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Variance approximation under balanced sampling

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Abstract

A balanced sampling design has the interesting property that Horvitz–Thompson estimators of totals for a set of balancing variables are equal to the totals we want to estimate, therefore the variance of Horvitz–Thompson estimators of variables of interest are reduced in function of their correlations with the balancing variables. Since it is hard to derive an analytic expression for the joint inclusion probabilities, we derive a general approximation of variance based on a residual technique. This approximation is useful even in the particular case of unequal probability sampling with fixed sample size. Finally, a set of numerical studies with an original methodology allows to validate this approximation.

Keywords: Sampling design; Balanced sampling; Unequal probability sampling; Variance approximation; Variance estimation; Sampling theory; Sample surveys; Sample; Sampling unequal probability

1. Introduction

A sample is said to be balanced on a set of balancing variables if the estimated totals of these variables are equal to the population totals. Several partial solutions had been presented in Deville et al. (1988), Deville (1992), Ardilly (1991), Hedayat and Majumdar (1995), and Valliant et al. (2000). The cube method proposed by Deville and Tillé (2002) provides a general non-enumerative solution to select balanced samples, and has been used at the *Institut National de la Statistique et des Etudes*

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Économiques (INSEE, French Bureau of Statistics) for its most important statistical projects: the renovated continuous census and the master sample (on this topic see Dumais and Isnard, 2000; Wilms, 2000). The use of balanced sampling in several projects has dramatically improved efficiency, allowing the reduction of the variance from 20% to 90% comparatively to simple random sampling in some cases (see for instance Deville et al., 1988).

An important question is the derivation of the variance of total estimators under balanced sampling. In balanced sampling it is hard to derive an analytic expression for balanced sampling. Firstly, we propose a class of approximations of the variance derived from theoretical arguments. These approximations are based on a residual technique and are related to previous works: Yates (1949), Hájek (1964, Chapters 4, 7 and 14), and Brewer (2002, Chapter 9).

These approximations show that the variance depends only on the residuals for a particular regression of the interest variable against the balancing variables. The variance is then equal to zero under a linear deterministic model. Secondly, we check the approximation by means of a set of numerical studies. We examine several cases of balanced sampling, and we look for the worst interest variable, i.e. the variable for which the approximation gives the largest overevaluation or underevaluation. We show that in most cases, the error due to the approximation does not exceed 10% of the value of the variance.

The notation is defined in Section 2. A class of variance approximations is given in Section 3. An original and new methodology to evaluate the accuracy of balanced design is developed in Section 4. In Section 5, we present the results of the numerical study. The question of estimation of the variance is discussed in Section 6. Mathematical technicalities are given in the appendices.

2. Balanced sampling

Consider a finite population U of size N whose units can be identified by a label $k \in \{1,\ldots,N\}$. The aim is to study the interest variable y that takes the values y_k, $k \in U$, on the units of the population. More precisely, we want to estimate the total $Y = \sum_{k\in U} y_k$. Suppose also that p balancing variables $x_1,\ldots,x_p$ are available, i.e. that the vectors of values $\mathbf{x}_k = (x_{k1} \ \ldots \ x_{kj} \ \ldots \ x_{kp})'$ taken by the p balancing variables are known for all the units of the population. Moreover, without loss of generality, the p vectors $(x_{1j}\ldots x_{kj}\ldots x_{Nj})'$, $j = 1,\ldots,p$, are assumed linearly independent.

A sampling design $p(.)$ is a probability distribution on the set Ω of all the subsets of U such that $\sum_{s\in\Omega} p(s) = 1$. The random sample S takes a value s with probability $\Pr(S = s) = p(s)$. The inclusion probability of unit k is the probability that unit k is in the sample $\pi_k = \Pr(k \in S)$ and the joint inclusion probability is the probability that two distinct units are together in the sample $\pi_{k\ell} = \Pr(k \text{ and } \ell \in S)$. The Horvitz–Thompson estimator given by $\hat{Y} = \sum_{k\in S} y_k/\pi_k$ is an unbiased estimator of Y. The Horvitz–Thompson estimator of the jth auxiliary balancing total $X_j = \sum_{k\in U} x_{kj}$ is $\hat{X}_{j\pi} = \sum_{k\in S} x_{kj}/\pi_k$. With a vectorial notation, the Horvitz–Thompson estimator vector $\hat{\mathbf{X}} = \sum_{k\in S} \mathbf{x}_k/\pi_k$, estimates without bias $\mathbf{X} = \sum_{k\in U} \mathbf{x}_k$.

We assume that $p(s)$ is a balanced sampling design defined as follows.

Definition 1. A sampling design $p(s)$ is said to be balanced on the variables $x_1,\ldots,x_p$, if and only if it satisfies the balancing equations given by

$$\hat{\mathbf{X}} = \mathbf{X} \tag{1}$$

which can also be written as

$$\sum_{k\in s} \frac{x_{kj}}{\pi_k} = \sum_{k\in U} x_{kj}$$

for all $s \in \Omega$ such that $p(s) > 0$, and for all $j = 1,\ldots,p$, or in other words

$$\mathrm{var}(\hat{\mathbf{X}}) = 0.$$

Remark. If the y_k are linear combinations of the $\mathbf{x}_k$, i.e. $y_k = \mathbf{x}_k'\mathbf{b}$ for all k, where $\mathbf{b}$ is a vector of constants, then $\mathrm{var}(\hat{Y}) = 0$. More generally, if the y_k are well explained by the $\mathbf{x}_k$, one can expect that $\mathrm{var}(\hat{Y}) \approx 0$.

Consider now the three following particular cases of balanced sampling.

Example 1. A sampling design of fixed sample size n is balanced on the variable $x_k = \pi_k$, $k \in U$:

$$\sum_{k\in S} \frac{x_k}{\pi_k} = \sum_{k\in S} 1 = \sum_{k\in U} \pi_k = n.$$

Example 2. Suppose that the design is stratified and that in each stratum U_h, $h = 1,\ldots,H$, of size N_h a simple random sample of size n_h is selected, then the design is balanced on variables δ_{kh} of values

$$\delta_{kh} = \begin{cases} 1 & \text{if } k \in U_h, \\ 0 & \text{if } k \notin U_h. \end{cases}$$

In this case, we have

$$\sum_{k\in S} \frac{\delta_{kh}}{\pi_k} = \sum_{k\in S} \delta_{kh} \frac{N_h}{n_h} = N_h$$

for $h = 1,\ldots,H$.

Example 3. In sampling with unequal probabilities, the Horvitz–Thompson estimator $\hat{N}_\pi = \sum_{k\in S} 1/\pi_k$. of the population size N is generally random. When the population size is known before selecting the sample, it could be interesting to select a sample such as

$$\sum_{k\in S} \frac{1}{\pi_k} = N. \tag{2}$$

Eq. (2) is a balancing equation, where the balancing variable is $x_k = 1$, $k \in U$.

Thus, stratified and unequal probability sampling are particular cases of balanced sampling. Nevertheless, an intricate problem with balanced sampling is that, in most of the cases, the balancing equations (1) cannot be exactly satisfied. Consider the following example.

Example 4. Suppose that $N = 10$, $n = 7$, $\pi_k = \frac{7}{10}$, $k \in U$, with $x_k = k$, $k \in U$. Then a balanced sample is such that

$$\sum_{k \in S} \frac{k}{\pi_k} = \sum_{k \in U} k,$$

that implies that

$$\sum_{k \in S} k = 55 \times \frac{7}{10} = 38.5$$

which is impossible as 38.5 is not an integer. The problem arises from the non-integer value of $1/\pi_k$, and from the small population size.

The previous example displays a problem of balanced sampling: there are situations where balanced equations cannot be exactly satisfied (see designs 7–9 in Section 5).

Remark 1. A balanced sampling design $p(.)$ with inclusion probabilities $\boldsymbol{\pi}=(\pi_1, \ldots, \pi_N)'$ can be exactly balanced, if given a set of auxiliary variables, there exists at least a set of balanced sample $\mathbf{s}_1, \ldots, \mathbf{s}_m$ such that

$$\sum_{\ell=1}^{m} \mathbf{s}_\ell = \boldsymbol{\pi}. \tag{3}$$

If condition (3) is not satisfied, then the sampling design cannot be exactly satisfied. There might exist a rounding problem that precludes meeting the constraints.

3. Variance approximations

The variance of the Horvitz–Thompson estimator is

$$\operatorname{var}(\hat{Y}) = \sum_{k \in U} \sum_{\ell \in U} \frac{y_k y_k}{\pi_k \pi_\ell} \Delta_{k\ell}, \tag{4}$$

where

$$\Delta_{k\ell} = \begin{cases} \pi_{k\ell} - \pi_k \pi_\ell & \text{if } k \neq \ell \\ \pi_k(1 - \pi_k) & \text{if } k = \ell \end{cases}$$

and $\boldsymbol{\Delta} = [\Delta_{k\ell}]$. Matrix $\boldsymbol{\Delta}$ will be called the variance–covariance operator. Thus the variance of $\hat{Y}$ can be expressed and estimated by using the joint (order two) inclusion probabilities.

