Spatial interpolation and kriging

EDS 222

Tamma Carleton
Fall 2023

Announcements/check-in

Final Projects

- 3-minute in-class presentation: 12/12, 4-7pm, Bren Hall 1424 -- with snacks! I will randomly allocate slots and post the presentation order by 12/07
- Blog post/write up: due 12/9, 5pm, send to me and Sandy via email in `.html` and `.pdf` formats
- See guidelines for details on expectations for presentation and write up
- If you are not a MEDS student and/or do not want a blog post, the `.pdf` alone is fine

Announcements/check-in

Course evaluations

- Incredibly valuable for me, this course, and for the development of MEDS more broadly!
- Some changes from previous years' feedback:
    - Added logistic regression
    - Integrated more code snippets into lecture materials
    - More environmental examples (too much economics...)
    - Slower pace of lecture content
    - More definitions of mathematical objects
    - More lectures on stats in practice

Announcements/check-in

Class plan for remainder of the quarter

- 11/28: time series + spatial data
- 11/30: spatial interpolation
- 12/05: spatial kriging in `R`
- 12/07: guest lecture -- stats in ecohydrology!

Today

Refresher: types of spatial data

Vectors/objects, rasters/fields

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A common challenge: spatial interpolation

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

Spatial Data can generally split into:

- **Vector** Data

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- **Object View**: The study region (and world) is a series of entities located in space. Examples: Points representing cities. Non-continuous polygons representing cities.

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- **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.

Spatial data

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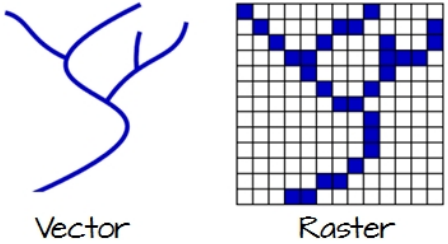
A: Usually, but it depends.



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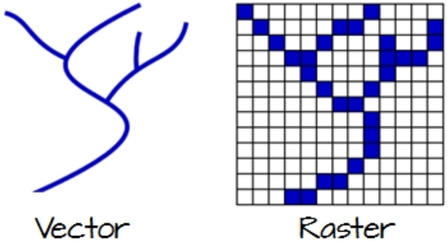

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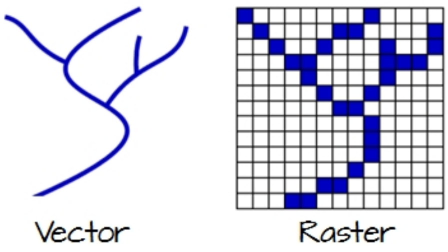
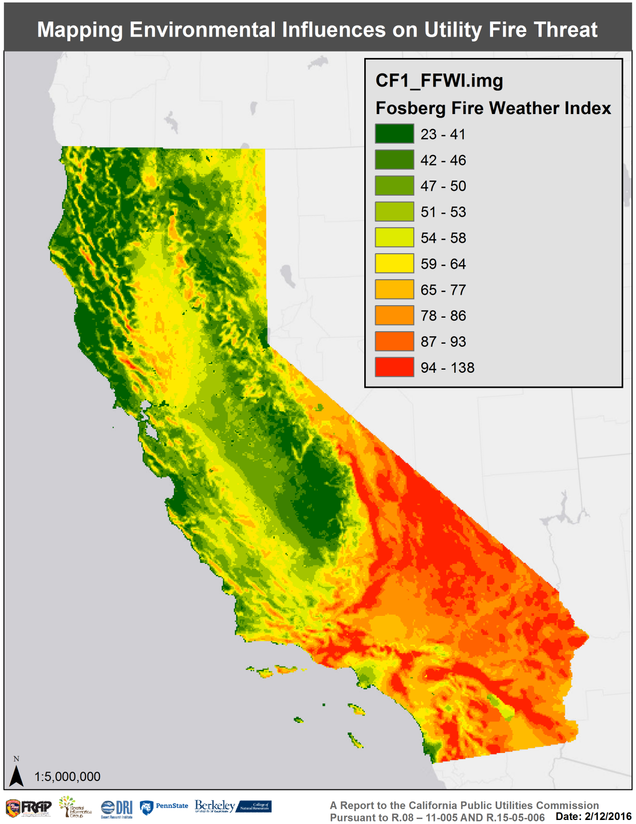


- Usually it will be easier to represent **objects** with **vector data** and **fields** with **raster** data, but ultimately this depends on what analysis you want to run
- Luckily, `R` makes it easy to switch back and forth (but we need to be careful and intentional when transforming!)

Spatial interpolation

Spatial interpolation

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



Spatial interpolation

But we are doing **statistics!**

Spatial interpolation

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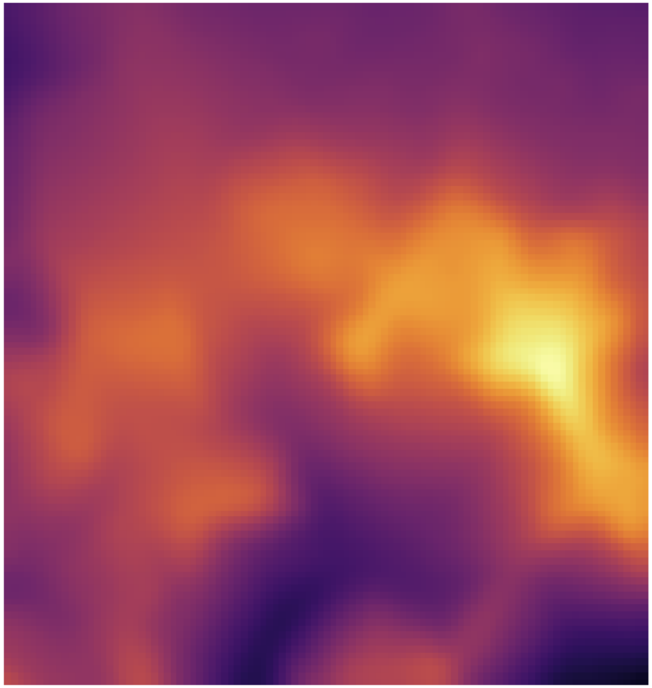
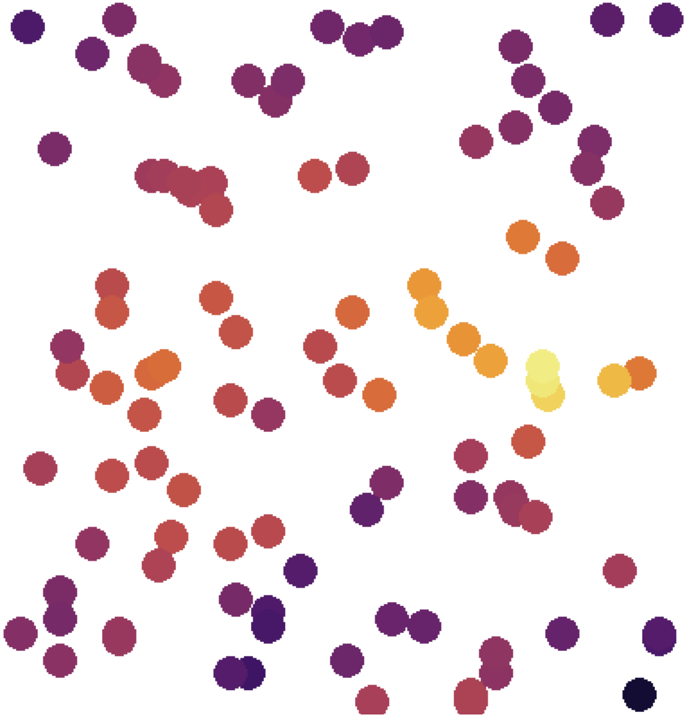
That means we only have data from a *sample*, not a census of the *population*





Spatial interpolation

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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
- ??

