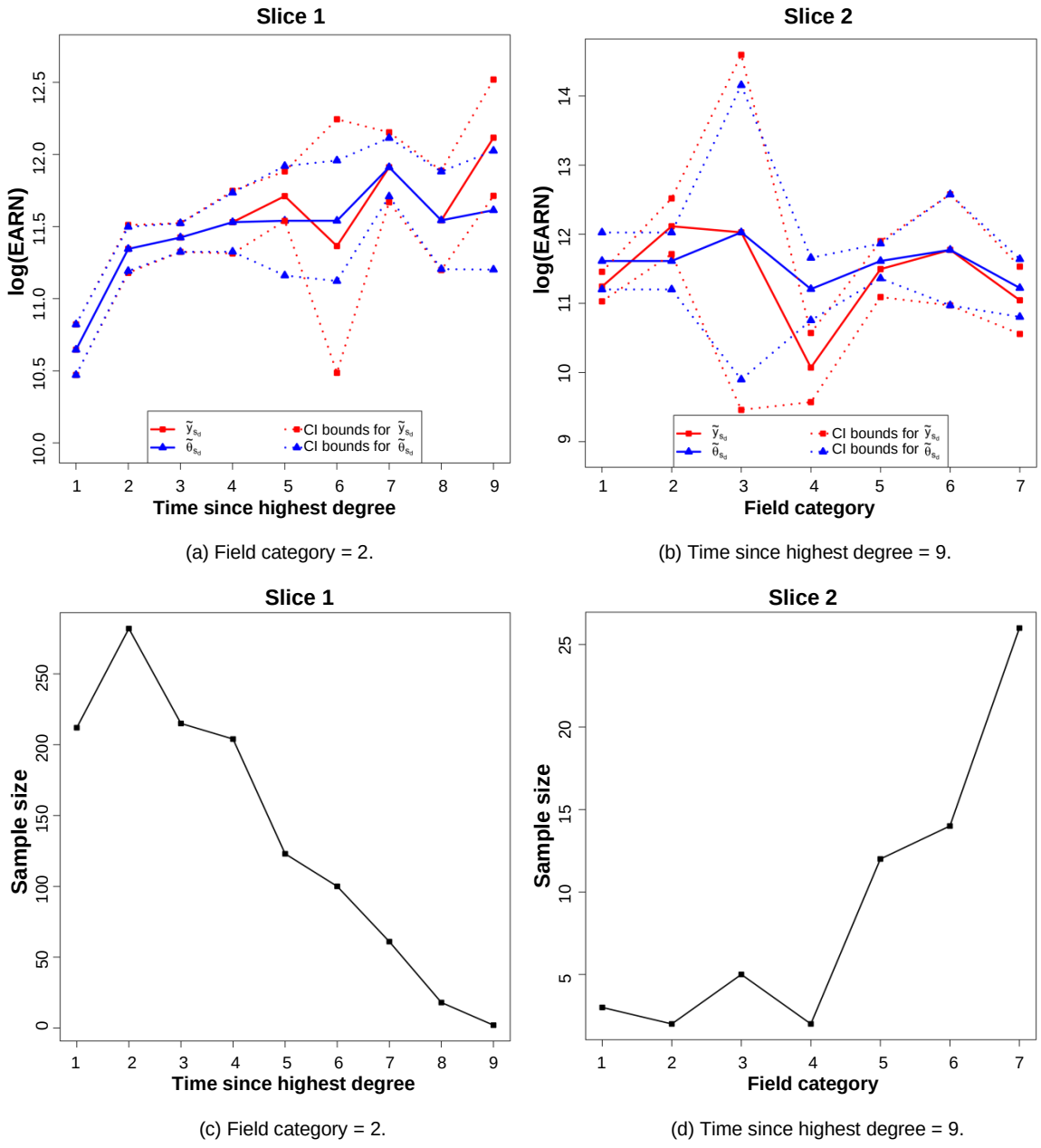


Figure 5.3 Ratio of the estimated standard errors of unconstrained estimates over those for constrained estimates for the 2015 NSCG data.

The first of these domains is displayed in Figure 5.4(a) and 5.4(c), indexed by 5. The unconstrained estimates for the domains indexed by 5 and 6 violate the monotonicity assumption, and thus, are being pooled to obtain the constrained estimates (additional pooling with domains in other "slices" is also occurring, but not visible in this plot). As can be seen in Figure 5.4(a), the confidence interval is narrower for the unconstrained estimates. However, the estimated standard error of the unconstrained estimator of domain 6 is very large, and pooling with domain 5 greatly stabilizes both the estimator and the estimated standard errors for that domain. Figure 5.4(c) shows that the samples sizes on these domains are reasonably large at approximately 100 observations each, implying that the noticed monotonicity violation might be in fact true in the population. The final decision on the balance between the improved stability of some domains with the potential for bias due to incorrect constraints would need to be carefully evaluated.

