The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

BAYESIAN SURROGATE ANALYSIS AND UNCERTAINTY PROPAGATION IN THE LIGHT OF MODEL (IN)ADEQUACY

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Keywords: *model adequacy, model inadequacy, uncertainty quantification, uncertainty propagation, surrogate models, meta-modeling, emulators, Bayesian probability theory, Bayesian inference*

We will take a Bayesian point of view on the inadequacy, or adequacy, of surrogate models as a substitute for full model evaluations that are too expensive for direct sampling. First, we introduce the surrogate's inadequacy (or trustworthiness, or uncertainty), as a continuous, unknown random variable. For generalized linear expansions (in the sense of linear in the expansion coefficients), we find (semi-) closed expressions for propagated uncertainties inferred through the surrogate [1]. In those closed forms, we identify additional inferential uncertainty that can be attributed solely to the inadequacy of the model. This means, that model inadequacy is not just always present, but that it also always has direct, meaningful and quantifiable consequences for the inference based on that model. Then, we consider model-form uncertainty by writing down explicit expressions for the probability for the surrogate model given the simulation data. From a Bayesian point of view, the most adequate surrogate model then is the average over all surrogate models weighted by their marginalized likelihoods. If time permits, the special cases of Polynomial Chaos Expansions, Gaussian Process Regression or Neural Networks are discussed. Lastly, we demonstrate a numerical example from the computational fluid dynamics of the human aorta, in which the consequences of surrogate model inadequacy on the inference, particularly uncertainty propagation, are quantified [2].

REFERENCES

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