Spatial interpolation in math

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

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

where λ_i are weights applied to each sampled location.

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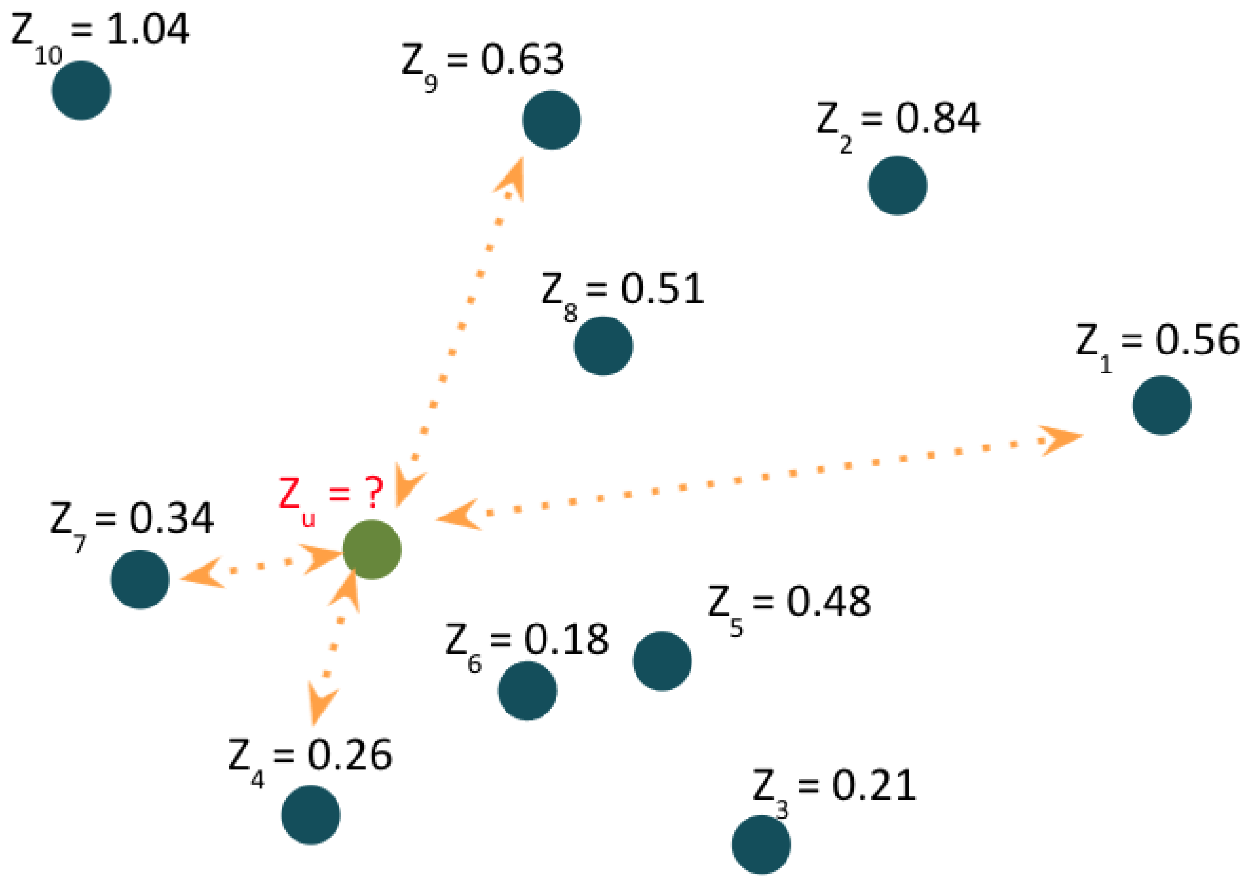
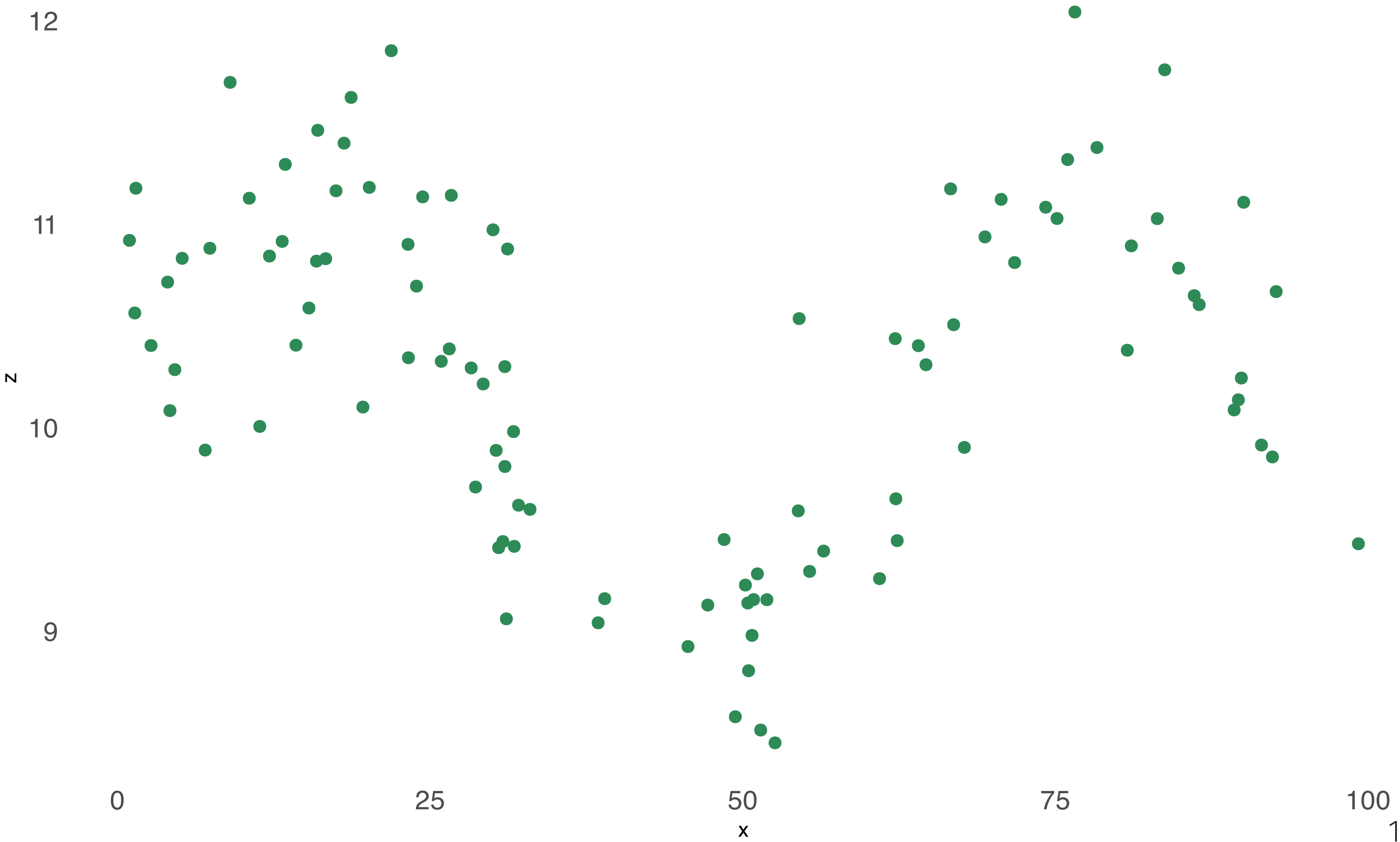
- All spatial interpolation methods assume or derive a set of λ's to compute $\hat{Z}$'s

