



Gaussian process simulation of soil Zn micronutrient spatial heterogeneity and uncertainty – A performance appraisal of three semivariogram models

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ABSTRACT

Geostatistical modelling has proven to be a good tool for decision making in soil nutrient management because it has the ability to map spatial heterogeneity and uncertainty. This study outlines a comparative approach to quantify the uncertainties and correlations in spatial process models as illustrated for the distribution of Zn in top soils of a semi-arid environment. The spatial correlation of Zn uncertainties is investigated by calculating the semi-variance of normalized Zn concentration residuals, for a sufficiently large dataset, as a function of distance between pairs of locations within the Zn field. Three semi-variogram models, namely: Exponential, Gaussian, and Spherical models were tested on the spatial correlation structure of the normalized residuals and further used as default input model for Sequential Gaussian Simulation. The Sequential Gaussian Simulation led to an improved description of spatial heterogeneity and uncertainty. The choice of semivariogram model is therefore critical for robust Sequential Gaussian Simulation and uncertainty analysis. A new criterion is proposed to inform the choice of default input model for sequential Gaussian simulation given by ratio of partial sill to square of major range. With this criterion, Exponential model performed better than both Gaussian and Spherical models. The results indicate spatial correlation in Zn field and it is suggested that the spatial correlation of Zn uncertainties should be considered to exclude inaccurate estimation for spatially distributed systems when performing nutrient distribution studies.

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Introduction

Soil micronutrients including zinc are important for plant growth. Even though micronutrients, unlike macronutrients, are required in small quantities they are known to be critical for growth and functioning of plants, animals and humans alike [2,5,26]. As such food source from Agricultural crops may provide pathway for Zn transfer to higher organisms. Notably, Zn is the only micronutrients present in all six classes of enzymes: transferases, hydrolases, oxido-reductases, lyases, isomerases and ligases [3]. An estimated 3000 proteins contain Zn prosthetic groups of higher animals including human

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[30]. Additionally, Zn ions are neurotransmitters, and cells in the salivary glands, prostate, immune system and the intestine utilize Zn signalling [17].

Micronutrients in soils, including Zn, derive mainly from pedogenic sources but other factors (e.g., pH, soil texture, organic matter and carbonate content) affect bioavailability and persistence of Zn within the crop rhizosphere. Owing to the immobile nature of Zn under a variety of soil conditions, it is common to observe Zn deficiency though high amounts ($>1000 \text{ mg Zn kg}^{-1}$) may be available [23]. In crop production systems specifically, low yield can be directly attributed to low bioavailable of Zn [6]. It is worthy of note that at-least a third of the cultivated soils globally are estimated to be low in bioavailable Zn [35]. It is therefore essential to manage agricultural soils for an important micronutrient such as Zn. This can be achieved by accurate measurement, monitoring and prediction of spatial patterns. This additionally presents an opportunity to formulate targeted nutrient deficit fertilizer supplements to support plant growth. Furthermore, environmental (geo) chemical budgets are dynamic and therefore justify the establishment of baseline studies to assess ecosystem evolution and the maintenance of soil health.

Advances in geographic information sciences complemented by fast but relatively accurate analysis of elemental composition has aided the collection of large spatio-temporal datasets that may be required for environmental assessment, monitoring and decision making. For example, this study assesses the spatial distribution of location-referenced Zn concentration first as a micronutrient that supports production food and fibre alongside ecosystem functioning and second to test the suitability of kriging-based estimators as basis for modelling spatial heterogeneity and uncertainty. Gaussian process simulation e.g. [11,15,20], have been suggested to be superior to standard kriging estimates. This is because standard kriging assumes a Gaussian process structure for the unknown spatial field with focus on calculating an optimal linear predictor of a sampling field. Deficiencies in this assumption are as follows: (1) the true covariance structure may be transient, (2) the estimated covariance structure may be unreliable, and (3) uncertainty in the spatial covariance structure may be unaccounted for. These issues have been addressed in a variety of ways. For example, Smith [27] suggests using likelihood-based methods for estimating the covariance structure, Handcock and Stein [16] proposed a Bayesian version of kriging that accounts for uncertainty in the spatial covariance structure, and Higdon [18], Higdon et al. [19], and Swall [28] have used Bayesian Gaussian Process analogues to kriging that account for uncertainty in the covariance structure. A Gaussian process model that has gained popularity within the geostatistics community is Sequential Gaussian Simulation (SGS) of which kriging serves as a default input e.g., [9,34]. To the best of our knowledge there is no laid down criteria for the choice of theoretical variogram model apart from the use of statistical indicators of model performance". Important questions to ask are whether the use of statistical indicators of model performance is "water-tight" and would SGS model produce a spatial process that differ significantly given differing default kriging inputs. The objective of this study is to test three semivariogram models: Exponential, Gaussian and Spherical models for their effectiveness at explaining spatial heterogeneity and uncertainty in Zn distribution in semi-arid top soils from Central Botswana. It is hypothesized that irrespective of kriging estimator as default Gaussian process input, the choice of a theoretical model for modeling the covariance function should lead to the same results.

