

MOD550 Applied Data Analytics and Statistics for Spatial and Temporal Modeling

05 - Kriging

Reidar B Bratvold

and

Enrico Riccardi

University of Stavanger

1

Recap - Variogram Estimation and Modeling

- What is a variogram?
 - A fundamental tool in geostatistics that quantifies spatial continuity.
 - Measures how spatial correlation changes with distance.
- o Key components of a variogram:
 - Nugget Effect: Measurement error or micro-scale variation.
 - Sill: The point where variance levels off.
 - Range: Distance at which spatial correlation disappears.
- Why is variogram modeling important?
 - Essential for spatial interpolation methods like kriging.
 - Helps understand anisotropy and spatial dependencies.

Insights from Variogram Analysis

- o Interpreting experimental variograms:
 - Spherical, exponential, and Gaussian models fit different spatial patterns.
 - Detecting anisotropy: Different correlation ranges in different directions.
 - Accounting for trends and cyclicity.
- o Challenges in variogram estimation:
 - Data scarcity and irregular sampling.
 - The need for positive-definite variogram models.
- o Best practices in variogram modeling:
 - Use the simplest model that captures key spatial characteristics.
 - Ensure consistency across directional variograms.

3

3

Kriging is a general term for a family of techniques that can be used to estimate the value of a regionalised variable from sample values

- o Why do we need Kriging?
 - Variograms provide a foundation for spatial interpolation.
 - Kriging optimally estimates values at unsampled locations while minimizing error.
- o Key steps in Kriging:
 - Variogram Fitting: Determines spatial correlation structure.
 - Weight Calculation: Assigns optimal weights based on distance and correlation.
 - Prediction and Uncertainty Estimation: Generates interpolated values with confidence intervals.
- o Comparison to other methods:
 - Unlike Inverse Distance Weighting (IDW), kriging accounts for spatial structure and provides uncertainty estimates.

Looking Ahead - Kriging in Action

- Types of Kriging:
 - Simple Kriging, Ordinary Kriging, (Universal Kriging).
 - Considerations for choosing the right approach.
- o Applications of Kriging:
 - Resource estimation in mining and petroleum.
 - Environmental monitoring (e.g., pollution dispersion).
 - Precision agriculture and soil property mapping.
- o This lecture focus:
 - Hands-on kriging implementation.
 - Practical examples and case studies.
 - Evaluating kriging performance and error assessment.

5

Kriging is BLUE

Best - minimises the variance

Linear - $Z^* = \sum \lambda Z$

Unbiased - $\overline{Z^*} = \overline{Z}$

Estimator - we are **not** trying to model all the

variability, but rather find the

best (minimum variance) estimate

c

Kriging

$$Z^* = \sum \lambda Z$$

- o The weights are a function of:
 - the spatial correlation of the variable (as summarized in the variogram)
 - the location of the sample data with respect to the location to be estimated, and with respect to each other (declustering)
 - the shape and size of the samples, and of the element being estimated (the support)
- and are computed by setting up and solving a set of simultaneous equations (the kriging equations) for each point to be estimated

7

7

Both distributions are unbiased O Error Variance Inverse distance Kriging Error variance for B is minimum

Kriging

- Relative to other estimation methods, kriging has the following advantages:
 - the estimate is unbiased
 - it honours the data (for point kriging with zero nugget)
 - it is optimal for the data used
 - it provides a measure of the error in the estimate
- o and the following disadvantages:
 - structural analysis (variography) must be performed before kriging
 - kriging itself can be computationally expensive
 - may require some assumption of stationarity
 - resulting map is "smoother" (has less variability) than the data (as are most other estimation techniques)

9

Simple Kriging

o Consider the residual data values about the mean m(u) (i.e. subtract the mean):

$$Y(u_i) = Z(u_i) - m(u_i), i=1,...,n$$

where $m(\mathbf{u})$ could be constant, locally varying, or constant but unknown.

