Calibration and Partial Calibration on Principal Components when the Number of Auxiliary Variables is Large

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Abstract: In survey sampling, calibration is a very popular tool used to make total estimators consistent with known totals of auxiliary variables and to reduce variance. When the number of auxiliary variables is large, calibration on all the variables may lead to estimators of totals whose mean squared error (MSE) is larger than the MSE of the Horvitz-Thompson estimator even if this simple estimator does not take account of the available auxiliary information. We study in this paper a new technique based on dimension reduction through principal components that can be useful in this large dimension context. Calibration is performed on the first principal components, which can be viewed as the synthetic variables containing the most important part of the variability of the auxiliary variables. When some auxiliary variables play a more important role than the others, the method can be adapted to provide an exact calibration on these important variables. Some asymptotic properties are given in which the number of variables is allowed to tend to infinity with the population size. A data driven selection criterion of the number of principal components ensuring that all the sampling weights remain positive is discussed. The methodology of the paper is illustrated, in a multipurpose context, by an application to the estimation of electricity consumption for each day of a week with the help of 336 auxiliary variables consisting of the past consumption measured every half an hour over the previous week.

Key words and phrases: dimension reduction; model-assisted estimation; multipurpose surveys; partial calibration; partial least squares; penalized calibration; ridge regression; survey sampling; variance approximation.

1. Introduction

Since the seminal work by Deville and Särndal (1992), calibration is one of the most popular and useful tools to improve Horvitz-Thompson estimators of totals in a design-based survey sampling framework. Roughly speaking, it consists in looking for a modification of the sampling weights so that the totals, in the population, of the auxiliary variables are perfectly estimated. Performing cal-

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ibration often leads to total estimators with smaller variances and this technique is routinely used by several national statistical agencies (see Särndal, 2007 for a review).

With the spread of automatic process for data collection as well as increasing storage capacities, it is not unusual anymore to have to analyze data coming from very large surveys with many auxiliary variables. In this finite population context, calibration on all the auxiliary variables may lead to estimators whose performances are worse than the simple Horvitz-Thompson estimator even if this latter estimator does not account for any auxiliary information (see *e.g.* Silva and Skinner, 1997). Several difficulties arise in this context such as instability of the calibration weights or variance inflation. There are different ways of dealing with these issues. One possibility is to choose only a subset of the auxiliary variables and to consider only the auxiliary variables that are expected to be the more pertinent, avoiding the problem of multicollinearity (see *e.g.* Silva and Skinner, 1997; Chambers, Skinner and Wang, 1999 and Clark and Chambers, 2008). Another way is to relax the calibration constraints, meaning that the too restrictive requirement of being exactly calibrated is dropped off and replaced by the requirement of being only approximately calibrated. A class of penalized estimators has been suggested by Bardsley and Chambers (1984) in a model-based setting and extended later by Chambers (1996), Rao and Singh (1997) and Théberge (2000) in a design-based (or model-assisted) setting. Usually, some auxiliary variables play a role that is more important than the others and it is required that their totals be estimated exactly. To fulfill this requirement, Bardsley and Chambers (1984) and Guggemos and Tillé (2010) suggested two different penalized optimization problems which lead in fact to the same system of weights (see Goga and Shehzad, 2014).

We present in this paper another way of dealing with this issue. Our estimator is based on dimension reduction of the auxiliary variables via principal components calibration. In multivariate statistics, principal component analysis (PCA) is a very popular tool for reducing the dimension of a set of quantitative variables (see *e.g.* Jolliffe, 2002) by transforming the initial data set into a new set of a few uncorrelated synthetic variables, called principal components (PC), which are linear combinations of the initial variables with the largest variance. Adopting a model-assisted point of view, the PCA calibration approach can also be viewed as a GREG estimator based on Principal Components Regression (PCR). PCR can be very useful to reduce the number of covariates in a linear regression

model especially when the regressors are highly correlated. As explained in Jolliffe (2002), even if PCR is a biased estimation method for estimating a regression coefficient, it is useful to overcome the problem of multicollinearity among the regressors. The method is easy to put into practice with classical softwares used for performing calibration.

Note that a natural alternative to principal components regression is partial least squares (PLS) which is also a popular dimension reduction regression technique that can be useful when there is a large number of auxiliary variables that are highly correlated (see for example Swold *et al.* 2001). Other model selection techniques such as the Lasso (Tibshirani, 1996) or the elastic net (Zou and Hastie, 2005) can be employed to deal with survey data with large number of auxiliary variables. The main drawback of all these model selection techniques is that they would give survey weights that would depend explicitly on the outcome variable, and this is generally not desired in surveys, particularly in multipurpose surveys, in which there can be many outcome variables under study. Consequently, all these alternative regression techniques have not been considered in this work.

The paper is structured as follows: we briefly recall in Section 2 the calibration method and the problems which may arise when the number of auxiliary variables is large. We introduce in Section 3 the suggested method and we give a model-assisted interpretation. When the auxiliary information is not complete, *i.e.* the values of the auxiliary variables are only known in the sample, we first estimate the PC's and then we perform calibration on the first estimated principal components (Section 4). In Section 5, under mild assumptions on the sampling design and on the study and auxiliary variables, we prove that the calibration estimator on true PC's as well as on estimated PC's are consistent. We present, in Section 6, how the method can be adapted to provide an exact calibration on the variables considered by the survey statistician more important than the other variables. Our method is illustrated in Section 7, in a multipurpose and large dimension context, on the estimation of the total electricity consumption for each day of a week with the help of the past consumption measured every half an hour over the previous week. Finally, a brief Section 8 gives some concluding remarks. The proofs as well as some additional results on the electricity data are available in a Supplementary file.

2. Calibration over a large number of auxiliary variables

We consider the finite population $U = \{1, \ldots, k, \ldots, N\}$ and we wish to estimate the total $t_y = \sum_{k \in U} y_k$, where y_k is the value of the variable of interest $\mathcal{Y}$ for the kth unit. Let s be a random sample, with fixed size n, drawn from U according to a sampling design that assigns to unit k a known inclusion probability $\pi_k = \Pr(\mathrm{k} \in \mathrm{s})$ satisfying $\pi_k > 0$. The corresponding sampling design weight is denoted by $d_k = 1/\pi_k$. We suppose that y_k is known for all $k \in s$ (complete response).

Without auxiliary information, the total t_y is estimated unbiasedly by the Horvitz-Thompson (HT) estimator $\hat{t}_{yd} = \sum_{k \in s} d_k y_k$. Consider now p auxiliary variables, $\mathcal{X}_1, \ldots, \mathcal{X}_p$, and let $\mathbf{x}_k^T = (x_{k1}, \ldots, x_{kp})$ be the transposed vector whose elements are the values of the auxiliary variables for the kth unit. The calibration method has been developed by Deville and Särndal (1992) to use as effectively as possible the known population totals of $\mathcal{X}_j, j = 1, \ldots, p$ at the estimation stage. The calibration estimator of t_y is a weighted estimator

$$\hat{t}_{yw} = \sum_{k \in s} w_k y_k, \tag{2.1}$$

whose (calibrated) weights w_k are chosen so that they are as close as possible to the initial sampling weights d_k, according to some distance Φ_s and subject to some constraints. More exactly,

$$(w_k)_{k \in s} = \mathrm{argmin}_w \Phi_s(w) \tag{2.2}$$

$$\text{subject to} \quad \sum_{k \in s} w_k \mathbf{x}_k = t_{\mathbf{x}}, \tag{2.3}$$

