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# The R Package forestinventory: Design-Based Global and Small Area Estimations for Multiphase Forest Inventories

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#### **Abstract**

Forest inventories provide reliable evidence-based information to assess the state and development of forests over time. They typically consist of a random sample of plot locations in the forest that are assessed individually by field crews. Due to the high costs of these terrestrial campaigns, remote sensing information available in high quantity and low costs is frequently incorporated in the estimation process in order to reduce inventory costs or improve estimation precision. With respect to this objective, the application of multiphase forest inventory methods (e.g., double- and triple-sampling regression estimators) has proved to be efficient. While these methods have been successfully applied in practice, the availability of open-source software has been rare if not non-existent. The R package **forestinventory** provides a comprehensive set of global and small area regression estimators for multiphase forest inventories under simple and cluster sampling. The implemented methods have been demonstrated in various scientific studies ranging from small to large scale forest inventories, and can be used for post-stratification, regression and regression within strata. This article summarizes the mathematical theory of this family of design-based estimators and demonstrates their application in the R environment.

*Keywords*: forest inventory, design-based, infinite population approach, two- and three-phase sampling, regression estimators, small area estimation.

#### 1. Introduction

In many countries, forest inventories have become an indispensable tool for evaluating the current state of forests as well as for tracking their development over time. They provide accurate quantitative information that can be used to define management actions, to adapt forest management strategies according to guidelines on national and international levels and to support in monitoring carbon change in the context of climate reporting and mitigation. As conducting a full census of all trees within any sizable forest area is clearly infeasible due to time and cost restrictions, forest inventories usually gather their information by means of statistical sampling methods. Typically this means that discrete sample locations (sample plots) are randomly chosen in the forest, making up the framework of a terrestrial inventory. This terrestrial sample data is then used to make estimates for the entire forested area and provide a measure of precision for those estimates in the form of confidence intervals. There is a broad

range of literature describing the concepts and methods regarding the choice of different estimators under various sample designs (Gregoire and Valentine 2007; Köhl, Magnussen, and Marchetti 2006; Schreuder, Gregoire, and Wood 1993; Mandallaz 2008).

Terrestrial inventories have the benefit of being very flexible in the sense that they can be used to produce high quality estimates for a wide-variety of different forest attributes. However, they have the downside of being very expensive. Improving the precision of the estimates by increasing the number of sample plots essentially means that travel costs will rise as trained inventorists are sent to more and more plot locations. This is why the number of terrestrial samples is often limited. Although national inventories usually possess a sufficiently large terrestrial sample size to provide high estimation accuracies for larger areas, this is often not the case for smaller areas, such as forest management units. As a result, there has been an increasing need for alternative inventory methods that can maintain the same estimation precision at lower costs, or achieve higher estimation precision at identical costs (von Lüpke 2013). A method which has become particularly attractive is called multiphase sampling. The core concept is to enlarge the sample size in order to gain higher estimation precision without enlarging the terrestrial sample size. This is done by using predictions of the terrestrial target variable at additional sample locations where the terrestrial information has not been gathered. These predictions are produced by regression models that use explanatory variables derived from auxiliary data, commonly in the form of spatially exhaustive remote sensing data in the inventory area. Regression estimators using this concept can consider either one additional sample of plot locations (two-phase or double-sampling) or two additional samples available in different sample sizes (three-phase or triplesampling) (Gregoire and Valentine 2007; Saborowski, Marx, Nagel, and Böckmann 2010; Mandallaz 2013a,d; von Lüpke, Hansen, and Saborowski 2012). Their application to existing forest inventory systems have already showed their efficiency in terms of cost reduction and gain in estimation precision (Breidenbach and Astrup 2012; von Lüpke and Saborowski 2014; Mandallaz, Breschan, and Hill 2013; Magnussen, Mandallaz, Breidenbach, Lanz, and Ginzler 2014; Massey, Mandallaz, and Lanz 2014).

Multistage and multiphase estimation has already been implemented in commercial as well as opensource software, such as the survey sampling procedures in SAS (SAS Institute Inc. 2015) and the survey package in R (Lumley 2016). However, both are targeted towards list-sampling as it is applied in official statistics. Available software providing multiphase sampling methods better suited for forest inventories has been rare. Two exceptions are the R package JoSAE by Breidenbach (2015) and the maSAE package by Cullmann (2016). However, a more comprehensive software package covering a larger variety of sample designs and estimators for forest inventories has not yet been available, which is the motivation behind the R package forestinventory. The package provides global and small area estimators for two-phase and three-phase forest inventories under simple and cluster sampling, which have been developed under the infinite population approach by Daniel Mandallaz at ETH Zurich between 2008 and 2017. The implemented methods have been demonstrated by case studies in Switzerland (Massey et al. 2014; Massey and Mandallaz 2015b; Mandallaz et al. 2013) and Germany (Hill, Mandallaz, and Langshausen 2018b). The implemented estimators cover 32 inventory scenarios and can be used for post-stratification, regression and regression within strata (Massey 2015). The long-term objective of **forestinventory** is to make the broad range of estimators available to a large user community and to facilitate their application in science as well as operational forest management.

The objectives of this article are to a) establish the link between the mathematical description of the estimators and their implementation in our package, b) illustrate their application to real-world inventory data sets and c) address special cases and demonstrate how the package-functions handle them.

# 2. Methods and structure of the package

#### 2.1. Forest inventory in the infinite population approach

Most forest inventories gather terrestrial information by sending field crews to randomly (or systematically) selected points in the forest area defined by coordinates. The crew then defines a sample plot by measuring individual trees located within one or multiple constructed inclusion circles around the sample point x, and aggregating their characteristics (e.g., timber volumes) to local plot densities (e.g., the timber density in m<sup>3</sup>/ha) including potential boundary adjustments (see Mandallaz (2008) for details). The estimators implemented in **forestinventory** use the so-called infinite population approach in order to bridge this inventory process to the mathematics behind the estimators. This approach assumes that the spatial distribution of the local density, Y(x), over the forest area is determined by a fixed piecewise constant function, as visualized in Fig. 1. The population total of the target variable (e.g., the total timber volume of the forest) is mathematically equivalent to the integral of that density function, which is depicted in Fig. 1 as the volume under the density surface. From this perspective, the practical challenge is that the form of this function is unknown. Theoretically, we could get the total timber volume by observing the function value, i.e., the local density Y(x), at each possible point x over the forest area and taking their sum. However, this is impossible because there is an infinite number of points in the forest area. Our strategy is thus to take a sample of  $n_2$  points,  $s_2$ , from an infinite population of possible points and use their associated local densities Y(x) to estimate the integral  $Y = \frac{1}{\lambda(F)} \int_F Y(x) dx$  with  $\hat{Y} = \frac{1}{n_2} \sum_{x \in s_2} Y(x)$ . The total timber volume can then be obtained by multiplying  $\hat{Y}$  by the known surface area of the forest,  $\lambda(F)$ . It should be noted  $\lambda(F)$  is often estimated in practice (see Mandallaz (2014)) for further explanation) but that is beyond the scope of this article. All estimators included in **forestinventory** rest upon this theoretical perspective. The key point in the infinite population approach is that a local density value Y(x) is associated with the sample point x, which constitutes the sample unit, and not with the sample plot area. Sampling the actual plot areas follows the so-called finite population approach, where the sample units are usually assumed to be either circular or rectangular plots. Although choosing between infinite and finite population schemas does not likely make much practical difference, the former does has some theoretical advantages. This is mainly due to the impossibility of a perfect tessellation over an amorphous forest area by any choice of plot shape. Hence, the population in the finite approach is, strictly speaking, not well defined with respect to the forest area. Also, cluster sampling is much more easily generalized in the infinite population approach. The consideration of an underlying infinite population of sample points will also play an important role when incorporating auxiliary information in the frame of two- and three-phase estimation methods.

#### 2.2. Two-phase sampling

The two-phase or double-sampling estimators use inventory information from two nested samples which are commonly referred to as phases (Fig. 2a). The first phase  $s_1$  comprises  $n_1$  sample locations that each provide a set of explanatory variables described by the column vector  $\mathbf{Z}(x) = (z(x)_1, z(x)_2, ..., z(x)_p)^{\top}$  at each point  $x \in s_1$ . These explanatory variables are derived from auxiliary information that is available in high quantity within the forest area F. The second phase  $s_2$  constitutes the terrestrial inventory conducted at  $n_2$  subsamples of the large phase  $s_1$  and provides the value of the target variable, i.e., the local density Y(x) (e.g., the timber volume per hectare). For every  $x \in s_1$ ,  $\mathbf{Z}(x)$  is transformed into a prediction  $\hat{Y}(x)$  of Y(x) using the choice of some model, which in **forestinventory** is always a linear model fit in  $s_2$  using ordinary least squares (OLS). The basic idea of this setup is to boost the sample size by providing a large sample of less precise but cheaper predictions of Y(x) in  $s_1$ 

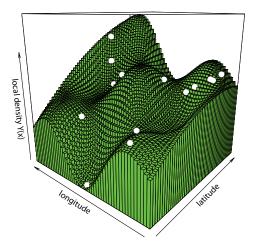


Figure 1: Artificial representation of a local density surface. The spatial distribution of a hypothetical density function for every point in a forested area is represented as a wavy piecewise constant green surface. Sample plots (white dots) inform the inventorist of the value of the density function at that point. Note that the plateaus of constant Y(x) values here have the shape of squares whereas in reality they are likely to be formed by the intersection of circles around trees.

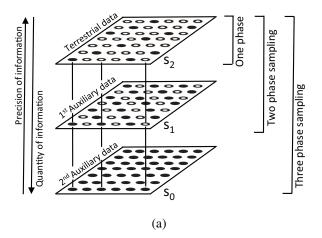
and to correct any possible model bias, i.e.,  $\mathbb{E}(Y(x) - \hat{Y}(x))$ , using the subsample of terrestrial inventory units where the value of Y(x) is observed. In the design-based context, the two-phase estimator is typically unbiased regardless of the model used to produce the predictions. This property comes from the assumption that each phase's sample is selected via simple random sampling (see Section 2.5).

#### 2.3. Three-phase sampling

Three-phase estimators extend the principle of two-phase sampling and use inventory information from three nested samples (phases) (Fig. 2a). The basic setup is that the explanatory variables calculated from the auxiliary information are available in two different frequencies. The phase  $s_0$  provides a large number  $n_0$  of auxiliary data, whereas the phase  $s_1$  provides additional auxiliary data that are only available at  $n_1$  subsamples of  $s_0$ . The terrestrial information is then collected at a further subsample  $s_2$  of  $s_1$ . The motivation for three-phase sampling is that the additional set of explanatory variables available at  $s_1$ , now denoted  $\mathbf{Z}^{(1)}(x)$ , adds considerable explanatory power to the set of variables available at all sample locations  $s_0$ , denoted  $\mathbf{Z}^{(0)}(s_0)$ . From that it follows that we can define two nested regression models. The full set of predictor variables  $\mathbf{Z}^{\top}(s) = (\mathbf{Z}^{(0)\top}(s), \mathbf{Z}^{(1)\top}(s))$  can be used to calculate the predictions  $\hat{\mathbf{Y}}(s)$  of  $\mathbf{Y}(s)$  at all sample locations  $s_0$ . The regression model applicable to the  $s_1$  phase is thus referred to as the full model. Less accurate predictions,  $\hat{\mathbf{Y}}^{(0)}(s)$ , can be produced at all the sample locations  $s_0$  using only the reduced set of explanatory variables  $\mathbf{Z}^{(0)}(s)$ . If there is a significant gain in model precision between the reduced and the full model and the sampling fraction between  $s_0$  and  $s_1$  is sufficiently large, the three-phase estimator normally leads to a further increase in estimation precision compared to the two-phase estimator.

#### 2.4. Small area estimation

Small area estimation does not necessarily refer to small spatial areas but rather to areas that contain little or no terrestrial sample. To formulate this mathematically, we want to make an estimate for a subregion G of the entire inventory area F (Fig. 2b). As the sample size in the small area,  $n_{2,G}$ , is usually too small to provide sufficient estimation precision, multiphase estimation can be efficient.



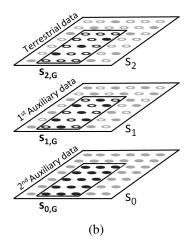


Figure 2: (a) Concept of multiphase sampling. The square represents the forest area for which an inventory is being conducted. The points denote the sample locations *x*. Filled points indicate available information. (b) Illustration of the small area estimation problem.

However,  $n_{2,G}$  may also be too small to justify fitting a separate regression model just for that area because the estimates produce undesirably large confidence intervals. The idea is then to borrow strength from the entire terrestrial sample  $s_2$  of F to fit the model, and to apply this model to the small area. The potential bias of applying that model in G is then corrected for by using the empirical model residuals derived from that small area. If there are no terrestrial plots in G (i.e.,  $n_{2,G} = 0$ ), one cannot correct for a potential model bias in G and has to accept a potential bias in the estimator. These are called synthetic estimates and despite their potential bias, it is usually still possible to calculate their design-based variance.

