POLITECNICO MILANO 1863

International Statistical Institute

Palacký University Olomouc

Spatial statistics for distributional observations

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1. **Spatial statistics for density data**
    - 1.1. Premiss: spatial statistics for object data
    - 1.2. Spatial statistics in Bayes spaces
    - 1.3. Case Studies

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1. **Spatial statistics for density data**
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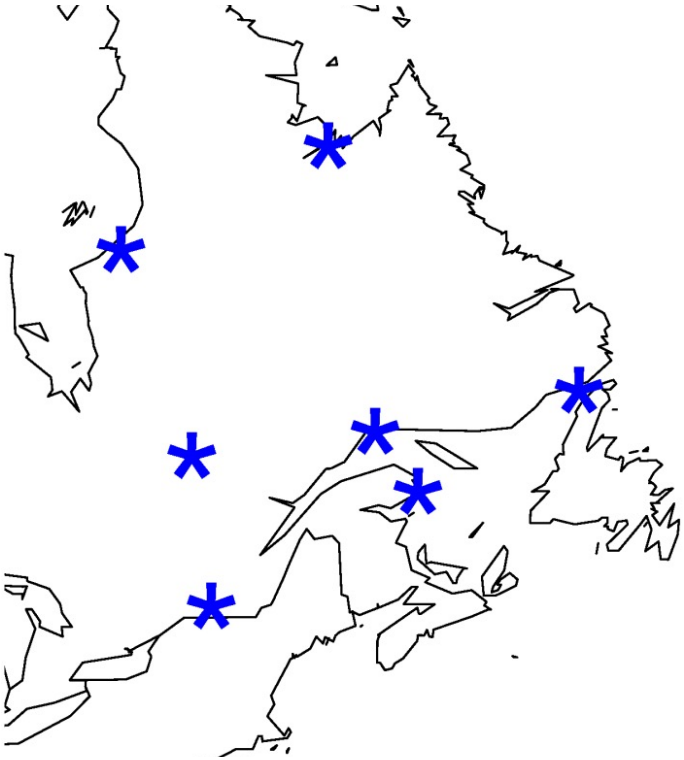
Premiss: object data with spatial dependence

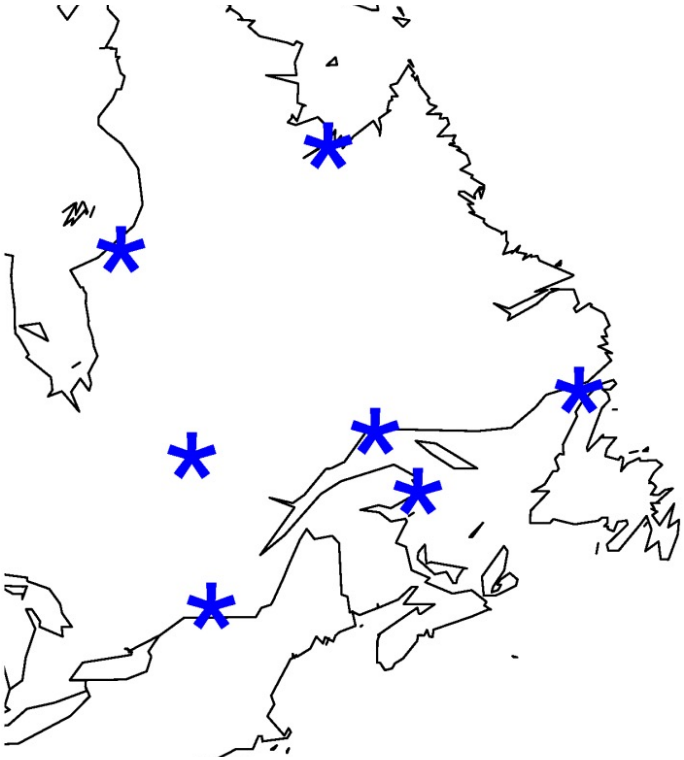
Spatially dependent data



Spatial location of meteorological stations in Quebec (Canada)

Premiss: object data with spatial dependence

Spatially dependent functional data



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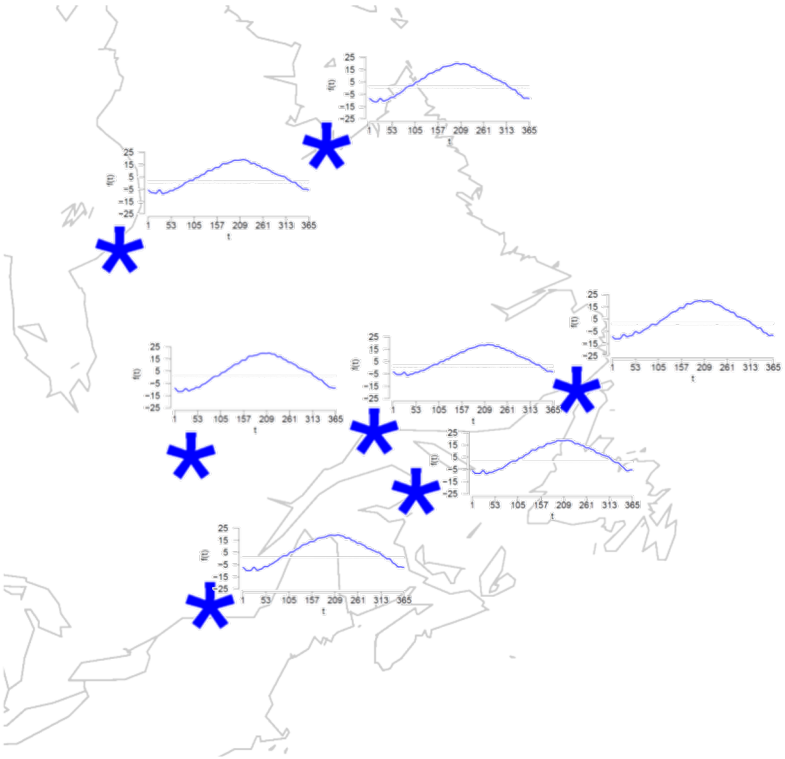
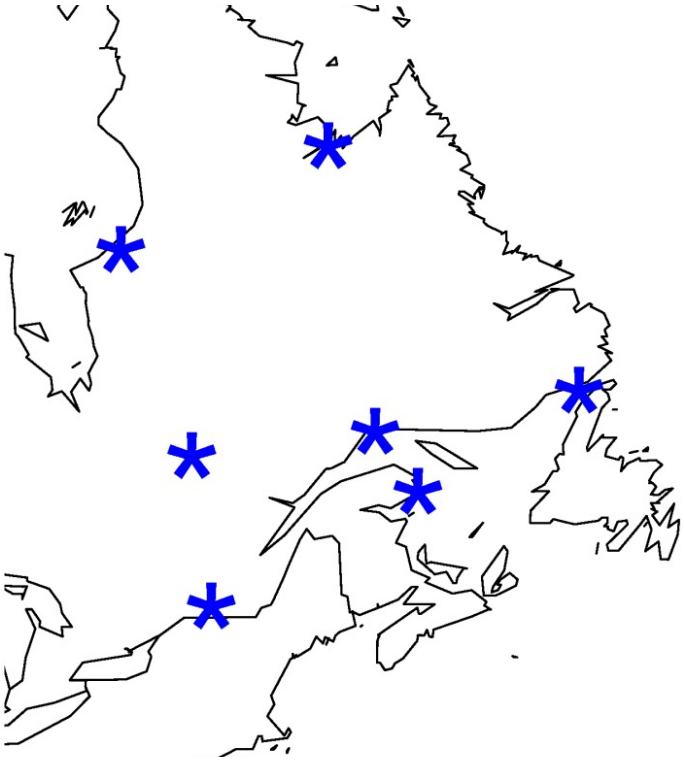


Daily mean temperatures along one year

Premiss: object data with spatial dependence

Spatially dependent constrained functional data



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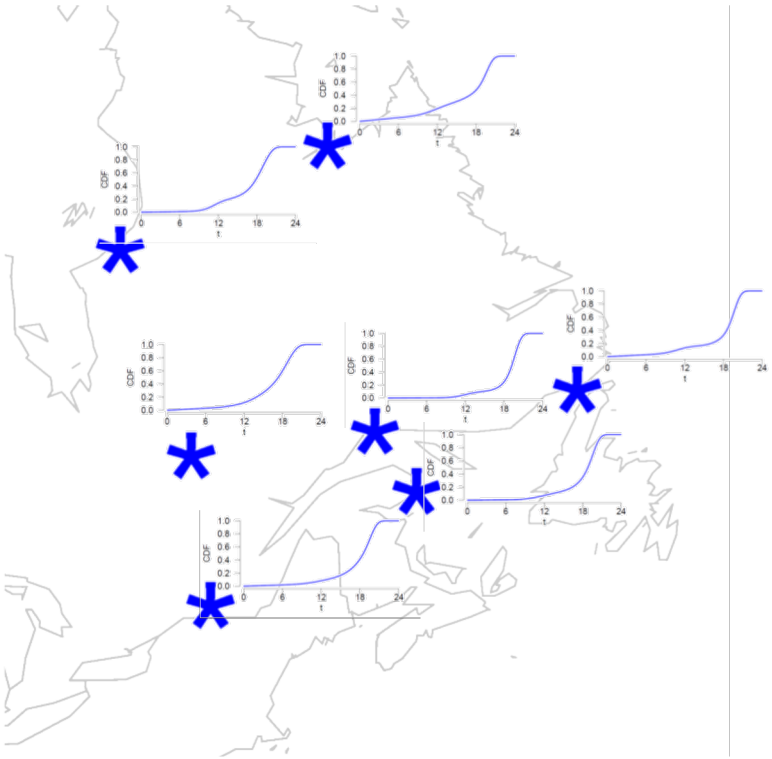
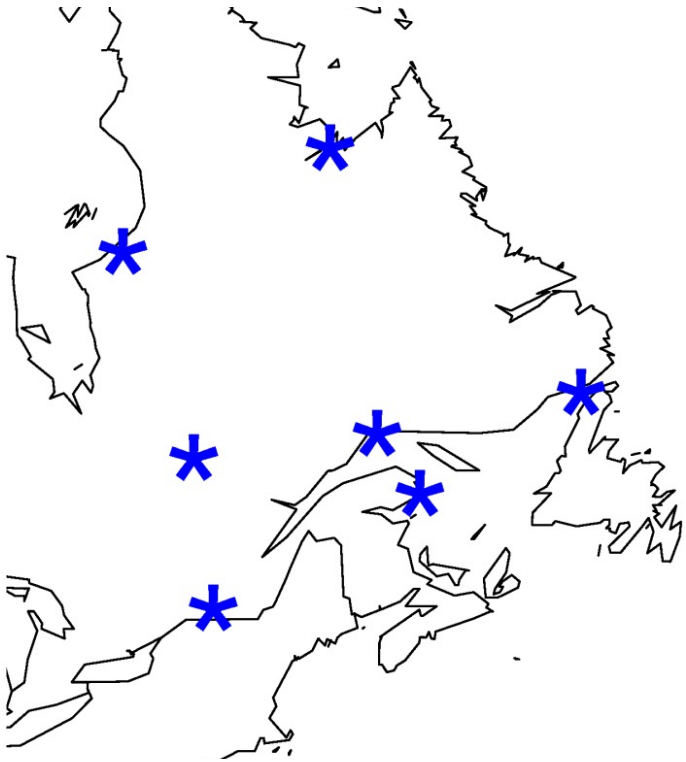