Variogram is defined as:

$$2 \gamma(h) = E\{ [Y(u) - Y(u+h)]^2 \}$$

o Covariance is defined as:

$$C(h) = E\{ Y(u) \cdot Y(u+h) \}$$

Simple Kriging

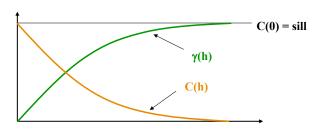
Link between the Variogram and Covariance under stationarity (as before):

$$2\gamma(h) = E\{Y^{2}(u)\} + E\{Y^{2}(u+h)\} - 2 \cdot E\{Y(u) \cdot Y(u+h)\}$$

$$= Var\{Y(u)\} + Var\{Y(u+h)\} - 2 \cdot C(h) \text{ (stationarity)}$$

$$= 2 [C(0) - C(h)]$$

SO,
$$C(h) = C(0) - \gamma(h)$$



11

Simple Kriging (1)

o Consider the linear estimator:

$$Y^*(u) = \sum_{i=1}^n \lambda_i \cdot Y(u_i)$$
 Known mear

 $Y(u_i)$ are the residual data (data values minus the mean) observed at locations u_i

 $Y^*(u)$ is the estimate of the residual at desired location u.

- o The estimation error variance in $Y^*(u)$ is $E\{[Y^*(u)-Y(u)]^2\}$
- o which can be expanded to:

=
$$E\{[Y^*(u)]^2\}$$
 $-2 \cdot E\{Y^*(u) \cdot Y(u)\}$ $+ E\{[Y(u)]^2\}$
 a^2 - 2ab + b^2

Simple Kriging (2)

The error variance in $Y^*(u)$ is

$$= E\{[Y^*(u)]^2\} -2 \cdot E\{Y^*(u) \cdot Y(u)\} + E\{[Y(u)]^2\}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j E\{Y(u_i) \cdot Y(u_j)\} -2 \cdot \sum_{i=1}^{n} \lambda_i E\{Y(u) \cdot Y(u_i)\} +C(0)$$

$$= \sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j C(u_i, u_j) - 2 \cdot \sum_{i=1}^n \lambda_i C(u, u_i) + C(0)$$

Data-Data Covariances (redundancy) Unknown-Data Covariances (closeness) Variance

14 14

Simple Kriging (3)

Error Variance =
$$\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j C(u_i, u_j) -2 \cdot \sum_{i=1}^{n} \lambda_i C(u, u_i) + C(0)$$

- o Optimal weights λ_i i=1,...,n are those that minimize the error variance.
- Determine these weights by taking partial derivatives of the error variance w.r.t. the weights

$$\frac{\partial [\boxed{\square}\boxed{\square}]}{\partial \lambda_i} = 2 \cdot \sum_{i=1}^n \lambda_j C(u_i, u_j) - 2 \cdot C(u, u_i), \quad i = 1, ..., n$$

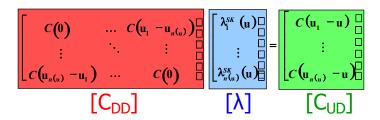
and setting them to zero

$$\sum_{i=1}^{n} \lambda_{j} C(u_{i}, u_{j}) = C(u, u_{i}), \quad i = 1, \dots, n$$

1!

Simple Kriging (4)

This system of n equations with n unknown weights is the simple kriging (SK) system. In matrix form



Solve for the weights, λ , by matrix inversion:

$$[C_{DD}]^*[\lambda] = [C_{UD}]$$
$$[\lambda] = [C_{DD}]^{-1} * [C_{UD}]$$

16

Simple Kriging: Example

Example using 3 data points

Red = data-data pairs
Green = unknown-data pairs

 $C_{1,3}$ $C_{1,2}$ $C_{0,3}$ $C_{0,1}$ $C_{0,2}$

- There are three equations to determine the three weights:
- $$\begin{split} &\lambda_{1} \cdot C(1,1) + \lambda_{2} \cdot C(1,2) + \lambda_{3} \cdot C(1,3) = C(0,1) \\ &\lambda_{1} \cdot C(2,1) + \lambda_{2} \cdot C(2,2) + \lambda_{3} \cdot C(2,3) = C(0,2) \\ &\lambda_{1} \cdot C(3,1) + \lambda_{2} \cdot C(3,2) + \lambda_{3} \cdot C(3,3) = C(0,3) \end{split}$$

o In matrix notation:

- C(1,1) C(1,2) C(1,3)
- C(2,1) C(2,2) C(2,3) C(3,1) C(3,2) C(3,3)
- $\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} C(0,1) \\ C(0,2) \\ C(0,3) \end{bmatrix}$
- o Since $C(h) = C(0) \gamma(h)$, the covariances can be computed from the modeled variogram $\gamma(h)$

In-Class Exercise

- Set up, and solve, the Simple Kriging equations for 3 arbitrary data points and one unknown point using a spherical variogram (of arbitrary parameters)
 - Use the Excel MMULT and MINVERSE functions
- Recall that $\hat{Z}(u) = m + \sum_{i=1}^{n} \lambda_i (Z(u_i) m)$
- o Compute the value of \overline{Z} at the unknown data point U for the following situations for spherical variogram range=10, sill=3

Lecture eg Data				
Point	Χ	Υ	Z	
1	-1.00	3.00	10	
2	1.00	5.00	30	
3	8.00	3.50	20	
J	0.00	0.00	?	

