Journées Sensibilisation au Problème des Incertitudes
Gaussian Processes for code validation

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Introduction

- Context of code validation : Is the code in agreement with a set of reference experiments ?
- Gaussian processes validation : Modelling of the error between the code and the physical system.
- Goals :
  - Calibration of the code
  - Completion of the code by a statistical term based on a set of experiments

Least square calibration

Gaussian processes notions

Gaussian Processes Validation Model

Calibration and prediction

Model selection

Application to the thermohydraulic code Flica IV

Computation code and reality

A computation code, or parametric numerical model, is represented by a function f :

$$\begin{aligned} f \quad : \mathbb{R}^d \times \mathbb{R}^m \quad &\rightarrow \mathbb{R} \\ (x, \beta) \quad &\rightarrow f(x, \beta) \end{aligned}$$

The physical system is represented by a function Y_{real}.

$$\begin{aligned} Y_{real} \quad : \mathbb{R}^d \quad &\rightarrow \mathbb{R} \\ x \quad &\rightarrow Y_{real}(x) \end{aligned}$$

- The inputs x are the experimental conditions.
- The inputs β are the calibration parameters of the computation code.
- The outputs $f(x, \beta)$ and $Y_{real}(x)$ are the quantity of interest.

A computation code models (gives an approximation of) a physical phenomenon.

Least square calibration

We dispose of a set of experimental results : x_1, $Y_{obs}(x_1)$, ..., x_n, $Y_{obs}(x_n)$.

Least Square calibration :

- Compute :
$$\hat{\beta}_{LS} \in \arg\min_{\beta} \sum_{i=1}^{n} (f(x_i, \beta) - Y_{obs}(x_i))^2$$
- For new experimental condition x_{new} we predict the quantity of interest by : $f(x_{new}, \hat{\beta}_{LS})$.

Least square calibration as a Maximum Likelihood estimation

Assume that there exist β so that for $1 \leq i \leq n$

$$Y_{obs}(x_i) = f(x_i, \beta) + z_i$$

With $z_i \sim_{iid} \mathcal{N}(0, \sigma^2)$. z_i's are either

- A measure error.
- A measure error and a model error

Then the maximum likelihood estimator $\hat{\beta}$ of β is

$$\begin{aligned}
\hat{\beta} \quad &\in \quad \arg\max_{\beta} \frac{1}{(2\pi)^{\frac{n}{2}}(\sigma^2)^n} \exp\left(-\frac{1}{2\sigma^2}\left(\sum_{i=1}^{n}(f(x_i,\beta) - Y_{obs}(x_i))^2\right)\right) \\
&\in \quad \arg\min \beta \sum_{i=1}^{n}(f(x_i,\beta) - Y_{obs}(x_i))^2
\end{aligned}$$

Least Square calibration : Case of insufficiency

When $\boldsymbol{z}_i$'s are only measure error :

- Problem when σ^2 (or an upper-bound) is known and when the errors $f(x_i, \hat{\beta}) - Y_{obs}(x_i)$ are too large. (Statistical tests available to detect).

When $\boldsymbol{z}_i$'s are model errors.

- The physical system $x \longrightarrow f(x, \beta) + z$ would be discontinuous
- It is reasonable to assume correlation between the model errors at two neighboor points

$\longrightarrow$ A Gaussian process model is a way to answer these issues

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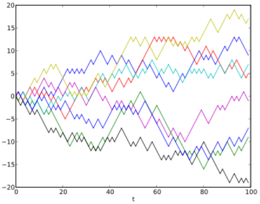
Gaussian processes (1/3)

A random function is a function $x \rightarrow F(x)$ such that $F(x)$ is a random variable. Alternalively a random function is a function that is unknown, or that depends of the hasard.