Sampling and methodology

Study site, sampling and elemental analysis

This study utilized dataset in *Data-in-Brief* repository [12] to assess heterogeneity and uncertainty in the spatial distribution of Zn in a semi-arid soil environment. The study site, Maibele Airstrip North (628200 and 631100 Easting; 759120 and 759680 Northing, 780–950 m above sea level), is located in the central part of Botswana (Fig. 1). The total area is about 2.64 km^2 and the dominant soil type is Haplic Luvisols [8] and mean annual rainfall amount is 600 mm. Detailed sampling protocol, analytical techniques can be found in Eze et al. [12]. A summary description is however as follows: (1) the sampling field was delineated into 30 parallel lines in a NE-SW orientation, (2) soil samples were collected at about 20 cm depth, intervals of 25 m and 35 sampling points on each row (Fig. 1) resulting in 1050 sampling points, (3), the soil samples were air-dried and analysed for elemental composition using Olympus Delta Sigma® portable X-ray fluorescence analyser (p-XRF) by the BML operations. Readings were taken in duplicates and for the purpose of this study, average Zn concentration were used. The p-XRF has 10 ppm limit of detection (LOD) for Zn. A summary statistics of the data set is presented in Table 2.

Pre-processing and statistical data analysis

A total of 1050 soil samples were analysed. The data was checked for integrity (i.e., duplicate measurements, outliers in terms of coordinates and numerical values, and zero or "not detected"). For values below detection limit ($< 10 \text{ ppm}$), one-half the detection limit for those values was applied since censored data are less than 15% of the total [33]. Python program (version 2.7) was used to perform a Kolmogorov–Smirnov (K–S) test for normality.

Geostatistical analysis and sequential Gaussian simulation

The dataset was tested for the following: (1) stationarity, (2) distribution and (3) spatial dependency. Then SGS was performed with the simulation pre-set to 100 realizations. To ensure stationarity (i.e., mean and variance known and constant),

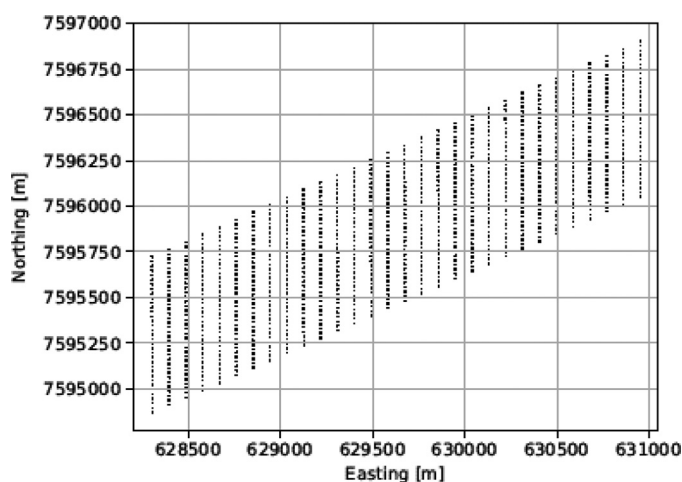


Fig. 1. Geographical location of the study area and sampling points. The dots represent the sampling points.

Table 1
Concentration of zinc in soils.

Micronutrient	Normal range found in soils ¹	Global average (mg kg ⁻¹)	Critical soil total concentration ²
Zinc (Zn)	1–900	90	70–400

¹ [4].

² [37].

Table 2
Descriptive statistics of Zn micronutrients in 0–20 cm soil profile ($n = 1050$).