Equi Distant Data			
Point	Χ	Υ	Z
1	-5.00	2.89	10
2	5.00	2.89	30
3	0.00	-5.77	20
Ū	0.00	0.00	?

2 Close Points			
Point	Х	Υ	Ζ
1	-5.00	0.50	10
2	5.00	0.00	30
3	-5.00	-0.50	20
U	0.00	0.00	?

In class: go thru Soln in: SOLN - Simple Kriging_3_data.xlsx

- Vary the data
- Vary the Variogram parameters

18

Ordinary Kriging

Ordinary Kriging

o General Simple Kriging (SK) estimator, m = global stationary mean

$$Z_{SK}^*(\mathbf{u}) - m = \sum_{\alpha=1}^n \lambda_{\alpha} (Z(\mathbf{u}_{\alpha}) - m)$$

- What if the mean is not (well) known or is not constant (= stationary)?
- o Solution

$$Z^*(\boldsymbol{u}) = \sum_{\alpha=1}^{n} \lambda_{\alpha} \ Z(\boldsymbol{u}_{\alpha}) - \left(1 - \sum_{\alpha=1}^{n} \lambda_{\alpha}\right) m$$

o Enforce the sum of the weights to be 1

$$Z_{OK}^*(\mathbf{u}) = \sum_{\alpha=1}^n \lambda_{\alpha} Z(\mathbf{u}_{\alpha})$$

20

20

Ordinary Kriging

- We also require the solution to satisfy the minimum variance condition
- Minimizing the variance with the condition that the weights must sum to 1 results in

$$\sum \lambda_i C\big(u_i,u_j\big) + \mu = C(u_i,u_0) \ for \ i=1,\dots,n$$

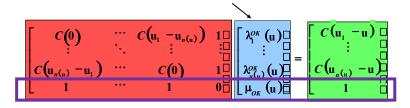
 \circ Where μ is called a Lagrange parameter

2

Ordinary Kriging

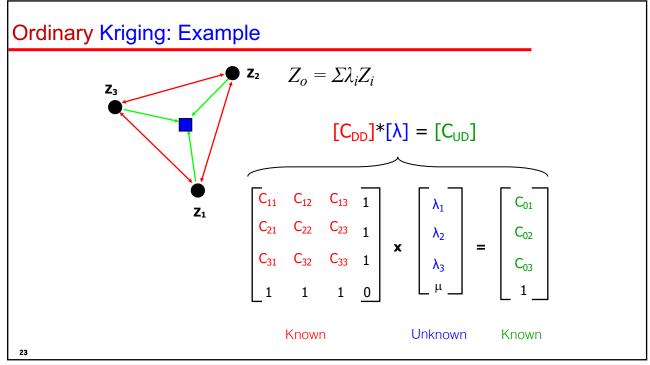
- Adds an additional equation which forces the sum of the weights to equal 1, ensuring that the estimate is unbiased.
 - Leads to ordinary kriging computing a local mean of the data points, which can vary across the area of interest – very useful
 - (Simple kriging uses the constant global mean)
- o The Ordinary Kriging equations are:

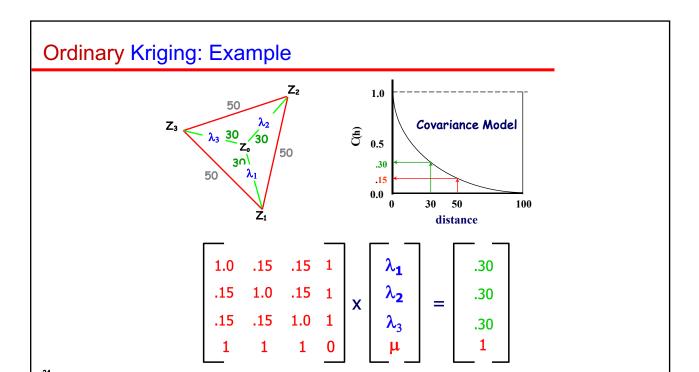
$$Z_{OK}^*(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{OK}(\mathbf{u}) Z(\mathbf{u}_i)$$



 \circ μ_{OK} is called the Lagrange parameter (not to be confused with the mean)

