

Mapping from point observations

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- 1 Problem
- 2 Spatial Prediction
- 3 Universal model
- 4 Mapping methods
 - Stratification
 - Global methods
 - Local methods
 - Locally-adaptive methods
- 5 Choosing a mapping method

- One or more **attributes** have been measured at a set of **“point” locations** with defined **coördinates** in geographic space.
 - 0-dimensional “point” actually has some spatial extent, its **support**
 - pH, organic C etc. in soil sample from an auger: 4 cm diameter (2D) + 10 cm length (3D)
 - biomass from vegetation plot 10 x 10 m (2D)
 - temperature, precipitation, relative humidity at a weather station (“point” instrument but variable is the same over some radius)
- The coördinates could also be or include **time**.

Example set of “point” observations

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point
observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification
Global methods
Local methods
Locally-adaptive
methods

Choosing a
mapping
method

318

O. Atteia, J.-P. Dubois, R. Webster

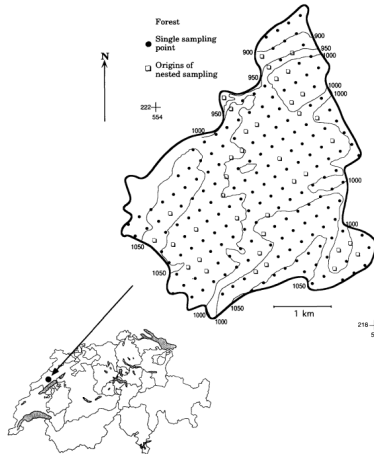
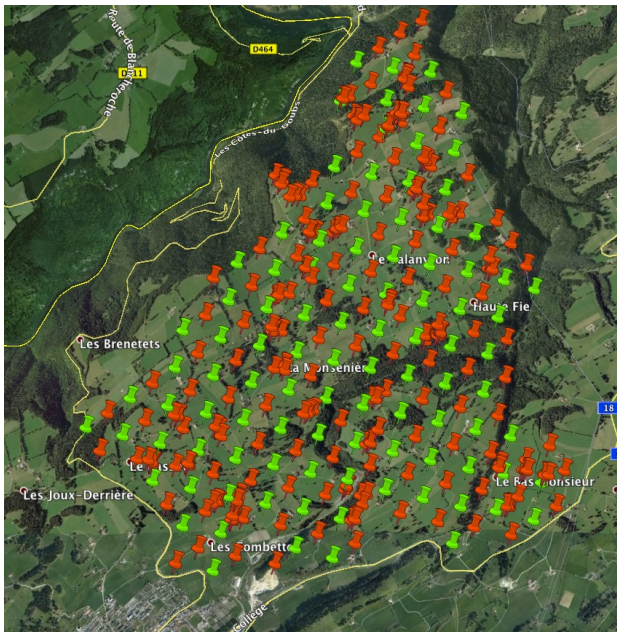


Fig. 1. Location of the region studied and of the sampling points.

Atteia, O., Dubois, J. P., & Webster, R. (1994). Geostatistical analysis of **soil contamination** in the Swiss Jura. *Environmental Pollution*, 86(3), 315–327.
[https://doi.org/10.1016/0269-7491\(94\)90172-4](https://doi.org/10.1016/0269-7491(94)90172-4)



Observed values of an attribute at “points”

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observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification

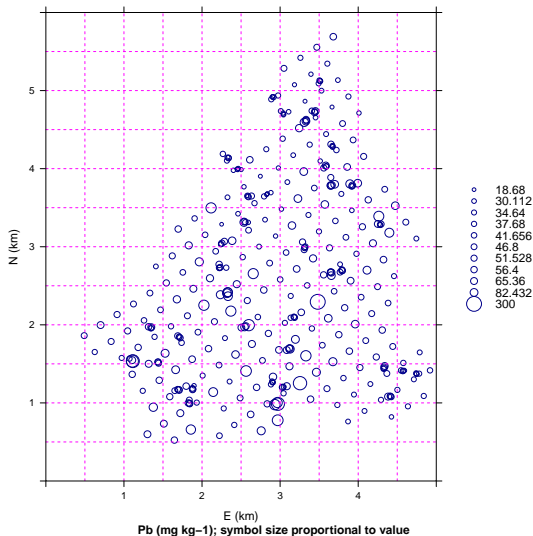
Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method

