Combining Kriging with optimal transport to estimate measure-valued data

Application to metamodeling in nuclear safety

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Introduction

- Analyzing complex industrial systems (e.g., nuclear reactors) relies on sophisticated computational codes
- Sophisticated $\rightarrow$ computationally intensive
- The amount of simulated data may be insufficient to accurately study a phenomenon across its entire domain of interest and also to quantify the uncertainty

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Goal : Build a fast-evaluating model (metamodel) to predict the output and thus generate new data

Ordinary kriging in $\mathbb{R}$ [1]

In this case, the computation code can be written as an unknown function:

$$f : \mathscr{D} \subset \mathbb{R}^d \to \mathbb{R}$$

and we consider the observations of f as realizations of a **spatially related** random process $\{\mathbf{Y}(x), x \in \mathscr{D}\}$. We denote by $(y(x_1), \ldots, y(x_n))$ the observations.

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Assumptions

- isotropic
- stationary
- unknown constant mean

BLUP

Given $(\mathbf{Y}(x_1), \ldots, \mathbf{Y}(x_n))$ coming from the stochastic process, the ordinary Kriging estimator of $\mathbf{Y}$ at a new point $x^\star \in \mathscr{D}$ is the Best Linear Unbiased Predictor (BLUP) written as:

$$\hat{\mathbf{Y}}(x^\star) = \sum_{i=1}^{n} \bar{\lambda}_i \mathbf{Y}(x_i) \tag{1}$$

where

$$\bar{\lambda} = \operatorname{argmin}_{\lambda=(\lambda_1,\ldots,\lambda_n)} \left\{ \mathbb{E}\left[\left\| \mathbf{Y}(x^\star) - \hat{\mathbf{Y}}_\lambda(x^\star) \right\|^2 \right], \sum_{i=1}^{n} \lambda_i = 1 \right\}, \tag{2}$$

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An estimation of $y(x^\star)$ denoted $\hat{y}(x^\star)$ is therefore given by (1) when replacing $\mathbf{Y}(x_i)$ by $y(x_i)$. This estimation can also be interpreted as a barycenter:

$$\hat{y}(x^\star) = \operatorname{argmin}_{y\in\mathbb{R}} \left\{ \sum_{i=1}^{n} \bar{\lambda}_i \| y(x_i) - y \|^2 \right\}. \quad (3)$$

Semivariogram

The spatial correlation can be obtained by estimating the semivariogram:

$$\gamma(\|x-x'\|) = \frac{1}{2}\mathbb{E}\left[\left\|\mathbf{Y}(x)-\mathbf{Y}(x')\right\|^2\right]$$

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By introducing a Lagrange multiplier α, we can show that $\bar{\lambda}$ is the solution of the following system:

$$\begin{bmatrix} \Gamma & \mathbb{1}_n \\ \mathbb{1}_n^T & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \alpha \end{bmatrix} = \begin{bmatrix} \gamma^\star \\ 1 \end{bmatrix}$$

where Γ is the $n \times n$ matrix with $\Gamma_{i,j} = \gamma(\|x_i - x_j\|)$, $\gamma^\star$ is the column vector of size n with $(\gamma^\star)_i = \gamma(\|x_i - x^\star\|)$ and $\mathbb{1}_n$ is the column vector of ones.

Matern semivariogram models

Experimental semivariogram:

$$\gamma_{exp}(h) = \frac{1}{2\,Card(N(h))} \sum_{(s,t)\in N(h)} \|y(x_s) - y(x_t)\|^2$$

with $N(h) = \{(s,t) \in \{1,\dots,n\}^2,\ h-\epsilon \leq ||x_s - x_t||_2 \leq h+\epsilon\}$ (ϵ depends on the problem)

The candidates for fitting models are classic semivariogram models like Matern functions:

$$\gamma_{\sigma,l,\nu}(h) = \sigma^2 \left(1 - \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\frac{h}{l}\right)^{\nu} K_\nu\left(\sqrt{2\nu}\frac{h}{l}\right)\right)$$

Ordinary Kriging in $\mathscr{P}_2(\mathbb{R})$ [2]

$$\mathscr{P}_2(\mathbb{R}) = \left\{ \mu \text{ proba measure} \mid \int_{\mathbb{R}} x^2 \, d\mu(x) < \infty \right\}$$

