# Spatial interpolation and kriging

**EDS 222** 

Tamma Carleton Fall 2022

#### Announcements/check-in

• Change in office hours next week: 12-1pm Monday 11/21 on Zoom (happy Thanksgiving!)

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- **Change in office hours** next week: 12-1pm Monday 11/21 on Zoom (happy Thanksgiving!)
- Remember to look at final project guidelines for details on presentation, writeup, etc.

# Today

Refresher: types of spatial data

Vectors/objects, rasters/fields

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Sample vs. population, points to fields

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A common challenge: spatial interpolation

Sample vs. population, points to fields

Kriging: a powerful form of interpolation

Variogram, kriging

# Types of spatial data

#### Spatial Data can generally split into:

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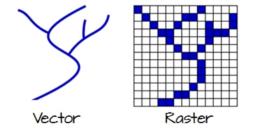
An **alternative framing**: object view versus field view

- **Object View**: The study region (and world) is a series of entities located in space. Examples: Points representing cities. Non-continuous polygons representing cities.
- **Field View**: Every location within the study region (and world) has a measurable value. Examples: Elevation. Temperature. Wind direction.

**Q**: Is there a *best* data type to represent objects or fields?

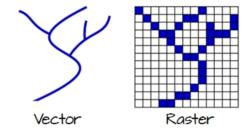
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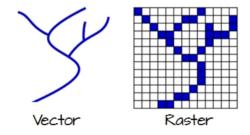
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 Usually it will be easier to represent objects with vector data and fields with raster data, but ultimately this depends on what analysis you want to run

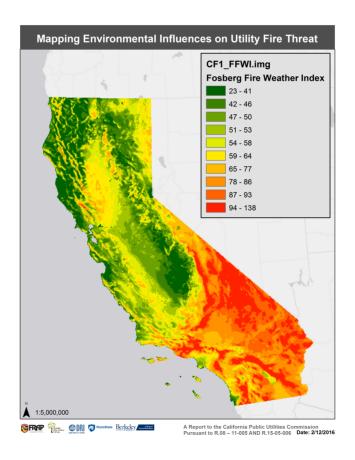
Q: Is there a *best* data type to represent objects or fields?

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- Usually it will be easier to represent objects with vector data and fields with raster data, but ultimately this depends on what analysis you want to run
- Luckily, R makes it easy to switch back and forth (but we need to be careful and intentional when transforming!)

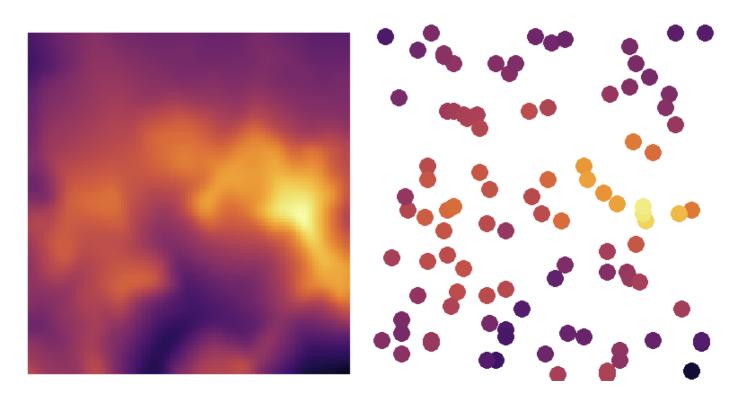
In environmental data science, we are **often interested in modeling fields** 



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That means we only have data from a *sample*, not a census of the *population* 



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#### **Definition:**

Spatial interpolation is the process of using a **sample** of observed points to estimate values for **all locations** in a study region

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#### For example:

- Predicting "gold grades" across South Africa using a few borehole samples (the problem of Daniel *Krige*!)
- Predicting depth to groundwater across California using monitoring wells
- Predicting air pollution across China using monitoring stations
- ??

