Can the SPDE approach replace traditional Geostatistics for industrial applications?

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MINES-ParisTech - Géosciences

Context

- The Geostatistics team of Mines-ParisTech
- Production of methodology for the society
- Production of softwares (RGeostats, Geovariances)
- Mineral ressources oriented

Constraints imposed by the industry

- Research of innovative solutions to increase productivity
- Quite conservative (changes allowed in a stable workflow)

Computational ressources

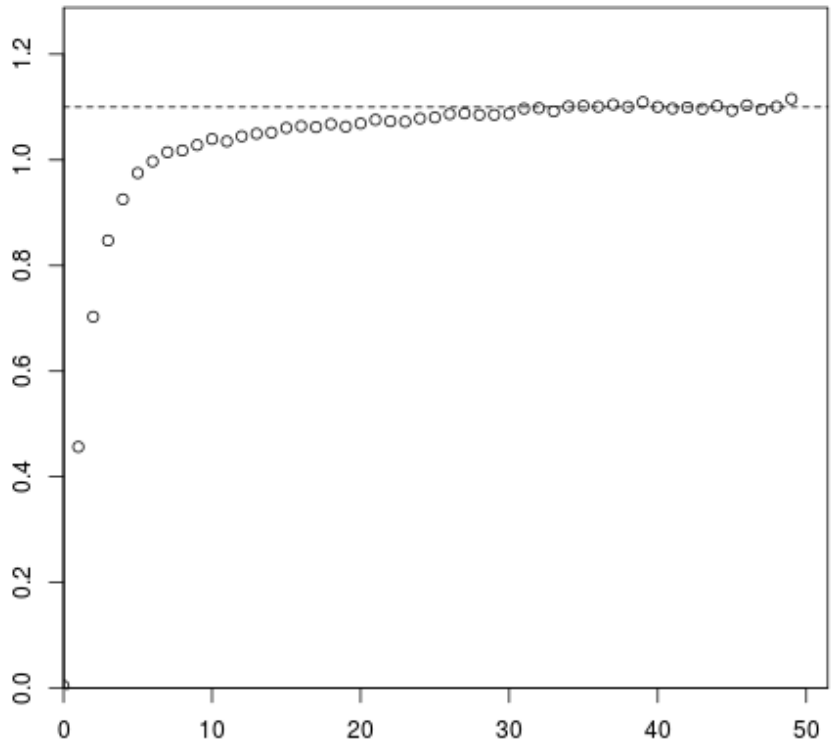
Computational ressources

Generally more limited

Uranium deposit - Arlit - Niger

Workflow

1) Modeling



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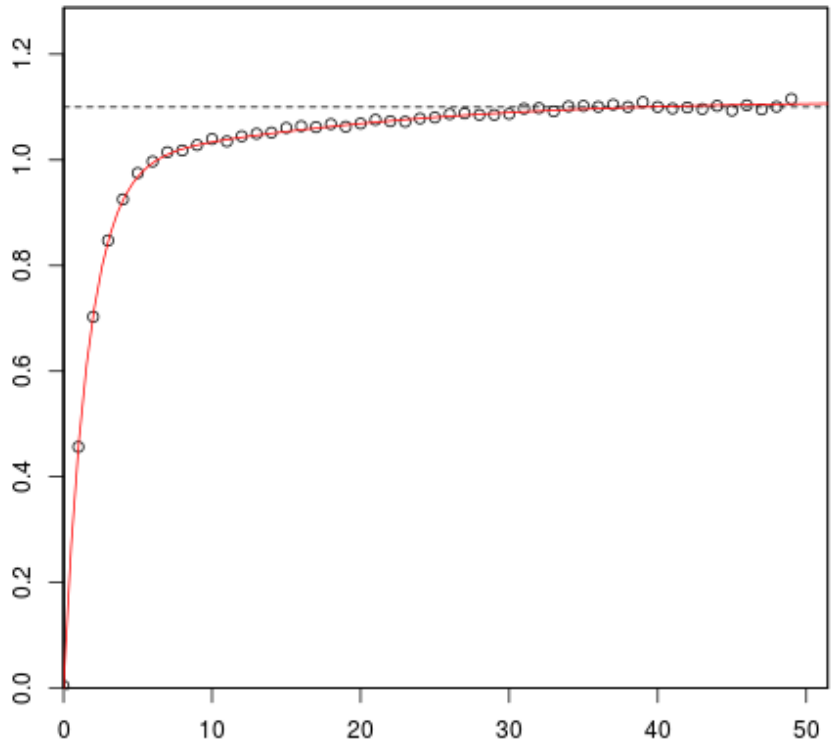

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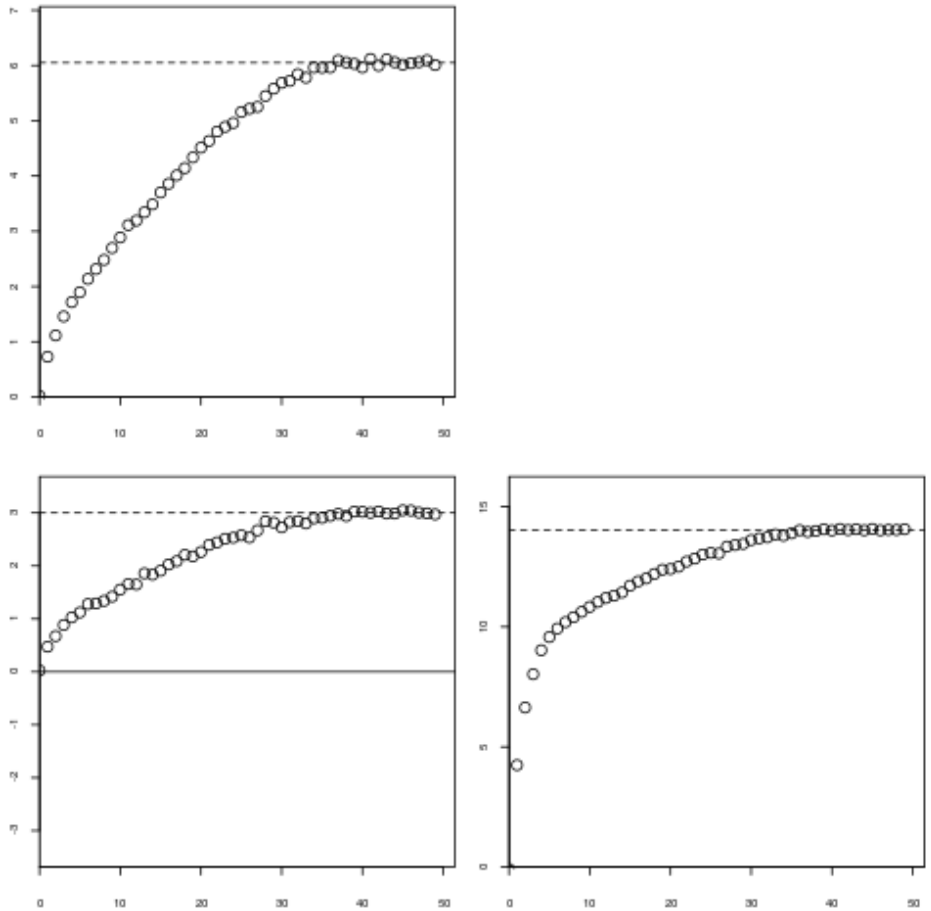

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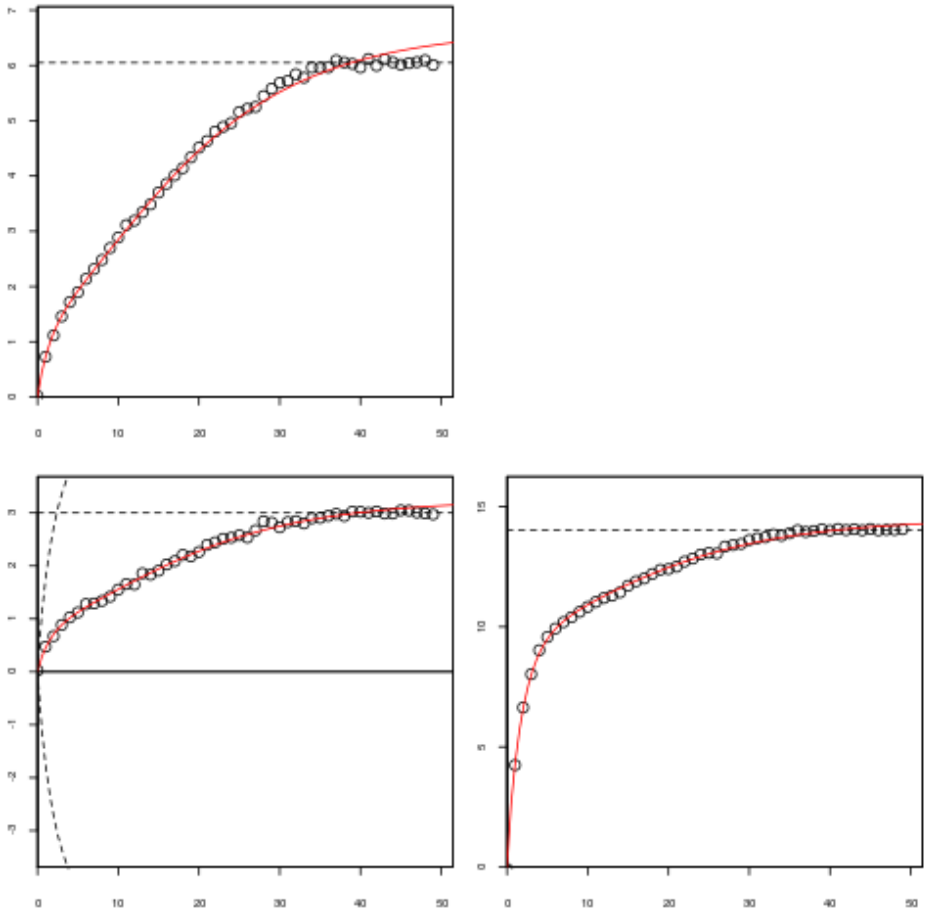

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- Conditional variance (covariance matrix of the errors)

$$Var[Z_T|Z_D] = \mathrm{Cov}(Z_T^\star - Z_T) = \Sigma_{TT} - \Sigma_{TD}\Sigma_{DD}^{-1}\Sigma_{DT}$$

Handling large data sets and large grid

- Kriging with large data sets is performed by using moving neighborhoods
- Conditional simulations are performed by using non conditional simulations and kriging of the residuals

Principle

Let

$$Z(x) = Z^{SK}(x) + Z(x) - Z^{SK}(x)$$

where

$Z^{SK}(x) = \sum_{j=1}^{n} \lambda_j(x) Z(x_j)$ simple kriging

$Z(x) - Z^{SK}(x)$ kriging residuals

Z^{SK} and $Z - Z^{SK}$ are two independent Gaussian random functions

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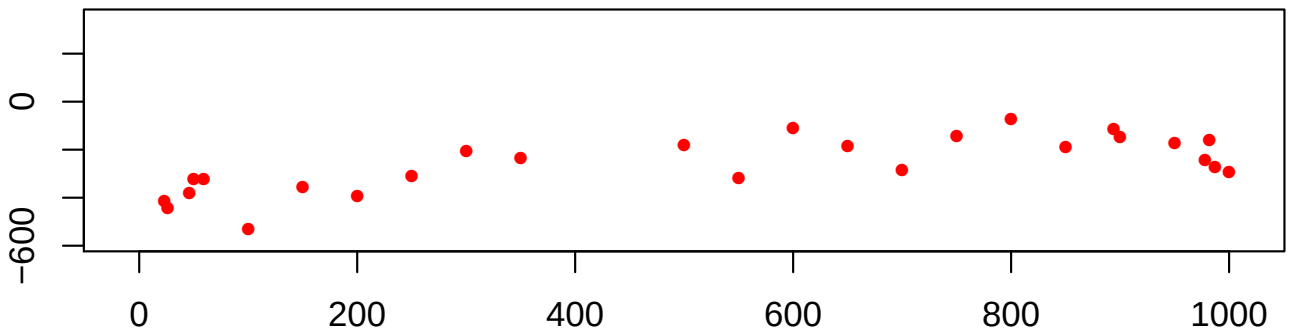

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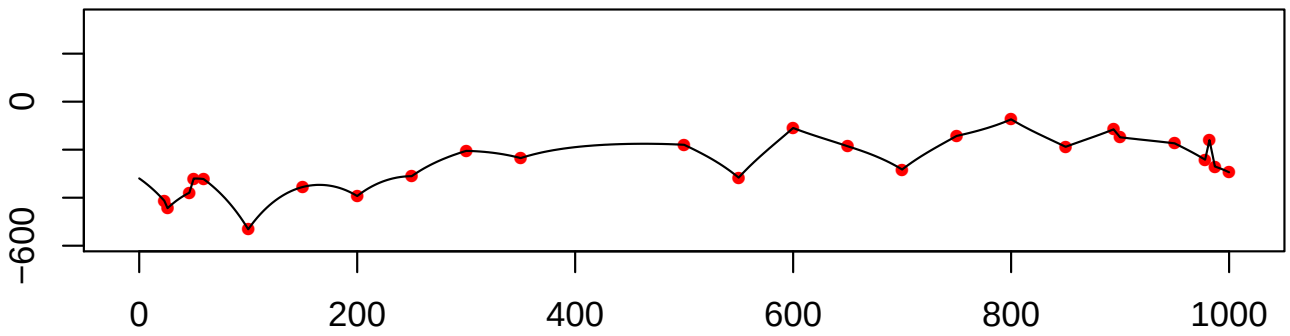

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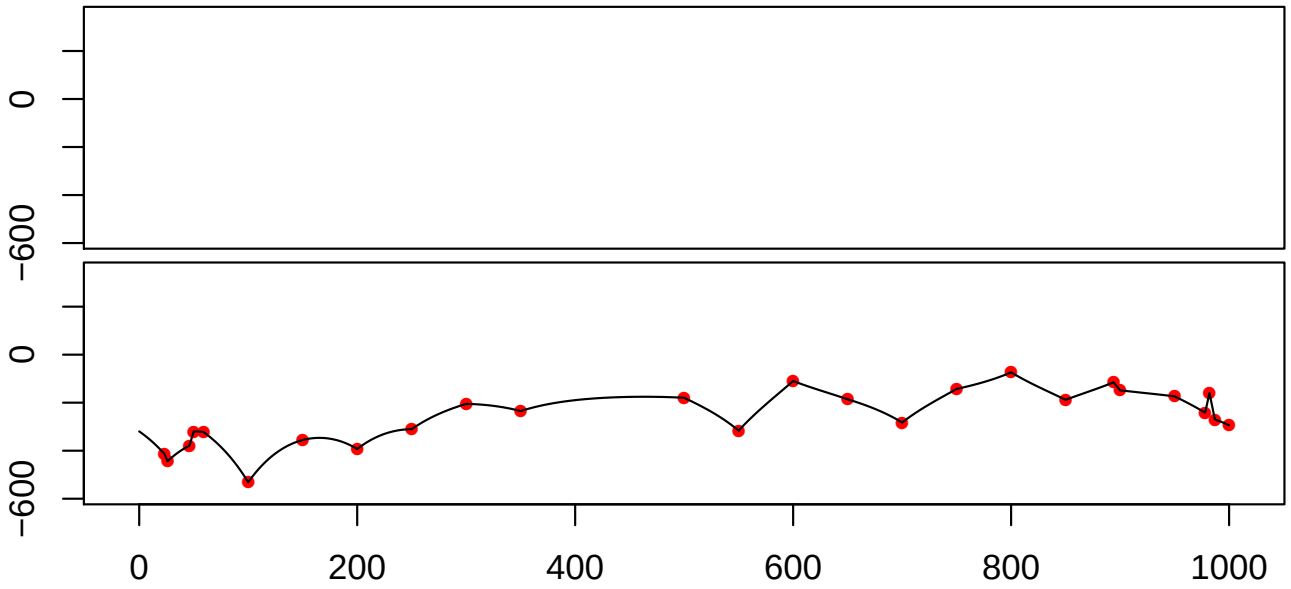

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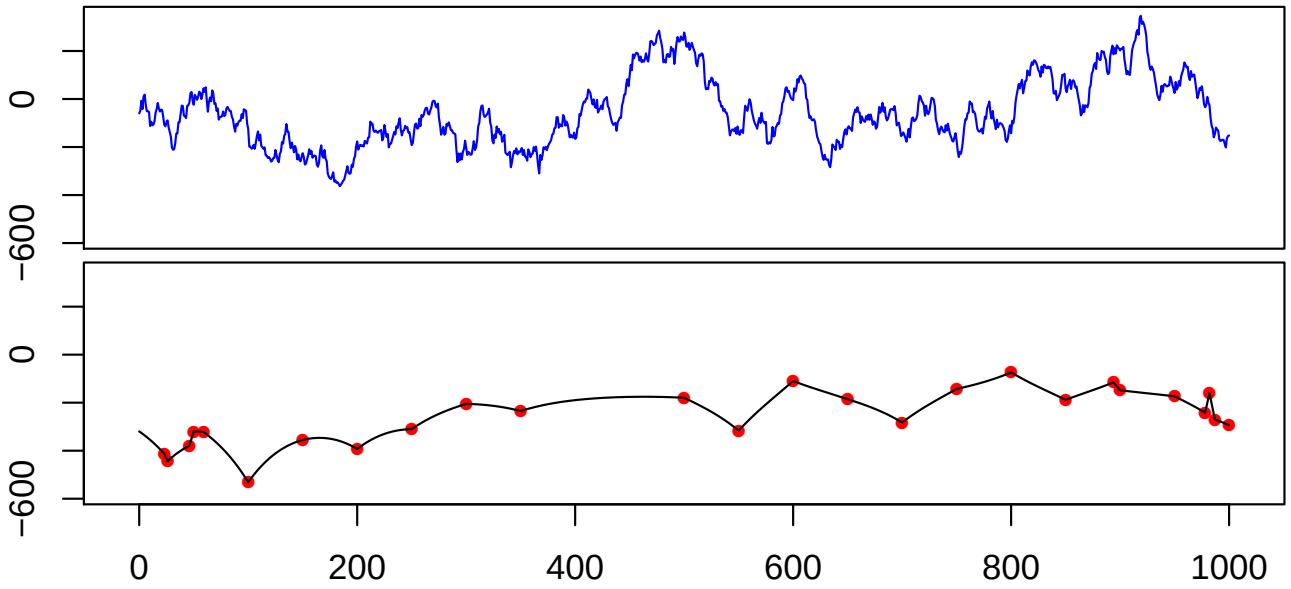