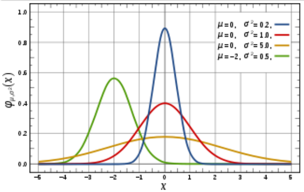
Finite dimensional distributions of a random function

Let us consider n points of $\mathbb{R}^d$: $x_1, \ldots, x_n$. By definition, the vector $(Z(x_1), \ldots, Z(x_n))$ is a random vector of $\mathbb{R}^n$. Its distribution is said to be a finite dimensional distribution of Z.

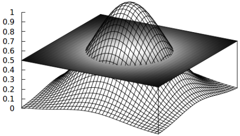
The finite dimensional distributions of Z are the set of these distributions with n et $x_1, \ldots, x_n$ varying.

Gaussian variables and vectors

A random variable is a Gaussian variable with mean μ and variance σ^2 when its probability density function is $f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$



A n dimensional random vector is a Gaussian vector with mean vector μ and covariance matrix R when its multidimensional probability density function is $f(x) =$
$\frac{1}{(2\pi)^{\frac{n}{2}}\sqrt{det(R)}} \exp\left(-\frac{1}{2}(x-\mu)^t R^{-1}(x-\mu)\right)$



Gaussian processes (1/2)

A random function Z on $\mathbb{R}^d$ is a Gaussian process when its finite dimensional distributions are Gaussian.

In the sequel, we only consider Gaussian processes :

- Gaussian variables : most commonly used to represent errors.
- Gaussian properties make the treatment of the problem simpler.

Mean function $M : x \rightarrow M(x) = \mathbb{E}(Z(x))$
Covariance function $C : (x_1, x_2) \rightarrow C(x_1, x_2) = cov(Z(x_1), Z(x_2))$

- A Gaussian process is caracterized by its mean and covariance functions.

Gaussian processes (2/2)

Examples of covariance functions

Nugget covariance function $C(x,y) = \sigma^2 \mathbf{1}_{x=y}$

Gaussian covariance function $C(x,y) = \sigma^2 \exp\left(-\frac{(x-y)^2}{l_c^2}\right)$

Exponential covariance function $C(x,y) = \sigma^2 \exp\left(-\frac{|x-y|}{l_c}\right)$

Examples of realizations with Gaussian covariance function

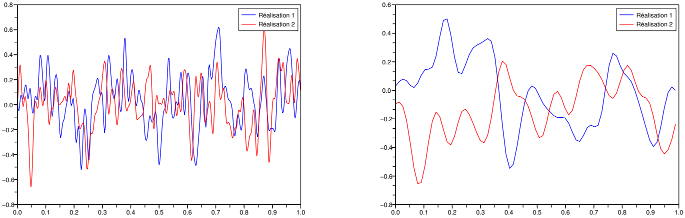


FIG.: Left : $\sigma = 0.2$, $l_c = 0.01$. Right : $\sigma = 0.2$, $l_c = 0.05$

Conditional distributions for Gaussian vectors

Theorem

Let

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m_1 \\ m_2 \end{pmatrix}, \begin{pmatrix} R_1 & R_{1,2} \\ R_{2,1} & R_2 \end{pmatrix}\right)$$

Then, conditionaly on $X_2 = x_2$, X_1 is a Gaussian vector with

$$\mathbb{E}(X_1|X_2 = x_2) = m_1 + R_{1,2}R_{2,2}^{-1}(x_2 - m_2)$$

and

$$cov(X_1|X_2 = x_2) = R_1 - R_{1,2}R_{2,2}^{-1}R_{2,1}$$

Illustration

Let

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$$

Then

$$\mathbb{E}(X_1|X_2 = x_2) = \rho x_2$$

and

$$var(X_1|X_2 = x_2) = 1 - \rho^2$$

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Model error

Statistical modelling : The physical phenomenon is one realization among a set of possible realizations. It is modeled as a realization of a random process.

Equation of the statistical model

$$Y_{real}(\omega, x) = f(x, \beta(\omega)) + Z(\omega, x)$$

- Equation that holds for a specific parameters vector β. Called "the" parameter of the numerical code.
  - No prior information case : β constant and unknown.
  - Prior information case (Bayesian case) : $\beta \sim \mathcal{N}(\beta_{prior}, Q_{prior})$
- Z is (a priori) a centered, stationary, Gaussian process. We denote by C_{mod} the covariance function of Z.

