A novel approach for estimating functions in the multivariate setting based on an adaptive knot selection for B-splines

StatMathAppli 2023

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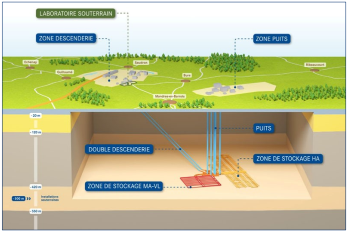
General context

Andra : French National Agency for Radioactive Waste Management

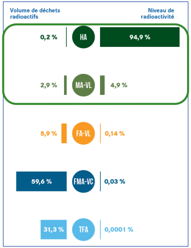
"Taking charge of radioactive waste produced by past and current generations to render it secure for future generations "

Location of Andra sites*

Cigéo Project*



Radioactive waste classification*



*Sources Andra

General context

To model the evolution of Cigéo components and the different interactions with their environment

Solving chemical reactions with **PHREEQC**, a computer program which takes x as inputs and gives output y such that $y = f(x)$ where f is an unknown function

Problem : time-consuming and costly simulations

IDEA : to estimate f (« black box »)

First solution : deep learning with **a deep neural network** exploiting a set of observations generated with PHREEQC

Problem : complex calibration of parameters, not yet optimized

Second solution : Implementation of a **statistical method** for estimating functions in a **multivariate nonparametric regression model** based on an **adaptive knot selection for B-splines.**

Definition of B-splines of order M

Let $\mathbf{t} = (t_1, \ldots, t_K)$ be a set of K points called **knots**. We define the augmented knot sequence τ such that:

$$\tau_1 = \ldots = \tau_M = x_{min},$$

$$\tau_{j+M} = t_j, \quad j = 1, \ldots, K,$$

$$x_{max} = \tau_{K+M+1} = \ldots = \tau_{K+2M},$$

$$\tau = (\tau_1, \ldots, \tau_{K+2M}) = \Big(\underbrace{x_{min}, \ldots, x_{min}}_{\text{M times}}, \underbrace{t_1, \ldots, t_K}_{\mathbf{t}}, \underbrace{x_{max}, \ldots, x_{max}}_{\text{M times}}\Big),$$

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B-splines are defined by De Boor (1978) by the following recursion: Denoting by $B_{i,m}(x)$ the ith B-spline basis function of order m for the knot sequence τ with $m \leq M$:

Definition of B-splines by recursion

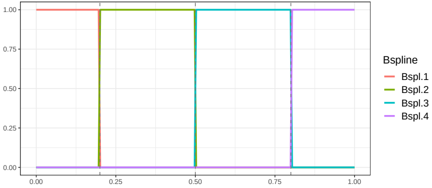
$$B_{i,1}(x) = \begin{cases} 1 & \text{if } \tau_i \leq x < \tau_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad \text{for} \quad i = 1, \ldots, K + 2M - 1,$$

and for $m \leq M$,

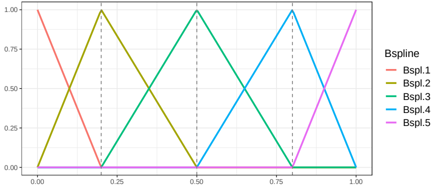
$$B_{i,m}(x) = \frac{x - \tau_i}{\tau_{i+m-1} - \tau_i} B_{i,m-1}(x) + \frac{\tau_{i+m} - x}{\tau_{i+m} - \tau_{i+1}} B_{i+1,m-1}(x),$$

for $i = 1, \ldots, (K + 2M - m)$.

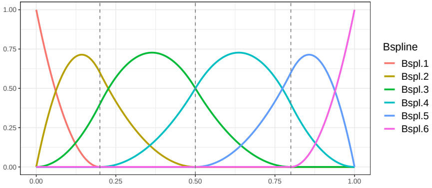
Visualization of B-splines of order M



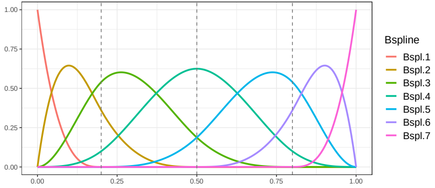
(a) B-spline basis of order $M = 1$



(b) B-spline basis of order $M = 2$



(c) B-spline basis of order $M = 3$



(d) B-spline basis of order $M = 4$

with $\mathbf{t} = (0.2, 0.5, 0.8)$

Nonparametric method to estimate function of one or two variables (1)

$$Y_i = f(x_i) + \varepsilon_i, \quad 1 \leq i \leq n, \quad \varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$$

where the x_i are observation points which belong to a compact set of $\mathbb{R}^d$, $d \geq 1$.
Approach : GLOBER inspired by MARS method introduced by Friedman (1991),
***d** $=$ **1** :