The second domain where unconstrained estimates produce smaller standard deviation estimates is displayed in Figure 5.4(b) and 5.4(d), indexed by 1. Here, this domain is being pooled with its neighboring domain to obtain the constrained estimate. However, as these two domains have very low sample sizes, the unconstrained estimates might be considered as unreliable, so that their estimated standard errors are

not a good indication of their precision. The constrained estimator appears to be preferred here because of the increase in the effective cell size.



(a) Field category = 2.

(b) Time since highest degree = 9.

(c) Field category = 2.

(d) Time since highest degree = 9.

Figure 5.4 Unconstrained and constrained estimates with Wald confidence intervals (top) and sample sizes (bottom) for the 2015 NSCG data, given that Postgrad = YES and Supervise = YES.

6 Conclusions

We have proposed a general methodology to estimate domain means which makes it possible incorporate natural restrictions between domains into design-based estimation. It was shown to improve estimation and inference, especially on small domains. As this new methodology covers a broad range of shape assumptions beyond univariate monotonicity, it aims to jointly take advantage of several types of qualitative information that arises naturally for survey data. Additional shapes that may be imposed include convexity or log-concavity; the latter might be imposed if the population domain means are believed to be increasing and then decreasing over a set of domains. Future work by the authors will include a "relaxed monotone" estimator to be used when the population domain means are "roughly" monotone in some sequence of domains. For the relaxed monotone estimator, a type of moving average over the domains is used to implement the constraints, allowing the estimator to have some departures from monotonicity.

We also proposed a design-based variance estimation method of the estimator, which only requires knowledge of the sample-specific constraint set. Replication-based methods are shown to behave similarly. From the computational side, the estimator is based on the Cone Projection Algorithm which is efficiently implemented in the package `coneproj` and freely available. In the important practical case of partial ordering, the constrained estimator is equivalent to a pooling of neighboring domains, so that once the constraint set is identified by CPA, subsequent computations of estimators and variance estimators can be done directly using traditional design-based estimation for the relevant domains.

An important practical issue, as illustrated in the NSCG analysis in Section 5, is the determination of when the imposed constraint might not be valid for a particular survey application. Recently, Oliva-Aviles, Meyer and Opsomer (2019) proposed the sample-based Cone Information Criterion as a criterion to choose between the constrained and unconstrained fits for the estimator of Wu et al. (2016). That approach is generalizable to the setting considered here, and is currently under development.

Appendix

The first part of this appendix contains lemmas used to obtain the theoretical results discussed in this paper. Proofs of the theorems are included at the end of this appendix.

Lemma 1. *If a non-zero vector can be written as the positive linear combination of linearly dependent non-zero vectors, then it can be expressed as the positive linear combination of a linearly independent subset of these.*

Proof. Let $\mathbf{v}$ be a non-zero vector such that it can be written as $\mathbf{v} = \sum_{i=1}^{k} a_i \ell_i$ where $\ell_1, \ell_2, \ldots, \ell_k$ are non-zero vectors and $a_i > 0$ for $i = 1, 2, \ldots, k$. If this set of vectors is not linearly independent, then there exist constants $b_1, \ldots, b_k$, not all zero, such that $\sum_{i=1}^{k} b_i \ell_i = \mathbf{0}$, and for any $c \in \mathbf{R}$, $\mathbf{v} = \sum_{i=1}^{k} (a_i + cb_i)\, \ell_i$. Let $c = -\min_{i:\, b_i \neq 0} a_i / b_i$; then $a_i + cb_i \geq 0$ for $i = 1, \ldots, k$ but for at least

one i, $a_i + cb_i = 0$. Then we have written $\mathbf{v}$ as a positive linear combination of a proper subset of the vectors. If this subset is still linearly dependent, the process can be repeated.

Lemma 2. *If* $\mathbf{A}$ *is a* $m \times D$ *irreducible matrix and* $\mathbf{B}$ *is a* $D \times D$ *nonsingular matrix, then* $\tilde{\mathbf{A}} = \mathbf{AB}$ *is also irreducible.*

Proof. Suppose $\tilde{\mathbf{A}}^\top \mathbf{c} = \mathbf{0}$ for some $\mathbf{c} \in \mathbb{R}^m, \mathbf{c} \geq \mathbf{0}$. Then $\mathbf{B}^\top \mathbf{A}^\top \mathbf{c} = \mathbf{0}$ implies that $\mathbf{A}^\top \mathbf{c} = \mathbf{0}$ by the non-singularity of $\mathbf{B}$. Because $\mathbf{A}$ is irreducible, we must have $\mathbf{c} = \mathbf{0}$, so the origin is not a positive linear combination of rows of $\tilde{\mathbf{A}}$. Next, suppose that one of the rows of $\tilde{\mathbf{A}}$ is a positive linear combination of other rows of $\tilde{\mathbf{A}}$. This means we can write $\tilde{\mathbf{A}}^\top \mathbf{b} = \mathbf{0}$, where $b_j = -1$ for some $j \in \{1, \ldots, m\}$ and $b_i \geq 0, i \neq j$. But $\tilde{\mathbf{A}}^\top \mathbf{b} = \mathbf{0}$ implies that $\mathbf{B}^\top \mathbf{A}^\top \mathbf{b} = \mathbf{0}$ implies that $\mathbf{A}^\top \mathbf{b} = \mathbf{0}$ by the non-singularity of $\mathbf{B}$. We can't have $\mathbf{A}^\top \mathbf{b} = \mathbf{0}$ for this $\mathbf{b}$, so we can't have a row of $\tilde{\mathbf{A}}$ is a positive linear combination of other rows of $\tilde{\mathbf{A}}$. Therefore, $\tilde{\mathbf{A}}$ is irreducible.

