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Spatial sampling methods modified by model use [1]

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ABSTRACT

Recent years have seen an intensive development in the field of spatial sampling methods, which generally focus on a balanced distribution of the sample in space. Adaptive sampling methods constitute another dynamic direction in the sampling theory. The issue raised in this article involves the combination of these directions. Five of the commonly known spatial sampling methods have been analysed. The experiment was designed to include statistical model in the sampling procedure. As in the case of adaptive methods, it serves to modify drawing probabilities during sampling. The necessary theory of this sampling modification has been developed and presented. An experiment using artificial data was conducted in order to analyse the efficiency of the model modification in comparison with the primary methods.

Key words: spatial sampling, drawn-by-drawn sampling, kriging, employees distribution

1. Introduction

Spatially balanced samples are samples in which units are well spread throughout the study area. They can be obtained by avoiding or reducing the number of contiguous units. For a long time the main aim in spatial surveys has been to achieve spatially balanced samples (Fattorini et al., 2015).

Wywiał (1996) proposed a sampling design based on the neighbourhood matrix. In this design the number of contiguous units in the sample is reduced using the information about neighbourhoods. After that several spatial designs were proposed (i.e. Bryant et al. (2002)). Stevens Jr and Olsen (2004) introduced the Generalized Random-Tessellation Stratified method (GRTS), which was based on the idea of transformation 2-dimensional space into 1-dimensional space. The Spatially Correlated Poisson Sampling method (SCPS) proposed by Grafström (2012) was an alternative to the GRTS method. It is a drawn-by-drawn sampling method which is a modification of the Correlated Poisson Sampling. Another drawn-by-drawn method, referred to as the Local Pivotal method, was proposed by Grafström et al. (2012). The authors presented two variants of this method, LPM1 and LPM2. Subsequently, the combination of LPM2 and Cube method (proposed by Deville and Tillé (2004)) was proposed by Grafström and Tillé (2013) and it was referred to as the Doubly Balanced Spatial Sampling (DBSS). GRTS, SCPS, LPM1 and LPM2 exploit the information provided by the location of the units in the study area with the purpose of achieving spatially balanced samples. DBSS uses the location in the space and, additionally, the information from auxiliary

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variables. It leads to a sample which is doubly balanced: spatially balanced and balanced with respect to the auxiliary variables.

Another approach to sampling from the space was proposed by (Thompson and Seber, 1996), who developed an adaptive sampling. In adaptive sampling methods, the sampling design may depend on the values of the survey variable which are observed during sampling. Primarily adaptive sampling designs were divided into two stages of sampling (Thompson and Seber, 1996). In the first stage a 'classical' sampling design, i.e. simple random sampling or stratified sampling is used. In the second stage, some additional elements which fulfilled a certain condition are added to the sample. The second stage is the adaptive part of sampling in the strict sense. Thompson (2006) introduced a new flexible class of adaptive sampling designs - Adaptive Web Sampling. In this method the second stage of sampling is redefined. With a certain probability the adaptive procedure is performed, otherwise a fixed (non-adaptive) design is used.

Model modification of spatial sampling is divided into two stages, as well as the adaptive sampling design. In the first stage it uses the primary sampling method in the way it was defined. In the experiment well-known sampling methods, like simple random sample, GRTS, SCPS, LPM1, LPM2 or DBSS, are considered. In the second stage, just like in the Adaptive Web Sampling, with a certain probability the adaptive procedure is performed, otherwise an initial design is used. For sampling modified by model use, the adaptive procedure is nothing more than rescaling probabilities for some elements and zeroing for others. The choice of whether the element's probability will be rescaled or zeroed depends on the predictions from the spatial interpolation model (i.e. kriging).

The main aim of this paper is to verify the potential of the presented modification. To achieve this, theoretical aspects are introduced in Section 2. Then, in Section 3 the model modification is evaluated using GRTS, SCPS, LPM1, LPM2 and DBSS on artificial data of employees' distribution. The method of data simulation was consistent with the real spatial characteristics of the employee population observed in the research. It should be mentioned that the approach to sampling from the space discussed in this paper is, to a certain extent, the development of the triangular method of spatial sampling (Bąk, 2014). It allows to stabilize the selected elements around a predetermined value.