Nevertheless, in the case of Poisson sampling, which is a sampling design with no balancing variables, the variance of $\hat{Y}$ is easy to derive and can be estimated because

only first-order inclusion probabilities are needed. If $\tilde{S}$ is the random sample selected by a Poisson sampling design and $\tilde{\pi}_k$, $k \in U$, are the first-order inclusion probabilities of the Poisson design, then

$$\mathrm{var}_{\mathrm{poiss}}(\hat{Y}) = \mathrm{var}_{\mathrm{poiss}}\left(\sum_{k\in\tilde{S}} \frac{y_k}{\pi_k}\right) = \sum_{k\in U} \frac{y_k^2}{\pi_k^2}\,\tilde{\pi}_k(1-\tilde{\pi}_k) = \mathbf{z}'\tilde{\boldsymbol{\Delta}}\mathbf{z}, \tag{5}$$

where $\mathbf{z}=(z_1 \ \ldots \ z_k \ \ldots \ z_N)'$, $z_k = y_k/\pi_k$, and $\tilde{\boldsymbol{\Delta}}=\mathrm{diag}[(\tilde{\pi}_k(1-\tilde{\pi}_k))]$. Note that expression (5) contains π_k, and $\tilde{\pi}_k$, because the variance of the usual estimator (function of π_k's) is computed under Poisson sampling (function of $\tilde{\pi}_k$'s). The π_k's are always known, but the $\tilde{\pi}_k$'s are not necessarily known.

Actually Poisson sampling maximizes the entropy measure:

$$I(p) = -\sum_{s\subset U} p(s)\log\, p(s) \tag{6}$$

under the constraints that $\sum_{s\ni k}\ p(s) = \tilde{\pi}_k$, $k \in U$. In the case of exact balanced sampling, we have the following theorem.

Theorem 1. *Let $p_{\mathrm{bal}}(.)$ be an exact balanced sampling design with inclusion probabilities π_k, $k \in U$, then*

(i) *There exists a unique maximum entropy sampling design $p(s)$ with inclusion probabilities π_k.*

(ii) *Let $\mathbf{c}=\mathbf{A}\boldsymbol{\pi}_0$, in $\mathbb{R}^p$, where $\boldsymbol{\pi}_0$ is an interior point of $C=[0,1]^N$, $\mathbf{A}=(\mathbf{a}_1 \ \ldots \ \mathbf{a}_k \ \ldots \ \mathbf{a}_N)$ and $\mathbf{a}_k = \mathbf{x}_k/\pi_k$, $k \in U$. There exists a uniquely defined Poisson sampling design $\tilde{p}^*(.)$ with inclusion probabilities $\tilde{\pi}_k$ such that $p(.)$ is the conditional of $\tilde{p}^*(.)$ conditionally to $\sum_{k\in\tilde{S}} \mathbf{x}_k/\pi_k = \mathbf{X}$ and that*

$$E_{\tilde{p}^*}\left(\sum_{k\in\tilde{S}} \frac{\mathbf{x}_k}{\pi_k}\right) = \mathbf{c},$$

where $E_{\tilde{p}^*}(.)$ is the expectation under the sampling design $\tilde{p}^*(.)$. In particular, one can take

$$\mathbf{c} = \mathbf{X} = \sum_{k\in U} \mathbf{x}_k.$$

The proof is given in Appendix B. It is important to point out that the inclusion probabilities $\tilde{\pi}_k$ of the sampling design $\tilde{p}^*(.)$ are generally unknown, except for the balanced sampling design described in Chen et al. (1994)

If we suppose that, through Poisson sampling, the vector $(\hat{Y}\hat{\mathbf{X}}')'$ has approximately a multinormal distribution, we obtain

$$\mathrm{var}_{\mathrm{poiss}}(\hat{Y}|\hat{\mathbf{X}} = \mathbf{X}) \approx \mathrm{var}_{\mathrm{poiss}}(\hat{Y} + (\mathbf{X} - \hat{\mathbf{X}})'\boldsymbol{\beta}), \tag{7}$$

where

$$\boldsymbol{\beta} = \mathrm{var}_{\mathrm{poiss}}(\hat{\mathbf{X}})^{-1}\,\mathrm{cov}_{\mathrm{poiss}}(\hat{\mathbf{X}}, \hat{Y}),$$

$$\mathrm{var}_{\mathrm{poiss}}(\hat{\mathbf{X}}) = \sum_{k\in U} \frac{\mathbf{x}_k \mathbf{x}_k'}{\pi_k^2}\,\tilde{\pi}_k(1-\tilde{\pi}_k)$$

and

$$\mathrm{cov}_{\mathrm{poiss}}(\hat{\mathbf{X}}, \hat{Y}) = \sum_{k\in U} \frac{\mathbf{x}_k y_k}{\pi_k^2}\,\tilde{\pi}_k(1-\tilde{\pi}_k).$$

Again $\mathrm{var}_{\mathrm{poiss}}(\hat{\mathbf{X}})$ and $\mathrm{cov}_{\mathrm{poiss}}(\hat{\mathbf{X}}, \hat{Y})$ is a function of π_k and $\tilde{\pi}_k$, because we compute the variance of the usual Horvitz–Thompson estimator (function of π_k) under the Poisson sampling design (function of $\tilde{\pi}_k$).

Observing that $\hat{\mathbf{X}} = \mathbf{A}\mathbf{s}$ and $\hat{Y} = \mathbf{z}'\mathbf{s}$, where $\mathbf{s}$ is a vector of $\mathbb{R}^N$ whose units take the value 1 if $k \in s$ and 0 if $k \notin s$, by (7) implies

$$\mathrm{var}(\hat{Y}|\hat{\mathbf{X}} = \mathbf{X}) \approx \mathbf{z}'(\mathbf{I}-\mathbf{P})'\tilde{\boldsymbol{\Delta}}(\mathbf{I}-\mathbf{P}),$$

where $\mathbf{P}' = \mathbf{A}'(\mathbf{A}\tilde{\boldsymbol{\Delta}}\mathbf{A}')^{-1}\mathbf{A}\tilde{\boldsymbol{\Delta}}$ i.e. that $(\mathbf{I}-\mathbf{P}')$ is the orthogonal projector on $\mathrm{Ker}\,\mathbf{A}$ according to the metrics defined by $\tilde{\boldsymbol{\Delta}}$, where

$$\mathrm{Ker}\,\mathbf{A} = \{\mathbf{u} \in \mathbb{R}^N | \mathbf{A}\mathbf{u} = \mathbf{0}\}.$$

If

$$b_k = \tilde{\pi}_k(1-\tilde{\pi}_k),$$

expression (7) can also be written as

$$\mathrm{var}_{\mathrm{app}}(\hat{Y}) = \sum_{k\in U} b_k(z_k - \ddot{z}_k)^2, \tag{8}$$

where

$$\ddot{z}_k = \mathbf{a}_k' \left(\sum_{\ell\in U} b_\ell \mathbf{a}_\ell \mathbf{a}_\ell'\right)^{-1} \sum_{\ell\in U} b_\ell \mathbf{a}_\ell z_\ell = [\mathbf{A}'(\mathbf{A}\tilde{\boldsymbol{\Delta}}\mathbf{A}')^{-1}\mathbf{A}\tilde{\boldsymbol{\Delta}}\mathbf{z}]_k$$

is a regression predictor of z_k for the suitable regression such that $z_k - \ddot{z}_k$ appears as a residual. When only one balancing variable $x_k = \pi_k$ is used, (see Example 1), $\ddot{z}_k$ is simply the mean of the z_k with the weights b_k. Unfortunately, the weights b_k are unknown, because they depend on $\tilde{\pi}_k$'s, which are not exactly equal to the π_k. We propose to approximate the b_k.

Note that expression (8) can also be written

$$\mathrm{var}_{\mathrm{app}}(\hat{Y}) = \mathbf{z}'\boldsymbol{\Delta}_{\mathrm{app}}\mathbf{z},$$

where $\boldsymbol{\Delta}_{\mathrm{app}} = \{\Delta_{\mathrm{app}k\ell}\}$ is the approximated variance operator where

$$\Delta_{\mathrm{app}k\ell} = \begin{cases} b_k - b_k\mathbf{a}_k' \left(\sum_{i\in U} b_i \mathbf{a}_i \mathbf{a}_i'\right)^{-1} \mathbf{a}_k b_k, & k = \ell, \\ b_k \mathbf{a}_k' \left(\sum_{k\in U} b_i \mathbf{a}_i \mathbf{a}_i'\right)^{-1} \mathbf{a}_l b_\ell, & k \neq \ell. \end{cases} \tag{9}$$

In Appendix C, we show that the proposed approximation is still valid for non-exact balanced sampling.

