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Interactive comment on "Efficiency and robustness in Monte Carlo sampling of 3-D geophysical inversions with Obsidian v0.1.2: Setting up for success" *by* Richard Scalzo et al.

Anonymous Referee #1

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General comments:

I have read the manuscript with interest and I think that it will be a good contribution to the field of integrated geophysical modelling and inversion. The manuscript is well written and well organized. The authors present an inversion code relying on Monte-Carlo sampling in a Bayesian framework. The theoretical background pertaining to the Parallel Tempered Markov-Chain Monte-Carlo (PTMCMC) that is provided allows a good understanding of the principles behind the implementation. The code they use is an extension of an existing software, and there is therefore not much information, for instance, about the way they calculate the forward geophysical problem. The manuscript is relatively de-attached from the software the authors introduce, which allows it to remain general and to provide a good introduction to Bayesian and Monte-Carlo techniques. However, I think that it is a little bit too detached from the code itself and more indications as to how users could use Obsidian in practice and to reproduce the work presented would be useful. The example they use to illustrate the methodology is appropriate.

The literature is generally well reviewed and well used but there are a few occurrences where references are miscited or should be added (in particular when it comes to less statistical and more geological considerations). I come back to it where necessary in the detailed comments below. This paper is used as a companion paper by Olierook et al. (2019) and is cited multiple times by them. The authors should consider citing Olierook et al. (2019) as an application example.

An aspect which is practically missing from the manuscript relates to the computational requirements of inverse modelling using Obsidian v.0.1.2. The model the authors are using as an illustration example seems small and yet I have the impression that carrying out the inverse modelling was relatively computationally intensive. A little bit more information would be welcome, and it would be useful to geoscientists planning to use Obsidian v.0.1.2.

Does the implementation restrict the modelling of one given property (say, density contrast) to one type of sensors (say, gravimeters)? I am asking this question because of the way equation 9 is formulated. It seems to imply that one physical property cannot be recovered from the joint inversion of two datasets. For instance, this would mean that, in its current version, Obsidian would not support an extension to the joint inversion of gravity anomaly measurements with tensor gravity gradiometry to recover density contrast?

Detailed comments:

The comments below follow a linear progression of the manuscript. ‘P’ indicates page number and ‘l’ indicates line number.

Title. ‘Sampling of [. . .] inversions’. I think that you cannot sample an inversion as it is a process, but that you can do sampling for 3-D inversions.

P2.l2-3. several works have recognised the issue. Consider adding a few references. P2.l6-7. ‘gravity, magnetic, and electrical measurements integrate data from the surrounding volume’. This is true for all geophysical methods, even high-frequency seismics. You can replace by something like ‘All geophysical measurements [. . .].’

P2.l13-14: In the work of A. Tarantola, non-uniqueness is clearly stated. It is one of the limitations of geophysical inversion and mitigating it is one of the motivations for integration and joint inversion as presented in this manuscript. Consider adding a word about non-uniqueness in geophysics to this sentence and perhaps another reference (for instance Sambridge (1998) might be relevant here).

P2.l22. ‘All input sources of information [. . .] are probability distributions’. This is not the case in all inversion schemes. If this is a general truth you are saying (and I think it is a general truth), and if this is how all inputs are treated in your work/Obsidian, then consider stating it clearly.

P3.l3-4. ‘posterior around each local maximum may in these cases significantly underestimate uncertainties’. This is a good point and it is often overlooked. Consider adding a reference to support this or an example illustrating this.

P3.l10-11. ‘Giraud et al. (2017, 2018) demonstrate an optimization-based Bayesian inversion framework for 3-D geological models, which finds the maximum of the posterior distribution (maximum a posteriori, or MAP), and expresses uncertainty in terms of the posterior covariance around the MAP solution; while they show that fusing data reduces uncertainty around this mode, they do not attempt to find or characterize other modes, or higher moments of the posterior’. This is partially true. Giraud et al. (2017, 2018) use uncertainty information and assess the reduction of uncertainty after inversion, and find the maximum of the MAP, but they do not show the posterior explicitely. Giraud et al. (2016) on the other hand, do calculate the posterior covariance matrix.

P6.l9. The shape of matrix Σ might be determined using probabilistic geological modelling (e.g, Wellmann et al. (2010), Pakyuz-Charrier et al. (2018a), de la Varga et al. (2018)). You could add that in the discussion.

P6.l16. “These authors found that in general updating blocks of parameters simultaneously was inefficient”. My impression is that you also refer to inversions schemes using graphic cuts to update the models. If this is the case please state it clearly/briefly.

P6.l31. “using information from ensembles of particles”, does the comment also extend to inversions using particle swarm optimization? If this is the case please state it clearly/briefly

P6.l26-30. You could consider making it clearer that this is what your version of Obsidian does so that readers/users are not wondering.

P8.l22. The acronym ‘IACT’ is used only in this place. Please remove.

P9.l29. I think that the usage of the word ‘layer’ is a bit confusing from a geological point of view as you later on refer to as an inclusion as a layer, which it is not. Please use more appropriate vocabulary.

P10.l8. Maybe you can state later in the manuscript that your implementation of geological structures is more suited to basin scenarii (and therefore oil and gas exploration cases), and that in hard rock / mining scenarii, different geological modelling approaches can be followed (as you do near the end of the manuscript when refering to gempy).

P10.l13. Equation 14. Just for the sake of completeness you may consider to specify what x’ and y’ are.

P10.l16. Typo: the bracket needs to be removed.

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P10.l25. Equation 12. Consider adding a short appendix detailing how it is derived.

P11.l34. – P12.l1. Note that drillhole uncertainty for control points can be modelled (Pakyuz-Charrier et al. (2018b)), as can seismic interpretation (Bond (2015), Schaaf and Bond (2019), Alcalde et al. (2017)).

P12.l4-5. I find this discretization a bit coarse. Is it because of the computation cost involved in PTMCMC or due to lack of information or to shorten run time?

P13.l1. Information entropy has been used in the geosciences after Wellmann and Regenauer-Lieb (2012) introduced it to the field, but it was initially introduced by Shannon (1948). Consider adding this reference, and possibly a brief statement explaining why it is appropriate to use it.

P14.l5-7. Please make this paragraph clearer.

P14.l32. The information about the number of computational hours is relevant only if the specs of the computer used are known. I think that more information about this aspect of the work presented and of Obsidian should be given: does it run on supercomputers, do it scale well? Just a little bit of information on this aspect would be useful to users and would strengthen the paper.

P16.l19-25. This paragraph is not very clear to me.

P17.l17: "Suppose that σ is unknown, however, and is allowed to vary alongside [theta]" does it mean you allow heteroscedasticity? If so this needs to be stated.

P17.l8. I'm not sure I understand the usage of the term 'fiducial' here.

P18.l3. "one potential weakness of this approach to balancing sensors". How would that relate to defining the relative weight of the different types of sensors in the joint inversion problem?

P18.l10. Equation number is missing.

P19. The models are shown only in 2D. A 3D view would be welcome.

P20.l24-25. You mention a number of interpolation techniques. Have you tried kriging, as it is widely used in geostatistics?

P23.l16-17. I am not sure that I understand the meaning of this sentence. Please clarify. By gradients, do you refer to the jacobian matrix? Or am I missing something?

P23.l30. the package proposed by de la Varga et al. (2018) offers the advantage of being open source but it is not the only one performing probabilistic geological modelling. For instance, other works using ideas introduced by Wellmann et al. (2010) such as Pakyuz-Charrier et al. (2018a) also achieves this.

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