Lemma 3. *Let* $\mathbf{A}$ *be a* $m \times D$ *matrix. Also, let* $\mathbf{S}_1$ *and* $\mathbf{S}_2$ *be* $D \times D$ *diagonal matrices with nonzero elements on the diagonal. For any set* $J \subseteq \{1, 2, \ldots, m\}$, *denote* $V_{i,J}$ *to be the set of vectors in rows* J *of* $\mathbf{A}_i = \mathbf{AS}_i$, $i = 1, 2$. *Then, for any* $J^* \subseteq J$,

$$\mathcal{L}(V_{1,J^*}) = \mathcal{L}(V_{1,J}) \Leftrightarrow \mathcal{L}(V_{2,J^*}) = \mathcal{L}(V_{2,J}).$$

Proof. Let $\mathbf{A}_{i,J} = \mathbf{A}_J \mathbf{S}_i$, $i = 1, 2$; where $\mathbf{A}_J$ denotes the submatrix of $\mathbf{A}$ that contains the rows in positions J. First, assume that $\mathcal{L}(V_{1,J^*}) = \mathcal{L}(V_{1,J})$. Since $J^* \subseteq J$, it is straightforward to see that $\mathcal{L}(V_{2,J^*}) \subseteq \mathcal{L}(V_{2,J})$. Now, consider any $\mathbf{v} \in \mathcal{L}(V_{2,J})$ so that $\mathbf{v} = \mathbf{A}_{2,J}^\top \mathbf{a} = \mathbf{S}_2 \mathbf{A}_J^\top \mathbf{a}$ for some vector $\mathbf{a}$. Then, we have $\mathbf{S}_1 \mathbf{S}_2^{-1} \mathbf{v} = \mathbf{S}_1 \mathbf{A}_J^\top \mathbf{a} \in \mathcal{L}(V_{1,J})$. By assumption, there exists a vector $\mathbf{b}$ such that $\mathbf{S}_1 \mathbf{S}_2^{-1} \mathbf{v} = \mathbf{S}_1 \mathbf{A}_{J^*}^\top \mathbf{b}$. Therefore, $\mathbf{v} = \mathbf{S}_2 \mathbf{A}_{J^*}^\top \mathbf{b} \in \mathcal{L}(V_{2,J^*})$. Thus, $\mathcal{L}(V_{2,J}) \subseteq \mathcal{L}(V_{2,J^*})$. Analogously, it follows that $\mathcal{L}(V_{2,J^*}) = \mathcal{L}(V_{2,J})$ implies $\mathcal{L}(V_{1,J^*}) = \mathcal{L}(V_{1,J})$.

Lemma 4. *Under Assumptions A1-A5, the following statements hold:*

(i) *The* $N^{-1}\hat{t}_d$ *are uniformly bounded.*

(ii) *The* $N^{-1}\hat{N}_d$ *are uniformly bounded above and uniformly bounded away from zero.*

(iii) $var(N^{-1}\hat{t}_d) = O(n^{-1})$ *and* $var(N^{-1}\hat{N}_d) = O(n^{-1})$.

(iv) $\mathbb{E}\left[(N^{-1}\hat{t}_d - r_d \mu_d)^2\right] = O(n^{-1})$ *and* $\mathbb{E}\left[(N^{-1}\hat{N}_d - r_d)^2\right] = O(n^{-1})$.

Proof.

(i) Note that

$$\frac{|\hat{t}_d|}{N} = \left| \frac{\sum_{k \in s_d} y_k / \pi_k}{N} \right| \leq \frac{\sum_{k \in U} |y_k|}{\lambda N}$$

which does not depend on s, and is bounded independently of N by Assumption A2.

(ii) From Assumptions A4 and A5, note that

$$\frac{\varepsilon n}{DN} \leq \frac{n_d}{N} \leq \frac{\hat{N}_d}{N} = N^{-1}\sum_{k\in s_d} 1/\pi_k \leq \lambda^{-1}N^{-1}N_d \leq \lambda^{-1},$$

where both lower and upper bounds do not depend on s, and are bounded for all N by Assumptions A1 and A4.