Four variance approximations will be tested numerically. All of them are obtained by various definitions of the b_k's. These four definitions are denoted b_{k1}, b_{k2}, b_{k3}, and b_{k4}, and permit the definition of four variance approximations denoted V_α, $\alpha = 1,2,3,4$ and four variance operators denoted $\mathbf{\Delta}_\alpha$, $\alpha = 1,2,3,4$ by replacing in (8) and (9), b_k by, respectively, b_{k1}, b_{k2}, b_{k3}, and b_{k4}.

(1) The first approximation is obtained by considering that at least for large sample size, $\pi_k \approx \tilde{\pi}_k$, $k \in U$. Thus we take $b_{k1} = \pi_k(1-\pi_k)$.

(2) The second approximation is obtained by applying a correction for loss of degrees of freedom

$$b_{k2} = \pi_k(1-\pi_k)\frac{N}{N-p}.$$

This correction allows obtaining the exact expression for simple random sampling with fixed sample size.

(3) The third approximation derives from the fact that the diagonal elements of the variance operator $\mathbf{\Delta}$ of the true variance are always known and are equal to $\pi_k(1-\pi_k)$. Thus by defining

$$b_{k3} = \pi_k(1-\pi_k)\frac{\operatorname{trace}\mathbf{\Delta}}{\operatorname{trace}\mathbf{\Delta}_1},$$

we can define the approximated variance operator $\mathbf{\Delta}_3$ that has the same trace as $\mathbf{\Delta}$.

(4) Finally, the fourth approximation derives from the fact that the diagonal elements $\mathbf{\Delta}_{\text{app}}$ can be computed and is given in (9). The b_{k4} are constructed in such a way that $\Delta_{k\ell} = \Delta_{\text{app}k\ell}$, or in other words that

$$\pi_k(1-\pi_k) = b_k - b_k\mathbf{a}_k'\left(\sum_{k\in U} b_k\mathbf{a}_k\mathbf{a}_k'\right)^{-1}\mathbf{a}_k b_k,\ k \in U. \tag{10}$$

The determination of the b_{k4} requires then the resolution of the non-linear equation system. This fourth approximation is the only one that provides the exact variance expression for stratification. A similar idea was already proposed by Hájek (1981, p. 26) for the fixed size constraint. However, there is a condition given by the following theorem.

Theorem 2. *For the fixed sample size constraint ($p = 1$, $x_k = \pi_k$, $a_k = 1$ for all $k \in U$), a necessary condition in order that a solution exists in (10) is that*

$$\max_k \frac{\pi_k(1-\pi_k)}{\sum_{\ell\in U}\pi_\ell(1-\pi_\ell)} < \frac{1}{2}.$$

The proof is given in Appendix D.

Fortunately, this condition holds rarely and has never appeared in the numerical study.

4. Measure of accuracy of the approximations of variance

The aim of numerical study is the evaluation of the approximation of variance for balanced sampling. The methodology is unusual because we do not evaluate an estimator but an approximation of an interest function. Moreover, our methodology consists of identifying the worst population vector of interest for a given sampling design. The worst vector is the one that provides the largest difference between the approximation and the true variance.

In the numerical study, the samples are generated by means of the cube method. This method is divided into a flight phase and a landing phase (see Deville and Tillé, 2002). Each phase can be applied with several options. For the flight phase, at each step of the algorithm, the direction has been selected in Ker $\mathbf{A}$ randomly by means of vector of independent standard reduced normal variables, which intuitively provides a large entropy to the sampling design. At the landing phase, the sample is selected by means of a linear program.

The π_k, $\pi_{k\ell}$ and $\boldsymbol{\Delta} = [\pi_{k\ell} - \pi_k \pi_\ell]$ are estimated by means of 10 000 iterations, these estimations are denoted, respectively, $\check{\pi}_k$, $\check{\pi}_{k\ell}$ and $\check{\boldsymbol{\Delta}}$. It is essential to use at least 10 000 iterations. For example, if $\pi_k = 0.5$, then

$$\operatorname{var}(\check{\pi}_k) = \frac{(0.5)^2}{10\,000} = (0.005)^2,$$

the length of the confidence interval of probability 0.95 is thus $2 \times 1.96 \times 0.005 \approx 0.02$. So, only a two-digit precision is ensured.

If V denotes the true variance i.e. $V = \operatorname{var}(\hat{Y}) = \mathbf{z}'\boldsymbol{\Delta}\mathbf{z}$, then the quality of a variance approximation could be measured by

$$R_\alpha = \frac{V_\alpha}{V} = \frac{\mathbf{z}'\boldsymbol{\Delta}_\alpha\mathbf{z}}{\mathbf{z}'\boldsymbol{\Delta}\mathbf{z}}, \quad \alpha = 1,2,3,4$$

and is estimated by means of a numerical study by

$$\check{R}_\alpha = \frac{\check{V}_\alpha}{\check{V}} = \frac{\mathbf{z}'\check{\boldsymbol{\Delta}}_\alpha\mathbf{z}}{\mathbf{z}'\check{\boldsymbol{\Delta}}\mathbf{z}}, \quad \alpha = 1,2,3,4, \tag{11}$$

where $\check{\boldsymbol{\Delta}}_\alpha$ denotes an estimation of $\boldsymbol{\Delta}_\alpha$ obtained by replacing the π_k by the $\check{\pi}_k$ in expression (8). Estimator $\check{V}_\alpha/\check{V}$, which is a ratio, is preferred to $V_\alpha/\check{V}$, that could also be computed.

The extreme values of $\check{R}_\alpha$ are given by

$$\max_{\mathbf{z}} \mathbf{z}'\check{\boldsymbol{\Delta}}_\alpha\mathbf{z} \quad \text{subject to } \mathbf{z}'\check{\boldsymbol{\Delta}}\mathbf{z} = \text{Constant}$$

and

$$\min_{\mathbf{z}} \mathbf{z}'\check{\boldsymbol{\Delta}}_\alpha\mathbf{z} \quad \text{subject to } \mathbf{z}'\check{\boldsymbol{\Delta}}\mathbf{z} = \text{Constant}$$

which gives $\check{\boldsymbol{\Delta}}_\alpha\mathbf{z} = \lambda\check{\boldsymbol{\Delta}}\mathbf{z}$ where λ is the Lagrange multiplier. The problem consists of finding the decomposition of $\check{\boldsymbol{\Delta}}_\alpha$ in $\check{\boldsymbol{\Delta}}$. Let λ_i be the ith eigenvalue of this decomposition (on this topic see Gabler, 1984; Harville, 1997, pp. 562, 581). Since $\check{\boldsymbol{\Delta}}_\alpha$ has

p eigenvalues equal to zero, then $\max_{\mathbf{z}} \check{R}_\alpha = \lambda_1$ and $\min_{\mathbf{z}} \check{R}_\alpha = \lambda_{N-p}$. Note that if $\operatorname{trace} \mathbf{\Delta}_\alpha = \operatorname{trace} \mathbf{\Delta}$, (this is the case for $\alpha = 3$ and 4) then

$$\frac{1}{N} \sum_{i=1}^{N} \lambda_i = 1.$$

These two eigenvalues $\lambda_{\max} = \lambda_1$ and $\lambda_{\min} = \lambda_{N-p}$ represent the worst cases for which the approximation gives, respectively, the largest overestimation or underestimation of the true variance. A good approximation should thus have a corresponding $\lambda_{\max}$ and $\lambda_{\min}$ very close to 1.

5. Results of the numerical studies

Except in the equal probability cases, the inclusion probabilities are generated by using the square of centered reduced normal variables (chi-square distribution with one degree of freedom). Nine numerical studies were carried out with balanced designs corresponding to the particular applications given in the previous sections. In some cases, the balancing equations can be exactly satisfied, in others not. Several applications are made on very small population sizes, which should provide the worst cases for the variance approximation.

Balanced design 1: Balancing the moments of the order number. The design has equal probabilities with $N = 40$, $n = 15$, $p = 4$, $x_{k1} = 1$, $x_{k2} = k$, $x_{k3} = 1/k$, and $x_{k4} = 1/k^2$, where $k = 1, \ldots, N$, is the order number. This sampling design is an exact balanced sampling design.

Balanced design 2: Triangular overlapping stratification. The design is defined by $N = 30$, $E(n) = 10$, $p = 3$,

$$x_{k1} = \begin{cases} 1, & k \in \{1, \ldots, 15\}, \\ 0, & k \notin \{1, \ldots, 15\}, \end{cases} \qquad x_{k2} = \begin{cases} 1, & k \in \{11, \ldots, 25\}, \\ 0, & k \notin \{11, \ldots, 25\}, \end{cases}$$

$$x_{k3} = \begin{cases} 1, & k \in \{21, \ldots, 30\} \cup \{1, \ldots, 5\}, \\ 0, & k \notin \{21, \ldots, 30\} \cup \{1, \ldots, 5\}. \end{cases}$$

This sampling design is not an exact balanced sampling design.

Balanced design 3: Cross-stratification or balanced quota sampling I. The design has equal probabilities with $N = 40$, $n = 10$. The constraints are the marginal totals of a 4×10 contingency table. The balancing equations can be exactly satisfied.

