



Optimal network design for spatial prediction of soil redistribution (^{137}Cs) based on a minimax approach

Firoozeh Rivaz ^{a,*}, Mohsen Hosseinalizadeh ^b, Edzer Pebesma ^c

^a Shahid Beheshti University, Faculty of Mathematical Sciences, Department of Statistics, Tehran, Iran

^b Gorgan University of Agricultural Sciences & Natural Resources, Department of Watershed & Arid Zone Management, Iran

^c University of Munster, Institute for Geoinformatics, Germany

Abstract

Measuring ^{137}Cs is considered an effective method to study soil redistribution rate and hence needs sampling at a number of sites. The spatial configuration of the network of sites to be sampled has a substantial effect on the soil redistribution assessment. Here, motivated by sampling ^{137}Cs , we adopted a model-based approach. For this, we chose the average kriging variance (AKV) as a design criterion. In fact, by minimizing the AKV of soil ^{137}Cs prediction in the paired sub-catchments of Iran's Golestan province, we determined the optimal sampling design in the case that no directly measured prior information of the primary variable of interest (^{137}Cs) is available. However, the AKV depends on some unknown parameters and preliminary estimates of model parameters are not available. To overcome this problem, we apply the minimax approach which minimizes the maximum value of design criterion over the misspecification of parameters. The method is illustrated taking into account the ancillary information (slope%) from representative Sub-catchments (Sample and Testifier, each around 190 ha in size). A simulated annealing algorithm is used to search for an optimal design from among all possible designs. Since, the number of sampling points is often limited by time and budgetary constraints, we use a sequential-based method for selecting the sample size. It is shown that 60 sites are sufficient for the proposed Sample and Testifier sub-catchments.

Keywords: ^{137}Cs , Golestan province, minimax approach, simulated annealing, spatial sampling.

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Introduction

Fallout radionuclides (FRNs), and more particularly ^{137}Cs , have been successfully used to quantify soil redistribution processes since the 1970s (Zapata, 2002). As demonstrated by some 4000 published research papers dealing with the use of ^{137}Cs , this technique has been shown an effective means to quantify soil redistribution rates (Ritchie and Ritchie, 2008). In fact, this technique has been validated successfully against other more conventional data provided by erosion plots, erosion pins, erosion– sedimentation modeling and catchment sediment yields, in a range of environments (e.g. Mabit et al. 2002; Wallbrink and Croke, 2002; Schuller et al. 2007). It should be noted that ^{137}Cs has been used to investigate soil redistribution over a range of scales, extending from experimental plots to large watershed of 217 km² in Quebec, Canada, reported by Mabit et al. (2007). So, the spatial configuration of the network of sites to be

* Corresponding author.

Shahid Beheshti University, Faculty of Mathematical Sciences, Department of Statistics, Tehran, Iran

Tel.: +982129903008

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E-mail address: f_rivaz@sbu.ac.ir

measured has a substantial effect on the soil redistribution assessment. Consequently, the first step in employing the ^{137}Cs technique involves the establishment of an appropriate sampling strategy. This involves the selection of both representative sampling areas and the sampling design, which in turn reflects the objectives of the proposed study as well as the characteristics of the local landscape. A literature review on the proposed aspect shows different views on sampling ^{137}Cs , but they generally focused on design-based sampling strategies rather than a model-based sampling. The most commonly used design for radionuclide studies is systematic, non-stratified sampling using either transects or grids (Zapata, 2002). Webster and Oliver (1992) argued that a minimum of 150 points is needed from each area of interest in order to identify the variogram model for geostatistical interpolation. Montgomery et al. (1997) used two sample networks, respectively with 110 and 48 samples, to estimate the variogram of the interested process. Lettner et al. (2000) applied three sampling networks with areas of 10m², 100m² and 1000m², each containing 81 sampling points. The smaller area networks of sampling were nested within the larger one, such that 235 samples were taken in their case study to perform an in-depth geostatistical analysis of the ^{137}Cs . Studying the spatial variability of ^{137}Cs in a single field in Germany, Bachhuber et al. (1987) concluded that at least 14 samples were required to obtain the mean activity of ^{137}Cs with 10% of tolerable error and 95% confidence limits. Based on ^{137}Cs measurements, Higgitt (1995) assessed the influence of sample number on soil redistribution map within a 3.2 ha cultivated field in Shropshire, England. A total of 83 samples were taken on a lattice with 20 × 20 m² cells, and a random-numbers generator was used to successively withdraw samples from the lattice to achieve sample sizes of 70, 60, 50, and 25. The interpolated maps maintain a broadly similar pattern until the sample size is reduced to 25. Yang et al. (2006) used transect-based sampling to study the spatial distribution of soil redistribution (^{137}Cs) at Loess Plateau of China's Shaanxi Province. Mabit et al. (2008) also applied the transect-based sampling, which in their study geostatistics and variography were considered as an indicator in validating sampling strategies. The semivariogram of ^{137}Cs indicated that the sampling strategy was adequate and adapted to reveal the spatial structures of the ^{137}Cs under investigation. Finally, a map of the soil redistribution was produced using the ordinary Kriging approach.

