Kriging

Statistical Learning Reading Group

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Gold Digging in Sofala, NSW

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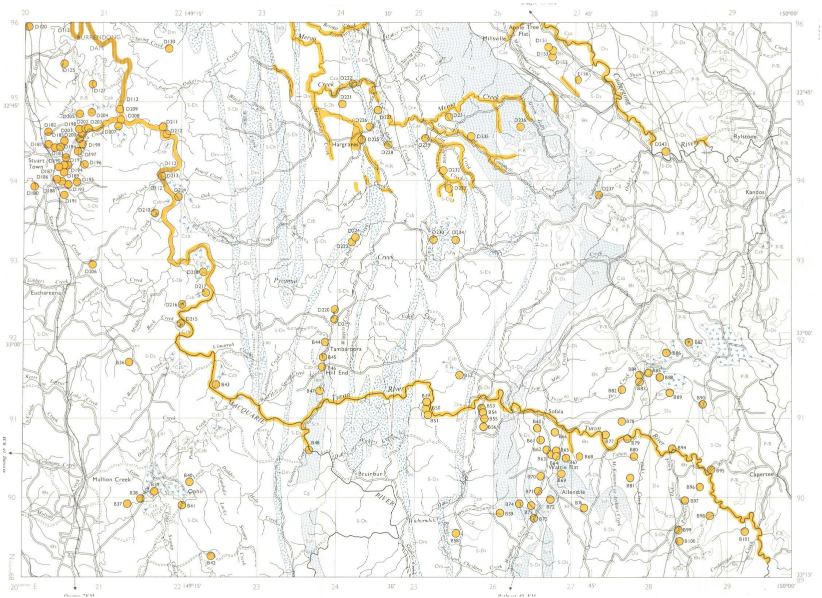
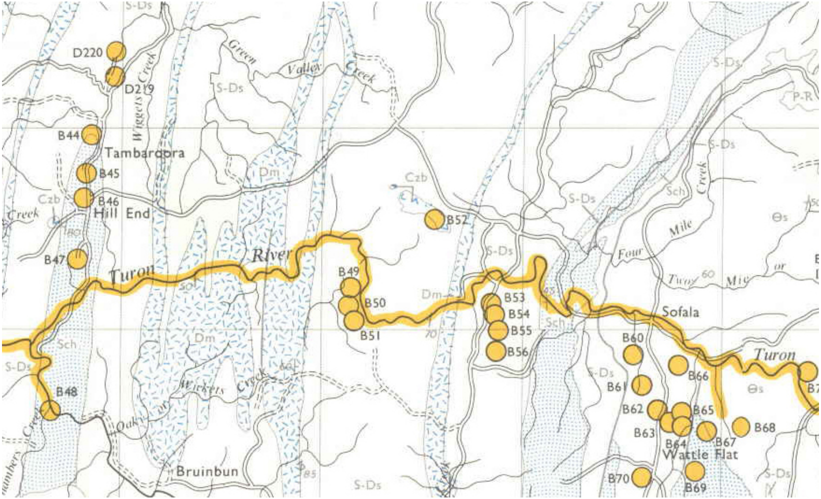
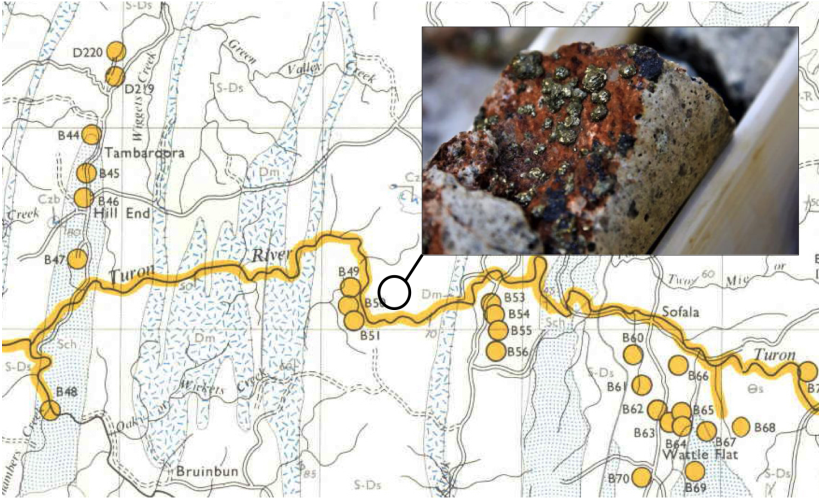


