

Calibration of computer models

A Closer Look at the Discrepancy Function

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INRAE

Outline

- 1 Validation
- 2 Robust Calibration
- 3 Model Selection
 - Bayes Factor
 - Mixture model
- 4 Posterior Inclusion Probabilities of input variables in the discrepancy

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Validation in [Bayarri et al., 2007] by examining the Discrepancy.

Estimate tolerance bounds by computing: For a fixed level γ , the tolerance bounds $\tau = \tau(\mathbf{x})$ are then computed such that $\gamma \cdot 100\%$ of the samples satisfy:

- for pure simulator predictions $\left| \hat{f}(\mathbf{x}_{new}, \hat{\theta}) - \zeta^{(i)}(\mathbf{x}_{new}) \right| < \tau$
- for bias-corrected predictions $\left| \hat{\zeta}(\mathbf{x}_{new}) - \zeta^{(i)}(\mathbf{x}_{new}) \right| < \tau$

where

- $\hat{f}(\mathbf{x}_{new}, \hat{\theta}) = m_D(\mathbf{x}_{new}, \hat{\theta})$ where $\hat{\theta}$ may refer to the posterior mean,
- $\zeta^{(i)}(\mathbf{x}_{new}) = F^{(i)}(\mathbf{x}_{new}, \theta^{(i)}) + \delta^{(i)}(\mathbf{x}_{new})$,
- $F^{(i)}(\mathbf{x}_{new}, \theta^{(i)})$ and $\delta^{(i)}(\mathbf{x}_{new})$ ($1 \leq i \leq N$) are obtained by an MCMC algorithm sampling from the joint posterior predictive distribution,
- $\hat{\zeta}(\mathbf{x}_{new}) = \frac{1}{N} \sum_{i=1}^N \left(F^{(i)}(\mathbf{x}_{new}, \theta^{(i)}) + \delta^{(i)}(\mathbf{x}_{new}) \right)$.

Note that the discrepancy can be estimated from the posterior model and discrepancy sampling on a set of new locations: \mathbf{X}_{new} :

$$\hat{\delta}_{\hat{\theta}} = \hat{\zeta}_{new} - \hat{f}(\mathbf{x}_{new}, \hat{\theta}).$$

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L_2 Calibration

Defined in [Tuo and Wu, 2016]:

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

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

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

[Tuo et al., 2015] proves the convergence $\hat{\theta}_{LS} \rightarrow \theta_{L_2}$
 [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]

$$y_i^e = f(\mathbf{x}_i^e, \boldsymbol{\theta}) + \mu^\delta(\mathbf{x}_i^e) + \delta_z(\mathbf{x}_i^e) + \epsilon_i$$

$$\mu^\delta(\mathbf{x}) = \sum_{i=1}^q h(\mathbf{x})\beta_i$$

$$\delta_z(\cdot) \sim GP(0, \sigma_\delta^2 c_\delta(\cdot, \cdot)) \text{ s.t. } \int_{\mathcal{X}} \delta_z(\mathbf{x})^2 d\mathbf{x} = Z$$

$$Z \sim p_{\delta_z}(\cdot), \quad p_{\delta_z}(Z) \propto f_z(Z = z|\lambda) \cdot p_\delta(z|\boldsymbol{\theta}, \Psi)$$

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

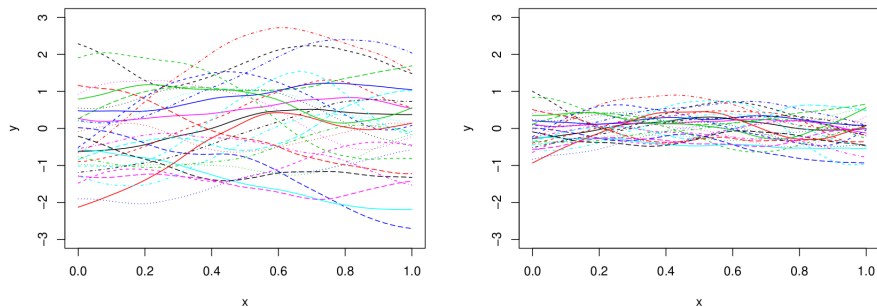


Figure 2. Fifty samples from the GaSP and discretized S-GaSP are graphed in the left and right panels, respectively, where x_i is equally spaced in $[0, 1]$. For both processes, we let $\mu^\delta = 0$, $\sigma_\delta^2 = 1$ and $\gamma^\delta = 1/2$. In the discretized S-GaSP, $\mathbf{x}_i^C = \mathbf{x}_i$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

from [Gu and Wang, 2018].