Steps of Gaussian processes code validation

- Step 1 : Estimation of the covariance function for the model error.
- Step 2 : With a given covariance function : calibration and prediction.
  - Calibration : gives a "posterior mean value" for the code parameter β and a "posterior variance".
  - Prediction : for a new experimental condition x_{new}, gives a "posterior mean value" for $Y_{real}(x_{new})$ and a "posterior variance".

Linear code and observations : notations

Linearization of the numerical model around the reference parameter :

$$\forall x : \; f(x, \beta) = \sum_{i=1}^{m} h_i(x)\beta_i$$

Observations

We observe the physical phenomenon $Y_{real}(x)$ for n inputs $x_1, \ldots, x_n$.
Define :

- $n \times m$ matrix of partial derivatives of the numerical model : H.
- Random vector of observations : y_{obs}.
- Random vector of measure error : ϵ.
- Random vector of model error : z.
- Covariance matrix of z : R_{mod}.

Matrix equation of the statistical model

The statistical model becomes, for the inputs $x_1, ..., x_n$:

$$y_{obs} = H\beta + z + \epsilon$$

Covariance matrix of $z + \epsilon$

$$R := cov(z + \epsilon) = R_{mod} + K$$

With $K := cov(\epsilon)$. K is diagonal. Most classical case : $K = \sigma^2_{mes} I$.

- No prior information case
  - When $R = \sigma^2 \mathbf{I}_n$: Classical linear regression model.
- Prior information case

$$y_{obs} \sim \mathcal{N}(H\beta_{prior}, R + HQ_{prior}H^T)$$

- Main interest of the correlation : Efficient prediction of the phenomenon when it does not have the same shape as the numerical code.

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Introduction

Assume we have fixed the covariance function C_{mod} of the model error.

- The statistical model is a linear regression model with a Gaussian process error.
- It is the same as the Kriging Model, well known e.g in Geostatistic and in analysis of computer experiments.
- We have closed form formulas for the calibration and the prediction.

Calibration (1/2)

Calibration problem = Statistical estimation problem

Estimation of β

- An estimator of β is a function $\hat{\beta} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$.
- $\hat{\beta}(y_{obs})$ is the estimation of β according to the vector of observations y_{obs}.
- $\hat{\beta}(y_{obs})$ is a random variable because y_{obs} is a random variable.
- Quality measure of an estimator : Mean square error : $\mathbb{E}_{y_{obs},\beta}\left[||\beta - \hat{\beta}(y_{obs})||^2\right]$.

Calibration (1/2)

No prior information case

The maximum likelihood estimator of β is

$$\hat{\beta} = (H^T R^{-1} H)^{-1} H^T R^{-1} y_{obs}$$

The covariance matrix of $\hat{\beta}$ is

$$cov(\hat{\beta}) = (H^T R^{-1} H)^{-1}$$

- $\hat{\beta}$ is unbiased : $\mathbb{E}(\hat{\beta}) = \beta$
- If $y_{obs} = H\beta$, $\hat{\beta} = \beta$

Calibration (2/2)

Prior information case

Recall the a priori probability law of β is normal with mean vector β_{prior} and covariance matrix Q_{prior}. Conditionally to the observations y_{obs}, β is Gaussian with mean vector β_{post} and covariance matrix Q_{post}.

$$\beta_{post} = \beta_{prior} + (Q_{prior}^{-1} + H^T R^{-1} H)^{-1} H^T R^{-1} (y_{obs} - H\beta_{prior}).$$

$$Q_{post} = (Q_{prior}^{-1} + H^T R^{-1} H)^{-1}$$

- Best predictor according to the mean square error.
- When $Q_{prior}^{-1} \rightarrow 0$ (Uninformative prior) we find the prediction of the no prior information case, even if $\beta_{prior} \neq 0$.
- When $Q_{prior} \rightarrow 0$ $\beta_{post} \rightarrow \beta_{prior}$.