Micronutrient	Minimum	Maximum	1st quartile	Mean	3rd quartile	SD	CV (%)	Skewness	Kurtosis	(k-s) ^a
Zn	3	174	56	71.95	85	21.92	30	0.49	4.20	0.03524

^a If the K-S < 0.05, then the distribution of soil micronutrient is not normal.

a pre-condition for SGS, a second order polynomial was used to remove trend in the dataset. The basis for SGS is that the data is normally distributed, therefore all further data analysis steps towards SGS included a normal score transformation as processing step. Overall our goal is to predict Zn values at un-sampled locations in the field; therefore the dataset was subject to spatial dependency test. To test spatial dependence of the dataset, the raw data was imported to ArcGIS, normal scored transformed and experimental semivariogram were calculated. Three variogram models (i.e., Experimental, Gaussian and Spherical) were fitted to the experimental semivariogram. A cross validation analysis was conducted to predict Zn values at sampled locations. Kriging was performed using the three semivariogram (i.e., Exponential, Spherical and Gaussian) models and the outputs were further used as input for SGS of soil micronutrient (Zn) distribution. The SGS was performed in ArcMap 10.6 software from Environmental Systems Research Institute, ESRI (ESRI, 2008). A flowchart of the SGS procedures is shown in Fig. 2.

Results

The average load of 71 mg Zn kg⁻¹ at the Maibele Airstrip North is below the average global 90 mg Zn kg⁻¹ value (Table 1). In Table 2 and Fig. 3, the descriptive statistics and probability distribution function (PDF) with a corresponding cumulative distribution function (CDF) are shown, respectively. Overall, Zn deficiency is expected to be widespread at the Maibele Airstrip North as indicated by Zn levels slightly skewed toward low values (Fig. 3(a)) as well as a low coefficient of variation (30%). Our idea is to test the performance of three different semivariogram models for their ability to explain uncertainty and spatial heterogeneity in Zn distribution by combining estimation and simulation. As required by SGS, symmetry was invoked by a normal score transform of the raw data (Fig. 3(a)) and the transformed data approaches a Gaussian distribution (Fig. 3(b)). In Fig. 4(a), (c) and (e), the simulated semivariogram for Spherical, Exponential and Gaussian models respectively are compared alongside their respective best fit results (Figs 4(b), (d) and (f)) for their performance to explain the spatial dependence of Zn distribution. Also, the parameters (nugget, partial sill and range) of the three semivariogram models are presented in Table 3. The resulting kriging estimates for Spherical, Exponential and Gaussian models (Fig. 5(a), (c) and (e), respectively) are presented alongside their respective SGS results for the 80th realization (Fig. 5(b), (d) and (f)). At this realization stability in model results was observed e.g., [34,36]. Since we consider only the influence of the

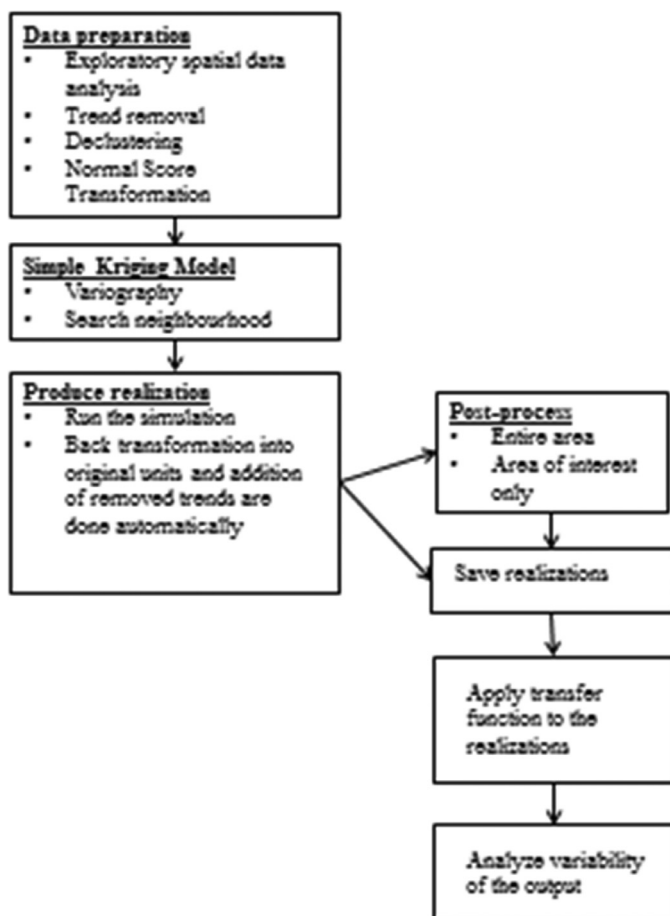


Fig. 2. Steps to creating a SGS in ArcGIS.