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**Spatial interpolation** aims to predict  $Z(x_0)$  using a linear combination of the values in the sampled locations:

$$\hat{Z}(x_0) = \sum_{i=1}^m \lambda_i Z(x_i)$$

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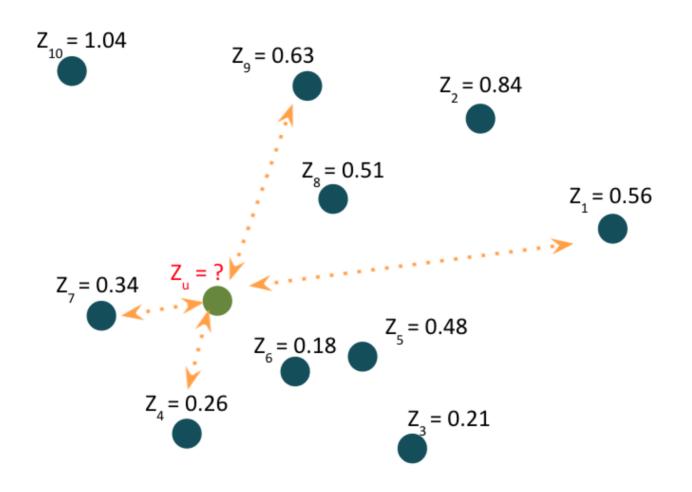
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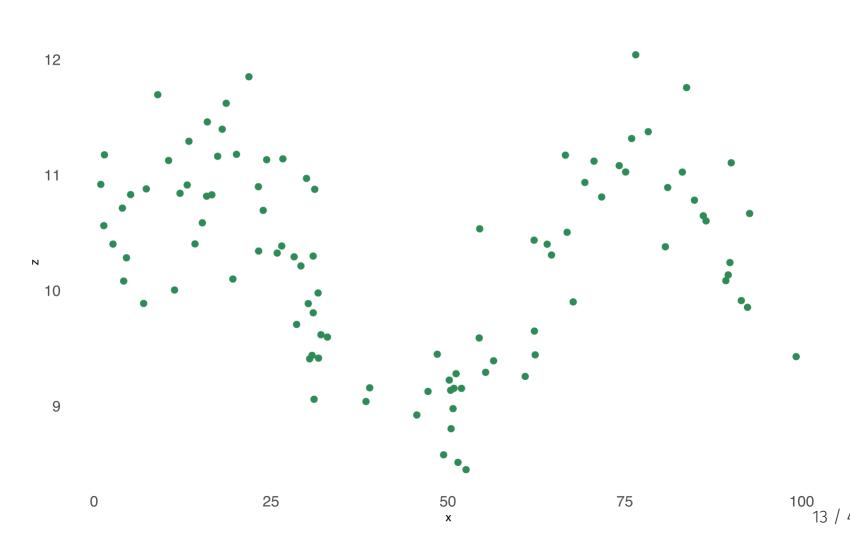
• All spatial interpolation methods assume or derive a set of  $\lambda$ 's to compute  $\hat{Z}$ 's

#### Interpolation in pictures



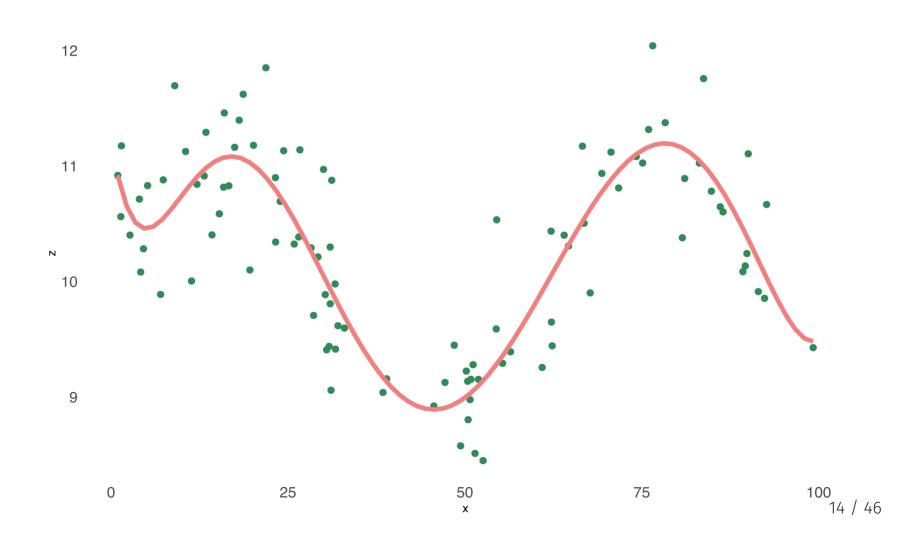
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Consider one-dimensional space where values z depend on location x