#### 2.5. Design-based vs. model-dependent approach

The subject of model selection gets a lot of attention in the field of forest inventory. This is why it is important to understand that the mathematical interpretation of how a model is used to produce estimates is fundamentally different between the design-based and model-dependent approach. In the model-dependent (also known as model-based) framework, the sample locations x are fixed and the observation Y(x) taken at location x is assumed to be a random variable as the forest is assumed to be the realization of a stochastic process. Although the model does not need to be fit from a probability sample, i.e., the sample locations could arbitrarily be chosen, the model should adequately describe the underlying stochastic process in order to efficiently ensure unbiased results. In practice this means that special attention must be made to ensure that the variable selection is appropriate to avoid overfitting, important variables are not omitted and all model assumptions are reasonably met through empirical verification. If a model is misspecified then estimation based on inference from that model may not be reliable. In the model-dependent framework one thus has to trust the model. In contrast, the designbased approach, on which all **forestinventory** estimators are based, rests upon the randomization of the sample locations x. While the sample locations x are independently and uniformly distributed in the forest, the forest itself and thus the values of the local density surface at any location  $x \in F$  are fixed and not the result of a stochastic process. A selected observation Y(x) still remains a random variable, but solely due to the random sample mechanism. A consequence of this approach is that the estimation properties of design-based regression estimators (e.g., unbiasedness) typically hold regardless of the model that is chosen. The philosophy of the design-based approach is thus to use prediction models to improve the efficiency of the estimators without having to rely on their correct specification, which

makes them very attractive to be used in official statistics. They are therefore also referred to as model-assisted. It should be noted that the randomization of sample locations upon which design-based inference depends, is in practice often replaced by systematic grids to achieve a more spatially balanced sample in the terrestrial survey. However, there is reasonable evidence that softening this assumption is acceptable for point and variance estimation as long as the grid does not interact with periodic features in the forest structure (Mandallaz 2008). The variance will in most cases be slightly overestimated and lead to wider, more conservative confidence intervals (Mandallaz 2013a).

#### 2.6. Package structure

In the **forestinventory** package, estimators for two-phase and three-phase sampling are applied with the twophase() and threephase() functions. From these two overall function calls, various estimators for specific inventory scenarios under the chosen sampling design can be applied (Fig. 3). Choosing an estimator follows a tree-like structure which can serve the user as a guideline throughout this article as well as in future applications. The basic decision to make is whether an estimate and its variance should be computed for an entire inventory area (global estimators) or only for subregions of the entire inventory area (small area estimators). In the second case, the package offers three small area estimators that will in detail be described in the following sections. The estimators are available under exhaustive and non-exhaustive use of the auxiliary data. Additionally, the package can also calculate one-phase estimates solely based on terrestrial samples. All estimators are also available for cluster sampling, in which case a sample unit consists of multiple, spatially agglomerated samples. The following sections describe the mathematical details and the application of the multiphase estimators implemented in the R package forestinventory. While Mandallaz (2008, 2013c,b, 2015) provides an extensive derivation of all estimators, we will provide the mathematical formulas that are actually implemented in the package. We will also restrict discussion to simple sampling, while the formulas for cluster sampling are available in the technical reports (Mandallaz, Hill, and Massey 2016; Mandallaz 2013c,b). A special case under cluster sampling is described in Section 6.

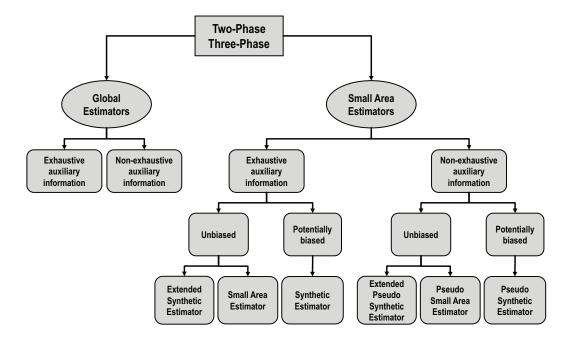


Figure 3: Structure of the multiphase estimators in the R package **forestinventory**. All estimators are also available for cluster sampling.

# 3. Two-phase estimators and their application

#### 3.1. Global estimators

#### Mathematical background

The vector of regression coefficients of the OLS regression model is found by using the following solution to the sample-based normal equation:

$$\hat{\boldsymbol{\beta}}_{s_2} = \left(\frac{1}{n_2} \sum_{x \in s_2} \mathbf{Z}(x) \mathbf{Z}^{\top}(x)\right)^{-1} \left(\frac{1}{n_2} \sum_{x \in s_2} Y(x) \mathbf{Z}(x)\right)$$
(1)

The individual predictions can then be calculated as  $\hat{Y}(x) = \mathbf{Z}^{\top}(x)\hat{\boldsymbol{\beta}}_{s_2}$  and the empirical model residuals, which are only available at all sample locations  $x \in s_2$ , are calculated as  $\hat{R}(x) = Y(x) - \hat{Y}(x)$ . Unless stated otherwise, **forestinventory** only uses internal models to calculate estimates. This means that the model fit, i.e.,  $\hat{\boldsymbol{\beta}}_{s_2}$ , is derived from the current inventory data that are passed to the twophase() and threephase() functions. While virtually all inventorists fit their models using the current inventory data, sometimes there is reason to use formulas derived from external models where the sample used to train the model is assumed to be taken from an independent source (Massey and Mandallaz 2015a). However, this usually occurs when using a model other than the OLS regression model and is beyond the scope of the package at this time.

The package provides the calculation of point estimates under exhaustive (EX) and non-exhaustive (NEX) use of the auxiliary information, which means to respectively apply  $\hat{\beta}_{s_2}$  to  $\bar{\mathbf{Z}}$ , i.e., the exact spatial mean of  $\mathbf{Z}(x)$ , or to  $\hat{\mathbf{Z}}$ , i.e., an estimate of the spatial mean of  $\mathbf{Z}(x)$ :

$$\hat{Y}_{reg2p,EX} = \bar{\mathbf{Z}}^{\top} \hat{\boldsymbol{\beta}}_{s_2} \tag{2a}$$

$$\hat{Y}_{reg2p,NEX} = \hat{\mathbf{Z}}^{\top} \hat{\boldsymbol{\beta}}_{s_2} \tag{2b}$$

Note that for internal linear models containing intercept terms, the mean of the empirical residuals  $\frac{1}{n_2}\sum_{x\in s_2}\hat{R}(x)$  is zero by construction (zero mean residual property) which is why it does not appear in the point estimate. More explanation about how to obtain the auxiliary means is given in the next subsection

The **forestinventory** package implements two kinds of variances for each of these point estimates: the g-weight formulation that accounts for the fact that our model is in fact internal, and the external variance formulation that assumes a true external regression model and thus neglects the uncertainty in the regression coefficients (Mandallaz *et al.* 2016).

The g-weight formulation is

$$\hat{\mathbb{V}}(\hat{Y}_{reg2p,EX}) := \bar{\mathbf{Z}}^{\mathsf{T}} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \bar{\mathbf{Z}}$$
(3a)

$$\hat{\mathbb{V}}(\hat{Y}_{reg2p,NEX}) := \hat{\bar{\mathbf{Z}}}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \hat{\bar{\mathbf{Z}}} + \hat{\boldsymbol{\beta}}_{s_2}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\bar{\mathbf{Z}}}} \hat{\boldsymbol{\beta}}_{s_2}$$
(3b)

where the g-weight variance-covariance matrix of  $\hat{\boldsymbol{\beta}}_{s_2}$  is calculated as

$$\hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} := \left(\frac{1}{n_2} \sum_{x \in s_2} \boldsymbol{Z}(x) \boldsymbol{Z}^{\top}(x)\right)^{-1} \left(\frac{1}{n_2^2} \sum_{x \in s_2} \hat{R}^2(x) \boldsymbol{Z}(x) \boldsymbol{Z}^{\top}(x)\right) \left(\frac{1}{n_2} \sum_{x \in s_2} \boldsymbol{Z}(x) \boldsymbol{Z}^{\top}(x)\right)^{-1}$$
(4)

and the uncertainty caused by using the  $s_1$  sample to estimate  $\bar{Z}$  by  $\hat{Z}$  is accounted for by the variance-covariance matrix of the auxiliary vector  $\hat{Z}$ 

$$\hat{\Sigma}_{\hat{\mathbf{Z}}} = \frac{1}{n_1(n_1 - 1)} \sum_{x \in s_1} (\mathbf{Z}(x) - \hat{\mathbf{Z}}) (\mathbf{Z}(x) - \hat{\mathbf{Z}})^{\top}$$

$$(5)$$

The external variance formulation for linear regression models is

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{reg2p,EX}) = \frac{1}{n_2} \hat{\mathbb{V}}_{s_2}(\hat{R}(x))$$

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{reg2p,NEX}) = \frac{1}{n_1} \hat{\mathbb{V}}_{s_1}(\hat{Y}(x)) + \frac{1}{n_2} \hat{\mathbb{V}}_{s_2}(\hat{R}(x))$$
(6a)

where  $\hat{\mathbb{V}}_{s_2}$  and  $\hat{\mathbb{V}}_{s_1}$  indicate taking the sample variance over  $s_2$  and  $s_1$  respectively.

Note that when applied to internal linear regression models, the external variance is asymptotically unbiased and usually slightly smaller than the g-weight variance, where the uncertainty of the regression coefficients is accounted for by the variance-covariance matrix (Eq. 4). The external variances are provided in the package **forestinventory** in case the user wants to compare linear models to another model type where no g-weight formulation is possible, as is the case with non-parametric models like kNN.

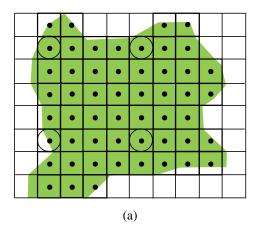
#### Calculation of explanatory variables

We will now draw our attention to the calculation of the explanatory variables from the auxiliary data for both the non-exhaustive and exhaustive cases. Fig. 4b depicts how the non-exhaustive case often looks like in practice: a regular terrestrial grid  $s_2$  is given by a terrestrial inventory (the points surrounded by dotted circles) and densified to a larger sample  $s_1$  (the points). For every point x, each explanatory variable in the vector  $\mathbf{Z}(x) = (z(x)_1, z(x)_2, ..., z(x)_p)^{\top}$  is calculated using a defined spatial extent of auxiliary information around that point called the support (the dark green square tiles). We emphasize that the value of the explanatory variables for  $\mathbf{Z}(x)$  are associated with the sample point whereas the support is the spatial extent of the auxiliary information used to calculate those values. So far this is in perfect agreement with the presented theory of the non-exhaustive estimator, except for using regular grids rather than randomly placed sample points. The **forestinventory** package calculates the empirical mean of  $\mathbf{Z}(x)$  automatically from the input data frame using  $\hat{\mathbf{Z}} = \frac{1}{n} \sum_{x \in s_1} \mathbf{Z}(x)$ .

The exhaustive case requires a closer look. In the infinite population approach,  $\mathbf{Z}(x)$  refers to the sample point x and not the area around it. Deriving the exact spatial mean,  $\bar{\mathbf{Z}} = \frac{1}{\lambda(F)} \int_F \mathbf{Z}(x) dx = (\frac{1}{\lambda(F)} \int_F z_1(x) dx, ..., \frac{1}{\lambda(F)} \int_F z_p(x) dx)^{\top}$ , implies that we need to calculate the spatial mean of each component of  $\mathbf{Z}(x)$  using all possible points in F. This is much like the situation we had with calculating the mean of the local density surface for Y(x) in that we need to find the mean of  $\mathbf{Z}(x)$  over an infinite number of sample points (i.e.,  $n_1 = \infty$ ). Although it is practically infeasible to assess  $\mathbf{Z}(x)$  for every x, there are few cases where the exact mean can in fact be precisely calculated. The first case is when the explanatory variables are provided by polygon layers (e.g., map of development stages). In this case, one can calculate the exact mean as the area-weighted average of each categorical variable. The second case is when the exact mean can be calculated in one step, e.g., taking the mean of all height pixels of a raster canopy height model will exactly equal the mean calculated by the use of an infinite number of supports (Mandallaz *et al.* 2013). However, for most types of explanatory variables, e.g. order statistics such as maximum or median canopy height in the spatial extent, this approach will fail. For example, the mean of the maximum pixel heights across all supports is clearly not equal to the

global maximum pixel height across the entire area. In such cases, we will try to get an approximation of  $\bar{\mathbf{Z}}$  that is only negligibly different.

One implementation to approximate the exact mean  $\bar{Z}$  is shown in Fig. 4a, where the spatial arrangement of the supports (the dark green tiles) are tessellated to form a perfect partition over the inventory area in order for all of the wall-to-wall auxiliary information to be exploited. Is has to be noted that this setup would allow for a perfect calculation of the exact mean  $\bar{Z}$  in the finite population approach, i.e., deriving Z(x) for the finite population of supports that are considered the sampling units. While in the infinite population approach this implementation probably does not produce the true exact mean  $\bar{Z}$ ,  $n_1$  is still expected to be reasonably large for the difference to be considered negligible as long as the size of the supports are not unreasonably large. However, the perfect tessellation implementation can also impose drawbacks. One is that a perfect tessellation by the supports strongly depends on the distance between the sample locations of  $s_1$  and the support size. Since in practice the support size should ideally be chosen to achieve a best possible explanatory power of the regression model (Hill, Buddenbaum, and Mandallaz 2018a) a perfect tessellation might often not be feasible. In the infinite population frame, the supports are allowed to overlap if this seems necessary to acquire a sufficiently large sample  $n_1$  to get a negligibly close approximation of  $\bar{Z}$ . With this respect, the infinite population approach provides more flexibility than the finite approach.



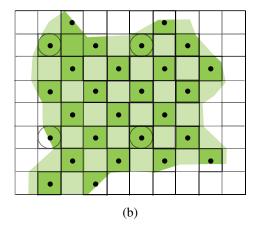


Figure 4: Concept of (a) exhaustive and (b) non-exhaustive calculation of explanatory variables including boundary adjustment at the support level. Auxiliary data are in both cases available over the entire inventory area marked by the large rectangle. A vector of explanatory variables  $\mathbf{Z}(x)$  is calculated within the supports (small squares) at each sample location x (points) that falls into the forest area (green underlying polygon).