where $w = (w_k, k \in s)$ is the vector of weights assigned to each unit in the sample and $t_{\mathbf{x}} = \sum_{k \in U} \mathbf{x}_k$ is the vector whose elements are the known totals of $\mathcal{X}_j$ for $j = 1, \ldots, p$. Several distance functions Φ_s have been studied in Deville and Särndal (1992). Under weak regularity assumptions these authors have shown that all resulting estimators are asymptotically equivalent to the one obtained by minimizing the chi-square distance function $\Phi_s(w) = \sum_{k \in s} (w_k - d_k)^2 / q_k d_k$, where the q_k's are known positive constants that can be used to take account of the variability of the observations and are unrelated to d_k. A common use in the applications is to consider uniform weights $q_k = 1$ for all units k and we will suppose, without loss of generality, that $q_k = 1$ in the following. We will only consider calibration estimators derived using the chi-square distance. The

calibration weights w_k, $k \in s$, are

$$w_k = d_k - d_k \mathbf{x}_k^T \left(\sum_{\ell \in s} d_\ell \mathbf{x}_\ell \mathbf{x}_\ell^T \right)^{-1} (\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}), \tag{2.4}$$

where $\hat{t}_{\mathbf{x}d} = \sum_{k \in s} d_k \mathbf{x}_k$ is the HT estimator of $t_{\mathbf{x}}$, and the corresponding calibration estimator is obtained by plugging-in w_k in (2.1).

With a different point of view, it can be shown that the calibration estimator obtained with the chi-squared distance is equal to the generalized regression estimator (GREG) which is derived by assuming a linear regression model between the study variable $\mathcal{Y}$ and the auxiliary variables $\mathcal{X}_1, \ldots, \mathcal{X}_p$,

$$\xi : \quad y_k = \mathbf{x}_k^T \boldsymbol{\beta} + \varepsilon_k, \tag{2.5}$$

where $\varepsilon = (\varepsilon_k, k \in U)$ is a centered random vector with a diagonal variance matrix, whose diagonal elements are equal to $1/q_k$. Cassel *et al.* (1976) suggested the generalized difference estimator

$$\tilde{t}_{y,\mathbf{x}}^{\text{diff}} = \hat{t}_{yd} - \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right)^T \tilde{\boldsymbol{\beta}}_{\mathbf{x}}, \tag{2.6}$$

where $\tilde{\boldsymbol{\beta}}_{\mathbf{x}} = (\sum_{k \in U} \mathbf{x}_k \mathbf{x}_k^T)^{-1} \sum_{k \in U} \mathbf{x}_k y_k$ is the ordinary least squares estimator of $\boldsymbol{\beta}$. Remark that $\tilde{t}_{y,\mathbf{x}}^{\text{diff}}$ can not be computed because $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}$ can not be computed unless we have observed the whole population. We estimate $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}$ by $\hat{\boldsymbol{\beta}}_{\mathbf{x}} = \left(\sum_{k \in s} d_k \mathbf{x}_k \mathbf{x}_k^T\right)^{-1} \sum_{k \in s} d_k \mathbf{x}_k y_k$ and obtain the GREG estimator of t_y : $\hat{t}_{yw} = \hat{t}_{yd} - \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right)^T \hat{\boldsymbol{\beta}}_{\mathbf{x}}$.

Under mild regularity assumptions, Deville and Särndal (1992) have proven that the calibration estimator $\hat{t}_{yw}$ and $\tilde{t}_{y,\mathbf{x}}^{\text{diff}}$ have the same asymptotic distribution. We have $N^{-1}\left(\hat{t}_{yw} - t_y\right) = N^{-1}\left(\tilde{t}_{y,\mathbf{x}}^{\text{diff}} - t_y\right) + o_{\text{p}}(n^{-1/2})$ and as a result, the asymptotic variance of $\hat{t}_{yw}$ is $AV(\hat{t}_{yw}) = \sum_{k \in U} \sum_{\ell \in U} (\pi_{k\ell} - \pi_k \pi_\ell) d_k d_\ell (y_k - \mathbf{x}_k^T \tilde{\boldsymbol{\beta}}_{\mathbf{x}})(y_\ell - \mathbf{x}_\ell^T \tilde{\boldsymbol{\beta}}_{\mathbf{x}})$, where $\pi_{k\ell} = \Pr(\text{k} \in \text{s} \;\&\; \ell \in \text{s})$ is the probability that both k and ℓ are included in the sample s, and $\pi_{kk} = \pi_k$. Calibration will improve the HT estimator, namely $AV(\hat{t}_{yw}) \leq V(\hat{t}_{yd})$, if the predicted values $\mathbf{x}_k^T \tilde{\boldsymbol{\beta}}_{\mathbf{x}}$ are close enough to the y_k's, that is to say if the model ξ stated in (2.5) explains sufficiently well the variable of interest. Nevertheless, when a very large number p of auxiliary variables are used, this result is no longer true as it was remarked by Silva and Skinner (1997) in a simulation study.

One way to circumvent the problems due to over-calibration such as extremely large weights and variance inflation, is to relax the calibration constraints, meaning that the too restrictive requirement of being exactly calibrated as in (2.3) is

dropped off and replaced by the requirement of being only approximately calibrated. Then, the deviation between $\sum_{k\in s} w_k \mathbf{x}_k$ and $\sum_{k\in U} \mathbf{x}_k$ is controlled by means of a penalty. Bardsley and Chambers (1984), in a model-based setting, and Chambers (1996), Rao and Singh (1997) in a design-based setting, suggested finding weights satisfying (2.2), subject to a quadratic constraint, as $w^{\text{pen}}(\lambda) = \arg\min_w \Phi_s(w) + \lambda^{-1} \left(\hat{t}_{\mathbf{x}w} - t_{\mathbf{x}}\right)^T \mathbf{C} \left(\hat{t}_{\mathbf{x}w} - t_{\mathbf{x}}\right)$, where $\hat{t}_{\mathbf{x}w} = \sum_{k\in s} w_k \mathbf{x}_k$, $\mathbf{C} = \text{diag}(c_j)_{j=1}^p$, and $c_j \geq 0$ is a user-specified cost associated with the jth calibration constraint. The tuning parameter $\lambda > 0$ controls the trade off between exact calibration ($\lambda \to 0$) and no calibration ($\lambda \to \infty$). With the chi-square distance, the solution is, for $k \in s$,

$$w_k^{\text{pen}}(\lambda) = d_k - d_k \mathbf{x}_k^T \left(\sum_{\ell \in s} d_\ell \mathbf{x}_\ell \mathbf{x}_\ell^T + \lambda \mathbf{C}^{-1} \right)^{-1} \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right),$$

and the penalized calibration estimator is a GREG type estimator, whose regression coefficient is estimated by a ridge-type estimator. For an infinite cost c_j, the jth calibration constraint is satisfied exactly (see Beaumont and Bocci, 2008). As noted in Bardsley and Chambers (1984), the risk of having negative weights (in the case of the chi-square distance) is greatly reduced by using penalized calibration. With an empirical likelihood approach, Chen *et al.* (2002) suggested to replace the true totals $t_{\mathbf{x}}$ with $t_{\mathbf{x}} + \Delta(\hat{t}_{\mathbf{x}w} - t_{\mathbf{x}})$ where Δ is a diagonal matrix depending on the costs c_j and a tuning parameter controlling the deviation between $\hat{t}_{\mathbf{x}w}$ and $\hat{t}_{\mathbf{x}}$.

