

Interactive comment on “Bayesian geological and geophysical data fusion for the construction and uncertainty quantification of 3D geological models” by Hugo K. H. Olierook et al.

Anonymous Referee #1

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1. General comments

Olierook et al. present a study where they integrate information from geological maps and observations, petrophysical measurements and geophysical data. They focus on a small area in Western Australia and use interpretation from a nearby seismic survey to constrain their modelling. Their aim is to present an example of holistic inverse modelling where gravity and magnetic data are constrained using all the available information.

There is some novelty in their approach and the study they show can be published after the authors address a series of comments about specific issues in the text and more

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general issues which, at the moment, is problematic. To date, Monte Carlo approaches for geological uncertainty have focussed on regional scale studies, while the work is clearly at a smaller scale. I think that this should be highlighted as one of the novelties of this paper.

I think that the formulation of the geophysical inversion problem should be described in more detail and that giving essential equations about geophysics and uncertainty assessment would improve the manuscript greatly. The only equation shown in the paper does not suffice to provide a good understanding of the basic mechanics of the methodology. Besides, after a quick manual derivation, I think that the right hand side of the equation provided might not be correct and may need revision. In any case, this derivation needs to be justified, by invoking an Eulerian integral of the first kind and the Beta function, using either the appropriate reference(s) and providing a succinct appendix.

Some references may be missing or are mis-cited. Several studies have been overlooked and have not been cited. This comment is relatively minor but addressing it would be important to show where the presented work stands in the literature. In my view, the introduction should emphasize the fact the idea of geology/geophysics integration is not new but that quantitative integration of both disciplines is an area of research that has received more and more attention recently. Some references need to be added, but I will come back to this in my detailed comments of the document. Please check that all the papers you cite as ‘in review’ are still in review and have not been published.

The hypotheses and assumptions that the authors made need to be clarified. They neglect the presence of some geological units on the basis that their relative coverage in previous interpretation amount to only a few percent of the total. This is a simplification that needs solid justification as it is sometimes the case that only a very small portion of a rock unit of interest is outcropping.

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Moreover, the area of the authors' study is known to be prospective for several minerals, the deposits of which is often not born by geological units making up most of the geology of the area, and are covered by regolith and outcrop only at a few locations.

An aspect of geophysical joint inversion that needs to be considered is the relative impact of the two different geophysical datasets inverted for when they present largely different spatial coverage and sampling. This is not clearly mentioned in the manuscript and I expect that there would be an imbalance as the magnetic dataset seems to have about 100x more points than the gravity one (see Kamm et al. (2015), Sun and Li (2016)). How do you cope with the fact that in such case your joint inversion may be dominated by magnetic data? State it clearly. The Figures are not all very informative and some could be grouped. Fig. 1 and Fig. 2 both refer to the geology of the area and are referred to next to each other in the manuscript. It may be a good idea to merge them. Fig. 3 is not very informative. In Figure 5, I think that it would be good to have the line of cross-section X-Y shown.

The authors rely a lot on Scalzo et al., in review, which is a good complement to the manuscript. However, it is submitted to a different journal and is still in review. For this reason, I suggest that they reduce the dependency of their manuscript to Scalzo et al., in review, and explain succinctly key concepts they refer to Scalzo for explanation. This would make the paper more readable and easier to understand as all key elements would be readily available. The manuscript also has a number of sentences or pieces of sentences that are either an exact match or are very close to what can be read in Scalzo et al., in review. This is not an accusation of plagiarism but a mere observation. There are a few occurrences that I noticed when reading Scalzo et al., in review.

Below are the detailed comments I have.

2. Detailed comments and technical corrections

You mention the fact that you use a global optimization technique only in 2.2. Maybe state it in the intro.

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P1 I14: "model results": results of the technique introduced here? Could be clearer.

P1 I16-18: "The boundaries between geological units are characterized by narrow regions with <95% certainty, which are typically 400–1000 m wide at the Earth's surface" what is the relation between these values and the sampling of gravity data? If I am correct the data sampling of gravity data guaranteed by GSWA is that there is a data point every 400 to 1000 m in the area?