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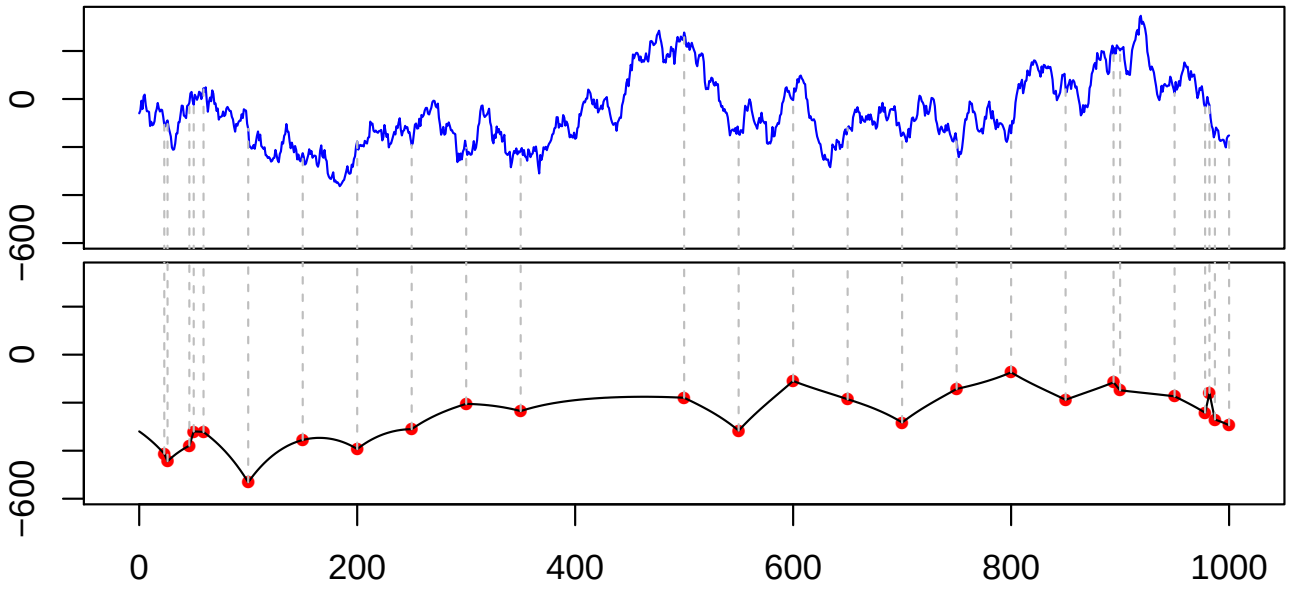

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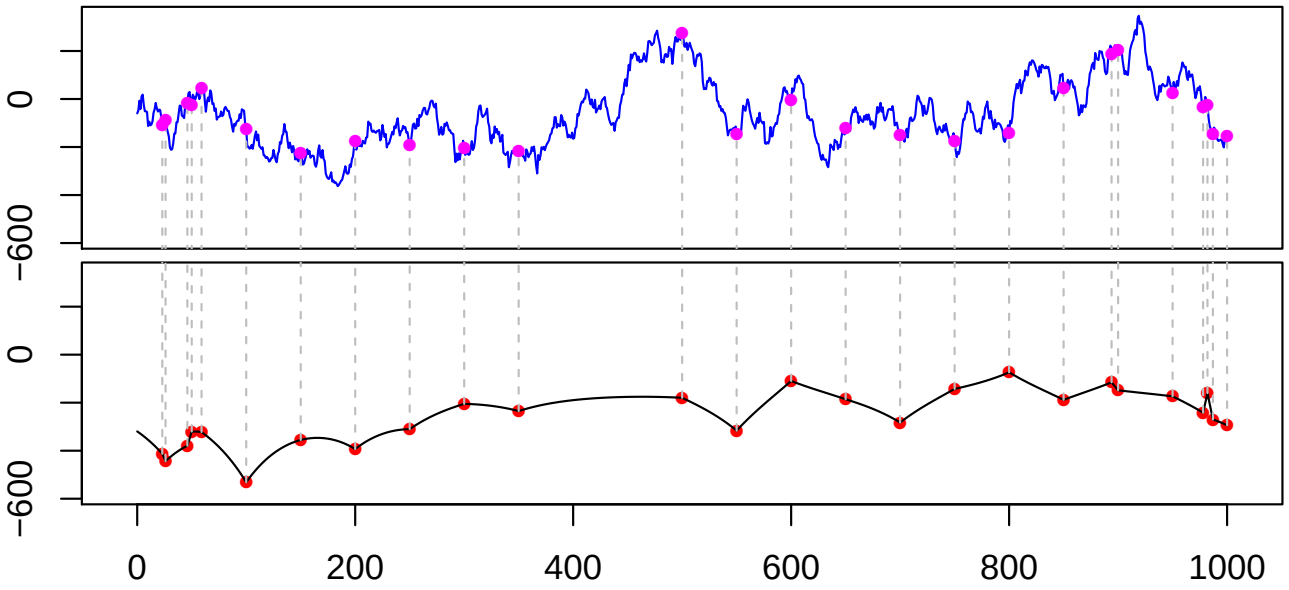

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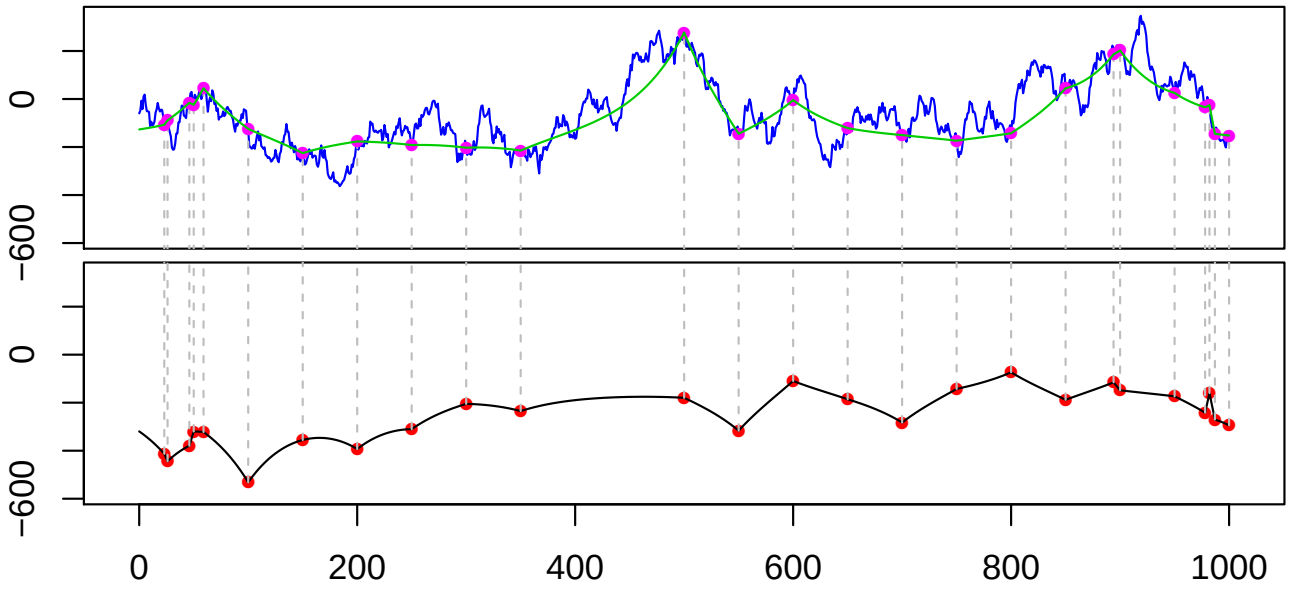

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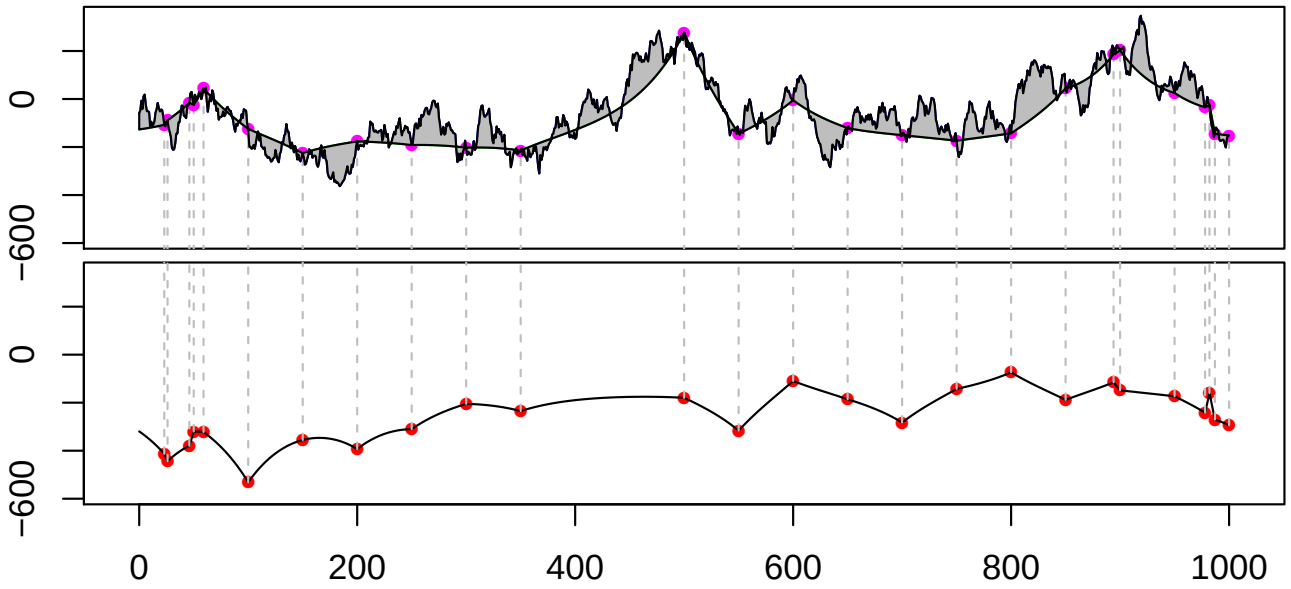

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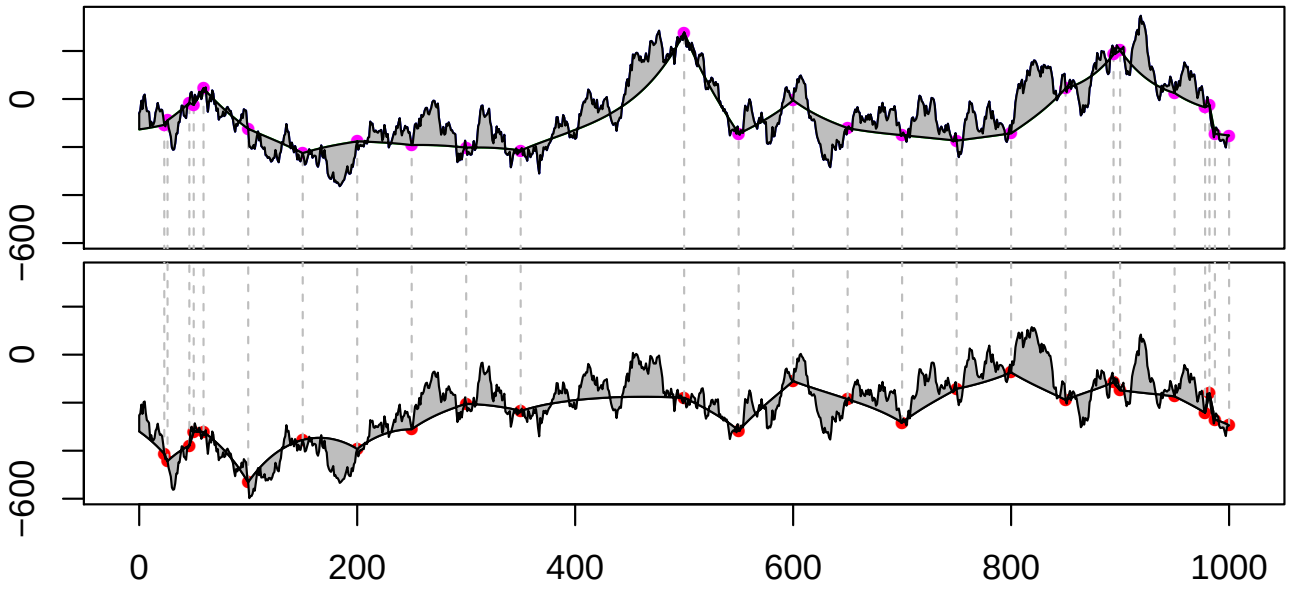

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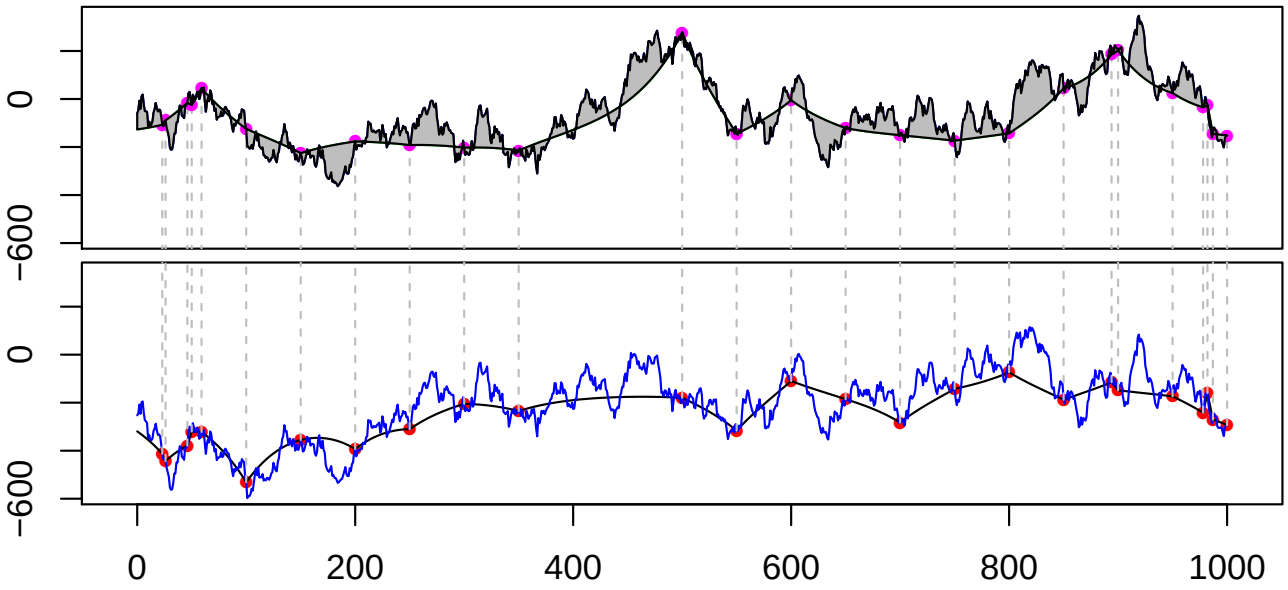