Soil samples, Swiss Jura



Support: 5 cm diameter tube, 0-25 cm depth

Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method

- The value of the attributes at **other** (unvisited) “point” locations, either ...
 - with the same **support** as the original observations, or ...
 - ...with some other support, usually larger (“block”)
- This requires **spatial prediction** based on the observed “point” observations

What is the value at this “point”?

Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification
Global methods
Local methods
Locally-adaptive
methods

Choosing a
mapping
method



With the same support as the observations.

What is the value over this block?

Mapping from
point
observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification
Global methods
Local methods
Locally-adaptive
methods

Choosing a
mapping
method



Mean, maximum, standard deviation ...

- The values of the attributes over a **grid** of other “point” locations → a **map** of the attributes
 - predict at **point** support at centre of grid, or ...
 - ... predict as **grid** support, i.e., average over the grid cell, or ...
 - ... predict as a **continous surface** which can be queried at any location
- Again, **spatial prediction** based on the observed “point” observations

“Point” predictions at centres of $(50m)^2$ grid cells

Problem

Spatial Prediction

Universal model

Mapping methods

Stratification

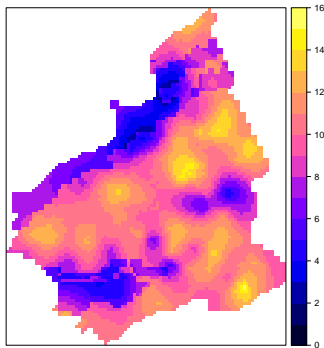
Global methods

Local methods

Locally-adaptive
methods

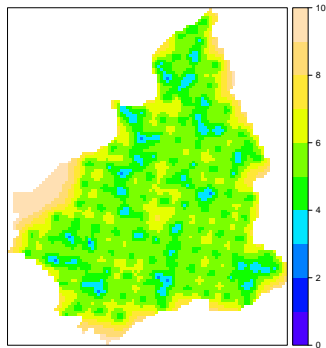
Choosing a mapping method

KED predictions



Co (ppm)

KED prediction variances



Co (ppm^2)

This prediction method also provides a **prediction variance** (uncertainty measure)

Discrete vs. Continuous predictions

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point
observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method

- **Points:** prediction at single locations (with some support)
 - **discrete**; can be any set of points, also on a regular **grid**
 - identified by coördinates in as many dimensions as the object (can be in space, time or both)
- **Surfaces:** conceptually, a **continuous, smooth** prediction; can be examined anywhere
 - often presented as a regular grid, but must be able to compute at any location given by coördinates
 - 1-D: lines, 2-D: surfaces; 3-D volumes or 2-D+time, 3-D+time

- Two objectives: (1) practical and (2) scientific
- **Objective 1** (*practical*): Given a set of **attribute values** at **known points**, **predict** the value of that attribute:
 - at other “points”,
 - over a block (area),
 - or over a surface.
 - Preferably with the **uncertainty** of the prediction.
- **Objective 2** (*scientific*): **Understand** why the attribute has its spatial distribution.
- These may require different methods

Modelling A **conceptual** and **statistical** representation of the **geographic distribution of the observations**

- **conceptual**: what geographic factors determine the geographic distribution?
- **statistical**: how are these represented in computation?

Mapping Using the statistical model to **predict** at unknown locations, typically regular-spaced across the study area

A taxonomy of spatial prediction methods

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observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method

Strata: divide area to be mapped into ‘homogeneous’ **strata**; predict **within each stratum** from all observations in that stratum.