As the goal in soil redistribution studies is to produce the prediction map, in this study, we intend to find the optimal sampling designs that are efficient for spatial prediction of soil redistribution using ^{137}Cs . To the best of our knowledge, actually there is no published paper using the model-based approach to determine optimal spatial network design for ^{137}Cs . Consequently, adopting a model-based approach, we chose average kriging variance as the design criterion. In fact, we determined optimal spatial network for two crop production Sub-catchments in Iran's Golestan province, with the same area but different shapes and distinctive management policies such as tillage and grazing management as well. It should be noted that Sample and Testifier sub-catchments are closed and open area for grazing, respectively. This is motivated by the fact that no directly measured prior information on the primary variable of interest is available. However, since, the design criterion depends on the correlation structure and no data is available providing partial knowledge of the unknown model, we concentrate on a rich and flexible family of correlation functions for modeling the spatial structure. Thereafter, to overcome the misspecification of model parameters we use the minimax approach (Wiens, 2005; Spöck, 2010). The optimal design in the minimax sense is the design that minimizes the maximum value of the design criterion over the misspecification of model parameters. For this, we first assume a range of plausible values for the parameters. Then, the optimal design is chosen when the parameters take the worst possible value within their respective ranges and thus the criterion be minimized. The least favorable parameter values are those that maximize the design criterion. For choosing the optimal design, we have discretized the parameter space and then apply simulated annealing (SA) algorithm (van Groenigen and Stein, 1998).

The use of auxiliary variables for soil properties is expected to systematically enhance prediction accuracies especially because soil data are generally scarce over large areas and auxiliary variables are readily available (Li, 2010). In this study, we use slope% as an auxiliary variable because slope plays a significant role on soil redistribution rate, and also because it is readily available at the stage when nothing is known about the primary variable in the proposed areas and in their proximity. Since no optimal number of samples is known, it becomes necessary to develop a methodology to determine the number of sampling points while maintaining its ability to describe the spatial soil redistribution across the field. For this reason, a sequential-based method is used to determine the sample size.

The rest of the paper is organized as follows. Section 2 discusses materials and methods including study area as well as the sampling approach. Section 3 deals with results whereas Section 4 contains discussion and concluding remarks.

Material and Methods

Study Area

The proposed areas of study are located in the north-east of Iran's Golestan province as paired Sub-catchments (Sample and Testifier; enclosed and open area respectively) of representative watershed, intensively exploited arable land with commonly cultivated crops such as, sun flower, barley, wheat, watermelon, artificial and natural forest and so and so forth. The above representative catchment of approximately 2,061,338 ha is affected by diverse water erosions types (sheet, rill, and splash) and intense agricultural activities over there. The soil in area is a silt loam and loam, varying from shallow to deep. The climate is typically semi-arid with an average annual temperature of about 16.7°C and an annual precipitation amount of 482mm. The landscape is gently undulate with an average altitude of approximately 800m. While Fig. 1 shows the location map of Sub-Catchments, Table 1 summarizes some characteristics of these Sub-Catchments.

