Batch simulations and uncertainty quantification in Gaussian process surrogate ABC

Marko Järvenpää .
Department of Biostatistics, University of Oslo, Norway.

1 October 2020, 11.30 UK time

Abstract
The computational efficiency of approximate Bayesian computation (ABC) has been improved by using surrogate models such as neural networks and Gaussian processes (GP). In one such promising framework the discrepancy between the simulated and observed data is modelled with a GP surrogate which is further used to form a model-based estimator for the intractable posterior and to select new simulation locations adaptively so as to maximise sample-efficiency. In this talk we show how to improve this approach in several ways. Most importantly, we develop batch-sequential Bayesian experimental design strategies to parallelise the expensive simulations. In earlier related work only sequential strategies have been used. Current surrogate-based ABC methods also do not fully account the uncertainty due to the limited budget of model simulations as they output only a point estimate of the ABC posterior. We propose a numerical method to fully quantify the uncertainty in, for example, ABC posterior moments. We call the resulting improved framework as "Bayesian ABC"and provide a detailed discussion on its connection to Bayesian optimisation, Bayesian quadrature and GP-based level set estimation methods. Experiments with toy and real-world simulation models are used demonstrate advantages of the proposed techniques.

This is joint work with Aki Vehtari and Pekka Marttinen. This work was done while the speaker was with Department of Computer Science, Aalto University, Finland.

References

M Järvenpää, A. Vehtari and P. Marttinen. Batch simulations and uncertainty quantification in Gaussian process surrogate approximate Bayesian computation. Proceedings of the 36th Conference on Uncertainty in Artificial Intelligence (UAI), PMLR volume 124, http://proceedings.mlr.press/v124/jarvenpaa20a.html