Global: (or “regional”) predictors: use **all observations** to build a model that allows to predict at **all points** or over a surface.

Local: predictors: use only ‘**nearby**’ observations to predict at each point.

Mixed: predictors: some of structure is explained by strata or globally, the **residuals** from this are explained **locally**

These are discussed in detail, below.

Universal model of spatial variation

Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method

$$Z(\mathbf{s}) = Z^*(\mathbf{s}) + \varepsilon(\mathbf{s}) + \varepsilon'(\mathbf{s}) \quad (1)$$

\mathbf{s} a location in space, designated by a **vector** of coördinates(1D, 2D, 3D)

$Z(\mathbf{s})$ **true** (unknown) value of some property at the location

$Z^*(\mathbf{s})$ **deterministic** component, due to a **non-stochastic** process

$\varepsilon(\mathbf{s})$ **spatially-autocorrelated stochastic** component

$\varepsilon'(\mathbf{s})$ pure (“white”) **noise**, no structure

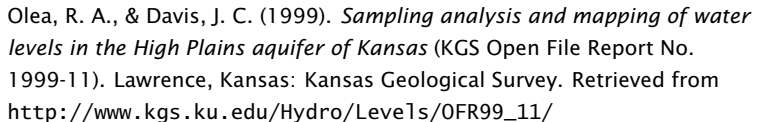
These components each require a **model**

adapted from: Matheron, G. (1969). Le krigeage universel. École nationale supérieure des mines de Paris; Cahiers du Centre de morphologie mathématique de Fontainebleau, fasc. 1.

- “Auto” = “self”, i.e., an attribute correlated to itself
- “Spatial”: the correlation depends on the **spatial relation** between points.
- Key idea: observations have a relation in both **geographic** and **feature** (attribute) spaces.
- Can be applied to an attribute (observation) $Z(\mathbf{s})$ or the **residuals** $\varepsilon(\mathbf{s})$ from some deterministic model

- **attribute to map**: elevation above sea level of the top of an aquifer in Kansas (USA)
- **observed** at a large number of wells (“points”)
- Q: What determines the spatial variation? (the **physical process**)
- Q: How can we **model** this from the observations? (using the **universal model** of spatial variation)
- Q: How can we **map** over a regular grid covering the region, using the model?

