Calibration of computer models

A Closer Look at the Discrepancy Function

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Outline

Validation in [Bayarri et al., 2007] by examinning the Discrepancy. tolerance bounds around the posterior predictive mean which should contain with a high probability the true real process. These bounds are computed by integrating the different sources of uncertainties on the simulator due to its emulation and its discrepancy with the real world process, its parameters, field data... The prediction for a new input variable location $\mathbf{x}_{new}$ can be either a pure-simulator prediction given as

$$\hat{f}(\mathbf{x}_{new}, \hat{\boldsymbol{\theta}}) = m_D(\mathbf{x}_{new}, \hat{\boldsymbol{\theta}})$$

where $\hat{\boldsymbol{\theta}}$ may refer to the posterior mean or the posterior mode and m_D is used instead of f if we consider an expensive simulator, or a bias-corrected (discrepancy-corrected) prediction given as the mean:

$$\hat{f}^R(\mathbf{x}_{new}) = \frac{1}{M} \sum_{j=1}^{M} \left(F^{(j)}(\mathbf{x}_{new}, \boldsymbol{\theta}^{(j)}) + \delta^{(j)}(\mathbf{x}_{new}) \right)$$

where $F^{(j)}$ are posterior realizations of the GP F given $f(D)$ (evaluations of f at the DoNE) and $(\boldsymbol{\theta}^{(j)}, \delta^{(j)})$ are sampled from the joint posterior predictive distribution deriving from Equation (**??**) given the field data $\mathbf{y}^e$. For a fixed level γ, the tolerance bounds $\tau = \tau(\mathbf{x})$ are then computed such that $\gamma \cdot 100\%$ of the samples satisfy:

$$\left| \hat{f}(\mathbf{x}_{new}, \hat{\boldsymbol{\theta}}) - m_D(\mathbf{x}_{new}, \hat{\boldsymbol{\theta}}) \right| < \tau$$

for the pure-simulator prediction. Similarly for the bias-corrected prediction, τ are computed such that $\gamma \cdot 100\%$ of the samples satisfy:

Outline

L_2 Calibration

Defined in [Tuo and Wu, 2016]:

$$\boldsymbol{\theta}_{L_2} = \underset{\Theta}{\operatorname{argmin}} \|\delta_{\boldsymbol{\theta}}(\cdot)\|_{L_2(\mathcal{X})} = \underset{\Theta}{\operatorname{argmin}} \left(\int_{\mathcal{X}} (\zeta(\mathbf{x}) - f(\mathbf{x}, \boldsymbol{\theta}))^2 d\mathbf{x} \right)^{1/2}.$$

[Tuo et al., 2015]proposes to first obtain an estimate $\hat{\zeta}$ of the reality ζ via a Gaussian stochastic stochastic process and then plug it into the minimization problem to get $\hat{\boldsymbol{\theta}}_{L_2}$.
Consistent estimation $\hat{\boldsymbol{\theta}}_{L_2} \rightarrow \boldsymbol{\theta}_{L_2}$ provided that $\hat{\zeta}$ is good approximation.
An alternative least square :

$$\hat{\boldsymbol{\theta}}_{LS} = \underset{\Theta}{\operatorname{argmin}} \left(\sum_{i=1}^{n_e} (y_{exp_i} - f(\mathbf{x}, \boldsymbol{\theta}))^2 \right)$$

[Tuo et al., 2015] proves the convergence $\hat{\boldsymbol{\theta}}_{LS} \rightarrow \boldsymbol{\theta}_{L_2}$
[Wong et al., 2017] uses LS calibration as a plug-in estimator for estimating the discrepancy function via a nonparametric regression