(iii) Note that

$$n\,\mathrm{var}\left(N^{-1}\hat{t}_d\right) = n\,\mathrm{var}\left(N^{-1}\sum_{k\in s_d} y_k/\pi_k\right) \leq \frac{\sum_{k\in U_d} y_k^2}{\lambda^2 N}\left(\frac{n}{N} + n\max_{k,l\in U_d:\, k\neq l}|\Delta_{kl}|\right)$$

which is bounded by Assumptions A2, A4 and A5. Setting $y_k \equiv 1$ and following an analogous argument, it can be shown that $n\,\mathrm{var}\left(N^{-1}\hat{N}_d\right) = O(1)$.

(iv) Since

$$\mathbb{E}\left[\left(N^{-1}\hat{t}_d - r_d\mu_d\right)^2\right] = \mathrm{var}\left(N^{-1}\hat{t}_d\right) + \left(\frac{N_d}{N}\bar{y}_{U_d} - r_d\mu_d\right)^2,$$

Assumption A3 and (iii) lead to the desired conclusion. Analogously, we find

$$\mathbb{E}\left[\left(N^{-1}\hat{N}_d - r_d\right)^2\right] = O(n^{-1}).$$

Proof of Theorem 1. First, suppose that $\Pi(\mathbf{z}|\Omega^0) = \Pi(\mathbf{z}|\mathcal{L}(V_J)) = \mathbf{0}$. In that case, any subset $J^* \subset J$ such that V_J is linearly independent will satisfy $\Pi(\mathbf{z}|\mathcal{L}(V_{J^*})) = \mathbf{0} \in \bar{\mathcal{F}}_{J^*}$. Hence, it is enough to choose $J^* \subset J$ such that V_{J^*} is linearly independent and spans $\mathcal{L}(V_J)$. Now, suppose that $\Pi(\mathbf{z}|\Omega^0) \neq \mathbf{0}$. Since $\Pi(\mathbf{z}|\Omega^0) = \Pi(\mathbf{z}|\mathcal{L}(V_J)) \in \bar{\mathcal{F}}_J$, $\Pi(\mathbf{z}|\mathcal{L}(V_J))$ can be written as the positive linear combination of vectors $\boldsymbol{\gamma}_j$, $j \in J$. Moreover, $\langle \mathbf{z} - \Pi(\mathbf{z}|\mathcal{L}(V_J)), \boldsymbol{\gamma}_j\rangle = 0$ for $j \in J$. From Lemma 1, there exists $J_0 \subset J$ such that V_{J_0} is linearly independent and $\Pi(\mathbf{z}|\mathcal{L}(V_J))$ can be written as a positive linear combination of the vectors in V_{J_0}, which implies that $\Pi(\mathbf{z}|\mathcal{L}(V_J)) \in \bar{\mathcal{F}}_{J_0}$. In addition, since $\langle \mathbf{z} - \Pi(\mathbf{z}|\mathcal{L}(V_J)), \boldsymbol{\gamma}_j\rangle = 0$ for $j \in J_0$, $\Pi(\mathbf{z}|\mathcal{L}(V_{J_0})) = \Pi(\mathbf{z}|\mathcal{L}(V_J))$. Thus, $\Pi(\mathbf{z}|\Omega^0) = \Pi(\mathbf{z}|\mathcal{L}(V_{J_0}))$. If $\mathcal{L}(V_{J_0}) = \mathcal{L}(V_J)$ then $J^* = J_0$ satifies all required conditions. Now, assume that $\mathcal{L}(V_{J_0}) \subset \mathcal{L}(V_J)$. The fact that $\Pi(\mathbf{z}|\mathcal{L}(V_{J_0})) = \Pi(\mathbf{z}|\mathcal{L}(V_J))$ implies that $\Pi(\mathbf{z}|\mathcal{L}(V_{J_1})) = \Pi(\mathbf{z}|\mathcal{L}(V_{J_0}))$ for any set J_1 such that $J_0 \subseteq J_1 \subseteq J$. Further, since $\Pi(\mathbf{z}|\mathcal{L}(V_{J_0})) \in \bar{\mathcal{F}}_{J_0}$ then $\Pi(\mathbf{z}|\mathcal{L}(V_{J_1})) \in \bar{\mathcal{F}}_{J_1}$. Thus, it is enough to choose the set J^* such that $J_0 \subset J^* \subset J$ and V_{J^*} is a linearly independent set that spans $\mathcal{L}(V_J)$.

Proof of Theorem 2. To prove this theorem, we start with a set $J \notin \mathcal{G}_\mu$ and find necessary conditions for such set to belong to $\mathcal{G}_s$. These necessary conditions, expressed as inequalities in terms of smooth and continuous functions of the $\hat{N}_d/N$ and the $\hat{t}_d/N$, are then used to bound the probability of interest.

Finally, we use Theorem 5.4.3 in Fuller (1996) to show that this probability converges to zero with a rate of $O(n^{-1})$.