Model modification of spatial sampling methods can be also applied to other spatial design-based sampling methods than the five chosen for the experiment. The theory presented in Section 2 can be simply adapted to other design-based sampling methods. Therefore this method can expand the range of design-based methods that can be used in research. It may prove useful in planning sample selection in some spatial studies.

2. Construction of spatial sampling modified by model use

Let us consider a finite population of N spatial locations in the study area, labelled by $1,\ldots,N$. Moreover denote by y_i the value of the characteristic Y under study and by x_i the value of an auxiliary variable X well correlated with Y corresponding to location $i = 1,\ldots,N$. Values of the Y characteristic which are observed during sampling are fixed but they are treated as the outcome of a random process just to perform a model-dependent prediction of these values:

$$\{Y(i) : i \in \{1,\ldots,N\}\}. \tag{1}$$

Two stages of spatial sampling modified by model use may be distinguished, as in the case of adaptive sampling. In the first stage an initial sample $\{i_1,\ldots,i_{n_0}\}$ consisted of n_0 elements is selected. Each of n_0 sampled elements is selected with drawing probabilities:

$$p = [p_1,\ldots,p_N]. \tag{2}$$

Furthermore, n_0 realizations of the Y process are obtained. Denote them by $y_{i_1},\ldots,y_{i_{n_0}}$. It means that for initial sample elements both values and locations are known. Therefore, it is possible to build statistical model to predict values of Y process for the whole population. Denote by $\hat{Y}_{n_0}(i)$, $i \in \{1,\ldots,N\}$ the predictions of the values of Y process which are based on the initial sample. These predictions modify drawing probabilities for next m elements. Then, the new predictor $\hat{Y}_{n_0+m}(i), i \in \{1,\ldots,N\}$ is constructed and then used to modify probabilities for elements $n_0+m+1,...,n_0+2m$.

Let us consider that the predictor $\hat{Y}_{n_0+(k-1)m}(i), i \in \{1,\ldots,N\}$ was constructed. Then, the sampling can be made in one of two ways: depending on the predictor $\hat{Y}_{n_0+(k-1)m}(i)$ or in the same way as selection of the elements $1,\ldots,n_0$ - using drawing probabilities (2). In other words a mixture of schemes is used (Thompson, 2006). Next, let us introduce the probability d_{k-1}. Then, the condition that determinates the sampling scheme choice in the k-th drawing is:

$$\exists_{i\in\{\{1,\ldots,N\}\setminus\{i_1,\ldots,i_{n_0+(k-1)m}\}\}} f(x_i,\hat{y}_i,\bar{x},\bar{\hat{y}}) \in A, \tag{3}$$

where $\hat{y}_i$, $i \in \{1,\ldots,N\}$ are predictions of Y characteristic from the model $\hat{Y}_{(k-1)m}(i)$, $i \in \{1,\ldots,N\}$, $\bar{\hat{y}}$ is the average value of those predictions and A is the subset of the range of f function. The construction of the function f is crucial for the efficiency of presented solution. For the purposes of description of the construction of spatial sampling modified by model use, we will limit ourselves to the general form of the f function. Some examples will be presented in the next section.

Depending on the satisfiability of the condition (3), the k-th drawing is conducted in one of two ways:

- Condition (3) is false. Then, a sampling method analogous to the one that has been used in the initial sampling stage is used. Drawing probabilities for k-th element are defined as $p_k = p$.

