Response to RC1 - Ashton Krajnovich AR = Authors Response

Thank you very much for the positive feedback and finding typos. We have corrected the text on the indicated locations.

Response to RC2 - Anonymous Reviewer AR = Authors Response

General Comments:

The reviewer writes: "The manuscript still reads like a draft version"

AR: After careful evaluation, we found some small typos that were fixed. We do not see this comment justified. Surely, different opinions about writing styles exist and the reviewers can use their preferred style in their manuscript.

The reviewer writes: "#3 has been ignored." (original #3 comment: Terms like observation, prior and likelihood are applied in an unclear manner often contradicting convention)

AR: After pondering about this comment for quite some time, we think that it relates to a misunderstanding about the application of probabilistic inference in this paper.

We do not see Bayes' equation as a strict separation between subjective knowledge and data, but as a way to combine conditional probabilities. This aspect is, in essence, obvious from the definition of conditional probabilities in the derivation of the Bayes equation. Of course, this is not our invention - but a mainstream view that is encapsulated in the use of probabilistic hierarchical models (e.g. Koller and Friedman, 2009). Also, we would like to refer to the interesting perspective in Nearing & Gupta (2018). We also included a clarification about this aspect in the manuscript (P6 L6).

We are still not sure if this is the point that led to the strong comments by the reviewer. It seems to be the case that this is a subject of philosophical debate for some - and that's surely fine and important, but outside of the topic of this paper and we firmly believe that any strong opinions in this direction should not hinder the publication about the aspect that *this* paper is about: including information about topological relationships in geological modeling frameworks. In the aim to stress the main theme of the paper, we have restructured the introduction with a stronger emphasis on how topological constraints can be used to encode geological knowledge in structural geology probabilistic inferences.

Koller, D., & Friedman, N. (2009). Probabilistic graphical models: principles and techniques. MIT press.

Nearing, G.S., Gupta, H.V. Ensembles vs. information theory: supporting science under
uncertainty.Front.EarthSci.12,653–660(2018).https://doi.org/10.1007/s11707-018-0709-9

Specific Comments

The reviewer writes: "I could not find the place in the revised manuscript where this change was made". (original comment: 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: When we use the term observation we refer to the parameter *y* of the Bayes Eq. 2 not to the literal semantic meaning of the word observation. Since it may lead to confusion to some readers we have added some extra clarification when observation is defined:

Notice that when the words "observation" or "observed data" are used in the context of a probabilistic model, we refer to this mathematical term \$y\$ instead to the literal semantic meaning of the words.

In addition we add a clarification about why derived the term "y" from the initial geological model topology:

The assumption is that this topological graph encapsulates some of the geological knowledge used during its construction by an expert and thus, geometrical configurations more similar to this graph can be considered more likely. This graph would be treated from this point on as a "observation" \$y\$ due to its use as a constraint within the probabilistic model.

The reviewer writes: This comment has not been addressed. All I asked is that you state that the initial graph is what is treated as an observation even though its derivation includes significant subjective steps. This ties in with specific comment 3 as the procedure behind the observation was never properly discussed. (original comment: 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 disagree that using the topological graph as the "observation" is a choice and could be considered as prior. In fact, it is in the nature of implicit representations that topology is not fixed (e.g. Wellmann and Caumon, 2018). The mathematical model M, used to relate model parameters, $p(\theta)$ and observations also limits which information (data) can be used as

model parameters or observation---analogous to an inverse problem. Topology---similar to some geophysical data---is a good example of information that cannot easily be used directly as input in this type of geological modeling algorithm.

There are many reasons to favour one probabilistic model over others. In this paper the main reason to select this specific probabilistic model is to obtain a set of parameters and parameter correlations capable of generating valid geological models---for the interpolation function used during the inference.

Someone could be tempted to think that if a model does not support information derived from human interpretation as a form of prior parameters, θ (as opposed to "observations", y), that this should be a clear indication that the selected model must be inadequate. However, in the authors opinion, such a distinction between "measured observations" and "human guesses" seems to treat the Bayesian equality as something more fundamental other than what it is: a mathematical tool to perform inference.

Gelman, A. and Hennig, C. (2017), Beyond subjective and objective in statistics. J. R. Stat. Soc. A, 180: 967-1033. https://doi.org/10.1111/rssa.12276

The reviewer writes: Still incorrect as I stated in the previous annotated document. (original: ABC does not learn prior distributions, it approximates posteriors over model parameters.)