### Boundary adjustment

An extension to the so-far published estimators by Mandallaz is the consideration of a boundary adjustment. In forest inventories, the sample is often restricted to those sample locations located within the forest area. In case a consistent forest definition can be applied to both the  $s_2$  and  $s_1$  sample (e.g., by a polygon forest mask layer), it might be desired to restrict the calculation of the explanatory variables to the forest area within the given support (see Fig. 4). This method was suggested in Mandallaz *et al.* (2013) and led to an improvement in estimation precision. In order to ensure an unbiased calculation of either  $\hat{\mathbf{Z}}$  or  $\bar{\mathbf{Z}}$ , the respective means have then to be calculated as the weighted mean (Eq. 7) where

the weight w(x) is equal to the percentage of forested area within the support of sample location x.

$$\hat{\bar{\mathbf{Z}}} = \frac{\sum_{x \in s_1} w(x) \mathbf{Z}(x)}{\sum_{x \in s_1} w(x)}$$
(7)

#### **Application**

To demonstrate the use of the global two-phase estimators, we will use the grisons data set that comes with installing the package from the CRAN repository. The data set contains data from a simple (i.e., non-cluster) two-phase forest inventory conducted in 2007 that was used in Mandallaz *et al.* (2013) as a case study. The  $s_1$  sample is comprised of 306 sample locations arranged on a systematic grid containing auxiliary information in the form of airborne laserscanning (LiDAR) canopy height metrics (mean, stddev, max, q75). For a systematic subsample of 67 ( $s_2$  sample), terrestrial information of the timber volume per hectare (tvo1) on the sample plot level is provided from a terrestrial survey. We can load **forestinventory** and examine the grisons data set in the R environment as follows:

```
R> library("forestinventory")
R> data("grisons", package = "forestinventory")
R> head(grisons)
```

	phase_id_2p	boundary_weights	mean	stddev	max	q75	smallarea	tvol
1	2	1.00	9.30	11.84	40.87	21.14	C	107.80
2	1	1.00	12.16	11.35	39.80	21.54	Α	NA
3	2	1.00	5.25	5.74	23.82	9.53	D	63.77
4	1	1.00	7.53	9.33	34.10	13.02	Α	NA
5	1	0.67	6.11	5.87	23.33	10.55	В	NA
6	1	1.00	12.15	10.16	33.76	20.97	C	NA
7	2	1.00	6.38	4.72	17.96	10.14	D	154.10
8	1	1.00	1.25	3.79	22.72	0.00	В	NA
9	1	1.00	21.56	7.49	32.66	27.81	A	NA
10	2	1.00	13.55	7.20	36.14	18.59	A	256.15

Estimates can be made using the onephase(), twophase() or threephase() functions. The data frame inputted to these functions must have the structure where each row corresponds to a unique sample location and the columns specify the attributes associated to that respective sample location. Attributes that are missing, e.g., because they are associated with sample locations that were not selected in the subsample for the subsequent phase, should be designated as NA and the phase membership is encoded as numeric.

For global two-phase estimation, we have to specify

- the regression model (formula) as specified in the lm()-function (R Core Team 2017).
- the inputted data.frame containing the inventory information (data).
- the list-object phase\_id containing: the phase.col argument identifying the name of the column specifying membership to  $s_1$  or  $s_2$ , and the terrgrid.id argument specifying which numeric value indicates  $s_2$  membership in that column. Note that **forestinventory** implicitly assumes that all rows not indicated as  $s_2$  belong to the  $s_1$  phase.
- the name of the column containing the weights w(x) of the boundary adjustments (optional).

The non-exhaustive estimator with boundary weight adjustment can thus be applied as follows:

```
R> reg2p_nex <- twophase(formula = tvol ~ mean + stddev + max + q75, data = grisons,
+ phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
+ boundary_weights = "boundary_weights")</pre>
```

The twophase() function creates an S3 object of class "twophase" with subclass "global". A readable summary of the estimation results can be obtained by passing this object to the summary() function, which automatically interprets what type of estimator was used and returns pertinent information such as the regression model formula, the point estimate (estimate), the g-weight and external variance (g\_variance and ext\_variance) as well as the sample sizes and the model R<sup>2</sup>:

```
R> summary(reg2p_nex)
Two-Phase global estimation
Call:
twophase(formula = tvol ~ mean + stddev + max + q75, data = grisons,
    phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
    boundary_weights = "boundary_weights")

Method used:
Non-exhaustive global estimator

Regression Model:
tvol ~ mean + stddev + max + q75

Estimation results:
    estimate ext_variance g_variance n1 n2 r.squared
383.5354 279.954 271.5057 306 67 0.6428771
```

'boundary\_weight'- option was used to calculate weighted means of auxiliary variables

For practical use, one should normally always prefer the g-weight variance over the external variance. This is because when we use internal models, the regression coefficients actually depend on the terrestrial sample realized by the sampling design. In contrast to the external variance, the g-weight variance accounts for this sampling variability which results in more reliable point and variance estimates and also enjoys better statistical calibration properties (g-weights). The external and g-weight variances are asymptotically equivalent but the external variance is really only included here in case the user wants to compare to another estimator where no g-weight variance exists.

The exhaustive estimator can be applied by additionally passing a vector containing the exact means of the explanatory variables, i.e.,  $\bar{Z}$ , to the optional argument exhaustive. This vector must be calculated beforehand in such a way that any desired boundary adjustment has already been applied. Note that the vector input to exhaustive must be in the same order that the lm()-function processes a formula object including the intercept term whose exact mean will always be 1. Particular caution must be taken if categorical variables are present because the lm()-function, which is internally used to set up the design-matrix, automatically creates dummy variables with one of the categories used as a reference. Using our grisons example, the correct order can always be extracted by the following R-code:

```
R> colnames(lm(formula = tvol ~ mean + stddev + max + q75, data = grisons, + x = TRUE)$x)
```

The exhaustive estimator can be applied after defining the vector of exact means  $\bar{Z}$  taken from Mandallaz *et al.* (2013), denoted as true.means.Z:

```
R> true.means.Z \leftarrow c(1, 11.39, 8.84, 32.68, 18.03)
R> reg2p_ex <- twophase(formula = tvol ~ mean + stddev + max + q75, data = grisons, + phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2), exhaustive = true.means.Z)
```

An alternative way to look at the estimation results without using the summary() is to query reg2p\_ex directly:

```
estimate ext_variance g_variance n1 n2 r.squared 1 376.7426 202.5602 187.2787 Inf 67 0.6428771
```

Note that both variances of the exhaustive estimation are smaller than those of the non-exhaustive estimation. This is essentially because we eliminated one component of uncertainty by substituting the estimated means of the explanatory variables  $\hat{Z}$  by their exact means  $\bar{Z}$ .

#### 3.2. Small area estimators

R> reg2p\_ex\$estimation

#### Mathematical background

The **forestinventory** package provides three types of small area estimators each of which has an exhaustive and non-exhaustive form. We will use a different nomenclature for the non-exhaustive case in small area estimation since much of the existing literature shows preference for the label pseudo to indicate that the mean of the explanatory variables within the small area was based on a finite sample. The main idea for all these small area estimators is to calculate the regression coefficient vector  $\hat{\boldsymbol{\beta}}_{s_2}$  and its variance-covariance matrix  $\hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}}$  on the entire  $s_2$  sample according to Eq. 1 and 4, and subsequently use that to make predictions for sample locations restricted to small area G.

We first introduce the small area estimator (SMALL), which uses exhaustively computed explanatory variables, and its non-exhaustive version, the pseudo small area estimator (PSMALL).

$$\hat{Y}_{G,SMALL,2p} = \bar{\mathbf{Z}}_G^{\mathsf{T}} \hat{\boldsymbol{\beta}}_{s_2} + \frac{1}{n_{2,G}} \hat{R}(x)$$
(8a)

$$\hat{Y}_{G,PSMALL,2p} = \hat{\mathbf{Z}}_{G}^{\top} \hat{\boldsymbol{\beta}}_{s_2} + \frac{1}{n_{2,G}} \hat{R}(x)$$
(8b)

In the equations for the point estimates (Eq. 8a and 8b), we see that the globally derived regression coefficients are applied to the exhaustively or non-exhaustively calculated means of the explanatory variables ( $\bar{Z}_G$ ,  $\hat{\bar{Z}}_G$ ) which are now only based on the first-phase sample  $s_{1,G}$  located within small area G. A potential bias of the regression model predictions in the small area G, due to fitting the regression model with data also outside of G, is then corrected by adding the mean of the empirical model residuals in G. This is called the bias or residual correction term.

The package provides the g-weight variance for SMALL and PSMALL respectively (Eq. 9a, 9b) as well as the external variance (Eq. 10a, 10b). Again note that all components are restricted to those available at the sample locations in the small area ( $s_{1,G}$  and  $s_{2,G}$ ), with exception of the regression coefficient components  $\hat{\boldsymbol{\beta}}_{s_2}$  and  $\hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}}$ .

$$\hat{\mathbb{V}}(\hat{Y}_{G,SMALL,2p}) := \bar{\mathbf{Z}}_{G}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \bar{\mathbf{Z}}_{G} + \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}(x))$$
(9a)

$$\hat{\mathbb{V}}(\hat{Y}_{G,PSMALL,2p}) := \hat{\bar{\mathbf{Z}}}_{G}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_{2}}} \hat{\bar{\mathbf{Z}}}_{G} + \hat{\boldsymbol{\beta}}_{s_{2}}^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\mathbf{Z}}_{G}} \hat{\boldsymbol{\beta}}_{s_{2}} + \frac{1}{n_{2 G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}(x))$$
(9b)

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{G,SMALL,2p}) := \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}(x))$$
 (10a)

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{G,PSMALL,2p}) := \frac{1}{n_{1,G}} \hat{\mathbb{V}}_{s_{2,G}}(Y(x)) + \left(1 - \frac{n_{2,G}}{n_{1,G}}\right) \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}(x))$$
(10b)

where  $\hat{\mathbb{V}}_{s_{2,G}}$  indicates taking the sample variance over  $s_{2,G}$ . If boundary adjustment is applied, the simple mean of the explanatory variable vector over the small area  $\hat{\mathbf{Z}}_G = \frac{1}{n_{1,G}} \sum_{x \in s_{1,G}} \mathbf{Z}(x)$  is replaced by its weighted version  $\hat{\mathbf{Z}}_G = \frac{\sum_{x \in s_{1,G}} w(x) \mathbf{Z}(x)}{\sum_{x \in s_{1,G}} w(x)}$ , and likewise for exhaustively used auxiliary information.

The synthetic estimator (SYNTH) and pseudo synthetic estimator (PSYNTH) are commonly applied when no terrestrial sample is available within the small area G (i.e.,  $n_{2,G} = 0$ ). In this case, the point estimates (Eq. 11a and 11b) are based only on the predictions generated by applying the globally derived regression model to the auxiliary vectors  $\mathbf{\bar{Z}}_G$  and  $\mathbf{\bar{Z}}_G$  respectively. However, the bias correction using the observed residuals  $\hat{R}(x)$  is not applied as was the case in the small and pseudo small area estimator (Eq. 8a and 8b). Thus, the (pseudo) synthetic estimator has a potentially unobservable design-based bias. Also note that the residual variation can no longer be considered in the g-weight variance (Eq. 11c and 11d). Therefore, the synthetic estimators will usually have a smaller variance than estimators incorporating the regression model uncertainties, but at the cost of a potential bias. Due to the absence of available residuals in G, there is also no external variance form for the synthetic and pseudo synthetic estimator.

$$\hat{Y}_{G,SYNTH,2p} = \bar{\boldsymbol{Z}}_{G}^{\top} \hat{\boldsymbol{\beta}}_{s_{2}} \tag{11a}$$

$$\hat{Y}_{G,PSYNTH,2p} = \hat{\mathbf{Z}}_{G}^{\top} \hat{\boldsymbol{\beta}}_{s_{2}} \tag{11b}$$

$$\hat{\mathbb{V}}(\hat{Y}_{G,SYNTH,2p}) = \bar{\mathbf{Z}}_{G}^{\mathsf{T}} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}} \bar{\mathbf{Z}}_{G}$$
(11c)

$$\hat{\mathbb{V}}(\hat{Y}_{G,PSYNTH,2p}) = \hat{\mathbf{Z}}_{G}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_{2}}} \hat{\mathbf{Z}}_{G} + \hat{\boldsymbol{\beta}}_{s_{2}}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\mathbf{Z}}_{G}} \hat{\boldsymbol{\beta}}_{s_{2}}$$
(11d)

where the variance-covariance matrix of the auxiliary vector  $\hat{\mathbf{Z}}_G$  is estimated by

$$\hat{\Sigma}_{\hat{\mathbf{Z}}_{G}} = \frac{1}{n_{1,G}(n_{1,G} - 1)} \sum_{x \in S_{1,G}} (\mathbf{Z}(x) - \hat{\mathbf{Z}}_{G})(\mathbf{Z}(x) - \hat{\mathbf{Z}}_{G})^{\top}$$
(12)

The synthetic estimators, SYNTH and PSYNTH, have attractively compact formulas but come with the downside of potential bias in their point estimates which can make the variances seem deceptively optimistic. The SMALL and PSMALL estimators overcome this issue by using a bias correction term, i.e.,  $\frac{1}{n_{2,G}}\sum_{x\in s_{2,G}} \hat{R}(x)$ . The motivation behind the extended synthetic and extended pseudo synthetic estimator (EXTSYNTH and EXTPSYNTH) is to use the same mathematically elegant formulas of the (pseudo) synthetic estimators while ensuring that the mean of the empirical prediction model residuals in the entire area F and the small area G are by construction both zero at the same time. This is

accomplished by extending the vector of auxiliary information  $\mathbf{Z}(x)$  by a binary categorical indicator variable  $I_G(x)$  which takes the value 1 if the sample location x lies inside the target small area G and is otherwise set to 0. Recalling that linear models fitted using OLS have zero mean residual property by construction also if categorical variables are used, this leads to unbiased point estimates. The new extended auxiliary vector thus becomes  $\mathbf{Z}^{\top}(x) = (\mathbf{Z}^{\top}(x), I_G^{\top}(x))$  and can be used to replace its non-extended counterpart  $\mathbf{Z}^{\top}(x)$  whereever it is used in Eq. 11 and 12. Note that the package functions internally extend the data set by the indicator variable if the EXTSYNTH or EXTPSYNTH estimator is called.