P1 I18: "Beyond ~4 km depth, the model requires drill hole data". You need to be clearer here. Drillhole data that reaches below 4km in the area is not likely in hard rock scenarios, although it might be in oil and gas exploration (basin scenarios). I suspect that you mean that for model cells below 4km the addition of constraints at depth such as drillhole data might help constrain the deeper regions better?

P1 I27: "faults or suture zones": how about unconformities in general?

P2 I13: You cite Pakyuz-Charrier et al 2018 but this is a conference abstract. There are two journal papers relating to their MC approach for geological modelling that appeared in 2018. Please replace that reference by the most appropriate one (or both if you want to be broader) of the following: Pakyuz-Charrier et al. (2018a), (2018b).

P2 I13-14: There have been metrological studies published in recent years that tackle the issue of modelling the uncertainty on geological measurements.

P2 I21-22: "However, there is still a paucity of work in fusing solid Earth geological observations and geophysical data in a Bayesian framework to develop robust 3D geological models". True, but you may need to consider Wellmann et al. (2017), who "...address these shortcomings here with an approach for the integration of structural geological and geophysical data into a framework that explicitly considers model uncertainties [...] in probabilistic programming in a Bayesian framework". Please cite this work. This also relates closely to de la Varga et al. (2018), which you cite earlier in this paragraph. Likewise, Jessell et al. (2010), (2014), (2018) highlight the need for

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robust geology-geophysics integration. I suggest to cite some of these as they strongly advocates for the kind study presented here.

P2 I31-33: “One useful addition to the current features of Obsidian would be the integration of geological and geophysical field observations made on the Earth’s surface, which are vital for surface and near-surface applications (< 1 km)” this statement sort of contradicts the 1st sentence of this paragraph where you say “The Obsidian software package provides a workflow to fuse disparate geological and geophysical data within a Bayesian framework”.

P3 I1-2: “geophysical observations” and “geophysical survey data”: how is it not the same thing?

P3 4-14: Maybe say somewhere that exploration undercover has been recognised to be important for the future of mineral exploration with a ref or two. The last sentence of this paragraph could also go in conclusion.

P3 section 2.1: Lead authors Johnson and Sheppard are cited a number of times - consider adding work from someone else.

P4 section 2.2: Sambridge and Mosegaard are cited many times here – maybe add some diversity with papers coming from other researchers.

P4 I14: “single unique” → “unique” is enough.

P4 I16: There are also other works you may want to cite when it comes to using information derived from geological measurements or modelling directly into geophysical inversion. For instance, Fullagar et al. (2008), Guillen et al. (2008), Scholl et al. (2016) integrate geological information or modelling in their inversion algorithm. Publications relating to works using level-set inversion also rely on geological models (see for example Bijani et al., 2017, and Zheglova et al., 2018, for joint inversion).

P4 I15-16: “Ways to introduce such constraints include regularization (Giraud et al., in review) but this technique fails to acknowledge alternative scenarios.” This statement in

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unclear as Giraud et al derive constraints from a collection of geological models, therefore using all realizations from MC sampling of geological model space. But because their inversion is deterministic, they obtain a single geophysical inverse model, which indeed represent a single scenario. I think that this is what you mean but it needs to be clarified.

P4 I21-30. “The Bayesian framework converts a deterministic model into a probabilistic one by using probability distributions to represent the free parameters rather than using optimal or single-point estimates.” To make this clear and unambiguous, you should remind the principle behind Bayesian approaches, when you invoke Bayes’ theorem. Solving a problem in a probabilistic way does not necessarily make it Bayesian. In this sentence you may want to stress the fact that you also use the prior distribution and sample the posterior, as it is a major difference with deterministic inversions. The utilisation of the priors is stated in the next sentence but I think that it could be made clearer overall. I would also not cite Oldenburg 2005 here, but perhaps one of A. Tarantola and others’ publications which are seminal to many inversion approaches.

P5 I1: I strongly suggest that you add the mathematical foundation of your Bayesian inversion methodology. Just a few of the equations centre to your modelling approach would do and I think be informative to the reader. P5 I10: “convergence can be challenging” rephrase. Something like: “convergence can be difficult to reach”

P5 I13-24: Please add other cites to your citations of works by M. Sambridge and his team’s. For instance, they may have brought lots of new ideas and methods to the field but the Metropolis-Hastings algorithm is not by them.