SCS precipitation distributions

Premiss: object data with spatial dependence

Spatially dependent manifold data



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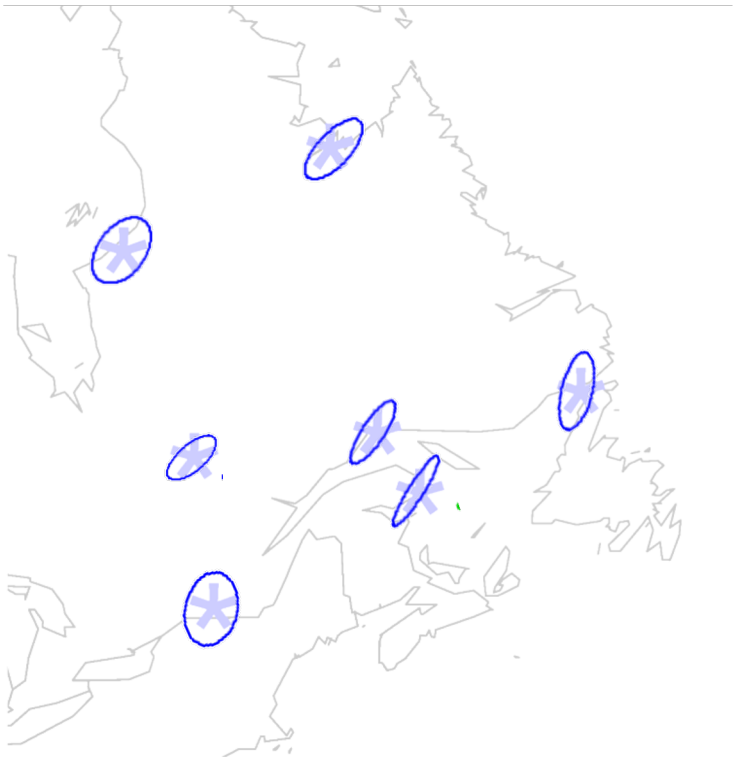
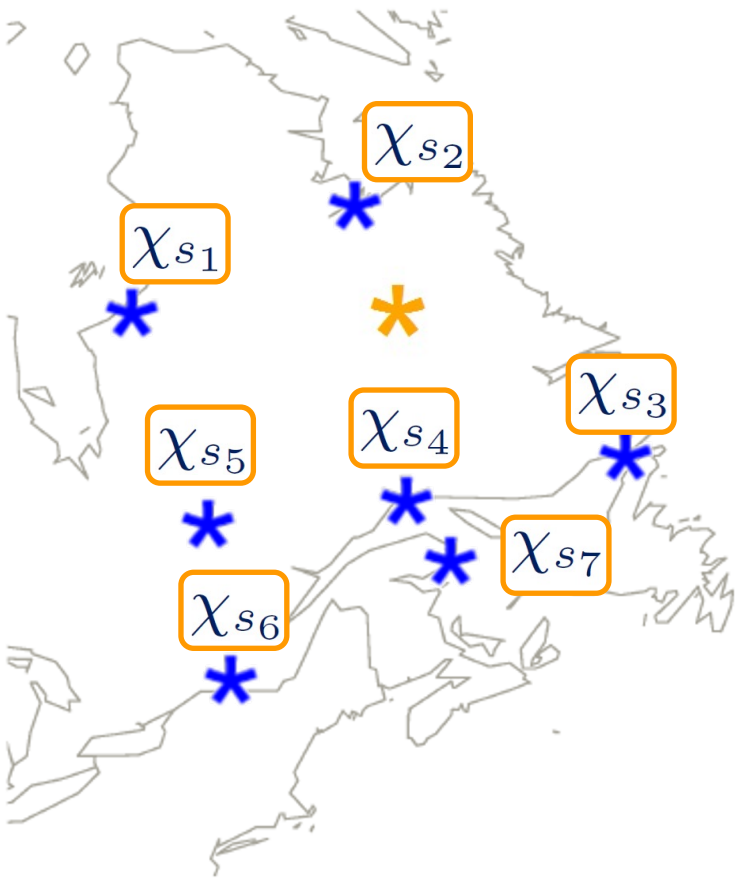


S=Cov(Temperature, Precipitation) covariance matrices in January

Geostatistics for Object data

Spatially dependent object data



Aim:

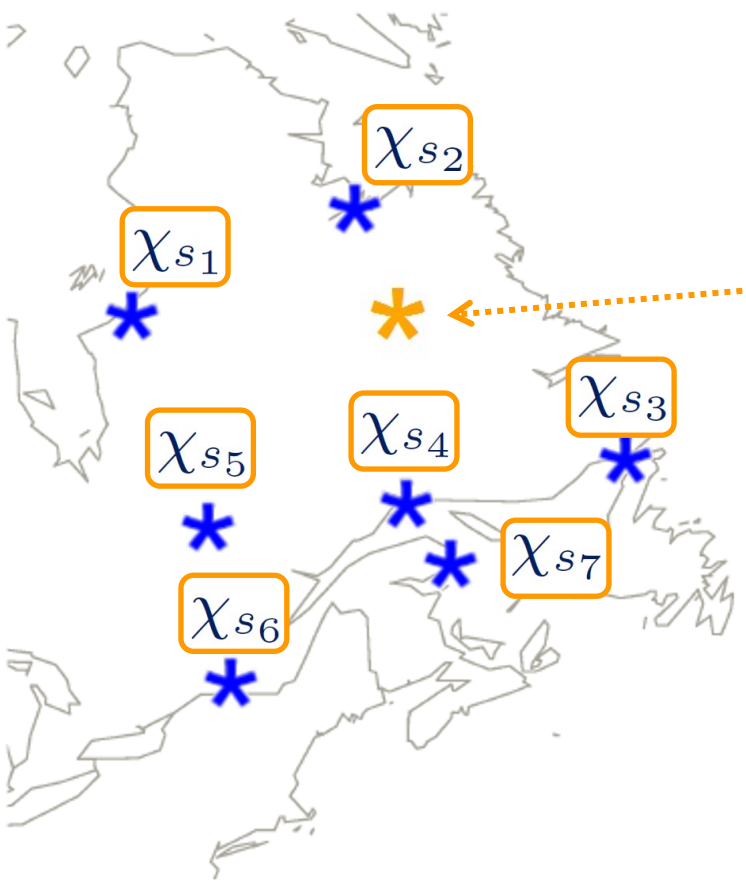
1) Estimate the **structure of spatial dependence**

First Law of Geography
"*Everything is related to everything else, but near things are more related than distant things.*"

Waldo Tobler (1970)

Geostatistics for Object data

Spatially dependent object data



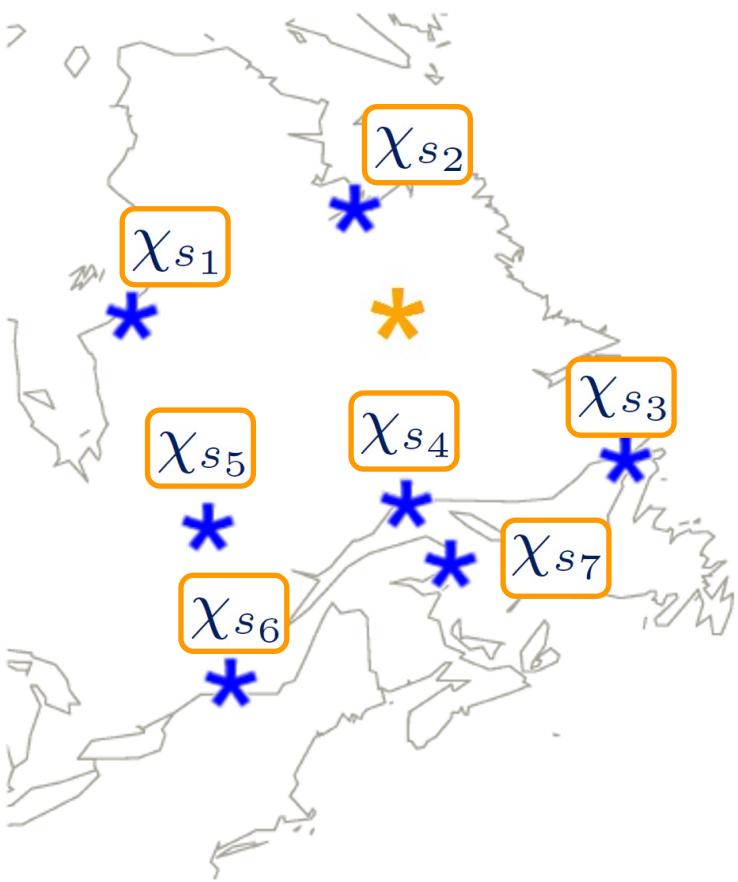
Aim:

1) Estimate the **structure of spatial dependence**

2) **Prediction** of an observation at an unsampled location s_0

Geostatistics for Object data

Spatially dependent object data



Aim:

1) Estimate the **structure of spatial dependence**
2) **Prediction** of an observation at an unsampled location
3) Uncertainty quantification

Geostatistics for Object data

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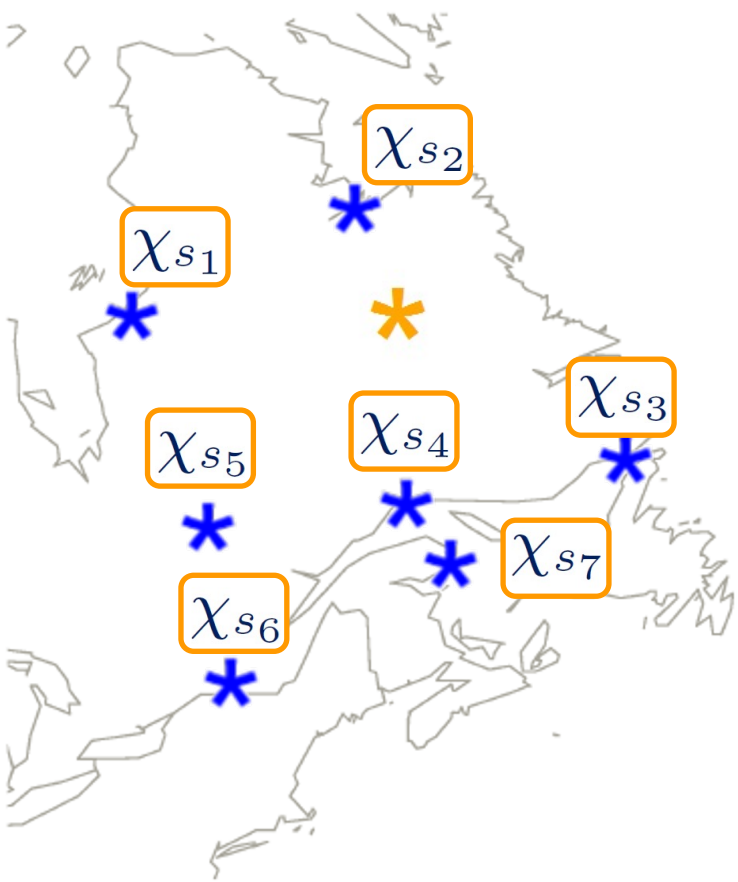


Aim:

1) Estimate the **structure of spatial dependence**
2) **Prediction** of an observation at an unsampled location
3) Uncertainty quantification

Methods: Object Oriented Geostatistics

a) **Object-oriented** approach:

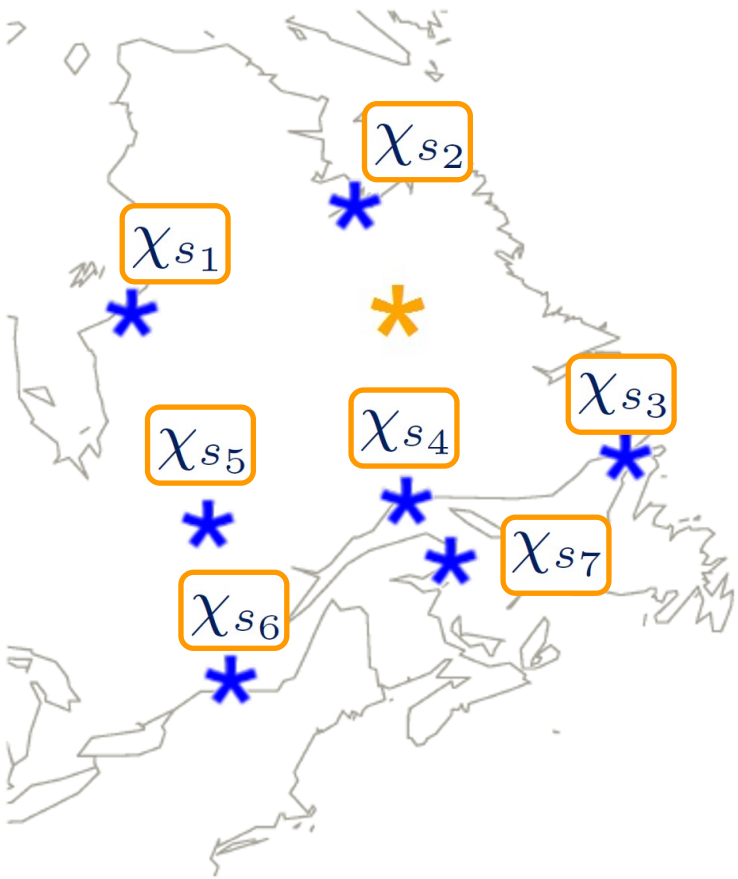
$$\chi_{s_1}, \ldots, \chi_{s_n} \in H$$

Space *H* should capture the **"appropriate geometry"** for the data objects (e.g., a Hilbert space)

b) **Geostatistical** approach (**kriging**) to treat the **spatial dependence**

Geostatistics for Object data

Spatially dependent object data



In this lecture:
spatial statistics for object data in Bayes spaces (i.e., density data)

Topics covered:

- Modelling spatial density data
- Estimate the spatial dependence
- Make (spatial) prediction

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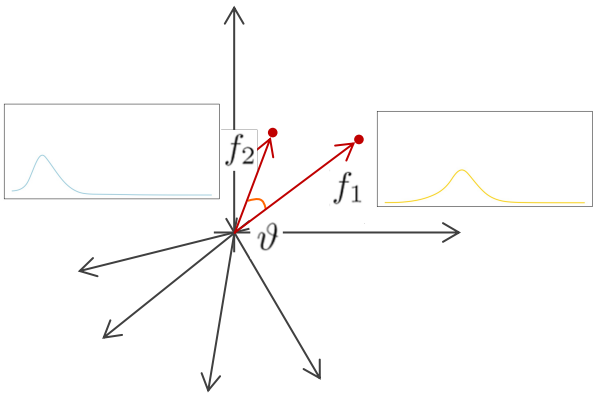
A Hilbert-space approach to the analysis of spatial data

Main idea:
The data objects are considered as points within a Hilbert space

Hilbert space *H*



Space whose points are objects of any dimension
(e.g., functions)

- Sum: $f_1 \oplus f_2$
- Product by a constant: $c \odot f$

Operations ($\oplus$,$\odot$)

- Norm: $\|f\|$
- Distance: $\|f_1 \ominus f_2\|$
- Angle: $\vartheta = \arccos \frac{\langle f_1, f_2 \rangle}{\|f_1\| \|f_2\|}$

Inner product $\langle f_1, f_2 \rangle$

A Hilbert-space approach to the analysis of spatial data

Main idea:
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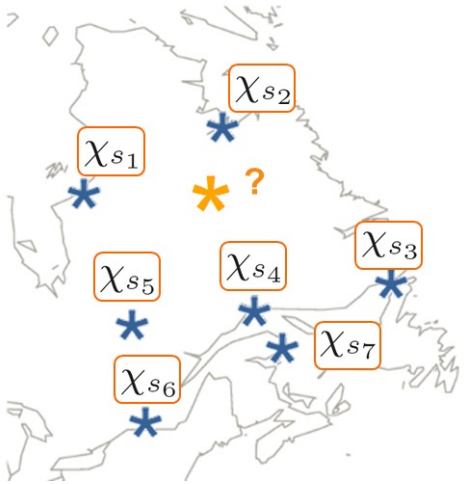
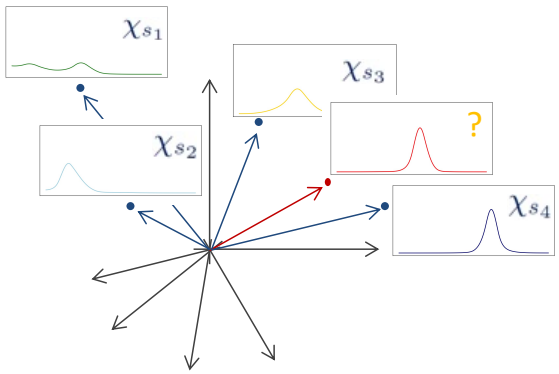
Strategy

Spatially dependent object data



Points of a Hilbert space



Geometry of the space

- Measure the **spatial dependence**: *similarities* between objects (distances)
- **Prediction** at unsampled locations through *linear combinations* of the data

A Hilbert-space approach to the analysis of spatial data

Classical Geostatistics framework

- $\{\chi_s : s \in D\}$: stochastic process indexed by a **continuous spatial variable** $s \in D \subset \mathbb{R}^d$
- $\chi_{s_1}, \ldots, \chi_{s_n}$: **observations** of the process in *n* **sampled locations**

Object-Oriented approach

- $\overline{\chi_s}$: random element of an **infinite-dimensional** separable Hilbert space *H* $(\oplus, \odot, \langle\cdot,\cdot\rangle, \|\cdot\|)$
- $\chi_{s_1}, \ldots, \chi_{s_n}$: set of **object data**

Menafoglio, Secchi, Dalla Rosa (2013)

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Strategy:

Extend classical geostatistics methods (e.g., variogram modeling, kriging) to object data, by analogy with the classical case, using the geometry of *H*

Menafoglio, Secchi, Dalla Rosa (2013)

A Hilbert-space approach to the analysis of spatial data

Menafoglio, Secchi, Dalla Rosa (2013)

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Extend classical geostatistics methods (e.g., variogram modeling, kriging) to object data, by analogy with the classical case, using the geometry of *H*

$\{\chi_s : s \in D\}$ ***real***-valued process:

- Spatial mean: $m_s = \mathbb{E}[\chi_s],$
- Covariogram: $$C(\boldsymbol{s}_i, \boldsymbol{s}_j) = \mathrm{Cov}_{\mathbb{R}}(\chi_{\boldsymbol{s}_i}, \chi_{\boldsymbol{s}_j}) = \\ = \mathbb{E}[(\chi_{\boldsymbol{s}_i} - m_{\boldsymbol{s}_i})(\chi_{\boldsymbol{s}_j} - m_{\boldsymbol{s}_j})]$$
- Variogram $$2\gamma(\boldsymbol{s}_i, \boldsymbol{s}_j) = \mathrm{Var}_{\mathbb{R}}(\chi_{\boldsymbol{s}_i} - \chi_{\boldsymbol{s}_j}) = \\ = \mathbb{E}[(\chi_{\boldsymbol{s}_i} - \chi_{\boldsymbol{s}_j})^2] - (m_{\boldsymbol{s}_i} - m_{\boldsymbol{s}_j})^2$$