MEASURED OBSERVATION WELLS IN THE HIGH PLAINS AQUIFER, JANUARY 1999



Observation wells

Problem

Spatial
Prediction

Universal
model

Mapping
methods

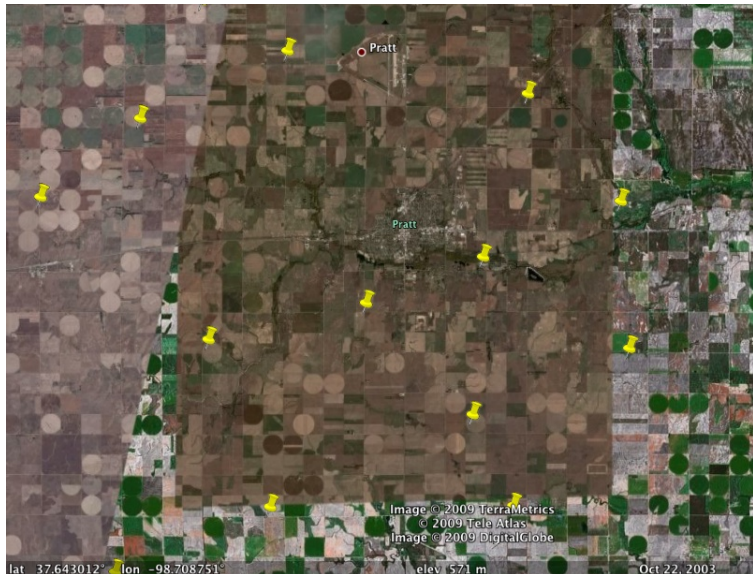
Stratification

Global methods

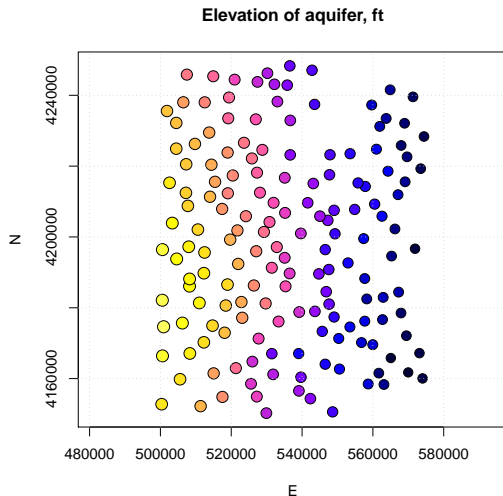
Local methods

Locally-adaptive
methods

Choosing a
mapping
method

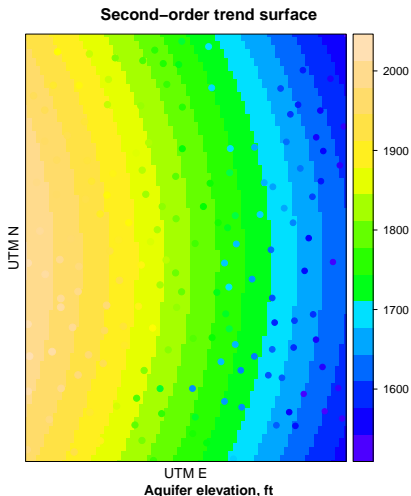


A study area



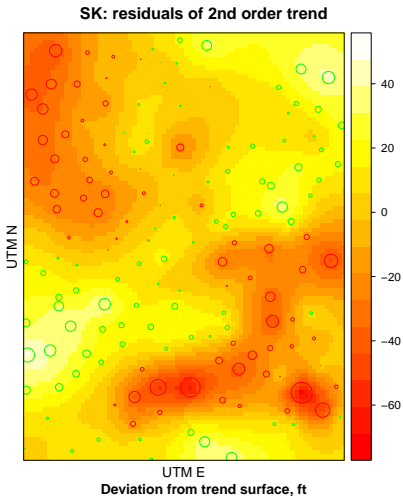
Model these observations $Z(\mathbf{s})$ by $Z^*(\mathbf{s})$, $\varepsilon(\mathbf{s})$, and $\varepsilon'(\mathbf{s})$?

A deterministic trend:



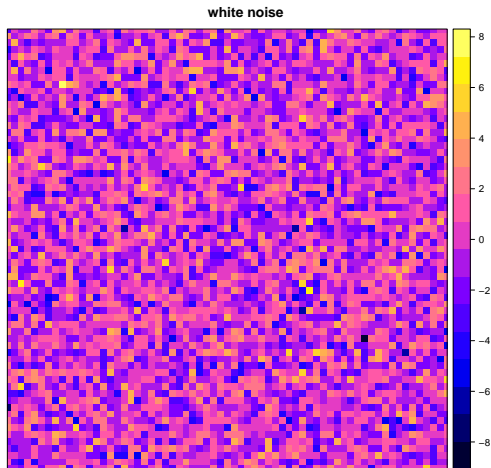
process: dipping and slightly deformed sandstone rock: $Z^*(\mathbf{s})$
modelled with a 2nd-order polynomial **trend surface**