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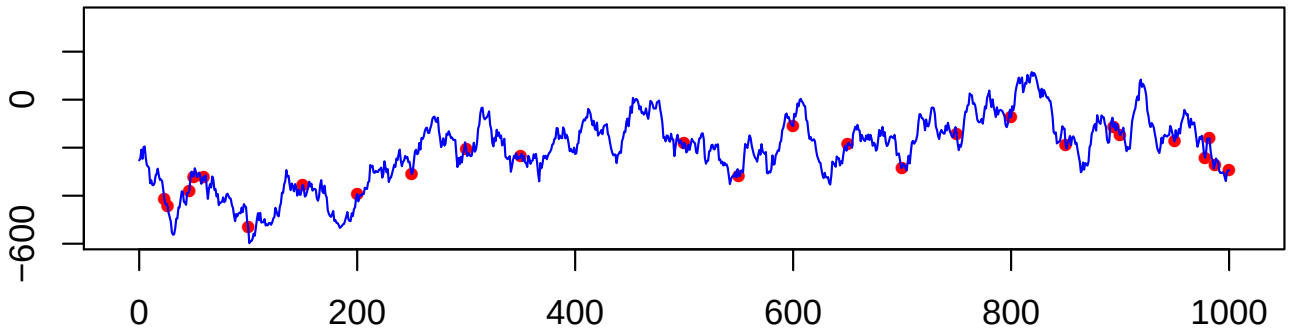
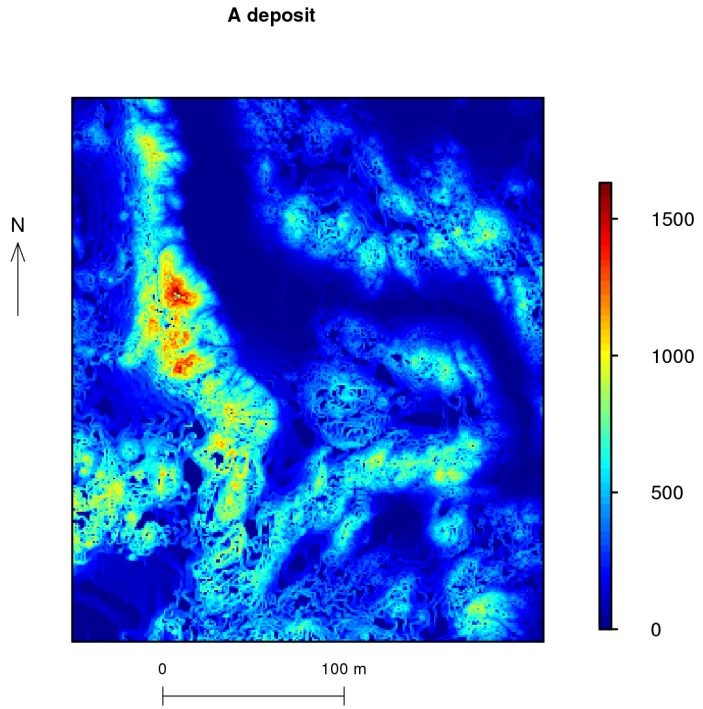


Selective exploitation

- Punctual grade

$$Z(x), x \in \mathcal{D}$$

with mean m and covariance function C



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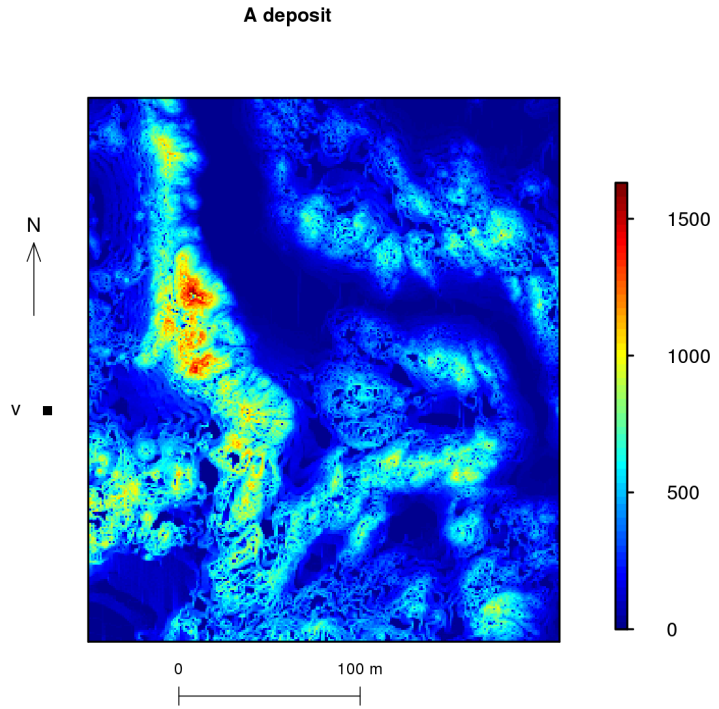

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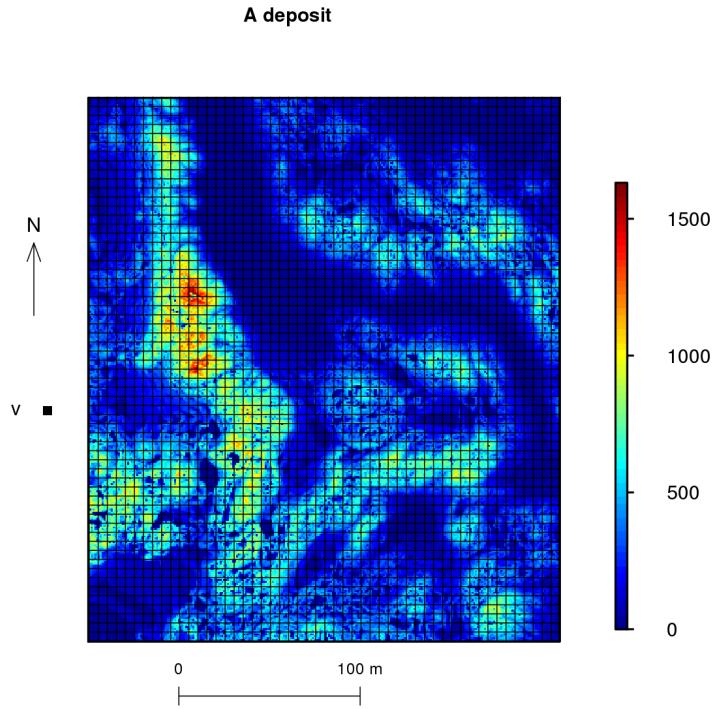

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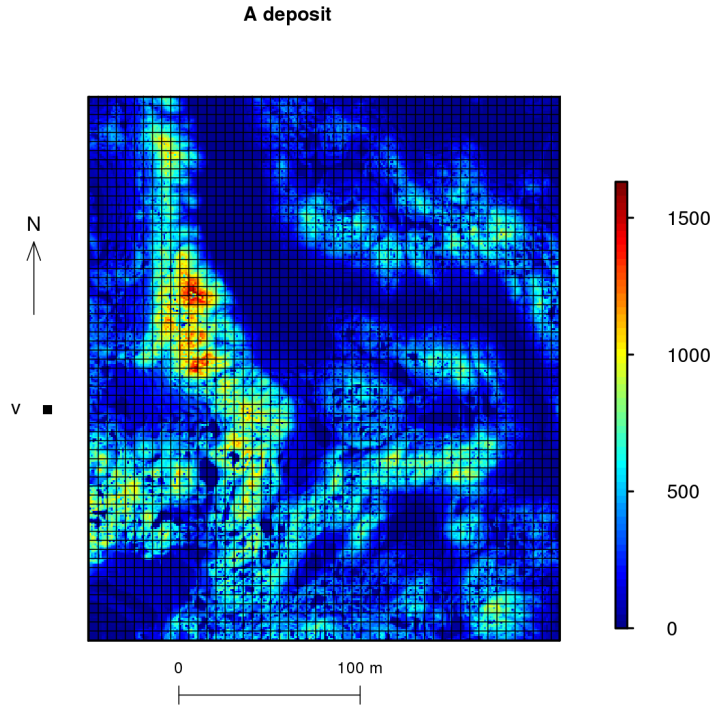

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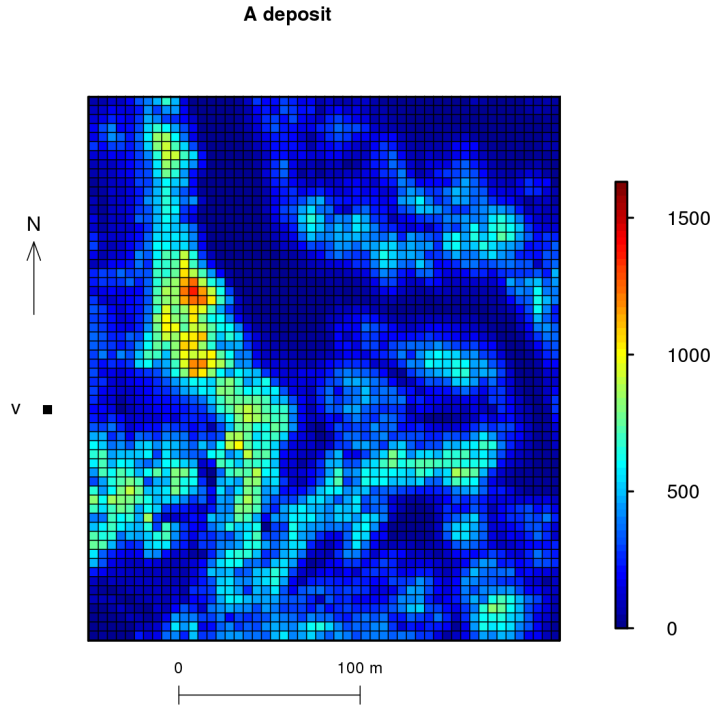

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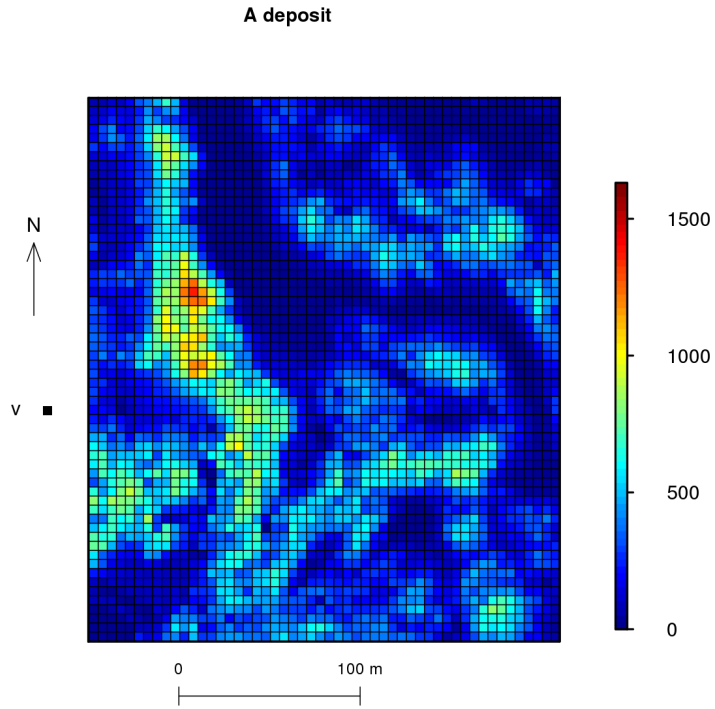

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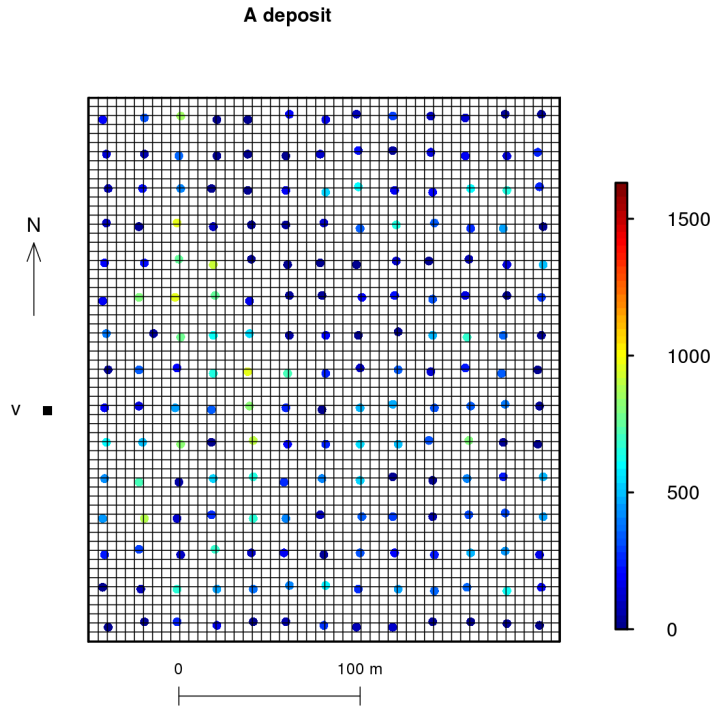

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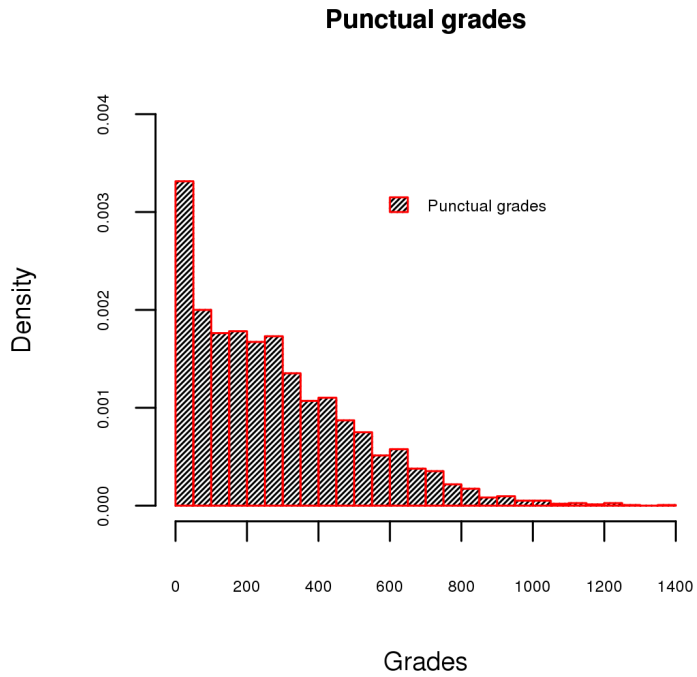

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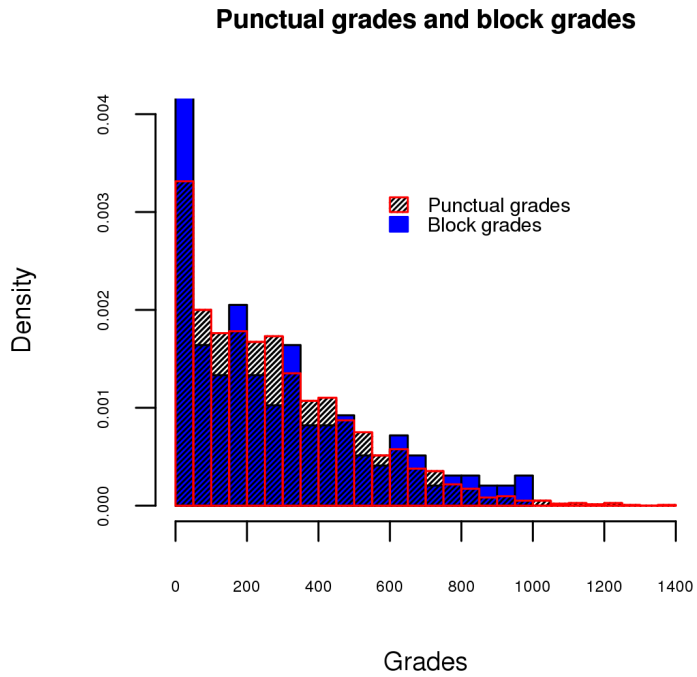

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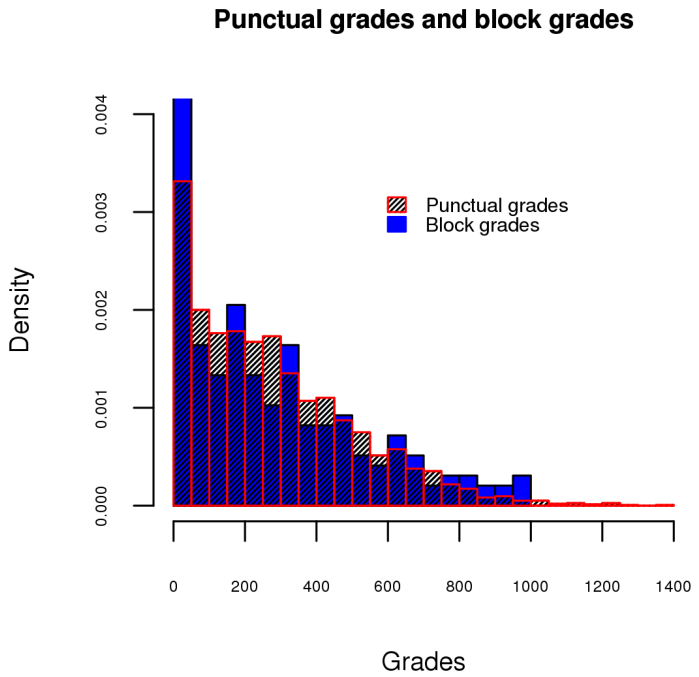
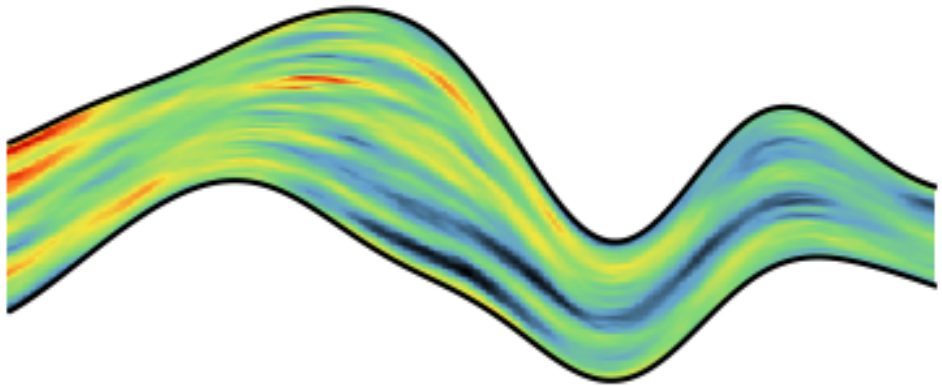
- Block simulations are required to generate several scenarios



