Optimization of Sample Configurations using Spatial Simulated Annealing

Congreso Escuela en Estadística Espacial

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Introduction – Spatial Modelling

Spatial Modelling

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Spatial models (should) serve the practical purpose of producing the spatial information needed to support many of our every-day decisions.

Modern Spatial Modelling

Modern spatial modelling is based on using **statistical models** that account for:

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- the **empirical correlation** of the target geographic phenomenon itself – autocorrelation

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This is the **mixed model of spatial variation**

Mixed Model of Spatial Variation

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- Y is the target geographic phenomenon at spatial location $\boldsymbol{s}$.
- $m(\boldsymbol{s})$ are the fixed effects, the **deterministic** environmental conditions – that can be modelled using a (linear) trend function
- $e(\boldsymbol{s})$ are the random effects, the seemingly **stochastic** spatial variation – that can be modelled using a covariance function

Spatial models – such as the mixed model – are a *simplification of reality* – they explain only a small part of the spatial variation of geographic phenomena.

The outcome of any spatial model – a (digital) map – will always deviate from the "truth", i.e. be in *error*.

Error and Uncertainty

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There are multiple **sources of uncertainty** in spatial modelling:

- Interpolation/extrapolation error
- Data errors (analytical error, sample design and size)
- Covariate errors (poor correlation with target phenomenon)
- Model structural error (linear or non-linear)

Today we will talk about **sample design**

Spatial Sampling

The usual spatial modelling **challenge**:

1. Multiple geographic phenomena have to be modelled/mapped
2. We know very little about the form of the models of spatial variation
   – **Terra Incognita**
3. Operational constraints limit sampling to a single phase

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In the mixed model context, we need an efficient spatial sample to meet three **conflicting objectives**:

1. Identify and estimate the spatial trend, $Y(\boldsymbol{s}) = m(\boldsymbol{s}) + e(\boldsymbol{s})$
2. Identify and estimate the covariance function, $Y(\boldsymbol{s}) = m(\boldsymbol{s}) + e(\boldsymbol{s})$
3. Make spatial predictions, $Y(\boldsymbol{s}) = m(\boldsymbol{s}) + e(\boldsymbol{s})$

Purposive Sampling – Free Survey

Traditional sampling method to produce area-class soil maps

- The surveyor is free to select the observation locations
- Selected based on conceptual and operational factors
- Goals: learn/verify spatial relationships and maximize the number of observations and geographic coverage
- Personal factors can play a role too, e.g. motivation

A chosen observation location

Purposive Sampling – Mixed Model

- *Purposive sampling* is a non-probability sampling mode
- Sampling locations are selected intentionally as to satisfy an *a priori* criterion
- Based on the **statistical model** that will be used to infer the structure of spatial variation of $Y(s)$

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The modelling framework needs to be made explicit – translate objective into a function, an **objective function**

- Mathematical and heuristic rules are formalized in the form of a computer algorithm
- Find the sampling locations that minimize (or maximize) that criterion

An example

Purposive Sampling – Simple Linear Regression

Suppose that we **know before hand** that the relation between a target geographic phenomenon and an auxiliary variable is linear

$$Y(\boldsymbol{s}) = \beta_0 + \beta_1 X(\boldsymbol{s}) + e(\boldsymbol{s})$$

- A sample is needed to estimate the parameters β_0 and β_1 of this linear model with **minimum variance** $- (X^T X)^{-1} \sigma^2$

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From statistical theory: determinant of information matrix $X^T X$

- Search for the sample configuration that maximizes $|X^T X|$
- We now have an **objective function**

Spatial Simulated Annealing

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Exhaustive search can be VERY time consuming

Spatial simulated annealing is a reasonable alternative

Spatial Simulated Annealing

A relatively simple algorithm that works by trial and error:

1. Start with a completely random sample configuration
2. Compute its objective function value
3. Select one sample and randomly shift its location
4. Compute the objective function value of the new sample configuration
5. **Decide** whether to accept or not the new sample configuration
6. Select another sample and randomly shift its location
7. Compute the objective function value, **decide** whether to accept
8. Continue till the optimum sample configuration is found

How to decide whether to accept or not the new sample configuration?