P5 I23: section 2.3. You need to give more information about Obsidian. It is too short and not sufficiently informative. The main reference you use (Schalzo et al in review) is still in review a basic summary of Obsidian should be self-contained in the paper.

P5 I31-32: This sentence is exactly the same as Scalzo et al., in review, beginning of section 2.4. Layers are not discrete if they have smooth boundaries. I suspect that

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what you try to say is that the outline of a given layer is not angular (i.e., that its representative functional would be differentiable)? If so this should be made clear.

P6 I2-4: "The layer boundaries are indexed in a strict order of increasing depth in the subsurface but are permitted to cross." The fact that they cross violates basic stratigraphic principles. You need to state explain briefly how you cope with that and how this is dealt with by your algorithm. This sentence is exactly the same as Scalzo et al., in review before they introduce equation 9.

P6 I10: "x and y correlation length" you haven't introduced what x and y are, except in Fig. 2. Just say that your RBF is anisotropic and I think that it's enough. The first sentence of this paragraph is very close to the one preceding equation 10 in Scalzo et al., in review.

P6 I13-15: please reformulate the last sentence. The parameter alpha and beta haven't been defined.

P6 I18: PTMCMC: this acronym has not been defined yet.

P6 I32: "and cross-cuts" you cannot rule out all uncertainty about the fact that it cross-cuts, but you are making the (reasonable) assumption that it does. Please add this information.

P7 I1: "ordering of layers". Say "stratigraphy" or "stratigraphic pile".

P7 I6-9: typo in line 6. I don't think that a lithology with 3% of occurrence is insignificant. You need to provide more information as to why you do not account for rock units except Halfway Gneiss and Durlacher Supersuite.

P7 I14-16: how do your values compare to literature values, or work reported in the area or similar settings? If you have only approx. 100 samples to characterize several rock units through mean and standard deviation you can assume that your uncertainty on these parameters is quite high.

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P7 I24-32 and 1st paragraph in P8: I don't think that it is necessary to give detailed information about the processing of the field measurements. You can keep it, but I recommend to put it in Appendix instead of the full text.

P8 I15: consider replacing 'acquired' by 'obtained'.

P8 I21: I think that you should replace ">" by plain text words.

P9 I2-3: please explain briefly how the shape parameters were obtained.

P9 I9: please number the equations.

P9 I13-14: the calculation of this integral is not straightforward. If you want to leave it in the manuscript as it is please add a short appendix explaining how it is calculated, and at least provide the appropriate references.

P9 I17: please define what 'ID dataset' is.

P9 I25: the 'iGRW' acronym is not used in the rest of the text. Delete.

P10 paragraph 1: please add a figure to help the reader to understand how this works. The readership of Solid Earth might not be specialist in MCMC techniques.

P10 I 13: This information is relevant only if you provide information about the computing resources you used.

P10 I17: please add in the methodology the definition of the indicators you use to analyse your results.

P10 I22: I can make an educated guess about what sigma means here, but it needs to be clearly stated.

P11 I13: the reference to Geweke score should come earlier in the text. The ref given might not be the best. I would cite the following instead: Geweke, Evaluating the accuracy of sampling based approaches to the calculation of posterior moments, 1992, Bayesian Statistics 4, pp. 169-193

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P11 section 4.2. Although it's not perfect as an indicator, I'd also give the root-mean-square error. As said above I do not provide review comments on the results section. From here I go straight to section 5.2.

P14 I20-21: "So, if higher resolution geophysical surveys and/or geological field observations are acquired, the model can then become more precise". This is not necessary as it is obvious.

P14 I24-25: "Where such regions are under cover and drilling is required to establish formation contacts, our results also aid in constraining which areas should be drilled first to maximize information gain". This is true as a first approximation but not always valid. You can imagine that adding more information in a certain part of the model may improve greatly a portion of the model that is equally uncertain because it is linked to that first structure in a structural or topologic sense.

3. References

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