Direct block simulations

- The number of SMU can be large (e.g 1 million)
- Conditional simulations by using discretization of the blocks can be time consuming
- Solution : use of a change of support model to describe the multivariate distribution of the points and the blocks and perform conditional simulations of the regularized variable without discretization
- Several hours for 100 simulations with around 100 000 observations

Handling covariance non-stationarities



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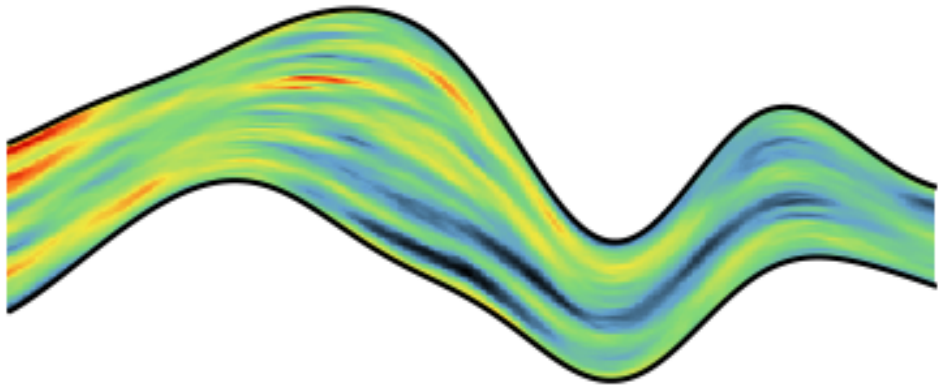
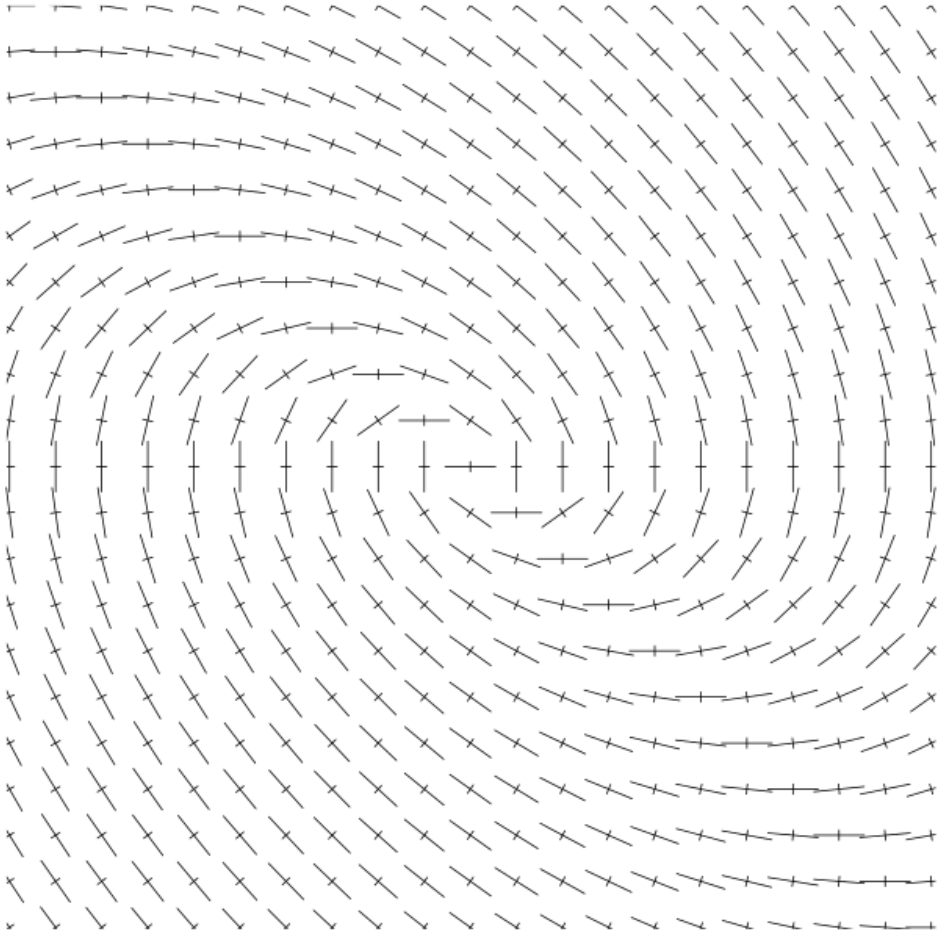


Current solutions

- Deform the space
- Cut the domain into several sub-domains in which stationarity is acceptable

More complex environments



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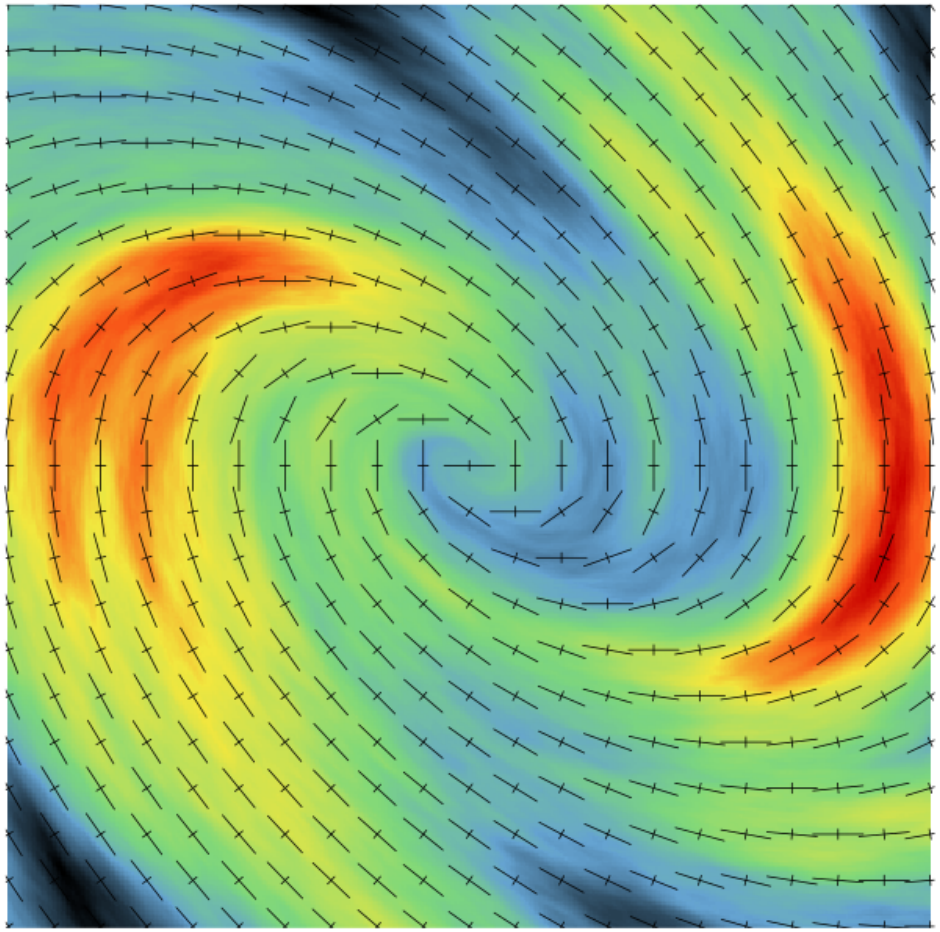

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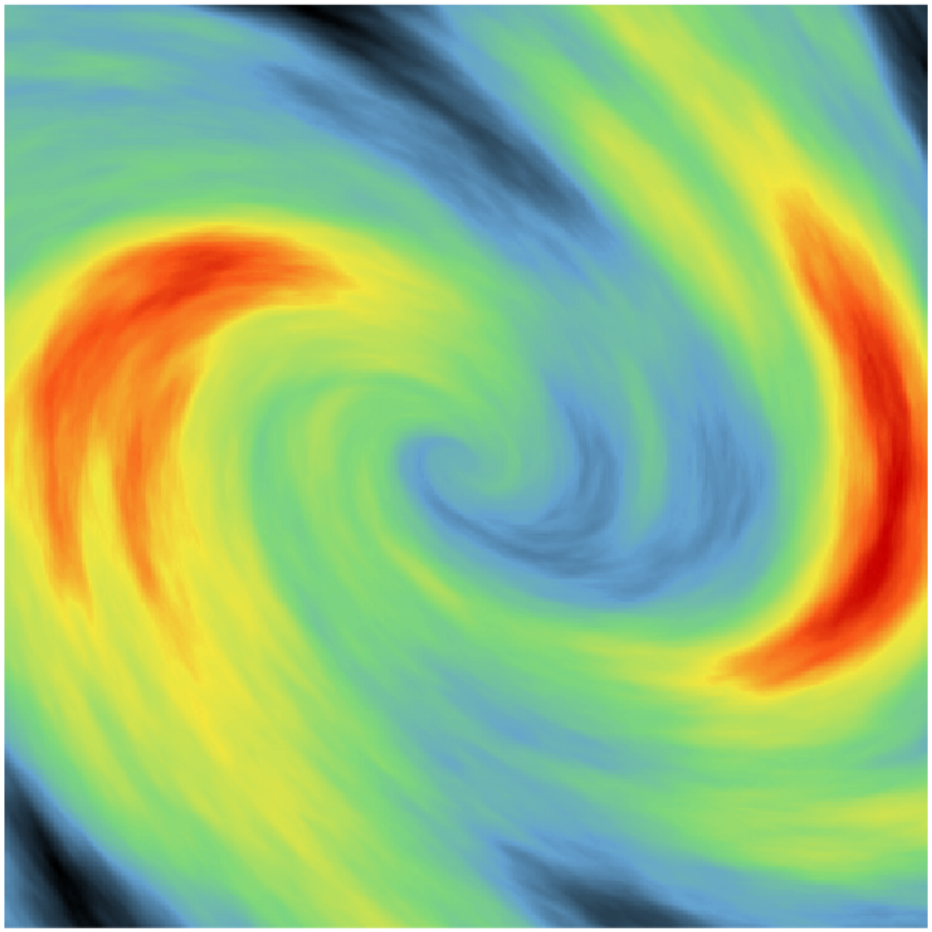

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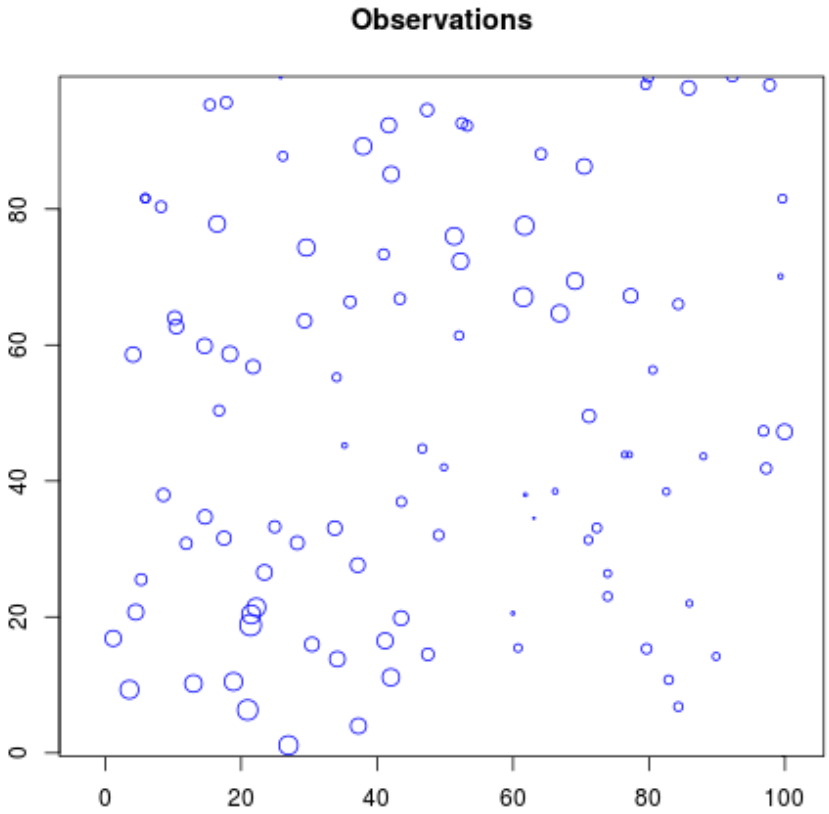
Comparison with classical approach



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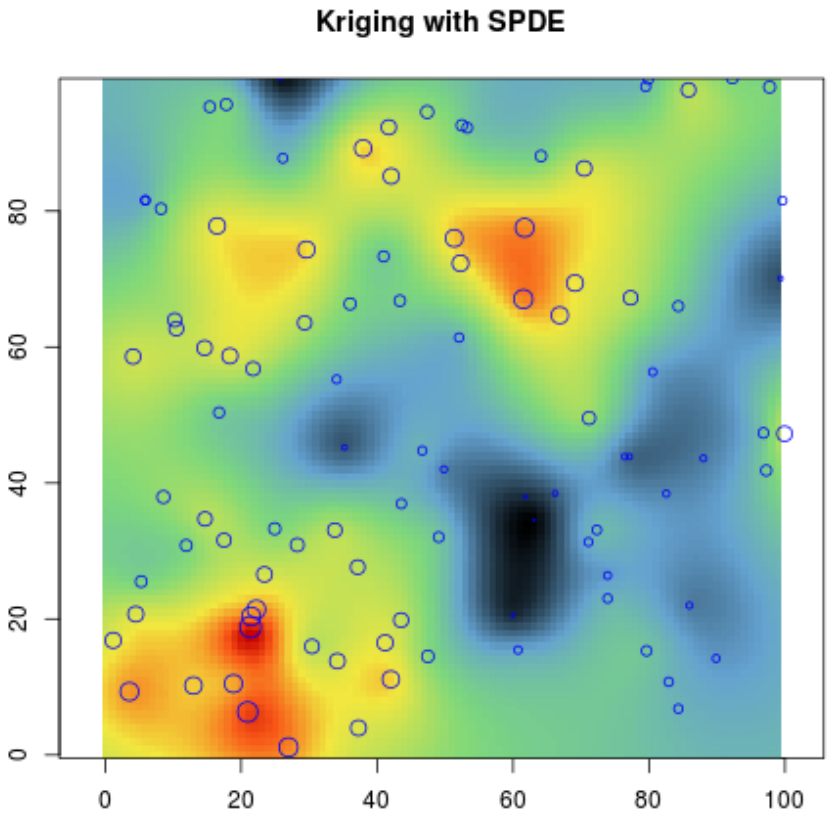

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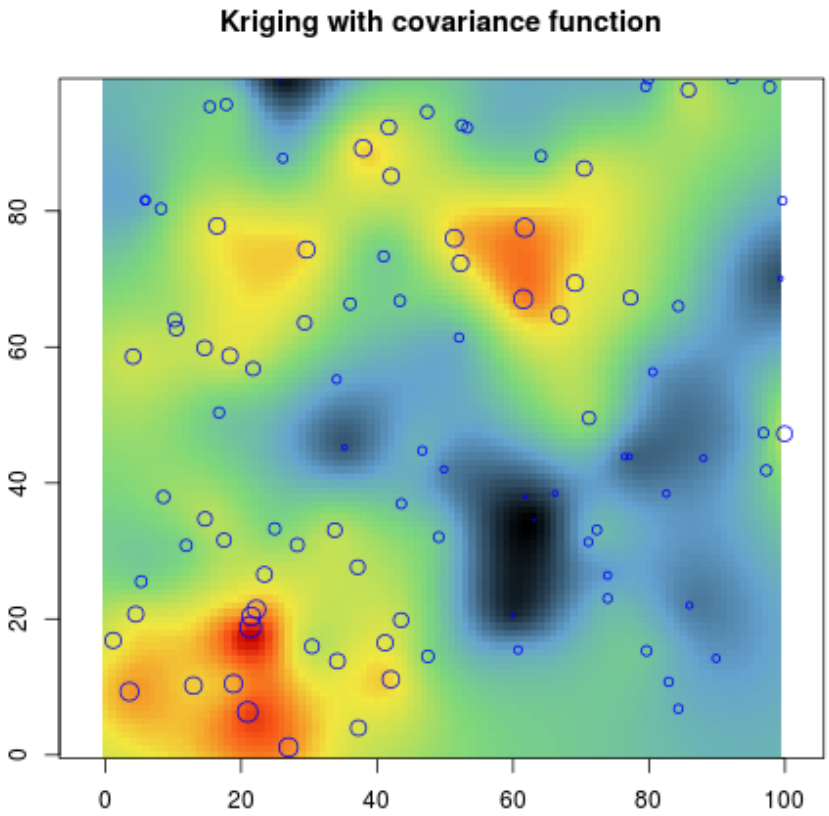