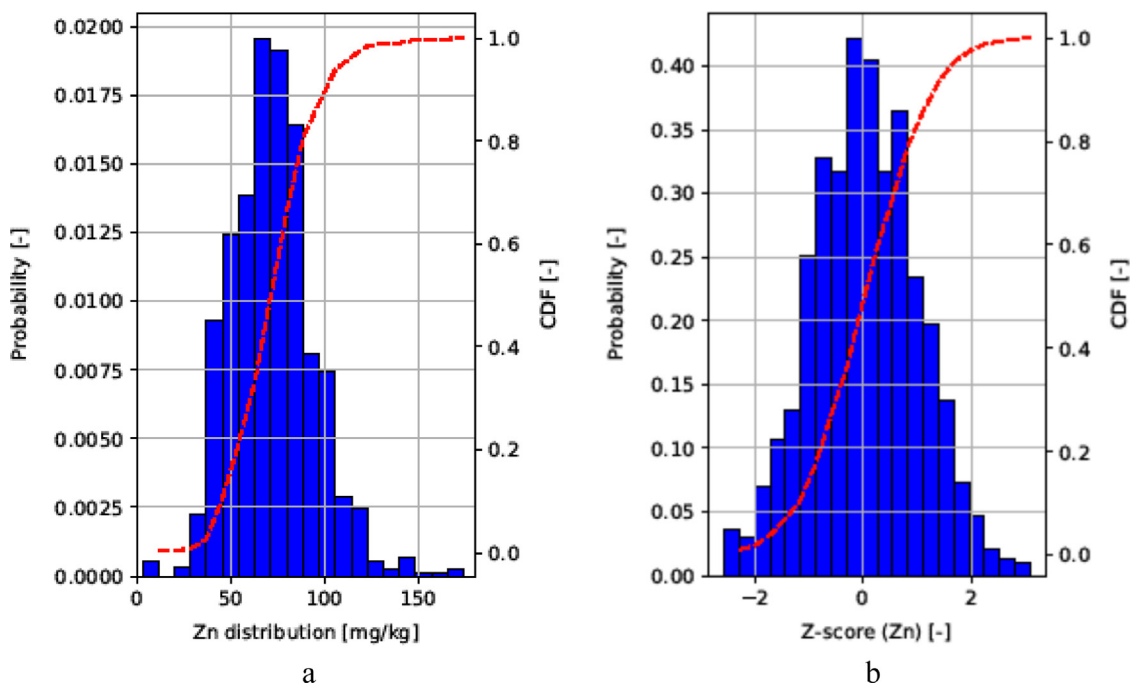


Fig. 3. Histogram of the raw (a) and normal score transform (b) for Zn content.