Not every equation needs to be re-written here, but to give an example of the notational change, the regression coefficient under extended model approach becomes

$$\hat{\boldsymbol{\theta}}_{s_2} = \left(\frac{1}{n_2} \sum_{x \in s_2} \mathbf{Z}(x) \mathbf{Z}^\top(x)\right)^{-1} \left(\frac{1}{n_2} \sum_{x \in s_2} Y(x) \mathbf{Z}(x)\right)$$
(13)

The point estimates and their g-weight variances can then be re-written as

$$\hat{Y}_{G,EXTSYNTH,2p} = \bar{\mathbf{Z}}_{G}^{\top} \hat{\boldsymbol{\theta}}_{s_{2}} \tag{14a}$$

$$\hat{Y}_{G,EXTPSYNTH,2p} = \hat{\mathbf{Z}}_{G}^{\top} \hat{\boldsymbol{\theta}}_{s_{2}}$$
 (14b)

$$\hat{\mathbb{V}}(\hat{Y}_{G,EXTSYNTH,2p}) = \bar{\mathbf{Z}}_{G}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\theta}}_{SS}} \bar{\mathbf{Z}}_{G}$$
(14c)

$$\hat{\mathbb{V}}(\hat{Y}_{G,EXTPSYNTH,2p}) = \hat{\bar{\mathbb{Z}}}_{G}^{\top} \hat{\pmb{\Sigma}}_{\hat{\boldsymbol{\theta}}_{s_{2}}} \hat{\bar{\mathbb{Z}}}_{G} + \hat{\boldsymbol{\theta}}_{s_{2}}^{\top} \hat{\pmb{\Sigma}}_{\hat{\bar{\mathbb{Z}}}_{G}} \hat{\boldsymbol{\theta}}_{s_{2}}$$
(14d)

While the formulas look similar to the synthetic estimators, note that a decomposition of  $\hat{\theta}_{s_2}$  reveals that the residual correction term is now included in the regression coefficient  $\hat{\theta}_{s_2}$  (Mandallaz *et al.* 2016) and thus the estimates are asymptotically design-unbiased.

The package also provides the external variance for both the extended synthetic and extended pseudo synthetic estimator. Note that neither the extended model approach nor external variance estimates are possible in the absence of terrestrial samples and thus model residuals in G, which is precisely when one must rely on the (pseudo) synthetic estimates. The external variance forms of EXTSYNTH and EXTPSYNTH are

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{G,EXTSYNTH,2p}) = \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{\mathbb{R}}(x))$$
 (15a)

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{G,EXTPSYNTH,2p}) = \frac{1}{n_{1,G}} \hat{\mathbb{V}}_{s_{2,G}}(Y(x)) + \left(1 - \frac{n_{2,G}}{n_{1,G}}\right) \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2_G}}(\hat{\mathbb{R}}(x))$$
(15b)

where  $\hat{\mathbb{R}}(x)$  are the empirical residuals under the extended auxiliary vector.

To summarize, the synthetic estimators SYNTH and PSYNTH can be applied whether terrestrial inventory sample is found in the small area or not, but has a deceptively small g-weight variance due to its potential bias. When terrestrial sample is observed in the small area, we can produce (asymptotically) design-unbiased estimates and variances using either SMALL or PSMALL which remove this bias explicitly with a mean residual term, or more elegantly with EXTSYNTH or EXTPSYNTH which simply use the same synthetic formulas while including an indicator variable for the small area in the model formula to remove the bias by construction in OLS.

#### Application

Small area estimates in the **forestinventory** package can be applied by specifying the optional argument small\_area. The input data set has to include an additional column of class factor that describes the small area membership of the sample location represented by that row. The argument small\_area requires a list-object that comprises

- the name of the column specifiying the small area of each observation (sa.col).
- a vector specifying the small area(s) for which estimations are desired (areas).
- the argument unbiased that controls which of the three available estimators is applied.

In order to apply the pseudo small area estimator (PSMALL) with boundary adjustment, we set unbiased=TRUE as well as the optional argument psmall=TRUE:

```
R> psmall_2p <- twophase(formula = tvol ~ mean + stddev + max + q75,
     data = grisons, phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     small\_area = list(sa.col = "smallarea", areas = c("A", "B"),
     unbiased = TRUE), psmall = TRUE, boundary_weights = "boundary_weights")
R> summary(psmall_2p)
Two-phase small area estimation
Call:
twophase(formula = tvol ~ mean + stddev + max + q75, data = grisons,
    phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
    small_area = list(sa.col = "smallarea", areas = c("A", "B"),
        unbiased = TRUE), boundary_weights = "boundary_weights",
    psmall = TRUE)
Method used:
Pseudo small area estimator
Regression Model:
tvol ~ mean + stddev + max + q75
Estimation results:
 area estimate ext_variance g_variance n1 n2 n1G n2G r.squared
    A 393.9713 1009.034 1308.117 306 67 94 19 0.6428771
                             1259.472 306 67 81 17 0.6428771
    B 419.6416
                 1214.035
```

'boundary\_weight'- option was used to calculate weighted means of auxiliary variables

The small area functions all return an S3 object of class "twophase" with subclass "smallarea". In addition to global estimation, the estimation object now comprises the estimates and variances for all small areas (column area). We can view the sample sizes by looking into the object itself

The extended pseudo synthetic estimator (EXTPSYNTH) can be applied by setting unbiased=TRUE and leaving the optional argument psmall to its default value of FALSE:

The **forestinventory** package automatically includes the indicator variable for the small area behind the scenes so there is no need for the user to implement it. Notice that the  $R^2$ s (r.squared) under the EXTPSYNTH estimator vary between the small areas, while they are identical under the PSMALL estimator. This is because under the EXTPSYNTH estimator, the regression model is recalculated for each small area estimation after adding the indicator variable for the respective small area in the globally derived design matrix. In case of the PSMALL estimator, the regression model stays the same for each small area estimation. Although the results of both estimators should always be close to each other, we recommend applying both estimators and compare the results afterwards in order to reveal unsuspected patterns in the data, particularly in the case of cluster sampling (see Section 6).

Setting the argument unbiased=FALSE applies the pseudo synthetic estimator to the selected small areas. Note that in the grisons data set, all small areas possess much more than the suggested minimum number of terrestrial observations (a rule of thumb is that  $n_{2,G} \ge 6$ ) required to produce reliable design-unbiased estimates. Hence, choosing to use PSYNTH is probably not desireable and is just applied here for demonstration purposes. In this case the residual correction will not be applied.

We see here that the PSYNTH variances are almost only half the variances of the PSMALL and EXTP-SYNTH estimator. However, PSMALL and EXTPSYNTH are design unbiased and their variances reflect the fact that they account for potential bias of the regression model predictions. The g-weight variance of PSYNTH completely neglects a potential bias and as a result risks severely overstating the estimation precision.

The exhaustive versions of the small area estimators (Eq. 8a, 9a, 10a, 11a, 11c) are specified via the optional argument exhaustive. Its application requires that we know the exact means of all explanatory variables within the small area(s) of interest. In contrast to the global estimators, the exact means have now to be delivered in the form of a data.frame, where each row corresponds to a small area, and each column specifies the exact mean of the respective explanatory variable. Note that likewise the case of global estimation, the order of the explanatory variables in the data frame has to match the order in which they appear in the design matrix defined by the lm()-function in R. In order

to tell R which row describes which small area, the row names have to match the respective names of the small areas specified in the areas argument.

For the grisons data set, the exact means of the explanatory variables for the small areas used in Mandallaz *et al.* (2013) are thus defined by

R> colnames(lm(formula = tvol ~ mean + stddev + max + q75, data = grisons,

```
x = TRUE(x)
R> true.means.Z.G <- data.frame(Intercept = rep(1, 4),
     mean = c(12.85, 12.21, 9.33, 10.45),
     stddev = c(9.31, 9.47, 7.90, 8.36),
     \max = c(34.92, 35.36, 28.81, 30.22),
     q75 = c(19.77, 19.16, 15.40, 16.91))
R> rownames(true.means.Z.G) <- c("A", "B", "C", "D")
R> true.means.Z.G
  Intercept mean stddev max
                                 q75
         1 12.85 9.31 34.92 19.77
В
         1 12.21 9.47 35.36 19.16
         1 9.33 7.90 28.81 15.40
          1 10.45 8.36 30.22 16.91
The extended synthetic estimator (EXTSYNTH) can then be applied by
R> extsynth_2p <- twophase(formula = tvol ~ mean + stddev + max + q75,</pre>
     data = grisons, phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     small_area = list(sa.col ="smallarea", areas = c("A", "B"),
     unbiased = TRUE), exhaustive = true.means.Z.G)
R> extsynth_2p$estimation
```

Just as in the global case, we see that the variance has again been significantly decreased by substituting the exact auxiliary means and both first phase sample sizes are now infinity. Note that the function extracts the required exact means for small area "A" and "B" from the complete set of exact means defined in true.means.Z.G.

744.3658 696.5739 Inf 67 Inf 19 0.6526503

708.1105 Inf 67 Inf 17 0.6428854

area estimate ext\_variance g\_variance n1 n2 n1G n2G r.squared

693.8576

A 372.6930

B 387.5116

# 4. Three-phase estimators and their application

#### 4.1. Global estimators

#### Mathematical background

Solving the sample-based normal equations, the vector of regression coefficients  $\hat{\boldsymbol{\alpha}}_{s_2}$  for the reduced model, i.e., using the reduced set of explanatory variables  $\mathbf{Z}^{(0)}(x)$  available at  $x \in s_0$ , and likewise the vector of regression coefficients  $\hat{\boldsymbol{\beta}}_{s_2}$  for the full model, i.e., using the full set of explanatory variables  $\mathbf{Z}^{\top}(x) = (\mathbf{Z}^{(0)\top}(x), \mathbf{Z}^{(1)\top}(x))$  available only at a subset  $x \in s_1 \subset s_0$ , are derived as

$$\hat{\boldsymbol{\alpha}}_{s_2} = \left(\frac{1}{n_2} \sum_{x \in s_2} \mathbf{Z}^{(0)}(x) \mathbf{Z}^{(0)\top}(x)\right)^{-1} \frac{1}{n_2} \sum_{x \in s_2} Y(x) \mathbf{Z}^{(0)}(x)$$
(16a)

$$\hat{\boldsymbol{\beta}}_{s_2} = \left(\frac{1}{n_2} \sum_{x \in s_2} \mathbf{Z}(x) \mathbf{Z}^\top(x)\right)^{-1} \frac{1}{n_2} \sum_{x \in s_2} Y(x) \mathbf{Z}(x)$$
(16b)

The package allows for the calculation of point estimates under exhaustive and non-exhaustive use of the auxiliary information in the  $s_0$  phase. Fitting the model using  $s_2$  (i.e., internally) ensures the zero mean residual property over  $s_2$ .

$$\hat{Y}_{reg3p,EX} = \frac{1}{\lambda(F)} \int_{F} \mathbf{Z}^{(0)\top}(x) \hat{\boldsymbol{\alpha}}_{s_{2}} + \frac{1}{n_{1}} \sum_{x \in s_{1}} (\mathbf{Z}^{\top}(x) \hat{\boldsymbol{\beta}}_{s_{2}} - \mathbf{Z}^{(0)\top}(x) \hat{\boldsymbol{\alpha}}_{s_{2}}) + \frac{1}{n_{2}} \sum_{x \in s_{2}} (Y(x) - \mathbf{Z}^{\top}(x) \hat{\boldsymbol{\beta}}_{s_{2}}) 
= (\bar{\mathbf{Z}}_{0}^{(0)} - \hat{\mathbf{Z}}_{1}^{(0)})^{\top} \hat{\boldsymbol{\alpha}}_{s_{2}} + \hat{\mathbf{Z}}_{1}^{\top} \hat{\boldsymbol{\beta}}_{s_{2}} 
\hat{Y}_{reg3p,NEX} = \frac{1}{n_{0}} \sum_{x \in s_{0}} \mathbf{Z}^{(0)\top}(x) \hat{\boldsymbol{\alpha}}_{s_{2}} + \frac{1}{n_{1}} \sum_{x \in s_{1}} (\mathbf{Z}^{\top}(x) \hat{\boldsymbol{\beta}}_{s_{2}} - \mathbf{Z}^{(0)\top}(x) \hat{\boldsymbol{\alpha}}_{s_{2}}) + \frac{1}{n_{2}} \sum_{x \in s_{2}} (Y(x) - \mathbf{Z}^{\top}(x) \hat{\boldsymbol{\beta}}_{s_{2}}) 
= (\hat{\mathbf{Z}}_{0}^{(0)} - \hat{\mathbf{Z}}_{1}^{(0)})^{\top} \hat{\boldsymbol{\alpha}}_{s_{2}} + \hat{\mathbf{Z}}_{1}^{\top} \hat{\boldsymbol{\beta}}_{s_{2}}$$
(17b)

Intuitively, the three phase estimator is simply the mean of the predictions using the reduced model (i.e.  $\frac{1}{n_0}\sum_{x\in s_0}\mathbf{Z}^{(0)\top}(x)\hat{\boldsymbol{\alpha}}_{s_2}$ ), corrected by the mean difference between the reduced model predictions and the more accurate full model predictions (i.e.  $\frac{1}{n_1}\sum_{x\in s_1}(\mathbf{Z}^\top(x)\hat{\boldsymbol{\beta}}_{s_2}-\mathbf{Z}^{(0)\top}(x)\hat{\boldsymbol{\alpha}}_{s_2})$ ), corrected by the mean difference between the ground truth and the full model predictions (i.e.  $\frac{1}{n_2}\sum_{x\in s_2}(Y(x)-\mathbf{Z}^\top(x)\hat{\boldsymbol{\beta}}_{s_2})$ ). For the compact version of the formula in the non-exhaustive case, the estimated means of  $\mathbf{Z}^{(0)}(x)$  over both the  $s_0$  and  $s_1$  phase, as well as the estimated mean of  $\mathbf{Z}(x)$  over the  $s_1$  phase are calculated according to Eq. 18. If the exact mean over  $s_0$  is known, the estimated mean  $\hat{\mathbf{Z}}_0^{(0)}$  can simply be replaced by the exact mean  $\bar{\mathbf{Z}}_0^{(0)}$ . Note that in case of applied boundary adjustment (Section 3), the simple mean is again replaced by the weighted mean analogous to Eq. 7.

