行政院國家科學委員會專題研究計畫成果報告

地理統計模擬與估計法評估土壤重金屬污染範圍

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一、摘要

土壤重金屬調查資料之空間特性有明顯差異，部份重金屬常顯現出許多的極端值或小區域內污染物濃度複雜的空間變異。本研究以彰化地區小樣區的鋅重金屬調查資料為例，以一般克利金與條件隨機模擬法，分別估計與模擬這些重金屬的濃度空間分佈，並比較分析、估計與模擬結果。結果顯示條件模擬法可模擬出多模擬域鋅重金屬，且這些模擬域之變異圖能吻合實際值之變異圖，因此這些模擬域可為此重金屬中樣區鋅重金屬大範圍聯合克利金估計時之第二變數，以增加其估計之精確度。

關鍵詞：條件隨機模擬法,克利金法,土壤重金屬,空間變異,極端值,聯合克利金

Abstract

Collected data in soil heavy metal investigations may contain significant levels of uncertainty, including complex and even unexplainable spatial variations at a small investigation site. Therefore, this study identifies the spatial structure of soil zinc in the northern part of Changhua County in Taiwan to generate multiple realization of soil zinc. The spatial maps of this heavy metal are simulated by using the geostatistical simulation, and estimated by using ordinary kriging and natural log kriging. The estimation and simulation results indicate that Sequential Gaussian Simulations can reproduce the spatial structure for investigated data. Furthermore, displaying a low spatial variability, the ordinary kriging can not fit the spatial structure and small-scale variation for the soil zinc investigated data. The multiple simulated realizations also can be used as secondary variable for cokriging to improve the accuracy of estimation.

Keywords: Geostatistical simulation, kriging, soil zinc, spatial variability, cokriging

1. INTRODUCTION

Geostatistics may be defined as a collection of techniques for solving estimation problems related to spatial variables (Journel and Huijbregts, 1978, and ASCE 1990). A geostatistcal technique, kriging is a linear interpolation procedure. It provides a best linear unbiased estimator (BLUE) for quantities that vary in space. Geostatistical approaches have recently been applied to analyze the spatial variability of pollutants, with notable examples including Yost et al. (1982), Keck et al. (1993), Samra and Gill (1993), Litaor (1995), Couto et al. (1997), Juang and Lee (1998), Wang and Zhang (1999), and White et al. (1999).

The estimated values based on kriging display a lower variation than the actual investigated values. To correct the above deficiency, geostatistical simulation can be performed. Simulation generates equally likely sets of values for a variable, which are consistent with available in-situ measurements.

Conditional simulation attempts not only to generate a set of values that have some specified mean and covariance, but also to reproduce observed data at several locations.

In this study, we employ ordinary kriging, and conditional simulation techniques to produce the maps and realizations of Zn in a case study. The descriptive statistics, spatial structure (experimental variogram), and spatial structure of estimated and simulated results are also discussed and compared in this study.

2. MATERIALS AND METHODS

(1) Data

This study develops maps illustrating the geographic distribution of Zn in surficial soil horizons in the northern part of Changhua County in Taiwan using geostatistical estimation, simulation and geographic information systems (GIS). Data were derived from the EPA studies described above. In this study area, 350 sampling points (Figure 1) are used for estimating and simulating the spatial distribution of Zn.Table 1 summarizes the descriptive statistics of Zn investigated data.

(2) Kriging

Geostatistics provides a variogram of data within a statistical framework, including spatial and temporal covariance functions. Kriging estimates are calculated as weighted sums of the adjacent sampled concentrations. These weights depend on the exhibited correlation structure. The criterion for selecting these weights is a minimization of the estimation variance. In this framework, kriging estimates can be regarded as the most accurate among all linear estimators (i.e. Best Linear Unbiased Estimator).

(3) Sequential Gaussian Simulation

A simulated value at visited point is randomly selected from the normal distribution function defined by the kriging mean and variance based on neighborhood values. Finally, the simulated normal values are back transformed into simulated values for an original variable. At the new randomly visited point, the simulated value is conditional on the original data and previously simulated values. This process is repeated until all points are simulated at each realization over the study area.

The simulations and estimations are performed into a square 34 columns by 38 rows grid consisting of 1292, 80m by 80m cells. Five simulations (Sim1, Sim2, Sim3, Sim4, Sim5) are performed at these 1292 cells.

Descriptive Statistics

The ordinary kriging estimates, ln kriging estimates and simulations are based on the above variogram models and 350 observations. Table 2 summarizes the descriptive statistics of ordinary kriging and Sequential Gaussian Simulation results. Above results indicate that ordinary kriging process may not preserve the variability of the investigated process. Sequential Gaussian Simulations can reproduce the statistics for investigated soil zinc.