Prediction (1/4)

Goal : to complete the prediction of $f(x_0, \hat{\beta})$ at a new point x_0.

Notations

- Physical phenomenon at x_0 : $y_0 := Y_{real}(x_0)$.
- (pseudo) new observation at x_0 : $y_{obs,0}$.
- Column vector of partial derivatives of the code : h_0.
- Random variable of the model error : z_0.
- Random variable of the measure error : ϵ_0.
- Column covariance vector r_0 : $r_{0,i} := cov((z+\epsilon)_i, z_0+\epsilon_0)$.

Prediction of y_0

- A predictor of y_0 is a function $\langle y_0 \rangle : \mathbb{R}^n \to \mathbb{R}$.
- $\langle y_0 \rangle(y_{obs})$ is the prediction of y_0 according to the vector of observations y_{obs}.
- $\langle y_0 \rangle(y_{obs})$ is a random variable because y_{obs} is a random variable.
- Quality measure of a predicor : Mean square error : $\mathbb{E}_{y_{obs},y_0}\left[|y_0 - \langle y_0 \rangle(y_{obs})|^2\right]$.

Prediction (2/4) : No prior information case

Prediction

The unbiased predictor of $y_{obs,0}$ at x_0, linear with respect to the vector of observations y_{obs}, which minimizes the mean square error (the BLUP) is :

$$\langle y_{obs,0} \rangle = (h_0)^T \hat{\beta} + (r_0)^T R^{-1} (y_{obs} - H\hat{\beta})$$

with $\hat{\beta}$ the no prior information case estimator of β.

- We do not have access to the best predictor, because its expression makes use of the unknown parameter β.
- The prediction expression is decomposed into a calibration term and a Gaussian inference term of the model error.

Predictive variance

The mean square error of the BLUP is :

$$\hat{\sigma}^2_{x_0} = \mathbb{E}((z_0 + \epsilon_0)^2) - \begin{pmatrix} h_0 \\ r_0 \end{pmatrix}^t \begin{pmatrix} 0 & H^t \\ H & R \end{pmatrix}^{-1} \begin{pmatrix} h_0 \\ r_0 \end{pmatrix}$$

Confidence intervals available

Prediction (3/4) : Prior information case

Prediction

The conditional law of $y_{obs,0}$ according to the observations y_{obs} is Gaussian with mean $\langle y_{obs,0} \rangle$, with :

$$\langle y_{obs,0} \rangle = (h_0)^T \beta_{post} + (r_0)^T R^{-1} (y_{obs} - H\beta_{post})$$

- Best predictor.

Predictive variance

Conditionally to y_{obs} the variance of $y_{obs,0}$ is :

$$\hat{\sigma}^2_{x_0} = \mathbb{E}((z_0 + \epsilon_0)^2) - \begin{pmatrix} h_0 \\ r_0 \end{pmatrix}^t \begin{pmatrix} -Q^{-1}_{prior} & H^t \\ H & R \end{pmatrix}^{-1} \begin{pmatrix} h_0 \\ r_0 \end{pmatrix}$$

- When $Q^{-1}_{prior} \to 0$ (uninformative prior) we find the no prior information case.

Prediction (4/4) : from $y_{obs,0}$ to y_0

No prior information case

The BLUP of the observation equals the BLUP of the physical phenomenon :

$$\forall \lambda \in \mathbb{R}^n : \quad \mathbb{E}\left((\lambda^t y_{obs} - y_{obs,0})^2 \right) = \mathbb{E}\left((\lambda^t y_{obs} - y_0)^2 \right) + \mathbb{E}\left((\epsilon_0)^2 \right)$$

Prior information case

The conditional means are the same and the conditional variances are the same up to the measure error :

- $\mathbb{E}(y_0 | y_{obs}) = \mathbb{E}(y_{obs,0} | y_{obs})$
- $var(y_{obs,0} | y_{obs}) = var(y_0 | y_{obs}) + \mathbb{E}\left((\epsilon_0)^2 \right)$

$\boxed{\longrightarrow}$ In both cases, we keep the same prediction, and remove $\mathbb{E}\left((\epsilon_0)^2 \right)$ to the predictive variance.

