Field-Scale Water and
Solute Flux in Soils
Monte Verità

KRIGING VERSUS ALTERNATIVE INTERPOLATORS: ERRORS AND SENSITIVITY TO MODEL INPUTS

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This study deals with interpolations through time and space. Two data sets are utilized, soil water content values at the 25 cm depth for a 45 hectare and an artificially-generated set of random but spatially correlated values. Interpolators include punctual kriging, a nonparametric estimator and co-kriging. Results show that although the model parameters depicting spatial interdependence (such as range and sill for a variogram) are highly dependent on the sample, the interpolations resulting from use of such models are not very sensitive to the model parameters. Co-kriging predictions were shown to be effective by using moisture content values for two different times as covariates. Additionally, an example illustrates the variogram for moisture content measured at one time can be adjusted and used for interpolations at a second time.

1. Objectives

Field-scale characterization of soils requires interpolations and extrapolations through time and space. Here we examine some alternative methods and compare performance based on a set of field-measured moisture contents and a set of simulated data. Questions addressed include:

a. How sensitive are the interpolator model parameters to the sample on which they are based? Included are considerations on numbers in a sample and spatial distribution.

b. How sensitive are estimated values to the model parameters?

c. How much help are auxiliary properties, such as are used by co-kriging or time invariance principles?

   Included in the analysis are the effects of sample number and locations. Also, the preservations of information from one time to another is examined as well as use of texture and water retention properties as supplementary information to predict water contents.

2. The Interpolators and the Data Sets

Interpolators chosen are kriging and a nonparametric regression model (NPR) (Watson, 1964; Yakowitz and Szidarovsky, 1985). For variogram models, parameters are determined in different ways, but for the main, are based on the negative log likelihood function and methodology outlined by Samper and Neuman (1989a):

$$\mathrm{NLL} = M \ln(2\pi) + \sum_{i=1}^{M} \ln\left(\sigma_i^2\right) + \sum_{i=1}^{M} \left(e_i / \sigma_i\right)^2 \tag{1}$$

with M the number of observations, e_i the difference between the observed and kriged values at point i based on the other M-1 observation and σ_i the kriging standard deviation at point i based on the other M-1 observations.

In order to minimize the NLL as given by Eq. 1, it is observed that

$$\begin{aligned} \mathrm{NLL} = M \ln(2\pi) + M \ln C + \sum_{i=1}^{M} \ln\left[\left(\sigma_{u,i}\right)^2\right] \\ + (1/C) \sum_{i-1}^{M} \left(e_i / \sigma_{u,i}\right)^2 \end{aligned} \tag{2}$$

where C is the sill and $\sigma_{u,i}{}^2$ is obtained from

$$\sigma_i^2 = C\, \sigma_{u,i}^2 \tag{3}$$

(cf. Warrick and Myers, 1987). Also, since e_i is independent of the sill C, then the minimum will occur when

$$C = (1/M) \sum_{i=1}^{M} \left(e_i / \sigma_{u,i}\right)^2 \tag{4}$$

For a zero nugget and C as in Eq. 4, the value of NLL in Eq. 2 depends only on the range of the variogram (or alternatively the integral scale). For simplicity, the effect of a nugget will not be considered, but the approach would remain the same if it were. Minimums of the NLL were found by using a golden section search to find the range and then the sill is evaluated from Eq. 4. The NPR estimator (Yakowitz and Szidarovsky, 1985) is given by

$$y_o = \frac{\sum_{i=1}^{M} y_i\, K\left(x_o - x_i,\ a\right)}{\sum_{i=1}^{M} K\left(x_o - x_i,\ a\right)} \tag{5}$$

where y_i and x_i refer to known values and locations, respectively and y_o and x_o are for the estimated value and location. The K is a kernel function of bandwidth "a" which we take here as an exponential function:

$$K(x, a) = (1/a) \exp(-x/a) \tag{6}$$

Other choices of the kernel could be made including a Gaussian distribution function. A discussion of the expected errors and variance of the error are given by Yakowitz and Szidarovsky (1985).

The field data was from the Maricopa Agricultural Center in central Arizona and consists of moisture content at 5, 10 and 25 cm at 45 sites on May 31 and 91 sites on June 12, 1988. Figure 1 shows the 45 sites which are on a 100 m regular grid as well as 46 additional sites chosen in two clusters to provide a more uniform distribution of couple distances of separation. Common sites for the two times were sampled with an Oakfield probe of 2.5 cm inner diameter. Supporting data for texture and moisture retention are also available but will not be used here. Figure 2 shows the sample variogram for both dates and a fitted spherical model with zero nugget and ranges of 650 m for May 31 and 550 m for June 12 with sills of 18 and 15.5, respectively. The variogram was based on the 45 data points. The artificial data set is that of Samper and Neuman (1989b) and consists of 200 "random" points on a 30 x 30 unit area generated with an exponential variogram with unit sill and range of 3.