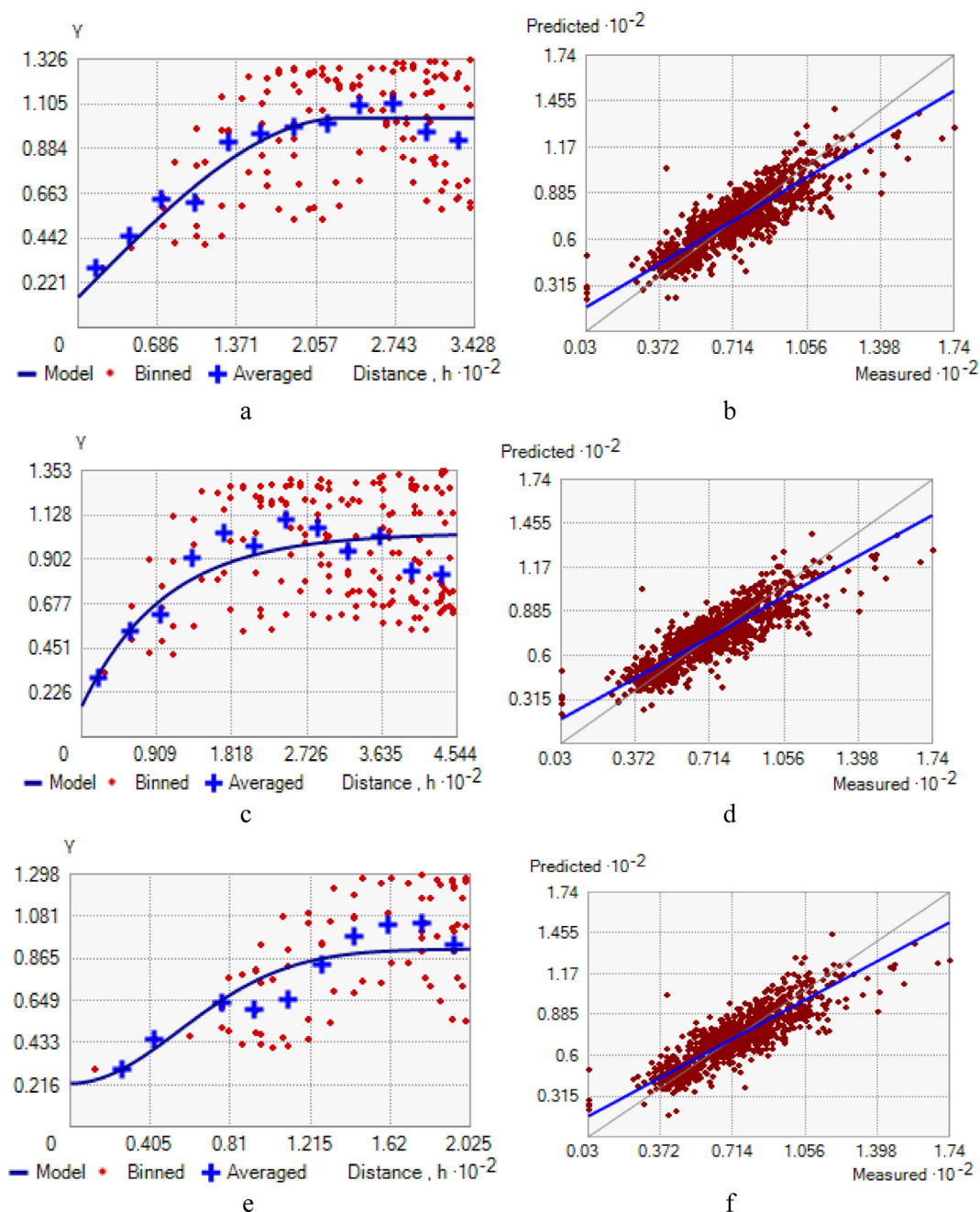


Fig. 4. Experimental semivariogram and best fit results obtained for (a) Spherical, (c) Exponential and (e) Gaussian models (estimated model parameters are show in Table 3) versus cross validation results obtained for (b) Spherical, (d) Exponential and (f) Gaussian models.

Table 3

Parameters of the fitted variogram models to Zn data.

Model structure	Nugget effect (mg kg^{-1}) ²	#Sill (mg kg^{-1}) ²	Range (m)	Mean Standardize Error	RMSS
Spherical	0.1507	0.8848	228.56	0.0054	0.9860
Exponential	0.1564	0.8797	302.94	0.0127	0.8926
Gaussian	0.2225	0.6898	135.02	0.0047	1.0246