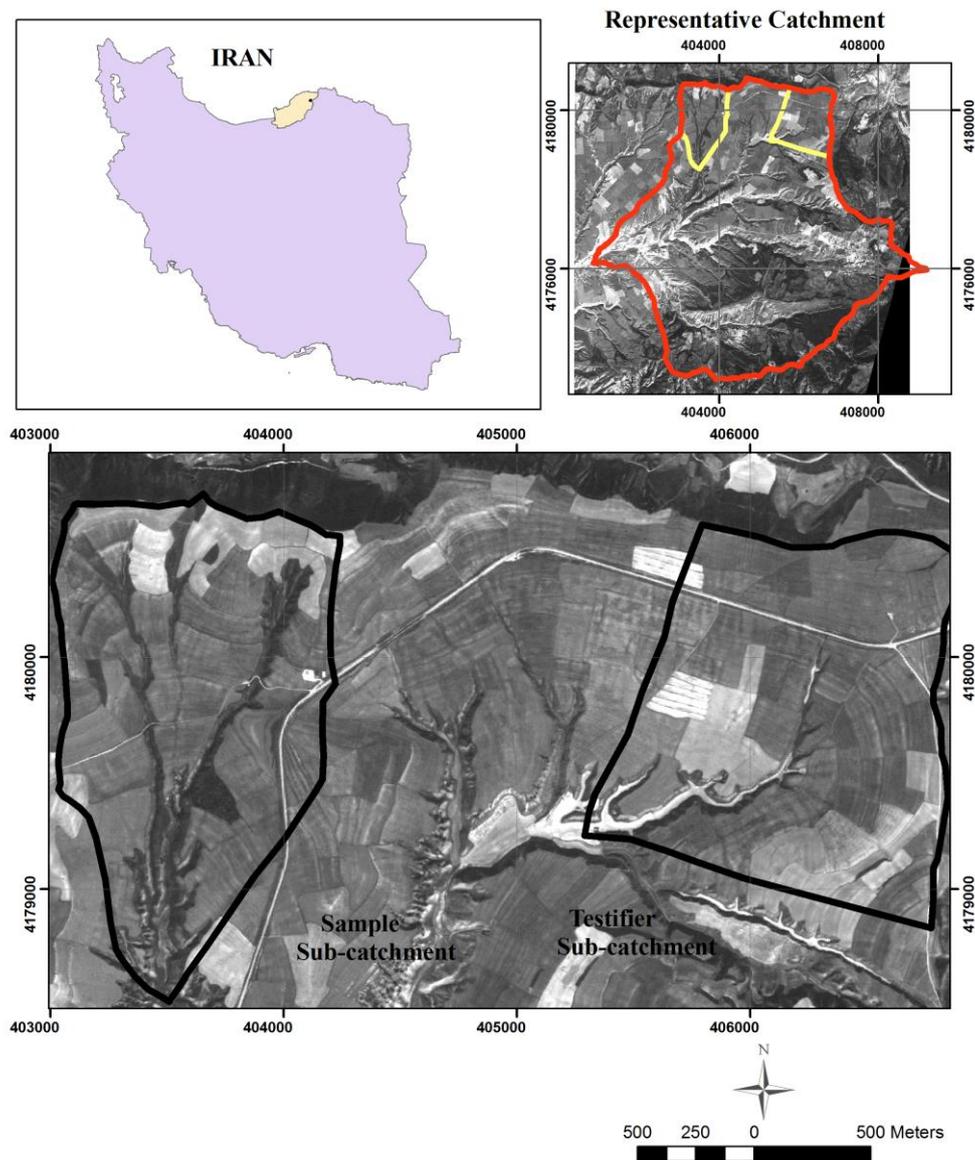


Figure 1. The location map of Sub-Catchments

Table 1. Some characteristics of Sub-catchments

Sub-catchment	Sample	Testifier
Slope (%)	0-166	0-90
Elevation (m)	700-900	755-850
Area (ha)	191	196

The design problem comes down to the following: choose a set of n points that optimizes the design criterion among all the sets of n points from the region of interest. To facilitate a search for the optimal points, we need to discretize the proposed Sub-catchments into two finite spaces. Sutherland (1994), Lu and Higgitt (1999) and Zapata (2002) suggested that sampling interval should be 10 to 25 m away from the adjacent samples. So, two fine square 20×20 grids are used to approximate the Sample and Testifier sub-catchments, with the total grid points $N_1 = 3060$ and $N_2 = 3141$, respectively. We therefore search for optimal design among the grid points in Sample and Testifier areas using simulated annealing algorithm. It must be noted that there was no prior measurement of ^{137}Cs in the proposed areas and the slope% is used as an auxiliary data influencing soil redistribution.