Scaled Gaussian Process

[Gu and Wang, 2018]

$$
\begin{aligned}
y_{exp_i} =& f(\mathbf{x}_i, \boldsymbol{\theta}) + \mu^{\delta}(\mathbf{x}_i) + \delta_z(\mathbf{x}_i) + \epsilon_i \\
\mu^{\delta} =& \sum_{i=1}^{q} h(\mathbf{x}_i)\beta_i \\
\delta_z(\cdot) \sim& GP(0, \sigma_\delta^2 c_\delta(\cdot,\cdot)) \text{ s.t. } \int_{\mathcal{X}} \delta_z(\mathbf{x})^2 d\mathbf{x} = Z \\
Z \sim& p_{\delta_z}(\cdot), \quad p_{\delta_z}(z) \propto f_z(Z = z|\lambda) \cdot p_\delta(z|\boldsymbol{\theta}, \Psi)
\end{aligned}
$$

where $p_\delta(z|\boldsymbol{\theta}, \Psi)$ is the implicit prior on Z for a GP on the discrepancy.
Then if f_z constant $\Rightarrow$ Model is equivalent to KOH model.

Comparison GP with SGP

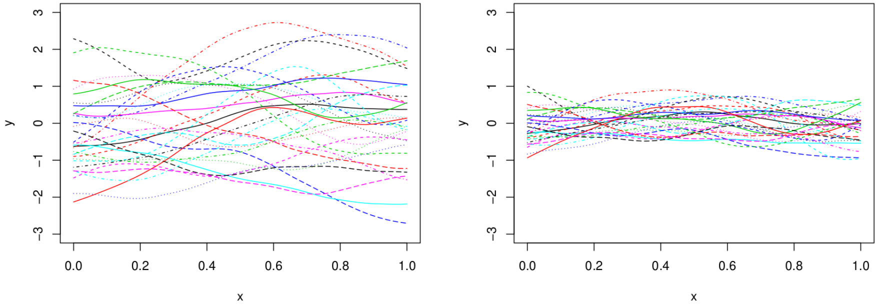

Figure 2. *Fifty samples from the GaSP and discretized S-GaSP are graphed in the left and right panels, respectively, where* x_i *is equally spaced in* $[0, 1]$*. For both processes, we let* $\mu^\delta = 0$, $\sigma^2_\delta = 1$ *and* $\gamma^\delta = 1/2$*. In the discretized S-GaSP,* $\mathbf{x}^C_i = \mathbf{x}_i$ *for* $i = 1, ..., N_C$, $N_C = n$ *and* $\lambda = n/2$ *are assumed..*

from [Gu and Wang, 2018].

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Model Comparison

- $\mathcal{H}_0 : \zeta(\cdot) = f(\cdot, \boldsymbol{\theta}^*)$ for a "true" $\boldsymbol{\theta}^*$:

$$y_i \quad = \quad f(\mathbf{x}_i, \boldsymbol{\theta}^*) + \epsilon_i^0 \,,$$

  where $\epsilon_i^0 \overset{iid}{\sim} \mathcal{N}(0, \lambda_0^2)$.

- $\mathcal{H}_1$: Code discrepancy term $\delta(\mathbf{x})$ s.t. $\zeta(\mathbf{x}) = f(\mathbf{x}, \boldsymbol{\theta}^*) + \delta(\mathbf{x})$:

$$y_i = f(\mathbf{x}_i, \boldsymbol{\theta}^*) + \delta(\mathbf{x}_i) + \epsilon_i^1 \qquad \begin{array}{ll} \text{where} & \delta(.) \sim \mathcal{GP}(0, \sigma^2 \Sigma_\psi(.,.)) \\ \text{and} & \epsilon_i^1 \overset{iid}{\sim} \mathcal{N}(0, \lambda_1^2) \end{array}$$

Bayes Factor

$$B_{0,1}(\boldsymbol{y}) := \frac{p(\boldsymbol{y}|\mathcal{H}_0)}{p(\boldsymbol{y}|\mathcal{H}_1)} \quad \text{where} \quad p(\boldsymbol{z}|\mathcal{H}_j) = \int_{\boldsymbol{p}_j} p(\boldsymbol{y}|\boldsymbol{p}_j, \mathcal{H}_j)\pi(\boldsymbol{p}_j) d\boldsymbol{p}_j \,.$$

Intrinsic Bayes Factor

Berger and Perrichi (1996).

Main issue: Evidence $p(\boldsymbol{y}|\mathcal{H}_j)$ sensitive to priors $\pi(\boldsymbol{p}_j)$.