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Model Comparison

[Damblin et al., 2016]

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

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

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

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

$$y_i = f(\mathbf{x}_i, \theta^*) + \delta(\mathbf{x}_i) + \epsilon_i^1 \quad \text{where } \delta(\cdot) \sim \mathcal{GP}(0, \sigma_\delta^2 \Sigma_\psi(\cdot, \cdot))$$

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

Bayes Factor

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

Intrinsic Bayes Factor

[Berger and Pericchi, 1996]

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

- Need to use compatible priors [Celeux et al., 2006] or objective priors [Casella and Moreno, 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:

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

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

$$B_{0,1}^A(\mathbf{y}^e) = \frac{B_{0,1}(\mathbf{z})}{C(n, n_0)} \sum_{|m|=n_0} B_{0,1}(\mathbf{y}^e(m))^{-1}.$$

IBF computation under linearization of the code

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

Prior choices and consequences:

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

$$\mathcal{H}_0 : \mathbf{y}^e \sim \mathcal{N}(G\theta_0; \lambda_0^2 \mathbf{I}_{n_e}); \quad \mathbf{p}_0 = (\theta_0, \lambda_0^2)$$

where $G = [g(\mathbf{x}_1^e), \dots, g(\mathbf{x}_{n_e}^e)]^\top$ the $n_e \times p$ design matrix.

→ Under Jeffreys prior: $\pi(\mathbf{p}_0) \propto \lambda_0^{-2}$, $p(\mathbf{y}^e | \mathcal{H}_0)$ explicit.

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

$$\mathcal{H}_1 : \mathbf{y}^e \sim \mathcal{N}(G\theta_1; \sigma_\delta^2 V_{k,\psi}); \quad \mathbf{p}_1 = (\theta_1, \sigma_\delta^2, \psi, k)$$

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

- Prior choice: $\pi(\mathbf{p}_1) \propto \pi(\psi|k)\pi(k)\sigma^{-2}$ with proper priors for $\pi(\psi|k)\pi(k)$,
- Integration of $p(\mathbf{y}^e | \mathbf{p}_1, \mathcal{H}_1)$: explicit over $(\theta_1, \sigma_\delta^2)$, by Gaussian quadrature over (ψ, k) .

Computation of the IBF

Proposition

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

$$B_{0,1}^A(\mathbf{y}^e) = \frac{B_{0,1}(\mathbf{z})}{C(n, n_0)} \sum_{|m|=n_0} B_{0,1}(\mathbf{y}^e(m))^{-1} = B_{0,1}(\mathbf{y}^e)$$

In the following,

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

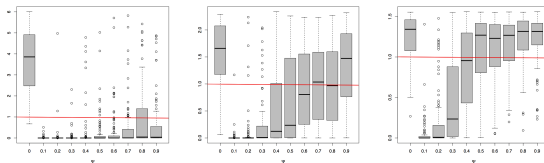
Synthetic data

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

$$\mathbf{x}_i^e = \left(\frac{i}{n_e} \right)_{1 \leq i \leq n}, \quad n_e = 30, \quad \sigma_\delta^2 = 0.1, \quad k = 0.1.$$

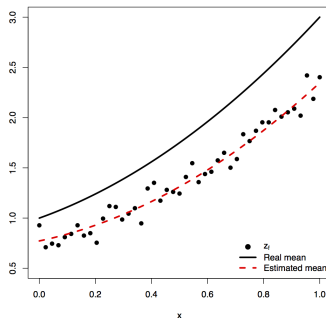
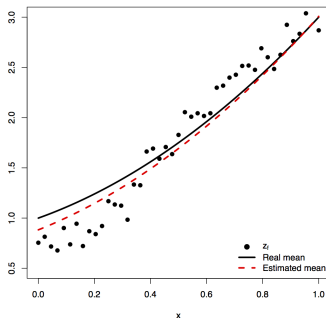
From left to right