Balanced design 4: Cross-stratification or balanced quota sampling II. The design has equal probabilities with $N = 60$, $n = 12$. The constraints are the marginal totals of a 5×12 contingency table (cross-stratification or balanced quota sampling). This sampling design is an exact balanced sampling design.

Balanced design 5: Cross-stratification or balanced quota sampling III. The design has unequal probabilities with $N = 48$, $n = 12$. The constraints are the marginal totals of a 3×4 contingency table (cross-stratification or balanced quota sampling). This sampling design is an exact balanced sampling design.

Table 1
Results of the numerical study

Approximation	b_{k1}		b_{k2}		b_{k3}		b_{k4}	
Balanced design	$\lambda_{\min}$	$\lambda_{\max}$	$\lambda_{\min}$	$\lambda_{\max}$	$\lambda_{\min}$	$\lambda_{\max}$	$\lambda_{\min}$	$\lambda_{\max}$
1	0.76	1.03	0.80	1.14	0.80	1.14	0.90	1.10
2	0.83	1.06	0.93	1.18	0.94	1.20	0.92	1.16
3	0.54	0.85	0.80	1.26	0.83	1.31	0.92	1.10
4	0.58	0.89	0.80	1.21	0.83	1.25	0.88	1.13
5	0.75	1.00	0.85	1.14	0.86	1.14	0.86	1.14
6	0.83	1.05	0.89	1.13	0.50	1.14	0.90	1.11
7	0.57	0.66	0.94	1.10	0.95	1.11	0.94	1.06
8	0.73	0.90	1.04	1.20	0.98	1.13	0.96	1.14
9	0.78	0.92	0.94	1.11	0.94	1.12	0.98	1.06

Balanced design 6: Two overlapping strata. The design has equal probabilities with $N = 30$, $E(n) = 15$, $p = 2$,

$$x_{k1} = \begin{cases} 1, & k \in \{1,\ldots,20\}, \\ 0, & k \notin \{1,\ldots,20\}, \end{cases} \qquad x_{k2} = \begin{cases} 1, & k \in \{11,\ldots,30\}, \\ 0, & k \notin \{11,\ldots,30\}. \end{cases}$$

This sampling design is an exact balanced sampling design.

Balanced design 7: Small population size. The design has equal probabilities with $N = 10$, $n = 5$, $p = 4$. This sampling design is not an exact balanced sampling design.

Balanced design 8: The design is Balanced on n and N with very small population size I, and $N = 8$, $n = 3$, $p = 2$, $x_{k1} = \pi_k$, $x_{k2} = 1$. This sampling design is not an exact balanced sampling design.

Balanced design 9: The design is Balanced on n and N with very small population size II, $N = 12$, $n = 5$, $p = 2$, $x_{k1} = \pi_k$, $x_{k2} = 1$. This sampling design is not an exact balanced sampling design.

Table 1 gives the smallest and the largest eigenvalues $\lambda_{\min}$ and $\lambda_{\max}$, for $\alpha = 1, 2, 3, 4$. In almost all the cases, the $\mathbf{\Delta}_4$ is the best approximation. Even when the balancing equations are not exactly satisfied, the ratio $\mathbf{z}'\mathbf{\Delta}_4\mathbf{z}/(\mathbf{z}'\mathbf{\Delta}\mathbf{z})$ remains close to 1. Note that $\lambda_{\min}$, and $\lambda_{\max}$ correspond to the worst ratio, the approximation will thus be better in any practical case. The correction for the loss of degrees of freedom can be important when the population size is small.

6. Variance estimation

In this section, we propose an estimator of (8). As (8) is a function of totals, we can substitute each total by its Horvitz–Thompson estimator (Deville, 1999). The resulting estimator for (8) is

$$\widehat{\mathrm{var}}(\hat{Y}) = \sum_{k \in S} c_k (z_k - \hat{\tilde{z}}_k)^2, \tag{12}$$

where

$$\hat{\tilde{z}}_k = \mathbf{a}_k' \left(\sum_{\ell \in S} c_\ell \mathbf{a}_\ell \mathbf{a}_\ell' \right)^{-1} \sum_{\ell \in S} c_\ell \mathbf{a}_\ell \mathbf{z}_\ell$$

is the estimator of the regression predictor of z_k.

Note that (12) can also be written as

$$\sum_{k \in S} \sum_{\ell \in S} z_k D_{k\ell} z_\ell,$$

where

$$D_{k\ell} = \begin{cases} c_k - c_k \mathbf{a}_k' \left(\sum_{i \in S} c_i \mathbf{a}_i \mathbf{a}_i' \right)^{-1} \mathbf{a}_k c_k, & k = \ell, \\ c_k \mathbf{a}_k' \left(\sum_{k \in S} c_i \mathbf{a}_i \mathbf{a}_i' \right)^{-1} \mathbf{a}_\ell c_\ell, & k \neq \ell. \end{cases}$$

The five definitions of the c_k's are denoted c_{k1}, c_{k2}, c_{k3}, c_{k5}, and c_{k5}, and allow to define five variance estimators by replacing in expression (12) c_k by, respectively, c_{k1}, c_{k2}, c_{k3}, c_{k4}, and c_{k5}.

(1) The first estimator is obtained by taking $c_{k1} = (1 - \pi_k)$.

(2) The second estimator is obtained by applying a correction for loss of degrees of freedom

$$c_{k2} = (1 - \pi_k) \frac{n}{n - p}.$$

This correction for the loss of degrees of freedom gives the unbiased estimator in simple random sampling with fixed sample size.

(3) The third estimator derives from the fact that the diagonal elements of the true matrix $\Delta_{k\ell}/\pi_{k\ell}$ are always known and are equal to $1 - \pi_k$. Thus we can use

$$c_{k3} = (1 - \pi_k) \frac{\sum_{k \in S} (1 - \pi_k)}{\sum_{k \in S} D_{kk}}.$$

(4) The fourth estimator can be derived from b_{k4} obtained by solving equation system (10),

$$c_{k4} = \frac{b_{k4}}{\pi_k} \frac{n}{n - p} \frac{N - p}{N}.$$

(5) Finally, the fifth estimator derives from the fact that the diagonal elements D_{kk} are known. The c_{k5} are constructed in such a way that

$$1 - \pi_k = D_{kk}, \quad k \in U \tag{13}$$

or in other words that

$$1 - \pi_k = c_k - c_k \mathbf{a}_k' \left(\sum_{i \in S} c_i \mathbf{a}_i \mathbf{a}_i' \right)^{-1} \mathbf{a}_k c_k, \quad k \in U.$$

This fifth approximation is the only one that provides the exact unbiased variance estimator for stratification. A necessary condition in order that a solution exists for equation system (13), is that

$$\max_k \frac{1-\pi_k}{\sum_{\ell\in S}(1-\pi_\ell)} < \frac{1}{2}.$$

7. Conclusion

We have shown that the variance of the Horvitz–Thompson estimator under balanced sampling can be approximated and estimated with a residual technique. Balanced sampling can be viewed as a calibration (Huang and Fuller, 1978; Deville and Särndal, 1992) at design stage. Like for calibration, the variance under balanced sampling can be approximated as a variance of residuals. Numerical results support our findings.

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Appendix A. Technical theorem

We need a following technical theorem in order to prove Theorem 1.

Theorem A.1. *Let m_0 be a probability measure on $\mathbb{R}^N$ with a compact support K, C the convex closure of K, and $\overset{\circ}{C}$ the interior of C assumed to be non-empty. Let m_λ, $\boldsymbol{\lambda}\in\mathbb{R}^N$ the exponential family of probability measures defined by*

$$m_\lambda(\mathrm{d}\mathbf{x}) = \exp[\boldsymbol{\lambda}'\mathbf{x} - \mu(\boldsymbol{\lambda})]m_0(\mathrm{d}\mathbf{x}),$$

where

$$\exp\mu(\boldsymbol{\lambda}) = \int \exp(\boldsymbol{\lambda}'\mathbf{x})m_0(\mathrm{d}\mathbf{x}).$$

The expectation of $m_\lambda(\mathrm{d}\mathbf{x})$ is the vector $\boldsymbol{\pi} = \mu'(\boldsymbol{\lambda})$ and the variance matrix is $\mu''(\boldsymbol{\lambda})$. The mapping $\boldsymbol{\lambda}\to\boldsymbol{\pi}=\mu'(\boldsymbol{\lambda})$ is a C^∞ diffeomorphism (i.e. a one-to-one and indefinitely differentiable) from $\mathbb{R}^N$ onto $\overset{\circ}{C}$.

Proof. The first statement is a standard fact. Moreover the fact that $\mu''(\boldsymbol{\lambda})$ is of full rank for every $\boldsymbol{\lambda}$ implies that the mapping is injective. Differentiability for all orders is obvious. It remains to prove that it is onto. For this purpose we need a following Lemma (which is actually the proof for the case $N = 1$).