Metropolis criterion: **acceptance probability** $P(\boldsymbol{X}_i \rightarrow \boldsymbol{X}_{i+1})$

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$$P(\boldsymbol{X}_i \rightarrow \boldsymbol{X}_{i+1}) = \begin{cases} 1, & \text{if } \boldsymbol{f}(\boldsymbol{X}_{i+1}) \leq \boldsymbol{f}(\boldsymbol{X}_i), \\ exp\left(\frac{\boldsymbol{f}(\boldsymbol{X}_i) - \boldsymbol{f}(\boldsymbol{X}_{i+1})}{T}\right), & \text{if } \boldsymbol{f}(\boldsymbol{X}_{i+1}) > \boldsymbol{f}(\boldsymbol{X}_i), \end{cases}$$

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- A better sample configuration is always accepted
- A worse sample configuration sometimes is accepted too – escape from **local optima**
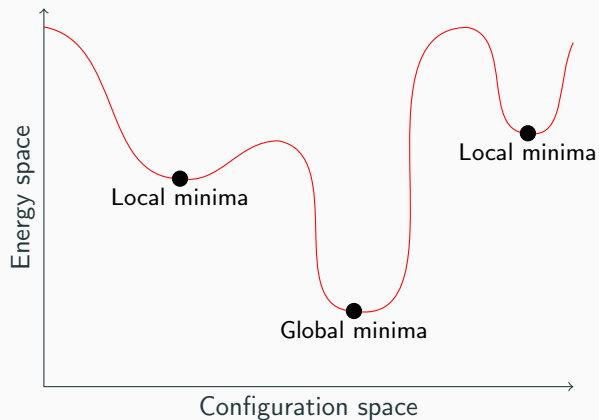
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The Metropolis criterion has a **temperature** parameter T

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- At the end of the optimization, only better sample configurations are accepted

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Spatial Simulated Annealing – Temperature

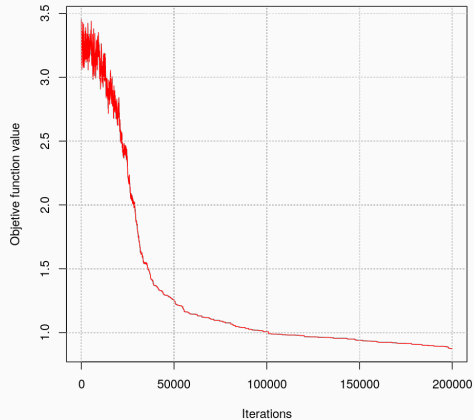The Metropolis criterion has a **temperature** parameter T

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- Worse sample configurations are more likely to be accepted in the beginning of the optimization
- At the end of the optimization, only better sample configurations are accepted

Also, shorter random shifts in samples as the optimization approaches its end – the optimal solution is expected to be nearby

Evolution of objective function values during the optimization

Back to *Terra Incognita*

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Objective Functions

Various objective functions have already been proposed

Is there room for improvement?

- Spatial (nonlinear) trend estimation ($m(\boldsymbol{s})$)
- Variogram estimation ($e(\boldsymbol{s})$)
- Spatial interpolation ($Y(\boldsymbol{s})$)

Objective Functions and the Mixed Model

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How to combine these conflicting objective functions – spatial modelling is a *multi-objective combinatorial optimization problem*

Variogram Estimation ($e(s)$)

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Space Variogram space, i.e. the unidimensional space defined by the distances between sample points.

Algorithm Point-pairs per lag-distance class.

Goal Uniform distribution of point-pairs per equidistant lag-distance class in the empirical variogram.