3. Calibration on Principal Components

We consider in this work another class of approximately calibrated estimators which are based on dimension reduction through principal components analysis (PCA). In multivariate statistics, PCA is one of the most popular techniques for reducing the dimension of a set of quantitative variables (see *e.g.* Jolliffe, 2002) by extracting most of the variability of the data by projection on a low dimension space. Principal components analysis consists in transforming the initial data set into a new set of a few uncorrelated synthetic variables, called principal components (PC), which are linear combinations of the initial variables with the largest variance. The principal components are "naturally" ordered, with respect to their contribution to the total variance of the data, and the reduction of the dimension is then realized by taking only the first few of PCs. PCA

is particularly useful when the correlation among the variables in the dataset is strong. These new variables can be also used as auxiliary information for calibration as noted in Goga *et al.* (2011).

Complete Auxiliary Information

We suppose without loss of generality that the auxiliary variables are centered, namely $N^{-1}t_{\mathbf{x}} = 0$ and to avoid heavy notations we do not include an intercept term in the model. Note that in applications this intercept term should be included. We suppose now that the auxiliary information is complete, that is to say the p-dimensional vector $\mathbf{x}_k$ is known for all the units $k \in U$.

Let $\mathbf{X}$ be the $N \times p$ data matrix having $\mathbf{x}_k^T, k \in U$ as rows. The variance-covariance matrix of the original variables $\mathcal{X}_1, \ldots, \mathcal{X}_p$ is given by $N^{-1}\mathbf{X}^T\mathbf{X}$. Let $\lambda_1 \geq \ldots \geq \lambda_p \geq 0$ be the eigenvalues of $N^{-1}\mathbf{X}^T\mathbf{X}$ associated to the corresponding orthonormal eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_p$,

$$\frac{1}{N}\mathbf{X}^T\mathbf{X}\mathbf{v}_j = \lambda_j \mathbf{v}_j, \quad j = 1, \ldots, p. \tag{3.1}$$

For $j = 1, \ldots, p$, the jth principal component, denoted by $\mathbf{Z}_j$, is defined as follows

$$\mathbf{Z}_j = \mathbf{X}\mathbf{v}_j = (z_{kj})_{k \in U}. \tag{3.2}$$

Each variable $\mathbf{Z}_j$ has a (population) variance equal to $N^{-1}\sum_{k \in U} z_{kj}^2 = \lambda_j$. We only consider the first r (with $r < p$) principal components, $\mathbf{Z}_1, \ldots, \mathbf{Z}_r$, which correspond to the r largest eigenvalues. In a survey sampling framework, the goal is not to give interpretations of these new variables $\mathbf{Z}_1, \ldots, \mathbf{Z}_r$ as it is the custom in PCA. These variables serve as a tool to obtain calibration weights which are more stable than the calibration weights that would have been obtained with the whole set of auxiliary variables.

More exactly, we want to find the principal component (PC) calibration estimator $\hat{t}_{yw}^{\mathrm{pc}}(r) = \sum_{k \in s} w_k^{\mathrm{pc}}(r) y_k$, where the vector of PC calibration weights $w_k^{\mathrm{pc}}(r), k \in s$, which depends on the number r of principal components used for calibration, is the solution of the optimization problem (2.2) and subject to $\sum_{k \in s} w_k^{\mathrm{pc}}(r)\mathbf{z}_{kr} = \sum_{k \in U} \mathbf{z}_{kr}$, where $\mathbf{z}_{kr}^T = (z_{k1}, \ldots, z_{kr})$ is the vector containing the values of the first r PCs computed for the k-th individual. The PC calibration weights $w_k^{\mathrm{pc}}(r)$'s are given by $w_k^{\mathrm{pc}}(r) = d_k - d_k \mathbf{z}_{kr}^T \left(\sum_{\ell \in s} d_\ell \mathbf{z}_{\ell r}\mathbf{z}_{\ell r}^T\right)^{-1} (\hat{t}_{\mathbf{z}_r d} - t_{\mathbf{z}_r}), k \in s$ where $\hat{t}_{\mathbf{z}_r d} = \sum_{k \in s} d_k \mathbf{z}_{kr}$ is the HT estimator of the total $t_{\mathbf{z}_r} = (0, \ldots, 0)$ since we have supposed that the original variables have mean zero.

The total t_y is again estimated by a GREG-type estimator which uses $\mathbf{Z}_1, \ldots, \mathbf{Z}_r$

as auxiliary variables

$$\hat{t}_{yw}^{\mathrm{pc}}(r) = \sum_{k\in s} w_k^{\mathrm{pc}}(r) y_k = \hat{t}_{yd} - \left(\hat{t}_{\mathbf{z}_r d} - t_{\mathbf{z}_r}\right)^T \hat{\boldsymbol{\gamma}}_{\mathbf{z}}(r), \tag{3.3}$$

where

$$\hat{\boldsymbol{\gamma}}_{\mathbf{z}}(r) = \left(\sum_{k\in s} d_k \mathbf{z}_{kr}\mathbf{z}_{kr}^T\right)^{-1} \sum_{k\in s} d_k \mathbf{z}_{kr} y_k. \tag{3.4}$$

The PC calibration estimator $\hat{t}_{yw}^{\mathrm{pc}}(r)$ depends on the number r of PC variables and it can be noted that if $r = 0$, that is to say if we do not take auxiliary information into account, then $\hat{t}_{yw}^{\mathrm{pc}}(0)$ is simply the HT estimator (or the Hájek estimator if the intercept term is included in the model) whereas if $r = p$, we get the calibration estimator which takes account of all the auxiliary variables.

A Model-Assisted Point of View

Consider again the superpopulation model ξ presented in (2.5) and denote by $\mathbf{G} = (\mathbf{v}_1, \ldots, \mathbf{v}_p)$ the matrix whose jth column is the jth eigenvector $\mathbf{v}_j$. Model ξ may be written in the equivalent form

$$\xi : \quad y_k = \mathbf{z}_k^T \boldsymbol{\gamma} + \varepsilon_k,$$

where $\boldsymbol{\gamma} = \mathbf{G}^T\boldsymbol{\beta}$ and $\mathbf{z}_k^T = (z_{k1}, \ldots, z_{kp})$ where z_{kj} is the value of $\mathbf{Z}_j$ for the kth unit. Principal components regression consists in considering a reduced linear regression model, denoted by ξ_r, which uses as predictors the first r principal components, $\mathbf{Z}_1, \ldots, \mathbf{Z}_r$, as follows

$$\xi_r : \quad y_k = \mathbf{z}_{kr}^T \boldsymbol{\gamma}(r) + \varepsilon_{kr}, \tag{3.5}$$

where $\boldsymbol{\gamma}(r)$ is a vector of r elements composed of the first r elements of $\boldsymbol{\gamma}$ and ε_{kr} is the appropriate error term of mean zero. The least squares estimation, at the population level, of $\boldsymbol{\gamma}(r)$, is

$$\tilde{\boldsymbol{\gamma}}_{\mathbf{z}}(r) = \left(\sum_{k\in U} \mathbf{z}_{kr}\mathbf{z}_{kr}^T\right)^{-1} \sum_{k\in U} \mathbf{z}_{kr} y_k, \tag{3.6}$$

which in turn can be estimated, on a sample s, by the design-based estimator $\hat{\boldsymbol{\gamma}}_{\mathbf{z}}(r)$ given by (3.4). We can see now that the PC calibration estimator given in (3.3) is in fact equal to a GREG-type estimator assisted by the reduced model ξ_r described in (3.5). Note also that since the principal components are centered

and uncorrelated, the matrix $\left(\sum_{k\in U}\mathbf{z}_{kr}\mathbf{z}_{kr}^T\right)$ is diagonal, with diagonal elements $(\lambda_1 N,\ldots,\lambda_r N)$.