Lemma A.1. *Let m_0^1 be a probability measure that has* [0, 1] *for convex closure of its support, and m_λ^1 the probability measure*

$$\exp[-\lambda x - \mu(\lambda)]m_0^1(\mathrm{d}x) \quad (\lambda, x \in \mathbb{R}).$$

Then $\int x\,\mathrm{d}m_\lambda^1(x)$ is a continuous decreasing function with limit equal to 0 when λ tends to infinity.

Proof. The function is obviously continuous and decreasing. Now let $\varepsilon > 0$ arbitrary small,

$$p_\lambda^0 = m_\lambda^1\left(\left[0, \frac{\varepsilon}{4}\right]\right), \quad p_\lambda^1 = m_\lambda^1\left(\left[\frac{\varepsilon}{2}, 1\right]\right).$$

As

$$\frac{p_\lambda^0}{p_\lambda^1} \geqslant \frac{p_0^0}{p_0^1}\exp\frac{\lambda\varepsilon}{4},$$

p_λ^1 tends to 0 when λ increases. We conclude by using the trivial majoration $\int x\,\mathrm{d}m_\lambda^1(x) \leqslant \varepsilon/2 + p_\lambda^1$. □

Let now $\mathbf{u}$ be any unit vector in $\mathbb{R}^N$ (with the standard metrics) and $t(\mathbf{u}) > 0$ such that

$$f_u(\mathbf{x}) = t(\mathbf{u})\mathbf{u}'(\mathbf{x} - \boldsymbol{\pi}_0) = 1, \qquad \left(\boldsymbol{\pi}_0 = \int \mathbf{x}\,\mathrm{d}m_0(\mathbf{x}) = \mu'(0)\right)$$

is the equation of a tangent hyperplan to C. As C is compact, $t(\mathbf{u})$ is a bounded function on the unit sphere of $\mathbb{R}^N$ and $C = \bigcap_{\mathbf{u}}\{f_u(\mathbf{x}) \leqslant 1\}$. Consider $C_\varepsilon = \bigcap_{\mathbf{u}}\{f_u(\mathbf{x}) \leqslant 1 - \varepsilon\}$, the homothetic of C by the homothety centered at $\boldsymbol{\pi}_0$ (which belongs always to C_ε) that has ratio $1 - \varepsilon$. Let B_r the ball of radius r in $\mathbb{R}^N$ and D_r its border, $C(r) = \mu'(B_r)$, $\bar{C}_r = \mu'(D_r)$ the border of $C(r)$. This set delimits two regions in $\overset{\circ}{C}$, the interior to which belongs $\boldsymbol{\pi}_0$ and the exterior. As μ' restrained to B_r define a homotopy, every point of the interior is also in $C(r)$. It remains to show that for ε given, we can find r such that $C_\varepsilon \subset C(r)$, or, which is the same, that $\bar{C}(r)$ is outside of C_ε. Note that f_u maps the probability measure $m_0(\mathrm{d}x)$ on a real probability measure $m_0^*(\mathrm{d}\boldsymbol{\xi})$ which has support for extreme points $-t(-\boldsymbol{\lambda})/t(\boldsymbol{\lambda})$ and 1. For $\boldsymbol{\lambda} = \alpha\mathbf{u}$, $m_\lambda(\mathrm{d}\boldsymbol{\xi})$ is mapped to the probability measure

$$m^*(\mathrm{d}\boldsymbol{\xi}) = \exp[\alpha\boldsymbol{\xi} - \mu(\alpha\mathbf{u})]\,\mathrm{d}m_0^*(\boldsymbol{\xi}).$$

We have

$$f_u(\boldsymbol{\pi}(\alpha\mathbf{u})) = \int \exp[\alpha\boldsymbol{\xi} - \mu(\alpha\mathbf{u})]\,\mathrm{d}m_0^*(\boldsymbol{\xi}).$$

From Lemma A.1, we get the existence of $\alpha(\mathbf{u})$ such that $f_u(\boldsymbol{\pi}(\alpha(\mathbf{u})'\mathbf{u})) = 1 - \varepsilon/2$ and $f_u(\boldsymbol{\pi}(\alpha\mathbf{u})) > 1 - \varepsilon/2$, if $\alpha > \alpha(\mathbf{u})$. All the $\boldsymbol{\pi}(\alpha\mathbf{u})$, $\alpha > \alpha(\mathbf{u})$ are therefore outside of C_ε. Moreover it can be seen that $\alpha(\mathbf{u})$ is a continuous function of $\mathbf{u}$ on the unit sphere of $\mathbb{R}^N$ which is compact. $\alpha(\mathbf{u})$ has a supremum $r(\varepsilon)$ and $\mu'(D_{r(\varepsilon)}) = \bar{C}(r(\varepsilon))$ is outside of C_ε, which completes the proof. □

Remark. When K is a finite set and m_0 the uniform measure on K, Theorem A.1 follows easily from the fact that every point $\boldsymbol{\pi}$ in $\overset{\circ}{C}$ is a convex combination of the extreme points of K (existence of a probability measure supported by K having $\boldsymbol{\pi}$ for mean) and from the existence of a maximum entropy probability on K with mean $\boldsymbol{\pi}$. This probability gives to the points $\mathbf{x}$ of K masses proportional to $\exp(\boldsymbol{\lambda}'\mathbf{x})$ for some $\boldsymbol{\lambda}$.

Appendix B. Proof of Theorem 1

(i) Let

$$\Omega_X = \left\{ s \in \Omega \,\middle|\, \sum_{k \in s} \frac{\mathbf{x}_k}{\pi_k} = \mathbf{A}\mathbf{s} = \mathbf{X} = \mathbf{A}\boldsymbol{\pi} \right\}.$$

This set is the set of extreme points of the convex compact $(\boldsymbol{\pi} + \operatorname{Ker}\mathbf{A}) \cap C$ and lies in a linear subspace of dimension $N - p$. From Theorem A.1 of Appendix A (or only the remark at the end of Appendix A), there exists a unique vector $\boldsymbol{\lambda}_0$ in $\operatorname{Ker}\mathbf{A}$ (satisfying $\mathbf{A}\boldsymbol{\lambda}_0 = 0$) such that with

$$p_X(s) = \frac{\exp \boldsymbol{\lambda}'\mathbf{s}}{\sum_{s \in \Omega_X} \exp \boldsymbol{\lambda}'\mathbf{s}}$$

we have

$$\pi_k = \sum_{s \in \Omega_X} \mathbf{s}\, p_X(s) = \sum_{s \ni k | s \in \Omega_X} p(s).$$

This plan is the maximum entropy sampling design with support Ω_X and inclusion probabilities π_k.

(ii) Observe that a Poisson sampling design can be defined by

$$\tilde{p}(s) = \frac{\exp \boldsymbol{\lambda}_0'\mathbf{s}}{\sum_{s \in \Omega} \exp \boldsymbol{\lambda}_0'\mathbf{s}}$$

and that $p_X(s)$ is $\tilde{p}(s)$ conditional on $s \in \Omega_X$. Let $\mathscr{A} = \{\mathbf{A}\mathbf{s} | \mathbf{s} \in \Omega\}$ and for $\mathbf{c} \in \mathscr{A}$, $\Omega_a = \{s | \mathbf{A}\mathbf{s} = \mathbf{c}\}$ and

$$q(\mathbf{c}) = \sum_{s \in \Omega_a} \tilde{p}(s).$$

Observe that the convex closure of $\mathscr{A}$ (in $\mathbb{R}^p$) is exactly $\mathbf{A}(C) = \{\mathbf{A}\mathbf{x} | \mathbf{x} \in C\}$, and that $q(\mathbf{c}), \mathbf{c} \in \mathscr{A}$, define a probability measure on $\mathscr{A}$. We can rewrite

$$\tilde{p}(s) = q(\mathbf{A}\mathbf{s})\, \tilde{p}(\mathbf{s} | \mathbf{A}\mathbf{s} = \mathbf{c}),$$

where $\mathbf{s} \in \Omega_a$, and

$$\tilde{p}(\mathbf{s} | \mathbf{A}\mathbf{s} = \mathbf{c}) = p_a(s) = \frac{\exp \boldsymbol{\lambda}_0'\mathbf{s}}{\sum_{s \in \Omega_a} \exp \boldsymbol{\lambda}_0'\mathbf{s}}. \tag{B.1}$$

(iii) By Theorem A.1 of Appendix A, we get that for any $\mathbf{c}$ lying in the interior of the convex set $\mathbf{A}(C)$, for $\mathbf{c}=\mathbf{X}$ for instance, since $\mathbf{X}=\mathbf{A}\boldsymbol{\pi}$ and $\boldsymbol{\pi}$ is in the interior of C, there exists a uniquely defined $\boldsymbol{v}\in\mathbb{R}^p$ such that

$$\mathbf{c}=\sum_{\mathbf{x}\in\mathscr{A}}\mathbf{x}\exp[\boldsymbol{v}'\mathbf{x}-\mu_A(\boldsymbol{v})]q(\mathbf{x}), \tag{B.2}$$

where

$$\mu_A(\boldsymbol{v})=\sum_{\mathbf{c}\in\mathscr{A}}q(\mathbf{c})\exp(\boldsymbol{v}'\mathbf{c}).$$