Illustration of calibration (1/3)

- Observation of the physical phenomenon : $Y_{obs}(x) = x^2 + \epsilon$. $\epsilon \sim \mathcal{N}(0, \sigma^2_{mes} = 0.1^2)$
- Numerical code : $f(x, \beta) = \beta_0 + \beta_1 x$.
- Model error as a realization of a Gaussian process with covariance function : $C_{mod}(x-y) = \sigma^2 \exp\left(-\frac{|x-y|^2}{l_c^2}\right)$. $\sigma = 0.3$, $l_c = 0.5$ (known).
- Bayesian case with :

$$\beta_{prior} = \begin{pmatrix} 0.2 \\ 1 \end{pmatrix}, Q_{prior} = \begin{pmatrix} 0.09 & 0 \\ 0 & 0.09 \end{pmatrix}$$

- Observations : $x_1 = 0.2$, $x_2 = 0.4$, $x_3 = 0.6$ and $x_4 = 0.8$.

Illustration of calibration (2/3) (unnoised case)

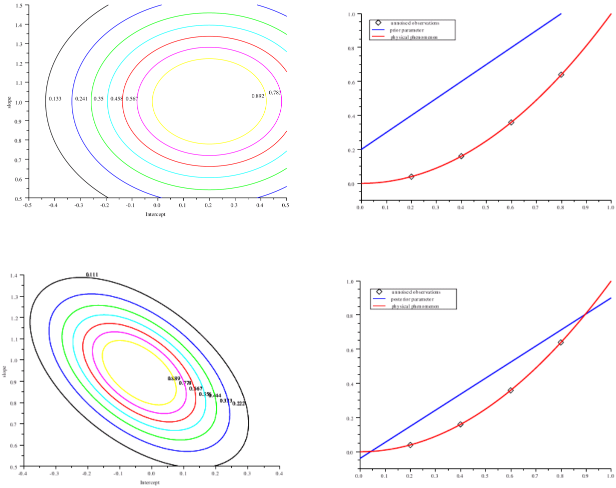


FIG.: Up-left : Prior distribution of the parameter β. Down-left : Posterior distribution of the parameter β. Right : plot of the code response corresponding to prior and posterior mean of the code parameter.

Illustration of calibration (3/3) (noised case)

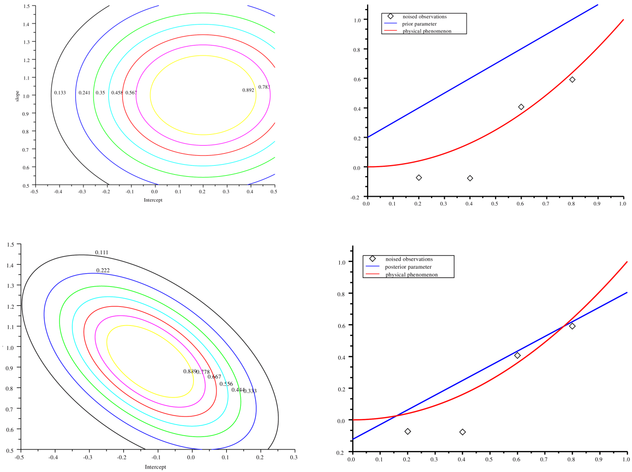
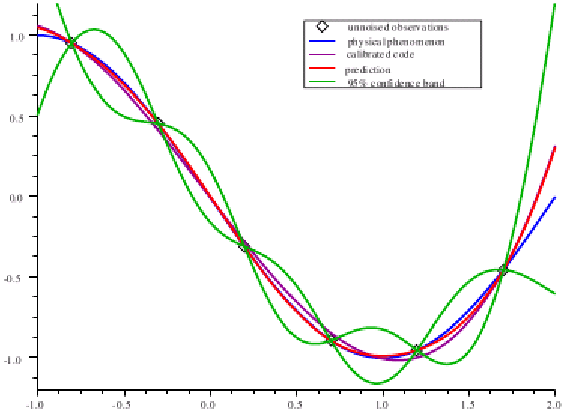