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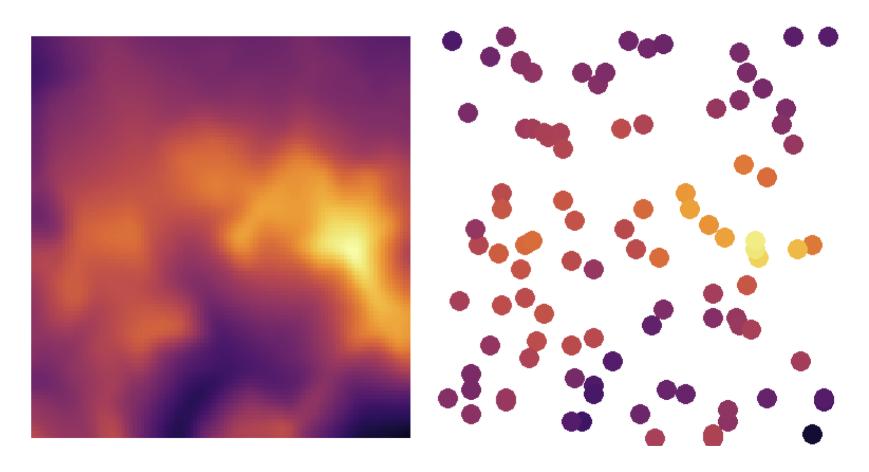


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Often we have data for an outcome z observed in 2-D space: z(x,y)

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#### Interpolation methods

#### Polynomial regression

• In one-dimensional space:

$$\hat{Z}(x_0) = \hat{eta}_0 + \hat{eta}_1 x_0 + \hat{eta}_2 x_0^2 {+} \ldots {+} \hat{eta}^p x_0^p$$

• In two-dimensional space with  $(x_0,y_0)$  the unknown location:

$$\hat{Z}(x_0,y_0) = \hat{eta}_0 + \hat{eta}_1 x_0 + \hat{eta}_2 y_0 + \hat{eta}_3 x_0 y_0 + \hat{eta}_4 x_0^2 + \hat{eta}_5 y_0^2 + \dots$$

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**Exact:** Predicts a value identical to the measured value.

**Inexact:** Does *not* predict a value identical to the measured value.

# Polynomial regression interpolation

This is just **multiple linear regression** using spatial information as the independent variables

```
mod = lm(z~poly(x,8))
predictions = augment(mod)$.fitted
```

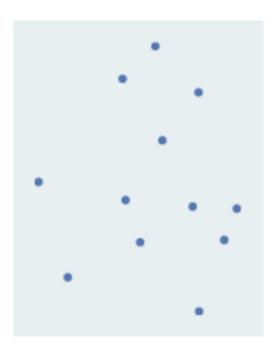
Nearest Neighbors (NN)

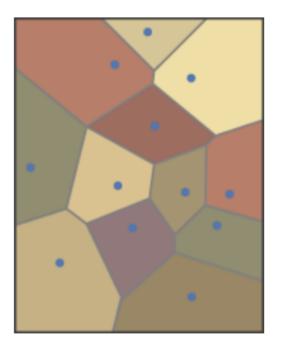
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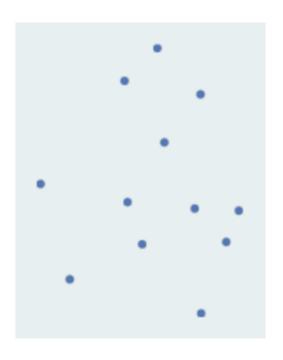
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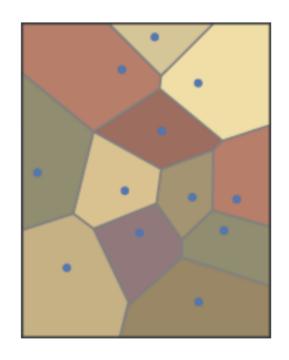