22





24

Ordinary Kriging: Simple Example

Solve for the weights by matrix inversion

$$[C_{DD}]^*[\lambda] = [C_{UD}]$$
$$[\lambda] = [C_{DD}]^{-1*}[C_{UD}]$$

All weights turn out to be, trivially, 0.333 therefore, the estimated value is

$$Z_0^* = \lambda_1 Z_1 + \lambda_2 Z_2 + \lambda_3 Z_3$$

$$Z_0^* = 0.333 Z_1 + 0.333 Z_2 + 0.333 Z_3$$

Kriging Variance

o In the computation of the kriging estimator, error minimization leads to the determination of a variance at each location, called the kriging variance

$$\sigma_{OK}^{2}(\boldsymbol{u}) = C(0) - \sum_{i=1}^{n(\boldsymbol{u})} \lambda_{i}^{OK}(\boldsymbol{u}) C(\boldsymbol{u}_{i} - \boldsymbol{u}) - \mu_{OK}(\boldsymbol{u})$$

- The term variance is misleading because this does not represent the variance of the data at each location but only the variance of the estimate
- Only dependent on the geometry of the data points and the spatial model, not the variance of actual data values
- True error could be greater

26

26

Ordinary Kriging

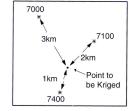
Returning to the initial example, the equations for Ordinary Kriging are:

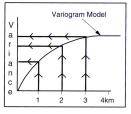
$$\gamma_{11} \lambda_{1} + \gamma_{12} \lambda_{2} + \gamma_{13} \lambda_{3} + \mu = \gamma_{1u}$$

$$\gamma_{12} \lambda_{1} + \gamma_{22} \lambda_{2} + \gamma_{23} \lambda_{3} + \mu = \gamma_{2u}$$

$$\gamma_{13} \lambda_{1} + \gamma_{23} \lambda_{2} + \gamma_{33} \lambda_{3} + \mu = \gamma_{3u}$$

$$\lambda_{1} + \lambda_{2} + \lambda_{3} + 0 = 1$$





To solve this, we must know $\gamma(h)$

Assume $\gamma(h) = C\{1.5(h/4) = 0.5(h/4)^3\}$, ie a spherical variogram with a range of 4 km, no nugget, and a sill value of C. We also need the distances separating each pair of sample points, and between each sample point and the point being estimated. These distances are:

 $h_{12} = 2.93 \text{ km}, h_{23} = 3.12 \text{ km} \text{ and } h_{13} = 3.77 \text{ km}$

 $h_{1u} = 1.00 \text{ km}, h_{2u} = 2.00 \text{ km} \text{ and } h_{3u} = 3.00 \text{ km}$

Ordinary Kriging

Then

$$\gamma_{11} = \gamma_{22} = \gamma_{33} = \gamma(0) = 0.00$$

$$\gamma_{12} = \gamma(2.93) = 0.902$$
C $\gamma_{13} = \gamma(3.77) = 0.995$ C $\gamma_{23} = \gamma(3.12) = 0.933$ C

$$\gamma_{1x} = \gamma(1.00) = 0.373C$$
 $\gamma_{2x} = \gamma(2.00) = 0.688C$ $\gamma_{3x} = \gamma(3.00) = 0.914C$

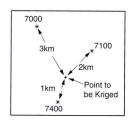
and the kriging equations are

$$0.000 \lambda_1 + 0.902 \lambda_2 + 0.955 \lambda_3 + \mu/C = 0.373$$

$$0.902 \lambda_1 + 0.000 \lambda_2 + 0.933 \lambda_3 + \mu/C = 0.688$$

$$0.955 \lambda_1 + 0.933 \lambda_2 + 0.000 \lambda_3 + \mu/C = 0.914$$

$$1.000 \lambda_1 + 1.000 \lambda_2 + 1.000 \lambda_3 + 0 = 1.000$$



The solution is $\lambda_1 = 0.636$, $\lambda_2 = 0.285$, $\lambda_3 = 0.079$, $\mu = 0.041$ C, so