Gold Digging in Sofala, NSW



Gold Digging in Sofala, NSW



History of Kriging

- Gold mining in South Africa in the 1940s
- Mines established in locations with surface exposure of ore ⇒ biased sampling
- Sample mean of assays times estimated ore-body volume used to predict recoverable ore
- Sample standard deviation used to estimate variability in ore quality throughout the ore body
- D. G. Krige in the 1950s noted three flaws:
  - Gold-assay data are log-normal
  - Local variability (block grade) is lower than global variability (core sample grade)
  - Block grade and core sample grade are correlated
- Similar techniques and models developed in meteorology, forestry, physics, geodesy

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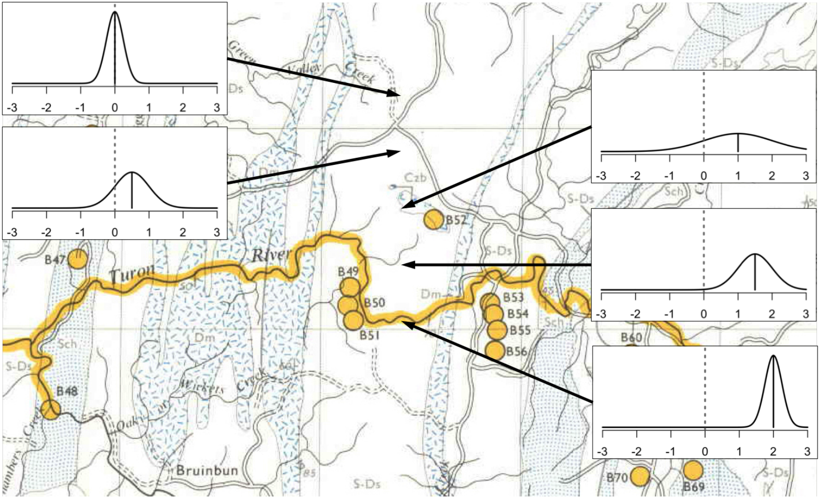


Gaussian Process

- Observations $Z(\mathbf{s}_1), \dots, Z(\mathbf{s}_N)$ at locations $\mathbf{s}_1, \dots, \mathbf{s}_N$ of random variable Z
- Here, each $\mathbf{s}_i$ is a 2-dimensional vector
- Data are a partial realisation of a stochastic process:

$$\{Z(\mathbf{s}) : \mathbf{s} \in D\} \tag{1}$$

  with $D \subset \mathbb{R}^2$
- Replications are not independent but are spatially correlated
- **Goal:** estimating $Z(\mathbf{s}_0)$ for location(s) $\mathbf{s}_0$
- Rewrite the model: $Z(\mathbf{s}) = \mu(\mathbf{s}) + \epsilon(\mathbf{s}) =$ drift + zero-mean residual
- **Estimation requires:**
  - Description of *drift* $\mathbb{E}[Z(\mathbf{s})] = \mu(\mathbf{s})$
  - Description of *spatial covariance* $\mathrm{Cov}(Z(\mathbf{s}_i), Z(\mathbf{s}_j))$