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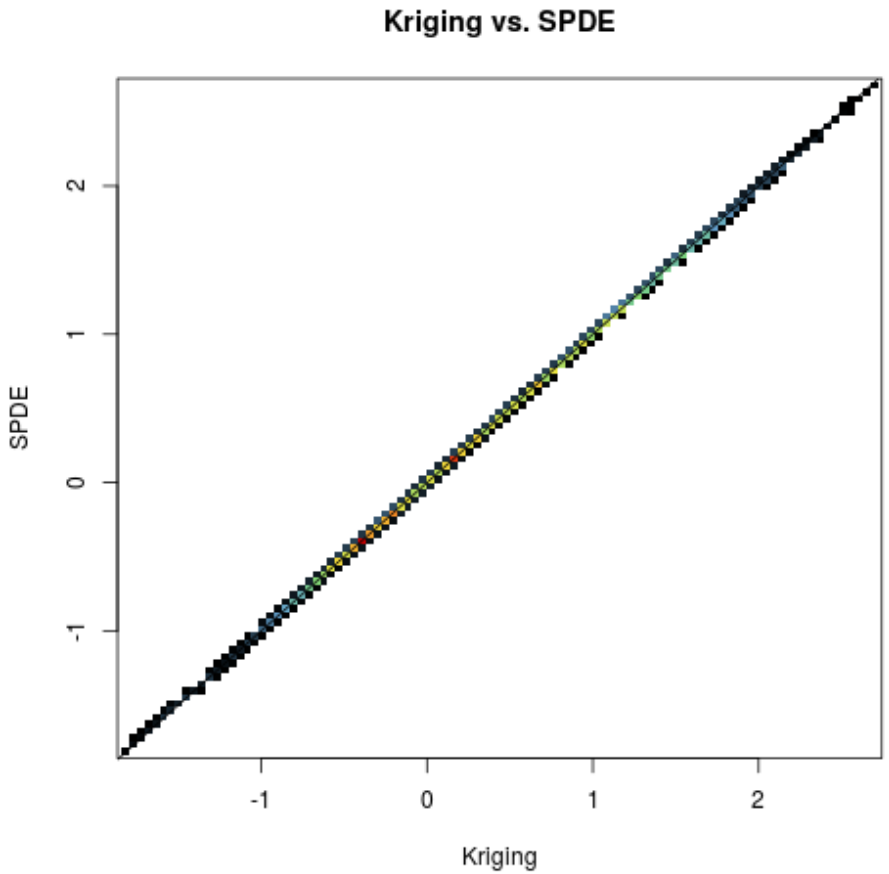

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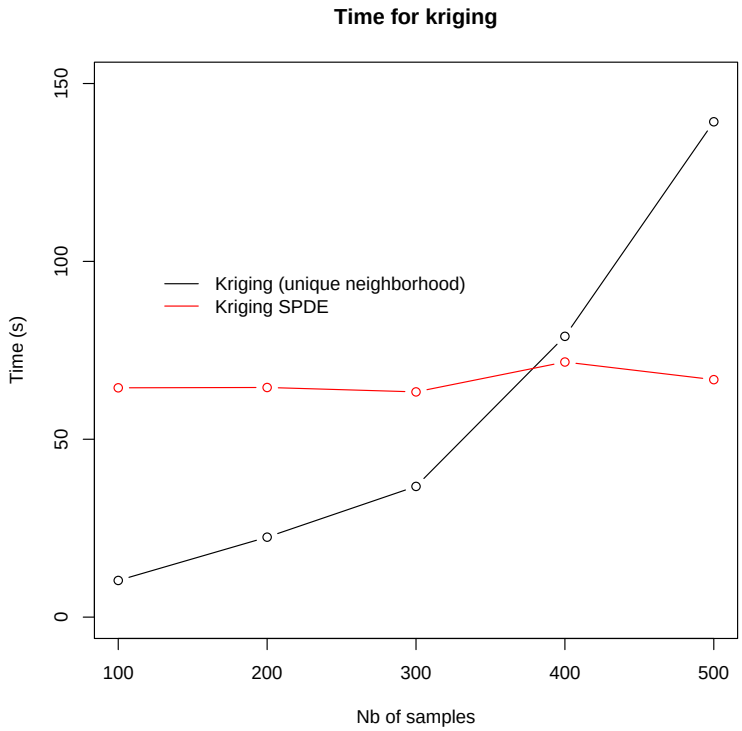

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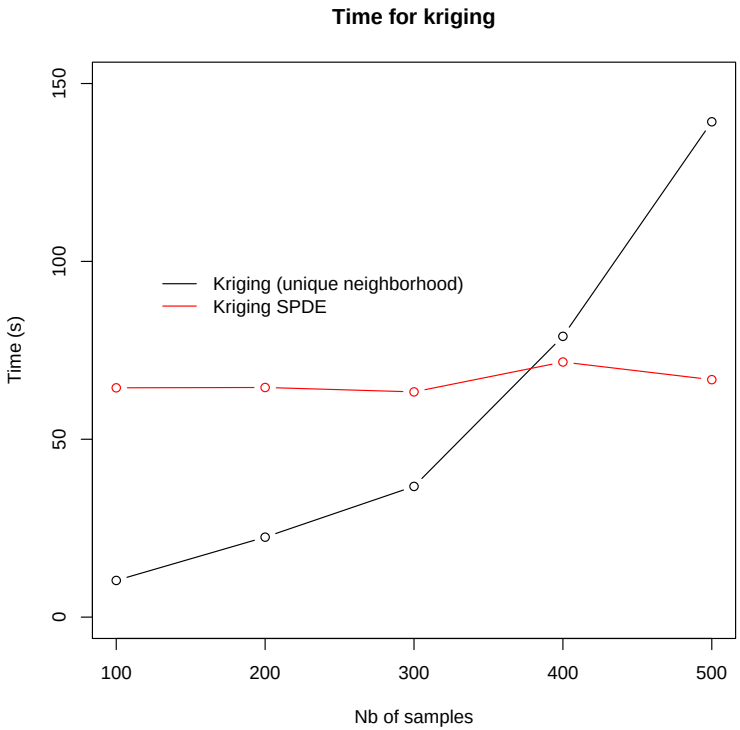
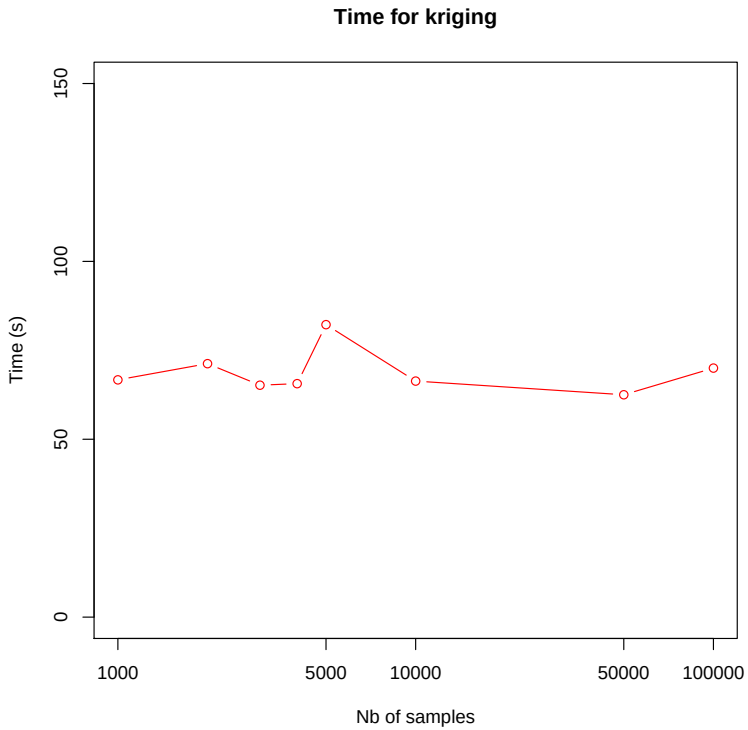
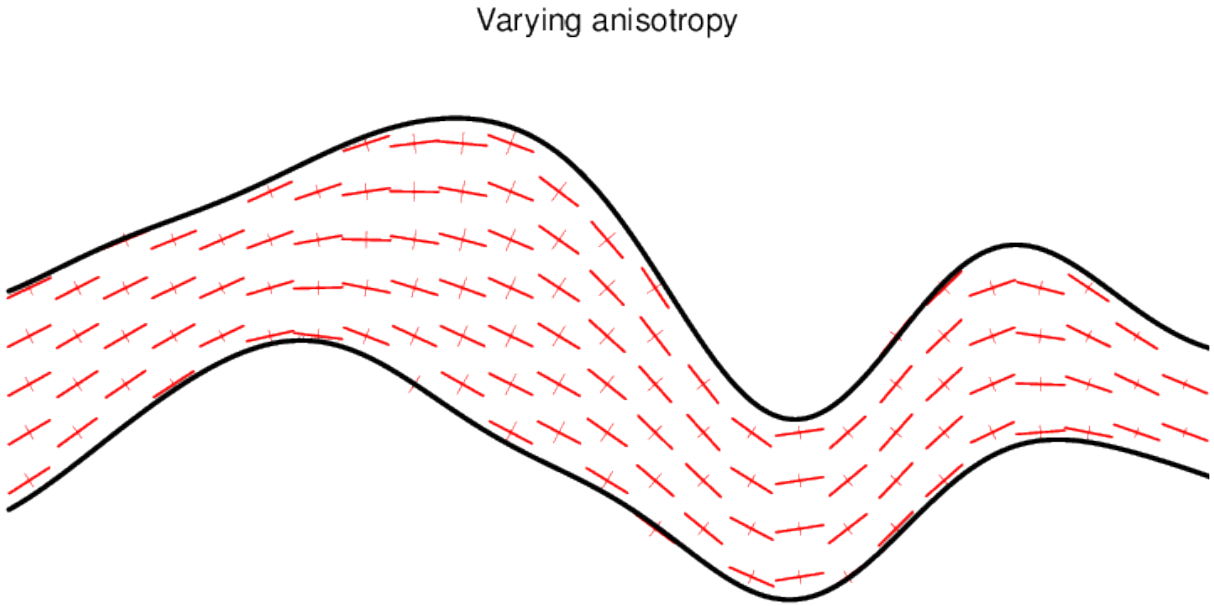
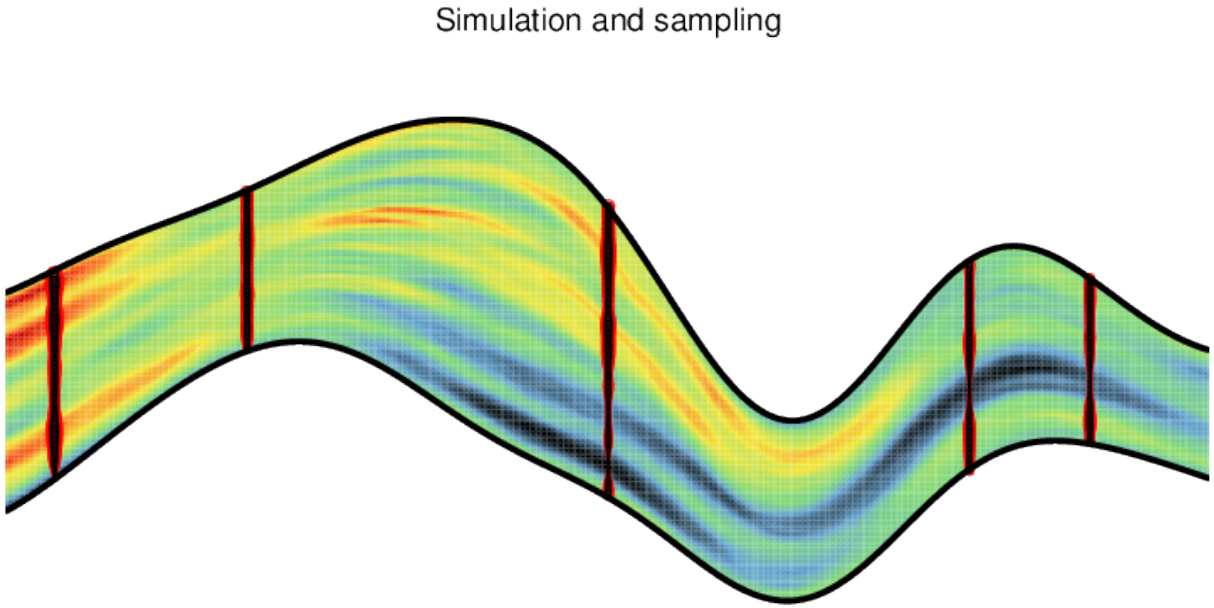