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



Boxplots of $B_{0,1}^A(\mathbf{y}^e)$ 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_δ^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

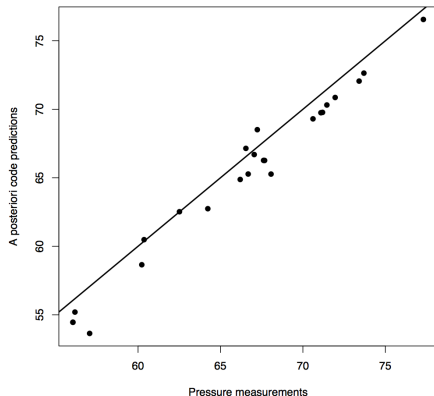
Main code features:

- $p = 20$ input variables ($\mathbf{x} \in \mathbb{R}^{20}$)
- $d = 2$ 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 θ^* :

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

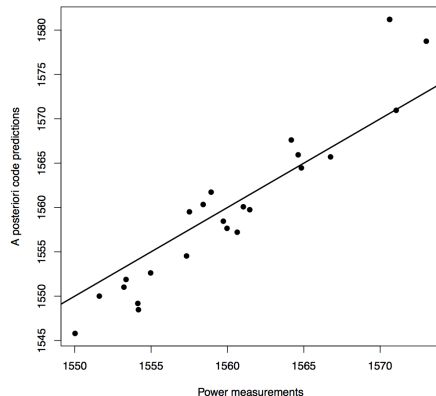
where $h(\mathbf{x}_i) = \nabla_\theta f(\mathbf{x}_i, \theta^*)$ evaluated numerically through finite difference

Calibrated code predictions vs measures



Pressure

$$B_{0,1}^A = 2 \times 10^{-18}$$



Power

$$B_{0,1}^A = 3 \times 10^{-3}$$

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

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Model selection as a mixture problem

[Kamary et al., 2019] inspired by [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 $\epsilon_i^0 \stackrel{iid}{\sim} \mathcal{N}(0, \lambda_0^2)$ and $\epsilon_i^1 \stackrel{iid}{\sim} \mathcal{N}(0, \lambda_1^2)$

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}_α 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: $f(\mathbf{x}, \boldsymbol{\theta}) = g(\mathbf{x})^\top \boldsymbol{\theta}$.

- GP prior for discrepancy function:

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

- 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 $g : \mathbb{R}^p \rightarrow \mathbb{R}^d$ be a finite-valued function and vector $\mathbf{x}_1^e, \dots, \mathbf{x}_n^e$ such that the rank of $\{g(\mathbf{x}_1^e), \dots, g(\mathbf{x}_n^e)\}$ 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_δ^2 of the discrepancy prior distribution is reparameterized as $\sigma_\delta^2 = \lambda^2/k$ 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 $t=1, \dots, T$ do

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

- a.1) For $i = 1, \dots, n; j = 0, 1$, generate auxiliary variable $\nu_i^{(t)}$ from

$$\mathbb{P}(\nu_i = j | \mathbf{y}_i^e, \mathbf{x}_i^e, \delta^{(t-1)}, \boldsymbol{\theta}^{(t-1)}, \lambda^{(t-1)}, k^{(t-1)}, \psi_{\delta}^{(t-1)}).$$

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

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

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

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

- d) Generate $\alpha^{(t)} | \mathbf{y}^e, \mathbf{X}^e, \nu^{(t)}, \delta^{(t)}, \boldsymbol{\theta}^{(t)}, \lambda^{(t)}, k^{(t-1)} \sim \text{Beta}(n - m + a_0, m + a_0).$

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

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

Synthetic example \mathfrak{M}_0

Code is a quadratic function.

50 datasets of size $n = 30$ from $\mathfrak{M}_0 : y_i = g(x)^\top \theta^* + \epsilon_i$.