Sampling Method

Two sampling approaches preferred widely for soil mapping are the design-based approach used in classical survey sampling and the model-based approach followed primarily in geostatistics (Brus and de Gruijter, 1997). They differ in assumptions with respect to properties of both population targets (value of soil property) and the sampling locations. The design-based approach is the most suitable for estimating the frequency distribution of soil property and one or more parameters of that distribution such as the global mean. In contrast, the local prediction through interpolation or simulation requires sampling schemes that allow quantification of the spatial dependence and provides good area coverage for the reliable prediction map. Since the goal of ^{137}Cs sampling is to produce a soil redistribution map, the model-based geostatistical sampling approach is often more appropriate (Brus et al. 2002). The geostatistical sampling chooses the optimal sample pattern by minimizing a design criterion such as the mean or maximum prediction variance, where predictions are computed by kriging assuming that the covariance model and all its parameters are known. More precisely, let a continuous spatially-varying quantity, Z , is to be observed at a predetermined number of points s_1, \dots, s_n in a region of interest D . Suppose $Z(s_1), \dots, Z(s_n)$ represent the observations taken at these points. These observations are modeled as a realization of a random field $\{Z(s), s \in D\}$ with mean $E[Z(s)] = f'(s)\beta$ and covariance function $C(s_1, s_2) = cov(Z(s_1), Z(s_2))$ where $f'(s) = (f_0(s), \dots, f_p(s))$ with $f_0(s) = 1$ is a known vector of observed covariates and $\beta = (\beta_1, \dots, \beta_p)'$ is unknown regression parameters. First, we assume that the covariance function is known. By the stated assumptions, the best linear unbiased predictor (BLUP) of Z at an arbitrary unsampled site $s_0 \in D$, is the so-called universal kriging predictor, which is given by

$$\hat{Z}(s_0) = [c + X(X'\Sigma^{-1}X)^{-1}(x - X'\Sigma^{-1}c)]'\Sigma^{-1}z,$$

where $X = (f'(s_1), \dots, f'(s_n))'$ is the full rank $n \times (p + 1)$ matrix, c is the vector whose i th element is $C(s_i, s_0)$, $\Sigma = (C(s_i, s_j))$, x is the vector whose j th element is $f_{j-1}(s_0)$ and $z = (z(s_1), \dots, z(s_n))'$ is the data vector. The minimized prediction error variance associated with $\hat{Z}(s_0)$, also called the kriging variance, is given by

$$\sigma^2_K(s_0) = var(\hat{Z}(s_0) - Z(s_0)) = C(s_0, s_0) - c'\Sigma^{-1}c + (x - X'\Sigma^{-1}c)'(X'\Sigma^{-1}X)^{-1}(x - X'\Sigma^{-1}c)$$

(1)

Suppose we wish to choose a subset of n points from D that are optimal, in some sense, for the purpose of kriging. As noted previously, the two most commonly used design criteria for this purpose are the average kriging variance (AKV):

$$\frac{1}{|S|} \int \sigma^2_K(s) ds$$

and the maximum kriging variance:

$$\max_{s \in S} \sigma^2_K(s)$$

where S is the set of all possible points that observations may be taken and $|S|$ is the volume of S . The optimal design with respect to these criteria is the one that minimizes the criterion over all possible designs taken from S . To calculate these criteria for any design, the covariance model and its parameters should be known. However, prior knowledge of the spatial variation of the primary variable is often not available or its gathering significantly increases the sampling cost. Thus the model-based sampling schemes that merely utilize measurements of the primary variable are likely to be costly and time-consuming, especially in cases when expensive laboratory procedures like Gamma ray spectrometry are involved or when the area to be investigated is large. In such a case, for determining the design criterion, we need to assume that there exists a preliminary estimate or guess of the unknown covariance structure. Since there is no any prior knowledge of the spatial structure, we concentrate on a rich and flexible family of covariance model. In this study, a general and flexible powered exponential family is used to model the covariance structure (Banerjee et al. 2004), which involves a shape parameter p in addition to the range parameter ϕ , and is given as:

$$c(h; \theta) = \tau^2 I_{\{h=0\}} + \sigma^2 e^{-|\phi h|^p} I_{\{h>0\}}; \quad 0 < p \leq 2, \phi \in \mathfrak{R}^+ \quad (2)$$

where $\theta = (\sigma, \tau, \phi, p)$ such that σ^2 and τ^2 are variance and nugget effect, respectively. The exponential and Gaussian covariance functions are special cases of the powered exponential covariance family with $p = 1$ and $p = 2$, respectively. The design criterion yet depends on the unknown parameters of powered exponential model. To overcome this problem, we used the minimax approach which minimizes the maximum value of design criterion over the misspecification of parameters. In other words, the minimax approach aims to obtain the best design for the worst possible case of the model misspecification. For this purpose, we first need to discretize the parameter space, Θ , into a finite space Θ_d and find optimal designs for all $\theta \in \Theta_d$. Then, we can evaluate the maximum of design criterion on $\theta \in \Theta_d$ for any design and search for the one that minimizes the maximum. Since slope% has influential effect on soil redistribution and due to easy application, it is considered as a covariate variable. In fact, we consider a linear trend of slope in prediction equations.