Interpolation in pictures



Interpolation in one dimension

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



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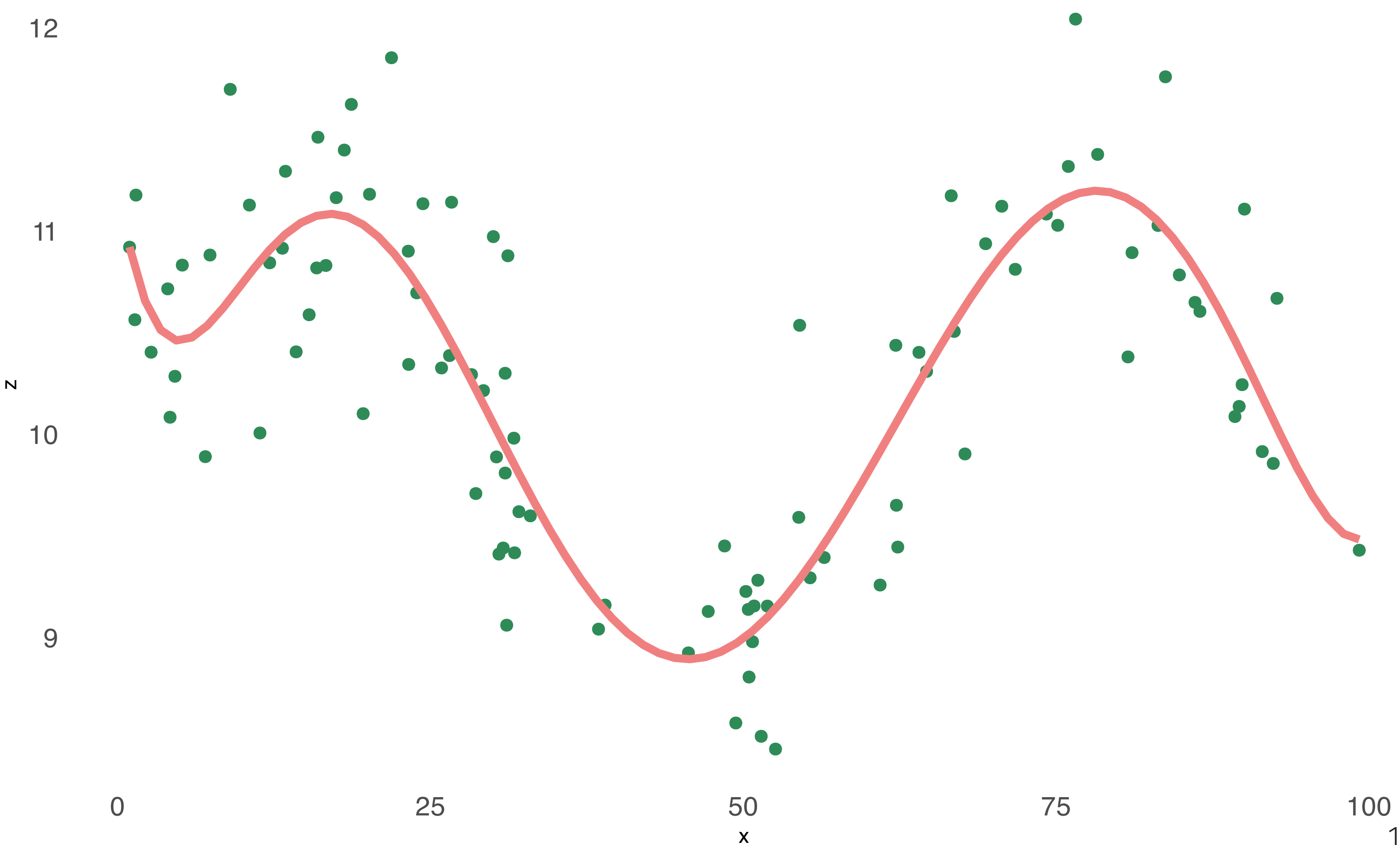

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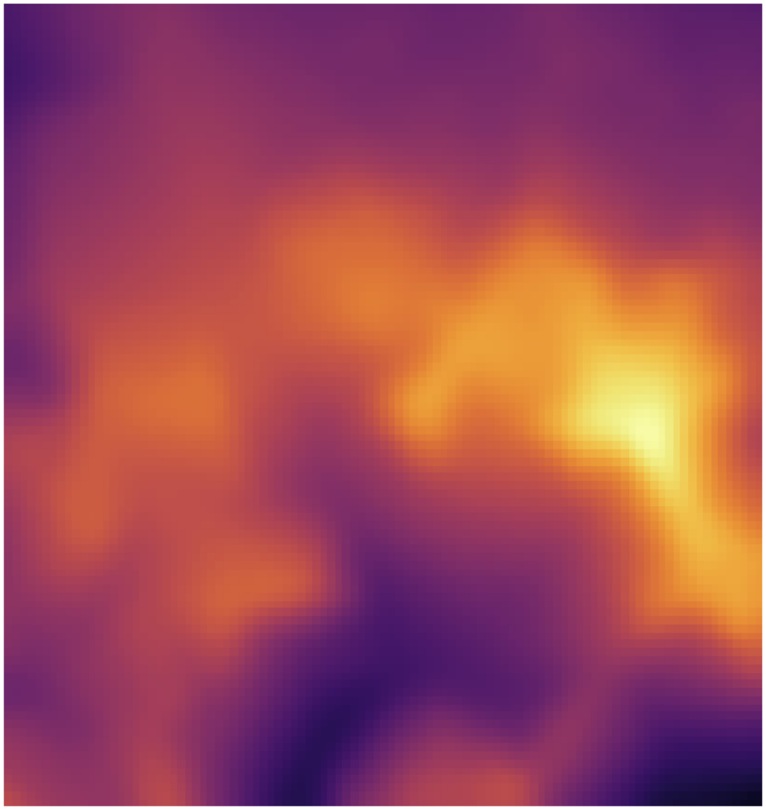

