

Fast Update of Conditional Simulation Ensembles

Clément Chevalier¹, David Ginsbourger¹ and Xavier Emery²

Chorus Workshop
Kriging and Gaussian processes for computer experiments
Institut Henri Poincaré, Paris, April 30th 2014.

¹IMSV, University of Bern

²University of Chile, Santiago

Outline

- 1 Motivations, context
- 2 Main result
- 3 Algorithm
- 4 Some perspectives

Outline

- 1 Motivations, context
- 2 Main result
- 3 Algorithm
- 4 Some perspectives

Motivations, context

General kriging settings: L^2 random field Z indexed by $D \subset \mathbb{R}^d$

- known covariance function $k(\cdot, \cdot)$
- mean function is a linear combination of known basis functions.

Motivations, context

General kriging settings: L^2 random field Z indexed by $D \subset \mathbb{R}^d$

- known covariance function $k(\cdot, \cdot)$
- mean function is a linear combination of known basis functions.

$n \geq 0$ obs. $Z(\mathbf{X}_n)$ at points $\mathbf{X}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$,

$q \geq 1$ new obs. $Z(\mathbf{X}_q)$ at points $\mathbf{X}_q = \{\mathbf{x}_{n+1}, \dots, \mathbf{x}_{n+q}\}$.

$M \geq 1$ conditional simulations of Z ; conditioned on the obs. $Z(\mathbf{X}_n)$.

Motivations, context

General kriging settings: L^2 random field Z indexed by $D \subset \mathbb{R}^d$

- known covariance function $k(\cdot, \cdot)$
- mean function is a linear combination of known basis functions.

$n \geq 0$ obs. $Z(\mathbf{X}_n)$ at points $\mathbf{X}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$,

$q \geq 1$ new obs. $Z(\mathbf{X}_q)$ at points $\mathbf{X}_q = \{\mathbf{x}_{n+1}, \dots, \mathbf{x}_{n+q}\}$.

$M \geq 1$ conditional simulations of Z ; conditioned on the obs. $Z(\mathbf{X}_n)$.

Update problem

Can we take advantage of previous computations to quickly obtain M conditional simulations conditioned on the $n + q$ observations $Z(\mathbf{X}_n), Z(\mathbf{X}_q)$?

Motivations, context

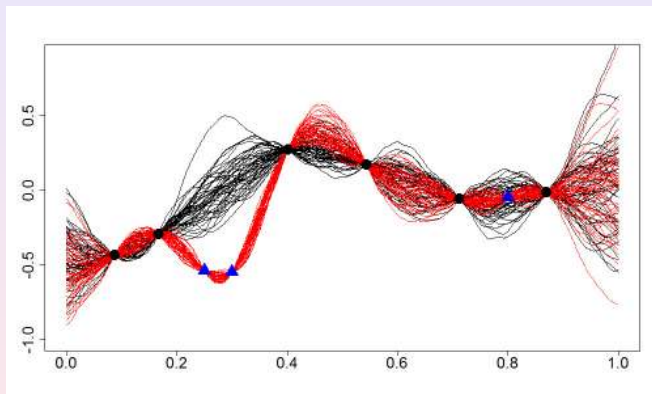


Figure: GRF simulations conditioned on $n = 6$ observations (black curves) and $n + q = 9$ observations (red curves). The black circles stand for $n = 6$ initial observations and the blue triangles represent $q = 3$ additional observations.

Outline

- 1 Motivations, context
- 2 Main result**
- 3 Algorithm
- 4 Some perspectives

Main result

Update of GRF conditional simulations

Let $Z^{(1)}, \dots, Z^{(M)}$ be independent replicates of $Z|Z(\mathbf{X}_n)$, i.e., simulations of Z conditioned on the n observations $Z(\mathbf{X}_n)$. Then, the random fields

$$Z^{*(i)} := Z^{(i)} + \lambda_{n,q}^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)) \quad (i \in \{1, \dots, M\}) \quad (1)$$

have the same conditional distribution as Z conditioned on the $n+q$ observations $Z(\mathbf{X}_n), Z(\mathbf{X}_q)$ for any conditioning values $\mathbf{z}_n \in \mathbb{R}^n$, $\mathbf{z}_q \in \mathbb{R}^q$.

Furthermore, the kriging weights $\lambda_{n,q}$ are given by:

$$\lambda_{n,q}(\mathbf{x}) = K_{n,q}^{-1} k_n(\mathbf{x}, \mathbf{X}_q),$$

where $K_{n,q} := k_n(\mathbf{X}_q, \mathbf{X}_q) = (k_n(\mathbf{x}_{n+i}, \mathbf{x}_{n+j}))_{1 \leq i, j \leq q}$.