Varying anisotropy

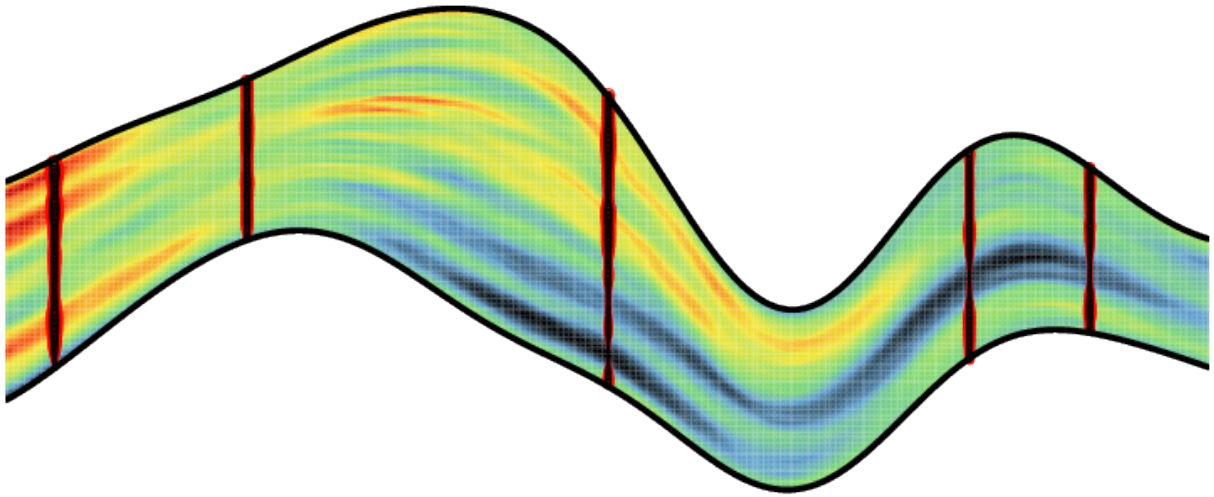


Varying anisotropy

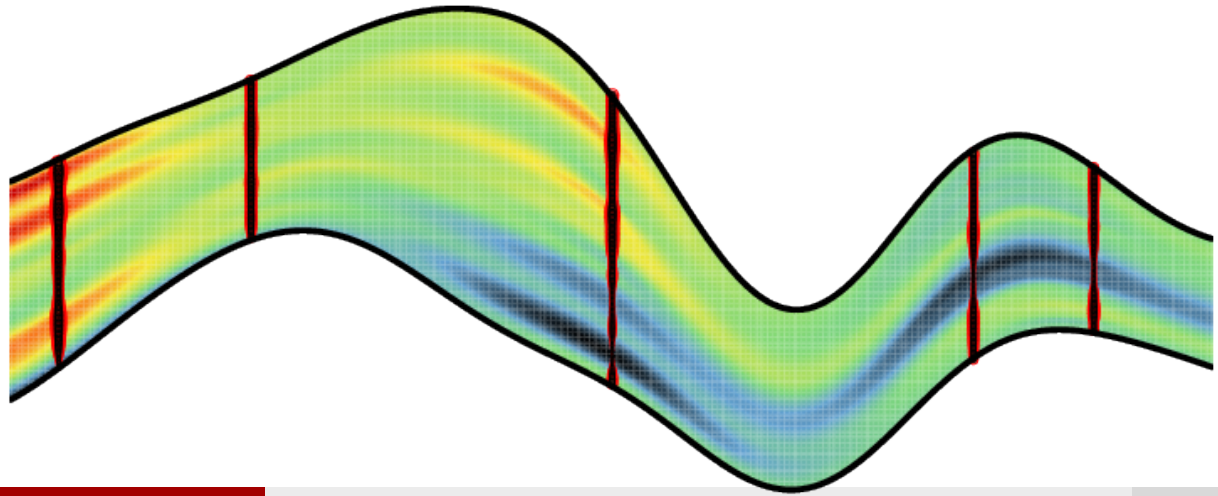


Varying anisotropy

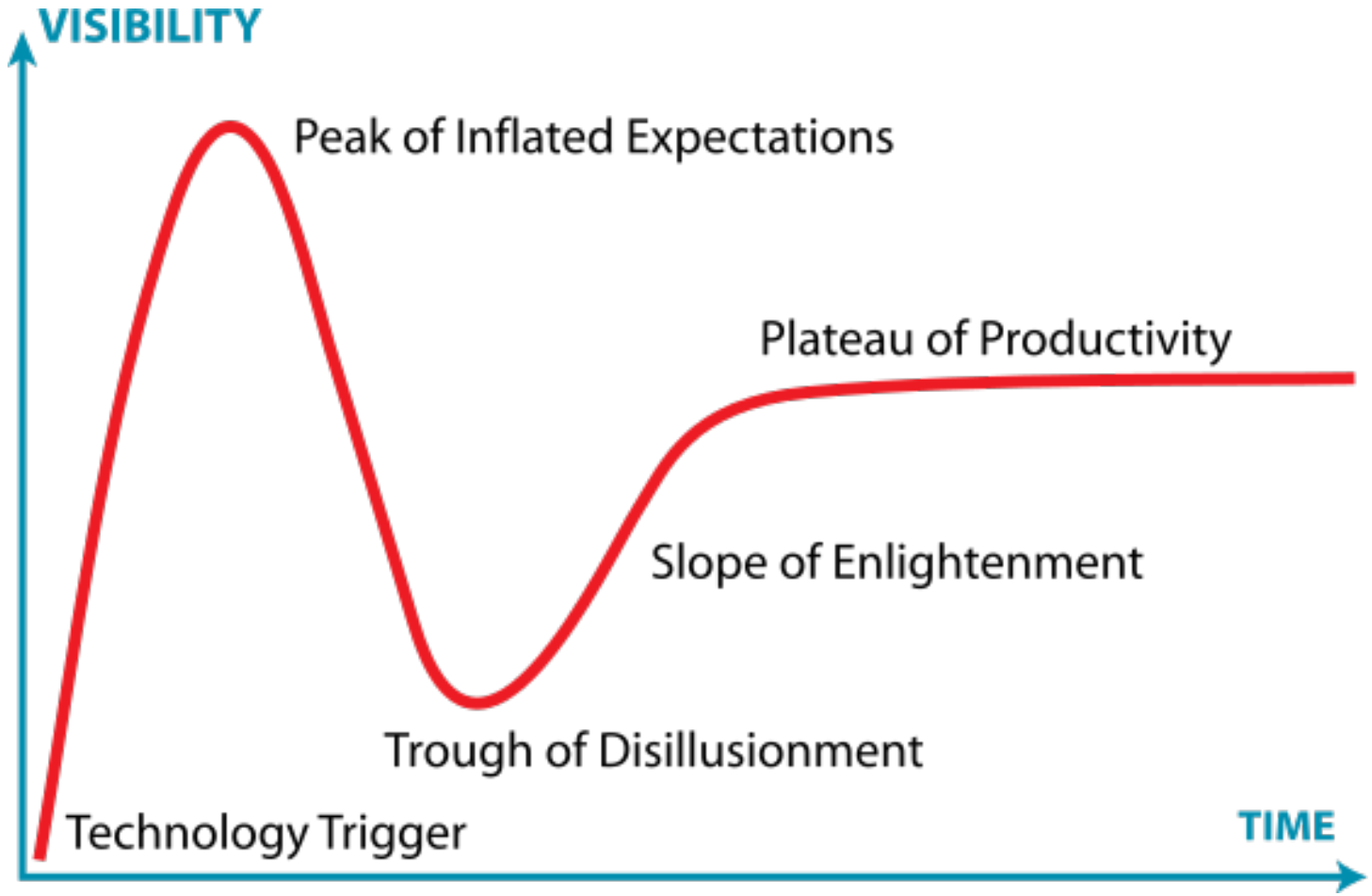
Simulation and sampling



Simple kriging with SPDE



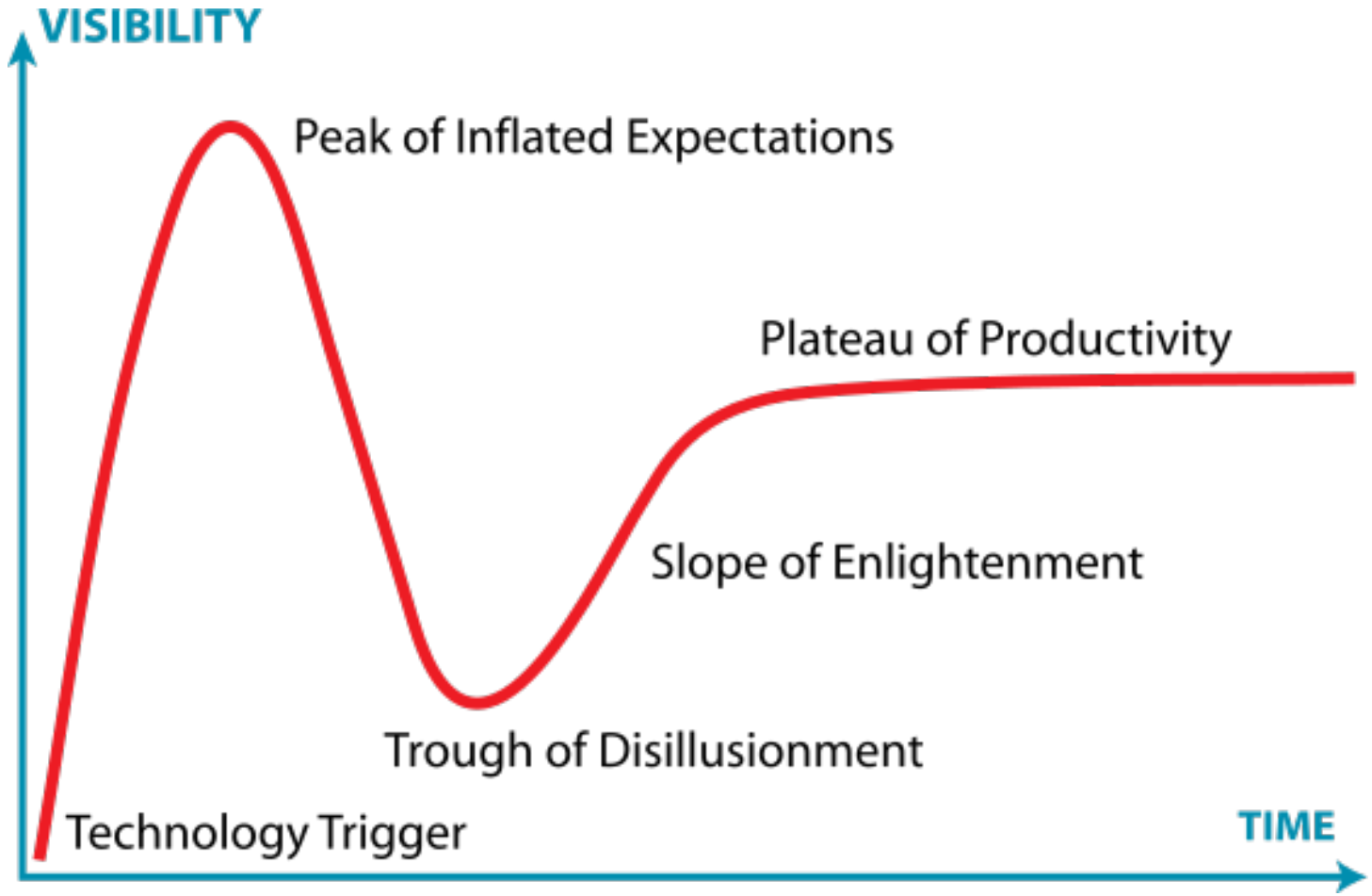
Gartner Hype Cycle



Expectations

- Outperform the time performances of "old geostatistics" in 3D
- Handle one million of targets
- OK to work with Matérn only (or Markovian approximations)
- Handle nested models (nugget effect + 2 basic structures)
- Handle several variables (co-kriging with linear model of coregionalisation)
- Develop block simulation
- Handle varying anisotropies

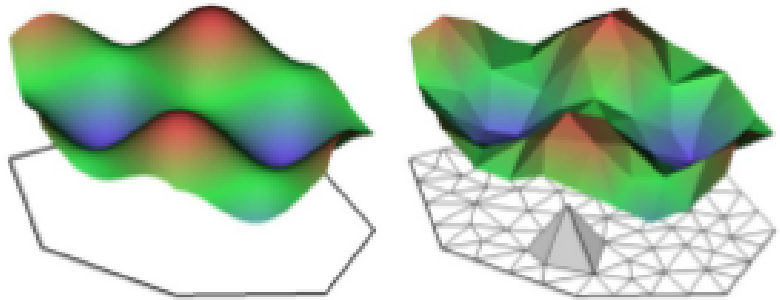
Gartner Hype Cycle



Issues with the 3D

- The system size quickly increases
- The sparsity of the precision matrix decreases
- The Cholesky factorization of Q_{TT} is not possible anymore for a system size greater than 200 000

Finite elements approximation

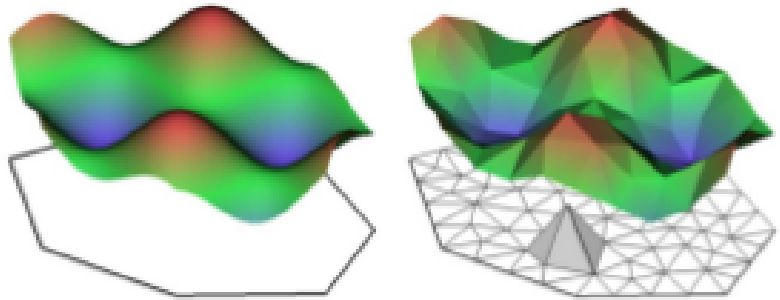


Cameletti et al. (2013)

- For kriging, we can use a coarse meshing to reduce the system size and interpolate the result inside the elements

$$Z(s) = \sum_{i=1}^{N} z_i \psi_i(s)$$

Finite elements approximation



Cameletti et al. (2013)

- For kriging, we can use a coarse meshing to reduce the system size and interpolate the result inside the elements

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- But simulations have to be performed on the final target grid in order to reproduce the local variability

Separate the problems

- Work with several meshings : one for the simulation (fine) and one for the kriging (coarse)
- Find an efficient algorithm to perform non conditional simulation on the fine meshing (Pereira and Desassis, 2018)
- Perform the kriging of the residuals on the coarse mesh and interpolate linearly the result on the fine mesh

Model

$$\tilde{Z}(s_i) = Z(s_i) + \varepsilon(s_i)$$

with

- Z solution of a SPDE
- $\varepsilon(s_i)$ is a measurement error with variance σ_i^2
- The errors are uncorrelated

We want to predict Z_T knowing the observations $\tilde{Z}_D$

- Problem: the precision matrix of $(Z_T, \tilde{Z}_D)$ is not sparse
- Solution: consider the larger vector $(Z_{T \cup D}, \tilde{Z}_D)$
- Its precision matrix is sparse
- The size of the system to solve is $N_T + N_D$
- Can we avoid to put vertices at data locations?

- Finite element formulation

$$Z(s) = \sum_{i=1}^{N} z_i \psi_i(s)$$

- $Z = (z_1, \ldots, z_N)$ has covariance matrix Σ and precision matrix Q
- $\varepsilon = (\varepsilon(s_1), \ldots, \varepsilon(s_n))$ has diagonal variance matrix E (with i^{th} term σ_i^2)
- The data model is

$$\tilde{Z}_D = A^T Z + \varepsilon$$

where A is the $N \times n$ sparse matrix with elements $a_{ij} = \psi_i(s_j)$

Covariance and precision matrices

The covariance matrix of $(Z, \tilde{Z}_D)$ is

$$\tilde{\Sigma} = \begin{pmatrix} \Sigma & \Sigma A \\ A^T \Sigma & A^T \Sigma A + E \end{pmatrix}$$

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And the precision matrix is

$$\tilde{Q} = \begin{pmatrix} Q + AE^{-1}A^T & -AE^{-1} \\ -E^{-1}A^T & E^{-1} \end{pmatrix}$$

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And the precision matrix is

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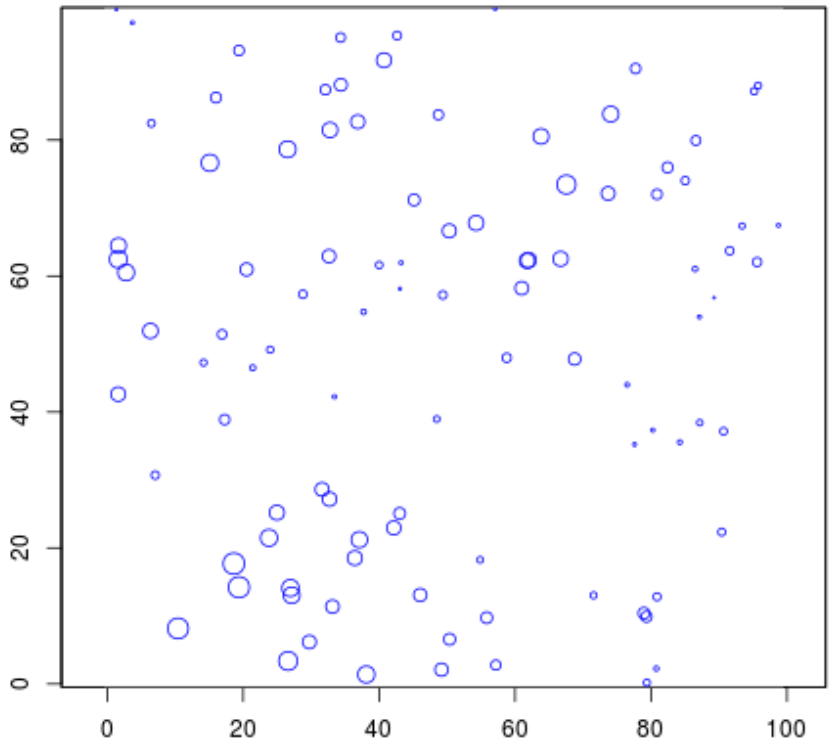
Therefore, the kriging of Z is given by

$$Z^\star = (Q + AE^{-1}A^T)^{-1}AE^{-1}\tilde{Z}_D$$

Does it work?

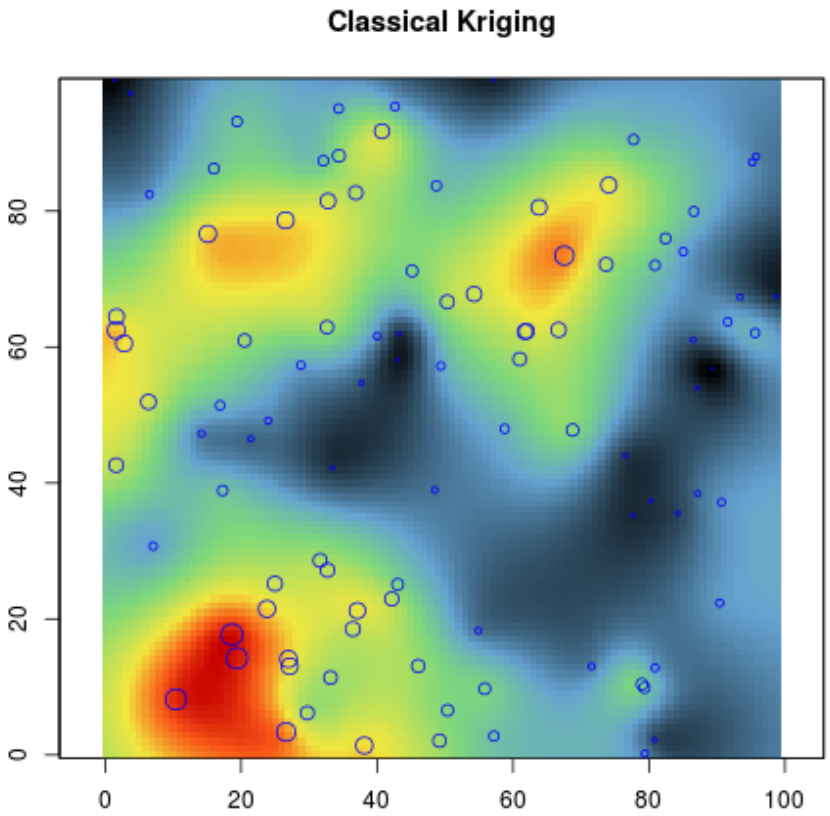
Comparison with kriging (Matérn with smoothness $\nu = 1$ and range $= 40$)



100 observations, 50×50 grid

Does it work?