- Need to use compatible priors Celeux et al. (2006) or objective priors Casella (2006),
- but marginal likelihood ill-defined (up to arbitrary constant) for improper priors (as objective priors often are).

Idea: using a part of data to obtain a proper prior:

- Partial Bayes Factor:

$$B_{0,1}(\boldsymbol{y}(-m)|\boldsymbol{y}(m)) = \frac{\int l(\boldsymbol{p}_0; \boldsymbol{y}(-m)|\boldsymbol{y}(m))\pi(\boldsymbol{p}_0|\boldsymbol{y}(m))d\boldsymbol{p}_0}{\int l(\boldsymbol{p}_1; \boldsymbol{y}(-m)|\boldsymbol{y}(m))\pi(\boldsymbol{p}_1|\boldsymbol{y}(m))d\boldsymbol{p}_1} = \frac{B_{0,1}(\boldsymbol{y})}{B_{0,1}(\boldsymbol{y}(m))}.$$

- $B_{0,1}(\boldsymbol{y}(-m)|\boldsymbol{y}(m))$ well-defined for $|m| \geq n_0$ large enough:
- Intrinsinc Bayes factor obtained by averaging over all $\boldsymbol{y}(m)$s :

$$B^A_{0,1}(\boldsymbol{y}) = \frac{B_{0,1}(\boldsymbol{z})}{C(n, n_0)} \sum_{|m|=n_0} B_{0,1}(\boldsymbol{y}(m))^{-1}.$$

IBF computation under linearization of the code

Linear assumption: $f(\boldsymbol{x}, \boldsymbol{\theta}) = g(\boldsymbol{x})^\top \boldsymbol{\theta}$, with $g(\boldsymbol{x}) \in \mathbb{R}^d$.

Prior choices and consequences:

- Model $\mathcal{H}_0$ boils down to:

$$\mathcal{H}_0 : \boldsymbol{y} \quad \sim \quad \mathcal{N}(G\boldsymbol{\theta}_0; \lambda_0^2 \mathrm{I}_\mathrm{n}); \quad \boldsymbol{p}_0 = (\boldsymbol{\theta}_0, \lambda_0^2)$$

  where $G = [g(\boldsymbol{x}_1), \cdots, g(\boldsymbol{x}_n)]^\top$ the $n \times p$ design matrix.
  $\hookrightarrow$ Under Jeffreys prior: $\pi(\boldsymbol{p}_0) \propto \lambda_0^{-2}$, $p(\boldsymbol{y}|\mathcal{H}_0)$ explicit.

- Model $\mathcal{H}_1$ boils down to:

$$\mathcal{H}_1 : \boldsymbol{y} \quad \sim \quad \mathcal{N}(G\boldsymbol{\theta}_1; \sigma^2 V_{k,\psi}); \quad \boldsymbol{p}_1 = (\boldsymbol{\theta}_1, \sigma^2, \psi, k)$$

$$V_{k,\psi}(i,j) = k\delta_{i,j} + e^{-||\boldsymbol{x}_i - \boldsymbol{x}_j||^2/\psi^2} \quad k = \lambda_1^2 \sigma^{-2}.$$

  - Prior choice: $\pi(\boldsymbol{p}_1) \propto \pi(\psi|k)\pi(k)\sigma^{-2}$ Berger et al. (2001) with proper priors for $\pi(\psi|k)\pi(k)$,
  - Integration of $p(\boldsymbol{y}|\boldsymbol{p}_1, \mathcal{H}_1)$: explicit over (θ_1, σ^2), by Gaussian quadrature over (ψ, k).

Computation of the IBF

Proposition

If $\pi(\boldsymbol{p}_1) = \pi(\theta_1, \sigma^2, \psi, k) = \pi(\psi|k)\pi(k)/\sigma^2$, $\pi(\psi, k)$ is proper and $m = d + 1$ then

$$B^A_{0,1}(\boldsymbol{y}) = \frac{B_{0,1}(\boldsymbol{z})}{C(n, n_0)} \sum_{|m|=n_0} B_{0,1}(\boldsymbol{y}(m))^{-1} = B_{0,1}(\boldsymbol{y})$$

Proof: Consequence of Berger et al. (1998).