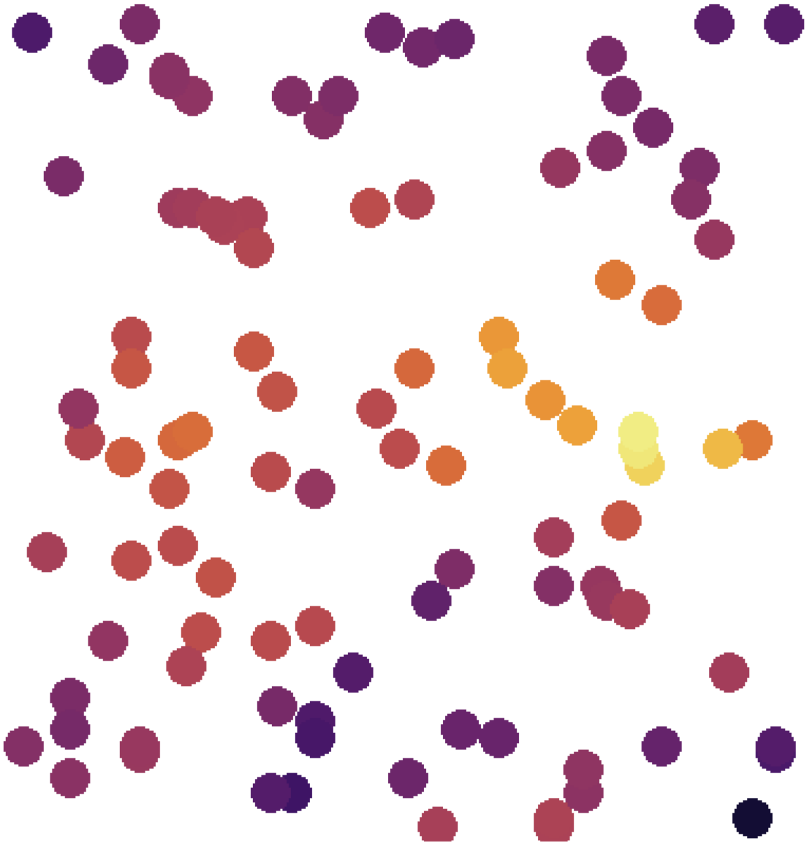

Interpolation methods

Polynomial regression

- In one-dimensional space:

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

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

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

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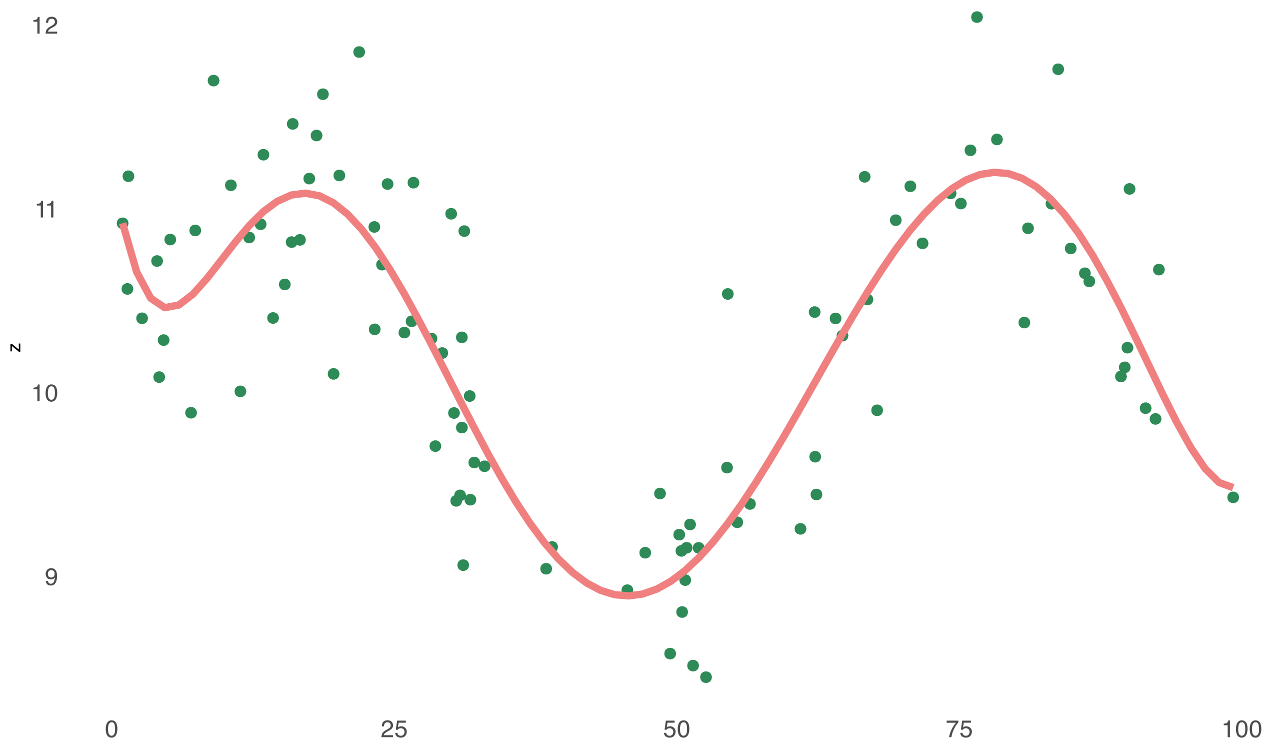
Exact: Predicts a value identical to the measured value.