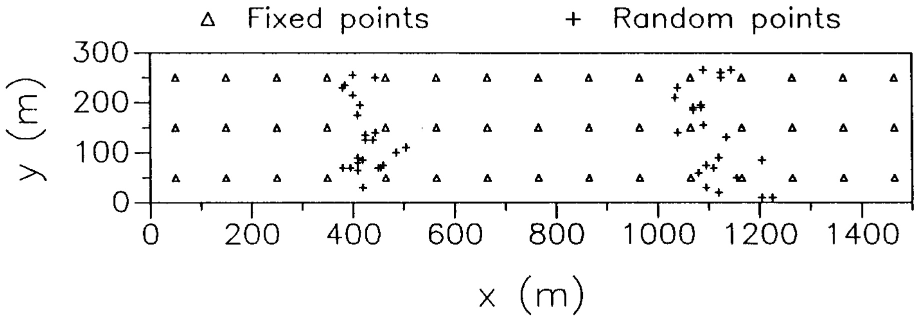

Figure 1: Sampling locations for moisture contents in the 45 hectare area.

3. Sensitivity of Model Parameters to the Specific Sample Chosen

The first example addresses the question of how the sample affects the model parameters of the interpolators. For this purpose, 30 subsamples were chosen:

10 for M = 15 points, 10 for M = 30 and 10 for M = 45 from the field moisture contents at 25 cm for June 12. Results are in Table I.

A spherical variogram model is used and Eq. 5 is used for the NPR kernel. Overall the estimates of the model parameters vary less from sample to sample as the sample size (M) increases. Both ranges and sills chosen by the maximum likelihood estimator in some cases are quite different from what would be estimated by a visual examination of Figure 2 although the tendency overall is consistent. For many of the subsamples, the range is shortened and the sill exaggerated, similar to the "Type I" error pointed out by Samper and Neuman (1989a, esp. Fig.20). The exercise was repeated for the synthetic data set for M of 25, 50 and 100 with similar results as shown in Table II. The fact that the NPR band width is different than the variogram range is not surprising, as they are selected on different principles.

4. Sensitivity of the Estimated Values to the Model Parameters

For the second example, the models given in Table II are used to calculate the root mean square errors (RMSE):

$$\mathrm{RMSE} = \sqrt{(1/N)\sum_{i=1}^{N}(y_i^* - y_i)^2} \tag{7}$$

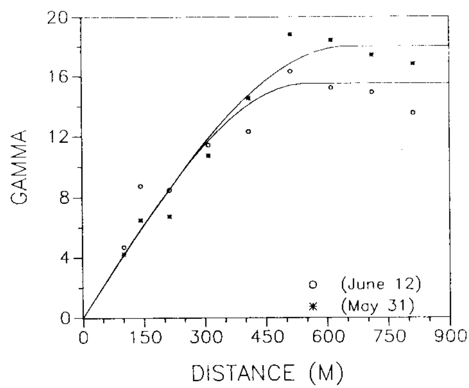

Figure 2: Variograms for May 31 and June 12 moisture contents.

where y_i^* and y_i are predicted values and measured values for points <u>not used</u> for the model determination, respectively. For all three values of M, the kriging values for the moisture contents (Table III) have a lower minimum and maximum value, although the upper values tend to be well within the range of the other interpolators. The NPR values drop steadily as M gets larger, which is a desirable feature. For small M, the inverse distance weighting (IDW) is as good as for the NPR, but for M = 45 it is not. In all cases, the spatial estimators offer an improvement over the sample standard deviations (Table I).

Table I: Range of values for 10 repeated samples for the June 12 water content data.

M	mean	Sample s.d.	Variogram range	(Spherical) sill	NPR bandwidth
15	18.4-21.1	2.72-3.85	80-554	7.94-45.1	0.48-63.8
30	18.5-20.2	2.70-3.95	274-483	8.12-29.8	15.8-49.7
45	19.0-19.8	2.88-3.36	245-673	9.64-38.7	14.6-25.0

Table II: Range of values for 10 repeated samples for the simulated data of Samper and Neuman (1989a).

M	mean	Sample s.d.	Variogram range	(Exponential) sill	NPR bandwidth
25	0.96-1-31	0.73-1.23	0.71-6.85	0.52-1.60	1.50-14.5[1]
50	0.88-1.30	0.78-1.10	1.81-6.01	0.67-1.40	0.888-3.86
100	0.84-1.17	0.82-0.99	2.00-4.40	0.65-1.04	0.585-1.47

[1] Does not inclde 1 sample which did not converge.