$$z*(u) = 0.636*7400 + 0.285*7100 + 0.079*7000 = 7283$$

28

Ordinary Kriging

The estimation variance for the kriged value is

$$\sigma_k^2 = \sum \lambda_i \gamma_{ix} + \mu$$

Substituting appropriate values gives

$$\sigma_k^2 = 0.636*0.373C + 0.285*0.688C + 0.079*0.914C + 0.041C$$

= 0.506C

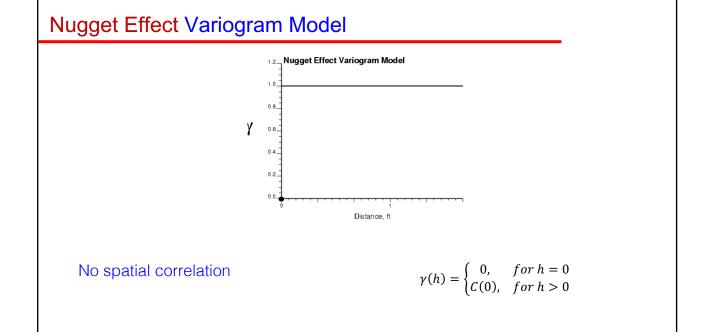
$$\sigma_k = (0.506\text{C})^{0.5} = 0.711\text{C}^{-1/2}$$

If the estimation errors are normally distributed, then the probability that the true value lies within $\pm 0.711C^{1/2}$ of the kriged value is 68%

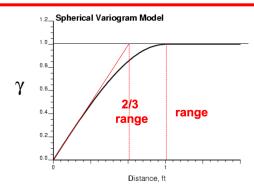
So kriging has determined a set of weights which are optimal (in the sense that the estimation variance is minimized) for the particular variogram and data configuration, and also gives a measurement of the error (ie the estimation variance itself).

29

Common Variogram Models



Spherical Variogram Model



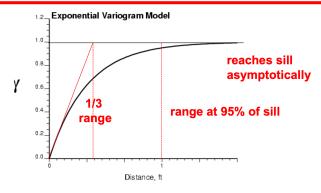
Most commonly used model

$$\gamma(h) = C(0) \cdot Sph\left(\frac{h}{a}\right) = \begin{cases} c \cdot \left[1.5\left(\frac{h}{a}\right) - 0.5\left(\frac{h}{a}\right)^{3}\right], & for \ h < a \\ c, & for \ h \ge a \end{cases}$$

32

32

Exponential Variogram Model

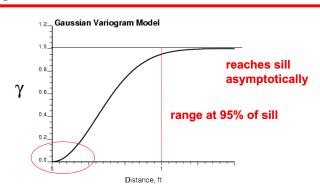


Similar to spherical but rises more steeply and reaches the sill asymptotically

$$\gamma(h) = C(0) \cdot Exp\left(\frac{h}{a}\right) = c \cdot \left[1 - exp\left(-\frac{h}{a}\right)\right]$$

33

Gaussian Variogram Model



Implies short scale continuity; parabolic behavior at the origin, instead of linear

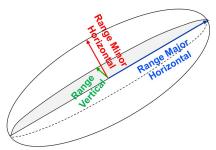
$$\gamma(h) = C(0) \cdot Gauss\left(\frac{h}{a}\right) = c \cdot \left[1 - exp\left(-\frac{h^2}{a^2}\right)\right]$$

34

34

2D / 3D Variogram Models

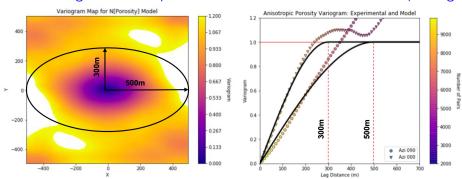
The variation of range along different directions is modeled using an ellipse in 2D and an ellipsoid in 3D



- There is an ellipsoidal variation in continuity (geometric anisotropy):
 - Parameters for a 2D variogram model:
 - direction, dip, major, minor and vertical range, type of variogram

2D Variogram Model

Calculate the variogram for all possible distances and directions (variogram map)



There is an ellipsoidal variation in continuity (geometric anisotropy):

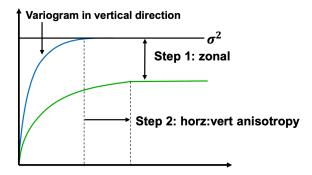
- Parameters for a 2D variogram model:
 - direction, major and minor range, type of variogram

36

36

Inference Given Sparse Data

- Calculate experimental variograms: the vertical variogram and the horizontal variogram lags that can be calculated
- Establish zonal anisotropy: estimate the fraction of variance explained "within zones" and "between zones"
- o Establish presence of vertical / horizontal trends.