- Condition (3) is true. Then, two situations are possible. With probability $1-d_{k-1}$, the k-th element is sampled in the same way as when condition (3) is false. Otherwise, with probability d_{k-1}, the k-th element is sampled among the elements of the set

$$H_{k-1} = \{i \in \{1,\ldots,N\}/\{i_1,\ldots, \quad i_{k-1}\} : \quad f(x_i,\hat{y}_i,\bar{x},\bar{\hat{y}}) \in A\}. \tag{4}$$

It means that the next element could be selected only among elements fulfilling the condition (3). Then, vector $p'_k = \left[p'_{k,1}, \ldots, p'_{k,N}\right]$ is defined as follows:

$$p'_{k,i} = \begin{cases} \frac{p_{k,i}}{\sum_{i \in H_{k-1}} p_{k,i}}, \text{ when } i \in H_{k-1}, \\ 0, \text{ when } i \notin H_{k-1}. \end{cases} \tag{5}$$

In other words, probabilities in p'_k vector are proportional to probabilities in p_k for the elements of the set H_{k-1} and equal to 0 for other elements of the population. The probabilities p'_k are used to sample the k-th element.

As we can see, the sampling plan which was used at the initial stage is used at the second stage of sampling too. Moreover, probabilities p'_k, $k = n_0 + 1, \ldots, N$ are based on the probabilities p_k, $k = n_0 + 1, \ldots, N$. Therefore, the choice of initial sampling has great impact on the spatial sampling modified by model use.

It should be emphasized that the construction of vector (5) implies that sampling without replacement is considered. However, spatial sampling modified by model use can be easily transformed into sampling with replacement. However, it was not done in this paper in order to keep the structure of the paper more transparent.

The basic feature of the d_k, $k = n_0, \ldots, n-1$ is that the higher the value of d_k, the greater 'adaptability' (ability to learn on already sampled elements) of the sampling scheme. On the other hand, the precision of the 'adaptability' is based on the precision of the model, which is mainly conditioned by the number of already sampled elements. It is well known that the precision of the spatial model increases with increasing sample size (Cressie, 1993). Therefore, a sequence of probabilities $d_k, k = n_0, \ldots, n-1$ should be increasing. In principle, the same assumption about the sequence $d_k, k = n_0, \ldots, n-1$ was made by Thompson (2006) in the Adaptive Web Sampling.

The sampling plan can be defined using the probabilities defined above. Let us denote final sample by $s = \{i_1, i_2, \ldots, i_n\}$. Then, the sampling plan is defined as:

$$P(s) = \sum_{\{j_1,\ldots,j_n\} \in S(s)} \prod_{m=1}^{n_0} p_{m,j_m}$$
$$\prod_{k=n_0+1}^{n} \left[P(\bar{\bar{H}}_{k-1} = 0) p_{k,j_k} + P(\bar{\bar{H}}_{k-1} \neq 0) \left(p'_{k,j_k} d_{k-1} + p'_{k,j_k} (1 - d_{k-1})\right)\right], \tag{6}$$

where $S(s)$ is a set of all permutation of s and $\bar{\bar{H}}_k$ is cardinality of the H_k set. The sampling plan (6) is conditioned by probabilities $P\left(\bar{\bar{H}}_k \neq 0\right)$ and $P\left(\bar{\bar{H}}_k = 0\right)$. In other words, the sampling plan is primarily defined by model predictions on unsampled elements.

The use of model modification results in unequal first-order probabilities of inclusion. They depend on the results of modelling and cannot be defined explicitly. Fattorini (2006) proposed the method of using Horvitz-Thompson estimator in the case when an explicit derivation of the first-order probabilities of inclusion is prohibitive. This approach was later developed in several papers (Thompson and Wu, 2008; Gamrot, 2014).

Let us assume that M samples from the population $\{1, \ldots, N\}$ are selected independently and by repeating the same rules. An invariably positive estimator of the first-order probabilities of inclusion $\pi_j,\ j=1,\ldots,N$ is

$$\hat{\pi}_j = \frac{m_j+1}{M+1}, \quad j=1,\ldots,N, \tag{7}$$

where m_j is the total number of samples in which the j-th element was drawn. Since $M \to \infty$, then the asymptotically unbiased modification of the primary Horvitz-Thompson estimator is

$$\hat{T} = \sum_{j=1}^{n} \frac{y_j}{\hat{\pi}_j}. \tag{8}$$

Another, much simpler method of first order probabilities of inclusion will be evaluated too. First order probabilities of inclusion will be proportional to the auxiliary variable X:

$$\pi_{X_j} = \frac{x_j}{\sum_{i=1}^{N} x_i}, \quad j=1,\ldots,N. \tag{9}$$

3. Example of spatial sampling modified by model use

Let us consider a spatial research of the average number of employees by district. Elements under study are districts of a region. An additional characteristic observed during research is the number of inhabitants. Artificially generated data were prepared to illustrate the usefulness of spatial sampling modified by model use in such research. In the first step the X matrix of the size 200×200 was generated. It contains simulated numbers of inhabitants. Each element of this matrix was sampled using one of three normal distributions:

$$\sim \begin{cases} \mathcal{N}(2500,120^2), \text{ when } (30 \le i \le 55 \text{ or } 155 \le i \le 190) \text{ and } 170 \le j \le 200, \\ \mathcal{N}(1500,80^2), \text{ when } (1 \le i \le 30 \text{ or } 165 \le i \le 200) \text{ and } 1 \le j \le 45, \\ \mathcal{N}(2000,100^2), \text{ in other cases,} \end{cases} \tag{10}$$

where i and j are row and column index in X matrix respectively. Then, the Y matrix of the size 200×200 was generated. Elements of the Y matrix are simulated values of the number of the employees. Values of the Y process were simulated in such a way that the correlation between Y and X was high (Pearson correlation coefficient equal to 0.928). Moreover, both matrices are identified with two-dimensional space $X_1 \times X_2$ size of $[0,200] \times [0,200]$. Each element of both matrices is related to the fragment of the two-dimensional space. The size of each fragment is 1×1 unit.

In practice, the spatial distribution of the employees, agglomerations is not as regular as Y matrix (Combes and Overman, 2004; Glaeser and Kerr, 2009). Therefore, from the two-dimensional space 300 fragments were sampled using uniform distribution. These 300 elements were treated as the population under study. Each population element is related to an appropriate element (realization of the random process) of X and Y matrices.. The average value of X characteristic in the final population was equal to 1990.794 inhabitants. It is assumed that the average value of X is known before sampling, but without the knowledge of the value of a X variable in specific elements. In the case of Y characteristic the average value was equal to 501.477 employees and is not known before sampling. The spatial distribution of the population under study is shown in Figure 1. The distribution of X and Y characteristics in the population is shown in Figure 2 and Figure 3 respectively. For both characteristics two aggregations of lower values and two aggregations of higher values can be observed. The purpose of these aggregations is to simulate spatial heterogeneity.

Spatial sampling modified by model use was used to draw a sample from this population. Five sampling methods were considered as the initial sampling method. Three of them were: Spatially Correlated Poisson Sampling method (SCPS) and both Local Pivotal methods (LPM1 and LPM2). Each of them exploits the information about spatial location of the population elements. The fourth of the methods was Cube method (CM), which is an example of balanced sampling, and the fifth was Unequal Probability Sampling (UPS). The last two methods use the information from auxiliary variables. The first-order inclusion probabilities were defined proportionally to the auxiliary variable for each initial sampling methods.

Ordinary kriging was chosen as a spatial data modeling method. The kriging model was built using *automap* package in R language (Hiemstra et al., 2008). Already sampled elements were used to variogram estimation. Spherical, exponential, Gaussian and Matern family models were considered as potential shape of the variogram. Finally, the sampling algorithm picked the variogram model that has the smallest residual sum of squares and used it in kriging modelling.

Kriging refers to making inferences on unobserved values of random process $X(i) : i \in \{1,\dots,N\}$ from data (Cressie, 1993)

$$\{x_{i_1},\dots,x_{i_n}\} \tag{11}$$

observed at n known spatial locations

$$\{i_1,\dots,i_n\}. \tag{12}$$

Ordinary kriging refers to spatial predictor $\hat{X}$, which fulfils the following two assumptions:

$$1.\ X(i) = \mu + \varepsilon(i), \tag{13}$$

where $i \in \{1,\dots,N\}$, $\varepsilon(i)$ is the error process with the expected value equal to 0 and μ is unknown.

$$2.\ \hat{X}(i) = \sum_{j=1}^{n} \lambda_j x_{i_j}, \tag{14}$$

where $\sum_{j=1}^{n} \lambda_j = 1$ and $i \in \{1,\dots,N\}$. Weights $\lambda_j, j = 1,\dots,n$ are determined by Lagrange multipliers so as to minimize the mean square error of the $\hat{X}$ predictor. As a result, the best linear unbiased predictor is obtained (Cressie, 1993).