(iv) Let

$$\tilde{p}^*(s)=\exp[\boldsymbol{v}'\mathbf{A}\mathbf{s}-\mu_A(\boldsymbol{v}'\mathbf{c}]q(\mathbf{A}\mathbf{s})p_{As}(s)$$

coming from the probability q_v on $\mathscr{A}$ used in (B.2) and the family of conditional probabilities (B.1). We can rewrite

$$\tilde{p}^*(s)=\frac{\exp[(\boldsymbol{\lambda}_0+\mathbf{A}'\boldsymbol{v})\mathbf{s}]}{\sum_{s\in\Omega}\exp[\boldsymbol{\lambda}_0'\mathbf{s}+\mu_A(\boldsymbol{v})]}.$$

Observe that $\boldsymbol{v}\to\boldsymbol{\lambda}_1=\mathbf{A}'\boldsymbol{v}$ is a bijection of $\mathbb{R}^p$ onto $\operatorname{Im}\mathbf{A}'$, the orthogonal subspace of $\operatorname{Ker}\mathbf{A}$ (for the standard metrics on $\mathbb{R}^N$) and $\boldsymbol{\lambda}=\boldsymbol{\lambda}_0+\boldsymbol{\lambda}_1$ is a uniquely defined vector of $\mathbb{R}^N$. Therefore

$$\tilde{p}^*(s)=\frac{\exp(\boldsymbol{\lambda}\mathbf{s})}{\sum_{s\in\Omega}\exp(\boldsymbol{\lambda}\mathbf{s})}$$

is a Poisson sampling design uniquely defined such that

$$\tilde{\pi}_k=\frac{\exp\lambda_k}{1+\exp\lambda_k},$$

$\tilde{p}^*(s)$ conditional to $s\in\Omega_a$ is $p_X(s)$ and

$$E_{\tilde{p}^*}\left(\sum_{k\in S}\frac{\mathbf{x}_k}{\pi_k}\right)=\mathbf{X}.$$

Remark B.1. This design has the interest of concentrating the probability on the vicinity of Ω_X, unlike to any choice of $\mathbf{c}\neq\mathbf{X}$.

Remark B.2. A nice purely algebraic way to see the mean and variance property of $\tilde{\boldsymbol{\pi}}$ is the following:

$$\tilde{\pi}_k=\sum_{s\ni k}\tilde{p}^*(s)=\exp\lambda_k\frac{\sum_{k\notin s}\exp\boldsymbol{\lambda}'\mathbf{s}}{\sum_{s\in\Omega}\exp\boldsymbol{\lambda}'\mathbf{s}}=\exp\lambda_k(1-\tilde{\pi}_k).$$

The mean for $\tilde{p}^*$ (from the first statement of Theorem A.1 in Appendix A) is computed from

$$\exp\mu(\boldsymbol{\lambda})=\sum_{s\in\Omega}\exp(\boldsymbol{\lambda}'\mathbf{s})$$

which gives

$$\exp \mu(\boldsymbol{\lambda}) \frac{\mathrm{d}\mu}{\mathrm{d}\boldsymbol{\lambda}} = \begin{bmatrix} \vdots \\ \exp \lambda_k \\ \vdots \end{bmatrix} \sum_{s \ni k} \exp (\boldsymbol{\lambda}' \mathbf{s})$$

and therefore

$$\frac{\mathrm{d}\mu}{\mathrm{d}\boldsymbol{\lambda}} = \begin{bmatrix} \vdots \\ \tilde{\pi}_k \\ \vdots \end{bmatrix}.$$

The variance operator for $\tilde{p}^*$ is

$$\frac{\mathrm{d}^2\mu}{\mathrm{d}\boldsymbol{\lambda}^2} = \left[\frac{\mathrm{d}\tilde{\pi}_k}{\mathrm{d}\lambda_k}\right] = \mathrm{diag}\,(\tilde{\pi}_k(1 - \tilde{\pi}_k)).$$

Appendix C. Elements for justifying the approximated variance in the non-exact case

We seek an approximation concerning the flight phase, assuming that the landing phase consists essentially of a kind of rounding. We have to set up a quite complicated construction.

C.1. p-faces

Let U^* be any subset of p co-ordinates amongst $[0, 1]$. A p-face f is a set indexed by a partition (U^0, U^1, U^*) of $[0, 1]$ such that $x_k = 0$, if $k \in U^0$, $x_k = 1$, if $k \in U^1$, $x_k \in [0, 1]$, if $k \in U^*$. Let C_p be the reunion of all the p-faces. This set can be canonically equipped with the probability measure

$$m = \frac{1}{2^{N-p} \binom{N}{p}} \sum_f m_f,$$

where m_f is the p-dimensional Lebesgue measure on $\mathbb{R}^N$.

By simplicity, assume that all square submatrices $\mathbf{A}_{U^*} = [\mathbf{a}_k,\, k \in U^*]$ of $\mathbf{A}$ have rank p. This is almost always the case if we can consider the $\mathbf{a}_k$ as drawn independently from some continuous multivariate distribution. The set Ω_a of extreme points of $C \cap \{\mathbf{Ax} = \mathbf{c}\}$ is exactly $C_p \cap \{\mathbf{Ax} = \mathbf{c}\}$. In particular, $\mathbf{A}(C_p) = \mathbf{A}(C) = \mathscr{A}$ (take $\boldsymbol{\pi} \in C$; $\Omega_{\mathbf{A}\boldsymbol{\pi}}$ is not empty). Every point $\mathbf{c}$ of $\mathscr{A}$ determines the convex polyhedron $C \cap \{\mathbf{Ax} = \mathbf{c}\}$ and Ω_a, its set of extreme points.

C.2. A family of maximum entropy probabilities

Like in Appendix B, we start with Ω_X. For simplicity, at once, assume that $\mathbf{X}$ is an ordinary point in $\mathscr{A}$ in this sense that $\Omega_X = \Omega_p = \bar{C}_p$ (with $\bar{C}_p = \bigcup_{q<p} C_q$). There exists a uniquely defined vector $\boldsymbol{\lambda}_0 \in \operatorname{Ker} \mathbf{A}$ such that the probability defined on Ω_X by

$$p_X(\boldsymbol{\pi}^*) = \frac{\exp[\boldsymbol{\lambda}_0' \boldsymbol{\pi}^* - \mu_X(\boldsymbol{\lambda}_0)]}{|\Omega_X|} \tag{C.1}$$

has for mean $\boldsymbol{\pi}$ (given). This is, as is easily seen, the maximum entropy probability measure on Ω_X.

Define now on C_p the probability measure

$$\tilde{p}^*(\boldsymbol{\lambda}' \boldsymbol{\pi}^*) = \exp[\boldsymbol{\lambda}_0' \boldsymbol{\pi}^* - \mu(\boldsymbol{\lambda}_0)]\, \mathrm{d}m(\boldsymbol{\pi}^*)$$

with

$$\mu(\boldsymbol{\lambda}_0) = \int_{C_p} \exp(\boldsymbol{\lambda}_0' \boldsymbol{\pi}^*)\, \mathrm{d}m(\boldsymbol{\pi}^*).$$

For every $\mathbf{c}$ in the set of ordinary points in $\mathscr{A}$, we can define a maximum entropy probability on Ω_a

$$\tilde{p}_a^*(\boldsymbol{\pi}^*) = \frac{\exp[\boldsymbol{\lambda}_0' \boldsymbol{\pi}^* - \mu_a(\boldsymbol{\lambda}_0)]}{|\Omega_a|}.$$

Let $\boldsymbol{\pi}_a^*$ be the mean on $\tilde{p}_a^*$ and $\mathbf{V}_a$ its variance operator. Let p_0^A be the probability measure $\tilde{p}^*$ 'projected' on $\mathbb{R}^p$ by $\mathbf{A}$:

$$p_0^A(\mathrm{d}\mathbf{c}) = \tilde{p}^*(\mathbf{A}^{-1}(\mathrm{d}a)).$$

The support of p_0^A is $\mathscr{A}$ which is a convex set (a zonoid in the terminology of Ziegler (1998)). Moreover p_0^A has density $\exp(\mu_a(\boldsymbol{\lambda}_0) - \mu(\boldsymbol{\lambda}_0))$ with respect to m^A, 'projection' of m and m^A can be written as

$$m^A(\mathrm{d}\mathbf{c}) = m(\mathbf{A}^{-1}(\mathrm{d}\mathbf{c})) = \sum_f \det(\mathbf{A}_{U^*(f)})^{-1}\, \mathrm{d}\mathbf{c},$$

where the sum is over all the p faces f such that $\mathbf{c} \in \mathbf{A}(f)$. It is clear that we have the desegregation

$$\tilde{p}^* = \sum_{\mathscr{A}} \tilde{p}_a^{*A}(\mathrm{d}a) \tag{C.2}$$

The family $\tilde{p}_A^*$ varies continuously when $\mathbf{c}$ varies in every open region on $\mathscr{A}$ on which no point of $\bar{C}_p$ is projected. This set of 'extraordinary' points has a measure 0 for m^A and p_0^A.