FIG.: Up-left : Prior distribution of the parameter β. Down-left : Posterior distribution of the parameter β. Right : plot of the code response corresponding to prior and posterior mean of the code parameter.

Illustration of prediction (1/3)

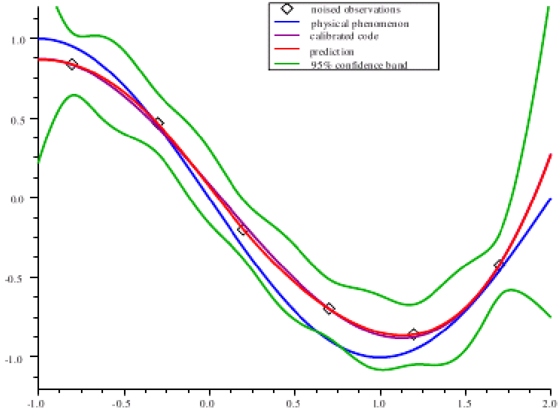
- Observation of the physical phenomenon : $Y_{obs}(x) = -sin(\frac{\pi x}{2}) + \epsilon$. $\epsilon \sim \mathcal{N}(0, \sigma_{mes}^2 = 0.1^2)$
- Numerical code : $f(x, \beta) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$.
- Model error as a realization of a Gaussian process with covariance function : $C_{mod}(x - y) = \sigma^2 \exp\left(-\frac{|x-y|^2}{l_c^2}\right)$. $\sigma = 0.3$, $l_c = 0.5$ (known).
- No prior information case.
- 6 observations regularly sampled between -0.8 and 1.7.

Illustration of prediction (2/3) (unnoised case)



- The use of the model error improves the prediction given by the numerical code.

Illustration of prediction (3/3) (noised case)



- The measure error deteriorates the quality of the predictions.
- The confidence intervals are however still reliable.

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Framework

- The calibration and prediction methods presented above give good results because we used a reasonable covariance function.
- The model selection is a statistical parameter estimation problem.

In our case, the covariance function of the measure error process ϵ is known for physical expertise. We want to take C_{mod} in a parametric set :

$$\left\{\sigma^2 C_{mod,\theta}\right\}$$

with $C_{mod,\theta}$ a correlation function.
Hence, with variance matrix $R_{\sigma,\theta} = \sigma^2 R_{mod,\theta} + K$, we have $(z+\epsilon) \sim \mathcal{N}(0, R_{\sigma,\theta})$ and we want to estimate σ and θ.
We present 2 methods for model selection : Restricted Maximum Likelihood and Leave One Out.

Restricted Maximum Likelihood

Principle : Estimate σ and θ independently of β (hence, same method with or without prior information).
Let C a $(n - m \times n)$ matrix of maximal rank such that $CH = 0$. Then we have :

$$w := Cy_{obs} \sim \mathcal{N}(0, CR_{\sigma,\theta}C')$$

We do maximum likelihood on the vector w.
The likelihood writes itself :

$$\ell_{\sigma,\theta}(w) \propto \frac{1}{det(CR_{\sigma,\theta}C^t)^{\frac{1}{2}}} \exp\left(-\frac{1}{2} w^t (CR_{\sigma,\theta}C^t)^{-1} w\right)$$

We maximize it :

$$\hat{\sigma}, \hat{\theta} \in \arg\max_{\sigma,\theta} \ell_{\sigma,\theta}(w).$$

Hence we estimate σ and θ to make the vector w the most probable.