Condition (3) was defined generally. To make it easier to interpret and use, let us con-

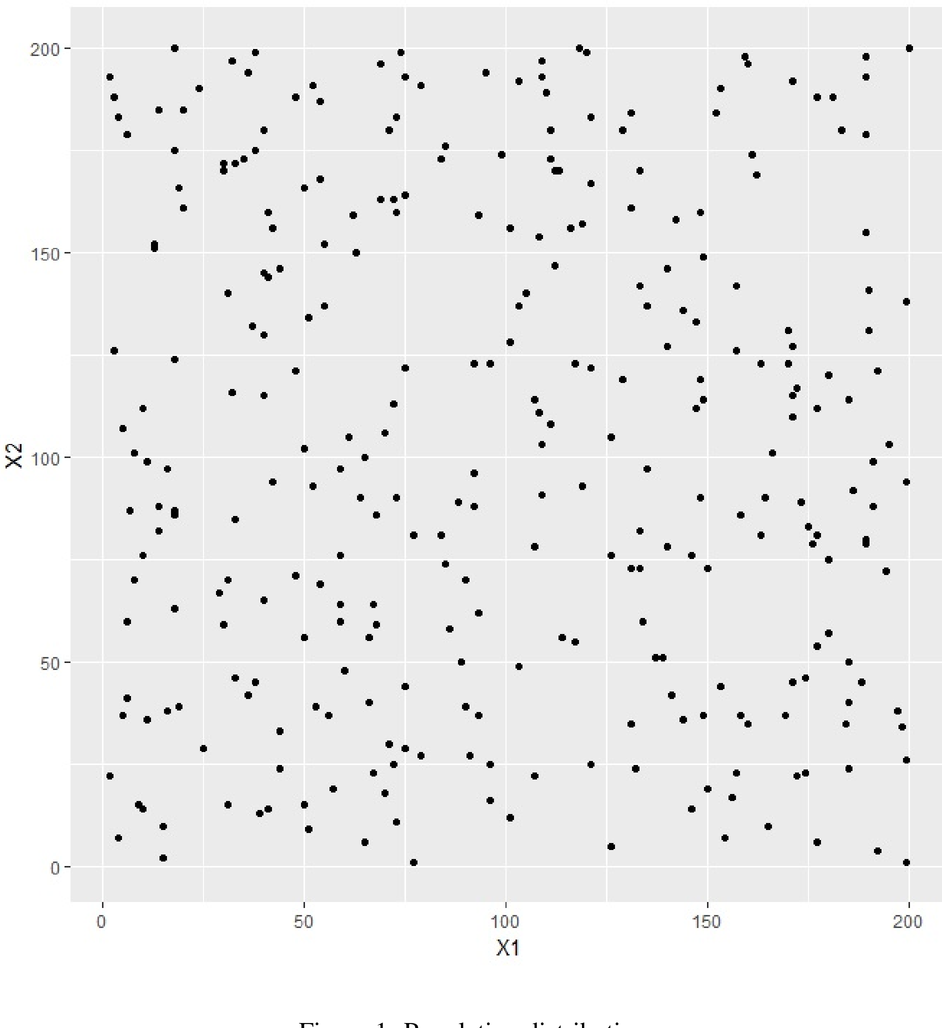

Figure 1: Population distribution.

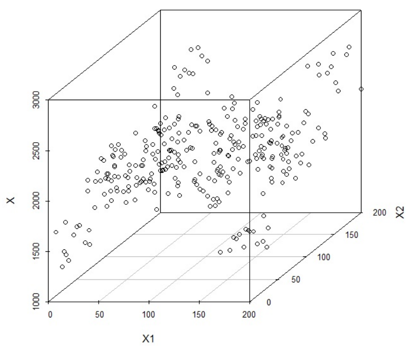

Figure 2: X characteristic distribution.