A Hilbert-space approach to the analysis of spatial data

Menafoglio, Secchi, Dalla Rosa (2013)

Classical Geostatistics framework

- $\{\chi_s : s \in D\}$: stochastic process indexed by a **continuous spatial variable** $s \in D \subset \mathbb{R}^d$
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Extend classical geostatistics methods (e.g., variogram modeling, kriging) to object data, by analogy with the classical case, using the geometry of *H*

$\{\chi_s : s \in D\}$ ***Hilbert space***-valued process:

- Spatial mean (Bochner integral): $m_s = \mathbb{E}[\chi_s]$,
- **Trace**-covariogram:

$$C(\boldsymbol{s}_i, \boldsymbol{s}_j) = \mathrm{Cov}_H(\chi_{\boldsymbol{s}_i}, \chi_{\boldsymbol{s}_j}) = \\ = \mathbb{E}[\langle \chi_{\boldsymbol{s}_i} \ominus m_{\boldsymbol{s}_i}, \chi_{\boldsymbol{s}_j} \ominus m_{\boldsymbol{s}_j} \rangle]$$

- **Trace**-variogram

$$2\gamma(\boldsymbol{s}_i, \boldsymbol{s}_j) = \mathrm{Var}_H(\chi_{\boldsymbol{s}_i} \ominus \chi_{\boldsymbol{s}_j}) = \\ = \mathbb{E}[\|\chi_{\boldsymbol{s}_i} \ominus \chi_{\boldsymbol{s}_j}\|^2] - \|m_{\boldsymbol{s}_i} \ominus m_{\boldsymbol{s}_j}\|^2$$

About the parameter estimation

Menafoglio, Secchi, Dalla Rosa (2013)

Second order stationarity

Process $\{\chi_s, s \in D\}$ is second-order stationary if:

i. $\mathbb{E}[\chi_{\boldsymbol{s}}] = m$ for all $s \in D$

ii. $Cov(\chi_{s_1}, \chi_{s_2}) = C(s_1 - s_2)$ for all $s_1, s_2 \in D$

Variogram estimate (under stationarity)

Classical Geostatistics

Variogram: $2\gamma(\boldsymbol{h}) = \mathbb{E}[(\chi_{\boldsymbol{s}} - \chi_{\boldsymbol{s}+\boldsymbol{h}})^2]$

1. Empirical estimate (MoM)

$$\widehat{\gamma}(h) = \frac{1}{2N(h)} \sum_{(i,j)\in N(h)} (\chi_{\boldsymbol{s}_i} - \chi_{\boldsymbol{s}_j})^2$$

2. Fit of a parametric model (LS) e.g., spherical, matérn

Object-Oriented geostatistics

Variogram: $2\gamma(\boldsymbol{h}) = \mathbb{E}[\|\chi_{\boldsymbol{s}} \ominus \chi_{\boldsymbol{s}+\boldsymbol{h}}\|^2]$

1. Empirical estimate (MoM)*

$$\widehat{\gamma}(h) = \frac{1}{2N(h)} \sum_{(i,j)\in N(h)} \|\chi_{\boldsymbol{s}_i} \ominus \chi_{\boldsymbol{s}_j}\|^2$$

2. Fit of a parametric model (LS) e.g., spherical, matérn

(Almost) the same modeling effort as in 1D geostatistics!

About the parameter estimation

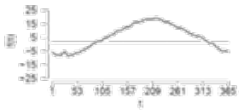
Menafoglio, Secchi, Dalla Rosa (2013)

Second order stationarity

Process $\{\chi_s, s \in D\}$ is second-order stationary if:

Key remark: data needs to be embedded in a **meaningful** Hilbert space

Data Object χ_s



...

2. Fit of a parametric model (LS) e.g., spherical, matérn

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(Almost) the same modeling effort as in 1D geostatistics!

Bayes spaces for PDF data

- If the data are densities, a miningflul Hilbert space embedding is given by the Bayes space
- In this case, all the above quantities need to be understood in terms of the Bayes operations and inner product

Bayes Hilbert space $B^2(I)$

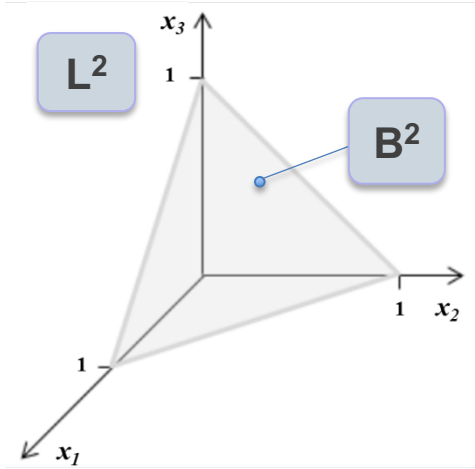
(van den Boogaart et al., 2014)

Space (of equivalence classes of) positive functions on I with square-integrable log

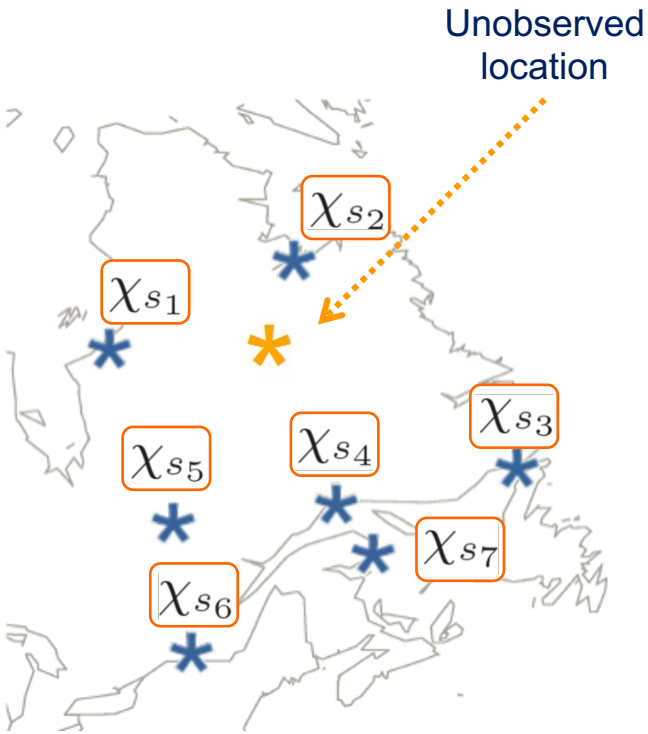
$$(f \oplus g)(t) = \frac{f(t)g(t)}{\int_I f(s)g(s)\,ds},$$

$$(\alpha \odot f)(t) = \frac{f(t)^\alpha}{\int_I f(s)^\alpha\,ds}, \quad t \in I.$$

$$\langle f, g \rangle_{\mathcal{B}} = \frac{1}{2\eta} \int_I \int_I \ln \frac{f(t)}{f(s)} \ln \frac{g(t)}{g(s)}\,dt\,ds$$



Spatial prediction: Kriging



Menafoglio, Secchi, Dalla Rosa (2013)

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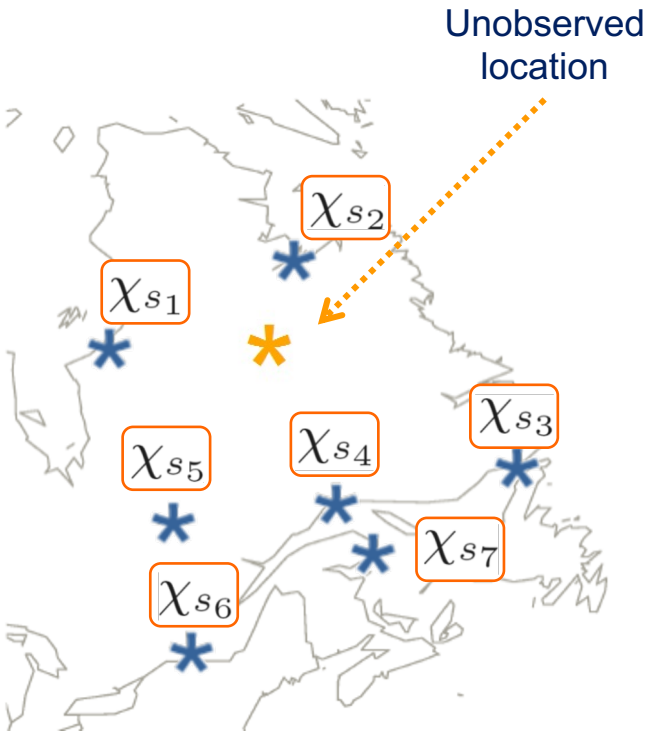
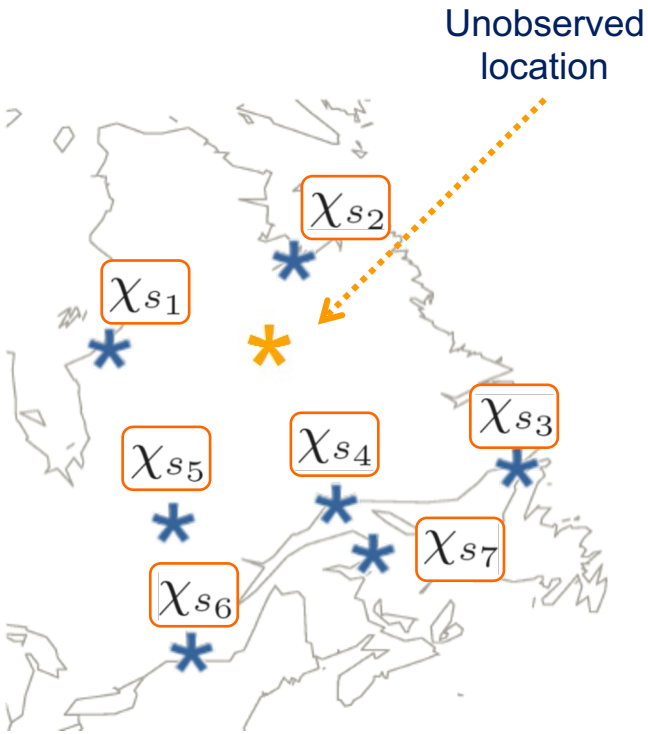