Gaussian Process

- Simplifying assumption 1 - *Stationarity*:

$$\mathbb{E}[Z(\mathbf{s})] = \mu \qquad \forall \mathbf{s} \in D$$

- Simplifying assumption 2 - *Second-order stationarity*:

$$\text{Cov}(Z(\mathbf{s}_i), Z(\mathbf{s}_j)) = C(Z(\mathbf{s}_i) - Z(\mathbf{s}_j)) \qquad \forall \mathbf{s}_i, \mathbf{s}_j \in D \quad (2)$$

- Covariance between observations depends on distance and direction but not location
- C is called the *covariance function*
- Even stronger assumption - *Isotropy*:

$$C(Z(\mathbf{s}_i) - Z(\mathbf{s}_j)) = C(Z(\mathbf{s}_k) - Z(\mathbf{s}_l)) \qquad \forall \mathbf{s}_i, \mathbf{s}_j, \mathbf{s}_k, \mathbf{s}_l \in D : \|\mathbf{s}_i - \mathbf{s}_j\| = \|\mathbf{s}_k - \mathbf{s}_l\|$$

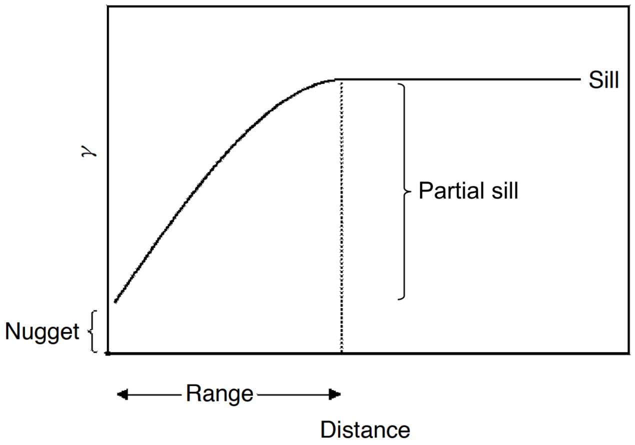
- Covariance between observations depends on distance but not on direction or location

Estimating Spatial Covariance - Semivariogram

- Alternative characterisation of spatial autocorrelation for isotropic processes (with some theoretical advantages)
- If:
$$\mathbb{V}[Z(\mathbf{s}_i) - Z(\mathbf{s}_j)] = 2\gamma(\mathbf{s}_i - \mathbf{s}_j)$$
$Z(\cdot)$ is called *intrinsically stationary* and $2\gamma(\cdot)$ is called the *variogram*
- $\gamma(\cdot)$ is the *semivariogram* and only depends on the spatial lag $\mathbf{h} = \mathbf{s}_i - \mathbf{s}_j$
- Properties:
  - $\gamma(-\mathbf{h}) = \gamma(\mathbf{h})$
  - $\gamma(\mathbf{0}) = 0$
  - $\gamma(\mathbf{h})/\|\mathbf{h}\|^2 \to 0$ as $\|\mathbf{h}\|^2 \to \infty$
  - $\gamma(\cdot)$ is conditionally negative definite for $\sum_{i=1}^{m} a_i = 0$:

$$\sum_{i=1}^{m}\sum_{j=1}^{m} a_i a_j \gamma(\mathbf{s}_i - \mathbf{s}_j) \leq 0$$

Semivariogram



Relationship with Covariance function

- For a second-order stationary process $Z(\cdot)$:

$$\gamma(\mathbf{h}) = C(\mathbf{0}) - C(\mathbf{h})$$

- If $C(\mathbf{h}) \to 0$ as $\|\mathbf{h}\| \to \infty$, then $\gamma(\mathbf{h}) \to C(\mathbf{0})$, so $C(\mathbf{0})$ is the variance of the process
- Range of the semivariogram in direction $\mathbf{r}_0/\|\mathbf{r}_0\|$ is the smallest value $\|r_0\|$ so that $\gamma(\mathbf{r}_0) = C(\mathbf{0})$
- Spatial correlogram: $\rho(\mathbf{h}) = C(\mathbf{h})/C(\mathbf{0})$
- So why do we need all three functions? Because the class of intrinsically stationary processes is larger than the class of second-order stationary processes (Brownian motion: $\gamma(\cdot)$ exists, $C(\cdot)$ does not)