Comparison with kriging (Matérn with smoothness $\nu = 1$ and range $= 40$)



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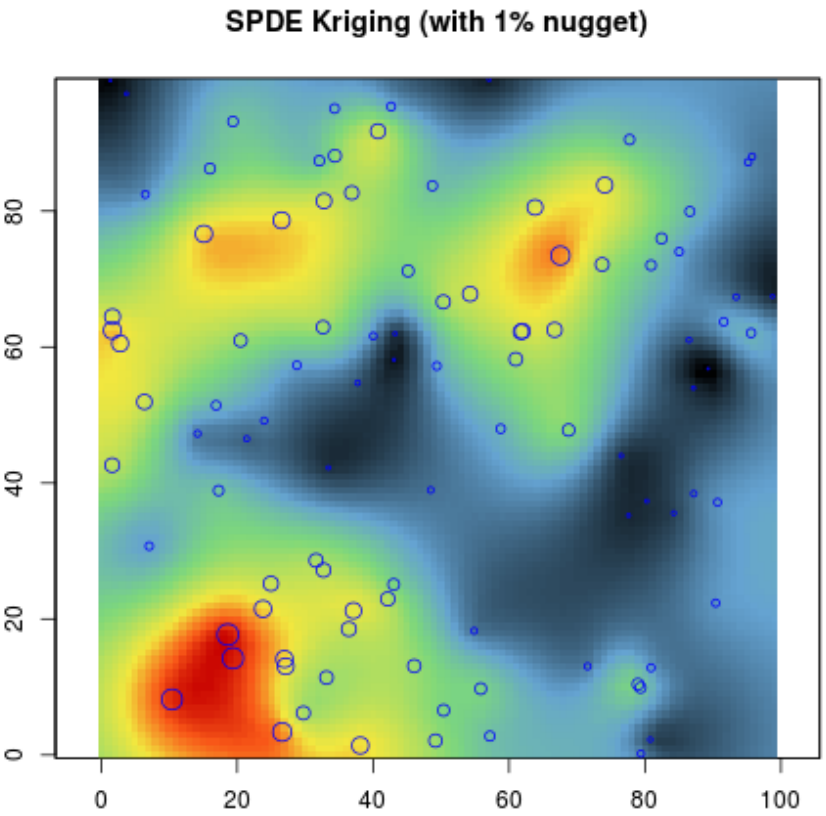

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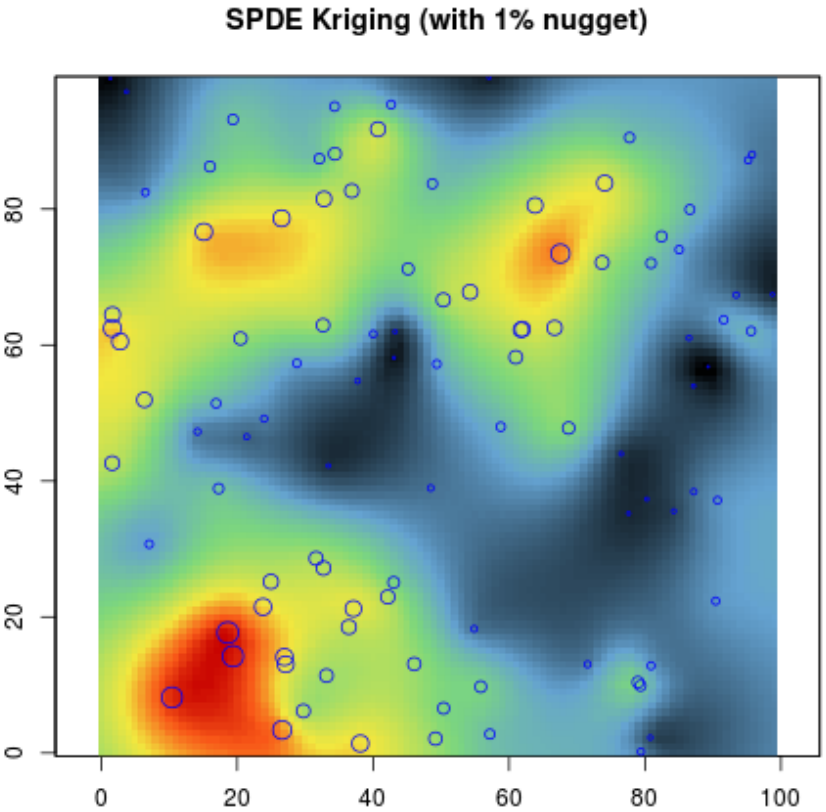

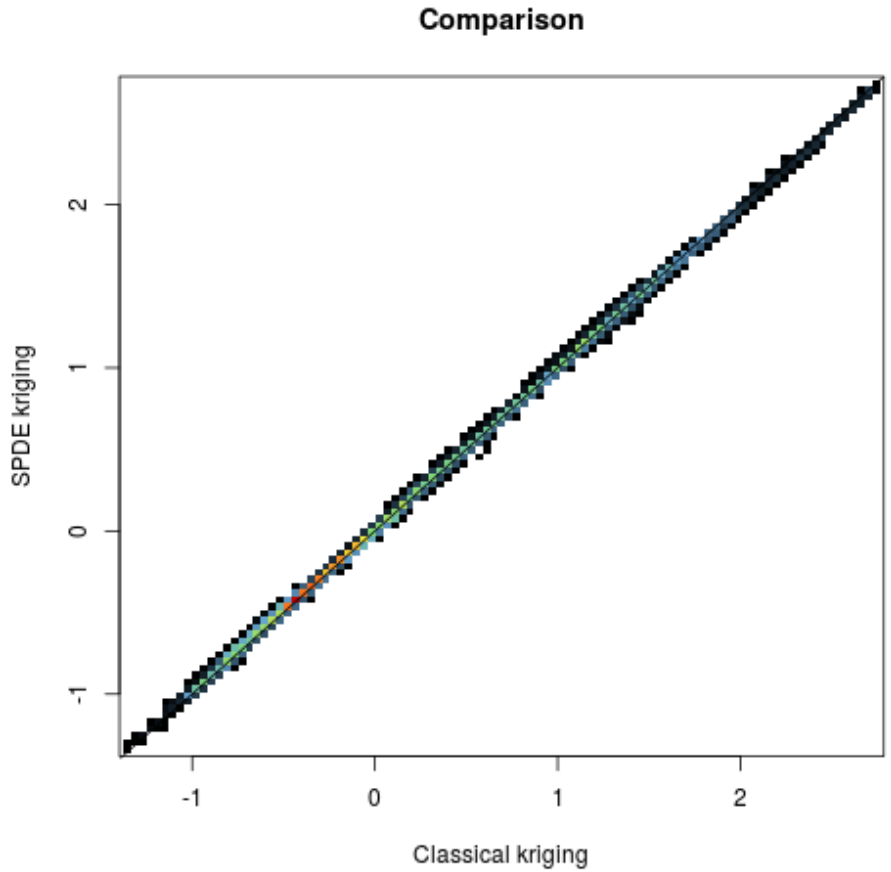

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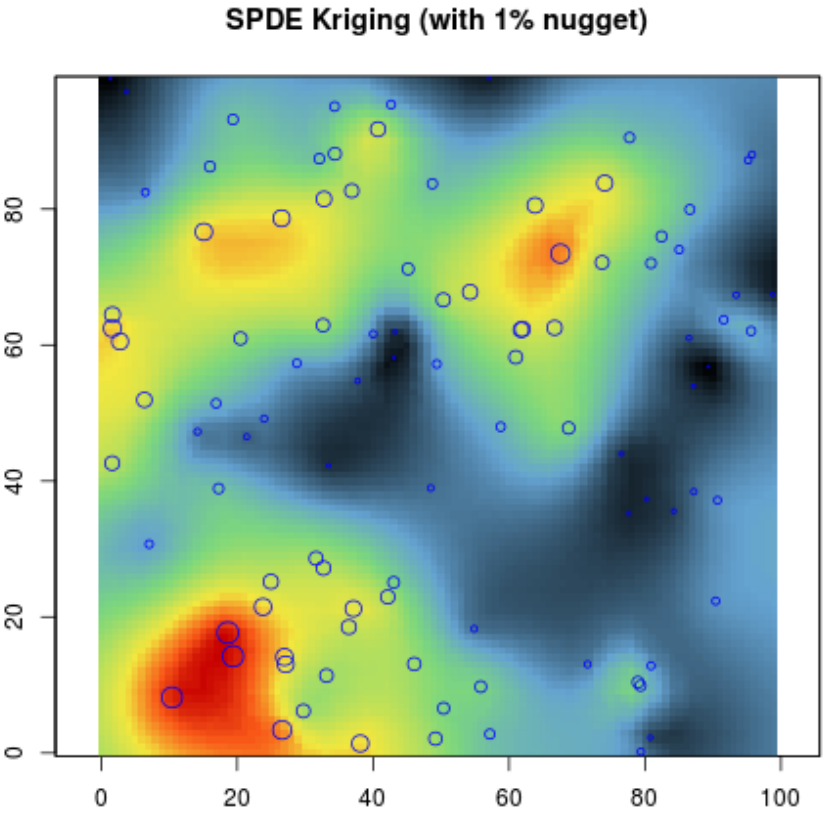
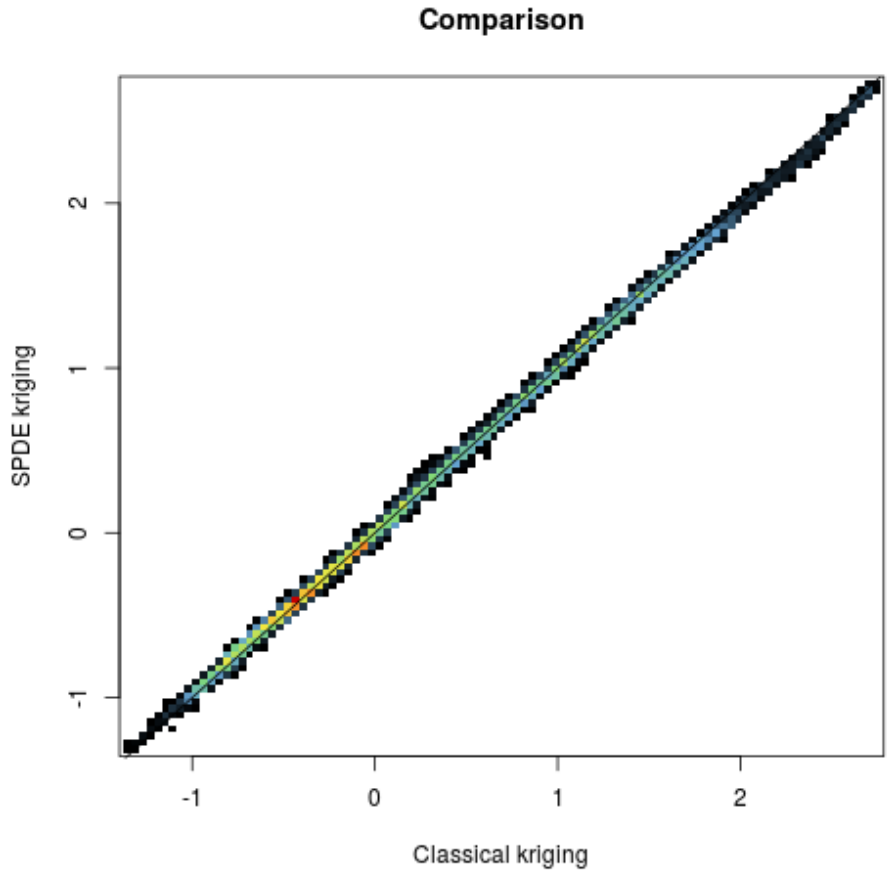
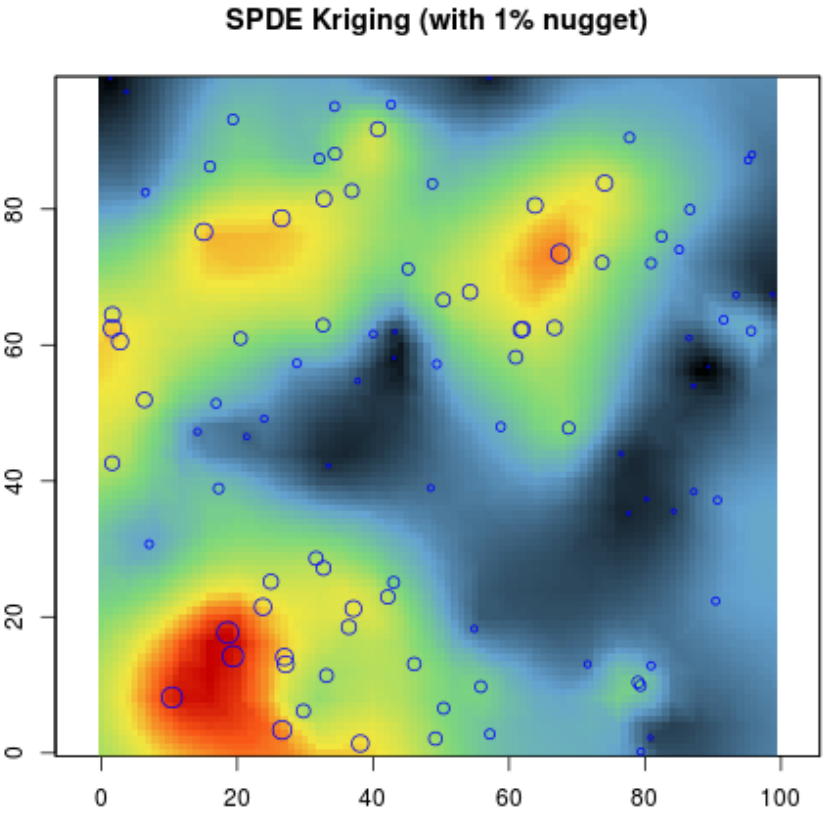


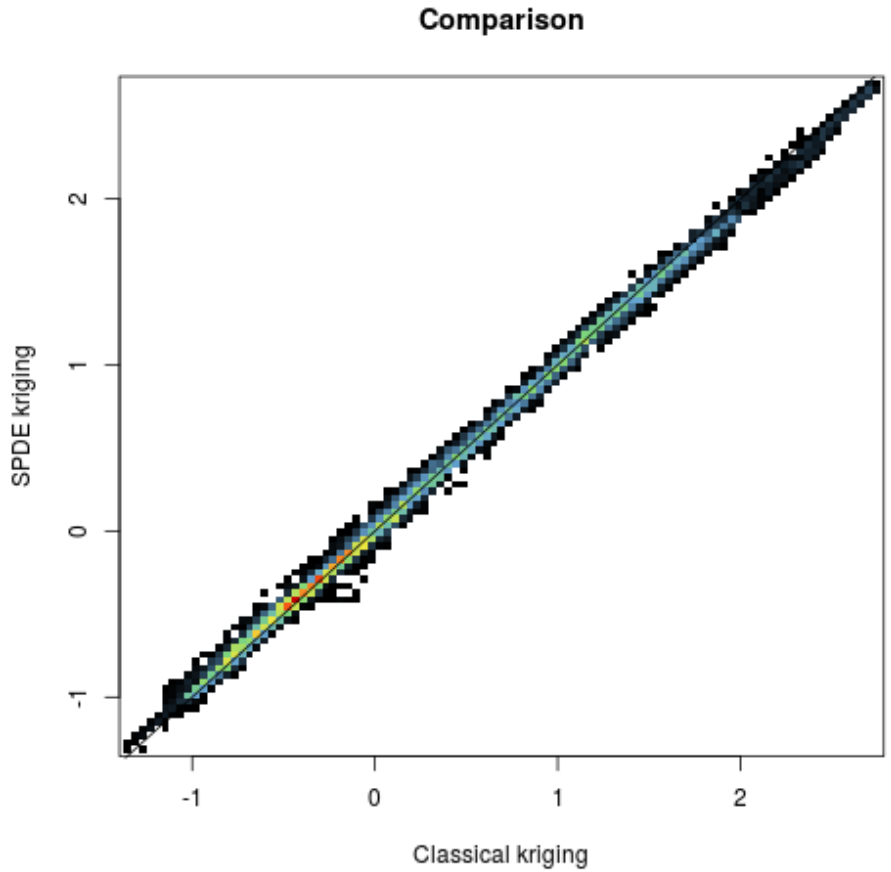


100 observations, 33×33 grid

Does it work?

Comparison with kriging (Matérn with smoothness $\nu = 1$ and range $= 40$)

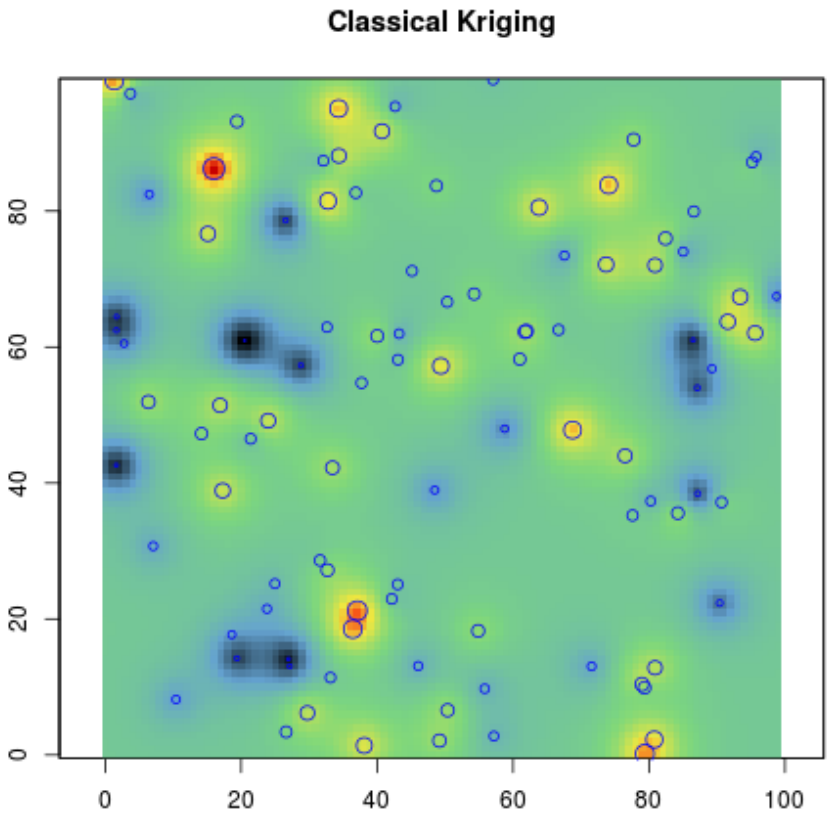




100 observations, 25×25 grid

Does it work?