$$\hat{\bar{Z}}_0^{(0)} = \frac{1}{n_0} \sum_{x \in s_0} Z^{(0)}(x), \quad \hat{\bar{Z}}_1^{(0)} = \frac{1}{n_1} \sum_{x \in s_1} Z^{(0)}(x), \quad \hat{\bar{Z}}_1 = \frac{1}{n_1} \sum_{x \in s_1} Z(x)$$
(18)

The package again provides the g-weight and external variances. The g-weight variance formulation is

$$\hat{\mathbb{V}}(\hat{Y}_{reg3p,EX}) = \frac{n_2}{n_1} \bar{\mathbf{Z}}^{(0)\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_2}} \bar{\mathbf{Z}}^{(0)} + (1 - \frac{n_2}{n_1}) \hat{\mathbf{Z}}_1^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \hat{\bar{\mathbf{Z}}}_1$$
(19a)

$$\hat{\mathbb{V}}(\hat{Y}_{reg3p,NEX}) = \hat{\boldsymbol{\alpha}}_{s_2}^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{Z}}_0^{(0)}} \hat{\boldsymbol{\alpha}}_{s_2} + \frac{n_2}{n_1} \hat{\boldsymbol{Z}}_0^{(0)\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_2}} \hat{\boldsymbol{Z}}_0^{(0)} + (1 - \frac{n_2}{n_1}) \hat{\boldsymbol{Z}}_1^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \hat{\boldsymbol{Z}}_1$$
(19b)

with the variance-covariance matrix of  $\hat{\mathbf{Z}}_0^{(0)}$  and the variance-covariance matrices of the regression coefficients  $\hat{\boldsymbol{\alpha}}_{s_2}$  and  $\hat{\boldsymbol{\beta}}_{s_2}$ :

$$\hat{\mathbf{\Sigma}}_{\hat{\mathbf{Z}}_0^{(0)}}^{(0)} = \frac{1}{n_0(n_0 - 1)} \sum_{x \in s_0} (\mathbf{Z}^{(0)}(x) - \hat{\mathbf{Z}}_0^{(0)}) (\mathbf{Z}^{(0)}(x) - \hat{\mathbf{Z}}_0^{(0)})^{\top}$$
(20a)

$$\hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_2}} = \left(\frac{1}{n_2} \sum_{x \in s_2} \mathbf{Z}^{(0)}(x) \mathbf{Z}^{(0)\top}(x)\right)^{-1} \left(\frac{1}{n_2^2} \sum_{x \in s_2} \hat{R}^{(0)2}(x) \mathbf{Z}^{(0)}(x) \mathbf{Z}^{(0)\top}(x)\right) \left(\frac{1}{n_2} \sum_{x \in s_2} \mathbf{Z}^{(0)}(x) \mathbf{Z}^{(0)\top}(x)\right)^{-1}$$
(20b)

$$\hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} = \left(\frac{1}{n_2} \sum_{x \in s_2} \boldsymbol{Z}(x) \boldsymbol{Z}^{\top}(x)\right)^{-1} \left(\frac{1}{n_2^2} \sum_{x \in s_2} \hat{R}^2(x) \boldsymbol{Z}(x) \boldsymbol{Z}^{\top}(x)\right) \left(\frac{1}{n_2} \sum_{x \in s_2} \boldsymbol{Z}(x) \boldsymbol{Z}^{\top}(x)\right)^{-1}$$
(20c)

Note that  $\hat{R}(x) = Y(x) - \mathbf{Z}^{\top}(x)\hat{\boldsymbol{\beta}}_{s_2}$  denotes the empirical residuals of the full model, whereas  $\hat{R}^{(0)}(x) = Y(x) - \mathbf{Z}^{(0)\top}\hat{\boldsymbol{\alpha}}_{s_2}$  denotes the empirical residuals of the reduced model. The external variance form under linear regression models is defined as

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{reg3p,EX}) = \frac{1}{n_1} \hat{\mathbb{V}}_{s_2}(\hat{R}^{(0)}(x)) + (1 - \frac{n_2}{n_1}) \frac{1}{n_2} \hat{\mathbb{V}}_{s_2}(\hat{R}(x))$$
(21a)

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{reg3p,NEX}) = \frac{1}{n_0} \hat{\mathbb{V}}_{s_0}(\hat{Y}^{(0)}(x)) + \frac{1}{n_1} \hat{\mathbb{V}}_{s_2}(\hat{R}^{(0)}(x)) + (1 - \frac{n_2}{n_1}) \frac{1}{n_2} \hat{\mathbb{V}}_{s_2}(\hat{R}(x))$$
(21b)

where  $\hat{\mathbb{V}}_{s_0}$  indicates taking the sample variance over  $s_0$ .

#### Application

In order to demonstrate the three-phase estimators in the package, we created an artificial three-phase scenario by recoding the phase indicators in the grisons data set (column phase\_id\_3p) according to the terminology used in this article (0 for  $s_0$ , 1 for  $s_1$ , 2 for  $s_2$ ). We now assume that the mean canopy height (mean) is available at all 306 sample locations  $x \in s_0$ , whereas we have the explanatory variables stddev, max and q75 only at 128 subsamples  $s_1$  of  $s_0$ . At 40 further subsamples  $s_2$  we have the observations Y(x) from the field inventory. Based on this setup, we can now define the reduced and full regression model formulas to be used in the threephase() function (note that the models are nested):

```
R> formula.rm <- tvol ~ mean
R> formula.fm <- tvol ~ mean + stddev + max + q75</pre>
```

Compared to the twophase()-function, we now have to specify two regression models, i.e., the nested reduced (formula.s0) and full (formula.s1) regression model. In addition, we also have to specify the indication of the  $s_1$  phase (s1.id) in the argument phase\_id (note that **forestinventory** implicitly assumes that all other rows in the input data set belong to  $s_0$ ). The global three-phase estimation can thus be applied by

R> summary(reg3p\_nex)

```
Three-phase global estimation
Call:
threephase(formula.s0 = formula.rm, formula.s1 = formula.fm,
    data = grisons, phase_id = list(phase.col = "phase_id_3p",
        s1.id = 1, terrgrid.id = 2), boundary_weights = "boundary_weights")
Method used:
Non-exhaustive global estimator
Full Regression Model:
tvol ~ mean + stddev + max + q75
Reduced Regression Model:
tvol ~ mean
Estimation results:
 estimate ext_variance g_variance n0 n1 n2 r.squared_reduced
            454.4064 451.3626 306 128 40
 372.0896
r.squared_full
      0.7166608
```

'boundary\_weight'- option was used to calculate weighted means of auxiliary variables

The summary() of a threephase()-function now recalls both regression model formulas and also gives the  $R^2$  for both the reduced (r.squared\_reduced) and the full (r.squared\_full) models. We are told that including stddev, max and q75 yields a 20 % improvement in  $R^2$ . When comparing to using only mean under a two-phase approach, we would see a considerable reduction in variance by the three-phase extension.

#### 4.2. Small area estimators

#### Mathematical background

The three two-phase small area estimators described in Section 3.2 can also be extended to the three-phase scenario. The general principle thereby stays the same, i.e., the regession coefficients of the reduced and full model and their variance-covariance matrices are calculated on the entire  $s_2$  sample according to Eq. 16a, 16b, 20b and 20c, and are subsequently used to make predictions for sample locations restricted to small area G.

The unbiased point estimates of the SMALL and PSMALL estimator are calculated by applying the globally derived reduced and full regression model coefficients to the small area means of the explanatory variables, and then corrected for a potential model bias in G by adding the small area mean of the full model residuals, i.e.,  $\hat{R}_G(x) = Y_G(x) - \mathbf{Z}_G^{\top}(x)\hat{\boldsymbol{\beta}}_{s_2}$ , to the point estimate. The difference between the mean  $\hat{\mathbf{Z}}_{1,G}^{(0)}$  and the more precise or exact mean  $\hat{\mathbf{Z}}_{0,G}^{(0)}$  and  $\bar{\mathbf{Z}}_{0,G}^{(0)}$  is again considered as a correction term likewise in the global estimation (Eq. 17).

$$\hat{Y}_{G,SMALL,3p} = (\bar{\mathbf{Z}}_{0,G}^{(0)} - \hat{\bar{\mathbf{Z}}}_{1,G}^{(0)})^{\top} \hat{\boldsymbol{\alpha}}_{s_2} + \hat{\bar{\mathbf{Z}}}_{1,G}^{\top} \hat{\boldsymbol{\beta}}_{s_2} + \frac{1}{n_{2,G}} \hat{R}_G(x)$$
(22a)

$$\hat{Y}_{G,PSMALL,3p} = (\hat{\bar{Z}}_{0,G}^{(0)} - \hat{\bar{Z}}_{1,G}^{(0)})^{\top} \hat{\alpha}_{s_2} + \hat{\bar{Z}}_{1,G}^{\top} \hat{\beta}_{s_2} + \frac{1}{n_{2,G}} \hat{R}_G(x)$$
(22b)

The g-weight variance is then calculated as

$$\hat{\mathbb{V}}(\hat{Y}_{G,SMALL,3p}) = \frac{n_2}{n_1} \bar{\mathbf{Z}}_{0,G}^{(0)\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_2}} \bar{\mathbf{Z}}_{0,G}^{(0)} + (1 - \frac{n_2}{n_1}) \hat{\bar{\mathbf{Z}}}_{1,G}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \hat{\bar{\mathbf{Z}}}_{1,G} + \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{\boldsymbol{R}}(x))$$
(23a)

$$\hat{\mathbb{V}}(\hat{Y}_{G,PSMALL,3p}) = \hat{\boldsymbol{\alpha}}_{s_2}^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{Z}}_{0,G}^{(0)}} \hat{\boldsymbol{\alpha}}_{s_2} + \frac{n_2}{n_1} \hat{\boldsymbol{Z}}_{0,G}^{(0)} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_2}} \hat{\boldsymbol{Z}}_{0,G}^{(0)} + (1 - \frac{n_2}{n_1}) \hat{\boldsymbol{Z}}_{1,G}^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \hat{\boldsymbol{Z}}_{1,G} + \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{\boldsymbol{R}}(x))$$
(23b)

with the variance-covariance matrix

$$\hat{\Sigma}_{\hat{\mathbf{Z}}_{0,G}^{(0)}} = \frac{1}{n_{0,G}(n_{0,G} - 1)} \sum_{x \in S_{0,G}} (\mathbf{Z}^{(0)}(x) - \hat{\mathbf{Z}}_{0,G}^{(0)}) (\mathbf{Z}^{(0)}(x) - \hat{\mathbf{Z}}_{0,G}^{(0)})^{\top}$$
(24)

The external variance is defined as:

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{G,SMALL,3p}) = \frac{1}{n_{1,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}^{(0)}(x)) + (1 - \frac{n_{2,G}}{n_{1,G}}) \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}(x))$$
(25a)

$$\hat{\mathbb{V}}_{ext}(\hat{Y}_{G,PSMALL,3p}) = \frac{1}{n_{0.G}} \hat{\mathbb{V}}_{s_{2,G}}(Y(x)) + (1 - \frac{n_{1,G}}{n_{0.G}}) \frac{1}{n_{1,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}^{(0)}(x))$$

$$+\left(1 - \frac{n_{2,G}}{n_{1,G}}\right) \frac{1}{n_{2,G}} \hat{\mathbb{V}}_{s_{2,G}}(\hat{R}(x)) \tag{25b}$$

where 
$$\hat{R}^{(0)}(x) = Y(x) - \hat{Y}^{(0)}(x)$$
 with  $\hat{Y}^{(0)}(x) = \mathbf{Z}^{(0)\top}(x)\hat{\boldsymbol{\alpha}}_{s_2}$ .