C.3. Continuity problems

For (C.2), we do not need to define $\tilde{p}_a^*$ when $\mathbf{c}$ is an 'extraordinary' point. However, from a statistical point of view, it is necessary to have a reasonable coherent definition. Let $\mathbf{c}_0$ be 'extraordinary' in $\mathscr{A}$. This point is the image by $\mathbf{A}$ of some point $\boldsymbol{\pi}_0^* \in C_q - \bar{C}_q$

with $q < p$ and belongs to a 'segment' of dimension q in $\mathscr{A}$. This segment is adjacent to

$$\begin{pmatrix} N-p+q \\ p-q \end{pmatrix}$$

p-faces. For instance, if $\boldsymbol{\pi}_0^* \in C_{p-1} - \bar{C}_{p-1}$, it belongs to a hyperplan delimiting two regions in $\mathbb{R}^p$ and there are $N-p+1$ p-faces adjacent to $\boldsymbol{\pi}_0^*$. When $\mathbf{c}$ varies on some lines in $\mathscr{A}$ crossing this Hyperplane at $\mathbf{c}_0$, the number of points Ω_a is a number $r \leqslant N-p+1$ before the crossing and $N-p+1-r$ after the crossing. The most 'continuous' way to define a weight at $\boldsymbol{\pi}_0^*$ (and $\mathbf{c}_0$) is to put $w(\boldsymbol{\pi}_0^*) = (N-p+1)/2$. By re-iterating the same argument, we obtain the weight

$$w(\boldsymbol{\pi}^*) = \begin{pmatrix} N-p+q \\ p-q \end{pmatrix} 2^{-(p-q)} \tag{C.3}$$

to a point $\boldsymbol{\pi}^*$ in $C_q - \bar{C}_q$, $0 \leqslant q \leqslant p$.

If $\mathbf{X}$ is an extraordinary point, we extend the definition given in (C.1) of p_X:

$$p_X(\boldsymbol{\pi}^*) = \frac{\exp[\boldsymbol{\lambda}_0' \boldsymbol{\pi}^* - \mu_X(\boldsymbol{\lambda}_0)] w(\boldsymbol{\pi}^*)}{\sum_{\Omega_X} w(\boldsymbol{\pi}^*)}.$$

With this construction extended to p_a, $\mathbf{c}$ extraordinary, we get a family of probabilities on the Ω_a such that p_{a_0} is always a mean between the limits of p_c when $\mathbf{c}$ tends to $\mathbf{c}_0$ coming from different directions.

In some cases, we achieve a complete continuity, for instance when $\mathbf{A} = (1, \ldots, 1)$ of rank 1, which occurs with the fixed sample size constraint, and $\mathbf{c}$ varies from 0 to N in $\mathbb{R}$. As a consequence, $\boldsymbol{\pi}_a^*$ and $\mathbf{V}_a$ are continuous functions of $\mathbf{c}$.

C.4. Exponential families on (C_p, m)

Again, the developments in this section are similar to Appendix B, although technically a bit more involved. As $\mathscr{A}$ is convex, compact in $\mathbb{R}^p$ and is the support of p_0^A, for every $\mathbf{c} \in \overset{\circ}{A}$ (interior of $\mathscr{A}$,) there exists a uniformly defined vector $\boldsymbol{v}_a \in \mathbb{R}^p$ such that

$$\mathbf{c} = \int_{\mathscr{A}} \mathbf{x} \exp(\boldsymbol{v}_a' \mathbf{x} - \mu^A(\boldsymbol{v}_a)) \, \mathrm{d} p_0^A(\mathbf{x}) = E_{p_{v_a}^A}(\mathbf{x}).$$

In particular, there is a uniquely defined value $\boldsymbol{v} = \boldsymbol{v}_X$ such that $\mathbf{X} = E_{p_v^A}(\mathbf{x})$. Consider now that exponential family in C_p indexed by $\boldsymbol{\lambda} \in \mathbb{R}^N$.

$$\tilde{p}_\lambda^*(\mathrm{d}\boldsymbol{\pi}^*) = \exp(\boldsymbol{\lambda}' \boldsymbol{\pi}^* - \mu(\boldsymbol{\lambda})) \, \mathrm{d} m(\boldsymbol{\pi}^*).$$

As $\boldsymbol{\lambda}$ has a unique decomposition $\boldsymbol{\lambda} = \boldsymbol{\lambda}_0 + \boldsymbol{\lambda}_1$ with $\boldsymbol{\lambda}_0 \in \operatorname{Ker} \mathbf{A}$ and $\boldsymbol{\lambda}_1 = \mathbf{A}' \boldsymbol{v}$ ($\boldsymbol{v} \in \mathbb{R}^p$), we have just proved (as in Theorem 1) that there exists a uniquely defined $\boldsymbol{\lambda} \in \mathbb{R}^N$ such that $E_{\tilde{p}_\lambda^*}(\mathbf{A}\boldsymbol{\pi}^*) = \mathbf{X}$, and $\tilde{p}_\lambda^*(\boldsymbol{\pi}^* | \mathbf{A}\boldsymbol{\pi}^* = \mathbf{X}) = p_X(\boldsymbol{\pi}^*)$. Moreover, we have

the desegregation

$$\tilde{p}_\lambda^* = \int_{\mathscr{A}} p_a \, \mathrm{d}\, p_v^A(\mathbf{c}).$$

We also have the standard decomposition for the variance operator $\mathbf{V}$:

$$\mathbf{V} = \mathbf{V}_I + \mathbf{V}_B$$

with

$$\mathbf{V}_I = \int_{\mathscr{A}} \mathbf{V}_a \, \mathrm{d}\, p_v^A(\mathbf{c}),$$

and

$$\mathbf{V}_B = \int_{\mathscr{A}} [\boldsymbol{\pi}_a^* - E(\boldsymbol{\pi}_a^*)][\boldsymbol{\pi}_a^* - E(\boldsymbol{\pi}_a^*)]' \, \mathrm{d}\, p_v^A(\mathbf{c}).$$

Operator $\mathbf{V}_I$ has for image $\operatorname{Ker}\mathbf{A}$ because it is already the case for every $\mathbf{V}_a$. Its kernel is the orthogonal supplement of $\operatorname{Ker}\mathbf{A}$ in the metric defined by $\mathbf{V}$, that is if $\mathbf{P} = \mathbf{I} - \mathbf{V}\mathbf{A}'(\mathbf{A}\mathbf{V}\mathbf{A}')\mathbf{A}$ is this projector, $\mathbf{V}_I = \mathbf{P}'\mathbf{V}\mathbf{P}$.

C.5. Variance approximation

We anticipate that $\mathbf{V}_I$ is a good approximation for $\mathbf{V}_X$. We rely on three other approximations which are very plausible for N large enough (which we can prove completely for the fixed sample size case).

(i) *First approximation*: $\mathbf{V}_a$ varies continuously with $\mathbf{c}$ when $\mathbf{c}$ varies in an open zone of $\mathscr{A}$. When $\mathbf{c}$ crosses a border at a point $\mathbf{c}_0 \in C_q$, $q < p$, the discontinuity on $\mathbf{V}_a$ has the order of magnitude of

$$\begin{pmatrix} N \\ p-q \end{pmatrix}$$

number of p faces projecting on $\mathbf{c}_0$. The denominator of this ratio is not easy to estimate (see Ziegler, 1998, Chapters 8 and 9 and the bibliography therein) but if $\mathbf{c}_0$ is 'central' enough, it is very large. Remark that, with our convention for discontinuity point in (C.3), $\mathbf{V}_a$ is continuous in the fixed sample size constraint case when $\mathbf{c}$ varies in $\mathbb{R}$ from 0 to N. A formal conclusion of this informal conclusion is that we should be correct when writing that for $\varepsilon > 0$ given, there exists some $r > 0$ such that $\|\mathbf{V}_X - \mathbf{V}_a\| < \varepsilon$ if $\|\mathbf{X} - \mathbf{c}\| < r$ (standard norm in $\mathbb{R}^p$ and an operator norm for the first inequality).

(ii) *Second approximation*: As the expectation of p_v^A is $\mathbf{X}$, we may think that the probability concentrates in a neighborhood of $\mathbf{X}$ when N is large. We could invoke a tendency to a normal distribution or a similar argument. For the fixed sample size constraint, $|\mathbf{s}| = n$, both $\boldsymbol{\lambda} = \lambda$, $\mathbf{c} = a$ are scalar. It is then easy to see that the density of p_v^A on the interval $]m-1, m[$, $m = 1, \ldots, N$, is proportional to $\binom{N}{m} \exp \lambda a$ and that $\exp \lambda$ is nearly equal to $n/(N-n)$. In this case, our assertion is easy to satisfy.