A spatially-correlated random field



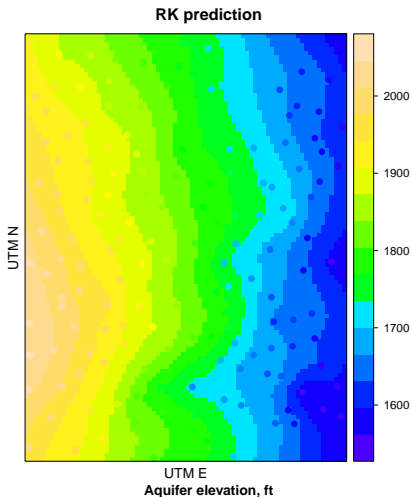
process: local variations from trend: $\varepsilon(\mathbf{s})$ (**model residuals**)
modelled by **variogram modelling** of the random field and
simple **kriging**

White noise: we do not know! but **assume** it looks like this:



quantified as **uncertainty** of the other fits

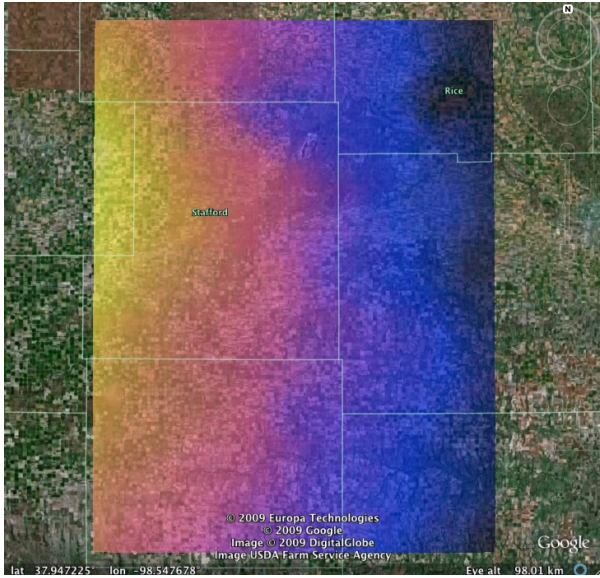
Model with both trend and local variations



$$Z^*(\mathbf{s}) + \varepsilon(\mathbf{s}); \text{ prediction uncertainty } \varepsilon'(\mathbf{s})$$

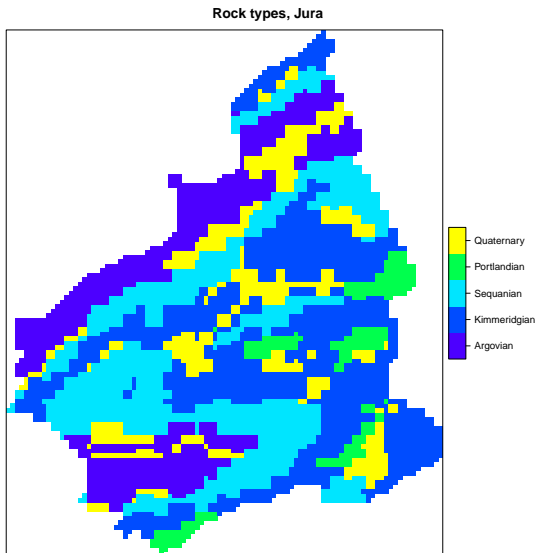
Predictions shown on the landscape

- Problem
- Spatial Prediction
- Universal model
- Mapping methods
 - Stratification
 - Global methods
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 - Locally-adaptive methods
- Choosing a mapping method



This models only $Z^*(\mathbf{s}) + \varepsilon'(\mathbf{s})$

- Divide the prediction area into **strata** based on objectives or pre-defined, e.g., political divisions
 - The stratum defines the deterministic $Z^*(\mathbf{s})$, each location \mathbf{s} is in exactly one stratum
- Divide the point set, each point into its stratum
- Compute appropriate statistics per-stratum based on its points, e.g., mean, total, standard deviation . . .
 - The s.d. is one measure of $\varepsilon'(\mathbf{s})$
- Present as a polygon map



