Manuscript: egusphere-2023-129

Object: answer to Anonymous Referee #3, 29 Mar 2023

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Dear Reviewer,

Thank you for taking the time to review our submission and for your constructive feedback. Below you will find our answers in blue.

Thank you!

The authors

After reviewing the manuscript titled "Integration of automatic implicit geological modelling in deterministic geophysical inversion," I was thoroughly pleased to see the development of new methodologies that address the problem of non-uniqueness in geophysical inverse problems. The manuscript is well-written and well-illustrated and has clear value that addresses the integration of geological and geophysical data. I look forward to seeing a field application of the proposed methods. Having said that, I do feel a few revisions would improve the quality of the manuscript.

First, equations (2) and (5) both present ways to map from signed-distances to physical properties, so which one is used in which stage of the inversion? The text (L 128 – 130) states that equation (5) is used to update the model, so when is equation (2) used then? Giraud et al. (2021a) suggest instead that equation (2) is used for the model update. Please clarify this, as equations (2) and (5) seem to be in conflict.

> We have brought clarifications to this, which indeed was a bit confusing. Eq. (2) is used to map signed distances to density contrast when the signed distance properties of $\boldsymbol{\phi}$ are initialised from a model of rock units, which is not the case after model update. Therefore, after each model update, we use equation (5) to obtain the new signed distances $\boldsymbol{\phi}$, which we recalculate at each iteration. Equation (2) is used for the calculation of the sensitivity matrix of the forward data to changes in signed distances. We have clarified this, in L100 of the original manuscript, we have modified the sentence introducing Eq. (2):
>
> "In our level-set inversions, $\boldsymbol{\phi}$ is the primary variable inverted for, which constitutes the proxy for a direct link mapping geophysical and geological representations of the subsurface. We map these signed distances to petrophysical properties using:
>
> (2)''

$$\boldsymbol{m}(\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_{n_r}) = \sum_{i=1}^{n_r} V_i H(\boldsymbol{\phi}_i) \left[\prod_{j=1, j \neq i}^{n_r} \left(1 - H(\boldsymbol{\phi}_j)\right) \right],$$

After the description of the cost function (Eg. 4), we have added the following:

"To solve for $\delta\boldsymbol{\phi}$, we build the system of equations given in Appendix 1, which requires the sensitivity matrix $\boldsymbol{S}^{\phi}$ of $\boldsymbol{d}^{calc}(\boldsymbol{m}(\boldsymbol{\phi}))$ with respect to changes in $\boldsymbol{\phi}$ using the chain rule:

$$\boldsymbol{S}^{\phi} = \frac{\partial \boldsymbol{d}^{calc}(\boldsymbol{m}(\boldsymbol{\phi}))}{\partial \boldsymbol{\phi}^k} = \frac{\partial \boldsymbol{d}}{\partial \boldsymbol{m}(\boldsymbol{\phi}^k)} \frac{\partial \boldsymbol{m}(\boldsymbol{\phi}^k)}{\partial \boldsymbol{\phi}^k} = \boldsymbol{S}^m \frac{\partial \boldsymbol{m}(\boldsymbol{\phi}^k)}{\partial \boldsymbol{\phi}^k}, \quad (4)$$

where $\frac{\partial \boldsymbol{m}(\boldsymbol{\phi}^k)}{\partial \boldsymbol{\phi}^k}$ is obtained analytically from Eq. (2-3) (see Giraud et al., 2021a for details)."

Second, I do feel that while the manuscript does make an effort to explain in detail the formulation of the inverse problems, it falls short in explaining how some of the parameters are determined. For example, the parameter "alpha" in equation (12) for the geological correction seems to be crucial in guiding the inversion, yet there is little mention on how "alpha" was determined. Results are shown for alpha = 0 and 0.5, but there is no explanation of how these values were determined. If "alpha" is a hyperparameter, then a sensitivity analysis that tests various values for "alpha" ranging between 0 and 1 would be appropriate.

Yes, the parameter "alpha" is a hyperparameter of the inversion. We did not perform extensive, rigorous testing of values for this parameter as we originally sought to balance the contribution of geological modelling and geophysical inversion in the search direction and a value of 0.5 gives a similar importance to both terms. We proceeded somewhat naively from manual fine tuning of alpha with values in the vicinity of 0.5. A value of 0.5 provides satisfactory results, which, at the time, did not warrant the need to perform any more advanced analysis such as, for example, the rigorous plot of an L-curve.

While adding a rigorous analysis of the importance of alpha would be interesting, we prefer to maintain the manuscript focussed and to its current length as much as possible. We added a couple of sentences explain the rationale behind a value of 0.5 in Sect. 5.2.1. (L408-410 of the updated manuscript):

"The value of α = 0.5 was chosen without a rigorous analysis of its impact on the results. A naïve trial and error approach revealed that a value of 0.5 effectively 'corrected' the course taken by un-corrected geophysical inversion and prevented the appearance of artefacts."