Leave One Out (1/4)

We have seen that the prediction procedure (Bayesian or non-Bayesian framework) leads to a simple stochastic metamodel :
$x_0 \rightarrow \mathcal{N}\left(\langle y_{obs,0}\rangle, \hat{\sigma}^2_{x_0}\right)$. This metamodel depends on σ and θ.

- It is built according to the observations ($\approx$ learning set).

Leave One Out

- Given a vector of hyper-parameters (σ, θ).
- For i from 1 to n we learn $x_0 \rightarrow \mathcal{N}\left(\langle y_{obs,0}\rangle, \hat{\sigma}^2_{x_0}\right)$ with the reduced observations vector
$\{(x_1, y_{obs,1}), \ldots, (x_{i-1}, y_{obs,i-1}), (x_{i+1}, y_{obs,i+1}), \ldots, (x_n, y_{obs,n})\}$
- we compute the LOO errors by :

$$\epsilon_{LOO,i}(\sigma, \theta) = y_{obs,i} - \langle y_{obs,i}\rangle(y_{obs,-i}).$$

- we compute the LOO predictive variance by :

$$\hat{\sigma}^2_{LOO,i}(\sigma, \theta) = \hat{\sigma}^2_{x_i}(y_{obs,-i})$$

General utility of the Leave One Out :

- See how large the errors are.
- Check that the predictive variance are of the right size.

Leave One Out (2/4) : closed form formulas

No prior information case

With :

$$Q^{-}(\sigma,\theta) = \left(R^{-1}_{\sigma,\theta} - R^{-1}_{\sigma,\theta}H(H^T R^{-1}_{\sigma,\theta}H)^{-1}H^T R^{-1}_{\sigma,\theta}\right)$$

We have :

$$\epsilon_{LOO}(\sigma,\theta) = (diag(Q^{-}))^{-1}Q^{-}y_{obs} \quad \text{and} \quad \hat{\sigma}^2_{LOO,i}(\sigma,\theta) = \frac{1}{(Q^{-})_{i,i}}$$

Prior information case

With :

$$Q = R_{\sigma,\theta} + HQ_{prior}H^t$$

We have :

$$\epsilon_{LOO}(\sigma,\theta) = (diag(Q^{-1}))^{-1}Q^{-1}y_{obs} \quad \text{and} \quad \hat{\sigma}^2_{LOO,i}(\sigma,\theta) = \frac{1}{(Q^{-1})_{i,i}}$$

Leave One Out (3/4) : closed form formulas

- The no prior information case is the limit of the prior information case when $Q_{prior}^{-1} \rightarrow 0$.
- From a computational point of view : computing the LOO errors and predictive variance has the same order of complexity than REML and Maximum Likelihood.
- $\boxed{\longrightarrow}$ Can be use as an alternative of Maximum Likelihood techniques.

Leave One Out (4/4) : A model selection method

General principle, optimize a quality criterion based on $\epsilon_{LOO}(\sigma,\theta)$ and the $\hat{\sigma}^2_{LOO,i}$. For instance :

- Minimize norm of LOO errors.
- Set number of valid LOO p-confidence intervals close to p.
- Set $\frac{1}{n}\sum_{i=1}^{n}\frac{\epsilon^2_{LOO,i}(\sigma,\theta)}{\hat{\sigma}^2_{LOO,i}(\sigma,\theta)}$ close to 1

When the covariance matrix K of the measure error is null and no prior information case, we have $R_{\sigma,\theta}=\sigma^2 R_{mod,\theta}$, hence :

- $\epsilon_{LOO}(\sigma,\theta)$ independent of σ
- $\hat{\sigma}^2_{LOO}(\sigma,\theta)=\sigma^2\hat{\sigma}^2_{LOO}(\theta)$

Hence a classical method is :

$$\hat{\theta}\in\arg\min_{\theta}||\epsilon_{LOO}(\theta)||^2 \quad \text{and} \quad \hat{\sigma}^2=\frac{1}{n}\sum_{i=1}^{n}\frac{\epsilon^2_{LOO,i}(\hat{\theta})}{\hat{\sigma}^2_{LOO,i}(\hat{\theta})}$$

When $K\neq 0$ or prior information case : no classical method.