Experimental Variogram

In this study, the experimental variograms of normalized estimated and simulated values are also performed with the same lag interval. According to Figure 2, the Sequential Gaussian Simulation can perform very well in terms of reproducing the spatial structure (experimental variogram) for the investigated values. The ordinary kriging values display a well-structured variogram with a low spatial variability and hole effect, but can not perform the spatial structure and small-scale variation for investigated values as shown in Figure 2.

4. CONCLUSION

Kriging provides the optimal estimation of Zn at unsampled sites. However, the estimated values based on ordinary kriging display lower variations than the actual investigated soil zinc. Sequential Gaussian Simulation can reproduce both the extreme measured soil zinc and overall zinc spatial distribution. Sequential Gaussian Simulation with multiple realizations has significant advantages at a site with high variation investigated data over ordinary kriging. The simulated results also can be used as secondary variable for cokriging.

5.References

ASCE Task Committee on Geostatistical Techniques in Geohydrology (S. Rouhani, Chairman and Principle Author), 116(5), 612-632 (1990).

Couto E. G., Stein, A. and Klamt, E., Agriculture, Ecosystems and Environment, 66, 139-152 (1997).

Deutsh C. and Journel, A. G., GSLIB, Geostatistical Software Library and User's

Guide, Oxford University Press., New York (1992).

Gamma Design Software, GS+: Geostatistics for the agronomic and biological sciences. Version 2.3. Gamma Design, Plainwell, MI, (1994).

Gotway, C.A. and Hergert, G.W., Soil Sci. Am. J., 61, 298-309 (1997).

Juang, K. W. and Lee, D. Y., J. Environ. Qaul., 27, 355-363 (1998).

Journel, A. G., Math. Geology, 12, 285-301 (1980).

Litaor, M.I., J. Environ. Qual., 24, 506-516 (1995).

Samra, J.S. and Gill, H.S., Soil Sci., 155, 148-153 (1993).

White J. G., Welch, R. M. and Norvell,W. A., Soil Sci. Soc. Am. (1998).

Wang, X. J. and Zhang, Z. P., J. of Environ. Sci. Health, Part A, 34, 73-89 (1999).

Yost, R.S., Uehara, G. and Fox,R. L., Soil Sci. Am. J., 46, 1033-1037 (1982). J., 61, 185-194 (1997).

TABLE 1　Descriptive Statistics of Investigated Zn

	Mean	Min	Max	Variance	Median	Kurtosis	Skewness
Zn	80.697 (mg/kg)	11.0 (mg/kg)	1095.0 (mg/kg)	12463.405 (mg/kg)^2	47.180 (mg/kg)	29.250	4.582

TABLE 2　Descriptive Statistics of Kriging estimates and Simulations

	Mean (mg/kg)	Variance (mg/kg)^2	Median (mg/kg)	Kurtosis	Skewness
Investigated	80.697	12463.405	47.180	29.250	4.582
Kriging	79.554	2696.932	65.740	3.269	1.750
Sim1	78.108	9883.386	43.273	15.623	3.419
Sim2	82.197	11144.131	48.000	18.695	3.724
Sim3	77.311	10321.810	41.410	15.957	3.499
Sim4	78.491	12762.762	41.000	22.502	4.203
Sim5	74.190	9979.634	41.000	37.602	4.656

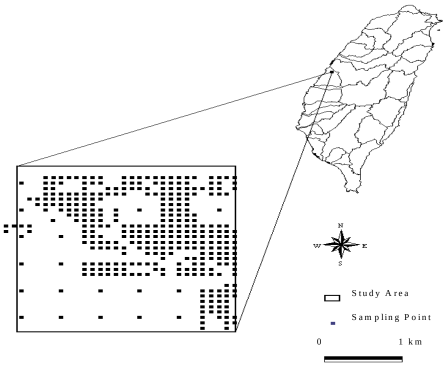

FIGURE 1 Study Area and Sampling Points

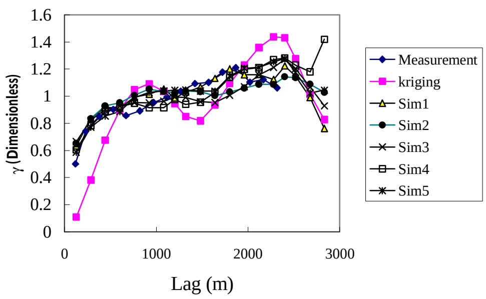

FIGURE 2　Experimental Variogram of Ordinary Kriging Estimation and Simulation