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 Creates what are called "Theissen Polygons", which allocate space to the nearest sampled point

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#### Implementation in R

• Easy with the voronoi() function from the dismo package:

```
library(dismo)
v ← voronoi(dta)
plot(v)
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Helpful tutorial here

#### Inverse distance weighting

Basic idea: weights are a decreasing function of distance from  $x_0$  to  $x_i$ 

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$$\hat{Z}(x_0) = \sum_{i=1}^m rac{Z(x_i) Dist(x_i, x_0)^{-p}}{\sum_{i=1}^m Dist(x_i, x_0)^{-p}}$$

Equivalently:

$$\lambda_i^{IDW} = rac{1/Dist(x_i,x_0)^p}{\sum_{i=1}^m 1/Dist(x_i,x_0)^p}$$

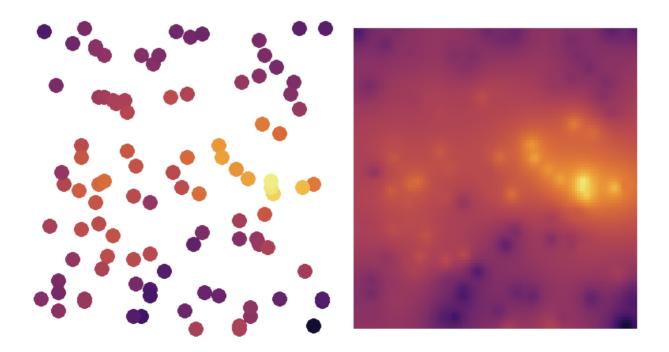
where p is the "power parameter" determining how fast the weight declines as the distance between the points grows larger

#### Inverse distance weighting

- **Pros:** Smooth, exact
- **Cons:** Difficult/computationally intensive (you need to compute distances for *all* pairs of points in the region!), all sampled observations influence  $\hat{Z}(x_0)$ , have to choose p somehow, result can be "clumpy"

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#### Inverse distance weighting

#### Implementation in R