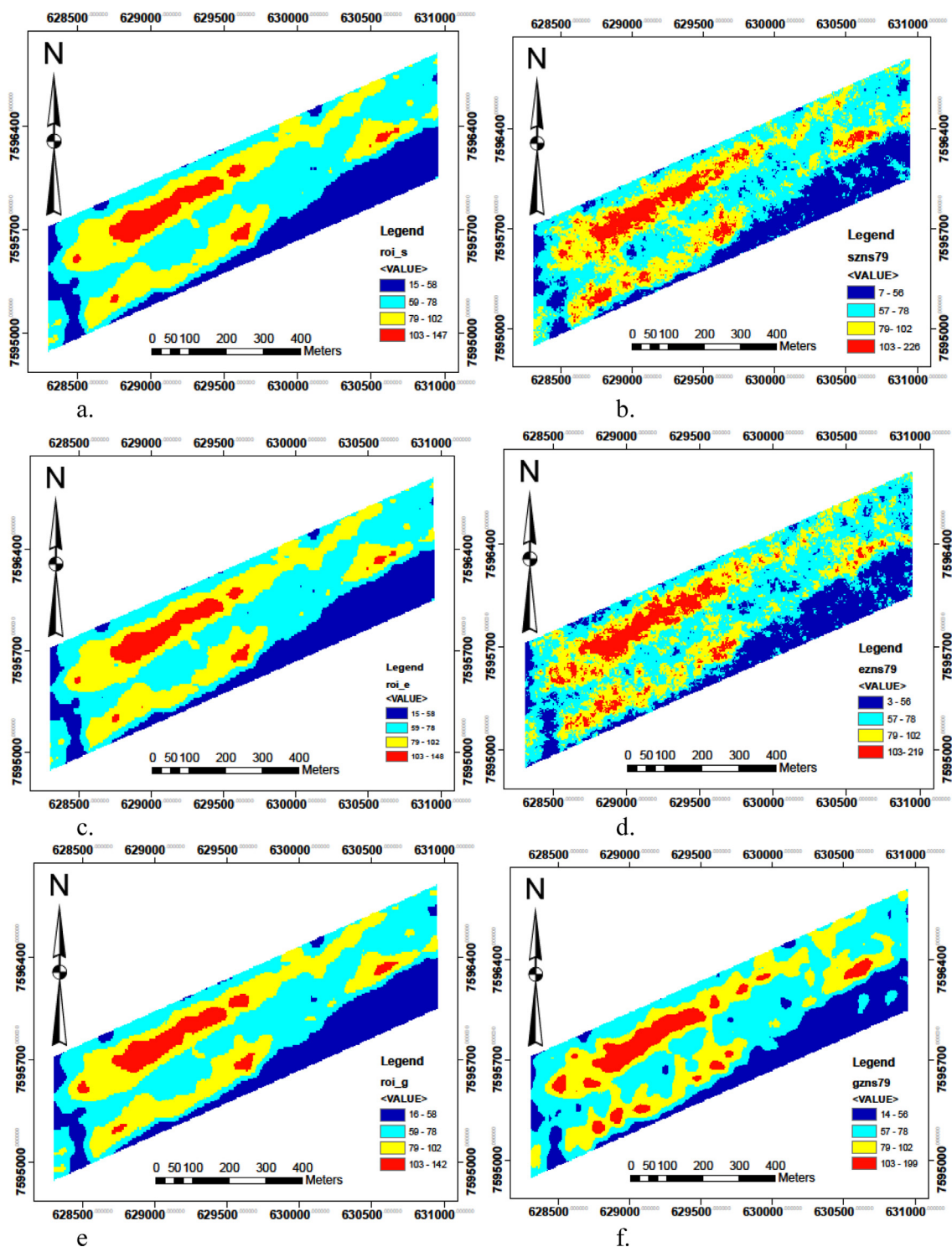


Fig. 5. Filled contour maps of Zn concentrations (mg kg⁻¹) obtained as simple kriging estimates (a), (c) and (e) versus SGS 80th realizations (b), (d), and (f). From top to bottom are Spherical, Exponential and Gaussian semivariogram models (left) versus SGS 80th realization.

Table 4

Statistical parameters of Zn data and outputs of different realizations, E-type and SK model.

Variable	Minimum	Maximum	Mean	SD
Actual	3.0	174	71.95	21.92
Simple kriging ^s	15.36	146.62	72.49	18.57
Simple kriging ^e	15.00	148.40	72.52	18.26
Simple kriging ^g	15.77	142.48	72.46	18.88
SGS-E-type (mean) ^s	13.56	149.67	72.59	18.49
SGS-E-type (mean) ^e	13.23	152.33	72.59	18.16
SGS-E-type (mean) ^g	16.08	141.22	72.53	18.78
SGS 80th realization ^s	7.49	225.75	72.82	20.40
SGS 80th realisation ^e	3.34	219.05	72.51	20.99
SGS 80th realisation ^g	14.10	199.16	72.78	20.58

^s Spherical.^e Exponential and,^g Gaussian models.**Table 5**Parameters of the simulation error for threshold values greater than 70 mg kg⁻¹.

	Spherical	Exponential	Gaussian
Mean	0.002668	0.002459	0.002853
Root-Mean-Square	0.366837	0.366808	0.367257
Mean Standardized	0.005538	0.004950	0.005886
Root-Mean-Square Standardized	1.004688	0.985694	1.010418
Average Standard	0.365261	0.372233	0.363668

choice of default model on the SGS outcome, we selected the 80th realization for comparison. Tang [29] noted that when an experimental variogram appears to have a sill value then Spherical, Exponential and Gaussian semivariogram models could be used as theoretical models. For the three models (Spherical, Exponential and Gaussian), the cross validation results (Fig. 4) and the statistical indicators (SE and RMSSE) of model performance (Table 3) suggest that any could be basis for SGS. We suggest that the use of statistical indicators (SE and RMSSE) of model performance may not be “water-tight”. We therefore propose a new criterion for the choice of theoretical semivariogram model:

$$\tau = \frac{\text{Partial sill}}{\text{Range}^2} \quad (1)$$

To test our proposed model in Eq. (1), we computed ratio of sill to square of range which follows the following order: [Exponential (9.58565E-06) < Spherical (1.69373E-05) < Gaussian (3.78379E-05)]. In Table 4, the summary statistics of both estimates and simulation results are presented. In Fig. 6, the probability maps of Zn distribution are shown based on a 70 mg kg⁻¹ Zn cut-off.

