Response to RC2 – Anonymous Reviewer

AR = Authors response

Thank you very much for your constructive review of our manuscript. We have incorporated many of your suggested improvements into our manuscript and believe this has significantly improved its quality and readability.

We have addressed many of the reviewer's suggestions to improve wording and grammar throughout the manuscript. We have mostly removed the term "likelihood-free" from the manuscript to not confuse the reader, except where we directly reference literature that uses this term. We have elaborated on our choice of prior parametrization, have improved the mathematical notation of the statistical methods used so that the reader can more clearly differentiate between what our priors are and what our constraint is (i.e. the ABC-equivalent to the likelihood). We have not significantly cut the ABC method description, as we believe it will be valuable to the geoscientific reader to read about it in the context of geological modeling.

Please find all our detailed responses to your comments in the supplementary material, along with both the revised and change-tracked manuscript.

General Comments

The reviewer writes: "ABC (both rejection and SMC) approximates likelihood in the following ways: Firstly, exact conformity to the the predictions of the model (theta) is relaxed using a distance measure and threshold. Secondly, if the simulation linking cause (theta) to observation (y) is stochastic then it uses a finite set of MC realisations instead of an integral over all outcomes of the random variables not of interest. Neither of these properties are used in the work presented here." **The reviewer confuses us with their statement: We relax exact conformity by using a distance measure and threshold (we use the Jaccard index as a distance measure between two topology graphs and allow an error threshold). The reviewer further states that** "Nothing what separates ABC from the traditional Bayesian approaches is used here**.", but then goes on to state that** "[…] it is ABC only in the most superficial sense**", providing us with a logical contradiction. It would have been helpful for us if the reviewer had provided us with literature references to properly understand their arguments.**

We have mostly removed the use of the term "likelihood-free" when referring to ABC, although this is often stated as such in literature. We have also clarified our choice of prior parametrization, as we agree that this will help the reader better understand the experiments despite the focus of the paper on the method itself.

Specific Comments

1) Remove claims all of circumventing or simplifying specification of topological knowledge due to ABC, these are untrue for the constraint presented here. I have highlighted these in the attached annotated pdf along with more detailed comments for each. Lines 60, 150, 155, 165.

AR: We have reworded our description of topological knowledge to make it more clear to the reader how we acquired it (through interpretation). In the supplement the reviewer writes "ABC is not a method for circumventing the subjectivity of specifying priors or likelihoods. It is likelihood-

free only in the sense of a likelihood never being explicitly calculated due to the nature of the approximation built into the samplers.”**, which we agree with. We hope our changes clarify this to the reader, as we never intended to claim that using ABC over conventional Bayesian inference makes the method somehow more objective.**

In the supplement the reviewer further notes that “the implicit probability function you use is simply the one that assigns uniform probability to all theta within the region where d < iota.”**. But as we *always* accept our parameter samples if they generate a model with a summary statistic within error, we would think that this does not constitute a uniform probability density function, as the area of the curve would be above 1.**

2) Remove all uses of the term ’likelihood-free’. There is no place in this article where its use helps clarify how the proposed approach works. Its only effect is as a potential source of misinterpretation. To avoid unneeded additional review rounds I am asking for complete removal and not fixing its use.

AR: We have removed the term “likelihood-free” in the manuscript to avoid confusion of the reader. It remains in two places where we directly refer to literature that describes Bayesian optimization for likelihood-free inference (Gutmann and Corander, 2016) and where we point the reader to literature that specifically describes ABC as a “likelihood-free” method (Marin et al, 2012). Again, it would have been really helpful for us if the reviewer had provided literature references for us to understand their issue with this specific term.

3) Do not refer to the initial connectivity graph as an observation. It is a semi-subjectice semi-empirically derived parameter to a subjectively chosen constraint family. Describe briefly how it is obtained and what the reasoning behind using the ’initial’ graph was.

AR: We have referred to the initial topology graph as an observation, as this is the terminology used in literature. We understand that this could potentially lead to certain confusion with the reader. We have thus added the clarification to the manuscript, that we treat our subjectively chosen topology graph as the observation in the terminology of ABC.

4) I am not asking that you replace ’likelihood’ with ’prior’ when referring to your topological constraint. Instead, please state somewhere that you choose to go with this label but that it could also be considered a prior or empirical prior and that the application of these terms is not always clear cut. State that you are simply treating the adjacency graph (y) as an observation.

AR: We already describe the topology graph (adjacency graph) as an observation --- something the reviewer has advised against in their previous comment.

5) Two topology distance measures are defined in section 2.4 which are never used. Since they are never discussed, analysed or compared, they serve no purpose. I suggest you remove them to simplify and shorten the already long paper, but feel free to ignore this suggestion.

AR: They are not used, but we think it serves the purpose of helping the reader think about different possible approaches to constrain geomodels using graph structures --- which we think has value.

6) Remove the mention of fuzzy sets in section 2.5, it is not relevant. Your posterior is probabilistic not fuzzy. It represents degrees of certainty concerning a single underlying truth, not degrees of membership to a category.

AR: We have removed the detailed explanations of information entropy in Section 2.5 and refer the reader to the relevant literature instead. Information entropy is used for assessing the prior and approximate posterior geomodel grids, not the posterior parameter distributions themselves.

7) Several sentences need to be reworded for clarity or readability. I have highlighted these in the annotated pdf. Please try to address most of them.

AR: We have reworded many parts of the manuscript given the suggestions by both reviewers.

References

Marin, J.-M., Pudlo, P., Robert, C. P., & Ryder, R. J. (2012). Approximate Bayesian computational methods. Statistics and Computing, 22(6), 1167–1180.

Gutmann, M. U., & Corander, J. (2016). Bayesian Optimization for Likelihood-Free Inference of Simulator-Based Statistical Models. Journal of Machine Learning Research, 17, 1–47.