```
library(phylin)
idw(values, coords, grid, method = "Shepard", p = 2, R = 2, N = 15,
    distFUN = geo.dist, ...)
```

- Note the method argument: "Shepard" follows the math on the previous slide
- Note the p argument: Need to specify power parameter

#### There are many more!

- Piecewise linear interpolation / Delany triangulation
- Local polynomial regression
- Radial basis function (RBF)
- Kriging (of many forms)
- Many new machine-learning based methods
- Learn more in Li and Heap (2014)

# Enter: Kriging

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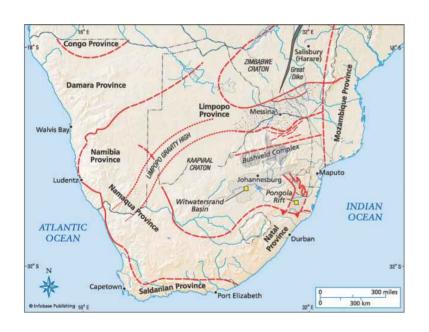
#### Why?

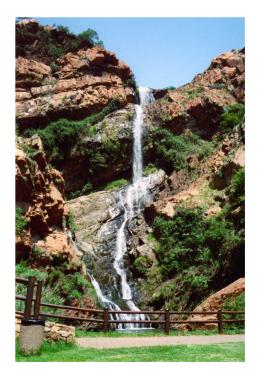
- It is *flexible* (i.e., less researcher decisions, more data-driven)
- Under certain assumptions it is the "best linear unbiased estimate" (sound like OLS yet??)
- You can recover an estimate and a standard error (i.e., it is stochastic)

Next up: Kriging details!

# Kriging

The Witwatersrand ("Rand") in South Africa is known for its gold content. Mining engineers wanted to know where in the Rand was most likely to have a high gold content per block of ore.





- Many individual ore samples have been taken (vector data -- points)
- Underlying data is the content of the rock (raster data -- field)

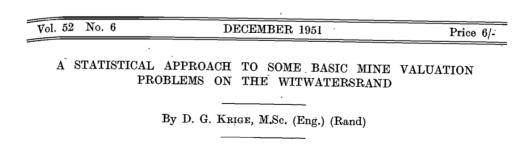
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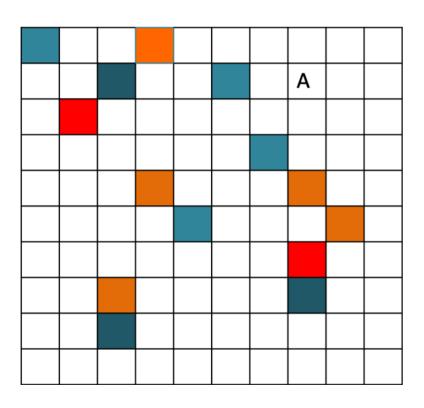
#### **Spatial interpolation** is highly valuable!

- Danie Krige's solution: [in his master's thesis!]
  - Use an estimator that minimizes the mean squared prediction error (very similar to OLS)
  - Show that it has a bunch of nice properties relative to other forms of spatial interpolation



## Correlations in space

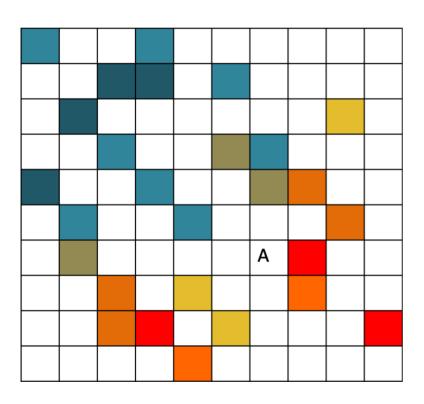
Q: If there is **no correlation** between values in nearby locations, can we predict new values based on our sample?



- Blue = low gold content; Red = high gold content
- **Zero** correlation between values in nearby locations
- Can you predict the gold content in location A based on this sample?

## Correlations in space

Q: If there is **no correlation** between values in nearby locations, can we predict new values based on our sample?



- Blue = low gold content; Red = high gold content
- **Positive** correlation between values in nearby locations
- Now can you predict the gold content in location A based on this sample?
- Why?

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**Key concept:** Variograms give us a way of understanding how correlated spatial observations are to those around them, and how that correlation "decays" as points get further apart

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A **variogram** shows the variance of values within groups of observations as a function of the *distance* between them

