Robustness analysis of gaussian process metamodels using Fisher density perturbations

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In recent years, a growing interest was taken in studying the robustness of a model output to a potential misspecification of input uncertainties [1, 2]. In a common uncertainty quantification (UQ) scheme, based on a numerical model G which uncertain inputs $X_1, \ldots, X_d$ are random variables, and a given QoI defined on the output $Y = G(X_1, \ldots, , X_d)$, this means considering a whole range of potential laws for the X_i. The idea initially proposed in [3] is to apply a perturbation to the density f_{i0} representing the baseline distribution of the i-th input X_i, and estimate the corresponding perturbed QoI.

This perturbation approach could be profitably extended to situations involving more advanced UQ tools such as sensitivity indices or metamodels. Here we propose a first exploration of how the perturbation method introduced in [4], which is based on the Fisher distance, could be applied in UQ studies involving gaussian process (GP) metamodels. To do so, we define $\mathcal{I}(\boldsymbol{\theta})$ the Fisher information Matrix (FIM) associated to the law of a GP $Z_{\boldsymbol{\theta}}$ with hyper-parameters $\boldsymbol{\theta} \in \Theta$:

$$\mathcal{I}(\boldsymbol{\theta}) = -\mathbb{E}\left[\frac{\partial^2 \ln f_Z(\boldsymbol{\theta}, \boldsymbol{z})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T}\right],$$

where $f_Z(\boldsymbol{\theta}, \cdot)$ is the (gaussian) density of the random process $Z_{\boldsymbol{\theta}}$, and $\boldsymbol{z} = [z^{(n)}]_{n=1,\ldots,N}$ the vector of observed outputs of the model at design points $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}$. This matrix induces a metric on Θ the parametric space in which the vector of hyper-parameters lies. The distance between two processes with parameters θ_0 and θ_1 is then given by:

$$d_F(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1) = \inf_{\gamma \in \mathcal{P}(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1)} \int_0^1 \sqrt{\dot{\gamma}(t)^T \mathcal{I}(t) \dot{\gamma}(t)} dt,$$

$\mathcal{P}(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1)$ denoting the set of path joining $\boldsymbol{\theta}_0$ to $\boldsymbol{\theta}_1$.

In this setting, each law at distance δ from the baseline one $f_Z(\boldsymbol{\theta}_0, \cdot)$ can be seen as a perturbed law at level δ. The principle of robustness analysis is then to consider Fisher spheres centered in $\boldsymbol{\theta}_0$ with growing radius, and find, for each perturbation level, the most impactful model towards the used QoI. It can be noted that in the specific case of GP surrogate models with stationary covariance kernels, the latter can be characterized by a probability density function in the Fourier space thanks to Bochner's theorem. Hence the described perturbation method could be implemented using this spectral representation of the law of the process.

In the most simple case, one can examine the robustness of an output probability when estimated through a GP emulator of a costly numerical model. But GP are also used to sequentially select numerical experiments, using some uncertainty reduction criteria, in order to estimate efficiently the target QoI with a limited computational budget. It is then possible to evaluate the robustness of the QoI as well as the employed criterion as regards the law of the GP. We will illustrate this principle on very simple toy-models as well as on well-known examples of the UQ community.

References:

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