When there is a strong multicollinearity among the auxiliary variables, it is well known that the ordinary least squares estimator of $\boldsymbol{\beta}$, is very sensitive to small changes in $\mathbf{x}_k$ and y_k and it has a very large variance (see *e.g* Hoerl and Kennard, 1970). To see better how small eigenvalues may affect $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}$, Gunst and Mason (1977) write the least squares estimator as follows: $\tilde{\boldsymbol{\beta}}_{\mathbf{x}} = \left(N^{-1}\sum_{k\in U}\mathbf{x}_k\mathbf{x}_k^T\right)^{-1}\left(N^{-1}\sum_{k\in U}\mathbf{x}_k y_k\right) = \sum_{j=1}^{p}\frac{1}{\lambda_j}\left[\mathbf{v}_j^T\left(N^{-1}\sum_{k\in U}\mathbf{x}_k y_k\right)\right]\mathbf{v}_j$. Approximating the covariance matrix $N^{-1}\sum_{k\in U}\mathbf{x}_k\mathbf{x}_k^T = N^{-1}\mathbf{X}^T\mathbf{X}$ by the rank r matrix $\left(\sum_{j=1}^{r}\lambda_j\mathbf{v}_j\mathbf{v}_j^T\right)$ leads to consider the following approximation to the regression estimator that is based on the first r principal components,

$$\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r) = \sum_{j=1}^{r}\frac{1}{\lambda_j}\left[\mathbf{v}_j^T\left(\frac{1}{N}\sum_{k\in U}\mathbf{x}_k y_k\right)\right]\mathbf{v}_j. \tag{3.7}$$

This means that $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)$ is obtained by subtracting from $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}$ the part of the data that belongs to the $p-r$ dimensional space with the smallest variance and by performing the regression in the r dimensional space that contains most of the variability of the data. Note that ridge-regression (Hoerl and Kennard, 1970), which is an alternative way of dealing with the multicollinearity issue, consists in adding a positive term λ to all eigenvalues $\lambda_j, j=1,\ldots,p$. More exactly, the ridge estimator of $\boldsymbol{\beta}$ may be written as $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}(\lambda) = (N^{-1}\sum_{k\in U}\mathbf{x}_k\mathbf{x}_k^T + \lambda\mathbf{I}_p)^{-1}\left(N^{-1}\sum_{k\in U}\mathbf{x}_k y_k\right) = \sum_{j=1}^{p}\frac{1}{\lambda+\lambda_j}\left[\mathbf{v}_j^T\left(N^{-1}\sum_{k\in U}\mathbf{x}_k y_k\right)\right]\mathbf{v}_j$, where $\mathbf{I}_p$ is the p-dimensional identity matrix. Both the ridge regression estimator $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}(\lambda)$ and the principal components estimator $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)$ are biased for $\boldsymbol{\beta}$ under the model ξ (Gunst and Mason, 1977).

The PC regression estimator $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)$ can be estimated under the sampling design by

$$\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r) = \mathbf{G}_r\hat{\boldsymbol{\gamma}}_{\mathbf{z}}(r), \tag{3.8}$$

where $\hat{\boldsymbol{\gamma}}_{\mathbf{z}}(r)$ is given in (3.4) and $\mathbf{G}_r$ is the $p\times r$ matrix whose jth column is equal to $\mathbf{v}_j$. Using relation (3.8) and the fact that $\mathbf{Z}_j = \mathbf{X}\mathbf{v}_j$, we obtain that $\left(\hat{t}_{\mathbf{z}_r d} - t_{\mathbf{z}_r}\right)^T\hat{\boldsymbol{\gamma}}_{\mathbf{z}}(r) = \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right)^T\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)$. Consequently $\hat{t}_{yw}^{\mathrm{pc}}(r)$ can also be written as follows, $\hat{t}_{yw}^{\mathrm{pc}}(r) = \hat{t}_{yd} - \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right)^T\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)$, and $\hat{t}_{yw}^{\mathrm{pc}}(r)$ may be seen as a GREG-type estimator assisted by the model ξ when $\boldsymbol{\beta}$ is estimated by $\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)$.

Calibration on the second moment of the PC variables

With complete auxiliary information, Särndal (2007) stated that "we are invited to consider $x_{kj}^2, j = 1, \ldots, p$ and other functions of x_{kj}^2 for inclusion in $\mathbf{x}_k$" especially when "the relationship to the study variable is curved". In our case, the PC variables $\mathbf{Z}_j$ satisfy $N^{-1}\mathbf{Z}_j^T\mathbf{Z}_j = N^{-1}\sum_{k\in U} z_{kj}^2 = \lambda_j, \quad \text{for all} \quad j = 1, \ldots, p.$ This means that in presence of complete auxiliary information, the totals of squares of the PCs are known. As a consequence, if we keep the first r variables $\mathbf{Z}_1, \ldots, \mathbf{Z}_r$ corresponding to the largest r eigenvalues, we can consider r additional calibration constraints on the second moment of these PCs. We look for the calibration weights $w^{\text{pc}}(r)$ solution to (2.2) and subject to $\sum_{k\in s} w_k^{\text{pc}}(r) \left(\mathbf{z}_{kr}, \mathbf{z}_{kr}^2\right)^T = \sum_{k\in U} \left(\mathbf{z}_{kr}, \mathbf{z}_{kr}^2\right)^T$ where $\mathbf{z}_{kr}^2 = (z_{k1}^2, \ldots, z_{kr}^2)$.

The estimator derived in this way is expected to perform better than the estimator calibrated only on the first moment of the principal components. Nevertheless, calibration on the second moment of the PCs requires r additional calibration constraints.

4. Calibration on Estimated Principal Components

The approach presented in the above Sections supposes that the values of the auxiliary variables $\mathcal{X}_j$, for $j = 1, \ldots, p$ are known for all units k in the population U. In practice, it often happens that the variables $\mathcal{X}_j$ are only known for the sampled individuals, but their population totals are known. Then, it is not possible anymore to compute the eigenvalues and the eigenvectors of the population variance-covariance matrix. We present in this section a way to perform principal components calibration when the auxiliary variables are only observed for the units belonging to the sample.

Let $\mathbf{\Gamma} = N^{-1}\mathbf{X}^T\mathbf{X}$ be the variance-covariance matrix estimated by

$$\hat{\mathbf{\Gamma}} = \frac{1}{\hat{N}} \sum_{k\in s} d_k (\mathbf{x}_k - \hat{\overline{\mathbf{X}}})(\mathbf{x}_k - \hat{\overline{\mathbf{X}}})^T = \frac{1}{\hat{N}} \sum_{k\in s} d_k \mathbf{x}_k \mathbf{x}_k^T - \hat{\overline{\mathbf{X}}}\hat{\overline{\mathbf{X}}}^T, \tag{4.1}$$

where $\hat{N} = \sum_{k\in s} d_k$ and $\hat{\overline{\mathbf{X}}} = \hat{N}^{-1}\sum_{k\in s} d_k \mathbf{x}_k$. Let $\hat{\lambda}_1 \geq \ldots \geq \hat{\lambda}_p \geq 0$ be the sorted eigenvalues of $\hat{\mathbf{\Gamma}}$ and $\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_p$ the corresponding orthonormal eigenvectors,

$$\hat{\mathbf{\Gamma}}\hat{\mathbf{v}}_j = \hat{\lambda}_j \hat{\mathbf{v}}_j, \quad j = 1, \ldots, p. \tag{4.2}$$

We have that $\hat{\lambda}_j$ and $\hat{\mathbf{v}}_j$ are the design-based estimators of λ_j and respectively, $\mathbf{v}_j$ for $j = 1, \ldots, p$. It is shown in Cardot *et al.* (2010) that with large samples and

under classical assumptions on the first and second order inclusion probabilities π_k, π_{kl} as well as on the variables $\mathcal{X}_j$, (see the assumptions (A1)-(A6) in Section 5), that the estimators $\hat{\lambda}_j$ and $\hat{\mathbf{v}}_j$ are asymptotically design unbiased and consistent for λ_j and respectively, for $\mathbf{v}_j$.