Goal: Prediction of a generic χ_{s_0} at site s_0 through the **Universal Kriging Predictor** (BLUP):

$$\chi^*_{s_0} = \bigoplus_{i=1}^{n} \lambda^*_i \odot \chi_{s_i}$$

Menafoglio, Secchi, Dalla Rosa (2013)

Spatial prediction: Kriging



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Assumptions

- $\{\chi_s : s \in D\}$ non-stationary random field of the form:

$$\chi_s = \underbrace{m_s}_{\text{deterministic drift}} \oplus \underbrace{\delta_s}_{\text{stochastic residual}}, \quad s \in D$$

- **Linear model** for the drift

$$m_s = \bigoplus_{l=0}^{L} (f_l(s) \odot a_l), \quad s \in D$$

- **Globally second-order stationary** residual (trace-variogram depending only on the increment vector between locations)

Menafoglio, Secchi, Dalla Rosa (2013)

Spatial prediction: Kriging

Goal: Prediction of a generic X_{s_0} at site s_0 through the **Universal Kriging Predictor** (BLUP):

$$X^*_{s_0} = \sum_{i=1}^{n} \lambda^*_i X_{s_i}$$

Assumptions

- $\{X_s, s \in D\}$ non-stationary random field of the form:

$$X_s = \underbrace{m_s}_{\text{deterministic drift}} + \underbrace{\boldsymbol{\delta}_s}_{\text{stochastic residual}}, \quad s \in D$$

- **Linear model** for the drift

$$m_s = \sum_{l=0}^{L} a_l \, f_l(s), \quad s \in D.$$

- **Second-order stationary** residual

Goal: Prediction of a generic $\boldsymbol{\chi}_{s_0}$ at site s_0 through the **Universal Kriging Predictor** (BLUP):

$$\boldsymbol{\chi}^*_{s_0} = \bigoplus_{i=1}^{n} \lambda^*_i \odot \boldsymbol{\chi}_{s_i}$$

Assumptions

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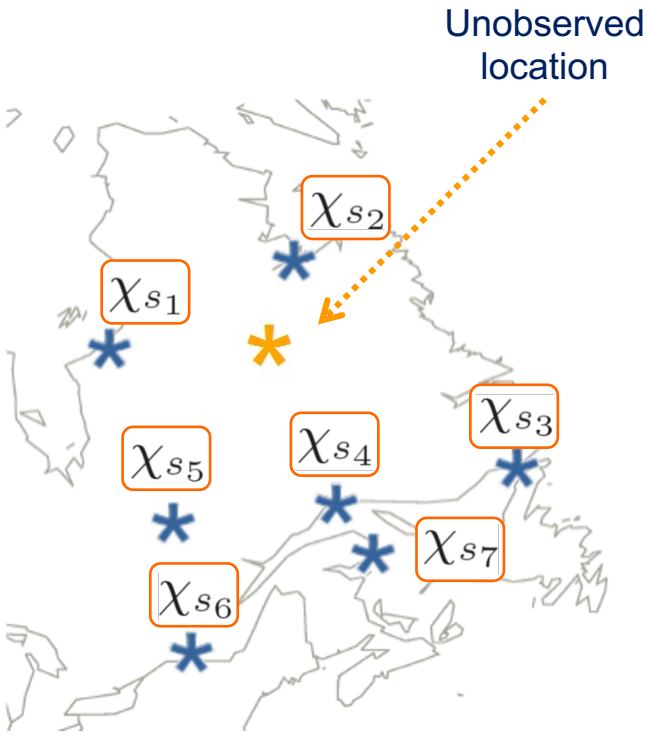
Spatial prediction: Kriging



Goal: Prediction of a generic χ_{s_0} at site s_0 through the **Universal Kriging Predictor** (BLUP):

$$\chi^*_{s_0} = \bigoplus_{i=1}^{n} \lambda^*_i \odot \chi_{s_i}$$

Formulation

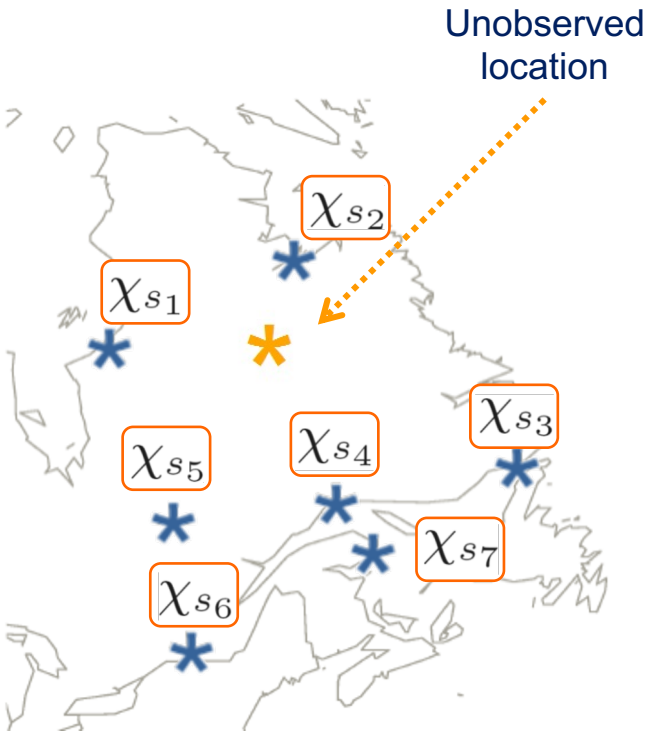
- Find $\lambda^*_1, \ldots, \lambda^*_n \in \mathbb{R}$ that solve

$$\min_{\lambda_1,\ldots,\lambda_n} \mathrm{Var}_H(\chi^*_{s_0} \ominus \chi_{s_0}),$$

$$\text{s. t.} \quad \mathbb{E}[\chi^*_{s_0} \ominus \chi_{s_0}] = 0.$$

Menafoglio, Secchi, Dalla Rosa (2013)

Spatial prediction: Kriging



Goal: Prediction of a generic $\boldsymbol{\chi}_{s_0}$ at site s_0 through the **Universal Kriging Predictor** (BLUP):

$$\boldsymbol{\chi}^*_{s_0} = \bigoplus_{i=1}^{n} \lambda^*_i \odot \boldsymbol{\chi}_{s_i}$$

Theorem

The optimal weights $\lambda^*_1, \ldots, \lambda^*_n \in \mathbb{R}$ are found by solving

$$\left(\begin{array}{c|c} \gamma(\boldsymbol{h}_{i,j}) & f_l(\boldsymbol{s}_i) \\ \hline f_l(\boldsymbol{s}_j) & 0 \end{array}\right) \left(\begin{array}{c} \lambda_i \\ \hline \zeta_l \end{array}\right) = \left(\begin{array}{c} \gamma(\boldsymbol{h}_{0,i}) \\ \hline f_l(\boldsymbol{s}_0) \end{array}\right)$$

Same as in 1D geostatistics!

Remark: the results generalizes that of Giraldo et al. (2011), Nerini et al (2008) [stationarity, H=L^2]

Menafoglio, Secchi, Dalla Rosa (2013)

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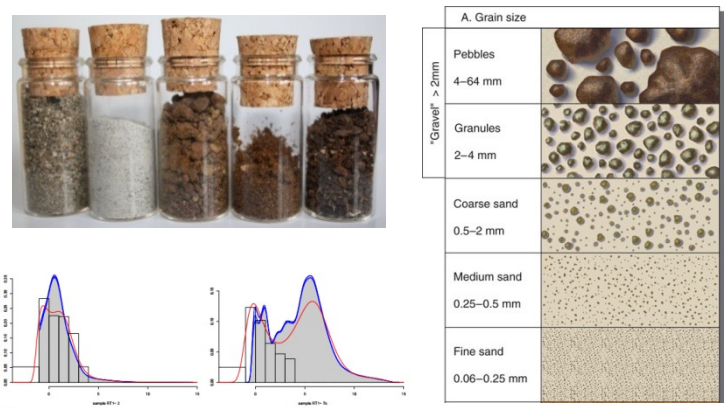
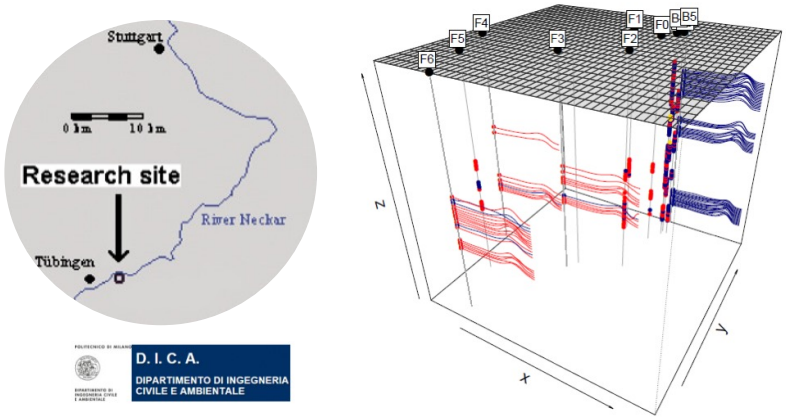
Analysis of particle-size curves in Heterogeneous Aquifers