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The experimental results for the friction model

The experiment consists in pressurized and possibly heated water passing through a cylinder. We measure the pressure drop between the two ends of the cylinder.
Quantity of interest : The part of the pressure drop due to friction : ΔP_{fro}
Two kinds of experimental conditions :

- System parameters : Hydraulic diameter D_h, Friction height H_f, Channel width e.
- Environment variables : Output pressure P_s, Flowrate G_e, Parietal heat flux Φ_p, Liquid enthalpy h_e^l, Thermodynamic title X_{th}^e, Input temperature T_e.

We dispose of 253 experimental results. 115 are in the isothermal domain and 138 in the monophasic (non-isothermal) domain.
Important : Among the 253 experimental results, only 8 different system parameters $\rightarrow$ Not enough to use the Gaussian processes model for prediction for new system parameters $\rightarrow$ We predict for new environment variables only.

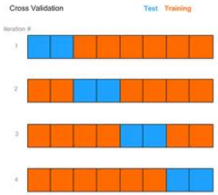
The Flica IV code for the friction model

Parameterized a_t and b_t.
Prior information (coming from previous studies) :

$$\beta_{prior} = \begin{pmatrix} 0.22 \\ 0.21 \end{pmatrix}, Q_{prior} = \begin{pmatrix} 0.11^2 & 0 \\ 0 & 0.105^2 \end{pmatrix}$$

Results

We compare predictions to observations using Cross Validation



We dispose of :

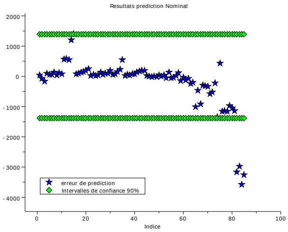
- The vector of posterior mean $\Delta\hat{P}_{fro}$ of size n.
- The vector of posterior variance σ^2_{pred} of size n.

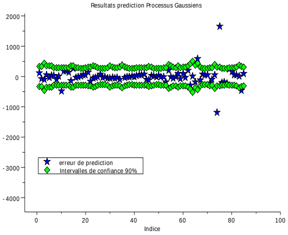
2 quantitative criteria :

- RMSE : $\sqrt{\frac{1}{n}\sum_{i=1}^{85}\left(\Delta P_{fro,i} - \Delta\hat{P}_{fro,i}\right)^2}$
- Confidence Intervals : proportion of observations that fall in the posterior 90% confidence interval.

Results : isothermal domain

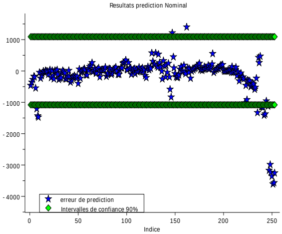
	RMSE	Confidence Intervals
Nominal code	$840Pa$	$80/85 \approx 0.94$
Gaussian Processes	$265Pa$	$79/85 \approx 0.93$

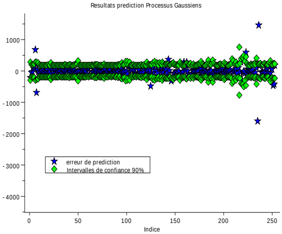




Results : isothermal and monophasic domain

	RMSE	Confidence Intervals
Nominal code	$661\,Pa$	$234/253 \approx 0.925$
Gaussian Processes	$189\,Pa$	$235/253 \approx 0.93$





Conclusion

- We can improve the prediction capability of the code by completing it with a statistical model based on the experimental results.
- Number of experimental results needs to be sufficient. No extrapolation.
- The choice of the covariance function is important.

Increasing use of probabilistic methods for numerical simulation : Kriging and Gaussian processes methods for surrogate models and code calibration and validation.

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