The unknown population principal components $\mathbf{Z}_j$ defined in (3.2) can be approximated as follows, $\hat{\mathbf{Z}}_j = \mathbf{X}\hat{\mathbf{v}}_j$, reminding that $\hat{\mathbf{Z}}_j = (\hat{z}_{kj})_{k\in U}$ is only known for the units in the sample. Nevertheless, its population total $t_{\hat{\mathbf{Z}}_j} = \sum_{k\in U} \hat{z}_{kj}$ is known and is equal to zero since $t_{\hat{\mathbf{Z}}_j} = t_{\mathbf{x}}^T \hat{\mathbf{v}}_j = 0, \quad j = 1, \ldots, p$. Note also that $\hat{\mathbf{Z}}_j$ are not exactly the principal components associated with the variance-covariance matrix $\hat{\mathbf{\Gamma}}$ because the original variables are centered in the population but not necessarily in the sample.

Consider now the first r estimated principal components $\hat{\mathbf{Z}}_1, \ldots, \hat{\mathbf{Z}}_r$, corresponding to the r largest eigenvalues $\hat{\lambda}_1 \geq \ldots \geq \hat{\lambda}_r \geq 0$ and suppose that $\hat{\lambda}_r > 0$. The estimated principal component (EPC) calibration estimator of t_y is $\hat{t}_{yw}^{\text{epc}}(r) = \sum_{k\in s} w_k^{\text{epc}}(r) y_k$, where the EPC calibration weights $w_k^{\text{epc}}, k \in s$ are the solution of the optimization problem (2.2) subject to the constraints $\sum_{k\in s} w_k^{\text{epc}}(r)\hat{\mathbf{z}}_{kr} = \sum_{k\in U} \hat{\mathbf{z}}_{kr}$, where $\hat{\mathbf{z}}_{kr}^T = (\hat{z}_{k1}, \ldots, \hat{z}_{kr})$ is the vector of values of $\hat{\mathbf{Z}}_j$, $j = 1, \ldots, r$ recorded for the kth unit. With the chi-square distance function Φ_s, the EPC calibration weights $w_k^{\text{epc}}(r)$ are given by

$$w_k^{\text{epc}}(r) = d_k - d_k \hat{\mathbf{z}}_{kr}^T \left(\sum_{\ell\in s} d_\ell \hat{\mathbf{z}}_{\ell r} \hat{\mathbf{z}}_{\ell r}^T \right)^{-1} (\hat{t}_{\hat{\mathbf{z}}_r d} - t_{\hat{\mathbf{z}}_r}), \tag{4.3}$$

where $\hat{t}_{\hat{\mathbf{z}}_r d} = \sum_{k\in s} d_k \hat{\mathbf{z}}_{kr}$ is the HT estimator of the total $t_{\hat{\mathbf{z}}_r} = \sum_{k\in U} \hat{\mathbf{z}}_{kr} = 0$. The EPC calibration estimator for t_y is given by $\hat{t}_{yw}^{\text{epc}}(r) = \sum_{k\in U} w_k^{\text{epc}}(r) y_k = \hat{t}_{yd} - \left(\hat{t}_{\hat{\mathbf{z}}_\mathbf{r} d} - t_{\hat{\mathbf{z}}_\mathbf{r}}\right)^T \hat{\boldsymbol{\gamma}}_{\hat{\mathbf{z}}}(r)$, where $\hat{\boldsymbol{\gamma}}_{\hat{\mathbf{z}}}(r) = \left(\sum_{k\in s} d_k \hat{\mathbf{z}}_{kr} \hat{\mathbf{z}}_{kr}^T\right)^{-1} \sum_{k\in s} d_k \hat{\mathbf{z}}_{kr} y_k$. The EPC calibration estimator may also be written with respect to the population totals of the original variables, $\mathcal{X}_1, \ldots, \mathcal{X}_p$, as follows $\hat{t}_{yw}^{\text{epc}}(r) = \hat{t}_{yd} - \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right)^T \hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\text{epc}}(r)$, where $\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\text{epc}}(r) = \widehat{\mathbf{G}}_r \hat{\boldsymbol{\gamma}}_{\hat{\mathbf{z}}}(r)$ and $\widehat{\mathbf{G}}_r$ is the $p \times r$ matrix whose jth column is equal to $\widehat{\mathbf{v}}_j$.

5. Some Asymptotic Properties of the Principal Components Calibration Estimators

We adopt in this section the asymptotic framework of Isaki and Fuller (1982). We consider a sequence of growing and nested populations U_N with size N tend-

ing to infinity and a sequence of samples s_N of size n_N drawn from U_N according to the fixed-size sampling designs $p_N(s_N)$. The sequence of subpopulations is an increasing nested one, whereas the sample sequence is not. For simplicity of notation, we drop the subscript N in the following when there is no ambiguity. The number p_N of auxiliary variables as well as the number r_N of principal components are allowed to tend to infinity. We suppose that the following assumptions hold.

(A1) $\lim_{N\to\infty} \frac{n}{N} = \pi \in (0,1)$.

(A2) $\pi_k > \delta > 0$ for all $k \in U_N$; $\overline{\lim}_{N\to\infty} n \max_{k\neq l} |\pi_{kl} - \pi_k\pi_l| < \infty$.

(A3) There is a constant C_y such that for all N, $\frac{1}{N}\sum_{U_N} y_k^4 < C_y$.

(A4) The largest eigenvalue λ_{1N} of $\mathbf{\Gamma}_N$ is bounded, $\lambda_{1N} \leq C_\lambda$.

(A5) There is a contant $c > 0$ and a non decreasing sequence of integers (r_N) such that for all $N \geq N_0$ we have $\lambda_{r_N} \geq c$.

(A6) There is a constant C_4 such that, $\forall \mathbf{v} \in \mathbb{R}^{p_N}$ satisfying $\|\mathbf{v}\| = 1$, we have $N^{-1}\sum_{k\in U_N} |\langle \mathbf{x}_k, \mathbf{v}\rangle|^4 \leq C_4$.

Conditions (A1), (A2) and (A3) are classical hypotheses for asymptotics in survey sampling. Condition (A4) is closely related to a moment condition on $\mathbf{x}_k$, for $k \in U_N$. If (A4) is fulfilled, $\frac{1}{N}\sum_{k\in U_N} \|\mathbf{x}_k\|^2 = \sum_{j=1}^{p_N} \lambda_{jN} \leq C_\lambda p_N$. Assumption (A5) ensures that there is no identifiability issue for the sequence $\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r_N)$ of regression coefficients defined at the population level. It only deals with λ_{r_N} and does not prevent λ_{p_N} from being equal to zero or from being very small. The finite population moment assumptions (A4) and (A6) indicate that the vectors $\mathbf{x}_k$ cannot be too concentrated in one direction (see Vershynin (2012) for examples in a classical statistical inference context). The proofs of Proposition 1 and Proposition 2 are given in a Supplementary file.