1. From the observation points, selection of specific points called **knots** by using the $(q+1)$th order generalized lasso defined by Tibshirani and Taylor (2011),
2. Definition of a B-spline basis of a certain order M,
3. Estimation of a one-dimensional function $(d = 1)$

$$\sum_{i=1}^{K+M} \gamma_i B_{i,M}(x), \tag{1}$$

where K is the number of knots defining the B-spline basis.

Nonparametric method to estimate function of one or two variables (2)

*$\mathbf{d = 2}$:

1. From the observation points, selection of **knots** for each dimension by fixing one dimension at a time so can be rewritten as an estimation problem in the one-dimensional framework ($d = 1$),
2. Definition of a B-spline basis for each dimension,
3. Estimation of a two-variable function ($d = 2$)

$$\sum_{i=1}^{Q_1} \sum_{j=1}^{Q_2} \gamma_{ij} B_{1,i,M}(x_1) B_{2,j,M}(x_2), \qquad (2)$$

where $B_{1,i,M}$ and $B_{2,j,M}$ are the B-spline basis of order M for the first and second dimension, respectively. In (2), $Q_1 = q + K_1 + 1$, $Q_2 = q + K_2 + 1$ with K_1 and K_2 the number of knots defined in the B-spline basis of the first and second variables, respectively and $M = q + 1$.

Selection of the knot set ($d = 1$)

Generalized lasso (Tibshirani et al, 2011)

$$\widehat{\beta}(\lambda) = \underset{\beta \in \mathbb{R}^n}{\text{argmin}} \{ ||\mathbf{Y} - \beta||_2^2 + \lambda ||D\beta||_1 \} \quad (3)$$

where $||y||_2^2 = \sum_{i=1}^n y_i^2$ for $y = (y_1, \ldots, y_n)$ and $||u||_1 = \sum_{i=1}^m |u_i|$ for $u = (u_1, \ldots, u_m)$, $\lambda > 0$ and $D \in \mathbb{R}^{m \times n}$ is a specified penalty matrix depending on the **order of differentiation** $(q + 1)$.

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Let $\Lambda = (\lambda_1, \ldots, \lambda_k)$ be a grid of penalization parameters λ_i. We define $\mathbf{a}(\lambda)$ by:

$$\boldsymbol{a}(\lambda) = D \cdot \widehat{\beta}(\lambda), \quad \lambda \in \Lambda$$

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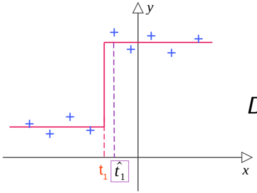

$$D = \begin{bmatrix} -1 & 1 & 0 & \ldots & 0 \\ 0 & -1 & 1 & \ldots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & \ldots & -1 & 1 \end{bmatrix}, \ \widehat{\beta}(\lambda_3) = \begin{bmatrix} 1.1 \\ 1.1 \\ 1.1 \\ 1.1 \\ 3.6 \\ 3.6 \\ 3.6 \\ 3.6 \\ 3.6 \end{bmatrix}, \ \mathbf{a}(\lambda_3) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2.5 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

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Generalized lasso (Tibshirani et al, 2011)

$$\widehat{\beta}(\lambda) = \underset{\beta \in \mathbb{R}^n}{\operatorname{argmin}} \{ ||\mathbf{Y} - \beta||_2^2 + \lambda ||D\beta||_1 \} \qquad (3)$$

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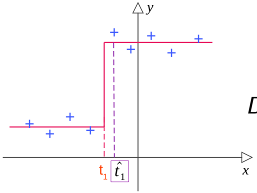

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Which penalization parameter λ to choose to get an optimal estimator of f?

Selection criterion of the parameter λ ($d = 1$)

EBIC criterion defined by Chen and Chen (2008)

$$\mathrm{EBIC}(\lambda) = \mathrm{SS}(\lambda) + (q + K_\lambda + 1)\log n + 2\log\binom{q + K_{\max} + 1}{q + K_\lambda + 1}, \quad (4)$$

where $K_{\max} = n$ and $\mathrm{SS}(\lambda)$ is the sum of squares defined by:

$$\mathrm{SS}(\lambda) = \|\mathbf{Y} - \widehat{\mathbf{Y}}(\lambda)\|_2^2\,, \quad (5)$$

where

$$\widehat{\mathbf{Y}}(\lambda) = \mathbf{B}(\lambda)\widehat{\gamma},$$

with $\widehat{\gamma}$ and $\mathbf{B}(\lambda)$ a $n \times (q + K_\lambda + 1)$ matrix having as ith column $(B_{i,M}(x_k))_{1 \le k \le n}$, i belonging to $\{1, \dots, q + K_\lambda + 1\}$.