Example: Particle-size distributions in heterogenous aquifer systems



Particle-size data



Data at the field site

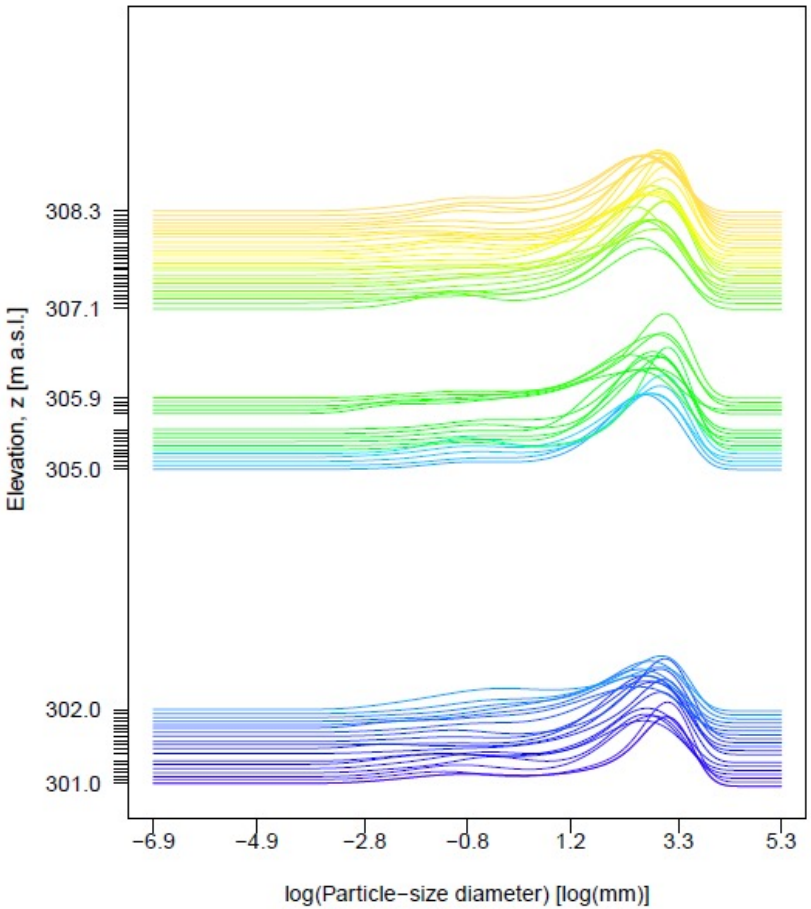
Menafoglio, Guadagnini, Secchi (SERRA, 2014, 2016; MATHGEO 2016, WRR 2016)

Analysis of particle-size curves in Heterogeneous Aquifers

A closer look to the data

- **Test site**:
  - part of an alluvial heterogeneous aquifer in the Neckar river valley (Germany)
  - we first focus on data at the borehole B5
- **The data at B5**: 60 particle-size distributions reconstructed through **grain sieve analysis** based on 12 sieve diameters
- **Idea:**
  - Model particle-size distributions as cumulative distribution functions
  - Analyze their densities (after smoothing) as **functional compositional data** through the **Bayes Hilbert geometry**

Particle-size distributions (Smoothed data)



Menafoglio, Guadagnini, Secchi (2014a,b)

Hilbert space geometry for particle-size densities

Bayes Hilbert space $B^2(I)$

(van den Boogaart et al., 2014)

Space (of equivalence classes of) positive functions on I with square-integrable log

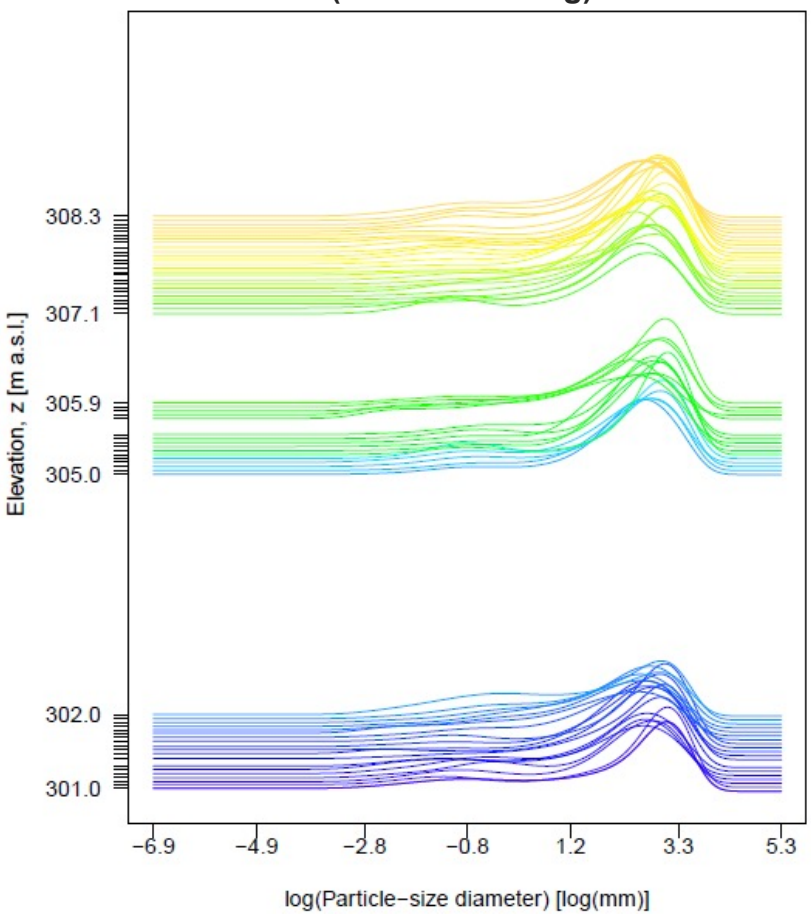
$$(f \oplus g)(t) = \frac{f(t)g(t)}{\int_I f(s)g(s)\,ds},$$

$$(\alpha \odot f)(t) = \frac{f(t)^\alpha}{\int_I f(s)^\alpha\,ds}, \quad t \in I.$$

$$\langle f, g \rangle_{\mathcal{B}} = \frac{1}{2\eta} \int_I \int_I \ln \frac{f(t)}{f(s)} \ln \frac{g(t)}{g(s)}\,dt\,ds$$

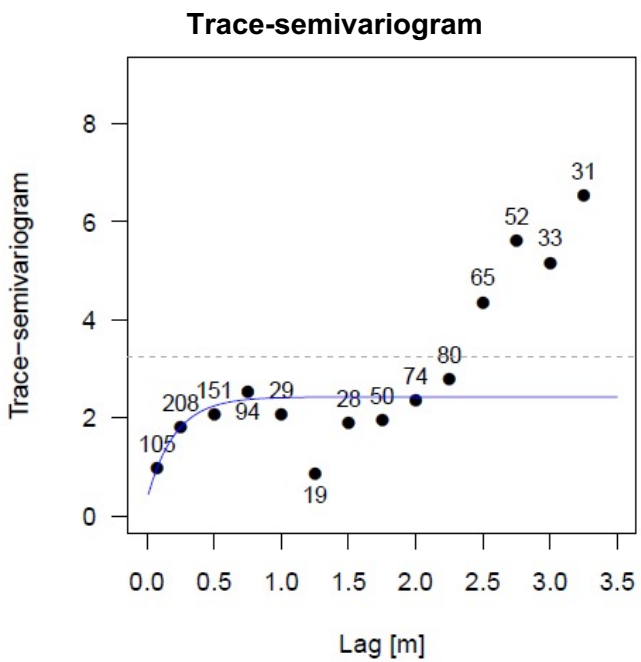
Data are embedded into the Hilbert space of functional compositions endowed with the generalized Aitchison geometry

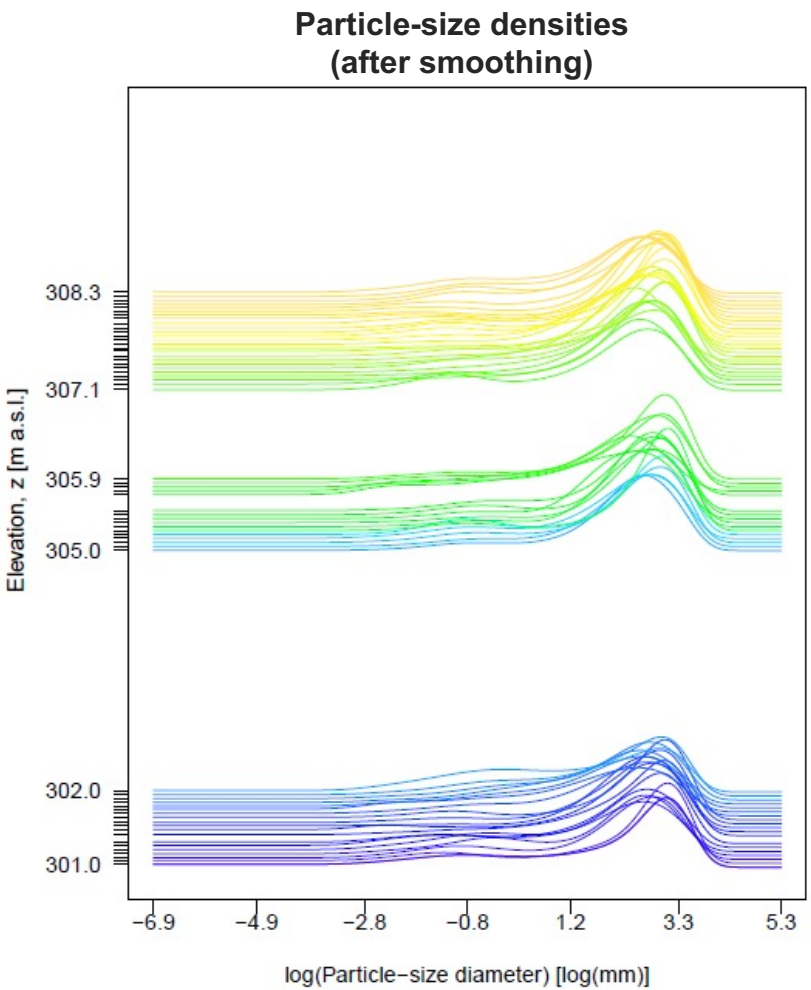
Particle-size densities (after smoothing)



Menafoglio, Guadagnini, Secchi (2014)