Now, we discretize the parameter space Θ into a four dimensional grid with $m = m[1] \times m[2] \times m[3] \times m[4]$ nodes. If the covariance model (1) is parameterized as

$$c(h; \eta) = \tau^2 I_{\{h=0\}} + \sigma^2 \phi^p I_{\{h>0\}},$$

it follows that $\eta = (\sigma, \tau, \phi, p) \in \mathfrak{R}^+ \times [0, \infty) \times (0, 1) \times (0, 2]$. The support of ϕ and p are bounded; hence discretization of them is straightforward. But it is not clear cut for σ and τ , because the support of them are unbounded. To apply the minimax method, it is necessary to determine a subset $(0, \sigma_0] \times [0, \tau_0]$ of $\mathfrak{R}^+ \times [0, \infty)$ and consider it as the practical support. To choose σ_0 and τ_0 , we apply a sensitivity analysis. In fact, the values of σ_0 and τ_0 are chosen in such a manner that the minimax design criterion be less sensitive to them. To do this, first two initial values for σ_0 and τ_0 , say $\sigma_0^{(ini)}$ and $\tau_0^{(ini)}$, are chosen. Then the parameter space is discretized and the minimax design is determined. Thereafter, we replace $\sigma_0^{(new)}$ and $\tau_0^{(new)}$ instead of old values of σ_0 and τ_0 , and minimax design is searched over the new parameter space. The algorithm continues until the design criterion is not sensitive to change of the values of σ_0 and τ_0 . We found that the design criterion is at all not sensitive for values greater than $\sigma_0 = 20$ and $\tau_0 = 25$. It must be noted that, a simulated annealing algorithm is employed to search for the optimal design.

By this way, we obtained $\Theta_d = \{1, 5, 10, 15, 20\} \times \{0, 5, 10, 15, 20, 25\} \times \{0.2, 0.45, 0.7, 0.95\} \times \{0.5, 1, 1.5, 2\}$. The parameter values at which we find minimax design for Sample and Testifier sub-catchments are $(20, 10, 0.2, 0.5)$ and $(15, 5, 0.45, 0.5)$, respectively.

So far, it was assumed that the sample size is known. Another aspect of this study is to determine the sample size due to the fact that the number of sampling points is limited by time and budgetary constraints. For this purpose, the optimal design criterion is determined for different sample sizes. Then, an appropriate sample

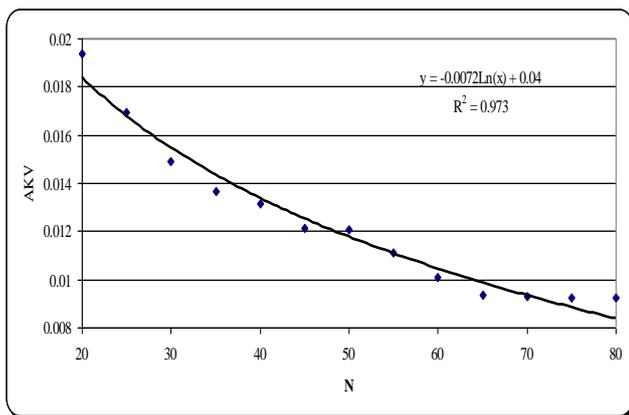
size is selected by accounting for the tradeoff between the prediction accuracy and the time and budgetary constraints. In other words, the optimal sample size is chosen in a way that the increasing sample size does not significantly impact on the value of design criterion.

Results

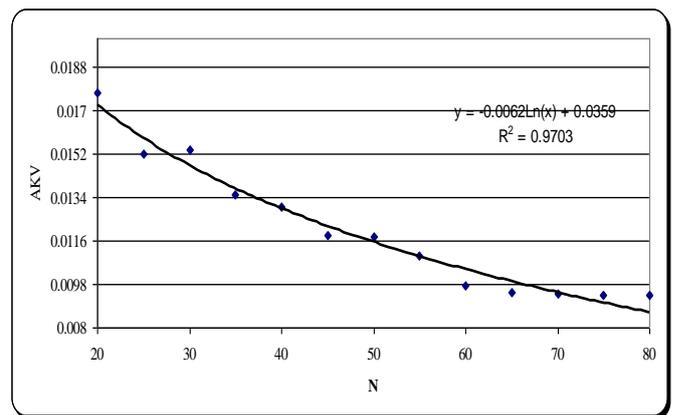
This section provides the results of the minimax method in determining the optimal design for paired Sub-catchments. It must be noted that the average kriging variance (AKV) has been considered as a design criterion. Table 2 summarizes the value of the AKV for different sample sizes. Moreover, Fig. 2 displays the result of Table 2 for the proposed Sub-catchments. As observed, the objective function improved during the increasing of the sample size. Although the objective function is yet decreasing after $n = 60$ in both Sub-catchments, but there is no sharp decline from 60 onward. Thus, a sample size of 60 seems to be reasonable in both Sub-catchments.