Consider

$$f : \mathscr{D} \subset \mathbb{R}^d \to \mathscr{P}_2(\mathbb{R})$$

Observations : $(\mu(x_1), \ldots, \mu(x_n))$

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Observations : $(\mu(x_1), \ldots, \mu(x_n))$
We extend the barycenter construction from the real case

$$\hat{\mu}(x^\star) = \operatorname{argmin}_{\mu \in \mathscr{P}_2(\mathbb{R})} \left\{ \sum_{i=1}^{n} \bar{\lambda}_i W_2^2(\mu(x_i), \mu) \right\}, \tag{4}$$

where:

$$\bar{\lambda} = \operatorname{argmin}_{\lambda = (\lambda_1, \ldots, \lambda_n)} \left\{ \mathbb{E}\left[W_2\left(\mu(x^\star), \hat{\mu}(x^\star)\right)^2 \right], \sum_{i=0}^{N-1} \lambda_i = 1 \right\}. \tag{5}$$

Wasserstein distance[3]

Second order Wasserstein distance:

$$W_2(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \left(\int_{\mathbb{R}\times\mathbb{R}} \|x-y\|^2 \, d\pi(x,y) \right)^{\frac{1}{2}},$$

In 1D ($\mathscr{P}_2(\mathbb{R})$), the Wasserstein distance of order 2 can be written:

$$W_2(\mu,\nu) = \left(\int_0^1 \left|F^{-1}(t) - G^{-1}(t)\right|^2 dt \right)^{\frac{1}{2}},$$

where F^{-1} and G^{-1} are the quantile functions of μ and ν

Predictor [4]

These statements allow us to introduce a new linear predictor based on quantile functions.

$$\hat{\mathbf{Q}}_{\mu(x^\star)} = \sum_{i=1}^{n} \bar{\lambda}_i \mathbf{Q}_{\mu(x_i)} \tag{6}$$

where

$$\bar{\lambda} = \text{argmin}_{\lambda=(\lambda_1,\dots,\lambda_n)} \left\{ \mathbb{E}\left[\int_0^1 \left(\mathbf{Q}_{\mu(x^\star)}(\xi) - \hat{\mathbf{Q}}_{\lambda,\mu(x^\star)}(\xi) \right)^2 d\xi \right], \sum_{i=1}^{n} \lambda_i = 1 \right\}, \tag{7}$$

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Experimental semivariogram for probability measures:

$$\gamma_{exp}^{W}(h) = \frac{1}{2Card(N(h))} \sum_{(s,t)\in N(h)} \left[\int_0^1 \left(Q_{\mu(x_s)}(\xi) - Q_{\mu(x_t)}(\xi) \right)^2 d\xi \right], \tag{8}$$

where $N(h)$ is as in the real case.

Cross validation[5]

- Limitation of the semivariogram: its estimation becomes unreliable when based on a limited number of observations.

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- We can estimate the model parameters by cross validation with the LOO MSE criterion :

$$\text{MSE}_{\text{LOO}} = \frac{1}{n}\sum_{i=1}^{n}\int_0^1 \left(Q_{\mu(x_i)}(\xi) - \hat{Q}^{(-i)}_{\mu(x_i)}(\xi)\right)^2 d\xi. \tag{9}$$

- Extension of virtual cross validation formulas for quantile functions.

Extension of virtual cross validation formulas [6]

Proposition

Let $\mathbf{Y}$ *be a stochastic process with values in* $\mathscr{P}_2(\mathbb{R})$ *with unknown constant mean, its semivariogram is denoted by* γ^W. *Let* $\mathbf{Y}(x_1),\ldots,\mathbf{Y}(x_n)$ *be observations of the process,* $(Q_1,\cdots,Q_n)$ *the quantile functions associated with the observation and* $(\Gamma_W)_{i,j} = \gamma^W(\|x_i - x_j\|)$. *Then* $\forall \xi \in [0,1]$ *and* $\forall i \in \{1,\cdots,n\}$ *we have:*

$$Q_i(\xi) - \hat{Q}_i(\xi) = \sum_{j=1}^{n} \frac{\tilde{\Gamma}_{ij}}{\tilde{\Gamma}_{i,i}} Q_j(\xi) \tag{10}$$

with:

- $\tilde{\Gamma} = {\Gamma_W}^{-1} - {\Gamma_W}^{-1}\mathbb{1}_n(\mathbb{1}_n^t {\Gamma_W}^{-1}\mathbb{1}_n)^{-1}\mathbb{1}_n^t {\Gamma_W}^{-1}$
- $\hat{Q}_i$ *is the estimator of* Q_i *based on all the other observations.*