Hilbert space geometry for particle-size densities



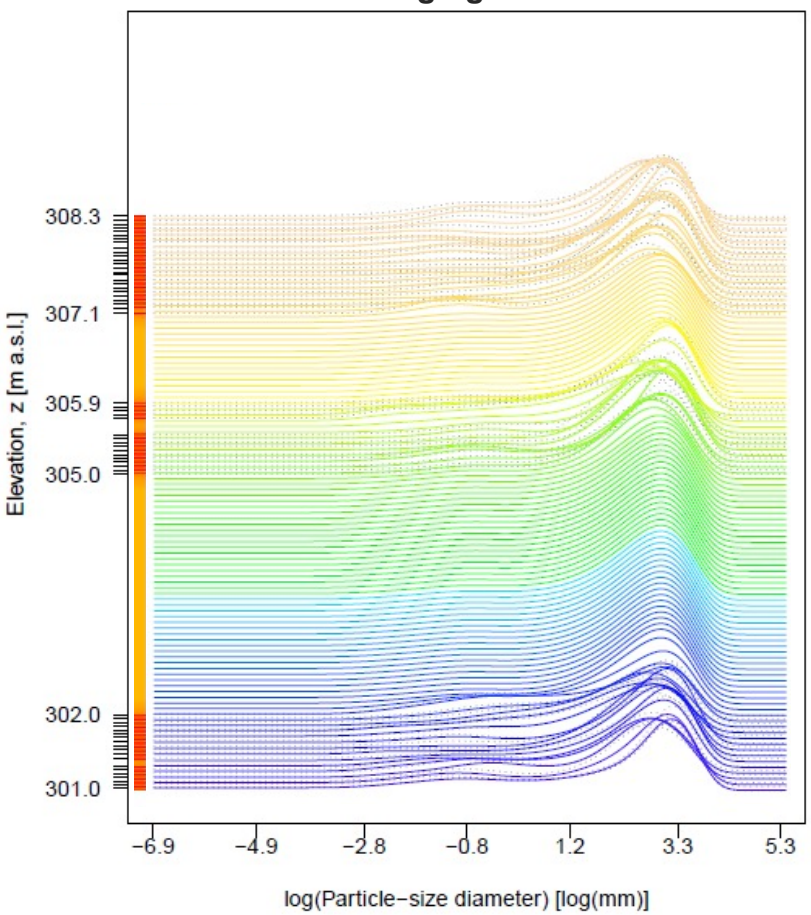


Estimate the spatial dependence
(trace-variogram)

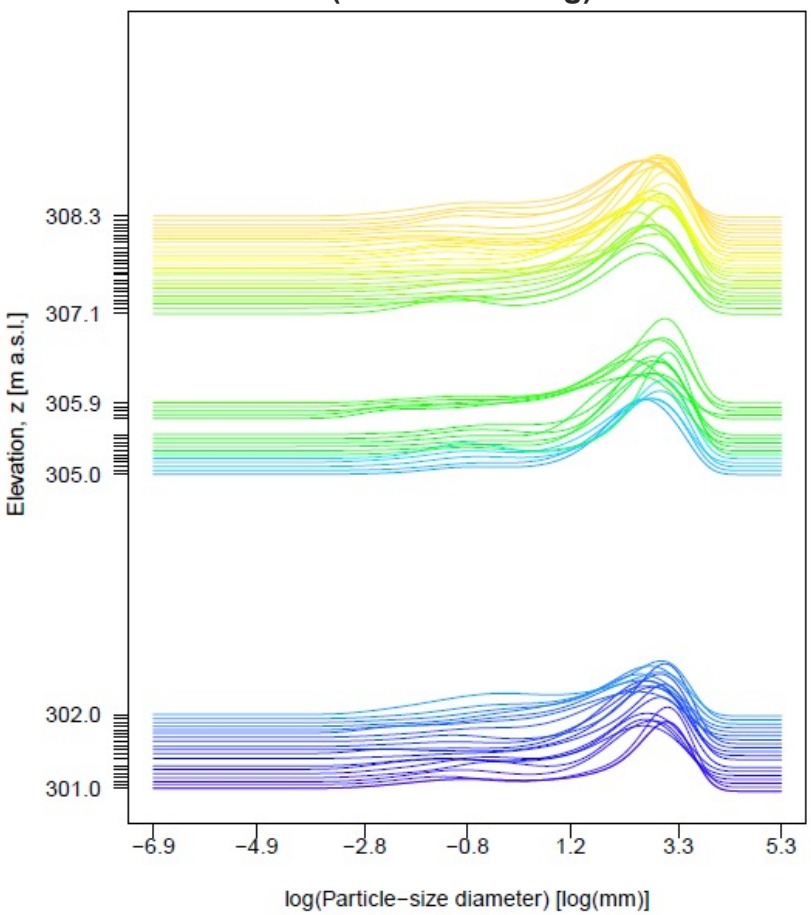
Menafoglio, Guadagnini, Secchi (2014)

Kriging prediction

Kriging predictions and Kriging Variance



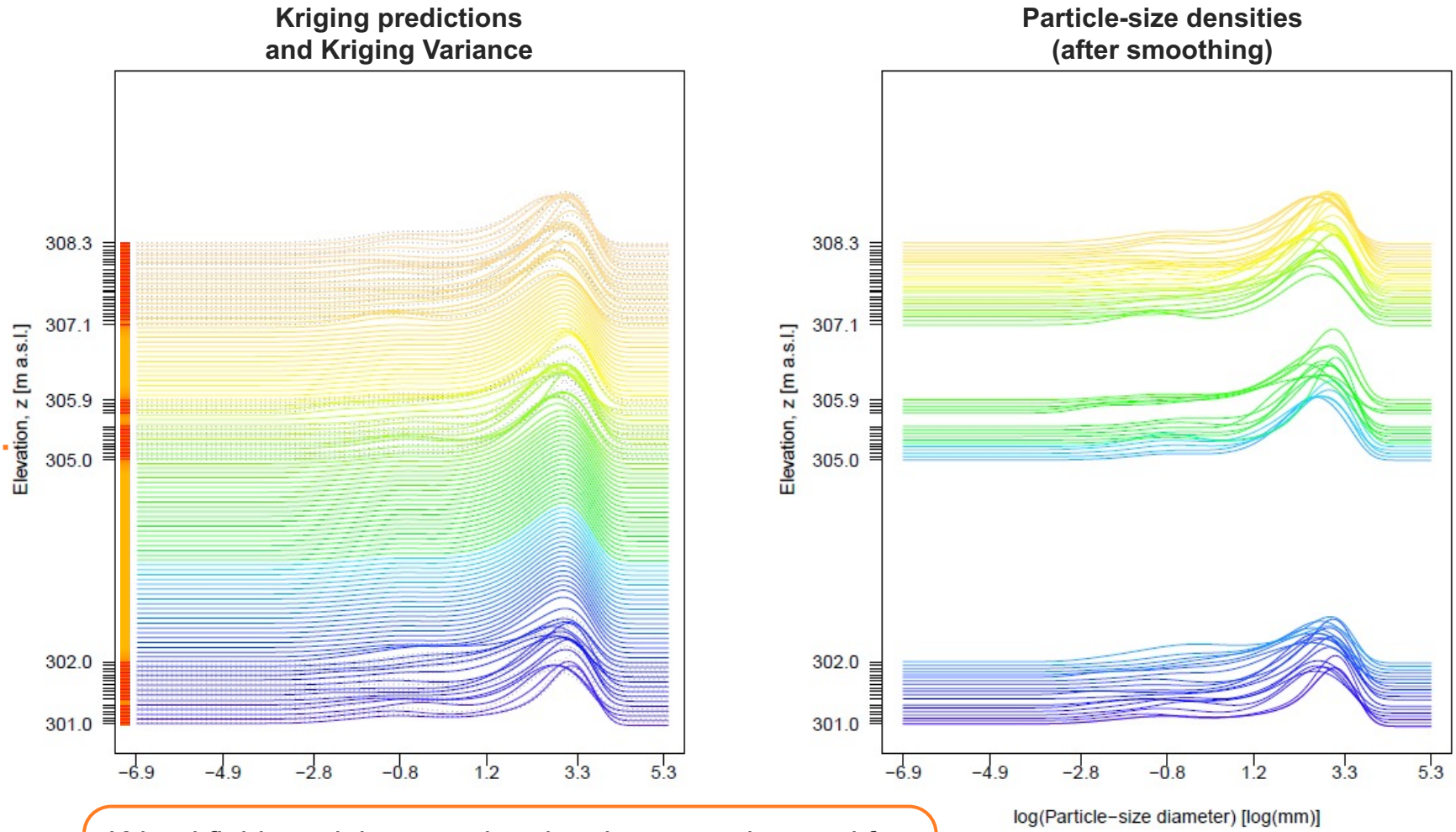
Particle-size densities (after smoothing)



Functional Compositional Kriging

Menafoglio, Guadagnini, Secchi (2014)

Kriging prediction



Kriged fields and the associated variance can be used for:

- Global quantile assessment
- Hydrofacies characterization in MC simulations

Menafoglio, Guadagnini, Secchi (2014)

We aim to compute **log-conductivities** by employing classical formulation based on the particle-size 10th and 60th quantiles (Kozeny-Carman equation, Hazen equation)

Formulations based on PSCs (Vukovic and Soro, 1992)

$$K = \frac{g}{v} C\, f(\phi)\, d_e^2$$

where: *g* is gravity, *v* is the fluid kinematic viscosity, *f(Φ)* is a function of porosity *Φ*, d_e is an effective particle diameter, and *C* is a sorting coefficient.
Porosity *Φ* is estimated as:

$$\phi = 0.255(1 + 0.83^U); \quad U = \left(\frac{d_{60}}{d_{10}}\right)$$

d10 and d60 being the 10th and 60th quantiles.