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
```



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In 2-D:

```
mod = lm(z~x + y + x*y + x2 + y2 + x2*y2)
```

Interpolation methods

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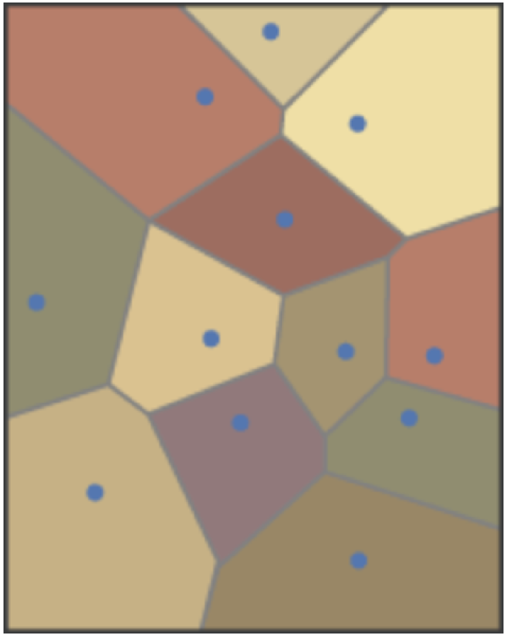

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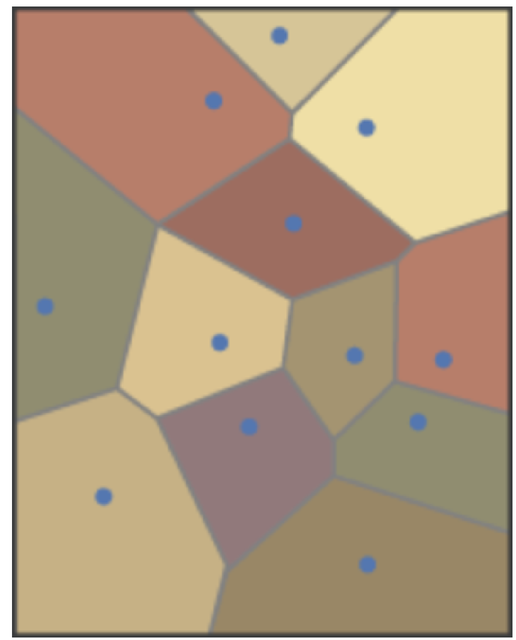

- Creates what are called "Theissen Polygons", which allocate space to the nearest sampled point

Nearest Neighbor interpolation

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library(dismo)
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plot(v)
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Inverse distance weighting

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

Equivalently:

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

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

Interpolation methods

Inverse distance weighting

- **Pros:** Smooth, exact
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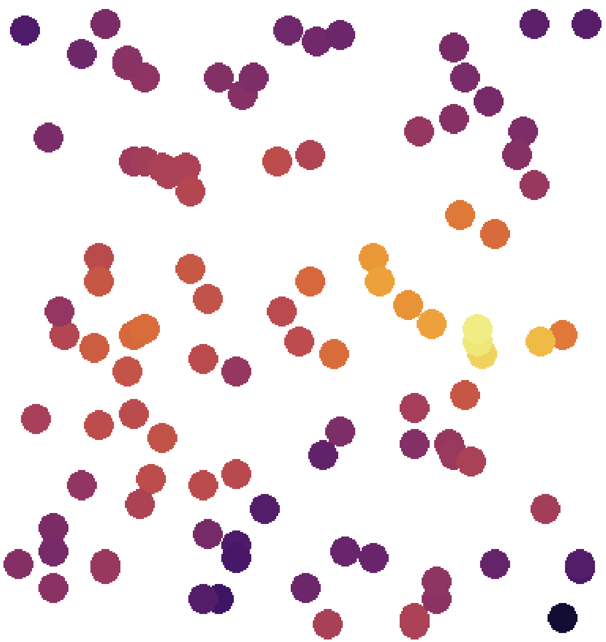

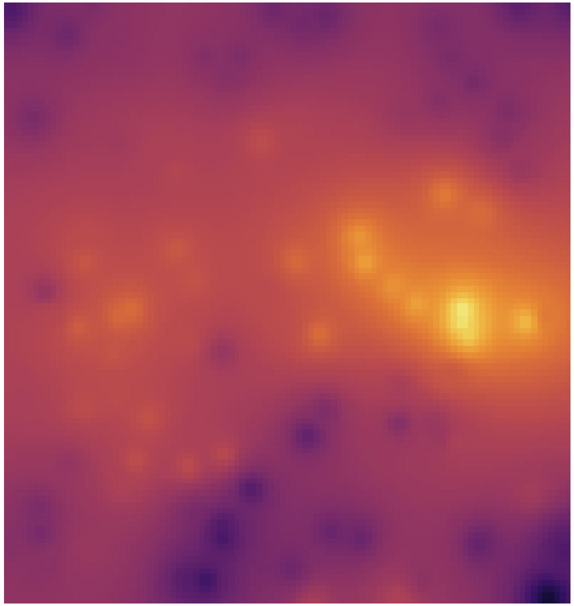

Inverse distance weighting

Implementation in `R`

```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

Interpolation methods

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?

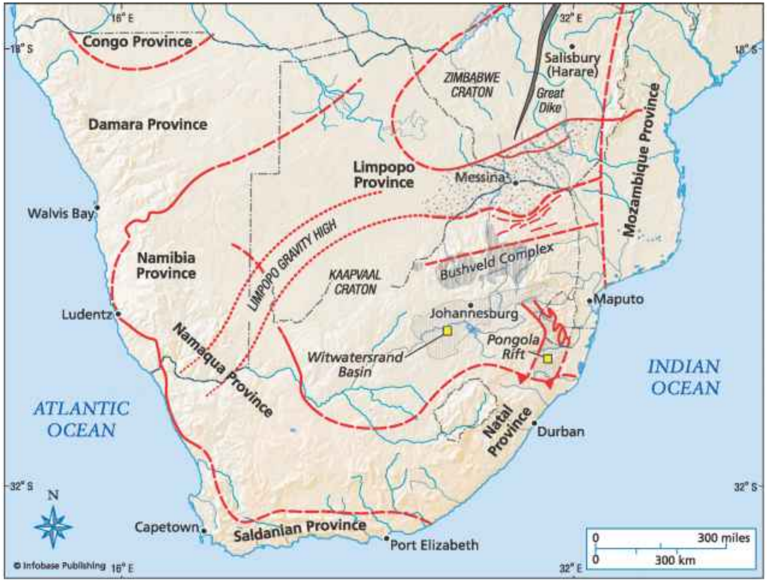
- It is *flexible* (i.e., less researcher decisions, more data-driven)
- Under certain assumptions it is the "best linear unbiased estimate" (sound like OLS yet??)
- You can recover an estimate *and* a standard error (i.e., it is *stochastic*)

Next up: Kriging details!

Kriging

Kriging: an origin story

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.



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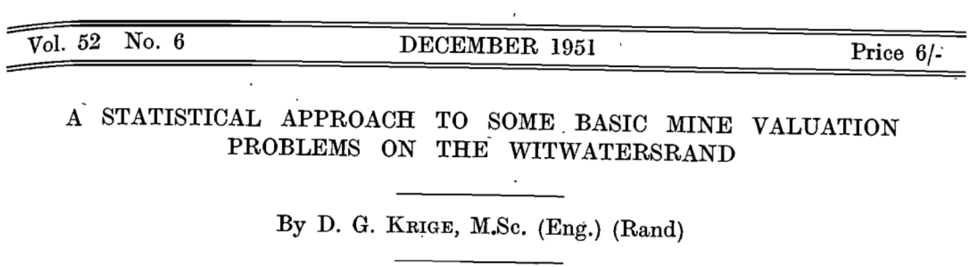
Spatial interpolation is highly valuable!