41

Influence of Variogram Parameters

- The slope of the variogram at the origin has a great influence on the continuity of the interpolation process. The gentler the slope, the smoother the interpolation.
- The estimation is very sensitive to the size of the nugget. Increasing the nugget component tends to make the data weights more similar and gives smoother maps which do not honour the data points.
 - A pure nugget variogram will produce purely random spatial variations.
- Rescaling the variogram by changing the sill has no effect on the kriging estimate but changes the kriging variance. This will then lead to increased variability in stochastic simulations using SGS.
- Increasing the range of the variogram will increase the influence of more distant data points and giving smoother maps

42

42

Kriging - 1

- Kriging is a procedure for constructing a minimum error variance linear estimate at a location where the true value is unknown
- The main controls on the kriging weights are:
 - closeness of the data to the location being estimated
 - redundancy between the data
 - the variogram
- Simple Kriging (SK) does not constrain the weights and works with the residual from the mean
- Ordinary Kriging (OK) constrains the sum of the weights to be 1.0, therefore, the mean does not need to be known
- There are many different types of kriging

43

Kriging - 2

- The implicit assumption is stationarity (work around with different types of kriging)
- Kriging is not used directly for mapping the spatial distribution of an attribute (sometimes when the attribute is smooth).
 - It is used, however, for building conditional distributions for stochastic simulation

44

Kriging - Review of Main Points

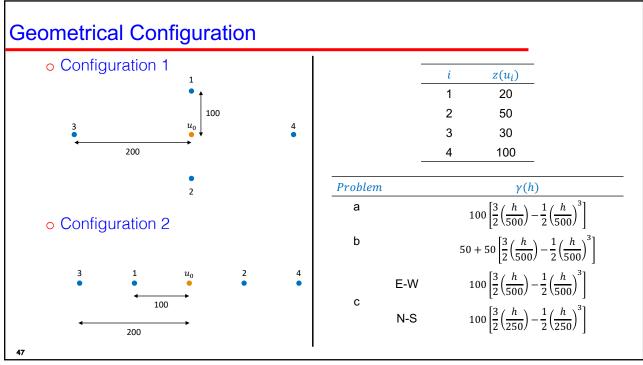
- Simple kriging (SK) is linear regression with some special properties:
 - Gives the mean and variance of conditional normal distribution
 - Best linear estimate for mean squared error criterion and variogram model
- Estimation variance is expected squared difference between estimate and truth that accounts for:
 - Initial variance if no data are available, the stationary variance of the property
 - The redundancy between the data
 - The closeness of the data to what is being estimated
- We derive simple kriging to minimize the error variance in expected value
- The use of SK estimates directly is somewhat limited, but it is used extensively under a multivariate Gaussian model for inference of conditional means and variances
 - We will discuss simulation later

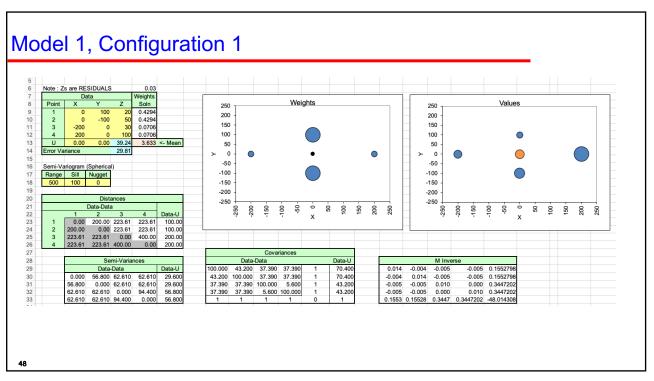
4

Ordinary Kriging

In Class Exercise

46





48

Model 1, Configuration 1

- o Weights:
 - Sum of weights = 1
 - Higher weights are assigned to the closest points
 - Symmetry of the configuration is maintained in the weights

Weights
Soln
0.4294
0.4294
0.0706
0.0706

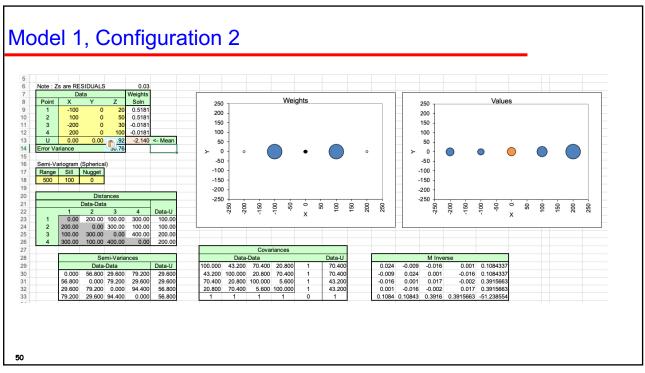
o Value:

 $-z(u_0) = 39.24$

o Error variance

 $-\sigma_E^2 = 29.81$

49



50

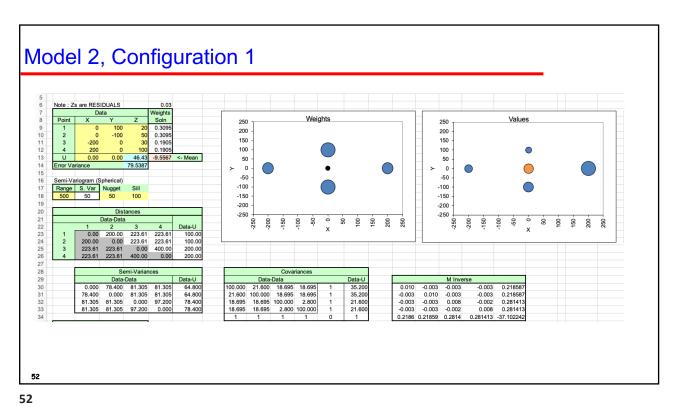
Model 1, Configuration 2

- o Slightly negative weights assigned to 3 and 4
- Because sample points 3 and 4 are directly behind points 1 and 2, the unsampled location does not "see" these samples, reducing their influence on the estimate
- Unlike conventional interpolation techniques (e.g. inverse distance methods), kriging accounts for the relative locations of the samples among themselves
- Higher error variance as this configuration does not provide as much information as the first configuration
- This illustrates that error variance is a reflection of surrounding data configuration
- More and well distributed samples will result in smaller error variance, whilst fewer and clustered samples will result in a bigger error variance

10/ 11/	
Weights	
Soln	
0.5181	
0.5181	
-0.0181	
-0.0181	

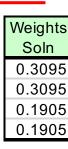
- o Value:
 - $-z(u_0) = 33.92$
- Error variance
 - $-\sigma_E^2 = 30.76$

5



Model 2, Configuration 1

- Compared with Model 1 for the same configuration, the weights assigned to the closest two sample points are reduced whilst the weights assigned to the farthest two points are increased
- o This is consistent with the model used
- A large nugget in the model indicates uncertainty about the spatial relationship
- Because we know less about the spatial relationship, the weights assigned to individual points are only partially influenced by the relative distances between sample points and the unsampled location
- In the limit of a pure nugget case, all weights will be equal as we have no prior information about the spatial relationship
- o Error variance is also higher
- o This also reflects the lack of spatial relationship



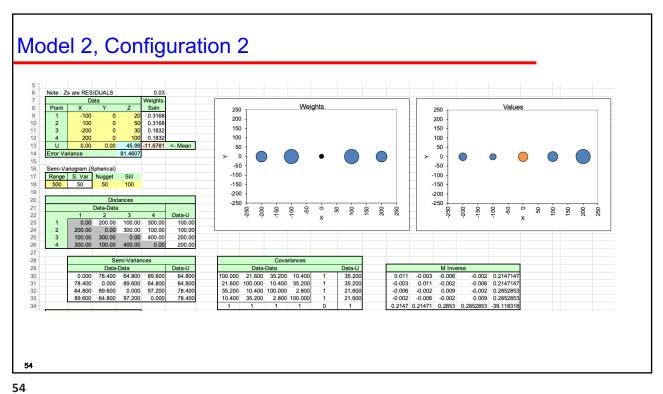
o Value:

 $-z(u_0) = 46.43$

Error variance

 $-\sigma_E^2 = 79.54$

53



77

Model 2, Configuration 2

- As for Model 1, the weights assigned to the two closest points increase
- This is because the two farthest point are being shielded by the nearest points
- However, in contract to Model 1, the differences in weights, compared to configuration 1, is small
- This is expected because we do not know as much about the spatial configuration
- The error variance compared with configuration 1 is higher which is also consistent

Weights
Weignis
Soln
0.3168
0.3168
0.1832
0.1832

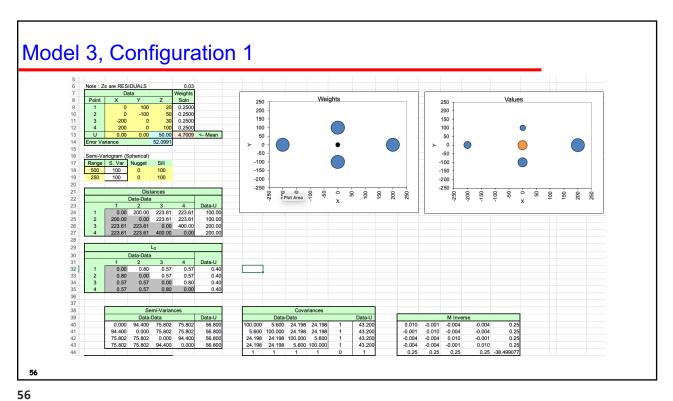
o Value:

 $-z(u_0) = 46.0$

o Error variance

 $-\sigma_E^2 = 81.5$

- 5



--

Model 3, Configuration 1

- The covariances between the sample points and the unsampled location are identical
- Because we have different ranges in different directions, the relative influences of sample points one and two, and three and four are identical
- The range in the north-south direction is smaller; therefore, the influence of sample points in that direction diminishes over a shorter distance, the weight assigned to each of the sample points is identical
- This is because the variogram distance for all four pints is the same
- o The error variance is higher than the error variance for Model 1
- This is because the range in the N-S direction is only half of what it was in Model 1
- Thus, the neighboring values in that direction do not provide as much information

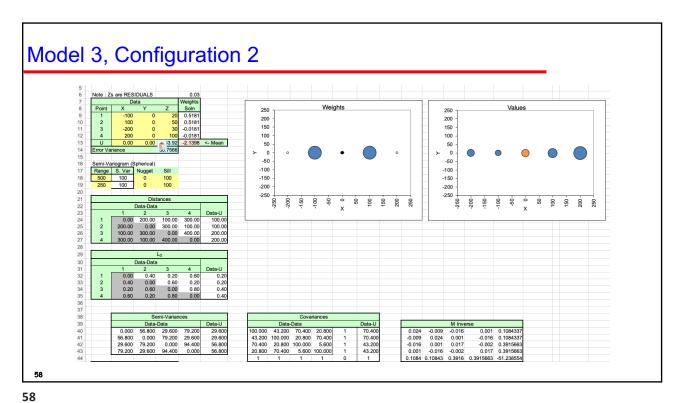
Weights	
Soln	
0.2500	
0.2500	
0.2500	
0.2500	

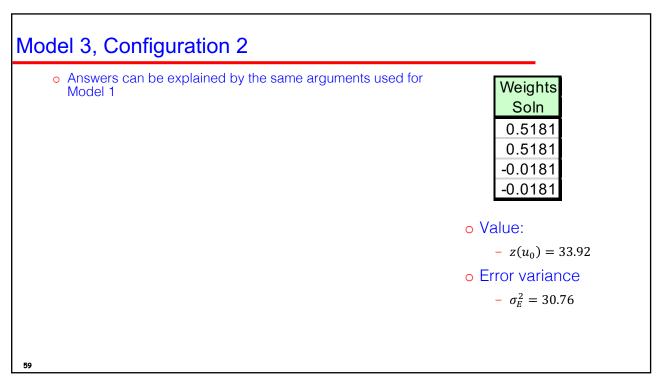
o Value:

 $-z(u_0) = 50.0$

Error variance

 $-\sigma_E^2 = 52.1$





Kriging

When to use SK versus OK

60

Kriging – When to Choose OK versus SK

- If the global mean is well known and known to be representative of the entire field, then SK is desired.
 - Remember that this requires no strong trends in the data.
- OK is a safe bet when the mean is not well known or in cases where the data contain trends.
 - How does OK get around the mean?

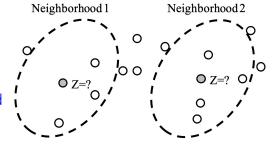
$$Z_{SK}^{*}(u) = \sum_{\alpha=1}^{n} \lambda_{\alpha} Z(u_{\alpha}) - \left(1 - \sum_{\alpha=1}^{n} \lambda_{\alpha}\right) m$$

Ordinary Kriging

$$\sum_{\alpha=1}^{n} \lambda_{\alpha} = 1 \quad \Longrightarrow \quad Z_{OK}^{*}(u) = \sum_{\alpha=1}^{n} \lambda_{\alpha} Z(u_{\alpha})$$

Kriging – When to Choose OK versus SK

- o Often, we use neighborhoods when kriging, i.e. to estimate a certain location only data within a certain search radius are used.
- To define a search radius we often use ellipses (why?):
- o In SK, we fix the mean, regardless of what neighboring points we use.
- In OK, since we do not fix the mean and we use different neighborhoods, then implicitly, the mean varies from neighborhood to neighborhood.



• The values in neighborhood 1 may give rise to a mean that is different from the values in neighborhood 2.