We first show that the estimator based on the true principal components is consistent and we give its asymptotic variance. Note that the assumption on the eigenvalues $\lambda_r > \lambda_{r+1} \geq 0$ ensures that there is no identifiability problem of the eigenspace generated by the eigenvectors associated to the r largest eigenvalues. The condition $r_N^3/n \to 0$ prevents the number of principal components from being too large and ensures that the remainder term, whose order is $r_N^{3/2}/n$, tends to zero and is negligible compared to the main term whose order is $1/\sqrt{n}$.

Proposition 1. *Assume that (A1)-(A6) hold and that* $\lambda_r > \lambda_{r+1} \geq 0$. *If* $r_N^3/n \to 0$ *when* N *goes to infinity, then*

$$N^{-1}(\hat{t}_{yw}^{\mathrm{pc}}(r_N) - t_y) = N^{-1}\left(\tilde{t}_{y,\mathbf{x}}^{\mathrm{diff}}(r_N) - t_y\right) + O_p\left(\frac{r_N^{3/2}}{n}\right)$$

and $\tilde{t}_{y,\mathbf{x}}^{\mathrm{diff}}(r_N) = \hat{t}_{yd} - \left(\hat{t}_{\mathbf{x}d} - t_{\mathbf{x}}\right)^T \tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r_N)$ *satisfies* $N^{-1}\left(\tilde{t}_{y,\mathbf{x}}^{\mathrm{diff}}(r_N) - t_y\right) = O_p\left(\frac{1}{\sqrt{n}}\right)$.

The condition $r_N^3/n \to 0$ could certainly be relaxed for particular sampling designs with high entropy under additional moment assumptions. Note also that the asymptotic variance of $\hat{t}_{yw}^{\mathrm{pc}}(r)$ is given by $AV(\hat{t}_{yw}^{\mathrm{pc}}(r)) = \sum_{k\in U}\sum_{l\in U}(\pi_{kl} - \pi_k\pi_l)\left(y_k - \mathbf{x}_k^T\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)\right)\left(y_l - \mathbf{x}_l^T\tilde{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)\right)$.

Before stating a consistency result for calibration on estimated principal components, let us introduce an additional condition on the spacing between adjacent eigenvalues.

(A7) There is a constant $c_\lambda > 0$ such that $\min_{j=1,\ldots,r_N+1}(\lambda_{jN} - \lambda_{j+1,N}) \geq c_\lambda r_N$.

This assumption ensures that the r_N largest eigenvalues are nearly equidistributed in $[c, C_\lambda]$.

Proposition 2. *Assume that (A1)-(A7) hold. If* $p_N^3 r_N^3/n \to 0$ *when* N *goes to infinity, then*

$$N^{-1}(\hat{t}_{yw}^{\mathrm{epc}}(r_N) - t_y) = N^{-1}\left(\tilde{t}_{y,\mathbf{x}}^{\mathrm{diff}}(r_N) - t_y\right) + O_p\left(\frac{p_N^{3/2} r_N^{3/2}}{n}\right)$$

A more restrictive condition on how r_N may go to infinity is imposed when the principal components are estimated. The condition $p_N^3 r_N^3/n \to 0$ ensures that the remainder term of order $p_N^{3/2} r_N^{3/2}/n$ is negligible compared to $1/\sqrt{n}$. If p_N is bounded, one gets back to classical $\sqrt{n}$-rates of convergence whether the population principal components are known or not.

If all the second-order inclusion probabilities $\pi_{k\ell}$ are strictly positive, the asymptotic variance of $\hat{t}_{yw}^{\mathrm{pc}}(r)$ can be estimated by the Horvitz-Thompson variance estimator for the residuals $y_k - \mathbf{x}_k^T\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r), k \in s$,

$$\widehat{Var}(\hat{t}_{yw}^{\mathrm{pc}}(r)) = \sum_{k\in s}\sum_{\ell\in s}\frac{\pi_{k\ell} - \pi_k\pi_\ell}{\pi_{k\ell}} d_k d_\ell \left(y_k - \mathbf{x}_k^T\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)\right)\left(y_\ell - \mathbf{x}_\ell^T\hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\mathrm{pc}}(r)\right),$$

while the asymptotic variance of $\hat{t}_{yw}^{\mathrm{epc}}(r)$ can be estimated by the Horvitz-Thompson

variance estimator for the residuals $y_k - \mathbf{x}_k^T \hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\text{epc}}(r), k \in s$:

$$\widehat{Var}(\hat{t}_{yw}^{\text{epc}}(r)) = \sum_{k\in s}\sum_{\ell\in s} \frac{\pi_{kl} - \pi_k\pi_l}{\pi_{kl}} d_k d_\ell (y_k - \mathbf{x}_k^T \hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\text{epc}}(r))(y_\ell - \mathbf{x}_\ell^T \hat{\boldsymbol{\beta}}_{\mathbf{x}}^{\text{epc}}(r)).$$

6. Partial Calibration on Principal Components

The calibration estimators derived before are not designed to give the exact finite population totals of the original variables $\mathcal{X}_j$, $j = 1, \ldots, p$. In practice, it is often desired to have this property satisfied for a few but important socio-demographical variables such as sex, age or socio-professional category.

We can adapt the method presented in the previous section in order to fulfill this requirement. We split the auxiliary matrix $\mathbf{X}$ into two blocks: a first block $\tilde{\mathbf{X}}_1$ containing the p_1 most important variables with p_1 small compared to p, and a second block $\tilde{\mathbf{X}}_2$ containing the remaining $p_2 = p - p_1$ variables. We have $\mathbf{X} = (\tilde{\mathbf{X}}_1, \tilde{\mathbf{X}}_2)$. Note that the constant term will generally belong to the first block of variables.