The synthetic (SYNTH) and pseudo synthetic (PSYNTH) estimator can be applied if no terrestrial samples are available in the small area, i.e.,  $n_{2,G} = 0$ . Consequently, the residual correction and the residual variation term of the full model can no longer be applied and drops from the point estimate (Eq. 26a and 26b) and g-weight variance (Eq. 26c and 26d) formulas. The point estimates are again potentially biased since  $\frac{1}{n_{2,G}} \sum_{x \in s_{2,G}} \hat{R}(x) = 0$  for the full model residuals can not be ensured within small area G. Also the variance will be small but to the cost of ignoring the model uncertainties. Note that there is again no external variance formula for the synthetic and pseudo synthetic estimation.

$$\hat{Y}_{G,SYNTH,3p} = (\bar{\mathbf{Z}}_{0,G}^{(0)} - \hat{\bar{\mathbf{Z}}}_{1,G}^{(0)})^{\top} \hat{\boldsymbol{\alpha}}_{2} + \hat{\bar{\mathbf{Z}}}_{1,G}^{\top} \hat{\boldsymbol{\beta}}_{s_{2}}$$
(26a)

$$\hat{Y}_{G,PSYNTH,3p} = (\hat{\bar{Z}}_{0,G}^{(0)} - \hat{\bar{Z}}_{1,G}^{(0)})^{\top} \hat{\alpha}_{2} + \hat{\bar{Z}}_{1,G}^{\top} \hat{\beta}_{s_{2}}$$
(26b)

$$\hat{\mathbb{V}}(\hat{Y}_{G,SYNTH,3p}) = \frac{n_2}{n_1} \bar{\mathbf{Z}}_{0,G}^{(0)\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_2}} \bar{\mathbf{Z}}_{0,G}^{(0)} + (1 - \frac{n_2}{n_1}) \hat{\mathbf{Z}}_{1,G}^{\top} \hat{\mathbf{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_2}} \bar{\mathbf{Z}}_{1,G}$$
(26c)

$$\hat{\mathbb{V}}(\hat{Y}_{G,PSYNTH,3p}) = \hat{\boldsymbol{\alpha}}_{2}^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{Z}}_{0,G}^{(0)}} \hat{\boldsymbol{\alpha}}_{2} + \frac{n_{2}}{n_{1}} \hat{\bar{\boldsymbol{Z}}}_{0,G}^{(0)\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\alpha}}_{s_{2}}} \hat{\bar{\boldsymbol{Z}}}_{0,G}^{(0)} + (1 - \frac{n_{2}}{n_{1}}) \hat{\bar{\boldsymbol{Z}}}_{1,G}^{\top} \hat{\boldsymbol{\Sigma}}_{\hat{\boldsymbol{\beta}}_{s_{2}}} \hat{\bar{\boldsymbol{Z}}}_{1,G}$$
(26d)

The extended synthetic (EXTSYNTH) and extended pseudo synthetic (EXTPSYNTH) estimator ensures that the residuals of the full model over both the entire inventory area F and the small area G are zero at the same time, i.e.,  $\frac{1}{n_2}\sum_{x\in s_2}\hat{R}(x)=\frac{1}{n_{2,G}}\sum_{x\in s_{2,G}}\hat{R}(x)=0$ . This is again realized by extending the vector of explanatory variables by a binary categorical indicator variable  $I_G(x)$  which takes the value 1 if the observation lies inside the small area G and is otherwise set to 0. The extended auxiliary vector is thus defined as  $\mathbf{Z}^{\top}(x)=(\mathbf{Z}^{(0)\top}(x),\mathbf{Z}^{(1)\top}(x))$ , where  $\mathbf{Z}^{(0)\top}(x)=(\mathbf{Z}^{(0)\top}(x),I_G^{\top}(x))$ . In other words, when the extended option is chosen, **forestinventory** automatically adds the binary indicator variable for the desired small area for all observations in the input data frame (i.e.,  $s_0$ ). The regression coefficients, point estimates and variance estimates are calculated by replacing  $\mathbf{Z}$  with  $\mathbf{Z}$  (and likewise

 $\mathbf{Z}^{(0)}$  with  $\mathbf{Z}^{(0)}$ ) into Eq. 16, 20, 25 and 26. Just as in the two-phase case, the resulting point estimates are now unbiased and have an associated g-weight variance that accounts for the variability of the regression coefficients resulting from the random sample  $s_2$ .

#### Application

We will demonstrate the use of three-phase small area estimation in the package **forestinventory** by applying the EXTSYNTH and SYNTH estimator to the grisons data set. The setup is thus exactly the same as in the example for global three-phase estimation (Section 4.1). However, this time will use the exact auxiliary mean of the mean canopy height variable (mean) and assume that we do not know the exact means of the remaining explanatory variables stddev, max and q75. We thus first define the true means for each small area just as we did in the twophase() example (Section 3.2):

```
R> truemeans.G \leftarrow data.frame(Intercept = rep(1, 4), + mean = c(12.85, 12.21, 9.33, 10.45))
R> rownames(truemeans.G) <- c("A", "B", "C", "D")
```

Three-phase small area estimation in the package can in general be applied by additionally specifying the small\_area list argument. The exhaustive estimators can be called by optionally passing a data.frame containing the exact auxiliary means to the exhaustive argument. The EXTSYNTH estimator can be applied by setting the argument unbiased to TRUE (default):

The SYNTH estimator can be applied by changing the argument unbiased to FALSE, which causes the function to not apply a bias correction in the respective small area.

```
R> synth_3p <- threephase(formula.rm, formula.fm, data = grisons,</pre>
     phase_id = list(phase.col = "phase_id_3p", s1.id = 1, terrgrid.id = 2),
+
     small\_area = list(sa.col = "smallarea", areas = c("A", "B"), unbiased = FALSE),
     exhaustive = truemeans.G, boundary_weights = "boundary_weights")
R> synth_3p$estimation
  area estimate ext_variance g_variance n0 n1 n2 n0G n1G n2G
                NA 410.7529 Inf 128 40 Inf 38 12
NA 461.8250 Inf 128 40 Inf 34 11
    A 409.3390
    B 375.4608
 r.squared_reduced r.squared_full
           0.527363 0.7166608
1
2
           0.527363
                        0.7166608
```

We see that the threephase()-function returns the sample sizes in the entire inventory area as well as within each small area. The value Inf for nOG indicates that the explanatory variables at  $s_0$  sample locations used in the reduced model were in our case derived exhaustively. If we compare the two results, we see that the SYNTH estimation again yields a much smaller variance than the EXTSYNTH estimation, but at the cost of a potential bias.

We can also analyse how the exhaustive derivation of mean performed compared to the case where mean is non-exhaustively available but at a very large  $s_0$  phase with  $n_{0,G} >> n_{1,G}$ . To do this, we additionally compute the EXTPSYNTH estimates. As we can see, the exhaustive derivation of mean only yielded a slightly smaller variance.

#### 5. Calculation of confidence intervals

Converting the estimated variance into a 95% confidence interval (CI) allows for a more practical interpretation of a point estimate's precision. The correct interpretation of a CI is not that there is a 95% probability that it contains the true value. In the design-based context, the true value of the population parameter we are trying to estimate, albeit unknown, is fixed and the sample is randomly generated under the sample design. Theoretically, if we were to repreatedly conduct the inventory using the same estimation method, estimator and auxiliary information under newly drawn random samples and calculate the 95% CI from each sample, then 95% of the CIs are expected to contain the true population parameter. The confidence level  $1 - \alpha$  (e.g., 95%) is thus the expected frequency or proportion of possible confidence intervals to contain the unknown population parameter under resampling and is therefore often also referred to as coverage rate. The CI is also linked to hypothesis testing in that its associated point estimate is considered statistically different from any given value that lies outside the CI boundaries.

Based on the central limit theorem it can be assumed that under hypothetical repeated sampling the point estimates will asymptotically follow a normal distribution. However, on the recommendation of Mandallaz (2013a), better confidence intervals can obtained using the Student's *t* distribution defined as

One-phase estimation:

$$CI_{1-\alpha}(\hat{Y}) = \left[ \hat{Y} - t_{n_2-1, 1-\frac{\alpha}{2}} \sqrt{\hat{\mathbb{V}}(\hat{Y})}, \hat{Y} + t_{n_2-1, 1-\frac{\alpha}{2}} \sqrt{\hat{\mathbb{V}}(\hat{Y})} \right]$$
(27)

Two-phase and three-phase global estimation:

$$CI_{1-\alpha}(\hat{Y}) = \left[ \hat{Y} - t_{n_2-p, 1-\frac{\alpha}{2}} \sqrt{\hat{\mathbb{V}}(\hat{Y})}, \hat{Y} + t_{n_2-p, 1-\frac{\alpha}{2}} \sqrt{\hat{\mathbb{V}}(\hat{Y})} \right]$$
(28)

Two-phase and three-phase small area estimation:

$$CI_{1-\alpha}(\hat{Y}) = \left[ \hat{Y} - t_{n_{2,G}-1,1-\frac{\alpha}{2}} \sqrt{\hat{\mathbb{V}}(\hat{Y})}, \hat{Y} + t_{n_{2,G}-1,1-\frac{\alpha}{2}} \sqrt{\hat{\mathbb{V}}(\hat{Y})} \right]$$
(29)

where  $\hat{Y}$  is the point estimate,  $\hat{\mathbb{V}}(\hat{Y})$  is the estimated variance,  $1-\alpha$  is the confidence level and p constitutes the number of parameters used in the (full) regression model. In case of cluster-sampling,  $n_{2,G}$  is the number of terrestrial clusters (a cluster constitutes the sample unit and comprises multiple sample plots). Note that in case of synthetic estimations (SYNTH, PSYNTH), the degrees of freedom are  $n_2-p$  as is the case for global estimation. In **forestinventory**, the confidence intervals for all estimation methods and estimators can be computed by the S3 generic method confint(), which requires an estimation object created by either the onephase(), twophase() or threephase() function. For example, the 95% confidence interval for the small area estimates by the EXTPSYNTH estimator (Section 3.2) are calculated by:

R> confint(extpsynth\_2p)

95% Confidence Intervals for twophase small area estimation

A commonly raised question of practitioners regarding the application of design-unbiased estimators is which minimum terrestrial sample size should be provided. Answering this question is highly related to ensuring the validity of the confidence coverage rates by a sufficiently large sample size. It has to be noted that giving a generally valid sample size for the asymptotic validity range is, unfortunately, infeasible because the convergence to the t- or normal distribution also depends on the hetereogeneity of the underlying population. However, simulation studies using an artificial local density surface were conducted in Mandallaz (2013a) and Mandallaz et al. (2013) to empirically check the asymptotic properties of the estimators. In order to develop the reader's intuition about when the sample size is too low to produce reliable results, we re-evaluated these simulations for a broader range of sample sizes. For each fixed sample size  $n_1$  and sampling fraction, 10000 samples were conducted by simple random sampling and the 95% confidence interval based on the g-weight variance was calculated for each sample after applying the global two-phase estimator (Section 3.1). The  $R^2$  of the regression model was 0.81. For further details on the simulation, the reader is referred to the original articles mentioned above. The results can also be reproduced or expanded using the R-code given in the Appendix.

From the simulation example for global estimation (Figure 5) it is obvious that the nominal coverage rate of 95% can expected to be met for large sample sizes (e.g.,  $n_2$ =50) regardless of the chosen sample size  $n_1$ . The realized coverage rate only drops significantly below 90% if considerably small sampling fractions (i.e., the ratio  $n_2/n_1$ ) < 0.1 are used that lead to small terrestrial sample sizes of 20 and less. The simulation examples also confirmed that in such cases, one should whenever possible consider one of the design-unbiased small area estimators (P)SMALL or EXT(P)SYNTH for which the nominal coverage rates in the simulations were already met for sample sizes  $n_{2,G} > 5$ . Finally, it should also be noted that applying the design-based estimators under systematic sampling will lead to an inflation of the estimated variance (Mandallaz 1993). This will also effect the actual coverage rates to be higher than those derived under simple random sampling.

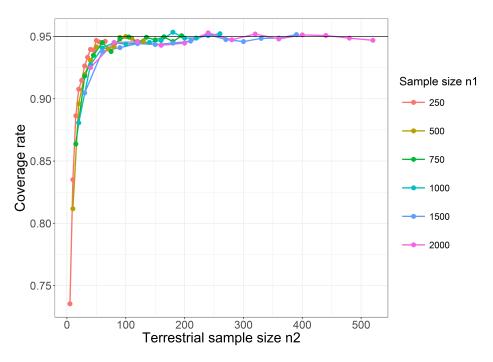


Figure 5: Coverage rates realized under varying sample sizes  $n_1$  and sampling fractions for an artificial simulation example given in Mandallaz (2013a). The nominal confidence level was 95% and for each setup, 10000 simulations were performed using simple random sampling.

# 6. Special cases and scenarios

#### 6.1. Post-stratification

A special case of multiphase regression estimation is post-stratification, which can further be divided into the cases of multiphase sampling for stratification and multiphase sampling for regression within strata. Both imply the use of one or more categorical variables in the regression model(s), leading to classical ANOVA and ANCOVA models.

To demonstrate post-stratification, we first create an artificial categorical variable development stage (stage) by clustering the mean canopy heights of the grisons data set into 3 height classes:

```
R> grisons$stage <- as.factor(kmeans(grisons$mean, centers = 3)$cluster)
```

Two-phase sampling for stratification is applied if the model only contains categorical variables, in this case the factor variable stage. Linear regression models only fitted with categorical variables produce ANOVA models, which when used in multiphase regression estimators, is equivalent to post-stratification. For our example, this means that the model predictions are simply the means of the terrestrial response values within each development stage (within-strata means).

```
R> twophase(formula = tvol ~ stage, data = grisons,
+ phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
+ boundary_weights = "boundary_weights")
```

Two-phase sampling for regression within strata implies the combination of continuous and categorical variables within the model (i.e., we have an ANCOVA model). If an interaction term is not present between categorical and continuous variables, the regression lines within the strata will have the same slope but different intercepts. If an interaction term is present, both the intercept and the slope are allowed to vary within the strata. Note that one can actually use the entire range of OLS regression techniques in the multiphase estimators, including higher order terms and transformations of the explanatory variables, which makes them very flexible.

```
R> twophase(formula=tvol ~ mean + stddev + max + q75 + stage, data = grisons,
+     phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
+     boundary_weights = "boundary_weights")
```

The variance of all design-based estimators included in **forestinventory** can be decreased by reducing the sum of squared residuals of the regression model. In case of post-stratification, this particularly implies minimizing the within strata residual square sum. Also, for post-stratification, the g-weight variance should be trusted over the external variance because it has the advantage that the strata weights are estimated from the large sample rather than the terrestrial sample  $s_2$ .

#### 6.2. Small area estimation under cluster sampling

As mentioned in Section 2.6, cluster sampling is a special case of sample designs where the sample consists of more than one spatially agglomerated sample points. One randomly places the sample location x in the inventory area as in the simple sampling design, but then M-1 additional sample locations  $x_2,...,x_M$  are created close to the cluster origin x by adding a fixed set of spatial vectors  $e_2,...,e_M$  to x. The idea of cluster sampling is to increase the amount of information without increasing the travel costs of the terrestrial campaign. However, the information gathered at all sub-locations of a cluster is then averaged on the cluster level, and this average value then references exactly one point,

i.e., the cluster origin x. Without going into too much mathematical detail, the estimators under simple sampling are thus extended in a way that all parameters (local density, mean vector of explanatory variables, mean model residuals) have to be calculated as the weighted cluster means with M(x) being the cluster weights. Whereas the geometric form and the number of sample locations per cluster M is fixed (i.e., defined by the inventorist), the actual number of points M(x) falling into the forest area F at sample location x is random because the cluster origin x is random. The **forstinventory** package identifies clusters via a unique cluster ID that is assigned to a column in the input data set. Its column name is passed to the argument cluster in the twophase() and threephase() function calls.