Main result

Two ingredients are used to prove this property:

Main result

Two ingredients are used to prove this property:

(1) Kriging residual (or kriging conditioning) algorithm:

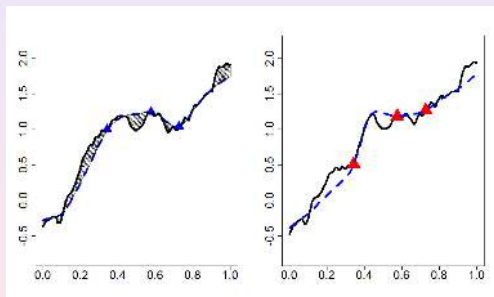


Figure: Left: kriging residual obtained by non-conditional simulation of a replicate $Z^{(i)}$ of a non-stationary GRF Z (black solid line) and its simple kriging mean (blue dashed line) based on $q = 3$ observations (blue triangles) at a design \mathbf{X}_q . Right: conditional simulation of Z (solid black line).

Main result

(2) The Kriging update formulas:

$$M_{n+q}(\mathbf{x}) = M_n(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - M_n(\mathbf{X}_q)) \quad (2)$$

$$k_{n+q}(\mathbf{x}, \mathbf{x}') = k_n(\mathbf{x}, \mathbf{x}') - \lambda_{n,q}(\mathbf{x})^\top K_{n,q} \lambda_{n,q}(\mathbf{x}') \quad (3)$$

$$\lambda_{n,q}(\mathbf{x}) = K_{n,q}^{-1} k_n(\mathbf{x}, \mathbf{X}_q) \quad (4)$$

Main result

(2) The Kriging update formulas:

$$M_{n+q}(\mathbf{x}) = M_n(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - M_n(\mathbf{X}_q)) \quad (2)$$

$$k_{n+q}(\mathbf{x}, \mathbf{x}') = k_n(\mathbf{x}, \mathbf{x}') - \lambda_{n,q}(\mathbf{x})^\top K_{n,q} \lambda_{n,q}(\mathbf{x}') \quad (3)$$

$$\lambda_{n,q}(\mathbf{x}) = K_{n,q}^{-1} k_n(\mathbf{x}, \mathbf{X}_q) \quad (4)$$

The kriging residual algorithm updates a GP realization Z by adding the **difference between two updated kriging mean function** to the “old” GP simulation. Thus, only this difference needs to be computed:

Main result

(2) The Kriging update formulas:

$$M_{n+q}(\mathbf{x}) = M_n(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - M_n(\mathbf{X}_q)) \quad (2)$$

$$k_{n+q}(\mathbf{x}, \mathbf{x}') = k_n(\mathbf{x}, \mathbf{x}') - \lambda_{n,q}(\mathbf{x})^\top K_{n,q} \lambda_{n,q}(\mathbf{x}') \quad (3)$$

$$\lambda_{n,q}(\mathbf{x}) = K_{n,q}^{-1} k_n(\mathbf{x}, \mathbf{X}_q) \quad (4)$$

The kriging residual algorithm updates a GP realization Z by adding the **difference between two updated kriging mean function** to the “old” GP simulation. Thus, only this difference needs to be computed:

This **difference** reduces to $\lambda_{n,q}^\top (Z(\mathbf{X}_q) - \mathbf{Z}^{(i)}(\mathbf{X}_q))$.

Outline

- 1 Motivations, context
- 2 Main result
- 3 Algorithm**
- 4 Some perspectives

Algorithm

Let's assume that we have M GRF simulations in p points
 $\mathbf{E}_p = (\mathbf{e}_1, \dots, \mathbf{e}_p)$ conditioned on n obs. at points \mathbf{X}_n .

Algorithm

Let's assume that we have M GRF simulations in p points
 $\mathbf{E}_p = (\mathbf{e}_1, \dots, \mathbf{e}_p)$ conditioned on n obs. at points \mathbf{X}_n .

Goal: "update" these simulations by conditioning on q additional obs.
at points \mathbf{X}_q .

Algorithm

Let's assume that we have M GRF simulations in p points
 $\mathbf{E}_p = (\mathbf{e}_1, \dots, \mathbf{e}_p)$ conditioned on n obs. at points \mathbf{X}_n .

Goal: “update” these simulations by conditioning on q additional obs.
 at points \mathbf{X}_q .