In the following,

$$\begin{aligned} \pi(\psi|k) &= \mathcal{U}([0,1]) \,, \\ \pi(k) &= Be(1,3) \,. \end{aligned}$$

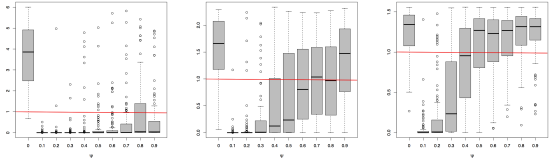
Synthetic data

Data simulated according to model $\mathcal{H}_1$, with $\delta \sim GP(0, \sigma^2 \Sigma_\psi)$:

$$\boldsymbol{x} = \left(\frac{i}{n}\right)_{1 \leq i \leq n}, \quad n = 30, \quad \sigma^2 = 0.1, \quad k = 0.1\,.$$

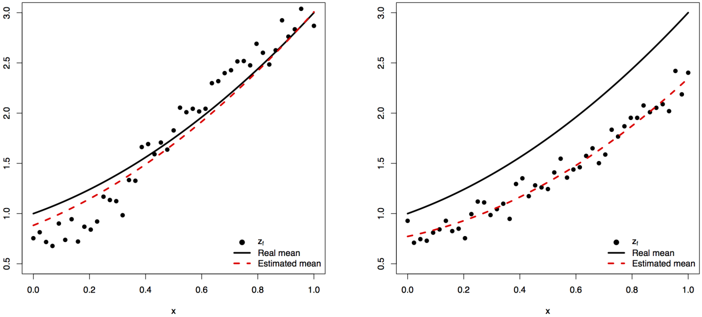
From left to right

- constant trend $g(\mathbf{x}) = 1$; $\theta_1 = 1$,
- linear trend $g(\mathbf{x}) = (1, x)$; $\boldsymbol{\theta}_1 = (1, 1)$,
- quadratic trend $g(\mathbf{x}) = (1, x, x^2)$; $\boldsymbol{\theta}_1 = (1, 1, 1)$.
- Bayes factor $B^A_{0,1}$ expected to decrease with ψ.



Boxplots of $B^A_{0,1}(\boldsymbol{y})$ values over 100 simulations with constant, linear and quadratic trends (left to right)

Confounding Effect



$\psi = 0.2$ left and $\psi = 0.7$ right

- ψ, k, σ^2 estimated by maximum likelihood.
- For $\psi = 0.7$, discrepancy indistinguishable from quadratic trend!

Case description

- Industrial computer code predicting the **productivity** of an electric power plant, based on measurements (temperature, pressure, discharge, ...) throughout the plant
- $n = 24$ available field measures (results of periodic testing) to validate code

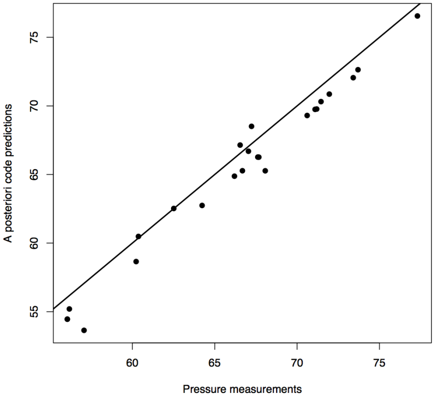
Main code features:

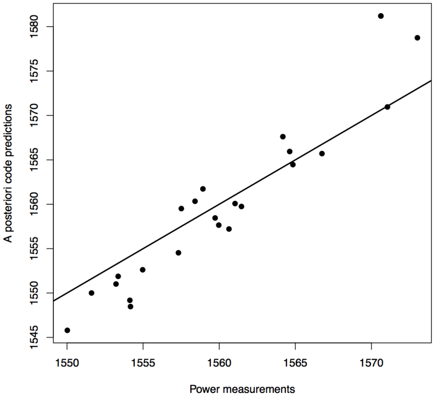
- $p = 20$ input variables ($\boldsymbol{x} \in \mathbb{R}^{20}$)
- $d = 2$ parameters: heat transfer coefficient of the condenser, yield of the main turbine 2 .
- Two outputs of interest (electric power, condenser pressure), seen here as two separate codes
- Code **linearized** in neighbourhood of reference value $\theta^\star$:

$$f(\boldsymbol{x}_i, \boldsymbol{\theta}) \approx f(\boldsymbol{x}_i, \boldsymbol{\theta}^\star) + h(\boldsymbol{x}_i)^\top (\boldsymbol{\theta} - \boldsymbol{\theta}^\star),$$

where $h(\boldsymbol{x}_i) = \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}_i, \boldsymbol{\theta}^\star)$ evaluated numerically through finite difference