The goal is to get calibration weights such that the totals of the p_1 auxiliary variables in $\tilde{\mathbf{X}}_1$ are estimated exactly while the totals of the p_2 remaining variables are estimated only approximately. The idea is to calibrate directly on the auxiliary variables from $\tilde{\mathbf{X}}_1$ and on the first principal components of $\tilde{\mathbf{X}}_2$, after having taken into account the fact that the variables in $\tilde{\mathbf{X}}_1$ and all their linear combinations are perfectly estimated. For that, we introduce the matrix $\mathbf{I}_N$ which is the N-dimensional identity matrix and $\mathbf{P}_{\tilde{\mathbf{X}}_1} = \tilde{\mathbf{X}}_1(\tilde{\mathbf{X}}_1^T\tilde{\mathbf{X}}_1)^{-1}\tilde{\mathbf{X}}_1^T$ the orthogonal projection onto the vector space spanned by the column vectors of matrix $\tilde{\mathbf{X}}_1$. We also define the matrix $\mathbf{A} = \left(\mathbf{I}_N - \mathbf{P}_{\tilde{\mathbf{X}}_1}\right)\tilde{\mathbf{X}}_2$, which is the projection of $\tilde{\mathbf{X}}_2$ onto the orthogonal space spanned by the column vectors of $\tilde{\mathbf{X}}_1$. Matrix $\mathbf{A}$ represents the residual part of $\tilde{\mathbf{X}}_2$ that is not "calibrated" when considering an estimator of the total of $\mathcal{Y}$ calibrated on the variables in $\tilde{\mathbf{X}}_1$. We define the residual covariance matrix $N^{-1}\mathbf{A}^T\mathbf{A} = N^{-1}\tilde{\mathbf{X}}_2^T\left(\mathbf{I}_N - \mathbf{P}_{\tilde{\mathbf{X}}_1}\right)\tilde{\mathbf{X}}_2$ and denote by $\tilde{\lambda}_1 \geq \ldots \tilde{\lambda}_{p_2}$ its eigenvalues and by $\tilde{\mathbf{v}}_1, \ldots, \tilde{\mathbf{v}}_{p_2}$ the corresponding orthonormal eigenvectors. Consider now, $\tilde{\mathbf{Z}}_j = \mathbf{A}\tilde{\mathbf{v}}_j$, for $j = 1, \ldots, p_2$, the principal components of $\mathbf{A}$. The calibration variables are $(\tilde{\mathbf{X}}_1, \tilde{\mathbf{Z}}_1, \ldots, \tilde{\mathbf{Z}}_r)$ of zero totals and the partial principal component (PPC) calibration estimator of t_y is $\hat{t}_{yw}^{\text{ppc}}(r) = \sum_{k\in s} w_k^{\text{ppc}}(r) y_k$, where the PPC calibration weights $w_k^{\text{ppc}}(r)$, for $k \in s$, are the solution of the optimization problem (2.2) subject to $\sum_{k\in s} w_k^{\text{ppc}}(r) \left(\tilde{\mathbf{x}}_k, \tilde{\mathbf{z}}_{kr}\right)^T = \sum_{k\in U} \left(\tilde{\mathbf{x}}_k, \tilde{\mathbf{z}}_{kr}\right)^T$, where $\tilde{\mathbf{x}}_k = (\tilde{x}_{k1}, \ldots, \tilde{x}_{kp_1})$ is the vector of the values of the variables in $\tilde{\mathbf{X}}_1$ and

$\mathbf{z}_{kr}^T = (\tilde{z}_{k1}, \ldots, \tilde{z}_{kr})$ is the vector whose elements are the partial principal components $\tilde{\mathbf{Z}}_1, \ldots, \tilde{\mathbf{Z}}_r$ for unit k. Note that with a different point of view, Breidt and Chauvet (2012) use, at the sampling stage, similar ideas in order to perform penalized balanced sampling.

Suppose now that we only have a sample s at hand and we know the totals of all the calibration variables. We denote by $\tilde{\mathbf{X}}_{s,1}$ (resp. $\tilde{\mathbf{X}}_{s,2}$) the $n \times p_1$ (resp. $n \times p_2$) matrix containing the observed values of the auxiliary variables. We can estimate the matrix $\mathbf{A}$ by $\hat{\mathbf{A}} = \left(\mathbf{I}_n - \hat{\mathbf{P}}_{\tilde{\mathbf{X}}_{s,1}}\right) \tilde{\mathbf{X}}_{s,2}$ where $\hat{\mathbf{P}}_{\tilde{\mathbf{X}}_{s,1}} = \tilde{\mathbf{X}}_{s,1} \left(\tilde{\mathbf{X}}_{s,1}^T \mathbf{D}_s \tilde{\mathbf{X}}_{s,1}\right)^{-1} \tilde{\mathbf{X}}_{s,1}^T \mathbf{D}_s$, is the estimation of the projection onto the space generated by the columns of $\tilde{\mathbf{X}}_1$ and $\mathbf{D}_s$ is the $n \times n$ diagonal matrix, with diagonal elements $d_k,\ k \in s$. Then, we can perform the principal components analysis of the projected sampled data corresponding to the variables belonging to the second group and compute the estimated principal components associated to the r largest eigenvalues as in Section 4. At last, the total estimator is calibrated on the totals of the variables in $\mathbf{X}_1$ and the first r estimated principal components.

7. Application to the estimation of the total electricity consumption

Description of the data

The interest of using principal components calibration is illustrated on data from the Irish Commission for Energy Regulation (CER) Smart Metering Project that was conducted in 2009-2010 (CER, 2011). In this project, which focuses on energy consumption and energy regulation, about 6000 smart meters have been installed in order to collect every half an hour, over a period of about two years, the electricity consumption of Irish residential and business customers.

We evaluate the interest of employing reduction dimension techniques based on PCA by considering a period of 14 consecutive days and a population of $N = 6291$ smart meters (households and companies). Thus, we have for each unit k in the population $(2 \times 7) \times 48 = 672$ measurement instants and we denote by $y_k(t_j), j = 1, \ldots 672$ the data corresponding to unit k where $y_k(t_j)$ is the electricity consumption (in kW) associated to smart meter k at instant t_j. We consider here a multipurpose setting and our aim is to estimate the mean electricity consumption of each day of the second week. For each day ℓ of the week, with $\ell \in \{1, \ldots, 7\}$, the outcome variable is $y_{k\ell} = \sum_{j=336+(\ell-1)\times 48}^{336+\ell\times 48} y_k(t_j)$ and our

The data are available on request at the address: `http://www.ucd.ie/issda/data/commissionforenergyregulation/`

target is the corresponding population total, $t_\ell = \sum_{k \in U} y_{k\ell}$.

The auxiliary information is the load electricity curve of the first week. This means that we have $p = 336$ auxiliary variables, which are the consumption electricity levels at each of the $p = 336$ half hours of the first week.

The condition number of the matrix $N^{-1}\mathbf{X}^T\mathbf{X}$, which is defined as the ratio λ_1/λ_{336}, is equal to 67055.78. This large value means that this matrix is ill-conditioned and there may exist strong correlations between some of the variables used for calibration. Indeed, the first principal component explains about 63% of the variance of the 336 original variables and about 83% of the total variability of the data is preserved by projection onto the subspace span by the first ten principal components.

Comparison of the estimators

To make comparisons, we draw $I = 1000$ samples of size $n = 600$ (the sampling fraction is about 0.095) according to a simple random sampling design without replacement and we estimate the total consumption t_ℓ over each day ℓ of the second week with the following estimators:

- Horvitz-Thompson estimators,
- Calibration estimators, denoted by $\hat{t}_{\ell w}$, that take account of all the $p = 336$ auxiliary variables plus the intercept term.
- Estimators calibrated on the principal components in the population (resp. in the sample) plus the constant term, denoted by $\hat{t}^{\mathrm{pc}}_{\ell w}(r)$ (resp. $\hat{t}^{\mathrm{epc}}_{\ell w}(r)$), for different values of the dimension r.

When performing principal components calibration, the dimension r plays the role of a tuning parameter. We also study the performances of an automatic and data-drive simple rule for selecting the dimension r which consists in selecting the largest dimension $\hat{r}$ such that all the calibrated principal component weights remain positive. Note that this selection strategy is the analogue of the strategy suggested in Bardsley and Chambers (1984) for choosing the tuning parameter in a ridge regression context.