Let $\mathbf{A}_{\mu}$, $\mathbf{A}_{\mu,J}$ and $\boldsymbol{\gamma}_{\mu_d}$ be the analogous versions of $\mathbf{A}_s$, $\mathbf{A}_{s,J}$ and $\boldsymbol{\gamma}_{s_d}$ obtained by substituting $\tilde{\mathbf{y}}_s$ and $\mathbf{W}_s$ by $\boldsymbol{\mu}$ and $\mathbf{W}_{\mu}$, respectively. Lemma 2 ensures that both $\mathbf{A}_s$ and $\mathbf{A}_{\mu}$ are irreducible since $\mathbf{A}$ is.

First, suppose $\varnothing \notin \mathcal{G}_{\mu}$ and let $J = \varnothing$. Then, from conditions in (2.8), $\varnothing \in \mathcal{G}_s$ if and only if $\langle \tilde{\mathbf{z}}_s, \boldsymbol{\gamma}_{s_j} \rangle \leq 0$ for $j = 1, 2, \ldots, m$. In contrast, suppose that $\langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_j} \rangle \leq 0$ for $j = 1, 2, \ldots, m$. Hence, $\varnothing \in \mathcal{G}_{\mu}$, which contradicts our choice of J. Therefore, there exists j_0 such that $\langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle > 0$. Then, we have

$$
\begin{aligned}
P(\varnothing \in \mathcal{G}_s) \leq P\left(0 \geq \langle \tilde{\mathbf{z}}_s, \boldsymbol{\gamma}_{s_{j_0}} \rangle\right) &= P\left(\langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle - \langle \tilde{\mathbf{z}}_s, \boldsymbol{\gamma}_{s_{j_0}} \rangle \geq \langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle\right) \\
&= P\left(\left[\frac{\langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle - \langle \tilde{\mathbf{z}}_s, \boldsymbol{\gamma}_{s_{j_0}} \rangle}{\langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle}\right]^2 \geq 1\right) \\
&\leq \frac{1}{\langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle^2} \mathrm{E}\left[\left(\langle \tilde{\mathbf{z}}_s, \boldsymbol{\gamma}_{s_{j_0}} \rangle - \langle \mathbf{z}_{\mu}, \boldsymbol{\gamma}_{\mu_{j_0}} \rangle\right)^2\right]
\end{aligned}
$$

where the last inequality is obtained by an application of Markov's inequality (see for example Casella and Berger (2002), Section 3.6.1). We show now that the expected value in the last term is $O(n^{-1})$. Note that the expression inside of the expected value in the above inequality is a function of vector $\hat{\mathbf{x}}_s = \left(N^{-1}\hat{t}_1, \ldots, N^{-1}\hat{t}_D, N^{-1}\hat{N}_1, \ldots, N^{-1}\hat{N}_D\right)^{\top}$. Let $f_1(\cdot)$ be such a function (which does not depend on N), and denote $\mathbf{x}_{\mu} = (r_1\mu_1, \ldots, r_D\mu_D, r_1, \ldots, r_D)$. To apply Theorem 5.4.3 in Fuller (1996) with $\alpha = 1$, $s = 2$ and $a_N = O(n^{-1/2})$, first we need to show that the following conditions are satisfied:

(a) $\mathrm{E}\left[\left(\hat{\mathbf{x}}_s - \mathbf{x}_{\mu}\right)^2\right] = O(n^{-1})$.

(b) f_1 is uniformly bounded in a closed and bounded sphere $\mathcal{S}$.

(c) $f_1^{(i_1, i_2)}(\mathbf{x})$ is continuous in $\mathbf{x}$ over $\mathcal{S}$, where

$$
f_1^{(i_1, \ldots, i_r)}(\mathbf{x}_0) = \frac{\partial^r}{\partial_{x_{i_1}} \ldots \partial_{x_{i_r}}} f_1(\mathbf{x})\big|_{\mathbf{x} = \mathbf{x}_0}.
$$

(d) $\mathbf{x}_{\mu}$ is an interior point of $\mathcal{S}$.

(e) There is a finite number K such that

$$
\begin{aligned}
&\left| f_1^{(i_1, i_2)}(\mathbf{x}) \right| \leq K \quad \text{for all} \quad \mathbf{x} \in \mathcal{S}, \\
&\left| f_1^{(i_1)}(\mathbf{x}_{\mu}) \right| \leq K \quad \text{and} \quad \left| f_1(\mathbf{x}_{\mu}) \right| \leq K.
\end{aligned}
$$