Calibrated code predictions vs measures





Pressure
$B^A_{0,1} = 2 \times 10^{-18}$

Power
$B^A_{0,1} = 3 \times 10^{-3}$

- Bias reduced by calibration, but not supressed
- strong evidence for code discrepancy

Outline

Model selection as a mixture problem

Kamary et al. (2014)

Model selection problem:

$$\mathfrak{M}_0 : y_i = f(\mathbf{x}_i, \boldsymbol{\theta}_0) + \epsilon_i^0$$
$$\mathfrak{M}_1 : y_i = f(\mathbf{x}_i, \boldsymbol{\theta}_1) + \delta(\mathbf{x}_i) + \epsilon_i^1 .$$

where $\epsilon_i^0 \overset{iid}{\sim} \mathcal{N}(0, \lambda_0^2)$ and $\epsilon_i^1 \overset{iid}{\sim} \mathcal{N}(0, \lambda_1^2)$

converted into a mixture model:

$$\mathfrak{M}_\alpha : y_i \sim \alpha \left(\ell_{\mathfrak{M}_0}(\boldsymbol{\theta}_0, \lambda_0^2; y_i, \mathbf{x}_i) \right) + (1 - \alpha) \left(\ell_{\mathfrak{M}_1}(\boldsymbol{\theta}_1, \lambda_1^2, \delta; y_i, \mathbf{x}_i) \right) .$$

- Model $\mathfrak{M}_\alpha$ is defined under the hypothesis that the likelihood of the model $\mathfrak{M}_1$ is conditioned on δ.
- δ is considered as a parameter of $\mathfrak{M}_1$.
- Conditionnally on δ, the y_i's are considered independent.
- Posterior distribution on α will provide a decision rule for $\mathfrak{M}_0$ against $\mathfrak{M}_1$.

Hypotheses and prior distribution

- Linear code: $f(\mathbf{x}, \boldsymbol{\theta}) = g(\mathbf{x})\boldsymbol{\theta}$.
- GP prior for discrepancy function:

$$\delta(.) \sim \mathcal{GP}(0, \sigma^2 \Sigma_\psi(.,.)) .$$

- Some parameters are common, $\boldsymbol{\theta}$ and λ^2 so a common prior distribution is chosen for both.

$$\mathfrak{M}_\alpha : y_i \sim \alpha \left(\ell_{\mathfrak{M}_0}(\boldsymbol{\theta}, \lambda^2; y_i, \mathbf{x}_i) \right) + (1-\alpha) \left(\ell_{\mathfrak{M}_1}(\boldsymbol{\theta}, \lambda^2, \delta; y_i, \mathbf{x}_i) \right) .$$

Posterior distribution

Theorem

Let $g : \mathbb{R}^p \to \mathbb{R}^d$ be a finite-valued function and vector $x_1, \ldots, x_n$ such that the rank of $\{g(x_1), \ldots, g(x_n)\}$ is d. The posterior distribution associated with the prior $\pi(\boldsymbol{\theta}, \lambda^2) = {}^1/_{\lambda^2}$ and with the likelihood is proper when

- for any $0 < k < 1$, the hyperparameter σ^2 of the discrepancy prior distribution is reparameterized as $\sigma^2 = {}^{\lambda^2}/_k$ and so $\Sigma_\psi = ({}^{\lambda^2}/_k)\text{Corr}_{\psi_\delta}$ when $\text{Corr}_{\psi_\delta}$ is the correlation function of δ.
- the mixture weight α has a proper beta prior $\mathcal{B}(a_0, a_0)$;
- ψ_δ has a proper Beta prior $\mathcal{B}(b_1, b_2)$.
- proper distribution is used on k.