Third, there is little mention of the robustness of the inverted models. Granted, this is a synthetic study, but how robust are some of the features that are consistently seen in the inverted models? Would changing the values of some parameters in the inversion result in different models, or would the features appear again (indicating some degree of robustness in the model)? This is also related to the fact that the method seems to be dependent on the starting model. How do the results change if the starting model changes? Ideally the proposed methods would give consistent results even when the parameters and starting model are changed. I would like to see some form of robustness test of the proposed methodologies.

Tests using starting models far from the reference models have been performed by Giraud et al. (2021), who tested starting models with a missing unit in the starting model and with erroneous density values. Rashidifard et al. (2021) also performed tests on synthetic data with starting models having a geometry that differs from the reference model. The issue you raise here was also raised by the other two reviewers and therefore this answer bear similarities with what we answered to RC1 and RC2. We ran tests using the first synthetic model:

- inversion with geological correction starting from the uncorrected case (added to 'Section 5.3. Improving the geological realism of a pre-existing model'.
- Inversion with under and over-estimated densities, added to 'Appendix 5: Appendix 5: Robustness to errors in the density of rock units'

We refer you to our answer to point 4 of RC1. Information about additional runs is now provided at the end Section 5.1.2. (see general answer).

While the robustness of level set inversion to noise in the data was shown by previous works cited in Introduction, an additional test with unrealistically high noise contamination is provided in Appendix 3 and 5.

We do not paste the associated appendix here not to dilute the focus of our answer. This new appendix is in the updated manuscript (Appendix 3 and Appendix 5).

We have also added the following to the manuscript, in the discussion section (Sect. 6.3):

"Previous work focusing on level set inversion following an approach similar to ours have investigated the importance of accurate knowledge on the geometry and the number of rock units a priori (Giraud et al., 2021a). Giraud et al., 2021a, and Rashidifard et al., 2021, suggest that inversion is somewhat robust to errors in the starting model geometry and in the petrophysics of the rock units. Nonetheless, relatively small deviations between, scenarios 2 and 5 illustrate that the proposed methodology is not sufficient to address the ill-posedness of the potential field problem. Moreover, results from Giraud et al., 2021a, suggest that level-set inversion "presents limitations when an important geologic unit is missing from the initial model". To alleviate this, ways to generate the 'birth' of new geological units for inversion to consider geological bodies previously not accounted due to lack of information may be devised. One possibility could be to use the sensitivity of geophysical data to changes in physical property"

In addition, one test with a starting model that is geologically unrealistic is shown in case (5) of synthetic model 2.

We have also added supplementary material as mentioned in our general answer.

Fourth, I would like to see the simulated synthetic data (i.e. gravity anomaly maps) and the predicted data from the inversions, as well as a data residual map. The data residual map would ideally show random patterns. A brief explanation on how the data was simulated would also be appropriate. Was the gravity data treated with random noise, or was it simply forward computed from the models? If the gravity data was treated with noise, how robust are the proposed methods to increasing levels of noise? In a field study, the observables would be gravity data maps and any additional geological information that may constrain the models. Yet, the manuscript does not address sufficiently in depth the data itself.

> The issue of noise was also raised by RC2. We use elements from our answer to RC2 here.
>
> In the second synthetic test, we assume that convergence was reached when data misfit reached 0.5 mGal. We chose this value accordingly with values obtained from the literature Barnes et al. (2011). We have added the following to the manuscript in section 5.2.1 Survey Setup (underlined text):
>
> "We run inversion corresponding to the four inversion scenarios proposed above. Inversions stop when reaching $ERR_d = 0.5$ mGal, which corresponds to values accepted for legacy data Barnes et al. (2011)"
>
> In the methodology section, we have added the following after the description of the cost function (eg. 4 in section 2.2).
>
> "We write the data misfit term as: $\|\boldsymbol{d}^{obs} - \boldsymbol{d}^{calc}\|_2^2$ instead of $\|\boldsymbol{W_d}(\boldsymbol{d}^{obs} - \boldsymbol{d}^{calc})\|_2^2$ with $\boldsymbol{W_d}$ would the data (co)variance matrix. In our current implementation, we simplify the problem by assuming that uncertainty (or noise) in the data is isotropic. This is equivalent to assuming an isotropic covariance matrix $\boldsymbol{W_d}$ and adjusting the other hyperparameters accordingly. An obvious extension of the work presented here is to consider a matrix $\boldsymbol{W_d}$ with values that can be set individually for each datum."
>
> In addition, in the tests that JG ran when developing the method, he observed that it showed good robustness to random noise. A possible explanation is that random noise may have an effect on physical property inversion as it can cause small scale anomalies in the recovered model. The severity of this is reduced in the case of geometrical inversion because the densities remain constant within the different rock units. Consequently, the risk of fitting random noise is reduced with this kind of inversion. However, it could be that longer wavelength correlated noise affect the inversion results, but is generally the case for many inversion schemes. As an example, we refer to the test with noisy data mentioned above and in the general answer (see Appendices 3 and 5) and also refer to the text added in relation to our answer to your third point.