Final estimator of f

$$\widehat{f}(x) = \widehat{f}_{\lambda_{\mathrm{EBIC}}}(x), \quad (6)$$

where $\widehat{f}_\lambda(x) = \sum_{i=1}^{q+K_\lambda+1} \widehat{\gamma}_i B_{i,M}(x)$ and

$$\lambda_{\mathrm{EBIC}} = \underset{\lambda \in \Lambda}{\mathrm{argmin}}\{\mathrm{EBIC}(\lambda)\}. \quad (7)$$

One-dimensional framework for the knot selection

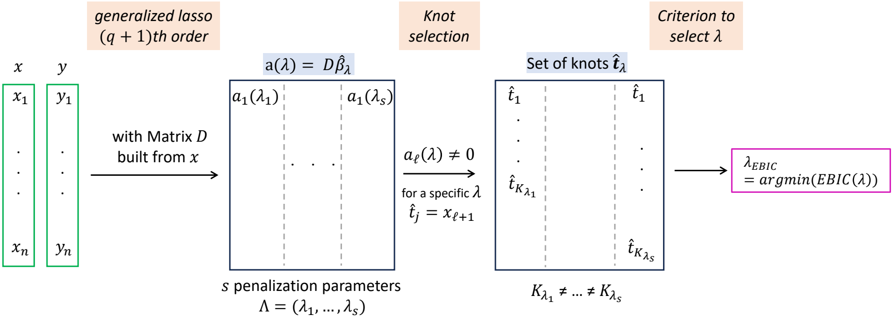

Figure 2: One-dimensional framework

Two-dimensional framework for the knot selection

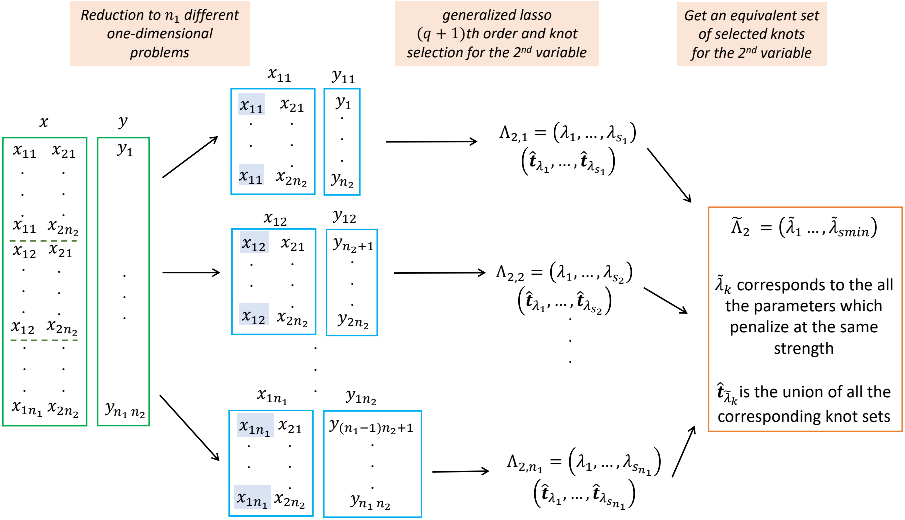

Figure 3: Two-dimensional framework

Selection of knot sets ($d = 2$)

Equivalent sets of knots – First dimension

$$\widetilde{\Lambda}_1 = \left\{\widetilde{\lambda}_{1,1}, \ldots, \widetilde{\lambda}_{1,s_{min_1}}\right\} \quad \text{and} \quad s_{min_1} = \min_{1 \leq i \leq n_2} s_i \ , \tag{8}$$

$$\widetilde{\lambda}_{1,k} = \left(\lambda_{(1,i),k}\right)_{1 \leq i \leq n_2}, \quad 1 \leq k \leq s_{min_1}. \tag{9}$$

In (9), $\widetilde{\lambda}_{1,k}$ can be seen as the vector of parameters which penalize (3) at an equivalent strength for each fixed value of x_2.