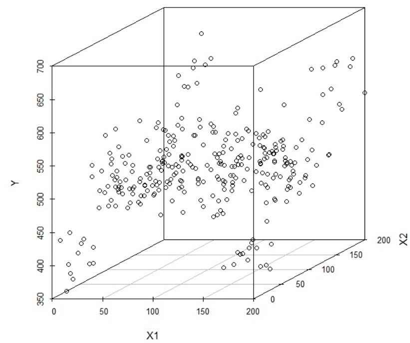

Figure 3: Y characteristic distribution.

sider $f(x_i, \hat{y}_i, \bar{x}, \bar{\hat{y}}) = \|\hat{x}_i - \bar{x}\|$ and $A = [0, c]$. Then, condition (3) can be represented as:

$$\|\hat{x}_i - \bar{x}\| \leq c, \tag{15}$$

and can be explained as a tendency to prefer elements for which the value of X is close to the average.

The sample size of $n = 100$, and the initial sample size of $n_0 = 50$ were considered. The sequence $\{d_k\}, k = 50, \ldots, n-1$ was defined as

$$d_k = \frac{k}{100}, k = 50, \ldots, 99. \tag{16}$$

The value of c coefficient was equal to 5, which was about 25% of standard deviation of X. Hereby, increased probabilities of the values of X characteristic which are close to the average value $\bar{x}$ was achieved. For each of five initial sampling methods, sampling of 100 elements was repeated 10 000 times to achieve, through the Monte Carlo method, estimation of the first-order inclusion probabilities.

Two different approaches to the first-order probabilities of inclusion definition were considered. The first was the empirical approach (7), which was based on Monte Carlo simulation. In this approach, the first-order probability of inclusion tends to increase when the $|X - \bar{x}|$ variable decreases. In the second approach, the first-order probabilities of inclusion were proportional to the auxiliary variable (9). For both approaches and each type of initial sampling method 1 000 samples were selected.

Results of spatial sampling modified by model use were compared to primary forms of sampling methods (the one which were used as initial sampling methods). Therefore, 1 000 samples, each consisting of 100 elements, were selected using all five sampling methods used for initial sampling. Estimation was based on the first-order probabilities of inclusion proportional to the auxiliary variable.

For each sampling method the Horvitz-Thompson estimators were calculated. Efficiency of spatial sampling modified by model use was verified using rRMSE of the estimator of the mean of Y. Results are presented in Table 1.

Table 1: rRMSE for different sampling methods, c=5.

Method	Spatial sampling modified by model usage - Probabilities of inclusion based on Monte Carlo	Spatial sampling modified by model usage - Probabilities of inclusion proportional to X variable	Spatial sampling method in primary form
CM	0.467%	0.298%	0.371%
LPM1	0.489%	0.306%	0.279%
LPM2	0.464%	0.275%	0.280%
SCPS	0.478%	0.276%	0.324%
UPS	0.494%	0.296%	0.310%

rRMSE for estimators based on the Monte Carlo first-order probabilities of inclusion was significantly higher than for the other two approaches. Spatial sampling modified by model use with the first-order probabilities of inclusion proportional to the auxiliary variable delivered lower rRMSE than the primary form for all methods except LPM1.

Simulation was repeated for c equal to 10, 15, 20 and 25. Results are presented in Tables from 2 to 5 respectively.

Table 2: rRMSE for different sampling methods, c=10.

Method	Spatial sampling modified by model usage - Probabilities of inclusion based on Monte Carlo	Spatial sampling modified by model usage - Probabilities of inclusion proportional to X variable	Spatial sampling method in primary form
CM	0.541%	0.299%	0.371%
LPM1	0.512%	0.276%	0.279%
LPM2	0.547%	0.267%	0.280%
SCPS	0.559%	0.285%	0.324%
UPS	0.491%	0.296%	0.310%

Table 3: rRMSE for different sampling methods, c=15.