For small area applications, the scenario might occur where the points of a cluster at sample locations x spread over more than one small area, i.e., only a subset  $M_G(x) < M(x)$  is included in the small area of interest. In this case, the zero mean residual property within the small area,  $\frac{\sum_{x \in s_{2,G}} M(x) \hat{R}_c(x)}{\sum_{x \in s_{2,G}} M(x)} = 0$ , is no longer guaranteed when using the extended and pseudo extended synthetic estimator (see EXTSYNTH and EXTPSYNTH in Sections 3.2 and 4.2). In this case, it is adviseable to use the (pseudo) small area estimator (SMALL or PSMALL) where the zero mean residual property is still ensured.

In order to keep track of such cases, **forestinventory** tells the user to do so by returning a warning message:

```
R> extpsynth.clust <- twophase(formula = basal ~ stade + couver + melange,
    data = zberg, phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     cluster = "cluster", small_area = list(sa.col = "ismallold", areas = c("1"),
    unbiased = TRUE))
Warning message:
At least one terrestrial cluster not entirely included within small area 1.
Zero mean residual assumption for small area maybe violated.
Check mean_Rc_x_hat_G and consider alternative estimator 'psmall'
R> psmall.clust <- twophase(formula = basal ~ stade + couver + melange,
     data = zberg, phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     cluster = "cluster", small_area = list(sa.col = "ismallold", areas = c("1"),
     unbiased = TRUE), psmall = TRUE)
R> extpsynth.clust$estimation
  area estimate ext_variance g_variance n1 n2 n1G n2G r.squared
   1 25.54748
                   14.03806
                             14.16853 298 73 29
                                                  8 0.205741
R> psmall.clust$estimation
  area estimate ext_variance g_variance n1 n2 n1G n2G r.squared
1
                    16.30509
                              15.69473 298 73 29
                                                     8 0.1873795
```

Comparing the EXTPSYNTH and PSMALL estimates, we see that in this particular case the point estimates are close and more important, the external as well as the g-weight variances only differ marginally. This can be taken as evidence that the violation of the zero mean residual property can here be expected to have negligible consequences.

#### 6.3. Violation of nesting in sample design

As explained in Section 2, a basic prerequisite for the application of multiphase estimators is that the sample phases  $(s_0, s_1, s_2)$  are nested in each other. The correct nesting thereby concerns the spatial arrangement of the sample phases (Fig. 2a) as well as the availability of terrestrial and auxiliary

information per phase and sample location. For the latter, **forestinventory** runs validity checks in the background, provides warning and error messages and, if possible, applies first-aid adjustments to the inventory data set to prevent the calculations from failing. We will demonstrate possible nesting violations by applying the global three-phase estimator to the grisons and zberg data sets.

#### Violation 1

Based on the nesting rule,  $s_2 \subset s_1 \subset s_0$ , each  $s_2$  and  $s_1$  sample location must have all explanatory variables available that are used in the full (and thus reduced) regression model. If e.g., an  $s_2$  and/or  $s_1$  point misses a variable which is used in the full and reduced model (in this case mean), the function will delete this sample point from the dataset and produce the following messages:

#### Violation 2

However, if an  $s_2$  and/or  $s_1$  point is missing a variable which is only used in the full regression model (in this example q75), the function will recode the phase indicator of that point to  $s_0$ , since the point still provides the required information for the reduced model. If this concerns an  $s_2$  sample location, the associated value of the response variable can no longer be used.

#### Violation 3

If an s<sub>0</sub> point misses at least one of the explanatory variables used in the reduced model, the sample

locations are deleted from the data set.

Note that all the automatic data adjustments (deletion, recoding) have to be accepted with caution. Recapitulating, the unbiasedness of estimators in the design-based framework is based on the uniform and independent randomization of the sample locations. This means that every possible location within the forest area F, as well as pairs of locations, have inclusion and joint inclusion probabilities greater than zero. Whereas this is already violated in practice by the use of regular grids, one can still expect that these grids do not exclude specific forest structures. If any information should be missing at the sample locations, one should clarify the reason for this and make sure that the information can reasonably be assumed to be completely missing at random.

#### Violation 4

If a categorical variable is used in the regression model(s) and the terrestrial sample  $s_2$  is considerably small compared to the  $s_1$  phase, it might occur that a category is only present in the  $s_1 \setminus s_2$  sample, and thus missing in the  $s_2$  sample. Therefore, an internal regression model cannot be calculated and the function stops with the following error message:

# 7. Analysis and visualization

#### 7.1. Analysis

We often want to compare the results and performances of different estimation methods and estimators for a given global or small area inventory, which can be easily accomplished in **forestinventory** using the estTable() function. This function restructures the results from the onephase(), twophase() and threephase() objects and merges them into one single data set that provides the basis for further analysis. For demonstration purposes, we will first recalculate the one-phase estimator as well as the two-phase and three-phase EXTPSYNTH and PSYNTH estimator for the grisons data set:

```
R> op <- onephase(formula = tvol~1, data = grisons,</pre>
     phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     area = list(sa.col = "smallarea", areas = c("A", "B", "C", "D"))
R> extpsynth_2p <- twophase(formula = tvol ~ mean + stddev + max + q75,</pre>
     data = grisons, phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     small\_area = list(sa.col = "smallarea", areas = c("A", "B", "C", "D"),
     unbiased = TRUE), boundary_weights = "boundary_weights")
R> psynth_2p <- twophase(formula = tvol ~ mean + stddev + max + q75,
     data = grisons, phase_id = list(phase.col = "phase_id_2p", terrgrid.id = 2),
     small_area = list(sa.col = "smallarea", areas = c("A", "B", "C", "D"),
     unbiased = FALSE), boundary_weights = "boundary_weights")
R> extpsynth_3p <- threephase(formula.s0 = tvol ~ mean,</pre>
     formula.s1 = tvol ~ mean + stddev + max + q75, data = grisons,
     phase_id = list(phase.col = "phase_id_3p", s1.id = 1, terrgrid.id = 2),
     small\_area = list(sa.col = "smallarea", areas = c("A", "B", "C", "D"),
     unbiased = TRUE), boundary_weights = "boundary_weights")
R> psynth_3p <- threephase(formula.s0 = tvol ~ mean,</pre>
   formula.s1 = tvol ~ mean + stddev + max + q75, data = grisons,
   phase_id = list(phase.col = "phase_id_3p", s1.id = 1, terrgrid.id = 2),
   small_area = list(sa.col = "smallarea", areas = c("A", "B", "C", "D"),
    unbiased = FALSE), boundary_weights = "boundary_weights")
```

We can then aggregate all estimation objects in a list and pass it to the estTable()-function:

The function merges the estimation results and returns a list object with the subclasses "esttable" "smallarea". The vartypes argument can be used to restrict the estTable() output to certain types of variances. If one prefers the data.frame format for further analysis, this can easily be done using as.data.frame(grisons.sae.table). Note however that **forestinventory** provides several S3 generic methods specifically for the class "esttable".

The structure of an esttable object is very similar to the objects created by the small area estimation functions of the package. However, the point estimates and variances from all estimation objects passed to estTable() have been stored in one single column (estimate and variance) and can be distinguished by the variables method, estimator and vartype which specify the estimation method

(one, two or three-phase), the estimator and the type of variance that was applied (g\_ for *g-weight* and ext\_ for external variance). By default, the confidence intervals are also added.

R> str(grisons.sae.table)

```
List of 20
                   : chr [1:28] "A" "A" "A" "A" ...
$ area
$ domain
                   : Factor w/ 2 levels "global", "smallarea": 1 2 2 2 2 2 1 2 ...
                   : Factor w/ 3 levels "onephase", "twophase", ...: 1 3 3 3 2 2 2 ....
$ method
$ estimator
                   : Factor w/ 3 levels "onephase", "psynth extended", ...: 1 2 2 3 ...
                   : Factor w/ 3 levels "ext_variance",..: 3 1 2 2 1 2 2 3 1 2 ...
$ vartype
 $ estimate
                   : num [1:28] 410 395 395 422 392 ...
                   : num [1:28] 1987 1901 1858 726 996 ...
 $ variance
                   : num [1:28] 44.6 43.6 43.1 26.9 31.6 ...
 $ error
                   : num [1:28] 10.86 11.03 10.91 6.39 8.05 ...
                   : num [1:28] 19 40 40 40 67 67 67 17 40 40 ...
$ n2
                   : num [1:28] NA 12 12 12 19 19 19 NA 11 11 ...
$ n2G
$ n1
                   : num [1:28] NA 128 128 128 306 306 306 NA 128 128 ...
$ n1G
                   : num [1:28] NA 38 38 38 94 94 94 NA 34 34 ...
$ n0
                   : int [1:28] NA 306 306 306 NA NA NA NA 306 306 ...
$ nOG
                   : int [1:28] NA 94 94 94 NA NA NA NA 81 81 ...
$ r.squared
                 : num [1:28] NA NA NA NA 0.653 ...
$ r.squared_reduced: num [1:28] NA 0.545 0.545 0.527 NA ...
$ r.squared_full : num [1:28] NA 0.724 0.724 0.717 NA ...
$ ci_lower
                   : num [1:28] 317 299 300 367 326 ...
                   : num [1:28] 504 491 490 476 458 ...
$ ci_upper
 - attr(*, "row.names")= int [1:28] 1 2 3 4 5 6 7 8 9 10 ...
- attr(*, "class")= chr [1:3] "list" "esttable" "smallarea"
```

Note that estTable() also returns the estimation error (error) that is defined as the standard error devided by the point estimate:

$$error_{[\%]} = \frac{\sqrt{\hat{\mathbb{V}}(\hat{Y})}}{\hat{Y}} \cdot 100 \tag{30}$$

As multiphase estimation techniques are primary intended to increase estimation precision, the function mphase.gain() can be applied to quantify the potential benefit of a multiphase global or small area estimate compared to its respective one-phase estimate. The function takes an esttable object as input and returns a summary of which multiphase method and estimator performed best using the precision from the one-phase estimator as a baseline. If the esttable object contains more than one multiphase estimation object, mphase.gain() identifies the one with the smallest variance and compares it to the one-phase estimation. The argument pref.vartype can be used to define what type of variance (g-weight or external) should be used for the comparison. Synthetic estimates (SYNTH and PSYNTH estimator) are not considered for the comparison under the default setting (exclude.synth = TRUE) since they usually have a much smaller variance at the cost of a potential bias.

R> mphase.gain(grisons.sae.table, pref.vartype = "g\_variance")

```
area var_onephase var_multiphase
                                      method
                                                   estimator gain rel.eff
          1987.117
                        1017.6327
                                    twophase psynth extended 48.8 1.952686
    Α
2
    В
          3175.068
                        1019.1913 twophase psynth extended 67.9 3.115281
3
    C
          1180.853
                        763.0731 threephase psynth extended 35.4 1.547496
          2290.652
                        1110.2454 twophase psynth extended 51.5 2.063194
```

The function call returns a data frame containing the one-phase variance (var\_onephase) and the variance of the best performing multiphase estimator (var\_multiphase). The multiphase estimation procedure is again specified in the method and estimator column. The last two columns quantify the potential benefit of the multiphase estimation. The gain is the reduction (if its value is positive) in variance when applying the multiphase as alternative to the one-phase estimation. For example, it is indicated that the two-phase extended PSYNTH estimation procedure for small area "B" leads to a 67.9 % reduction in variance compared to the one-phase procedure. The column rel.eff specifies the relative efficiency which is defined as the ratio between the one-phase variance and the multiphase variance:

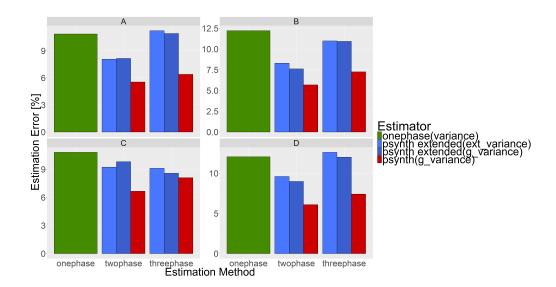
$$rel.eff = \frac{\hat{\mathbb{V}}_{onephase}(\hat{Y})}{\hat{\mathbb{V}}_{multiphase}(\hat{Y})}$$
(31)

The relative efficiency can be interpreted as the relative sample size of the one-phase estimator needed to achieve the variance of the multiphase estimator. For small area "B" we can thus see that we would have to increase the terrestrial sample size by factor 3 in the one-phase approach in order to get the same estimation precision as the two-phase EXTPSYNTH estimator. If the average costs for a terrestrial sample plot survey are known, the relative efficiency can thus be a simple means of quantifying the financial benefit of using multiphase estimation for forest inventories.

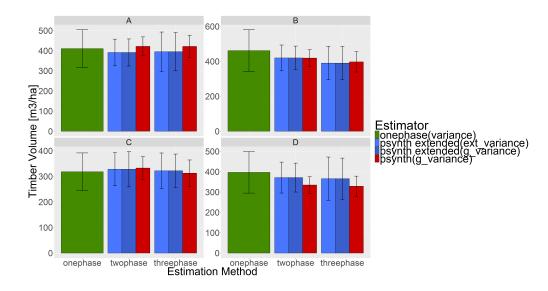
#### 7.2. Visualization

The **forestinventory** package also provides a S3 generic plot method based on the **ggplot2** package (Wickham 2009) to visualize the estimation results in two ways: 1) the point estimates with overlayed confidence intervals, and 2) the estimation errors. Both plots can be obtained by passing the esstable object to the plot() function.