Condition (a) is directly met by Lemma 4 (iv). In addition, Lemma 4 (i)-(ii) guarantees that there exist a constant $M > 1$ such that $\left| N^{-1}\hat{t}_d \right| \leq M$ and $M^{-1} \leq N^{-1}\hat{N}_d \leq M$. Hence, there exists a closed and bounded sphere $\mathcal{S}$ that it is contained within these constant bounds. Moreover, from Assumption A3, we can conclude that $\mathbf{x}_{\mu} \in \mathcal{S}$, so condition (d) is satisfied. To show that condition (b) is met, note that f_1 is

a continuous function in $\mathcal{S}$ since both $W_s^{-1/2}$ and $\tilde{y}_{s_d}$ exist for any $\mathbf{x} \in \mathcal{S}$. Therefore, the Extreme Value Theorem (see Theorem 4.15 in Rudin (1976)) ensures that f_1 is uniformly bounded in $\mathcal{S}$. Conditions (c) and (e) are satisfied since f_1 is a continuous rational function in $\mathcal{S}$, implying that f_1 is infinitely differentiable and its derivatives are bounded in $\mathcal{S}$. Finally, all conditions (a)-(e) are fulfilled. Therefore, from Theorem 5.4.3 in Fuller (1996), we can conclude that $\mathbb{E}[f_1(\mathbf{x})] = O(n^{-1})$, since f_1 and its first derivative with respect to the $N^{-1}\hat{t}_d$ and $N^{-1}\hat{N}_d$ evaluate to zero at $\mathbf{x}_\mu$.

Now, take any $J \neq \varnothing$ such that $J \notin \mathcal{G}_\mu$, and assume that $J \in \mathcal{G}_s$. Theorem 1 guarantees that we can always choose a subset $J^* \subseteq J$ such that $J^* \in \mathcal{G}_s$, V_{s,J^*} is linearly independent, and $\mathcal{L}(V_{s,J^*}) = \mathcal{L}(V_{s,J})$. Note that $\Pi(\tilde{\mathbf{z}}_s \,|\, \mathcal{L}(V_{s,J^*})) = \mathbf{A}_{s,J^*}^\top \left(\mathbf{A}_{s,J^*}\mathbf{A}_{s,J^*}^\top\right)^{-1}\mathbf{A}_{s,J^*}\tilde{\mathbf{z}}_s$. Let $\tilde{\mathbf{b}}_{s,J^*} = \left(\mathbf{A}_{s,J^*}\mathbf{A}_{s,J^*}^\top\right)^{-1}\mathbf{A}_{s,J^*}\tilde{\mathbf{z}}_s$. Hence, from conditions in (2.8), we have that $J \in \mathcal{G}_s$ implies that $\tilde{\mathbf{b}}_{s,J^*} \geq \mathbf{0}$, and $\left\langle \tilde{\mathbf{z}}_s - \mathbf{A}_{s,J^*}^\top \tilde{\mathbf{b}}_{s,J^*}, \boldsymbol{\gamma}_{s_j} \right\rangle \leq 0$ for any j. Define $\mathbf{b}_{\mu,J^*} = \left(\mathbf{A}_{\mu,J^*}\mathbf{A}_{\mu,J^*}^\top\right)^{-1}\mathbf{A}_{\mu,J^*}\mathbf{z}_\mu$ and assume that $\mathbf{b}_{\mu,J^*} \geq \mathbf{0}$, and $\left\langle \mathbf{z}_\mu - \mathbf{A}_{\mu,J^*}^\top \mathbf{b}_{\mu,J^*}, \boldsymbol{\gamma}_{\mu_j} \right\rangle \leq 0$ for $j = 1, 2, \ldots, m$. These conditions would imply that $J^* \in \mathcal{G}_\mu$, contradicting the original assumption that $J \notin \mathcal{G}_\mu$, since $\mathcal{L}(V_{\mu,J^*}) = \mathcal{L}(V_{\mu,J})$ from Lemma 3. Therefore, either there is an element of $\mathbf{b}_{\mu,J^*}$ that is strictly negative or there exists j_0 such that $\left\langle \mathbf{z}_\mu - \mathbf{A}_{\mu,J^*}^\top \mathbf{b}_{\mu,J^*}, \boldsymbol{\gamma}_{\mu_{j_0}} \right\rangle > 0$. Hence, proving that $P(J \in \mathcal{G}_s) = O(n^{-1})$ in any of these two scenarios will conclude the proof.

Suppose the $j_0{}^{\text{th}}$ element of $\mathbf{b}_{\mu,J^*}$ is strictly negative. That is, $\mathbf{e}_{j_0}^\top \mathbf{b}_{\mu,J^*} < 0$, where $\mathbf{e}_j$ denotes the indicator vector that is 1 for entry j and 0 otherwise. Then, we have

$$
\begin{aligned}
P(J \in \mathcal{G}_s) \leq P\left(\mathbf{e}_{j_0}^\top \tilde{\mathbf{b}}_{s,J^*} \geq 0\right) &= P\left(\mathbf{e}_{j_0}^\top \tilde{\mathbf{b}}_{s,J^*} - \mathbf{e}_{j_0}^\top \mathbf{b}_{\mu,J^*} \geq -\mathbf{e}_{j_0}^\top \mathbf{b}_{\mu,J^*}\right) \\
&\leq \frac{1}{\left(\mathbf{e}_{j_0}^\top \mathbf{b}_{\mu,J^*}\right)^2} \mathbb{E}\left[\left(\mathbf{e}_{j_0}^\top \tilde{\mathbf{b}}_{s,J^*} - \mathbf{e}_{j_0}^\top \mathbf{b}_{\mu,J^*}\right)^2\right].
\end{aligned}
$$