AR: Reworded to be extra precise:

We demonstrate how we can infer the posterior distributions of the model parameters using topology information in two experiments

The reviewer writes: Likelihood relates data to model parameters. This reads if the likelihood function is that data. The function is a relation not data in itself.

AR: Agree, this paragraph can be misleading. We have reworded the sentences involved:

In other words, by conditioning the probability of model parameters to some additional data, we are able to increase the overall information of the probabilistic model. Additional data can be, for example, a range of possible layer thicknesses in a depositional setting, geophysics or arguably geological knowledge in the form of valid geometrical configurations.

While the overall idea has been demonstrated in some specific cases, the general question of how to define suitable likelihood functions for specific type of observations---given a specific geological systems and diverse types of prior geological knowledge---still remains.

The reviewer writes: Using ABC to indirectly specify a likelihood function is your choice. The claim that obtaining such a function is intractable is untrue for the one you use.

If 'theta' is the model parameters and 'y' is the initial graph. Define a binary statistic of 'theta', call it 'x', as true if the topology graph of 'theta' is within distance 'iota' of 'y', and false otherwise. If we then formulate the likelihood in terms of 'x' being the observation 'f(x|theta)' and sample from posterior 'p(theta|x)', this samples from the same posterior as what your ABC method does in algorithm 1 and approximates in algorithm 2. Replacing data with a statistic of it to simplify a problem is a very old practice. So I will repeat this, the claim that the use of ABC solves an intractable likelihood specification is not true for this specific work.

AR: It is true that the problem can be formulated using a likelihood function instead of an ABC distance function. Arguably most of the ABC Inferences could be constructed using likelihood functions for that matter. Probabilistic or not, many functions have the necessary properties to perform inference. In any case, since this is not the subject of the paper we have reformulated the sentence trying to demystify the use of ABC:

The origin of topological information is generally qualitative. For this reason, choosing a likelihood function, trying to connote any probabilistic meaning to the comparison of topological graphs, does not seem to enhance the inference \citep{curtis_optimal_2004}. This work, favouring model simplicity, adopts an Approximate Bayesian Computation (ABC) approach to compute the posterior using a distance function instead of a likelihood function.

The reviewer writes: The definition of model parameters is still too vague and poorly written. The author conflates parameters with probability distributions as I pointed out in the previous annotated document.

AR: We refer here to parameters of the interpolation function, not the parameters of the probability distributions. Any geomodeling interpolator requires different types of parameters---geometric parameters (e.g. x coordinate), abstract parameters (e.g. the degree of a Matérn kernel used for one of several scalar fields used for the interpolation), and semantic parameters (e.g. faults). We refer the reviewer to Wellmann & Caumon, 2018, for a more detailed overview. Due to this level of complexity, we need to select a subset of the geomodeling parameters to be stochastic. We do not claim to perform an exhaustive analysis of all possible uncertainty in this manuscript.

We clarified this aspect in the text to avoid further confusion:

For case study 1, Figure 4 b) and Table 1 shows which geological modeling parameters are function of the probabilistic model parameters -- i.e. prior distributions of the Gaussian Family defined by the parameters mean and standard deviation.

For case study 2, since the geometry is harder (thus the existence of case 1) we only provide Table 2. However, the nature of the probabilistic model parameters are exactly the same as case study 1: *(i) vertical location of the layer interfaces for within each fault block; (ii) the lateral location of the fault interfaces.* (P12 L10 and P11 L3)

The reviewer writes: "chosen emperically" how?

AR: Added some extra information about the threshold value:

The initial topology graph is used as a constraining summary statistics using ABC with rejection sampling (ABC-REJ) using a threshold of \$\epsilon=0.025\$. The absolute threshold value will be directly proportional to the sensitivity of the model geometry with respect to the stochastic parameters. This prevents the selection of a value independent of the actual geological model under study. In this case study, the value of \$\epsilon\$ has been chosen empirically by performing several predictive simulations. Results were evaluated based on their correspondence to the geological setting.

The reviewer writes: "while reducing the number of required iterations through use of advanced sampling techniques."

Sampling technique efficiency was not presented as the focus in the preceding parts of this paper and should not as there is very little here on that topic

AR: Removed the sentence about sampling techniques.