Problem

Spatial

Prediction

Universal
model

Mapping
methods

Stratification

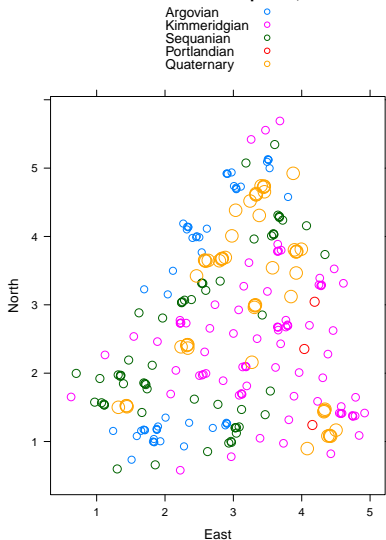
Global methods

Local methods

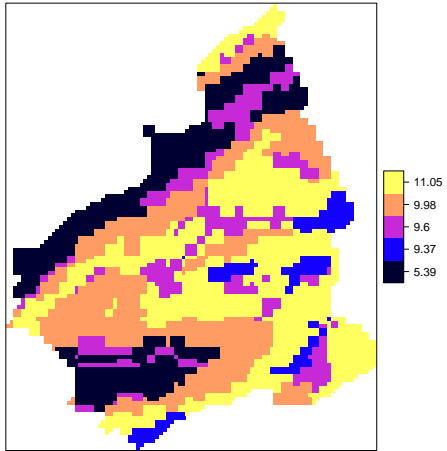
Locally-adaptive
methods

Choosing a
mapping
method

Co concentration in topsoils, Jura



Predicted Co concentration in topsoils, Jura



Can compute standard errors from the linear model (one-way ANOVA).

These model only $Z^*(\mathbf{s}) + \varepsilon'(\mathbf{s})$

- **Trend surface:** one equation (linear model) using the coördinates of all the observations as predictors
 - The model can be used to map because the coördinates are also known at each prediction location
- **Multiple regression from covariates** one equation (linear model) using the attribute values of **environmental covariates** as predictors
 - These must be known at each prediction location, so covariate maps must cover the prediction area
- **Data-driven:** machine learning, e.g., random forests, using the attribute values of **environmental covariates** and/or coördinates as predictors

These model only $\varepsilon(\mathbf{s}) + \varepsilon'(\mathbf{s})$

- **model-based** (“geostatistical”) local interpolation, e.g., Ordinary Kriging
 - requires a **model** of local spatial correlation
- ***ad-hoc*** local interpolation, e.g., inverse distance
 - Note: **no theory**, just intuition
- **closest point**: Thiessen polygons

Prediction by Ordinary Kriging – at points

Mapping from
point
observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

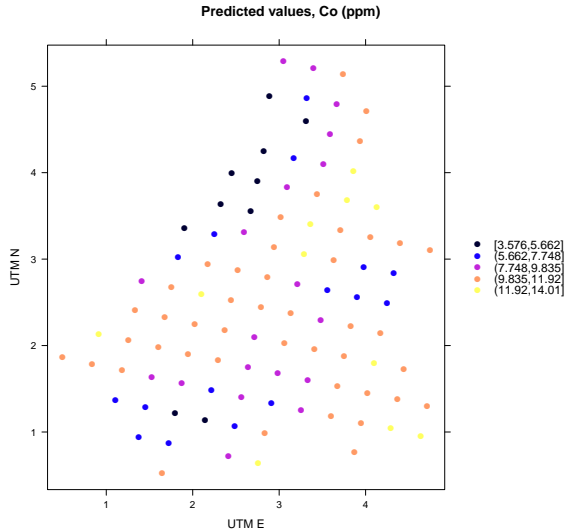
Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method



