Fast Update of Conditional Simulation Ensembles

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Outline

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

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Motivations, context

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

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$q \geq 1$ new obs. $Z(\boldsymbol{X}_q)$ at points $\boldsymbol{X}_q = \{\boldsymbol{x}_{n+1}, \ldots, \boldsymbol{x}_{n+q}\}$.
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Update problem

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

Motivations, context

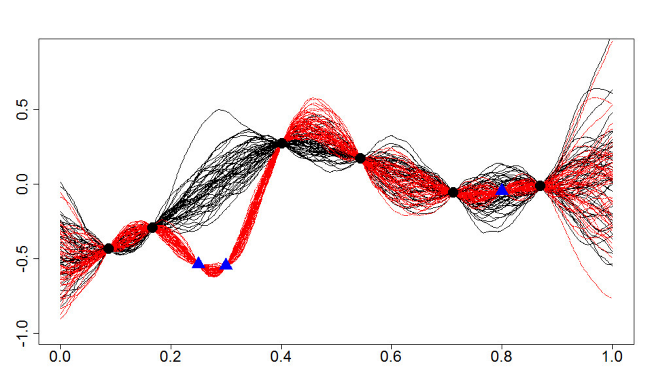

Figure: GRF simulations conditioned on $n = 6$ observations (black curves) and $n+q = 9$ observations (red curves). The black circles stand for $n = 6$ initial observations and the blue triangles represent $q = 3$ additional observations.

Outline

Main result

Update of GRF conditional simulations

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

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

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

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

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

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

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

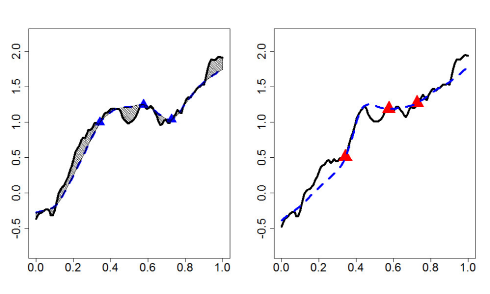

Figure: Left: kriging residual obtained by non-conditional simulation of a replicate $Z^{(i)}$ of a non-stationary GRF Z (black solid line) and its simple kriging mean (blue dashed line) based on $q = 3$ observations (blue triangles) at a design $\boldsymbol{X}_q$. Right: conditional simulation of Z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

Main result

(2) The Kriging update formulas:

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

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

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

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Algorithm

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Algorithm in 3 steps:

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

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Step 1: Simulate $Z^{(i)}(\boldsymbol{X}_q)$ in the case $\boldsymbol{X}_q \not\subseteq \boldsymbol{E}_p$.

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

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

- Remember that: $\lambda_{n,q}(\boldsymbol{x}) = k_n(\boldsymbol{X}_q, \boldsymbol{X}_q)^{-1} k_n(\boldsymbol{x}, \boldsymbol{X}_q)$
- 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 $O(n/q)$.

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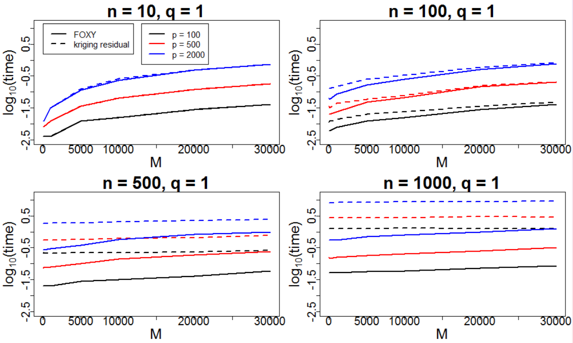

Figure: Computation times in function of M, n, p, q. (favorable case)

Outline

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).

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