Table 2. Average kriging variance for different sample sizes in proposed Sub-catchments

Testifier Sub-catchment		Sample Sub-catchment	
Sample numbers	Design criterion	Sample numbers	Design criterion
20	0.01936	20	0.01775
25	0.01696	25	0.01520
30	0.01490	30	0.01539
35	0.01364	35	0.01354
40	0.01313	40	0.01301
45	0.01216	45	0.01182
50	0.01206	50	0.01179
55	0.01110	55	0.01096
60	0.01011	60	0.00974
65	0.00938	65	0.00945
70	0.00933	70	0.00940
75	0.00926	75	0.00938
80	0.00922	80	0.00935



(a)



(b)

Figure 2. Average kriging variance for different sample sizes in Sample (a) and Testifier (b) sub-catchments

For fixed sample size and powered exponential correlation structure with parameters specified in section 2.2, the minimax designs in both catchments were determined using SA algorithm. Fig. 3 shows the spatial configuration of optimal design for Sample (left map) and Testifier (right map) sub-catchments. As observed, there is no specific regularity in sampling pattern like systematic, cluster and nested in both Sub-catchments. Meanwhile the sample locations are scattered in the whole area of two catchments.

Detailed slope characteristics for the selected sites in paired Sub-catchments (Table 3) show no any significant difference. Histogram and scatter plot of the slop values for the selected sites in both Sub-catchments (Fig. 4 and Fig. 5) illustrate more than 50% of sample sites (39 sites) belong to slope<18 % and 34 sample sites belong to slop<33%, in Sample and Testifier sub-catchments, respectively. It seems minimax design depends on auxiliary variable. Although the range of slope in Sample catchment is greater than Testifier catchment, but slope frequency distribution in the optimal designs have approximately the same behavior. In particular, the average slope is 28% in both Sub-catchments.