Metropolis within Gibbs

Algorithm 1: Metropolis-within-Gibbs algorithm

for t=1,...,T **do**

a) $\delta^{(t)}$ is sampled from $\pi(\delta|\boldsymbol{y}, \mathbf{x}, \boldsymbol{\theta}^{(t-1)}, \lambda^{(t-1)}, k^{(t-1)}, \psi_\delta^{(t-1)}, \alpha^{(t-1)})$ as follows.

   a.1) For $i = 1, \ldots, n$; $j = 0, 1$, generate auxiliaire variable $\zeta_i^{(t)}$ from

$$\mathbb{P}(\zeta_i = j|y_i, x_i, \delta^{(t-1)}, \boldsymbol{\theta}^{(t-1)}, \lambda^{(t-1)}, k^{(t-1)}, \psi_\delta^{(t-1)}) .$$

   a.2) Generate $\delta^{(t)}$ according to the conditional posterior distribution

$$\delta^{(t)}|\boldsymbol{y}, \mathbf{x}, \zeta^{(t)} = 1, \boldsymbol{\theta}^{(t-1)}, \lambda^{(t-1)}, k^{(t-1)}, \psi_\delta^{(t-1)}, \alpha^{(t-1)} \sim \mathcal{N}_n(\hat{\mu}_\delta, \hat{\Sigma}_\delta) .$$

b) Generate $\boldsymbol{\theta}^{(t)}|\boldsymbol{y}, \mathbf{x}, \boldsymbol{\zeta}^{(t)}, \delta^{(t)}, \lambda^{(t-1)}, k^{(t-1)}, \alpha^{(t-1)} \sim \mathcal{N}_d(\hat{\mu}_{\boldsymbol{\theta}}, \hat{\Sigma}_{\boldsymbol{\theta}})$.

c) Generate $\lambda^{(t)}|\boldsymbol{y}, \mathbf{x}, \boldsymbol{\zeta}^{(t)}, \delta^{(t-1)}, \boldsymbol{\theta}^{(t)}, k^{(t-1)}, \alpha^{(t-1)} \sim \mathcal{IG}(\hat{a}_\lambda, \hat{b}_\lambda)$.

d) Generate $\alpha^{(t)}|\boldsymbol{y}, \mathbf{x}, \boldsymbol{\zeta}^{(t)}, \delta^{(t)}, \boldsymbol{\theta}^{(t)}, \lambda^{(t)}, k^{(t-1)} \sim \mathcal{B}eta(n - m + a_0, m + a_0)$.

e) Generate $k^{(t)}$ from a random walk Metropolis-Hastings algorithm conditionally to $(\boldsymbol{y}, \mathbf{x}, \boldsymbol{\zeta}^{(t)}, \delta^{(t)}, \boldsymbol{\theta}^{(t)}, \lambda^{(t)}, \alpha^{(t)}, \psi_\delta^{(t-1)})$.

f) Generate $\psi_\delta^{(t)}$ from a random walk Metropolis-Hastings algorithm conditionally to $(\boldsymbol{y}, \mathbf{x}, \boldsymbol{\zeta}^{(t)}, \delta^{(t)}, \boldsymbol{\theta}^{(t)}, \lambda^{(t)}, \alpha^{(t)}, k^{(t)})$.

Synthetic example $\mathfrak{M}_0$

Code is a quadratic function.
50 datasets of size $n = 30$ from $\mathfrak{M}_0 : y_i = g(x)\boldsymbol{\theta}^* + \epsilon_i$.
Priors as in the theorem, $\alpha \sim \mathcal{B}eta(1,1)$, $\delta \sim \mathcal{GP}(0_n, \Sigma_\psi)$, $\psi_\delta \sim \mathcal{B}eta(1,1)$ and $k \sim \mathcal{B}eta(1,1)$.
Number of MCMC iterations is 10^4 with a burn-in of 10^3 iterations