Prediction variances by Ordinary Kriging – at points

Problem

Spatial
Prediction

Universal
model

Mapping
methods

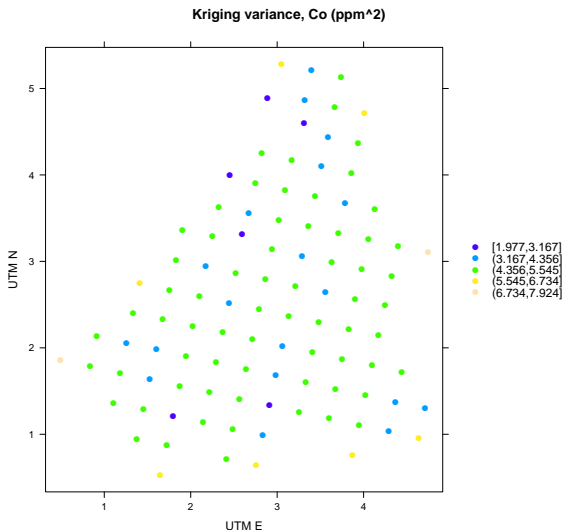
Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method



Prediction by Ordinary Kriging – at grid centres

Problem

Spatial
Prediction

Universal
model

Mapping
methods

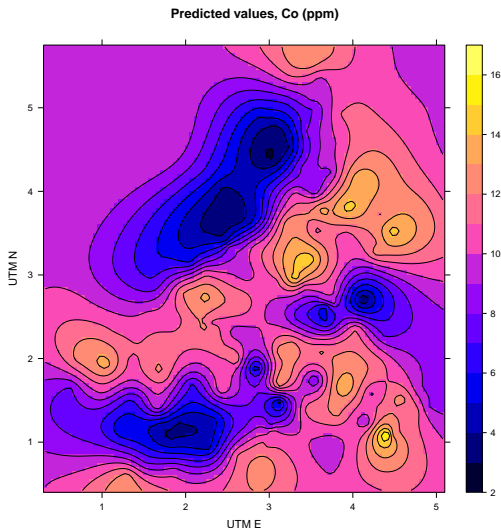
Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method



Contours calculated after surface, for visualization

Prediction variances by Ordinary Kriging – at grid centres

Problem

Spatial
Prediction

Universal
model

Mapping
methods

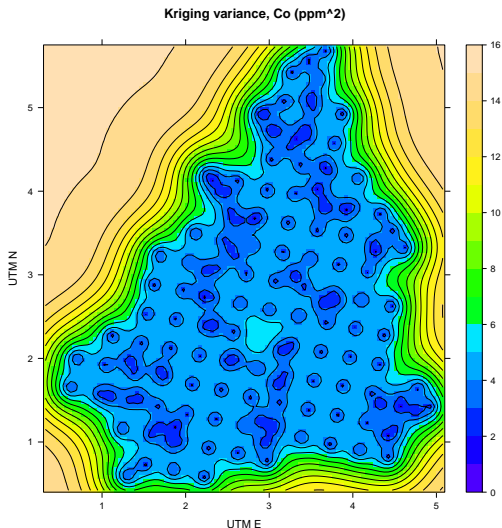
Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method



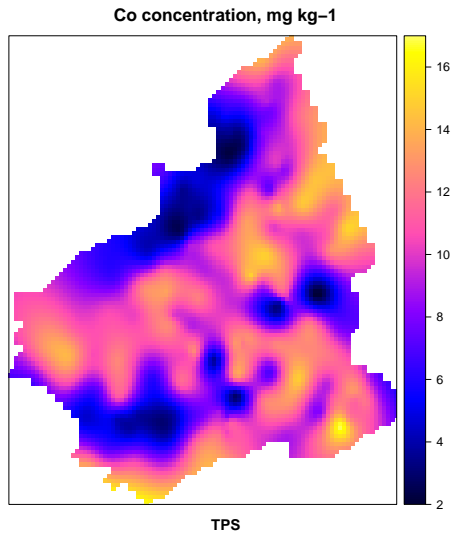
Mapping methods – locally-adaptive methods

These model only $Z^*(\mathbf{s}) + \varepsilon'(\mathbf{s})$ but use **locally-adaptive** functions for $Z^*(\mathbf{s})$