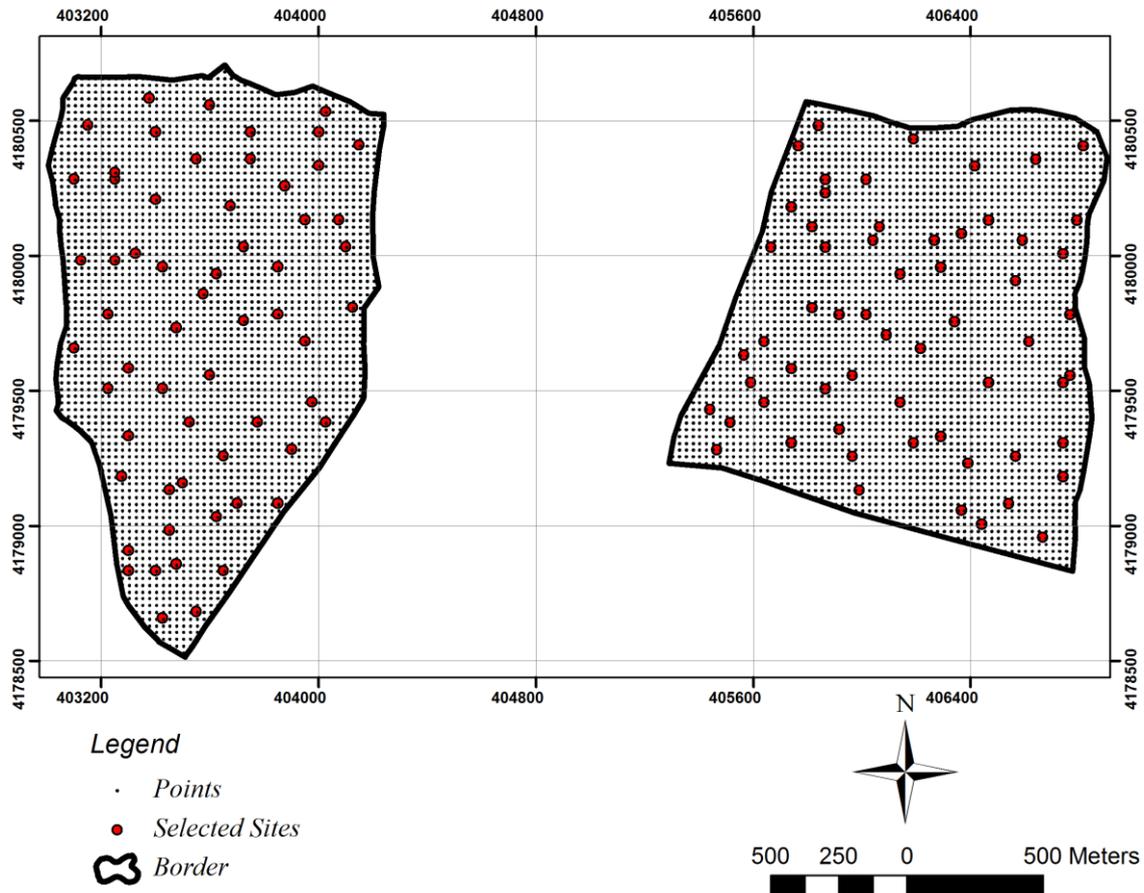


Figure 3. Location map of minimax design in Sample (left map) and Testifier (right map) sub-catchments

Table 3. Slope characteristics of the optimal network of sites in paired Sub-catchments

Sub-catchment	Slope (%)						
	Mean	Min.	Max.	SD	1 st quartile	Median	3 rd quartile
Sample	28	0	100	34	2	24	77
Testifier	28	4	88	24	8	11	41

Discussion

^{137}Cs as retrospective method in soil redistribution studies is a reliable technique for assessment of the past soil redistribution process. However, sampling of ^{137}Cs is still a debatable issue. This article has proposed a minimax method for finding the optimal sampling design that is efficient for spatial prediction of soil redistribution using ^{137}Cs when no directly measured prior information of the primary variable of interest is available. The study area was two sub-catchments called as paired Sub-catchments which have important roles in soil and water conservation. We also addressed an important issue, which has somewhat been ignored in the past literature, on how to select an appropriate sample size by accounting for the tradeoff between accuracy of prediction and time and budgetary constraint.

It was obtained that 60 samples (about 1 sample per 3ha) are enough for two Sub-catchments. In this study, the slope% was used as an auxiliary data influencing soil redistribution. As expected according to equation (1), the optimal designs depend on the auxiliary variable. As a result we came to conclude that more auxiliary variables increase information in selecting the optimal design. So it is suggested, when feasible, to use other auxiliary variables in determining optimal design.

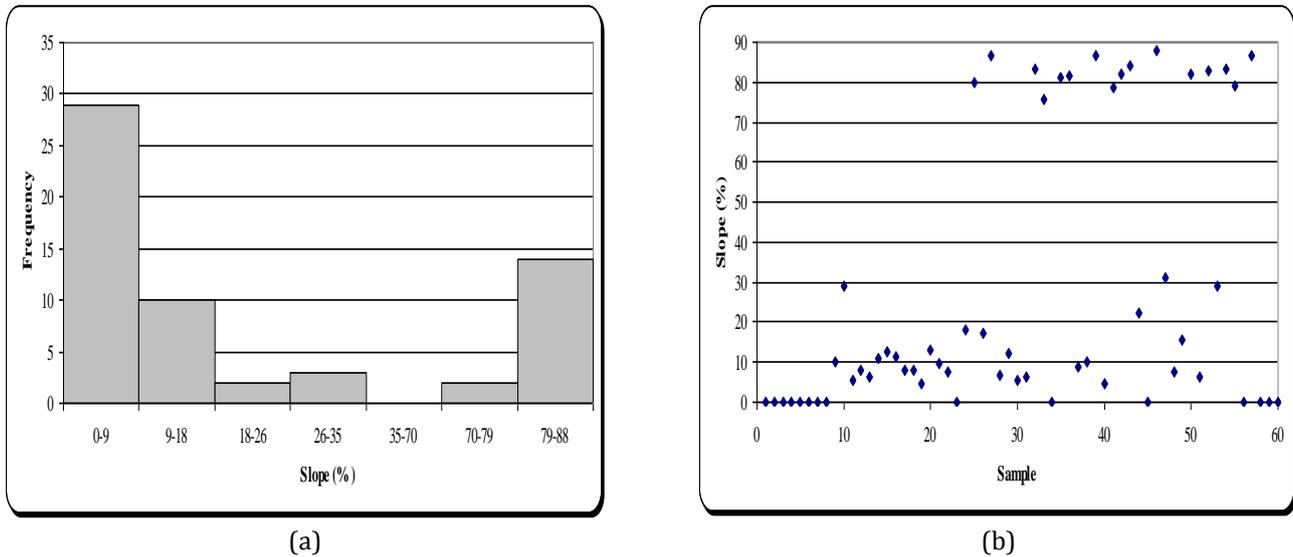


Figure 4. Histogram and scatter plot of the slop values for network sites in Sample sub-catchment

