Regret-based calibration using GPs
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How to calibrate a numerical model so that it performs reasonably well for different random operating conditions?

Objectives
▶ Define the notion of regret in a calibration context
▶ Develop efficient methods and algorithms in order to estimate those parameters

Background: estimation of the bottom friction in a shallow water model

Let \( u \) be some operating conditions (configuration, boundary conditions...)

\[
G: \Theta \rightarrow \mathbb{R}^2, \quad u \rightarrow G(\theta, u) \quad \text{bottom friction}
\]

Given some observations \( y_{\text{obs}} \), the MSE is

\[
J(\theta) = \frac{1}{2} \| G(\theta, u) - y_{\text{obs}} \|^2,
\]

and the estimate \( \hat{\theta} \) is defined as

\[
\hat{\theta} = \arg \min_{\theta} J(\theta)
\]

Now, \( u \in U \sim U \) of density \( p_U \)

For all \( \theta \), the loss function is now

\[
J(\theta, U) = \frac{1}{2} \| G(\theta, U) - y_{\text{obs}} \|^2,
\]

or equivalently,

\[
(J(\theta, U) | \theta \in \Theta) \text{ is a family of random variable indexed by } \theta.
\]
▶ How to choose a \( \tilde{\theta} \in \Theta \), such that "\( \tilde{\theta} = \arg \min_{\theta} J(\theta, U) " ?

(\text{Relative})-regret based calibration

▶ For a fixed \( u \in U \), the best attainable value is

\[
J^*(u) = \min_{\theta \in \Theta} J(\theta, u)
\]

We want to find \( \tilde{\theta} \) so that

\[
J(\tilde{\theta}, U) \rightarrow J^*(U) \quad \text{with high probability}
\]

\( \alpha \)-acceptability [TAVD20]

Given \( u \in U \),

\( \hat{\theta} \) is \( \alpha \)-acceptable if \( J(\hat{\theta}, U) \leq \alpha \cdot J^*(u) \)

▶ Find \( \hat{\theta} \) which is \( \alpha \)-acceptable with the highest probability:

\[
\hat{\theta}_\alpha = \arg \max_{\theta \in \Theta} P\{ J(\theta, U) \leq \alpha \cdot J^*(U) \}
\]

Large \( \alpha \): Conservative, performances controlled with high probability
Small \( \alpha \): Optimistic, good performances but less frequently
Good knowledge of \( J \) globally and around the conditional minimisers is required.

Computing regret-based estimates using GP regression

Two approaches:
▶ Reduce approximation error of \( J - \alpha J^* \)
▶ Improve estimation of the set \( \Delta_\alpha = \{ J - \alpha J^* \leq 0 \} \)

Let \( Z \sim \text{GP}(m_z, \Sigma_z) \) modelling \( J \) over \( \Theta \times U \)
▶ Define \( \Delta_\alpha(\theta, u) = Z(\theta, u) - \alpha Z^*(u) \) with \( Z^*(u) \) approximation of \( J^* \) computed using \( m_2^* \):

\[
Z^* \sim \text{GP}(m_2^*, \Sigma_z^2)
\]

Reduction of the expected IMSE

Approximation error \( \theta, u \) comes from:
▶ Uncertainty on the value of the function \( J: \Theta \times U \rightarrow \mathbb{R} \)
▶ Uncertainty on the conditional minimiser \( J^*: \Theta \times U \rightarrow \mathbb{R} \)

\[
\text{IMSE}(\Delta_\alpha) = \int_{\Theta \times U} \alpha^2 \text{P}(\theta, u) \text{d}(\theta, u)
\]

→ global measure of the approximation error. We want the smallest IMSE once a point is added to the design:

\[
(\hat{\theta}_{\text{new}}, U_{\text{new}}) = \arg \min_{\theta, U} \text{P}(\text{IMSE}(\Delta_\alpha \cup Z(\theta, u)))
\]

\( k \)-batch approach ([DSB11])

Improve the "classifier" \( \tilde{\theta}, u \in \Delta_\alpha \) by sampling in margin of uncertainty based on \( \Delta_\alpha 
▶ Define the probability of coverage

\[
\mathbb{P}(\tilde{\theta}, u \in \Delta_\alpha) = \mathbb{P}[ Z(\theta, u) - \alpha Z^*(u) \leq 0]
\]

▶ Define \( M = \{ \mathbb{E} \in [0,1] - \alpha \} \) – points where the classifier is not too "confident"
▶ Sample points in \( M \), and find centers of clusters using \( k \)-means.
▶ Adjust centroids to reduce either uncertainties on \( \Theta \) or on \( Z^* \)

Conclusion and perspectives
▶ Many criteria of robustness can be defined
▶ We propose adaptive enrichment methods to compute those estimates
▶ Alternatively, we can consider the optimization of the quantile \( Q_{u}(\frac{\text{IMSE}}{\text{IMSE}^*}) \)
▶ Similar iterative methods can be derived using a GP approximation of \( Z^* / Z^* \)

References