- **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



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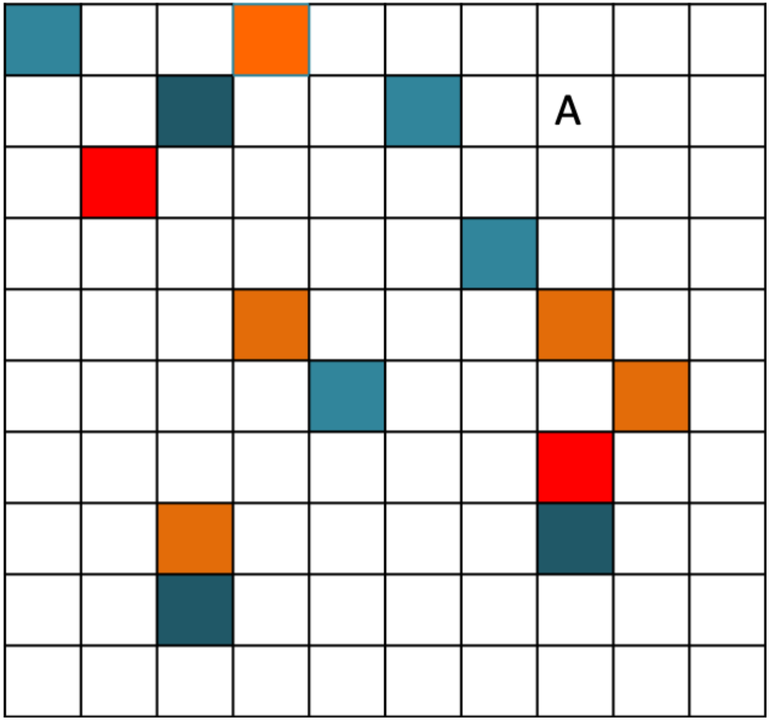
A STATISTICAL APPROACH TO SOME BASIC MINE VALUATION PROBLEMS ON THE WITWATERSRAND

By D. G. KRIGE, M.Sc. (Eng.) (Rand)

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

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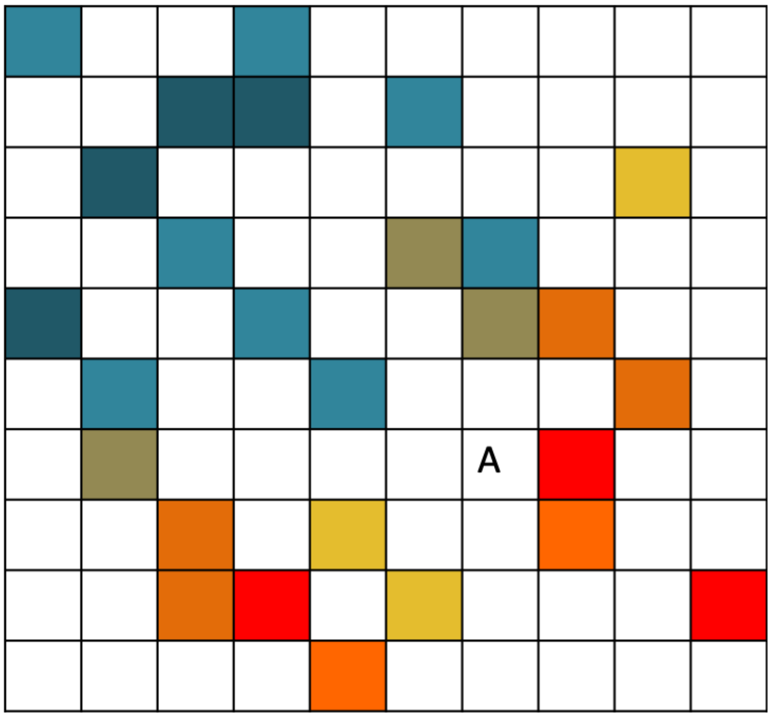

- Blue = low gold content; Red = high gold content
- **Positive** correlation between values in nearby locations
- Now can you predict the gold content in location A based on *this* sample?
- *Why?*

Variogram

Key takeaway: quantifying spatial dependence is key to spatial interpolation

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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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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.

Variogram

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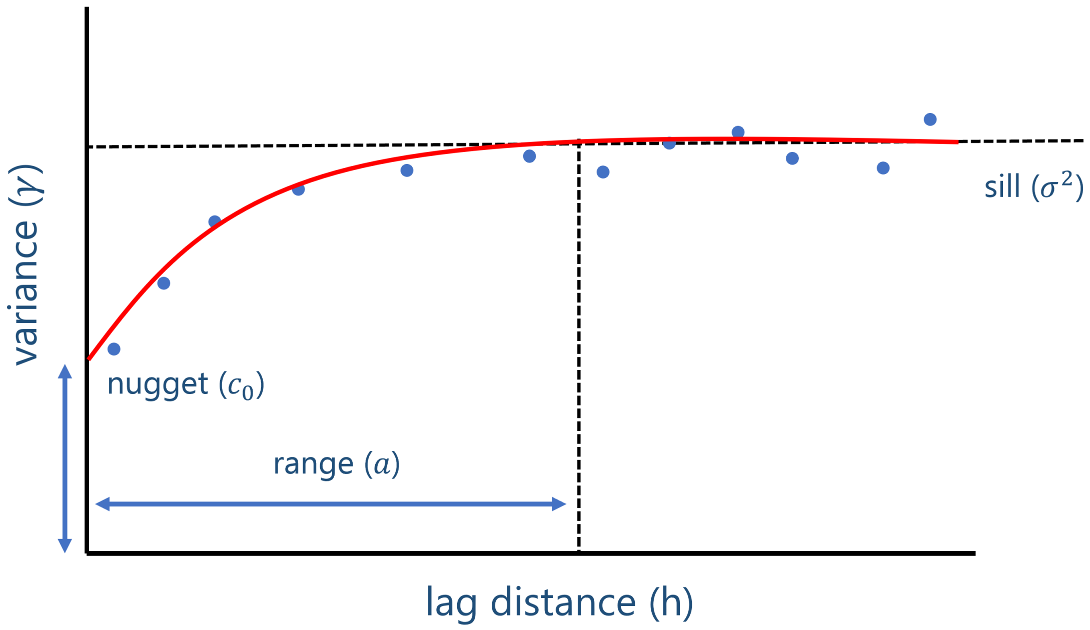
Why? Recall:

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

So, for a "stationary" variogram, we have
$\gamma(x+h, x) = var(Z(x)) - cov(Z(x), Z(x+h))$