Equivalent sets of knots – Second dimension

$$\widetilde{\Lambda}_2 = \left\{\widetilde{\lambda}_{2,1}, \ldots, \widetilde{\lambda}_{2,s_{min_2}}\right\} \quad \text{and} \quad \widetilde{\lambda}_{2,\ell} = \left(\lambda_{(2,i),\ell}\right)_{1 \leq i \leq n_1}, \quad 1 \leq \ell \leq s_{min_2}.$$

Let us consider two generic penalization parameters $\widetilde{\lambda}_1$ belonging to $\widetilde{\Lambda}_1$ and $\widetilde{\lambda}_2$ belonging to $\widetilde{\Lambda}_2$.

Selection of knot sets ($d = 2$)

Equivalent sets of knots – First dimension

$$\widetilde{\Lambda}_1 = \left\{ \widetilde{\lambda}_{1,1}, \dots, \widetilde{\lambda}_{1,s_{min_1}} \right\} \quad \text{and} \quad s_{min_1} = \min_{1 \le i \le n_2} s_i \ , \tag{8}$$

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Let us consider two generic penalization parameters $\widetilde{\lambda}_1$ belonging to $\widetilde{\Lambda}_1$ and $\widetilde{\lambda}_2$ belonging to $\widetilde{\Lambda}_2$.

Which combination of penalization parameters $(\widetilde{\lambda}_1, \widetilde{\lambda}_2)$ to choose to get an optimal estimator of f ?

Selection criterion of the parameters $(\widetilde{\lambda}_1, \widetilde{\lambda}_2)$ $(d = 2)$

EBIC criterion

$$\text{EBIC}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) = \text{SS}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) + \widetilde{Q}_1 \widetilde{Q}_2 \log n + 2\log\left(\frac{(q+n_1+1)(q+n_2+1)}{\widetilde{Q}_1 \widetilde{Q}_2}\right). \tag{10}$$

where $\widetilde{Q}_1 = q + K_{\widetilde{\lambda}_1} + 1$ and $\widetilde{Q}_2 = q + K_{\widetilde{\lambda}_2} + 1$ and $\text{SS}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right)$ is the sum of squares.

Final estimator of f

$$\widehat{f}(x_1, x_2) = \widehat{f}_{\widetilde{\lambda}_{1,\text{EBIC}}, \widetilde{\lambda}_{2,\text{EBIC}}}(x_1, x_2),$$

with $\widehat{f}_{\widetilde{\lambda}_1, \widetilde{\lambda}_2}$ defined as:

$$\widehat{f}_{\widetilde{\lambda}_1, \widetilde{\lambda}_2}(x) = \widehat{f}_{\widetilde{\lambda}_1, \widetilde{\lambda}_2}(x_1, x_2) = \sum_{i=1}^{\widetilde{Q}_1} \sum_{j=1}^{\widetilde{Q}_2} \widehat{\gamma}_{ij} B_{1,i,M}(x_1) B_{2,j,M}(x_2). \tag{11}$$

Metrics

One-dimensional form

$$\text{Normalized MAE}(\lambda) = \frac{1}{N}\sum_{k=1}^{N} \frac{\left|f(x_k) - \widehat{f}_\lambda(x_k)\right|}{f_{max} - f_{min}}. \quad (12)$$

$$\text{Normalized sup norm}(\lambda) = \max_{1\leq k\leq N} \frac{\left|f(x_k) - \widehat{f}_\lambda(x_k)\right|}{f_{max} - f_{min}}, \quad (13)$$

where $\widehat{f}_\lambda$ is defined in (1). In (13), N ($N > n$) is the cardinality of the set of evenly-spaced points $\{x_1, \dots, x_N\}$ of $[0, 1]$ which contains the observation points $x_1, \dots, x_n$ as well as additional points where f has not been observed.
f_{min} and f_{max} denote the minimum and maximum values of f evaluated on $\{x_1, \dots, x_N\}$, respectively.

Two-dimensional form

(12) and (13) with λ becomes $\widetilde{\lambda}_1$ and $\widetilde{\lambda}_2$ and $\widehat{f}_\lambda$ is replaced by $\widehat{f}_{\widetilde{\lambda}_1,\widetilde{\lambda}_2}$.

Results on geochemical applications ($d = 1$)

Function to estimate: Simple case of precipitation, we consider here one input (Spa) and one output (Amount of Salt) Savino et al. (2022). Real evaluations of f have been obtained with PHREEQC.