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Algorithm

Let's assume that we have M GRF simulations in p points $\mathbf{E}_p = (\mathbf{e}_1, \dots, \mathbf{e}_p)$ conditioned on n obs. at points \mathbf{X}_n .

Goal: “update” these simulations by conditioning on q additional obs. at points \mathbf{X}_q .

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Algorithm in 3 steps:

- 1 Simulate $Z^{(i)}(\mathbf{X}_q)$ in the case $\mathbf{X}_q \not\subseteq \mathbf{E}_p$
- 2 Compute the q kriging weights $\lambda_{n,q}(\mathbf{x})$ for all $\mathbf{x} \in \mathbf{E}_p$.
- 3 Update the GRF simulations.

Algorithm

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Algorithm

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Step 1: Simulate $Z^{(i)}(\mathbf{X}_q)$ in the case $\mathbf{X}_q \notin \mathbf{E}_p$.

- Requires to simulate conditionally on $n + p$ observations.
- $(n + p) \times (n + p)$ matrix inversion: $O(n + p)^3$ cost.

Algorithm

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Step 1: Simulate $Z^{(i)}(\mathbf{X}_q)$ in the case $\mathbf{X}_q \notin \mathbf{E}_p$.

- Requires to simulate conditionally on $n + p$ observations.
- $(n + p) \times (n + p)$ matrix inversion: $O(n + p)^3$ cost.

Step 2: Compute the q kriging weights $\lambda_{n,q}(\mathbf{x})$ for all $\mathbf{x} \in \mathbf{E}_p$.

- Remember that: $\lambda_{n,q}(\mathbf{x}) = k_n(\mathbf{X}_q, \mathbf{X}_q)^{-1} k_n(\mathbf{x}, \mathbf{X}_q)$
- Thus, only kriging covariances need to be computed. No big matrix storage or inversion.
- This step is where the new algorithm is much faster than a “classical” kriging residual algorithm. Essentially, we gain a factor $O(n/q)$.

Algorithm

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Algorithm

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Step 3 has a $O(Mpq)$ cost in both the new and “classical” algorithm.

Algorithm

$$Z^{*(i)}(\mathbf{x}) := Z^{(i)}(\mathbf{x}) + \lambda_{n,q}(\mathbf{x})^\top (Z(\mathbf{X}_q) - Z^{(i)}(\mathbf{X}_q)), \quad i \in \{1, \dots, M\}, \quad \mathbf{x} \in \mathbf{E}_p$$

Step 3 has a $O(Mpq)$ cost in both the new and “classical” algorithm.

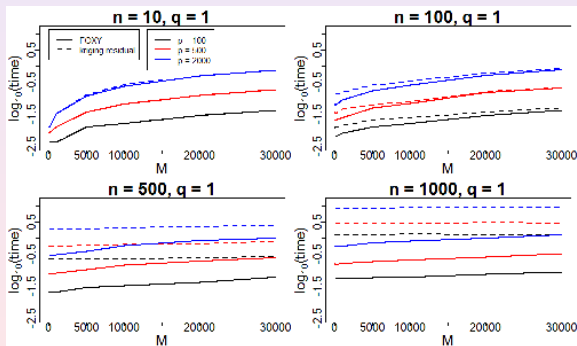


Figure: Computation times in function of M, n, p, q . (favorable case)

Outline

- 1 Motivations, context
- 2 Main result
- 3 Algorithm
- 4 Some perspectives**

Some perspectives

- Benefits of the update formula beyond computational savings.
- The formulas explicitly quantify the effect of the q newly assimilated observations on the sample paths.
- **Limitations:** covariance parameters need to be known.
- **Limitations:** numerical instabilities when applied recursively ?
- **Perspectives:** Efficient computations of Monte-Carlo estimates based on GRF simulations in sequential settings (e.g. IAGO algorithm of Villemonteix et. al. 2009).

References



C. Chevalier, X. Emery, D. Ginsbourger
Fast Update of Conditional Simulation Ensembles
submitted, preprint available on HAL.



J.P. Chilès and P. Delfiner
Geostatistics: Modeling Spatial Uncertainty
Wiley, New York, 2012.



X. Emery
The Kriging update equations and their application to the selection of
neighbouring data
Computational Geosciences, 13, 269–280, 2009.



C. Chevalier
Fast Uncertainty reduction strategies relying on Gaussian process models
Ph.D. thesis, University of Bern, 2013.



J. Villemonteix, E. Vazquez and E. Walter
An informational approach to the global optimization of expensive-to-evaluate
functions
Journal of Global Optimization 44(4):509–534 (2009).