Comparison with kriging (Matérn with smoothness $\nu = 1$ and range $= 5$)



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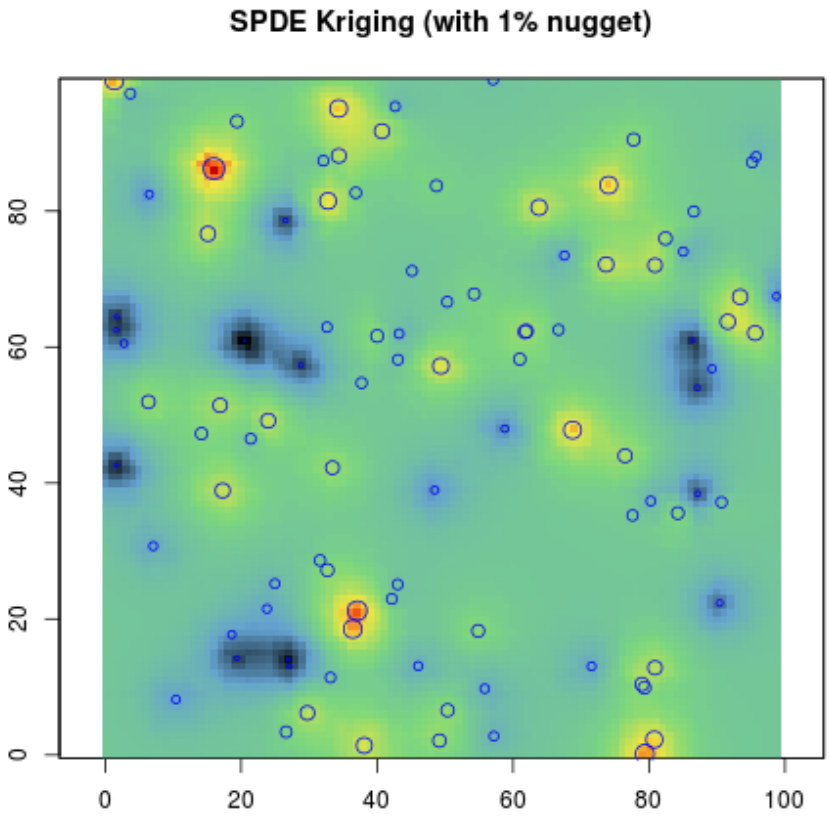

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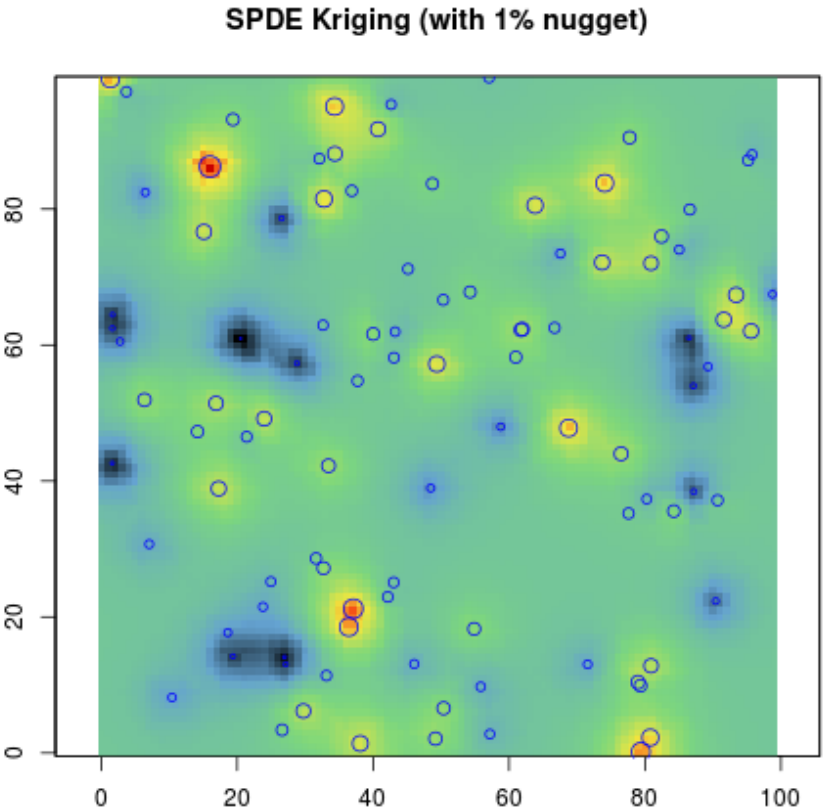

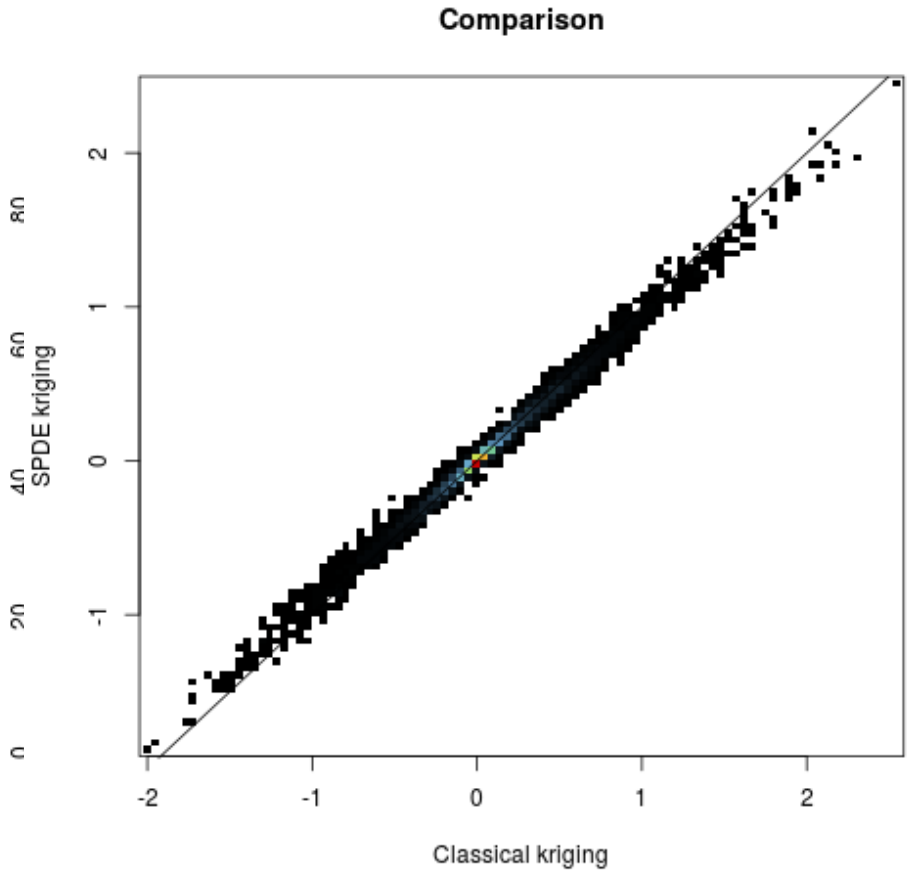

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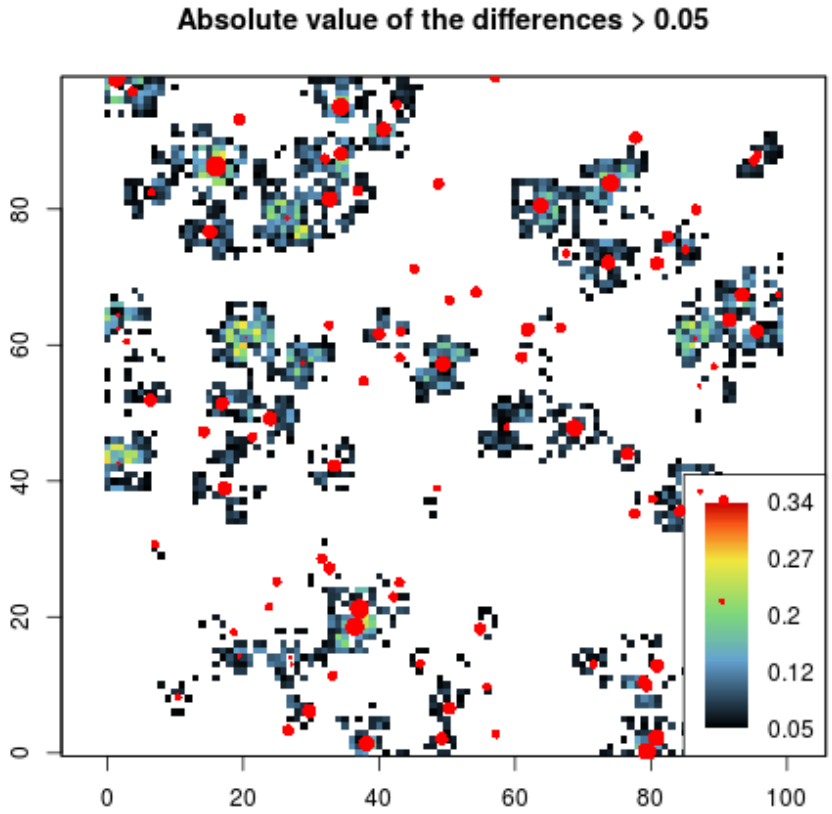

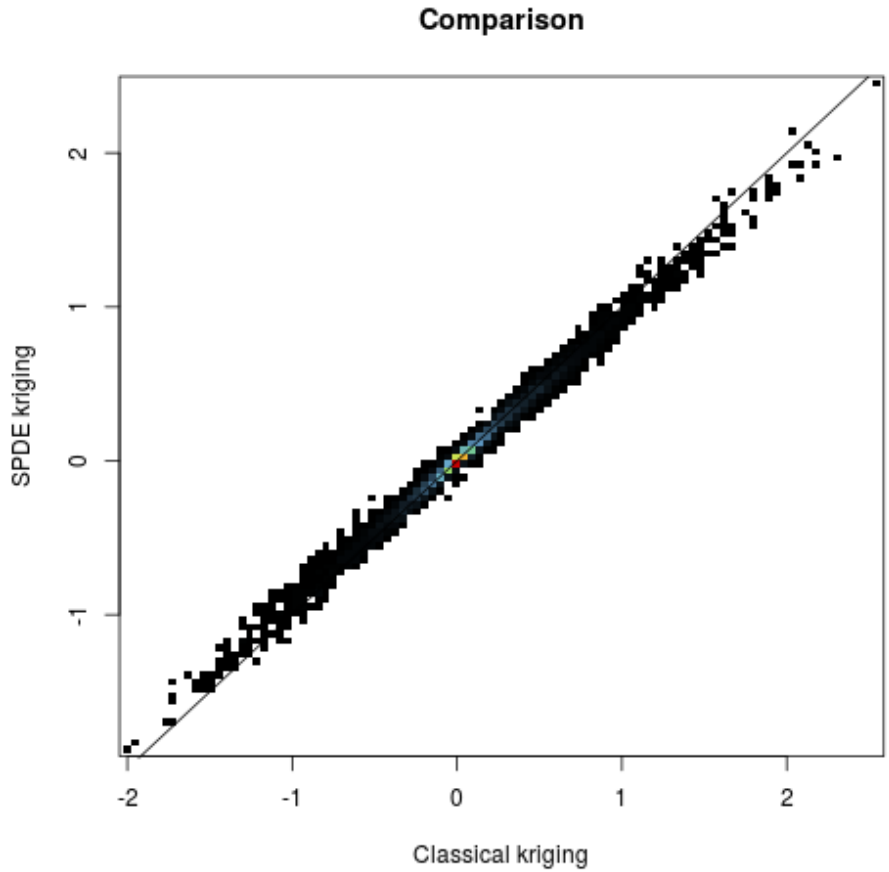

100 observations, 33×33 grid

First conclusions

- When the range (or ν) is large, the meshing can be coarse
- When the range is small, it is useless to put vertices far from data locations (or we can patch the vertices with the mean)

Nested Models

$$Z(s) = \sum_{k=1}^{K} Z_k(s)$$

where the Z_k are independant random fields with covariance C_k

- Z has covariance $C = \sum_{k=1}^{K} C_k$
- We don't know how to approximate Z with a Markovian Random Field

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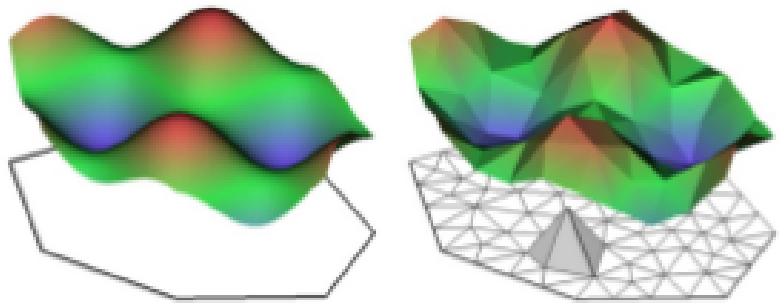

Cameletti et al. (2013)

$$Z(s) = \sum_{k=1}^{K} \sum_{i=1}^{N_k} z_i^{(k)} \psi_i^{(k)}(s)$$

Model

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- The data model is

$$\tilde{Z}_D = A_k^T Z_k + \varepsilon$$

where A_k is the $N_k \times n$ sparse matrix with elements $a_{ij} = \psi_i^{(k)}(s_j)$

Covariance and precision matrices of $(Z_1, \ldots, Z_K, \tilde{Z}_D)$

$$\tilde{\Sigma} = \begin{pmatrix} \Sigma_1 & 0 & \ldots & 0 & \Sigma_1 A_1 \\ 0 & \Sigma_2 & \ldots & 0 & \Sigma_2 A_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \Sigma_K & \Sigma_K A_K \\ A_1^T \Sigma_1 & A_2^T \Sigma_2 & \ldots & A_K^T \Sigma_K & \sum_{k=1}^K A_k^T \Sigma_k A_k + E \end{pmatrix}$$

Covariance and precision matrices of $(Z_1, \ldots, Z_K, \tilde{Z}_D)$

$$\tilde{Q} = \begin{pmatrix} Q_1 + A_1 E^{-1} A_1^T & A_1 E^{-1} A_2^T & \ldots & A_1 E^{-1} A_K^T & -A_1 E^{-1} \\ A_2 E^{-1} A_1^T & Q_2 + A_2 E^{-1} A_2^T & \ldots & A_2 E^{-1} A_K^T & -A_2 E^{-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ A_K E^{-1} A_1^T & A_K E^{-1} A_2^T & \ldots & Q_K + A_K E^{-1} A_K^T & -A_K E^{-1} \\ -E^{-1} A_1^T & -E^{-1} A_2^T & \ldots & -E^{-1} A_K^T & E^{-1} \end{pmatrix}$$

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- Use block Gauss-Seidel algorithm to solve the system
- Each subsystem is solved from the Cholesky factorization of

$$Q + A_k E^{-1} A_k^T$$

- The algorithm converges in a few iterations

Direct Block Simulation (stationary case)

The Discret Gaussian Model

We consider $v_1, \ldots, v_N$ a partition of the domain D where the sets v_i are equal up to a translation

Hypothesis and notations

- x is a fixed location and $\underline{x}$ is a uniform location within a block v
- $Z(\underline{x}) = \varphi(Y(\underline{x}))$ where $Y(\underline{x})$ is a standard Gaussian variable
- C_Y is the covariance of the stationary random field $\{Y(x), x \in D\}$
- $Z(v) = \varphi_v(Y_v)$ where Y_v is a standard Gaussian variable

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- If the observation locations $\underline{x_1}, \ldots, \underline{x_n}$ are uniform within their block and mutually independant then $(Y(\underline{x_1}), \ldots, Y(\underline{x_n}), Y_{v_1}, \ldots, Y_{v_N})$ is a Gaussian vector

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- $Y(\underline{x_i})$ and $Y(\underline{x_j})$ are independant conditionally to $Y_{v(i)}$ and $Y_{v(j)}$ the Gaussian values of the blocks in which $\underline{x_i}$ and $\underline{x_j}$ belongs

Consequences (Emery, 2007)

- The correlation r between $Y(\underline{x_i})$ and $Y_{v(i)}$ is deduced from the covariance function of the punctual Gaussian Y :

$$r^2 = \frac{1}{|v|^2} \int_v \int_v C_Y(x-y)dxdy$$

- The covariance $C_v(h)$ between Y_v and Y_{v+h} is given by

$$C_v(h) = \mathrm{Cov}(Y_v, Y_{v+h}) = \frac{1}{r^2|v|^2} \int_v \int_{v+h} C_Y(x-y)dxdy$$

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- $\mathrm{Cov}(Y(\underline{x}_i), Y_v) = r\mathrm{Cov}(Y_{v(i)}, Y_v)$
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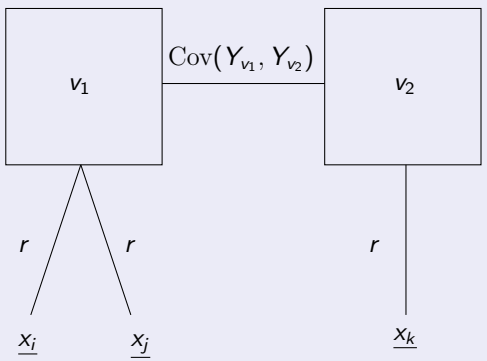

Covariance matrix of $(Y_{v_1}, \ldots, Y_{v_N}, Y(\underline{x}_1), \ldots, Y(\underline{x}_n))$

$$\begin{pmatrix} \Sigma_v & r\Sigma_v A^T \\ rA\Sigma_v & r^2 A\Sigma_v A^T + (1-r^2)I \end{pmatrix}$$

where

- Σ_v is built from the block covariance C_v
- A is the $n \times N$ matrix defined by $a_{ij} = 1_{\underline{x}_i \in v_j}$

Precision matrix of $(Y_{v_1}, \ldots, Y_{v_N}, Y(\underline{x}_1), \ldots, Y(\underline{x}_n))$

$$\frac{1}{1-r^2}\begin{pmatrix} (1-r^2)Q_v + r^2 A^T A & -rA^T \\ -rA & I \end{pmatrix}$$

where

- Q_v is the precision matrix built from SPDE
- A is the $n \times N$ matrix defined by $a_{ij} = 1_{\underline{x}_i \in v_j}$

Conclusions

- The SPDE approach should be able to replace traditional geostatistics
- Direct Block Simulation for non-stationary models has to be developped
- Inference for varying parameters should be developped
- It should allow to integrate geological knowledge

References

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