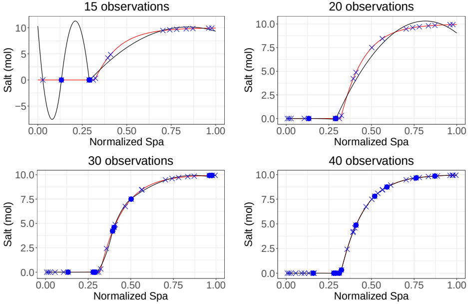

Figure 4: Illustration of the method over an increasing number of observations

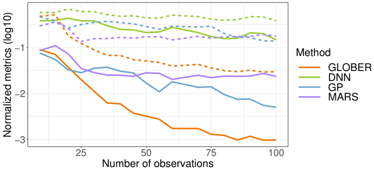

Figure 5: Statistic performance of our method (GLOBER) and of the state-of-the-art methods.The dashed (resp. solid) line displays the average of the Normalized Sup Norm (resp. Normalized MAE) values obtained from 10 replications.

Results on geochemical applications ($d = 2$)

Function to estimate: Simple case of precipitation, we consider here two inputs (Ca and Mg) and one output (Amount of Dolomite). Real evaluations of f have been obtained with PHREEQC.

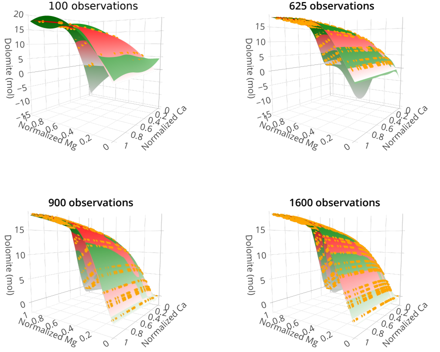

Figure 6: Illustration of the method over an increasing number of observations

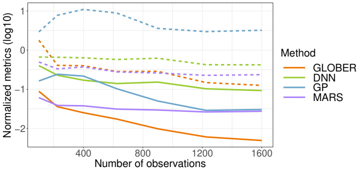

Figure 7: Statistic performance of our method (GLOBER) and of the state-of-the-art methods.The dashed (resp. solid) line displays the average of the Normalized Sup Norm (resp. Normalized MAE) values obtained from 10 replications.

Discussion and perspectives

- New way of estimating univariate and bivariate functions with B-splines
- Application to the one and two-dimentional settings
- Submitted article: M. E. Savino, C. Lévy-Leduc. **A novel approach for estimating functions in the multivariate setting based on an adaptive knot selection for B-splines with an application to a chemical system used in geoscience**, *arxiv:2306.00686, 2023.*
- Implementation of the method: R package `glober` available on the CRAN, by using the `genlasso` R package (Arnold and Tibshirani, 2016).
- Extension to higher dimensional settings and to general grid ongoing

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Friedman, J. H. (1991). Multivariate Adaptive Regression Splines. The Annals of Statistics 19(1), 1–67.

Savino, M., C. Lévy-Leduc, M. Leconte, and B. Cochepin (2022). An active learning approach for improving the performance of equilibrium based chemical simulations. Computational Geosciences 26(2), 365–380.

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Back-up slides

Definition of penalty matrix D

Case of evenly-spaced observations

$$D = D_{tf,q+1} = D_0 \cdot D_{tf,q} \quad q \geq 0, \tag{14}$$

with $D_{tf,0} = \mathrm{Id}_{\mathbb{R}^n}$, the identity matrix of $\mathbb{R}^n$

D_0 is the penalty matrix for the one-dimensional fused Lasso:

$$D_0 = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & -1 & 1 \end{bmatrix}.$$

Case of unevenly-spaced observations

$$D = \Delta^{(q+1)} = \mathbf{W}_{(q+1)} \cdot D_0 \cdot \Delta^{(q)}, \quad q \geq 0,$$

where $\Delta^{(0)} = \mathrm{Id}_{\mathbb{R}^n}$ and $\mathbf{W}_{(q+1)}$ is the diagonal weight matrix defined by:

$$\mathbf{W}_{(q+1)} = \mathrm{diag}\left(\frac{1}{(x_{(q+1)+1} - x_{(q+1)})}, \frac{1}{(x_{(q+1)+2} - x_{(q+1)+1})}, \dots, \frac{1}{(x_n - x_{n-1})} \right).$$