R> plot(grisons.sae.table, ncol = 2)



Whereas the estimation errors are plotted by default, the point estimates and confidence intervals are returned when setting the argument yvar = "estimate". Note that the graphics can arbitrarily be extended by additional **ggplot2** parameterizations.



# 8. Future plans

The **forestinventory** package currently provides a fairly well-rounded toolkit for forestry inventorists to integrate auxiliary information into their estimates using the model-assisted methods under the design-based approach. Although 32 combinations of inventory scenarios, estimators and sample designs are covered, there are still potential improvements planned for the future. As this is an open-source project, everyone is encouraged to give feedback and/or make contributions on the package's development page on GitHub (Hill 2017). Currently planned extensions include:

- Implement parallel procedures for efficiently calculating many small areas.
- Allow functions to accept objects of class data.table from the **data.table** package (Dowle and Srinivasan 2017) to improve memory efficiency.
- Enable the user to choose other types of models than linear regressions fitted with OLS.

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# **Appendix**

#### Simulation for global two-phase estimation

```
R> # function to create density surface:
R> target.suface <- function(x0, y0){</pre>
     30 + 13*x0 - 6*y0 - 4*x0^2 + 3*x0*y0 + 2*y0^2 + 6*cos(pi*x0)*sin(pi*y0)
R> # --- True spatial mean for Global and Small Area Surface Area: --- #
R> library(rmutil)
R> int2(target.suface, a = c(0,0), b=c(3,2))/6 # 39.17
R> int2(target.suface, a = c(0.5, 0.3), b=c(2, 1.3))/(1*1.5) # 37.16243
R> # --- sample generator for simple sampling: --- #
R> sample.generator<- function(n1, n2, target.surface=target.surface){</pre>
     realization <- matrix(NA,n1,7)</pre>
    for(i in 1:n1){
      x0=2*runif(1)
       y0=3*runif(1)
       realization[i,1] <- target.suface(x0, y0)</pre>
       realization[i,2]<-x0
      realization[i,3]<-y0
     realization[i,4]<-x0*x0
      realization[i,5]<-x0*y0
       realization[i,6]<-y0*y0
+
       realization[i,7]<-0
     }
+
     realization <- as.data.frame(realization)</pre>
     names(realization) <- c("response", "x", "y", "xx", "xy", "yy", "area")</pre>
     realization$phase <- 1
     realization$phase[sample(nrow(realization), n2)] <- 2</pre>
     realization$response[realization$phase == 1]<- NA
     realizationx >= 0.3 \& realization <= 1.3 \&
                       realization$y >= 0.5 & realization$y <= 2]<- 1
     return(realization)
  }
R> # --- function for global simulations --- #
R> run.global.sim <- function(num_replications, n1.vec){</pre>
     sfrac \leftarrow seq(0.02, 0.26, by=0.02) # sampling fractions
     true_value<- 39.17 # true population mean
     # data.frame to store results:
     coverage_rates <- data.frame(n1=integer(), n2=integer(),</pre>
                                   sampling_fractions=numeric(),
                                   avg.error.ext=numeric(),
                                   avg.error.g=numeric(),
                                   covrate.ext=numeric(),
                                   covrate.g=numeric(),
                                   no.valid.sims = integer())
     # ----- #
     # simulation loop:
```

```
for(i in 1:length(sfrac)){
       # variables to store temporary results:
       n2 <- integer()</pre>
       error.ext <- numeric()</pre>
       error.g <- numeric()</pre>
       ci.ext.logical <- logical()</pre>
       ci.g.logical <- logical()</pre>
       no.valid.sims. <- integer()</pre>
       for(j in 1:num_replications){
         realization <- sample.generator(n1 = n1.vec, n2 = round(n1.vec*sfrac[i]))
         est <- twophase(formula = response ~ y + x + xx, data=realization,</pre>
                           phase_id = list(phase.col = "phase", terrgrid.id = 2))
         ci <- confint(est)</pre>
         ci.ext.logical <- append(ci.ext.logical,</pre>
                                     ci$ci$ci_lower_ext <= true_value &</pre>
                                     true_value <= ci$ci$ci_upper_ext)</pre>
         ci.g.logical <- append(ci.g.logical,</pre>
                                   ci$ci$ci_lower_g <= true_value &</pre>
                                   true_value <= ci$ci$ci_upper_g)</pre>
         error.ext <- append(error.ext,</pre>
                               sqrt(est$estimation$ext_variance)/est$estimation$estimate)
         error.g <- append(error.g,</pre>
                             sqrt(est$estimation$g_variance)/est$estimation$estimate)
         n2 <- append(n2, est$estimation$n2)</pre>
         no.valid.sims. \leftarrow sum(n2 > 1)
       }
       # calculate cove.rates, avg. n2G etc:
       coverage_rates <- rbind(coverage_rates,</pre>
                                 data.frame(n1=n1.vec, n2=round(mean(n2)),
                                              sampling_fractions=sfrac[i],
                                              avg.error.ext=mean(error.ext, na.rm = TRUE),
                                              avg.error.g=mean(error.g, na.rm = TRUE),
                                              covrate.ext=mean(ci.ext.logical, na.rm = TRUE),
                                              covrate.g=mean(ci.g.logical, na.rm = TRUE),
                                              no.valid.sims=no.valid.sims.))
     } # end of sim
  return(coverage_rates)
+ } # end of function
```

```
R> # --- run global simulations --- #
R> library(forstinventory)
R> global.sims<- data.frame()
R> n1_sims<- c(250, 500, 750, 1000, 1500, 2000) # n1 sample sizes
R> for (i in 1:length(n1_sims)){
    res<- run.global.sim(num_replications = 10000, n1.vec = n1_sims[i])
    global.sims <- rbind(global.sims, res)
+ }</pre>
```

#### References

- Breidenbach J (2015). **JoSAE**: Functions for some Unit-Level Small Area Estimators and their Variances. R package version 0.2.3, URL https://CRAN.R-project.org/package=JoSAE.
- Breidenbach J, Astrup R (2012). "Small Area Estimation of Forest Attributes in the Norwegian National Forest Inventory." *European Journal of Forest Research*, **131**(4), 1255–1267. doi: 10.1007/s10342-012-0596-7.
- Cullmann AD (2016). *maSAE*: Mandallaz' Model-Assisted Small Area Estimators. R package version 0.1-5, URL https://CRAN.R-project.org/package=maSAE.
- Dowle M, Srinivasan A (2017). *data.table*: Extension of 'data.frame'. R package version 1.10.4-1, URL https://CRAN.R-project.org/package=data.table.
- Gregoire TG, Valentine HT (2007). Sampling Strategies for Natural Resources and the Environment. CRC Press.
- Hill A (2017). forestinventory. GitHub repository, URL https://github.com/AndreasChristianHill/forestinventory.
- Hill A, Buddenbaum H, Mandallaz D (2018a). "Combining canopy height and tree species map information for large-scale timber volume estimations under strong heterogeneity of auxiliary data and variable sample plot sizes." *European Journal of Forest Research*, **137**(4), 489–505. doi: https://doi.org/10.1007/s10342-018-1118-z.
- Hill A, Mandallaz D, Langshausen J (2018b). "A Double–Sampling Extension of the German National Forest Inventory for Design-Based Small Area Estimation on Forest District Levels." *Remote Sensing*, **10**(7), 1052. doi:https://doi.org/10.3390/rs10071052.
- Köhl M, Magnussen SS, Marchetti M (2006). Sampling Methods, Remote Sensing and GIS Multire-source Forest Inventory. Springer-Verlag Berlin Heidelberg.
- Lumley T (2016). survey: Analysis of Complex Survey Samples. R package version 3.32.
- Magnussen S, Mandallaz D, Breidenbach J, Lanz A, Ginzler C (2014). "National Forest Inventories in the Service of Small Area Estimation of Stem Volume." *Canadian Journal of Forest Research*, **44**(9), 1079–1090. doi:10.1139/cjfr-2013-0448. URL https://doi.org/10.1139/cjfr-2013-0448.
- Mandallaz D (1993). Geostatistical methods for double sampling schemes. Habilitation, ETH Zurich.
- Mandallaz D (2008). *Sampling Techniques for Forest Inventories*. CRC Press. doi:10.1201/9781584889779. URL https://doi.org/10.1201/9781584889779.
- Mandallaz D (2013a). "Design-Based Properties of Some Small-Area Estimators in Forest Inventory with Two-Phase Sampling." *Canadian Journal of Forest Research*, **43**(5), 441–449. doi:10.1139/cjfr-2012-0381. URL https://doi.org/10.1139/cjfr-2012-0381.
- Mandallaz D (2013b). "Regression Estimators in Forest Inventories with Three-Phase Sampling and Two Multivariate Components of Auxiliary Information." *Technical report*, Department of Environmental Systems Science, ETH Zurich. doi:10.3929/ethz-a-009990020. URL https://doi.org/10.3929/ethz-a-009990020.

- Mandallaz D (2013c). "Regression Estimators in Forest Inventories with Two-Phase Sampling and Partially Exhaustive Information with Applications to Small-Area Estimation." *Technical report*, Department of Environmental Systems Science, ETH Zurich. doi:10.3929/ethz-a-007623322. URL https://doi.org/10.3929/ethz-a-007623322.
- Mandallaz D (2013d). "A Three-Phase Sampling Extension of the Generalized Regression Estimator with Partially Exhaustive Information." *Canadian Journal of Forest Research*, **44**(4), 383–388. doi:10.1139/cjfr-2013-0449. URL https://doi.org/10.1139/cjfr-2013-0449.
- Mandallaz D (2014). "Note on the design-based estimation of densities, totals and goodness of fit in extensive inventories." *Technical report*, Department of Environmental Systems Science, ETH Zurich. doi:10.3929/ethz-a-010151635. URL https://doi.org/10.3929/ethz-a-010151635.
- Mandallaz D (2015). "Mathematical Details of Two-Phase/Two-Stage and Three-Phase/Two-Stage Regression Estimators in Forest Inventories. Design-based Monte Carlo Approach." *Technical report*, Department of Environmental Systems Science, ETH Zurich. doi:10.3929/ethz-a-010441361. URL https://doi.org/10.3929/ethz-a-010441361.
- Mandallaz D, Breschan J, Hill A (2013). "New Regression Estimators in Forest Inventories with Two-Phase Sampling and Partially Exhaustive Information: a Design-Based Monte Carlo Approach with Applications to Small-Area Estimation." *Canadian Journal of Forest Research*, **43**(11), 1023–1031. doi:10.1139/cjfr-2013-0181. URL https://doi.org/10.1139/cjfr-2013-0181.
- Mandallaz D, Hill A, Massey A (2016). "Design-Based Properties of Some Small-Area Estimators in Forest Inventory with Two-Phase Sampling Revised Version." *Technical report*, Department of Environmental Systems Science, ETH Zurich. doi:10.3929/ethz-a-010579388. URL https://doi.org/10.3929/ethz-a-010579388.
- Massey A, Mandallaz D (2015a). "Comparison of Classical, Kernel-Based, and Nearest Neighbors Regression Estimators using the Design-Based Monte Carlo Approach for Two-Phase Forest Inventories." Canadian Journal of Forest Research, **45**(11), 1480–1488. doi:10.1139/cjfr-2015-0151. URL https://doi.org/10.1139/cjfr-2015-0151.
- Massey A, Mandallaz D (2015b). "Design-Based Regression Estimation of Net Change for Forest Inventories." Canadian Journal of Forest Research, 45(12), 1775–1784. doi:10.1139/cjfr-2015-0266. https://doi.org/10.1139/cjfr-2015-0266, URL https://doi.org/10.1139/cjfr-2015-0266.
- Massey A, Mandallaz D, Lanz A (2014). "Integrating Remote Sensing and Past Inventory Data under the New Annual Design of the Swiss National Forest Inventory using Three-Phase Design-Based Regression Estimation." *Canadian Journal of Forest Research*, **44**(10), 1177–1186. doi:10.1139/cjfr-2014-0152. URL https://doi.org/10.1139/cjfr-2014-0152.
- Massey AF (2015). Multiphase Estimation Procedures for Forest Inventories under the Design-Based Monte Carlo Approach. Ph.D. thesis, ETH Zurich. doi:10.3929/ethz-a-010536381. URL https://doi.org/10.3929/ethz-a-010536381.
- R Core Team (2017). R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria. URL https://www.R-project.org/.
- Saborowski J, Marx A, Nagel J, Böckmann T (2010). "Double Sampling for Stratification in Periodic Inventories-Infinite Population Approach." *Forest ecology and management*, **260**(10), 1886–1895. doi:10.1016/j.foreco.2010.08.035. URL https://doi.org/10.1016/j.foreco.2010.08.035.

SAS Institute Inc (2015). SAS/STAT Software, Version 9.4. Cary, NC. URL http://www.sas.com/.

Schreuder HT, Gregoire TG, Wood GB (1993). Sampling Methods for Multiresource Forest Inventory. John Wiley & Sons.

von Lüpke N (2013). Approaches for the Optimisation of Double Sampling for Stratification in Repeated Forest Inventories. Ph.D. thesis, University of Göttingen.

von Lüpke N, Hansen J, Saborowski J (2012). "A Three-Phase Sampling Procedure for Continuous Forest Inventory with Partial Re-measurement and Updating of Terrestrial Sample Plots." European Journal of Forest Research, 131(6), 1979–1990. ISSN 1612-4677. doi:10.1007/ s10342-012-0648-z.

von Lüpke N, Saborowski J (2014). "Combining Double Sampling for Stratification and Cluster Sampling to a Three-Level Sampling Design for Continuous Forest Inventories." European journal of forest research, 133(1), 89-100. doi:10.1007/s10342-013-0743-9. URL http: //dx.doi.org/10.1007/s10342-013-0743-9.

Wickham H (2009). ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag New York. ISBN 978-0-387-98140-6. URL http://ggplot2.org.

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