In Table 4, both kriging and SGS-E-type results over estimated the lower bound and under estimated the upper bound. The SGS 80th realization on the other hand predicted values much closer to the lower bound in the exception of the Gaussian model whereas values for the upper bound were generally overestimated (Table 4). The SGS 80th realization based on the exponential model as default input outperformed all the other models with the prediction the lower bound. On the other hand the SGS 80th realization based on the Gaussian model as default input outperformed all the other models with the prediction of the upper bound. In Fig. 6, the probability of Zn values greater than 70 mg kg⁻¹ is compared for three models. Also the indicator prediction performance is presented as supplementary information (SI). The Spherical and Exponential models looked similar except for the slight difference in patches in Zn distribution. On the contrary, the Gaussian model predicted smaller areas of potential Zn deficiency. Both the indicator prediction and probability maps suggest widespread Zn deficiency. It is expected that the mean error and the root mean square standardized errors values (Table 5) of prediction equal to 0 and 1, respectively. The variance of the simulation standardized error measures the ratio between the experimental estimation error and the simulation variance. Consequently, the standardized results showed reasonably prediction of Zn deficiency.

Discussion

According to the widely cited [4], normally observable values for Zn in soil are in the range of 1–900 mg kg⁻¹. When values are lower than 70 mg Zn kg⁻¹, the soil can be considered critically deficient of micronutrient Zn. Based on the critical concentration range of 70–400 reported by Kabata-Pendias [21], the study area can be considered low in Zn content. A total soil Zn concentration below 70 mg kg⁻¹ is the level below which crop yield, quality, or performance is unsatisfactory. It should be noted however that, total concentration in excess of 400 mg Zn kg⁻¹ could possibly pose toxicity problem to crops. In this study, the total soil Zn concentration suggests that levels may be insufficient to support plant growth. This result needs to be reconciled with further measurement of other soil parameters and batch and speciation experiments

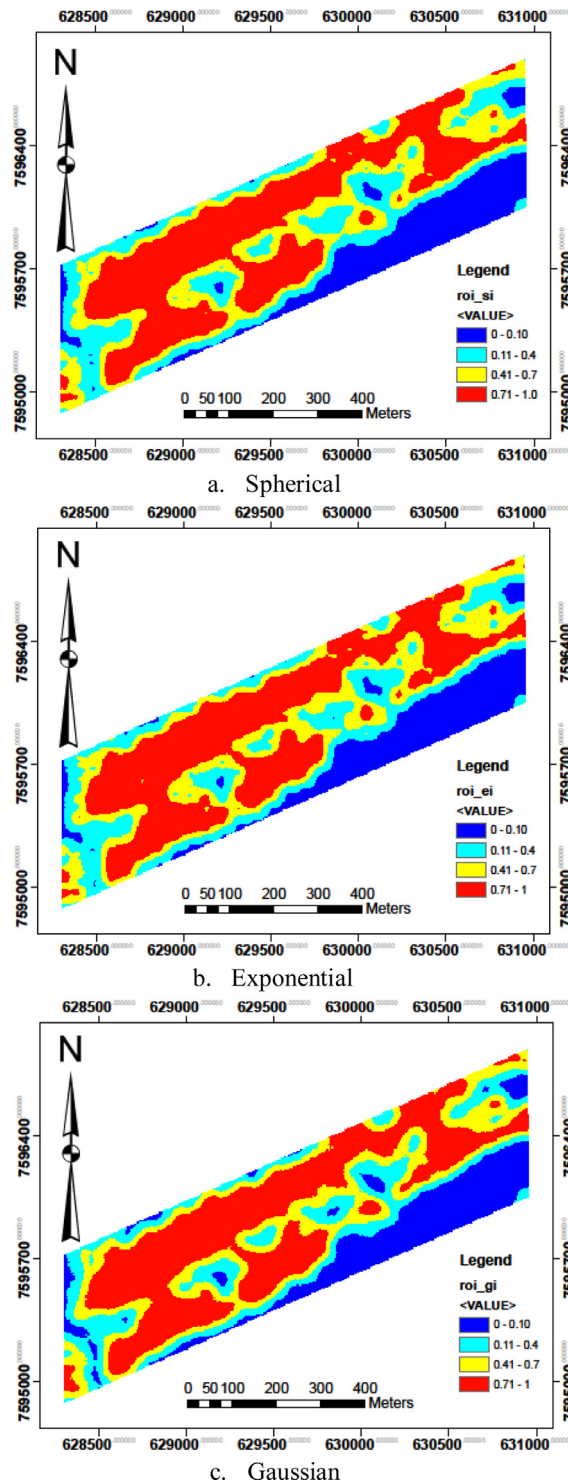


Fig. 6. Probability maps for soil Zinc $> 70 \text{ mg kg}^{-1}$ based on (a) Spherical, (b) Exponential and (c) Gaussian models versus their respective indicator predictions.

since sorption processes dominate the bioavailability of Zn [23]. Zinc deficiency as observed on such a relatively large scale (Fig. 6) in this study is however not completely unforeseen. Thus at-least a third of the cultivated soils globally are estimated to be low in bioavailable Zn [35].