Denote $f_2(\hat{\mathbf{x}}_s)$ to the expression inside the above expected value. An analogous argument to the one used for the function f_1 can be applied to the rational continuous function f_2 over $\mathcal{S}$, to conclude that $\mathbb{E}[f_2(\hat{\mathbf{x}}_s)] = O(n^{-1})$. Note that we also used the fact that $\mathbf{A}_{s,J^*}\mathbf{A}_{s,J^*}^\top$ is an invertible matrix for any $\mathbf{x} \in \mathcal{S}$.

Lastly, suppose there exists j_0 such that $\kappa_{\mathbf{z}_\mu, j_0} = \left\langle \mathbf{z}_\mu - \mathbf{A}_{\mu,J^*}^\top \mathbf{b}_{\mu,J^*}, \boldsymbol{\gamma}_{\mu_{j_0}} \right\rangle > 0$, and denote $\kappa_{\tilde{\mathbf{z}}_\mu, j_0} = \left\langle \tilde{\mathbf{z}}_s - \mathbf{A}_{s,J^*}^\top \tilde{\mathbf{b}}_{s,J^*}, \boldsymbol{\gamma}_{s_{j_0}} \right\rangle$. Then, we have

$$
\begin{aligned}
P\left(J \in \tilde{\mathcal{G}}_s\right) \leq P\left(0 \geq \kappa_{\tilde{\mathbf{z}}_s, j_0}\right) &= P\left(\kappa_{\mathbf{z}_\mu, j_0} - \kappa_{\tilde{\mathbf{z}}_s, j_0} \geq \kappa_{\mathbf{z}_\mu, j_0}\right) \\
&\leq \frac{1}{\kappa_{\mathbf{z}_\mu, j_0}^2} \mathbb{E}\left[\left(\kappa_{\tilde{\mathbf{z}}_s, j_0} - \kappa_{\mathbf{z}_\mu, j_0}\right)^2\right].
\end{aligned}
$$

Denote $f_3(\hat{\mathbf{x}}_s)$ to the expression inside the above expected value. An analogous argument to the one used for the functions f_1, f_2 is applied to conclude that $\mathbb{E}[f_3(\hat{\mathbf{x}}_s)] = O(n^{-1})$.

Proof of Theorem 3. Take any $J \in \mathcal{G}_s$ and any domain d. Note that the condition $\mathbf{A}\boldsymbol{\mu} \geq \mathbf{0}$ implies that $\varnothing \in \mathcal{G}_\mu$. Then, we can write $\tilde{\theta}_{s_d} - \bar{y}_{U_d}$ as

$$\tilde{\theta}_{s_d} - \bar{y}_{U_d} = (\tilde{y}_{s_d} - \bar{y}_{U_d})\,1_{J=\varnothing} + \sum_{J_G \in \mathcal{G}_\mu \setminus \varnothing} (\tilde{\theta}_{s_d, J_G} - \bar{y}_{U_d})\,1_{J_G = J} + \sum_{J_G \in \mathcal{G}_\mu^c} (\tilde{\theta}_{s_d, J_G} - \bar{y}_{U_d})\,1_{J_G = J},$$

where we used that $\tilde{\theta}_{s_d, \varnothing} = \tilde{y}_{s_d}$. Now, an unfeasible variance estimator $\mathrm{AV}(\tilde{\theta}_{s_d, J})$ can be written as

$$\mathrm{AV}(\tilde{\theta}_{s_d, J}) = \mathrm{AV}(\tilde{y}_{s_d})\,1_{J=\varnothing} + \sum_{J_G \in \mathcal{G}_\mu \setminus \varnothing} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})\,1_{J=J_G} + \sum_{J_G \in \mathcal{G}_\mu^c} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})\,1_{J=J_G}.$$