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Goal Uniform distribution of point-pairs per equidistant lag-distance class in the empirical variogram.
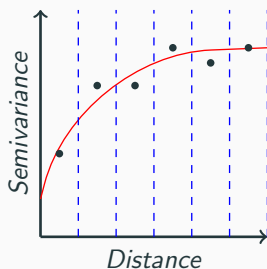
Example: six lag-distance classes.
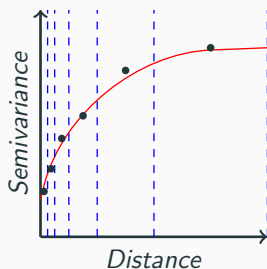

Equidistant lags.

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Algorithm **P**oints **P**er **L**ag-distance class (**PPL**).
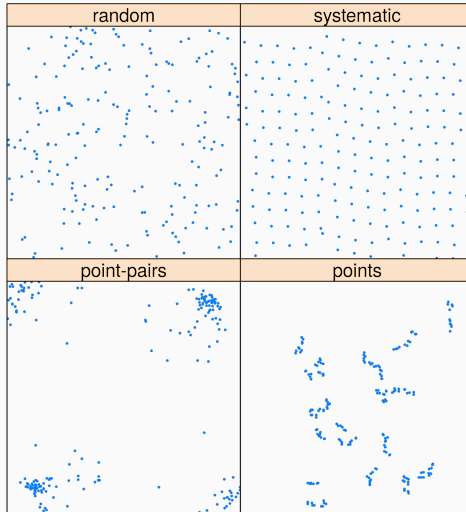
Goal Uniform distribution of points per exponential lag-distance class in the empirical variogram.

Example: six lag-distance classes.

Exponential lags.

Spatial samples in a square of 500×500.
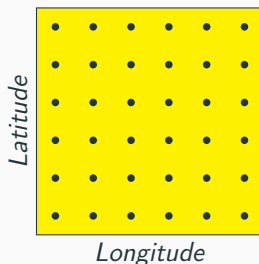
Spatial Interpolation ($Y(s)$)

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Space Geographic space, i.e. the bi-dimensional space defined by the boundaries of the sampling region.

Algorithm Spatial Coverage Sampling (k-means algorithm, SPCOSA).

Goal Minimize the overall distance between sample and prediction points.

Spatial Interpolation ($Y(s)$)

Space Geographic space, i.e. the bi-dimensional space defined by the boundaries of the sampling region.

Algorithm **M**ean **S**quared **S**hortest **D**istance (**MSSD**).

Goal Minimize the overall distance between sample and prediction points.

Example: Regular grid with 36 observations.

Longitude

Latitude

Uniform coverage.

Multi-Objective Combinatorial Optimization Problem

Completely different sample configurations for

- Variogram identification and estimation
- Spatial interpolation

Multi-Objective Combinatorial Optimization Problem

When solving a MOCOP, one aims at minimizing the vector of k objective functions

$$\boldsymbol{f}(\boldsymbol{X}) = (f_1(\boldsymbol{X}), f_2(\boldsymbol{X}), \ldots, f_k(\boldsymbol{X})), \qquad (1)$$

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To find a single optimum solution, one can aggregate the objective functions into a single *utility function*

$$U = \sum_{i=1}^{k} w_i f_i(\boldsymbol{X}), \tag{2}$$

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$$U = \sum_{i=1}^{k} w_i f_i(\boldsymbol{X}), \qquad (2)$$

Objective functions need to be scaled to the same approximate range of values – eliminate any potential numerical dominance

How do we scale the objective functions?

The **upper-lower bound approach**:

$$f_i'' = \frac{f_i(\boldsymbol{X}) - f_i^{\circ}}{f_i^{max} - f_i^{\circ}}, \tag{3}$$

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These can be found empirically (takes time), approximated numerically (sub-optimal) or (rarely) calculated

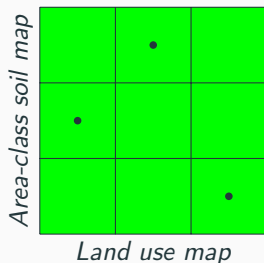# Spatial (Nonlinear) Trend Estimation ($m(s)$)

Spatial (Nonlinear) Trend Estimation ($m(s)$)

Space
Attribute space, i.e. the multi-dimensional space defined by the covariates (auxiliary variables).