- **Thin-plate splines** (“minimum curvature”) warped surfaces (local fitting of a trend surface)
- **Geographically-weighted regression** (GWR): multiple regression from covariates, with locally-adapted coefficients
- **Generalized additive models** (GAM): like multivariate regression, but allow smooth functions of covariates as predictors

Prediction by thin plate splines – continuous surface

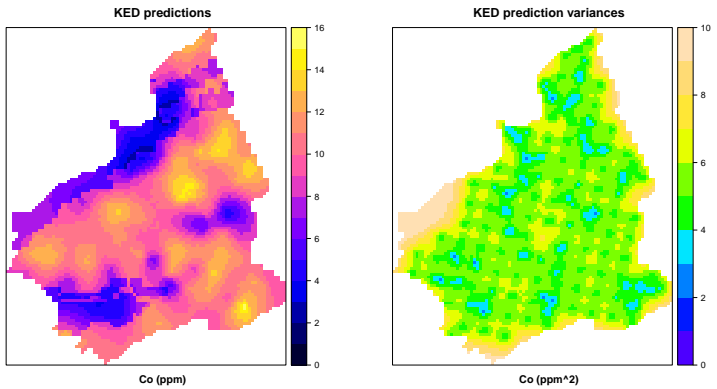
- Problem
- Spatial Prediction
- Universal model
- Mapping methods
 - Stratification
 - Global methods
 - Local methods
 - Locally-adaptive methods
- Choosing a mapping method



These model $Z^*(\mathbf{s}) + \varepsilon'(\mathbf{s})$ first and then $\varepsilon(\mathbf{s}) + \varepsilon'(\mathbf{s})$ from the **residuals** of the global model

- **Regression Kriging** (RK) with any of the global predictors for $Z^*(\mathbf{s})$
- **Kriging with External Drift** (KED), one-step method of RK
- **Stratified Kriging** (StK): separate geostatistical model per stratum

Prediction by Kriging with External Drift, rock type as covariate



The pattern of rock types is modified by kriging the residuals from the linear model.

- Is **prediction** or **understanding** more important?
 - if **prediction**, may favour machine-learning or locally-adaptive methods
 - if **understanding**, may favour explicit models (local, global or mixed)
- What do you know or suspect about the spatial variability of the target attribute?
 - e.g., should there be local spatial dependence?
 - e.g., do we suspect a regional trend? of what form?
 - e.g., are there covariates related to the target variable? do we have maps of these?
- For prediction, try various methods and compare **evaluation statistics**

Which prediction method is “best”?

Mapping from
point
observations

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Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification
Global methods
Local methods
Locally-adaptive
methods

Choosing a
mapping
method

- There is **no theoretical answer**.
- It depends on how well the approach models the ‘**true**’ **spatial structure**, which is unknown (but we may have **prior evidence**).
- The method should correspond with what we know about the **process** that created the spatial structure.
 - e.g., relation with environmental covariates or stratifying factor
- It should also be achievable with the **available data**.
 - e.g., for OK need “closely-”spaced observations, closer than the range of spatial dependence, to take advantage of local spatial structure $\varepsilon(\mathbf{s})$
 - e.g., for RF or MLR need observations covering the feature-space range

(continued . . .)

Which prediction method is “best”?

(continued)

Problem

Spatial
Prediction

Universal
model

Mapping
methods

Stratification

Global methods

Local methods

Locally-adaptive
methods

Choosing a
mapping
method

- Check against an independent **evaluation** (“validation”) dataset
 - **Mean squared error** (“precision”) of **prediction** vs. **actual** (residuals)
 - **Bias** (“accuracy”) of predicted vs. actual mean
- External vs. internal evaluation
 - With **large** datasets, model with one part and hold out the rest for **validation**
 - For **small** datasets use **cross-validation**
- How well it reproduces the **spatial variability** (pattern) of the calibration dataset
 - Difficult statistical problem