Variogram: in pictures



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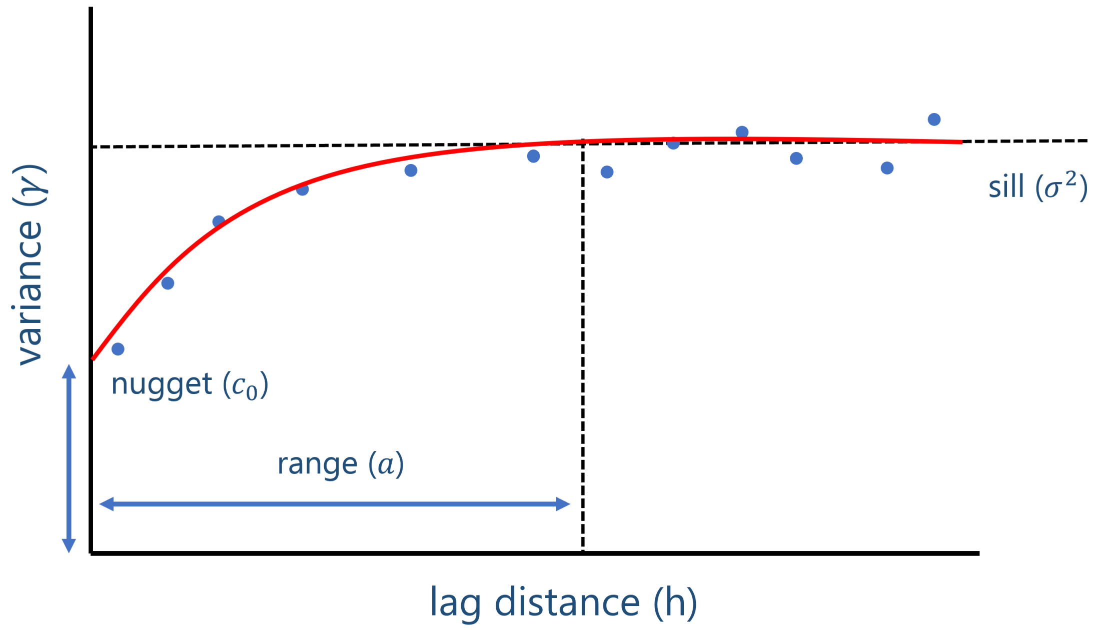

- **Nugget:** At $h = 0$, residual variance is from microscale effects or measurement error
- **Sill:** The stationary maximum variance -- no more covariance
- **Range:** Separation distance beyond which there is no covariance

Estimating a (semi)variogram

Empirical semivariogram

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

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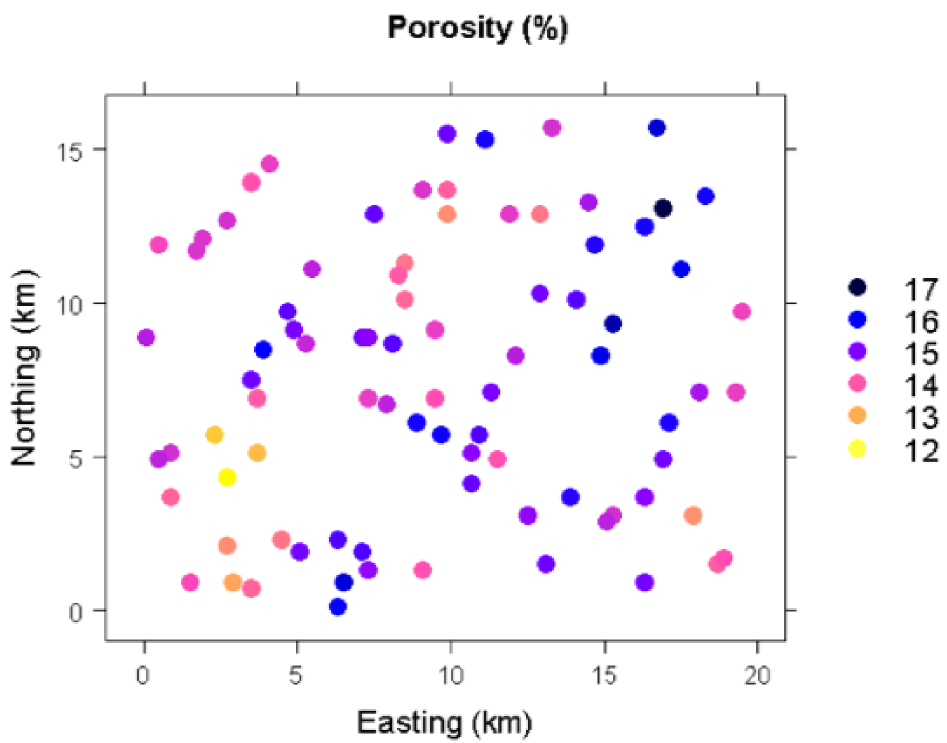
How?

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

Empirical variogram example

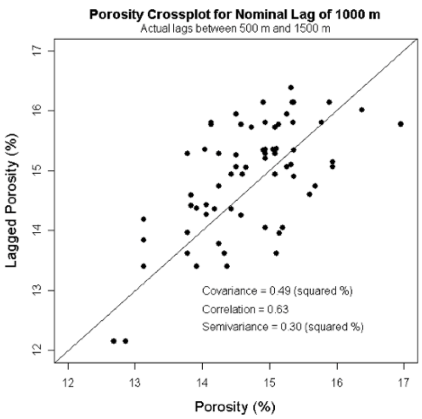
- Bohling's *Introduction to Geostatistics and Variogram Analysis*
- Porosity values in a bean field
- 85 wells sampled



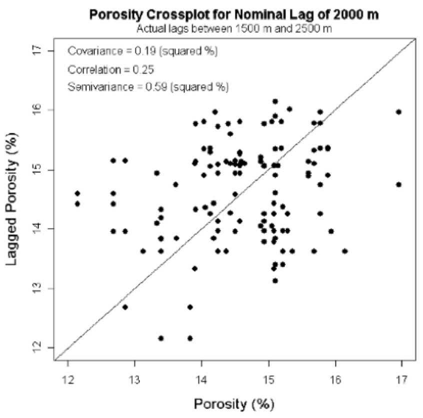
Empirical variogram example

For various values of h and a fixed δ, compute semivariance:

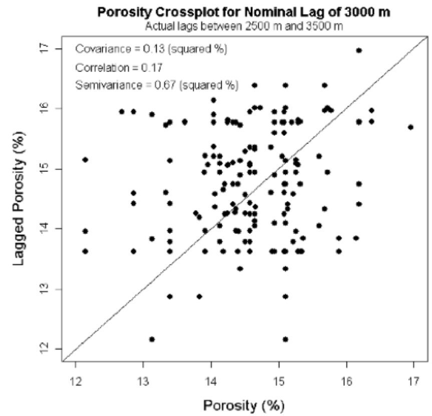
Separation: 500 - 1500 m



Separation: 1500 - 2500 m

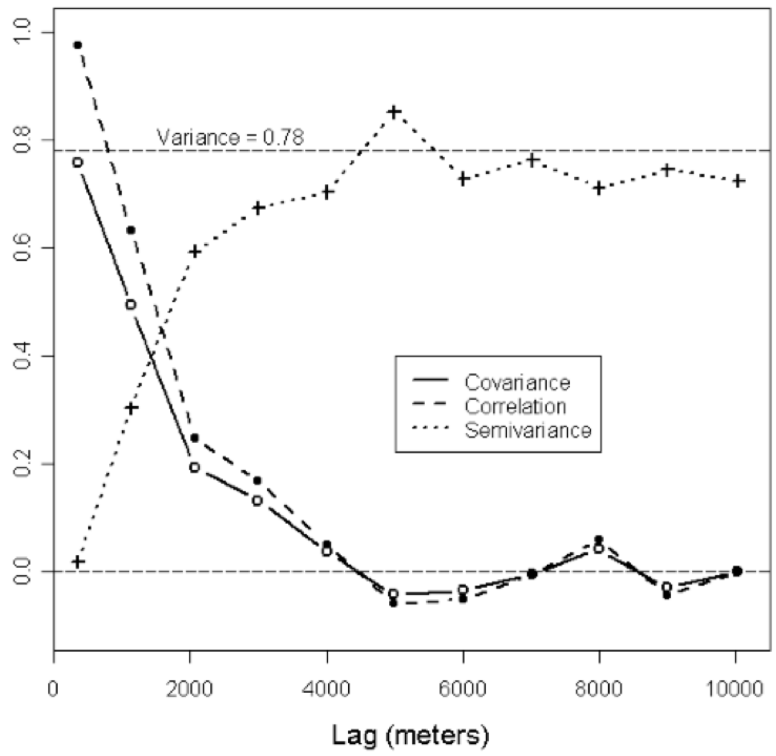


Separation: 2500 m - 3500 m



Empirical variogram example

Plot your semivariances:



Empirical variogram example

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 λ_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?

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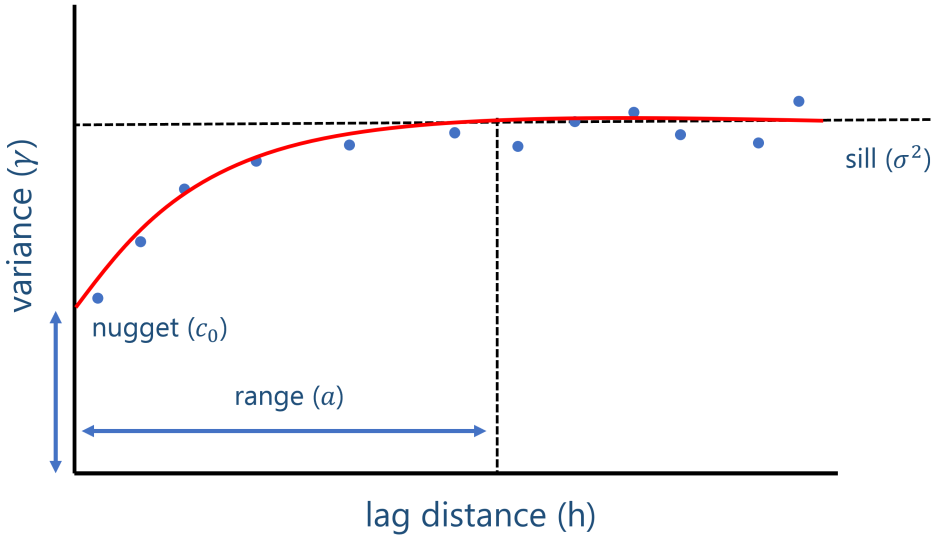
Hint:



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.

Deriving the kriging solution

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

Goal: minimize mean squared prediction error

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

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To solve:

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

Deriving the kriging solution

Result:

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

- where $\tilde{\gamma}(x_0)$ is the vector containing the semivariogram evaluated between x_0 and every other point, and
- $\mathbf{\Gamma}_Z$ is the $m \times m$ matrix containing all semivariogram evaluations for all sampled point pairs.

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Other helpful resources here

Forms of kriging

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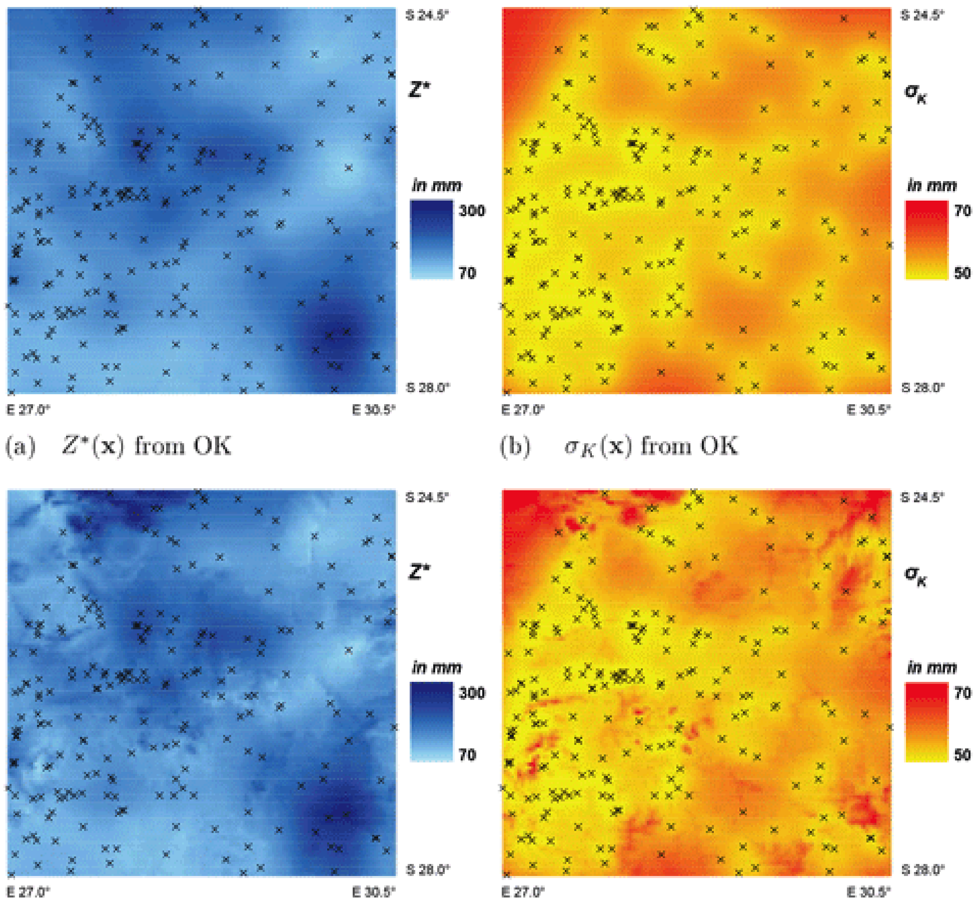
- We will work on implementation in `R` in the next lab.

Forms of kriging



(a) $Z^*(\mathbf{x})$ from OK
(b) $\sigma_K(\mathbf{x})$ from OK
(c) $Z^*(\mathbf{x})$ from EDK
(d) $\sigma_K(\mathbf{x})$ from EDK

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

A note of caution on interpolation

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All spatial interpolation approaches should be used cautiously, especially if:

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- You don't have very many observations

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