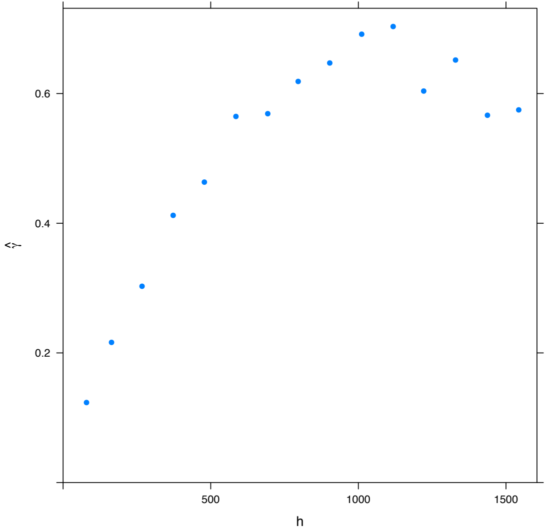
Estimating the Semivariogram

- Classic semivariogram estimator:
- Requires sufficient observations for each spatial lag
- With irregularly spaced data, pool data over tolerance regions
- Under intrinsic stationarity ($\mathbb{E}[Z(\mathbf{s})]$ constant):

$$
\begin{aligned}
2\gamma(\mathbf{h}) &= \mathbb{V}[Z(\mathbf{s}+\mathbf{h}) - Z(\mathbf{h})] \\
&= \mathbb{E}[(Z(\mathbf{s}+\mathbf{h}) - Z(\mathbf{h}))^2] - (\mathbb{E}[Z(\mathbf{s}+\mathbf{h}) - Z(\mathbf{h})])^2 \\
&= \mathbb{E}[(Z(\mathbf{s}+\mathbf{h}) - Z(\mathbf{h}))^2]
\end{aligned}
$$

- Estimate $\mathbb{E}[(Z(\mathbf{s}+\mathbf{h}) - Z(\mathbf{h}))^2]$ by averaging squared differences across pairs of observations

Estimating the Semivariogram



Parametric Isotropic Semivariogram Models

- Several parametric families can be fitted to estimated semivariogram
- Models typically assume isotropy but can be modified to fit well-defined anisotropy types:
  - Geometric anisotropy: range changes with direction, shape and sill remain constant
  - Zonal anisotropy: sill changes with direction, range remains constant
- Several fitting methods (NLS, ML)
- Methods for model comparison (single-parameter tests, chi-squared tests, AIC)
- Sum of models that are valid in $\mathbb{R}^d$ is again a valid model; model addition used for complex processes

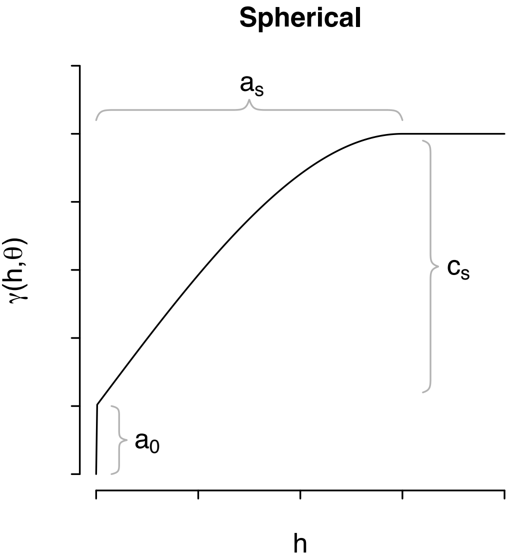
Spherical Semivariogram Model

- A semivariogram model is valid if it satisfies negative-definiteness
- *Spherical model*:

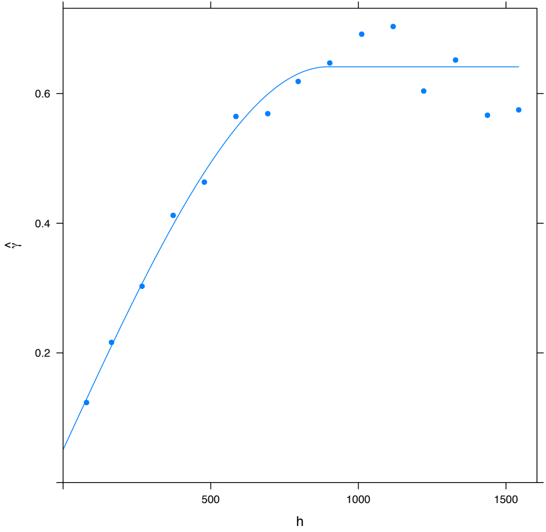
$$\gamma(h,\theta) = \begin{cases} 0, & h = 0 \\ c_0 + c_s[\frac{3}{2}\frac{h}{a_s} - \frac{1}{2}\left(\frac{h}{a_s}\right)^3], & 0 < h \leq a_s \\ c_0 + c_s, & h > a_s \end{cases}$$

  where $\theta = (c_0, c_s, a_s)$; $c_0, c_s \geq 0, a_s > 0$.
- c_0: nugget effect, c_s: partial sill, a_s: range
- Valid in 1, 2, and 3 dimensions

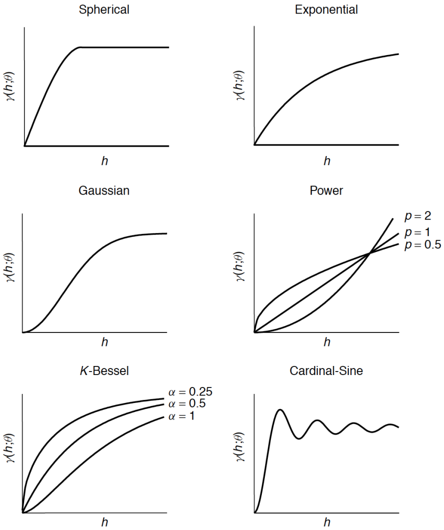
Spherical Semivariogram Model



Example Spherical Semivariogram Fit



Other Models



Estimating the Mean - Kriging

- Once we know how observations are related across space we can use these to:
  - Estimate $\mathbb{E}[Z(\mathbf{s}_0)]$ at some location $\mathbf{s}_0$
  - Obtain uncertainty bounds for our estimate
- Types of kriging:
  - *Simple*: mean known
  - *Ordinary*: mean constant but unknown
  - *Universal*: mean nonstationary and unknown
  - *Filterd*: smoothing and prediction for noisy data
  - *Lognormal*: optimal spatial estimation for lognormal data

Simple Kriging

- Let $S = \{\mathbf{s}_1, \ldots, \mathbf{s}_n\}$ be a set of locations at which we have observed realisations $z(\mathbf{s}_1), \ldots, z(\mathbf{s}_n)$ of the random variable $Z(\mathbf{s}) = \mu(\mathbf{s}) + \epsilon(\mathbf{s})$
- Assume $\mu(\mathbf{s})$ is known and $\gamma(\mathbf{s}_i - \mathbf{s}_j)$ is independent of the location
- We use the shorthand notation $Z_i = Z(\mathbf{s}_i)$ and $\mu_i = \mu(\mathbf{s}_i)$
- We want to estimate $Z_0 = Z(\mathbf{s}_0)$ using a linear estimator:

$$Z^* = \sum_{i=1}^{n} \lambda_i Z_i + \lambda_0$$

that minimises the *mean-squared prediction error* (MSPE):

$$\mathbb{E}[(Z^* - Z_0)^2] = \mathbb{V}[Z^* - Z_0] + (\mathbb{E}[Z^* - Z_0])^2$$