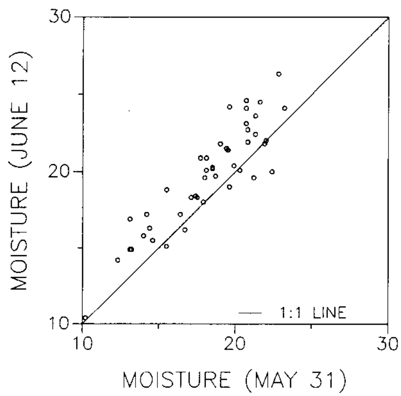

Fig. 3: Scatter diagram of soil moisture data for May 31 and June 12.

Results for the synthetic data set are in Table IV and are similar to those for moisture content results. As the original model is known for the synthetic data, the RMSE values were recalculated using an exponential model of unit sill and range of three. The results are given in Table IV and show that the RMSE is about the same as using the individually determined models.

5. Use of Auxiliary Properties

For the final comparison, 61 moisture contents for June 12 were estimated by using 30 values and 45 values from May 31 as a co-variate. Figure 2 shows the variogram models. The values tend to be time invariant (Vachaud, et al., 1985) with wet sites remaining wetter and drier staying drier for each of the two times. This is shown by the scatter diagram of Figure 3 which had a correlation r = 0.91 between the two times. Although the surface was considerably drier for May 31 than for June 12, the moisture contents at the 25 cm depth are close. One choice of using time-invariance is to simply use co-kriging, which greatly improves the results both for the RMSE and the kriging variance (see Table V).

Table III:Range of RMSE for the June 12 water content. In all cases N = 46 in Eq. 7.

M	Kriging	NPR	IDW[1]
15	1.88-3.12	2.13-3.54	2.13-3.33
30	1.79-2.36	1.92-2.81	2.03-2.77
45	1.74-2.21	1.87-2.31	2.04-2.60

[1] Inverse distance weighting with the same M known values.

Table IV: Range of RMSE for the simulated data. In all cases N = 100 in Eq 7.

M	Kriging	NPR	IDW[1]
25	0.784-0.998 (0783-0.977)[2]	0.822-1.02	0.771-1.00
50	0.700-0.898 (0.700-0.899)[2]	0.784-0.925	0.712-0.893
100	0.711-0.815 (0.692-0.811)[2]	0.719-0.828	0.746-0.850

[1] Inverse distance weighting with the same M known values.
[2] Using the original model.

As a final exercise, a variogram model for the June 12 data was obtained by multiplying the May 31 by the ratio of the sample variance. As shown in Table V (for the scaled variogram) the results are comparable to those for the original variogram, in fact, by chance the RMSE values are even lower.

Table V: Root mean square errors for June 12 moisture contents for predicting 61 points from 30 points

	RMSE	Kriging variance
kriging	2.92	13.6
co-kriging	1.81	8.6
inverse distance weighting	3.19	N/A
kriging (scaled variogram)	2.69	14.1

6. Summary and Conclusions

For the first objective, parameters for both the kriging and non-parametric models were found to be sensitive to the sample chosen. For the small samples (M=15 and 25), the range and sill varied by about an order of magnitude. The bandwidth varied by about two orders of magnitude (0.48-63.8) for the water content data. The range and bandwidth are less variable as M becomes larger and vary more typically by a factor of 1 to 2 or 1 to 3.

The kriging results for the RMSE were better in all cases as the sample size increased, although the accuracy was more influenced by the sample on which the interpolations are made than by the exact model. This is demonstrated most clearly for the synthetic results, for which the exact model gave results no better than the individually fitted models.

The final results illustrate two methods for interpolating spatially for different times. The first is by co-kriging with the moisture contents at the two times as co-variates. This is analogous to time-invariance methods although spatial interpolations can be included as well as site comparisons and rankings. The second method assumes the variograms are comparable and the sills adjusted with respect to the sample variance. Of course, the RMSE values are independent of the sills, but the scaling of the sills should lead to better overall performance.

A question often raised is whether kriging is worth the extra effort over more simple interpolators. These results show that RMSE values are only slightly better for kriging than for the other two interpolators. Similar results were found earlier (Warrick et al., 1988) for a larger variety of measured properties. The advantages of kriging exist primarily in the provision for additional error information, ability to include auxiliary information and the framework to predict from alternative sample support values. A final point to be made is the tendency towards "user friendly" software which allows easier and easier calculations.

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