Application in reflooding studies for nuclear safety

Loss of primary coolant accident

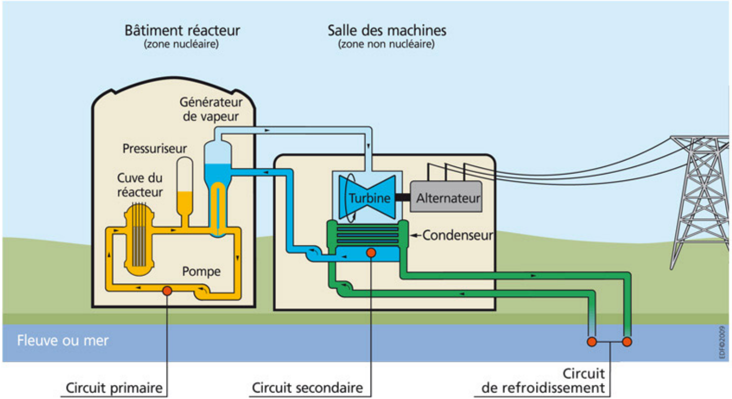

Figure 1: Scheme of a nuclear plant

Application in reflooding studies for nuclear safety

DRACCAR : Déformation et Renoyage d'un Assemblage de Crayon de Combustibles pendant un Accident de Refroidissement (ASNR software)

Figure 2: DRACCAR Process

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Figure 2: DRACCAR Process

Quantities of interest

- Average temperature
- 95% quantile
- Entire distribution (error measured with the wasserstein distance)

Models

Model based on ordinary kriging in $\mathbb{R}$ (prediction of the map then computation of the quantities of interest)

- Principal Component Analysis over the 100 discretization points of the maps [7]
- Kriging on the first three components
- Method for semivariogram estimation: Max likelihood under Gaussian assumption (model 1)

Models

Models based on ordinary kriging in $\mathscr{P}_2(\mathbb{R})$ (prediction of the distribution)

- Transform temperature maps into histograms
- Kriging based on quantile functions
- Method for semivariogram estimation:
  - Least squared with empirical semivariogram and positives weights (model 3)
  - Least squared with empirical semivariogram and no constrains on the weights (model 4)
  - Cross validation (model 5)

Results

- Model 1 : Ordinary kriging in $\mathbb{R}$ variogram parameters optimisation : Max likelihood
- Model 2 : Ordinary kriging in $\mathscr{P}_2(\mathbb{R})$ variogram parameters optimisation : Least squared + $\lambda > 0$
- Model 3 : Same + no constraints on λ
- Model 4: Odinary kriging + Cross validation

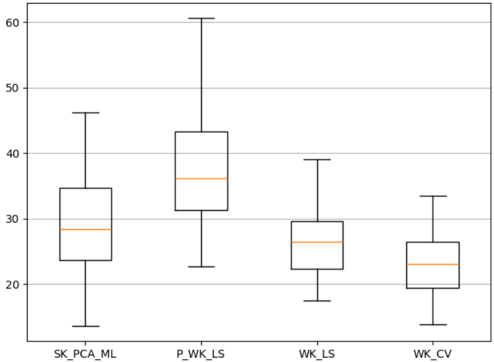

Figure 3: Boxplots of $\text{RMSE}_{\text{mean}}$ for each model.

Results

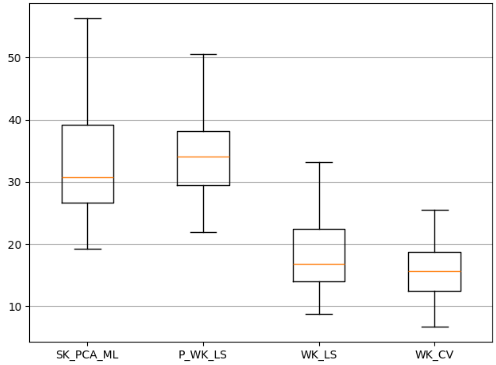

Figure 4: Boxplots of RMSE_{q95} for each model.

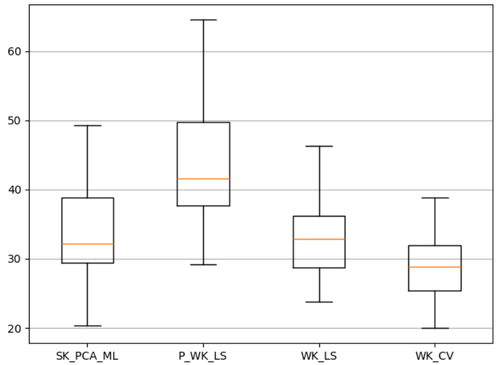

Figure 5: Boxplots of RMSE_W for each model.

Conclusion

- We proposed an extension of kriging for probability measures
- We also extended the virtual cross validation formulas for quantile functions
- These methods produce better results on the prediction of statistical parameters in thermohydraulic studies

Perspectives

- Build new kriging models for map prediction
- Predict the location of the temperature maxima on each map
- Predict the configurations that lead to critical situations
- Design and plan new experiments

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