The distribution of the coefficient of variation (CV) of the calibration weights for the I=1000 Monte Carlo experiments is presented in Figure 7.1 for different values of the dimension r. Recall that these weights do not depend on the variable of interest. It is clearly seen that those calibration weights have larger dispersion and are more and more heterogeneous as the number of principal components used

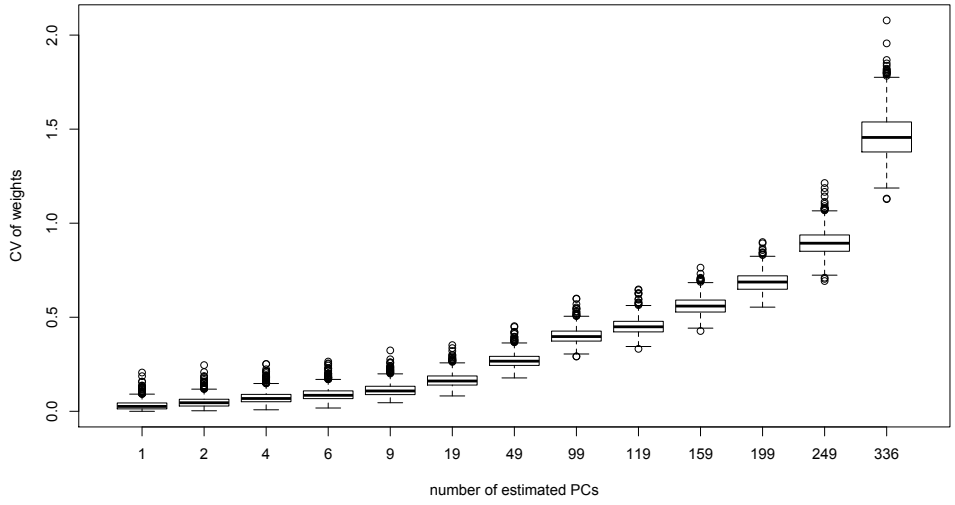

Figure 7.1: Distribution of the coefficient of variation (CV) of the sampling weights for different values of the dimension r. The sample size is $n = 600$.

for calibration increases. Calibrating with a large number of correlated auxiliary variables may lead to instable estimations and to a lack of robustness with respect to measurement errors or misspecification in the data bases, with for example the presence of strata jumpers. Note also that when all the auxiliary variables are used for calibration, around 25 % of the sampling weights take negatives values which is generally not desirable.

Our benchmarks are the estimators $\hat{t}_{\ell w}$ which are calibrated on all the $p = 336$ auxiliary variables. For each day ℓ, the performances of an estimator $\widehat{\theta}$ of the total t_ℓ are measured by considering the relative mean squared error,

$$R_\ell(\widehat{\theta}) = \frac{\sum_{i=1}^{I}(\widehat{\theta}^{(i)} - t_\ell)^2}{\sum_{i=1}^{I}(\hat{t}_{\ell w}^{(i)} - t_\ell)^2}. \tag{7.1}$$

Better estimators will correspond to small values of criterion $R_\ell(\widehat{\theta})$.

The values of this relative error for several values of r, as well as for the estimators obtained with the data driven dimension selection are given in Table 7.1. This relative error has also been computed for the ridge-type estimators derived with the sampling weights w^{pen} given in Section 2 and a penalty $\hat{\lambda}$ chosen to be the smallest value of λ such that all the resulting weights remain positive.

Estimators		Days monday	tuesday	wednesday	thursday	friday	saturday	sunday
Horvitz-Thompson		14.4	13.9	11.8	10.8	12.5	6.4	5.4
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 1$	0.65	0.62	0.50	0.47	0.64	1.17	1.57
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 2$	0.64	0.62	0.50	0.47	0.57	0.80	0.63
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 5$	0.52	0.47	0.40	0.50	0.51	0.53	0.52
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 50$	0.50	0.50	0.43	0.44	0.54	0.48	0.48
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 100$	0.57	0.60	0.59	0.51	0.58	0.60	0.64
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 200$	0.60	0.64	0.58	0.66	0.69	0.68	0.63
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$r = 300$	0.82	0.85	0.83	0.86	0.84	0.85	0.87
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 1$	0.75	0.73	0.61	0.56	0.73	1.23	1.59
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 2$	0.66	0.64	0.53	0.50	0.61	0.85	0.74
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 5$	0.53	0.47	0.40	0.41	0.53	0.59	0.53
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 50$	0.45	0.46	0.40	0.41	0.48	0.46	0.47
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 100$	0.46	0.47	0.42	0.45	0.52	0.49	0.50
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 200$	0.57	0.55	0.51	0.58	0.62	0.60	0.57
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$r = 300$	0.78	0.80	0.77	0.84	0.80	0.81	0.83
$\hat{t}_{\ell w}^{\mathrm{pc}}$	$\hat{r}$, $w(\hat{r}) > 0$	0.51	0.49	0.41	0.41	0.52	0.55	0.50
$\hat{t}_{\ell w}^{\mathrm{epc}}$	$\hat{r}$, $w(\hat{r}) > 0$	0.49	0.48	0.41	0.40	0.50	0.53	0.49
Ridge Calibration	$\hat{\lambda}$	0.44	0.46	0.40	0.41	0.48	0.48	0.43

Table 7.1: Comparison of the mean relative mean squared errors of the different estimators, according to criterion (7.1).

We can first note that the naive Horvitz-Thompson estimator can be greatly improved, for all the days of the week, by considering an over-calibration estimator which takes account of all the (redundant) auxiliary information. Indeed, the mean square error of the HT estimator is between five times and fourteen times larger than the MSE of this reference estimator. We can also remark that reducing the number of effective auxiliary variables through principal components, estimated on the sample or deduced from the population, can still improve estimation compared to calibration on all the variables and permits to divide by two the MSE. Another remarkable feature is the stability of the principal components calibration techniques with respect to the choice of the dimension r. Indeed, in this application, choosing between 5 and 100 principal components permits to divide by two, for all the outcome variables, the MSE compared to the calibration estimator based on the whole auxiliary information.

We noted that the mean number of selected principal components with the data driven selection rule is equal to 17.3 for the population principal components

and 21.3 for the sample principal components, explaining in each case about 85% of the variance of the original variables. As expected, the variability of the number of selected components is slightly larger when considering calibration on the estimated principal components (interquartile range of 26 versus 17 for the population principal components).

As seen in Table 7.1, the performances of the resulting estimators are good and comparable to the estimators based on ridge calibration with a selection rule for λ based on the same principle. The advantage of the principal components is that it permits to divide by more than 15 the final number of effective variables used for calibration and it can directly be used in classical survey sampling softwares.

Note that complementary information on this application can be found in the Supplementary File.

8. Discussion and concluding remarks

A simple dimension reduction technique based on principal components calibration has been studied in this article. It provides an effective technique for approximate calibration, when the number of auxiliary variables is large, that can improve significantly the estimation compared to calibration on the whole set of initial auxiliary variables. Furthermore this simple technique can also be modified so that calibration can be exact for a set of a few important auxiliary variables. A very simple rule which consists in choosing the largest number of principal components such that all the resulting sampling weights remain positive allows the construction of estimators with very good performances in terms of MSE. Furthermore, in our case study, this automatic selection technique permits, in average, to divide by 15 the number of effective calibration variables and to reduce by a half the mean squared error of estimation compared to calibration over all the auxiliary variables.

Some asymptotic justifications of this dimension reduction technique are given with a number p_N of auxiliary variables as well as a number r_N of principal components used for calibration that are allowed to grow to infinity as the population size N increases. Nevertheless, our conditions on the asymptotic behavior of r_N appear to be rather restrictive and could probably be relaxed (see for example the results presented in Vershynin (2012) on the estimation of covariance matri-

ces for independent observations in an infinite population). However, this would require to have at hand exponential inequalities for Horvitz-Thompson estimators in order to control very accurately their deviations around their target.

Note finally that borrowing ideas from Marx and Smith (1990) and Wu and Sitter (2001), it would be not too difficult to extend the principal component calibration approach in order to deal with non linear model-calibration.

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