Formally, we would write that for N large

$$p_v^A(\{\mathbf{c}; \|\mathbf{X} - \mathbf{c}\|\}) > 1 - \varepsilon.$$

Putting together the assumptions in (i) and (ii), we get that for N large and $\mathbf{X}$ sufficiently 'central' in $\mathscr{A}$. $\mathbf{V}_I$ is a close approximation of $\mathbf{V}_X$.

(iii) *Third approximation*: Concerning $\tilde{p}_\lambda^*$ (and therefore $\mathbf{V}$), for each co-ordinate λ_k of $\boldsymbol{\lambda}$, set

$$\tilde{\pi}_k = \frac{\exp \lambda_k}{1 + \exp \lambda_k}.$$

The density $\mathrm{d}\tilde{p}_\lambda^*/\mathrm{d}m$ is proportional to

$$\prod_{k \in U} \tilde{\pi}_k^{\pi_k^*} (1 - \tilde{\pi}_k)^{1 - \pi_k^*}.$$

If $\boldsymbol{\pi}^* = \mathbf{s}$ is a sample (a point that has integer co-ordinates), we find exactly the probability $\tilde{p}^*(s)$ of the Poisson sampling design with inclusion probabilities $\tilde{\pi}_k$. It remains to see that the probability $\tilde{p}_\lambda^*(\mathrm{d}\boldsymbol{\pi}^*)$ on C_p is well approximated by

$$\sum_s \tilde{p}^*(\mathbf{s})\, \delta_s,$$

where δ_s is the unit Dirac mass at $\mathbf{s}$. It is easy to see that it is true and in particular, that $\mathbf{V}$ can be approximated by $\tilde{\boldsymbol{\Delta}} = \mathrm{diag}\,(\tilde{\pi}_k(1 - \tilde{\pi}_k))$, the variance operator of the Poisson sampling design.

As it is seen in Section 5, this heuristic reasoning is completely confirmed by the numerical study.

Appendix D. Proof of Theorem 2

The problem consists of finding some numbers $\omega_k > 0$ of vector $\boldsymbol{\omega}$ of $\mathbb{R}^N$ with $\sum_{k=1}^N \omega_k = 1$, and a constant Ω such that

$$\mathrm{d}\rho_k = \mathrm{d}\Omega(\omega_k - \omega_k^2), \tag{D.1}$$

with $\mathrm{d} = \sum_{k=1}^N \pi_k(1 - \pi_k)$, and

$$\rho_k = \frac{\pi_k(1 - \pi_k)}{d}.$$

By summing the equations we find that

$$\Omega = \frac{1}{1 - \sum_{k=1}^N \omega_k^2} = \frac{1}{1 - \Omega_2}.$$

When $N = 3$, after some algebra, one can find the algebraic solution

$$\omega_k = 1 - \frac{2\rho_k(1-2\rho_k)}{1-2\sum_{i=1}^{3}\rho_i^2}$$

and a closer look shows the solution is acceptable only if $\max \rho_k < \frac{1}{2}$.

In the general case, we shall prove that the mapping

$$F(\boldsymbol{\omega}) = \begin{bmatrix} \vdots \\ \dfrac{\omega_k - \omega_k^2}{1-\Omega_2} \\ \vdots \end{bmatrix}$$

is a bijection from the open set

$$D = \left\{ \omega_k \left| \sum_{k=1}^{N} \omega_k = 1, \omega_k > 0 \right. \right\}$$

onto the open set

$$E = \left\{ \rho_k \left| \sum_{k=1}^{N} \rho_k = 1, \omega_k < \frac{1}{2} \right. \right\}.$$

The proof is completed in three steps: (1) F is injective; (2) F maps D into E; (3) F maps D onto E.

Step 1: *F is injective*. We have

$$(1-\Omega_2)\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\omega}} = \mathrm{diag}\,(1-2\omega_k) + 2F(\boldsymbol{\omega})\boldsymbol{\omega}'.$$

F is injective, if $\mathrm{d}F/\mathrm{d}\boldsymbol{\omega}$ is off full rank $N-1$ on the plane $\sum_{k=1}^{N} u_k = 0$ for every $\boldsymbol{\omega} \in D$. Therefore, we have to prove that we cannot find numbers u_k not simultaneously equal to 0 satisfying $\sum u_k = 0$ and for every k:

$$(1-2\omega_k)u_k + 2\frac{\omega_k - \omega_k^2}{1-\Omega_2}\sum_{\ell}\omega_\ell u_\ell = 0. \tag{D.2}$$

(1) $\sum_\ell \omega_\ell u_\ell = 0$ is impossible because:
   (a) If $\omega_k = \frac{1}{2}$ for all k, (D.2) gives $u_k = 0$.
   (b) At most one $\omega_k = \frac{1}{2}$ say ω_1. All the $u_k = 0$ for $k \geqslant 2$ because of (D.2). Moreover, u_1 is also equal to 0 because $\sum_k u_k = 0$.

(2) The u_k are defined up to an arbitrary multiplier and we can normalize by

$$\sum_k \omega_k u_k = 1.$$

Then
   (a) If some $\omega_k = \frac{1}{2}$, there is no solution for (D.2).
   (b) If all $\omega_k < 1/2$, all $u_k > 0$ and $\sum_k \omega_k u_k \neq 0$.

(c) One of the ω_k say $\omega_1 > \frac{1}{2}$ and therefore $u_1 < 0$ and $u_k > 0$, for all the other k. Let $\omega_+ = \max_{k \geqslant 2} \omega_k$, $\omega_+ < 1 - \omega_1 < \frac{1}{2}$. Moreover,

$$\begin{aligned}\sum_{k=1}^{N} \omega_k u_k &= -\omega_1 |u_1| + \sum_{k=2}^{N} \omega_k u_k \\ &\leqslant -\omega_1 |u_1| + \omega_+ (1 + |u_1|) \\ &\leqslant \omega_+ - (\omega_1 - \omega_+)|u_1| \\ &< 1/2,\end{aligned}$$

which concludes Step 1.

Step 2: *F maps D in E*. We prove for instance that $\rho_1 < \frac{1}{2}$. Set $\omega_1 = (1 - t)$ and for any $k \geqslant 2$, $\omega_k = t v_k$ ($\sum_{k=2}^{N} v_k = 1$, $v_k > 0$). Then

$$\rho_1 = \frac{t(1-t)}{1 - (1-t)^2 - t^2 \sigma} = \frac{1}{2} - \frac{1}{2} \times \frac{t(1-\sigma)}{2 - t(1+\sigma)},$$

where

$$\sigma = \sum_{k=2}^{N} v_k^2 < 1.$$

Therefore $\rho_1 < \frac{1}{2}$ but $\lim_{t \to 0} \rho_1 = \frac{1}{2}$. For others k,

$$\rho_k = \frac{v_k}{2} + \frac{1}{2} \times \frac{t v_k (1 + \sigma - 2 v_k)}{2 - t(1+\sigma)}$$

and thus $\lim_{t \to 0} \rho_k = v_k/2$, $k \geqslant 2$.

Step 3: *F maps D onto E*. We follow a similar method as in the proof of Theorem A.1 of Appendix A, and give only a sketch.

(1) Let

$$D_r = \{\boldsymbol{\omega} : \min \omega_k \geqslant r \text{ and } \max \omega_k \leqslant 1 - r\}$$

and $\bar{D}_r$, the border of this set. Those sets form an increasing family (when r decreases) of compact in D of which the union is D.

(2) Let

$$E_\varepsilon = \left\{ \mathbf{c} : \max \rho_k \leqslant \frac{1}{2} - \varepsilon \text{ and } \min \rho_k \geqslant \varepsilon \right\}.$$

Using the equations of Step 2, one can show that for all ε there exists an r such that $F(\bar{D}_r)$ is outside E_ε; like in the proof of Theorem A.1 in Appendix A, we conclude that E is covered.

Remark on Theorem 2. Theorem 2 is also related to a very classical sampling problem. Suppose that a sample of size $n = 2$ is selected with replacement using unequal probabilities p_k for each drawn, where $\sum_{k \in U} p_k = 1$. The rejective sampling design

consists of selecting the first sample that has two distinct units. Then the probability to select the sample $s = \{i, j\}$ is given by

$$p(s) = \pi_{ij} = \frac{2\,p_i\,p_j}{\sum_{k\in U}\sum_{\ell\neq k}\ p_k\,p_\ell} = \frac{2\,p_i\,p_j}{1-\sum_{k\in U}\ p_k^2}.$$

Since $n = 2$ the first-order inclusion probabilities are given by

$$\pi_i = \sum_{j\neq i}\pi_{ij} = \frac{2\,p_i(1-\ p_i)}{1-\sum_{k\in U}\ p_k^2}. \tag{D.3}$$

If the π_i are given, and the aim is the determination after the p_i, we have to solve equation system (D.3), which is exactly the same as (D.1). Note that since $\sum_i\ \pi_i = 2$, Theorem 2 shows that a solution always exists.

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