**Key concept:** Variograms give us a way of understanding how correlated spatial observations are to those around them, and how that correlation "decays" as points get further apart

**Mining example:** Variogram gives a measure of how much two samples taken from the mining area will vary in gold percentage depending on the distance between the samples. Samples farther apart will vary more than those taken close together.

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We often discuss the **semi-variogram**, which is:

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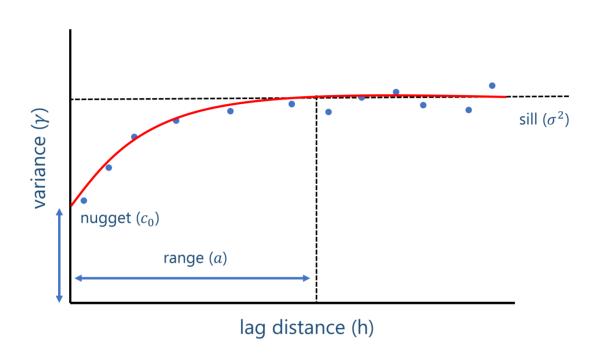
Why? Recall:

$$var(a-b) = var(a) + var(b) - 2cov(a,b)$$

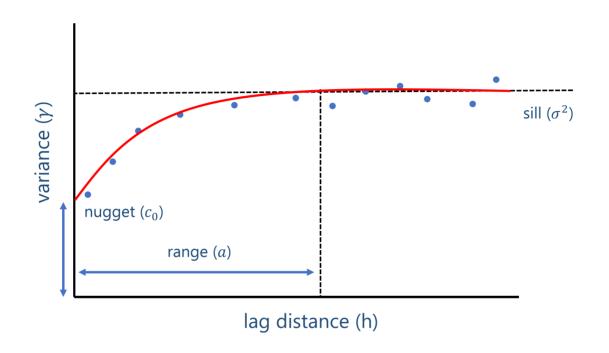
So, for a "stationary" variogram, we have

$$\gamma(x+h,x) = var(Z(x)) - cov(Z(x),Z(x+h))$$

# Variogram: in pictures



## Variogram: in pictures



- **Nugget:** At h=0, residual variance is from microscale effects or measurement error
- Sill: The stationary maximum variance -- no more covariance
- Range: Separation distance beyond which there is no covariance

# Estimating a (semi)variogram

#### Empirical semivariogram

$$\hat{\gamma}(h\pm\delta) = rac{1}{2N(h\pm\delta)} \sum_{(i,j)\in N(h\pm\delta)} \left|z_i-z_j
ight|^2.$$

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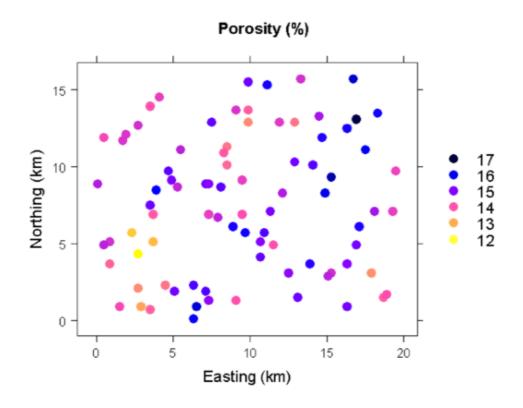
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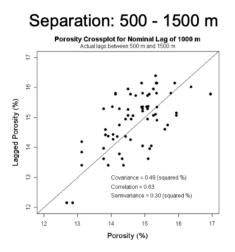
#### How?

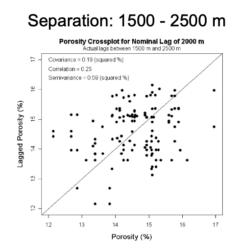
- ullet Draw "donuts" of width  $\delta$  and average distance h around each point
- Compute differences in values for each pair of points, square them
- Take an average!

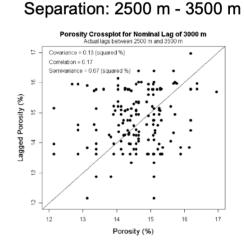
- Bohling's Introduction to Geostatistics and Variogram Analysis
- Porosity values in a bean field
- 85 wells sampled



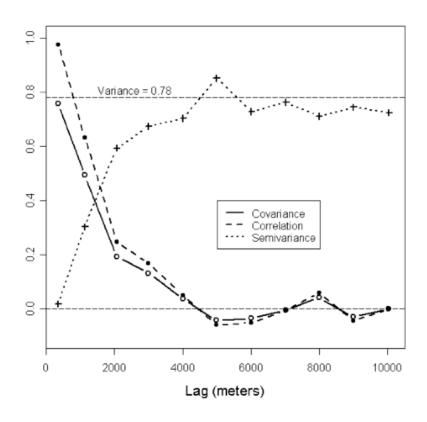
For various values of h and a fixed  $\delta$ , compute semivariance:







#### Plot your semivariances:



Then choose (or optimize) a **variogram model** to fit through the semivariance points:

- Exponential
- Spherical
- Gaussian
- ...

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- ...

**Many more details** on variograms here or in any geostatistics textbook (e.g., Cressie and Wikle, 2011)

### Back to kriging

Recall that our goal is a prediction of a value  $\hat{Z}(x_0)$  based on observations in all sampled locations:

$$\hat{Z}(x_0) = \sum_i^m \lambda_i Z(x_i)$$

## Back to kriging

Recall that our goal is a prediction of a value  $\hat{Z}(x_0)$  based on observations in all sampled locations:

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In **kriging** (and many spatial interpolation methods), the  $\lambda_i$  weights **decay** as distance between  $x_0$  and  $x_i$  grows larger