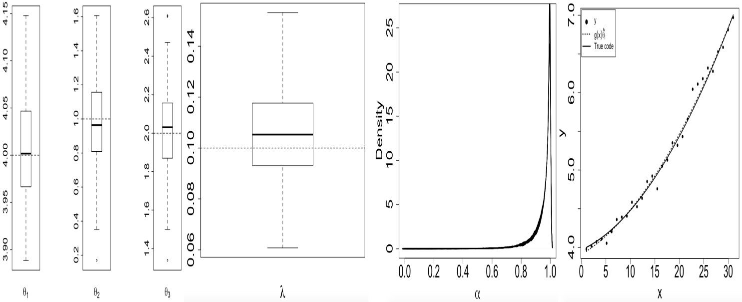


Figure: Posterior mean estimates of $\boldsymbol{\theta}, \lambda^2$, Posterior densities of α, Posterior prediction of the code.

Synthetic example $\mathfrak{M}_1$

Code is a quadratic function.
50 samples of size 50 simulated from $\mathfrak{M}_1$ when ψ_δ^* varies between 0.01 and 0.9, $\delta^*(x) \sim \mathcal{GP}(0_n, \Sigma_\psi)$, $\lambda^2* = 0.1$ and $k^* = 0.1$.
Priors as in the theorem, $\alpha \sim \mathcal{B}eta(1,1)$, $\delta \sim \mathcal{GP}(0_n, \Sigma_\psi)$, $\psi_\delta \sim \mathcal{B}eta(1,1)$ and $k \sim \mathcal{B}eta(1,1)$.
Number of MCMC iterations is 10^4 with a burn-in of 10^3 iterations.

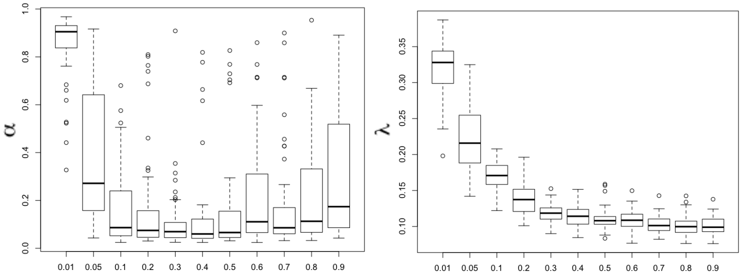


Figure: Posterior mean estimates for α and λ^2.

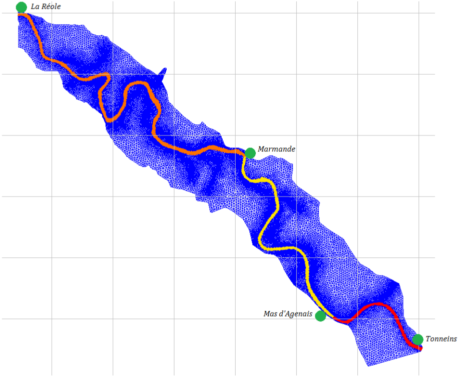
Hydraulic application: Garonne river

- TELEMAC 2D models the flow of the Garonne between Tonneins and la Réole:

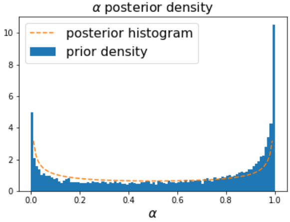
$$h_i = f(q_i, \mathbf{K_s}),$$

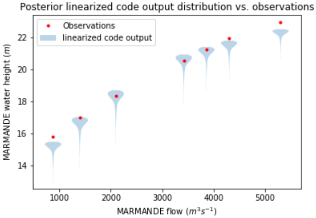
with:

- $\mathbf{h}_i$ water heights,
- $\mathbf{K_s} = (K_{s1}, \ldots, K_{s5})$ Strickler coefficients (5 friction coefficients)
- q_i river flow at Tonneins
- Linearization of the model around a reference value for the Strickler coefficient (limited to the most inflential ones).
- Only 7 data points available.



Results





Observation nb.	1	2	3	4	5	6	7
Bias probability	0.513	0.473	0.452	0.448	0.451	0.472	0.514

Table: Probability of a code bias for each observation in Marmande

Damblin + Kaniav

Outline

Variable Selection in the Discrepancy

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