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Peer Review

Review of: "Active Sequential Posterior Estimation for Sample-Efficient Simulation-Based Inference"

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Review of the Manuscript "Active Sequential Posterior Estimation for Sample-Efficient Simulation-Based Inference" by Griesemer et al. (preprint v1)

The manuscript introduces Active Sequential Neural Posterior Estimation (ASNPE), a novel extension of simulation-based inference (SBI) that incorporates active learning into the inference loop. The method is motivated by the challenges of computational inefficiency and scaling issues in high-dimensional simulation-based problems. The authors demonstrate ASNPE's performance on a real-world traffic demand calibration problem and benchmark scenarios, showing improved sample efficiency and posterior estimation accuracy compared to state-of-the-art methods.

The manuscript is well-written, clearly structured, and provides a compelling argument for the proposed method. The justification for the chosen acquisition function is well-motivated and tied to the goal of maximizing sample efficiency with minimal computational overhead. However, some aspects of the methodology and evaluation raise questions that require further clarification or exploration.

1. The manuscript suggests that the prior remains unchanged despite filtering during active learning. This claim warrants mathematical proof to reassure that the selection process does not implicitly alter the proposal prior: the acquisition mechanism could only select a certain subset of the prior and thereby also reduce the support.
2. The manuscript would benefit from a discussion part after the results section: here, one could at least briefly discuss how the method would work with other sequential methods than APT and if the method does work with neural likelihoods or ratios.

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3. Although ASNPE consistently reaches a lower RMSN, it does not always outperform SNPE in early iterations (Figures 3 and 4). Given the emphasis on sample efficiency, it would be helpful to discuss why the performance advantage emerges only after multiple rounds in some cases (maybe this is related to a poor approximation of the model's posterior at the beginning, which reduces the informativeness of the acquisition mechanism?)
4. The traffic calibration problem is a specific and computationally intensive application. While it is a strong demonstration of ASNPE's capabilities, the title does not reflect this specificity. Although other applications are considered, they only play a minor role in the main manuscript.
5. The manuscript introduces Monte Carlo dropout as an optional approximation for the posterior over model parameters but does not discuss alternative approaches. A discussion or comparison with other techniques (e.g., ensembles, variational methods) would provide valuable context. Potentially, one could also discuss the computational costs of estimating the posterior of the model.
6. Moreover, the authors reference Appendix C for details on consistent sampling and log probability evaluation in MAFs under MC dropout. However, these details are not provided, just a reference to the code.

Declarations

Potential competing interests: No potential competing interests to declare.

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