Method	Spatial sampling modified by model usage - Probabilities of inclusion based on Monte Carlo	Spatial sampling modified by model usage - Probabilities of inclusion proportional to X variable	Spatial sampling method in primary form
CM	0.507%	0.302%	0.371%
LPM1	0.522%	0.342%	0.279%
LPM2	0.494%	0.270%	0.280%
SCPS	0.483%	0.273%	0.324%
UPS	0.477%	0.295%	0.310%

The results show that for Cube method, Spatially Correlated Poisson Sampling method and Unequal Probability Sampling model modification increases sampling efficiency (in terms of rRMSE reduction) and it is independent from the c value. Modification of UPS method delivered quite stable rRMSE values for different c values. Model modification of SCPS and CM methods had generally higher rRMSE values for higher c values. LPM1

Table 4: rRMSE for different sampling methods, c=20.

Method	Spatial sampling modified by model usage - Probabilities of inclusion based on Monte Carlo	Spatial sampling modified by model usage - Probabilities of inclusion proportional to X variable	Spatial sampling method in primary form
CM	0.485%	0.336%	0.371%
LPM1	0.549%	0.286%	0.279%
LPM2	0.538%	0.322%	0.280%
SCPS	0.497%	0.316%	0.324%
UPS	0.465%	0.298%	0.310%

Table 5: rRMSE for different sampling methods, c=25.

Method	Spatial sampling modified by model usage - Probabilities of inclusion based on Monte Carlo	Spatial sampling modified by model usage - Probabilities of inclusion proportional to X variable	Spatial sampling method in primary form
CM	0.452%	0.331%	0.371%
LPM1	0.507%	0.326%	0.279%
LPM2	0.408%	0.304%	0.280%
SCPS	0.472%	0.309%	0.324%
UPS	0.441%	0.293%	0.310%

modified by model use achieved a better rRMSE value than primary LPM1 only for $c = 10$ and the difference was negligible. As a rule, model modification was inefficient for this sampling method. In the case of LPM2, model modification delivered better efficiency for low values of c parameter. However, the gain was smaller than the ones obtained on CM, SCPS and UPS model modifications.

4. Conclusions

The choice of modelling method determines the efficiency of the presented sampling modification. The precision of the model is a key to achieve the main advantage of this sampling modification - stabilization of sampling elements around the global average value of the additional variable. In the presented example a very basic type of model - ordinary kriging, was chosen. It did not give a full picture of the influence of modelling method on sampling efficiency. The aim of the example was, however, to evaluate the potential of the presented modification rather than in-depth analysis of how changes in values of different parameters (n_0, m, d_k) impact the rRMSE on different populations. Such an analysis would require rather a more multi-aspect approach than the one used in the above example and need more research.

The aim of this paper was to evaluate the potential of model modification. Considering the results of the experiment in which the model modification often improved the quality of the underlying method, it can be concluded that model modification can also be used for other design-based methods. From a theoretical point of view, the presented solution can easily be translated into other methods. As a results, we obtained quite an effective method, which expands the range of design-based methods, which can be used in spatial research.

Spatial sampling modified by model use requires ongoing access to statistical program which allows to construct kriging or other spatial models. This requirement could be fulfilled in two ways: by using mobile devices with the access to statistical software or by sending the information about sampled elements to a PC which works as a computational station. Both solutions increase the cost of research. However, both solutions should be treated as long-term investments in research equipment. Then, learning on the elements selected to the sample could be ongoing. Generally, real-time observation and analysis of the sample seems to be an interesting direction in the development of sampling methods.

The presented sampling modification gives a possibility to adjust the sampling method to the analysed population and its different characteristics. Adjustment could be introduced quite straightforwardly, by changes in the coefficients of spatial sampling modified by model use. It could also have other, more complex aspects, such as definition of probabilities of inclusion or modelling method choice. One can also think about further modification, which have not been discussed yet. One of more interesting in the author's opinion is to substitute $\bar{x}$ value of the additional variable, which is known before sampling, by an average value $\bar{y}$ of the characteristic under study, which is calculated during sampling process. After this change the sampling could be conducted without using the additional variable.

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