The simulation approach, SGS, require data which otherwise is not Gaussian to be transformed to follow a Gaussian distribution such that the entire multivariate distribution is then assumed to be Gaussian [10,13]. During Kriging, the dataset was excluded of trend following a second order polynomial. That way the precondition for a stochastic simulation, stationarity, was achieved. A closer look at the semivariogram parameters suggests some unique characteristics given by differences in the respective nugget, partial sill and major range values. For instance, the smaller the nugget, the smaller the proportion of the variability that can be explained by random behaviour. Also, the smaller the partial sill and major range values, the less variable and the shorter the distance after which no correlation exist in Zn field, respectively. In other words, the sampling design and data analysis protocols specifies that an average data at each of n ($=1050$) distinct locations was used for the assessment, and therefore the nugget effect captures spatial heterogeneity at a scale smaller than the closest distance between any two points in the sampling design whereas the partial sill captures variability at a scale larger than the distance between two closest sampling points. It could also be thought that the slope (or derivative) of the curve at any point in between the nugget and sill values should somehow translate into degree of spatial heterogeneity. The proposed new criteria for the choice of theoretical model (τ) actually provides as a measure of degree of spatial heterogeneity. In essence, τ is dispersion in physical quantity (i.e., Zn) per unit area. The smaller the value of τ , the better the tendency of the model to describe heterogeneity at the scale larger than the distance between two closest sampling points. Thus, larger τ value leads to smearing and can be observed for the Gaussian model (Fig. 5(e)). Following the above synthesis, it could be suggested that the three models (Fig. 4(a), (c), and (e)) have the tendency of capturing spatial heterogeneity at the larger scale in the order: $G < S < E$. The estimates have been largely smeared out (Table 4 and Fig. 5) leading to either over-estimation of lower values and under-estimation of higher values e.g., [14,22,24]. Though all three models over-estimated the lower bound and under-estimated the upper bound, the exponential model performed best for both the lower and upper bound while the Gaussian model performed worse (Table 4 and Fig. 5). The observation agrees with our proposed model in Eq. (1). The Gaussian model performed poorly in the lower range, and the maximum value obtained for the 80th realization is the closest to the actual value. Remarkably, the exponential model predicted a lower bound value of $3.34 \text{ mg Zn kg}^{-1}$ which is the closest of three models to the lower bound of the dataset ($3.0 \text{ mg Zn kg}^{-1}$). Integrating estimation and simulation and careful choice of default input model for simulation, therefore leads to more detailed description of spatial heterogeneity in the spatial process.

Since a greater proportion of the sampled area is low in Zn concentration, it is critical to ascertain whether the right conditions for Zn bioavailability persist. This is because, pure Zn minerals (carbonates, silicates, hydroxides) have been detected at high total soil Zn concentrations ($>1000 \text{ mg Zn kg}^{-1}$) but sorption reactions are known to largely control Zn solubility and bioavailability in soils [23]. Also, other factors including pH [31,32], type and quality of soil organic matter [1], carbonate content [23], soil texture or clay content [7] and the hydraulic properties of soil [1] are known to control Zn level in soils. Consequently, it would be prudent to conduct a further study into the factors controlling Zn level in such soils to propose a restoration module. Such systematic studies shall include: soil texture analysis, characterization of soil hydraulic functions, and further chemical analysis including pH, concentration of organic carbon, carbonates, silicates and hydroxides, Zn speciation [25] and sorption studies and partitioning coefficient determination [23].

Conclusion

Quantifying and mapping spatial distribution and uncertainty for micronutrients including Zn is essential for site-specific nutrient management in agro-ecological systems. An exploratory and multi-criteria geostatistical data analysis procedure that combines both estimation and simulation approaches to assess the uncertainty and spatial distribution of Zn is presented. In this approach, three semivariogram models (Spherical Exponential and Gaussian) used for estimation (kriging) and as input for modeling (SGS) spatial process in Zn distribution did not yield same results. Exponential and Spherical models provide better estimates of the lower bound but performed poorly at the upper bound. Gaussian model performed poorly at the lower bound but provides better estimates at the upper bound. In combination with the statistical indicators of model performance, we propose a ratio of partial sill to the square of the range as a guide to the choice of default input model for simulation studies. Thus, Exponential with the least partial sill to the square of the range ratio fulfils this criterion.

CRedit authorship contribution statement

Peter N. Eze: Conceptualization, Data curation, Formal analysis, Writing - original draft. **Samuel K. Kumahor:** Formal analysis, Writing - original draft, Writing - review & editing.

Conflict of interest

None.

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