Eliminating Bias

- To minimise $\mathbb{V}[Z^* - Z_0] + (\mathbb{E}[Z^* - Z_0])^2$ we first eliminate the bias term, that is, we choose:

$$\lambda_0 = \mu_0 - \sum_{i=1}^{n} \lambda_i \mu_i$$

- This gives for the estimator:

$$Z^* = \mu_0 + \sum_{i=1}^{n} \lambda_i \left(Z_i - \mu_i\right)$$

- Without loss of generality $\mu_0 = 0$

Minimising Mean Squared Prediction Error

- We expand:

$$\mathbb{V}[Z^* - Z_0] = -\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j\gamma(\mathbf{s}_i - \mathbf{s}_j) + 2\sum_{i=1}^{n}\lambda_i\gamma(\mathbf{s}_i - \mathbf{s}_0)$$

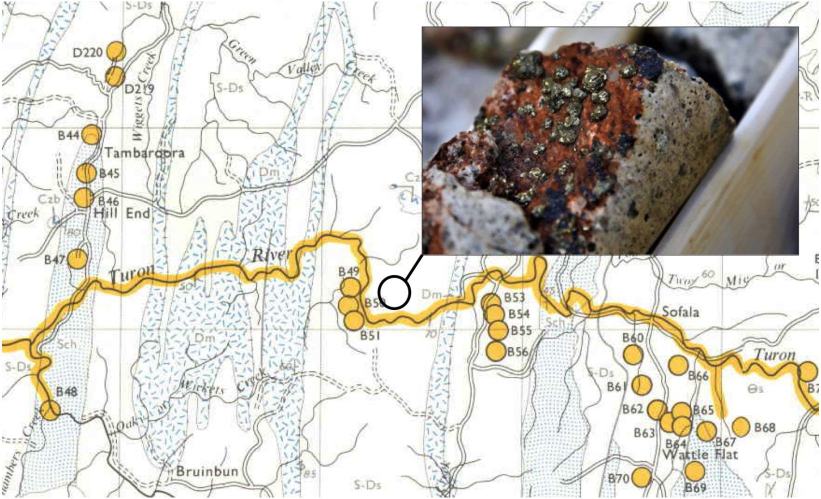
- Since we know/estimated $\gamma(\cdot)$, we can minimise the MSPE
- Taking derivatives wrt. λ_i and equating with 0 gives a system of equations, the *Simple Kriging System*:

$$\sum_{j=1}^{n}\lambda_j\gamma(\mathbf{s}_i - \mathbf{s}_j) = \gamma(\mathbf{s}_i - \mathbf{s}_0)$$

- Solution is the BLUP
- Measure of the error is given by simple kriging variance:

$$\sigma^2_{\mathrm{SK}} = \mathbb{E}[(Z^* - Z_0)^2] = C(\mathbf{0}) - \sum_{i=1}^{n}\lambda_i\gamma(\mathbf{s}_i - \mathbf{s}_0)$$

What if we don't know the mean?



Universal Kriging

- Basic idea: mean is a linear combination of 'nice' basis functions:

$$\mu(\mathbf{s}) = \sum_{\ell=0}^{L} a_\ell f^\ell(\mathbf{s}),$$

  mostly monomials in **s** of low degree
- We use the shorthand notation $f_i^\ell = f^\ell(\sim_i)$
- We again want to minimise the MSPE $\mathbb{E}[(Z^* - Z_0)^2] = \mathbb{V}[Z^* - Z_0] + (\mathbb{E}[Z^* - Z_0])^2$ using a linear predictor of the form:

$$Z^* = \sum_{i=1}^{n} \lambda_i Z_i,$$

Eliminating Bias

- Expanding the bias term we get:

$$\begin{aligned}\mathbb{E}[Z^* - Z_0] &= \sum_{i=1}^{n} \lambda_i \sum_{\ell=0}^{L} a_\ell f_i^\ell - \sum_{\ell=0}^{L} a_\ell f_0^\ell \\ &= \sum_{\ell=0}^{L} a_\ell \left(\sum_{i=1}^{n} \lambda_i f_i^\ell - f_0^\ell \right)\end{aligned}$$