--

How do we find the weights in kriging?

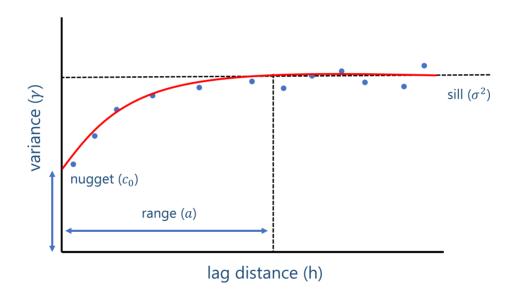
# Kriging weights

How do we find the weights in kriging?

## Kriging weights

How do we find the weights in kriging?

#### Hint:



The **variogram** tells us how correlated values are with other values near them, and how this correlation falls as distance grows. It is a **key input** into the kriging solution.

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Note: full derivation in Cressie and Wikle (2011) [this is a very shorthand version]

Goal: minimize mean squared prediction error

$$min_{\lambda} \ E[(Z(x_0) - \sum_i^m \lambda_i Z(x_i))^2] ext{ subject to } \sum_i^m \lambda_i = 1$$

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To solve:

- 1. Take derivatives with respect to each  $\lambda_i$
- 2. Set each first order condition = 0
- 3. Solve system of equations for  $\lambda_i^*$  values that minimize mean squared error

#### Result:

$$\hat{Z}(x_0) = \underbrace{\{ ilde{m{\gamma}}(x_0) + \mathbf{1}(1 - \mathbf{1}'m{\Gamma}_Z^{-1} ilde{m{\gamma}}(x_0))/(\mathbf{1}'m{\Gamma}_Z^{-1}\mathbf{1})\}'m{\Gamma}_Z^{-1}}_{\hat{\lambda}}Z$$

- where  $ilde{\gamma}(x_0)$  is the vector containing the semivariogram evaluated between  $x_0$  and every other point, and
- $\Gamma_Z$  is the m imes m matrix containing all semivariogram evaluations for all sampled point pairs.

#### Result:

$$\hat{Z}(x_0) = \underbrace{\{ ilde{m{\gamma}}(x_0) + \mathbf{1}(1 - \mathbf{1}'m{\Gamma}_Z^{-1} ilde{m{\gamma}}(x_0))/(\mathbf{1}'m{\Gamma}_Z^{-1}\mathbf{1})\}'m{\Gamma}_Z^{-1}}_{\hat{\lambda}}Z$$

- where  $ilde{\gamma}(x_0)$  is the vector containing the semivariogram evaluated between  $x_0$  and every other point, and
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Other helpful resources here

There are **three** main forms of kriging:

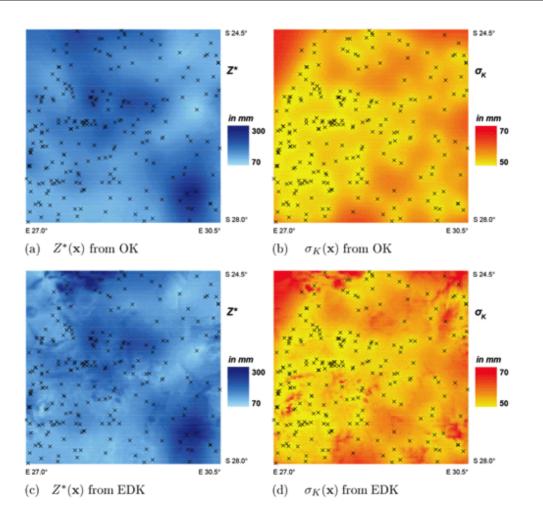
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- There are also other forms! E.g., quantile kriging, log-normal kriging, IRFk-kriging, etc.
- We will work on implementation in R in the next lab.



Source: Lebrenz and Bardossy (2019)

### Kriging summary

#### Pros:

- Under each set of assumptions specific to the kriging form, kriging is the best linear unbiased predictor ("BLUP")
- Weights are determined almost entirely by the data, instead of a-priori assumptions
- Exact
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#### Cons:

- Nonlinear methods may perform better (e.g., ML methods)
- Variogram has to be approximated/estimated
- Complex/computationally intensive

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Slides created via the R package **xaringan**.