Hence,

$$\begin{aligned}
\mathrm{AV}(\tilde{\theta}_{s_d, J})^{-1/2}(\tilde{\theta}_{s_d} - \bar{y}_{U_d}) &= \mathrm{AV}(\tilde{y}_{s_d})^{-1/2}(\tilde{y}_{s_d} - \bar{y}_{U_d})\,1_{J=\varnothing} \\
&\quad + \sum_{J_G \in \mathcal{G}_\mu \setminus \varnothing} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\tilde{\theta}_{s_d, J_G} - \bar{y}_{U_d})\,1_{J=J_G} \\
&\quad + \sum_{J_G \in \mathcal{G}_\mu^c} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\tilde{\theta}_{s_d, J_G} - \bar{y}_{U_d})\,1_{J=J_G} \\
&= \Bigg[\mathrm{AV}(\tilde{y}_{s_d})^{-1/2}(\tilde{y}_s - \bar{y}_{U_d})\,1_{J=\varnothing} \\
&\qquad + \sum_{J_G \in \mathcal{G}_\mu \setminus \varnothing} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\tilde{\theta}_{s_d, J_G} - \theta_{U_d, J_G})\,1_{J=J_G} \\
&\qquad + \sum_{J_G \in \mathcal{G}_\mu^c} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\tilde{\theta}_{s_d, J_G} - \theta_{U_d, J_G})\,1_{J=J_G} \Bigg] \\
&\quad + \left[\sum_{J_G \in \mathcal{G}_\mu \setminus \varnothing} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\theta_{U_d, J_G} - \bar{y}_{U_d})\,1_{J=J_G} \right] \\
&\quad + \left[\sum_{J_G \in \mathcal{G}_\mu^c} \mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\theta_{U_d, J_G} - \bar{y}_{U_d})\,1_{J=J_G} \right] \\
&= c_{1N} + c_{2N} + c_{3N},
\end{aligned}$$

where θ_{U_d, J_G} is the population version of $\tilde{\theta}_{s_d, J_G}$. A first order term Taylor expansion of $\tilde{\theta}_{s_d, J_G}$ and Assumption A6 allow to conclude that each term of the form

$$\mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\tilde{\theta}_{s_d, J_G} - \theta_{U_d, J_G})$$

converges in distribution to a standard normal distribution. Therefore, c_{1N} also converges to a standard normal distribution. Note that for each $J_G \in \mathcal{G}_\mu^c$,

$$\mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\theta_{U_d, J_G} - \bar{y}_{U_d}) = \left[n\mathrm{AV}(\tilde{\theta}_{s_d, J_G})\right]^{-1/2}\left[n^{1/2}(\theta_{U_d, J_G} - \bar{y}_{U_d})\right] = O(n^{1/2}),$$

while $1_{J=J_G} = O_p(n^{-1})$ by Theorem 2 (since $J \in \mathcal{G}_s$). Thus, $c_{3N} = O_p(n^{-1/2})$. Now, note that $\theta_{U_d, J_G} - \bar{y}_{U_d} = O(N^{-1/2})$ when $J_G \in \mathcal{G}_\mu \setminus \varnothing$ by Assumption A3. Hence, for any $J_G \in \mathcal{G}_\mu \setminus \varnothing$,

$$\mathrm{AV}(\tilde{\theta}_{s_d, J_G})^{-1/2}(\theta_{U_d, J_G} - \bar{y}_{U_d}) = \left[n\mathrm{AV}(\tilde{\theta}_{s_d, J_G})\right]^{-1/2}\left[n^{1/2}(\theta_{U_d, J_G} - \bar{y}_{U_d})\right] = O\left(\sqrt{\frac{n}{N}}\right),$$

which implies that $c_{2N} = O\left(\sqrt{\frac{n}{N}}\right)$ (bias term). Thus, by combining these properties of c_{1N}, c_{2N} and c_{3N}, we conclude that

$$\mathrm{AV}\left(\tilde{\theta}_{s_d, J}\right)^{-1/2}\left(\tilde{\theta}_{s_d} - \bar{y}_{U_d}\right) \xrightarrow{\mathcal{L}} \mathcal{N}(B, 1),$$

where $B = O\left(\sqrt{\frac{n}{N}}\right)$.

Now, write the feasible variance estimator $\hat{V}\left(\tilde{\theta}_{s_d, J}\right)$ as

$$\hat{V}\left(\tilde{\theta}_{s_d, J}\right) = \hat{V}\left(\tilde{y}_{s_d}\right) 1_{J=\varnothing} + \sum_{J_G \in \mathcal{G}_\mu \setminus \varnothing} \hat{V}\left(\tilde{\theta}_{s_d, J_G}\right) 1_{J=J_G} + \sum_{J_G \in \mathcal{G}_\mu^c} \hat{V}\left(\tilde{\theta}_{s_d, J_G}\right) 1_{J=J_G}.$$

By Assumption A6, we have that $\hat{V}\left(\tilde{\theta}_{s_d, J_G}\right) - \mathrm{AV}\left(\tilde{\theta}_{s_d, J_G}\right) = o_p\left(n^{-1}\right)$ for any J_G, which implies that $\hat{V}\left(\tilde{\theta}_{s_d, J}\right)^{1/2} - \mathrm{AV}\left(\tilde{\theta}_{s_d, J}\right)^{1/2} = o_p\left(n^{-1/2}\right)$. Hence, an application of Slutsky's theorem allows to replace $\mathrm{AV}\left(\tilde{\theta}_{s_d, J}\right)^{-1/2}$ by $\hat{V}\left(\tilde{\theta}_{s_d, J}\right)^{-1/2}$.

To prove the last part of this theorem, just note that $\mathbf{A}\boldsymbol{\mu} > \mathbf{0}$ implies $\mathcal{G}_\mu = \{\varnothing\}$. Thus, the term c_{2N} does not exist and the bias term vanishes.

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