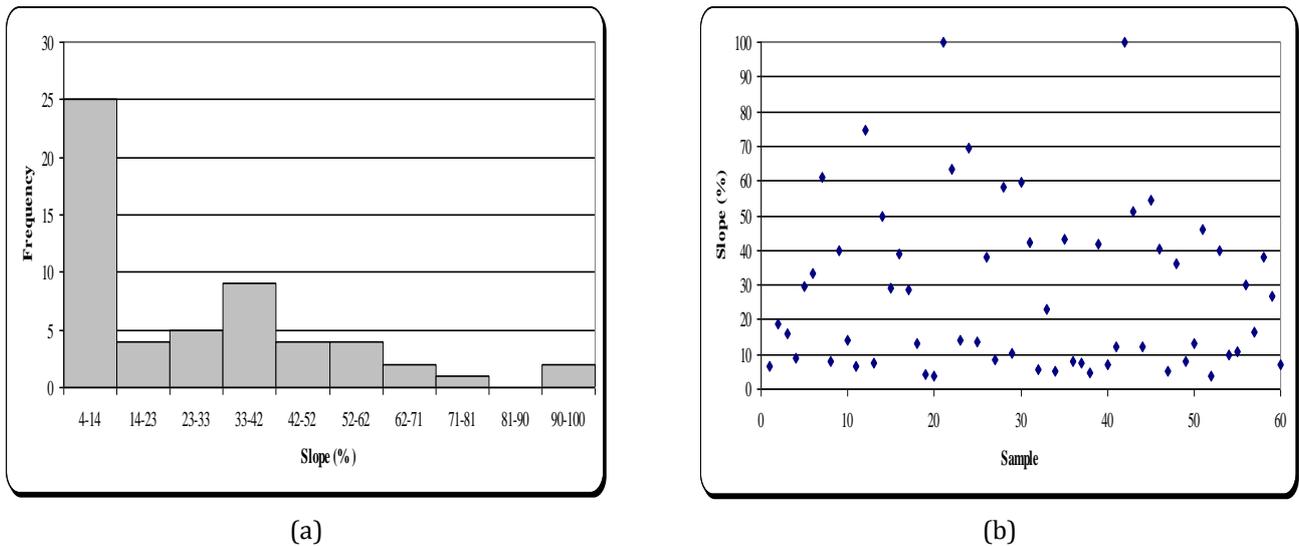


Figure 5. Histogram and scatter plot of the slop values for network sites in Testifier sub-catchment

In contrast to what [Zapata \(2002\)](#) found, we tried to show that the number and location of samples are determined effectively using the model-based approach. Further, this approach can use the budgetary constraint effectively and can be obtained without the exact knowledge of the true parameters, and thus can be applied in practice. Contrary to [Webster and Oliver \(1992\)](#) we illustrated that the sample size of the region of interest can be less than 150 points. This approach can conquer limitation on the use of ^{137}Cs (sampling pattern) in large areas.

The tillage erosion, as a calm and dangerous soil redistribution effect, is likely gain importance in the near future and FRNs technique will be considered for tillage cultivation results as well and spatial sampling of them would be a crucial issue. It must be noted that ^{137}Cs technique also considers tillage erosion that represent as much as 70% of total soil erosion ([Lobb et al. 1999](#)) dissimilar to other soil erosion methods.

As such, through the aforementioned methods and integrated Portable HpGe, soil redistribution will be measured in negligible time span and in a large area specifically cultivable land involved with plowing and soil redistribution. The special case in this paper includes ^{137}Cs , one of the FRNs. The approach could be embedded in a multivariate framework, where ^{137}Cs could be replaced by all three fallout radionuclides: ^7Be , ^{137}Cs and $^{210}\text{Pb}_{\text{ex}}$. Although, in such setting, a reasonable criterion that takes into account all three FRNs, is required.

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