Selection of the knot set $(d = 1)$

Let $\Lambda = (\lambda_1, \dots, \lambda_k)$ be a grid of penalization parameters λ_i. We define $\mathbf{a}(\lambda)$ by:

$$\boldsymbol{a}(\lambda) = D \cdot \widehat{\beta}(\lambda), \quad \lambda \in \Lambda$$

Approach to find the selected knots associated to λ

$$\widehat{\mathbf{t}}_\lambda = \left(\widehat{t}_j\right)_{j=1,\dots,K_\lambda} = \left(x_{p_j}\right)_{j=1,\dots,K_\lambda}, \quad \text{avec } p_j \in \mathcal{P}_\lambda,$$

where

$$\mathcal{P}_\lambda = \{\ell + 1, \ a_\ell(\lambda) \neq 0 \ \} \quad \text{et} \quad K_\lambda = \sum_{\ell=1}^{m} \mathbb{1}\{a_\ell(\lambda) \neq 0\},$$

$a_\ell(\lambda)$ denotes the ℓth component of $\mathbf{a}(\lambda)$ and $\mathbb{1}\{A\} = 1$ if the event A holds and 0 if not.

Sum of square detailed for two-dimensional case

Definition of SS $\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right)$

$$\mathrm{SS}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) = \left\| \mathbf{Y} - \widehat{\mathbf{Y}}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) \right\|_2^2,$$

where

$$\widehat{\mathbf{Y}}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) = \mathbf{B}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) \widehat{\gamma}, \tag{15}$$

and $\mathbf{B}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right)$ is defined as:

$$\mathbf{B}\left(\widetilde{\lambda}_1, \widetilde{\lambda}_2\right) = \mathbf{B}\left(\widetilde{\lambda}_1\right) \otimes \mathbf{B}\left(\widetilde{\lambda}_2\right), \tag{16}$$

$E \otimes F$ denoting the Kronecker product of the matrices E and F. In (16), $\mathbf{B}\left(\widetilde{\lambda}_1\right)$ is a $n_1 \times \widetilde{Q}_1$ matrix having as ith column $(B_{1,i,M}(x_{1k}))_{1 \leq k \leq n_1}$, i belonging to $\{1, \ldots, \widetilde{Q}_1\}$ and $\mathbf{B}\left(\widetilde{\lambda}_2\right)$ is a $n_2 \times \widetilde{Q}_2$ matrix having as jth column $(B_{2,j,M}(x_{2\ell}))_{1 \leq \ell \leq n_2}$, j belonging to $\{1, \ldots, \widetilde{Q}_2\}$.

State-of-the-art methods

- **Gaussian Processes (GP)**: squared exponential covariance function, implementation by using `scikit-learn` Python package,
- **Multivariate Adaptive Regression Splines (MARS):** interaction terms are included, implementation by using `earth` R package,
- **Deep Neural Networks (DNNs):** arbitrarily chosen since our goal is not to optimize it:
  - 2-hidden-layered structure composed of 10 neurons per layer
  - Activation function of the hidden layers: RELU function since it is one of the most used functions.
  - Optimizer: stochastic gradient descent method Adam
  - Loss function: the Mean Squared Error (MSE).
  - Number of epochs: 300 epochs for functions of $d = 1$ and 50 epochs for functions of $d = 2$ to avoid overfitting,

  implementation by using `keras` R package.

Suppplementary application for the two-dimensional framework

Function to estimate: Simple case of precipitation, we consider here two inputs (Spa and Spb) and one output (Amount of Halite). Real evaluations of f have been obtained with PHREEQC.

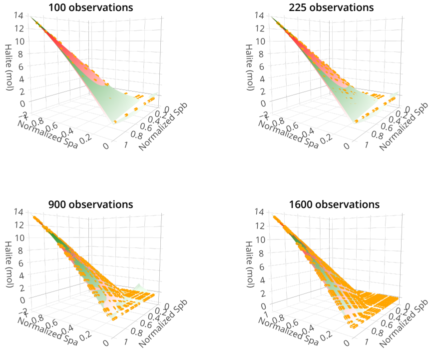

Figure 8: Illustration of the method over an increasing number of observations

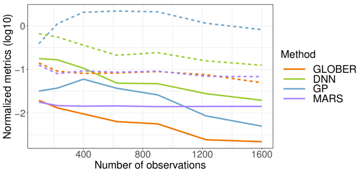

Figure 9: Statistic performance of our method (GLOBER) and of the state-of-the-art methods.The dashed (resp. solid) line displays the average of the Normalized Sup Norm (resp. Normalized MAE) values obtained from 10 replications.