Abstract submission for SAMO 2016 conference - Adaptive numerical designs for the calibration of computer codes

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Abstract

After having performed a sensibility analysis for screening influential inputs of a computer code, practitionners should aim at making the code outputs as close as possible to a set of field experiments in order to improve its predictive capability. That issue is called *calibration* (Campbell, 2006).

Our framework deals with a scalar physical quantity of interest, referred to as $r(\mathbf{x})$, where $\mathbf{x}$ is a vector of control variables and with a computer code $y_{\boldsymbol{\theta}}(\mathbf{x})$ where $\boldsymbol{\theta} \in \mathcal{T}$ is a vector of parameters having no observable counterpart in the reality and thus most often uncertain. The goal of statistical calibration consists in reducing the uncertainty affecting $\boldsymbol{\theta}$ with the help of a statistical model which links the code outputs with the field measurements, denoted by $\mathbf{z}^f := (z_1^f, \cdots, z_n^f)$ which are related to n experimental sites $\mathbf{X}^f = \left[\mathbf{x}_1^f, \cdots, \mathbf{x}_n^f\right]^T$. By assuming no code discrepancy can occur between $y_{\boldsymbol{\theta}}(\mathbf{x})$ and $r(\mathbf{x})$ for any $\mathbf{x} \in \mathcal{X}$, we have for $1 \leq i \leq n$:

$$z_i^f = y_{\boldsymbol{\theta}}(\mathbf{x}_i^f) + \epsilon_i, \tag{1}$$

where

$$\epsilon_i \sim \mathcal{E}_i \underset{i.i.d.}{=} \mathcal{N}(0, \lambda^2)$$

statistically encodes both the residual variability and the measurements error of the physical experiment (Kennedy and O'Hagan, 2001). In a Bayesian setting, where λ^2 is assumed known, the posterior distribution of $\boldsymbol{\theta}$ is then written as

$$\begin{aligned} \pi(\boldsymbol{\theta}|\mathbf{z}^f) &\propto \mathcal{L}(\mathbf{z}^f|\boldsymbol{\theta})\pi(\boldsymbol{\theta}), \\ &\propto \frac{1}{(\sqrt{2\pi}\lambda)^n} \exp\Big[-\frac{1}{2\lambda^2} SS(\boldsymbol{\theta})\Big]\pi(\boldsymbol{\theta}), \end{aligned} \tag{2}$$

where

$$SS(\boldsymbol{\theta}) = ||\mathbf{z}^f - y_{\boldsymbol{\theta}}(\mathbf{X}^f)||^2 \tag{3}$$

is the sum of squares of the residuals between the simulations and the field measurements. It is usually sampled using MCMC methods that become infeasible when the simulations are highly time-consuming. A way to circumvent this issue consists in replacing the computer code with a Gaussian Process Emulator (GPE) (Santner et al., 2003). It is built thanks

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to a learning sample of simulations $y(\mathbf{D}_M)$ run over a design of experiments $\mathbf{D}_M$. Then, a surrogate posterior distribution π^S based on the GPE can be established:

$$\pi^S(\boldsymbol{\theta}|\mathbf{z}^f, y(\mathbf{D}_M)) \propto \mathcal{L}^S(\mathbf{z}^f|y(\mathbf{D}_M), \boldsymbol{\theta})\pi(\boldsymbol{\theta}). \tag{4}$$

where

$$\mathcal{L}^S(\mathbf{z}^f|y(\mathbf{D}_M), \boldsymbol{\theta}) \propto |V^M_{\hat{\boldsymbol{\Psi}},\hat{\sigma}^2}(\boldsymbol{\theta}) + \lambda^2\mathbf{I}_n|^{-1/2} \exp\Bigg\{ -\frac{1}{2}\Big[(\mathbf{z}^f - \mu^M_{\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\Psi}}}(\mathbf{D}_{\boldsymbol{\theta}}))^{\mathrm{T}}) \\ (V^M_{\hat{\boldsymbol{\Psi}},\hat{\sigma}^2}(\boldsymbol{\theta}) + \lambda^2\mathbf{I}_n)^{-1}(\mathbf{z}^f - \mu^M_{\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\Psi}}}(\mathbf{D}_{\boldsymbol{\theta}}))\Big]\Bigg\} \tag{5}$$

is the conditionnal likelihood of $\mathbf{z}^f$ with respect to $y(\mathbf{D}_M)$ where $(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\Psi}}, \hat{\boldsymbol{\sigma}}^{\mathbf{2}})$ are plug-in estimators of the GPE's parameters. The surrogate posterior (4) and the target posterior (2) are different in that $y_{\boldsymbol{\theta}}(\mathbf{X}^f)$ is replaced by the mean vector of the GPE $\mu^M_{\boldsymbol{\beta}}(\mathbf{D}_{\boldsymbol{\theta}})$ and the conditional covariance matrix $V^M_{\hat{\boldsymbol{\Psi}},\hat{\sigma}^2}(\boldsymbol{\theta})$ is added up to $\lambda^2\mathbf{I}_n$.

By doing so, the surrogate posterior can be sampled using MCMC methods instead of the target one, but this is subject to an error which strongly depends on the numerical design of experiments $\mathbf{D}_M$ used to fit the GPE. The most used default strategy consists in building a Space Filling Design (SFD), such as an optimized Latin Hypercube (Morris and Mitchell, 1995). Our numerical tests have actually shown that they do not work well, leading to large errors in terms of the Kullback Leibler (KL) divergence (Cover and Thomas, 1991) between the surrogate posterior and the target posterior, that is written:

$$\mathrm{KL}\big(\pi(\boldsymbol{\theta}|\mathbf{z}^f)||\pi^S(\boldsymbol{\theta}|\mathbf{z}^f, y(\mathbf{D}_M))\big) = \int_{\mathcal{T}} \pi(\boldsymbol{\theta}|\mathbf{z}^f)\Big(\log\left(\pi(\boldsymbol{\theta}|\mathbf{z}^f)\right) - \log\left(\pi^S(\boldsymbol{\theta}|\mathbf{z}^f, y(\mathbf{D}_M))\right)\Big)\mathrm{d}\boldsymbol{\theta}. \tag{6}$$

Instead of using SFD, we propose to build in an adaptive fashion a proper design limited to $\mathbf{X}^f \times \mathcal{T}$ by means of the Expected Improvement criterion (Jones et al., 1998). Our simulation studies performed on several toy functions in 2d and 6d have shown the efficiency of the sequential strategies for reducing the KL divergence (6).

References

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