- **Kozeny-Carman** equation

$$C = 8.3 \cdot 10^{-3}; \quad f(\phi) = \left[\frac{\phi^3}{(1-\phi)^2}\right]; \quad d_e = d_{10}$$

- **Hazen** equation

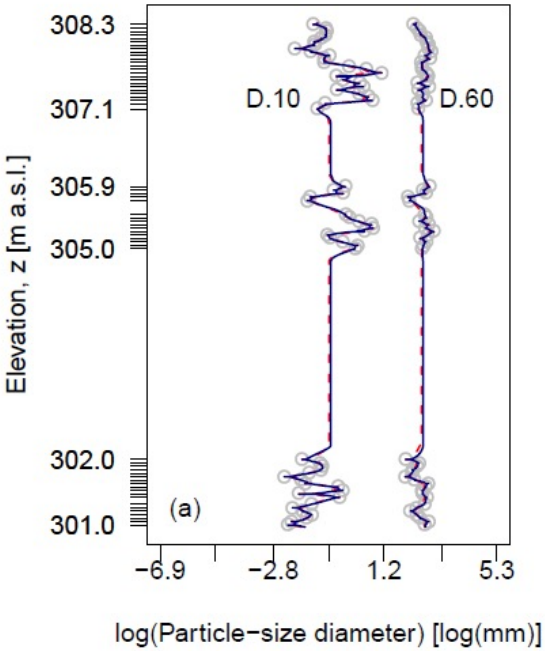
$$C = 6 \cdot 10^{-4}; \quad f(\phi) = 1 + 10(\phi - 0.26).$$

We consider OOK for global quantile assessment as opposed to classical kriging methods which focus on local quantile assessment (of D10 and D60 only)

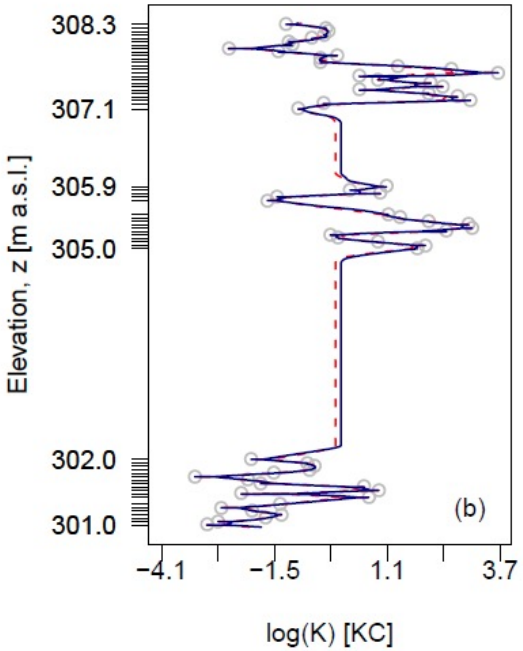
Kriging in Bayes spaces for Quantiles and Hydraulic log-conductivity assessment

We consider OOK for global quantile assessment as opposed to classical kriging methods which focus on local quantile assessment (of D10 and D60 only)

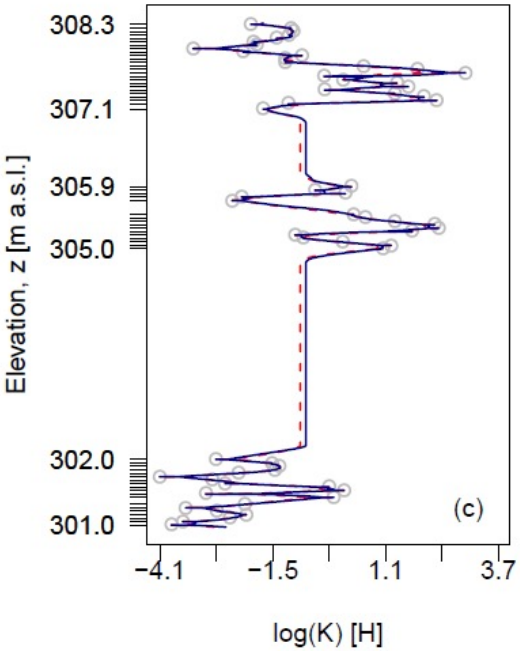
D10 and D60



[KC] hydraulic log-conductivity



[H] hydraulic log-conductivity

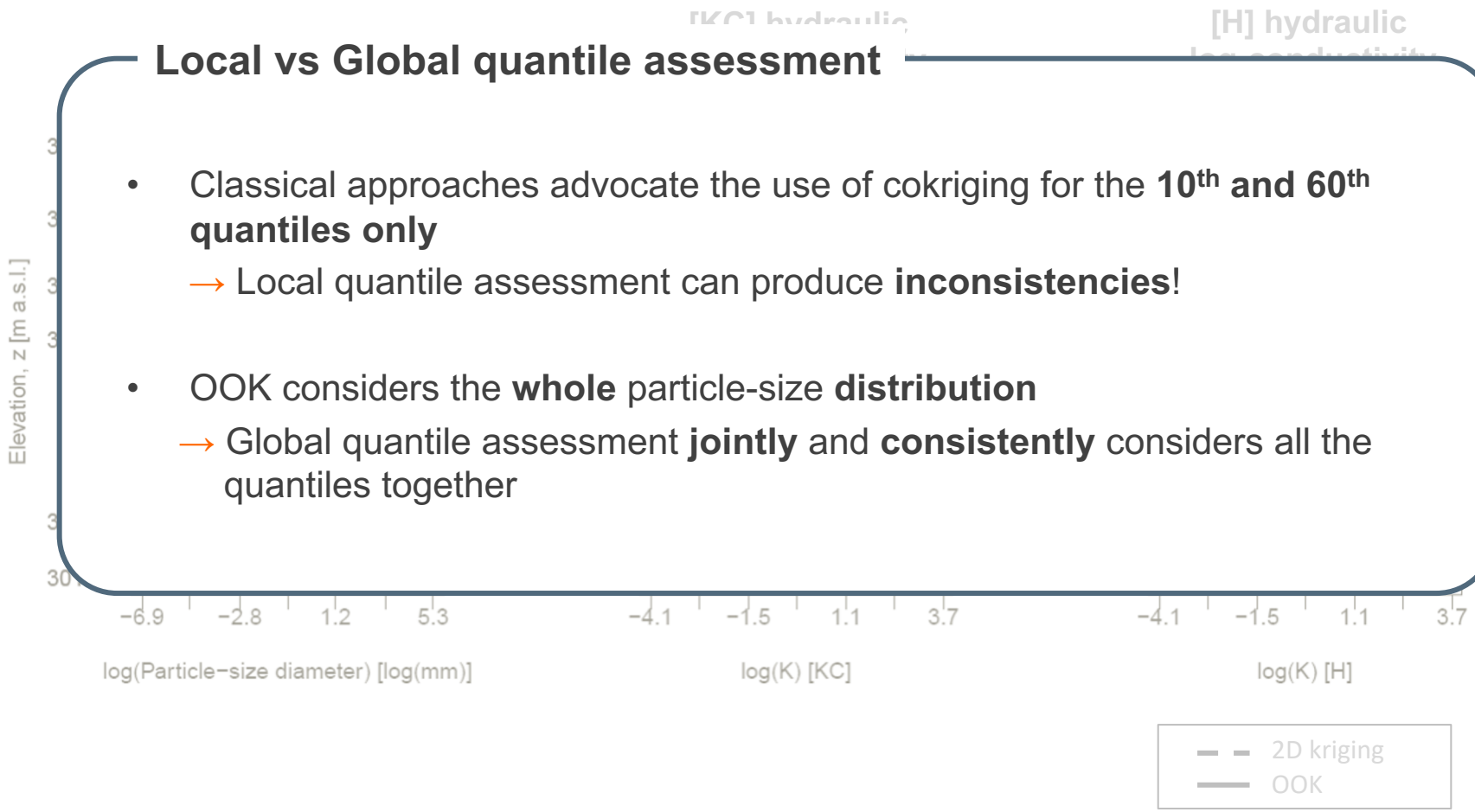


2D kriging
OOK

We consider OOK for global quantile assessment as opposed to classical kriging methods which focus on local quantile assessment (of D10 and D60 only)

Local vs Global quantile assessment

- Classical approaches advocate the use of cokriging for the **10th and 60th quantiles only**
  → Local quantile assessment can produce **inconsistencies**!
- OOK considers the **whole** particle-size **distribution**
  → Global quantile assessment **jointly** and **consistently** considers all the quantiles together



CONCLUSIONS

Conclusions and take home messages

- Data with dependence arise in several environmental applications
- Neglecting the dependence may generate sub-optimal results, when this is actually non-negligible
- When the data objects are densities, Bayes spaces embeddings can be used, and data modeled within the context of Object Oriented Spatial Statistics (O2S2)
- Bayes spaces offer an appealing viewpoint, because of the Hilbert space structure, which allows defining the spatial covariance through the inner product
- Analysing quantiles separately is an alternative approach, not always a good idea
- Alternative non-Hilbert approaches based on Wasserstein metric, which however does not allow for linear prediction and direct covariance modelling

Conclusions and take home messages

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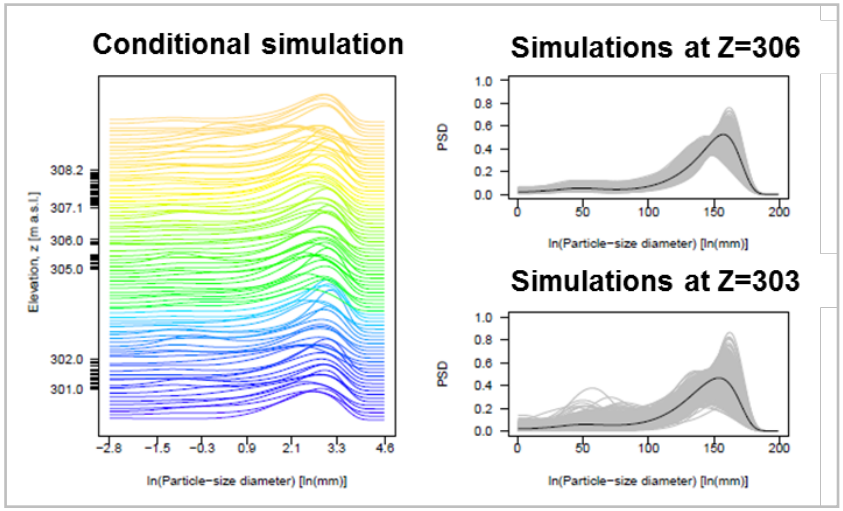
- Topics not covered in the module (still relevant): methods for uncertainty quantification (today mostly based on geostatistical stochastic simulation)

R-package for functional geostatistics: fdagstat (github.com/ogru/fdagstat)
[for data in L^2 but the same routines can be applied after clr transformation]



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Spatial statistics for distributional observations

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An Introduction to Functional Data Analysis for Density Functions in Bayes spaces

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