Priors as in the theorem, $\alpha \sim \text{Beta}(1, 1)$, $\delta \sim \mathcal{GP}(0_n, \Sigma_\psi)$, $\psi_\delta \sim \text{Beta}(1, 1)$ and $k \sim \text{Beta}(1, 1)$.

Number of MCMC iterations is 10^4 with a burn-in of 10^3 iterations

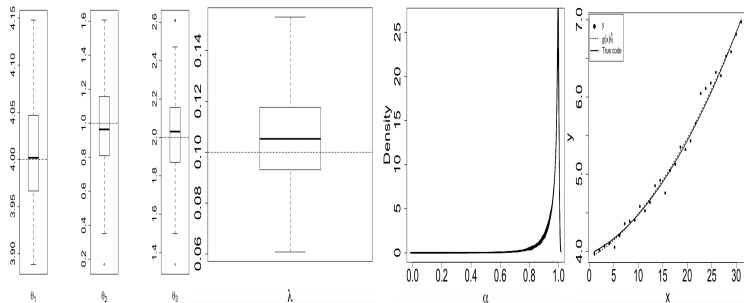


Figure: Posterior mean estimates of θ , λ^2 , Posterior densities of α , Posterior prediction of the code.

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, $\alpha \sim \text{Beta}(1, 1)$, $\delta \sim \mathcal{GP}(0_n, \Sigma_\psi)$, $\psi_\delta \sim \text{Beta}(1, 1)$ and $k \sim \text{Beta}(1, 1)$.

Number of MCMC iterations is 10^4 with a burn-in of 10^3 iterations.

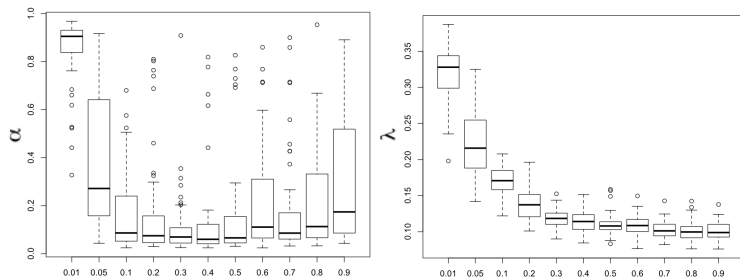


Figure: Posterior mean estimates for α and λ^2 .

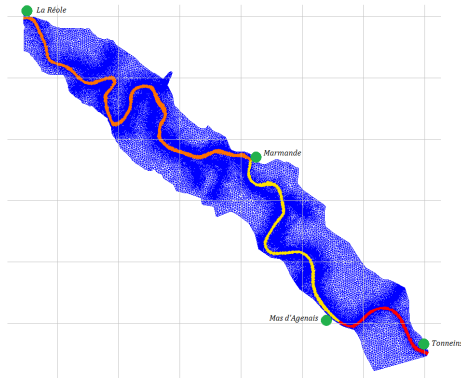
Hydraulic application: Garonne river

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

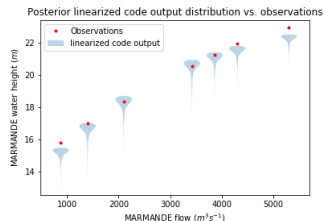
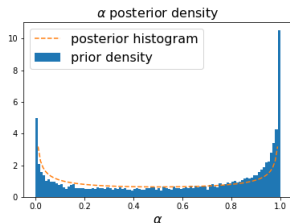
$$h_i = f(q_i, \mathbf{K}_s),$$

with:

- h_i water heights,
- $\mathbf{K}_s = (K_{s1}, \dots, K_{s5})$ 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 influential 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

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Variable selection in the discrepancy function

[Joseph and Yan, 2015]

- perform a sensitivity analysis on the discrepancy function,
- two-step procedure: i) find an optimal $\hat{\theta}$, ii) run an SA on the discrepancy (consequence of the fixed $\hat{\theta}$)

[Barbillon et al., 2021]

- run an MCMC algorithm to obtain posterior distribution,
- post-process the posterior samples to compute probabilities of inclusion for each of the input variable in the discrepancy.



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