- To minimise the MSPE we need to eliminate the bias, that is, we must have:

$$\sum_{i=1}^{n} \lambda_i f_i^\ell = f_0^\ell \qquad \forall \ell = 0, 1, \ldots, L,$$

called the *universal kriging conditions*

Minimising Mean Squared Prediction Error

- With these conditions in place, we expand the remaining term of the MSPE:

$$\mathbb{V}[Z^* - Z_0] = -\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i \lambda_j \gamma(\mathbf{s}_i - \mathbf{s}_j) + 2\sum_{i=1}^{n} \lambda_i \gamma(\mathbf{s}_i - \mathbf{s}_0)$$

- Our objective function now is:

$$Q = \mathbb{V}[Z^* - Z_0] + \sum_{\ell=0}^{L} a_\ell \left(\sum_{i=1}^{n} \lambda_i f_i^\ell - f_0^\ell \right)$$

where we need to estimate both, the a_ℓ and the λ_i

Minimising Mean Squared Prediction Error

- Taking partial derivatives wrt. a_ℓ and λ_i and equating to 0 gives:

$$\begin{cases} \sum_{j=1}^n \lambda_j \gamma(\mathbf{s}_i - \mathbf{s}_j) + \sum_{\ell=0}^L a_\ell f_i^\ell = \gamma(\mathbf{s}_i - \mathbf{s}_0), & i = 1, \dots n \\ \sum_{i=1}^n \lambda_i f_i^\ell = f_0^\ell, & \ell = 0, \dots L, \end{cases}$$

  the *Universal Kriging System*

- Measure of the error is given by universal kriging variance:

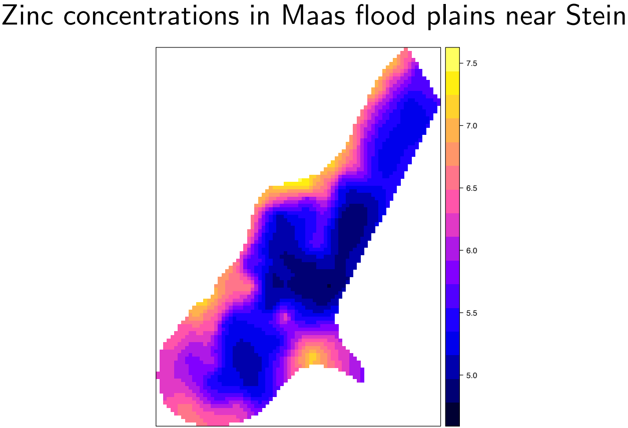
$$\sigma^2_{\mathrm{UK}} = \mathbb{E}[(Z^* - Z_0)^2] = \sum_{i=1}^n \lambda_i \gamma(\mathbf{s}_i - \mathbf{s}_0) + \sum_{\ell=0}^L a_\ell f_0^\ell$$

Misspecification of the Variogram

- Effect on kriging estimates is largely negligible as long as the behaviour near the origin is correct
- Effect on kriging variance can be substantial; sensitivity analysis is recommended

Predicting Zinc Concentrations

Predicting Zinc Concentrations



Thank You

More about kriging:

Waller, L.A. & Gotway, C. A. (2004). *Applied Spatial Statistics for Public Health Data*. Wiley.
Chiles, Jean-Paul & Delfiner, P. (1999). *Geostatistics: Modeling Spatial Uncertainty*. Wiley.

Kriging tutorial:

https://rpubs.com/nabilabd/134781

Image sources:

https://www.resourcesandenergy.nsw.gov.au/__data/assets/image/0007/526246/sofala-hill-end-stuart-town-1-250-000-gold-deposits-map.jpg
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