Algorithm
Conditioned Latin hypercube sampling (CLHS).

Goal
Reproduce (1) the marginal distribution of the numeric and (2) factor covariates, and (3) the linear correlation between numeric covariates.
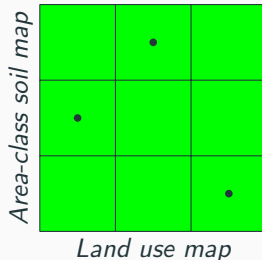
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Example: three samples from two covariates with three classes each.

Land use map

A Latin square.

Spatial (Nonlinear) Trend Estimation ($m(s)$)

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Algorithm **A**ssociation/**C**orrelation measure and marginal **D**istribution of the **C**ovariates (**ACDC**).
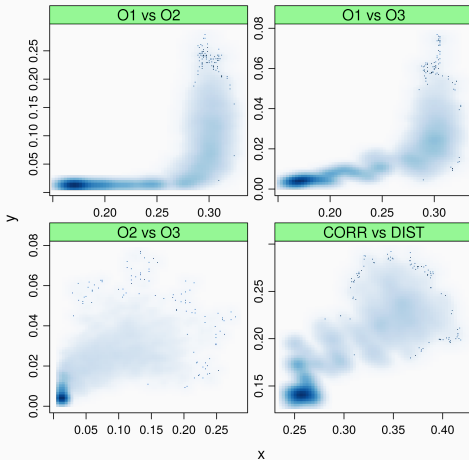
Goal Reproduce (1) the marginal distribution of the covariates, and (2) the linear association/correlation between covariates.

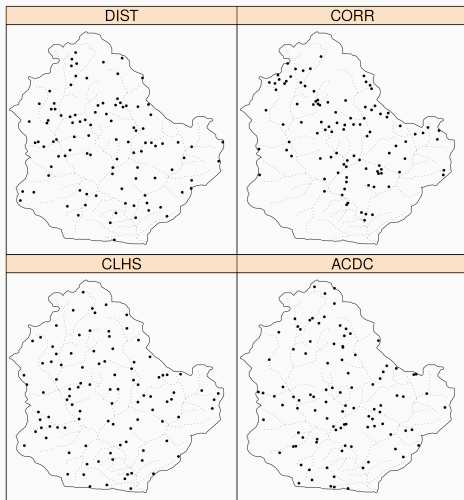Example: three samples from two covariates with three classes each.

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A Latin square.

Numerical behaviour.

Optimized spatial sample configurations.

Sampling in *Terra Incognita*

Three sampling algorithms to meet each sampling objective:

ACDC Spatial trend estimation, $Y(\boldsymbol{s}) = m(\boldsymbol{s}) + e(\boldsymbol{s})$

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General-purpose method to design sample configurations[1]

Space Attribute, variogram, and geographic spaces.

Algorithm $\mathbf{SPAN} = w_1\mathbf{ACDC} + w_2\mathbf{PPL} + w_3\mathbf{MSSD}$

Goal Uniformly cover the feature, variogram and geographic spaces.

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Final Thoughts

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1. Existing sampling algorithms can be improved, but it is not clear if this always translates into improved prediction accuracy.

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Optimization of Spatial Samples

Spatial sample optimization and simulated annealing are relatively well known techniques

1. Existing sampling algorithms can be improved, but it is not clear if this always translates into improved prediction accuracy.
2. Larger sample size seems to improve prediction quality irrespective of the sampling algorithm used – is there a limit?
3. It is not clear what is the best sample configuration for highly nonlinear models such as random forests.

I will be happy to try answering your questions