Fifth, this is somewhat addressed in the last case (5) of the second synthetic study, but what happens if a geological correction is applied to the inverted model from case (1)? This is also related to what is mentioned in L 57 – 60, where an a posteriori ad hoc process could also ensure geological plausibility of an inverted model. Could it be possible that applying a geological correction after geophysical inversion (not every iteration) gives similar results? Then, an argument could be made that the cumulative geological corrections applied at each iteration could be summed into one single geological correction applied at the end of the geophysical inversion. Or perhaps a geological correction is not necessary at every iteration. A plot showing the evolution of the geological correction with every iteration would be appropriate here.

We break this point into its main logical parts and answer separately:

"Fifth, this is somewhat addressed in the last case (5) of the second synthetic study, but what happens if a geological correction is applied to the inverted model from case (1)? Fifth, this is somewhat addressed in the last case (5) of the second synthetic study, but what happens if a geological correction is applied to the inverted model from case (1)? This is also related to what is mentioned in L 57 – 60, where an a posteriori ad hoc process could also ensure geological plausibility of an inverted model. Could it be possible that applying a geological correction after geophysical inversion (not every iteration) gives similar results?"

Similar to the second synthetic case, if we apply a geological correction term to the first synthetic, starting from the uncorrected case, it lead to a model misfit that is intermediate between the case with geological correction applied from the beginning of inversion and no correction at all. We point out that in the case without correction, the geological realism of the inversion result without geological correction is seriously compromised. This makes the geological correction quite substantial as compared to the corrections made during the iterative process.

There is the risk that once starting from a geologically unrealistic model, the geological correction term might propose the closest geological model, which could be from a family of geological model different from the true model.

We have run inversions with geological correction with a starting model equal to the inversion results of the uncorrected case. The result is shown below (Figure 1 in this document and Figure 13 in the new version of the manuscript):

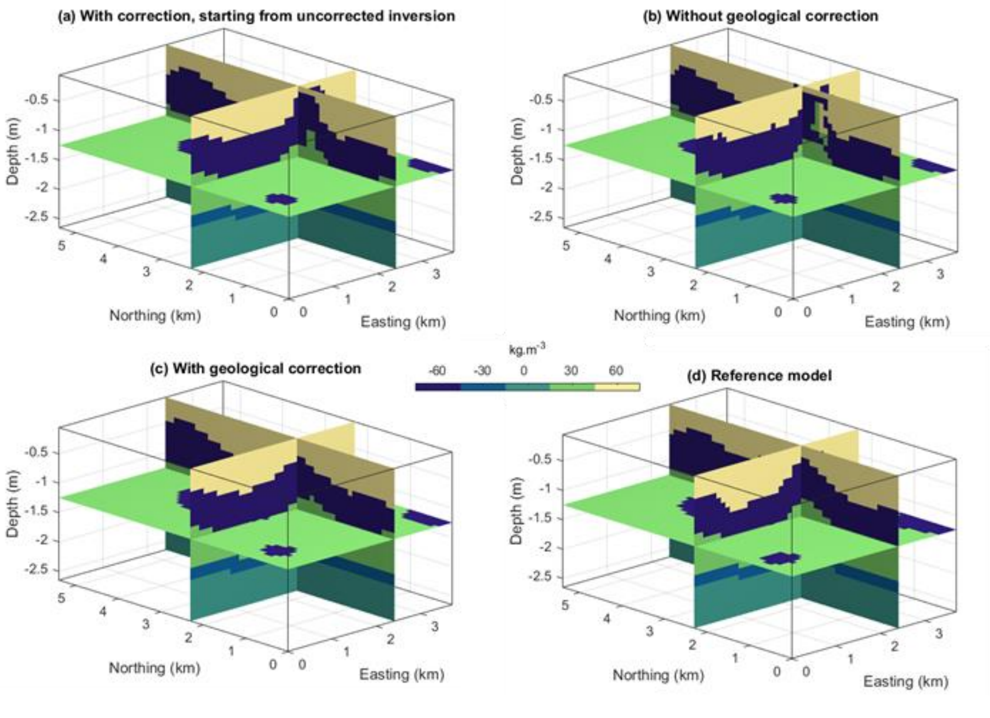

Figure 1. Comparison of inversion results with (a) geological correction starting from inverted model obtain without geological correction, as shown in (b); results with geological correction (c) and reference model (d).

While there are some obvious improvements, some unrealistic features remain. This indicates that in this case, the inversion starts from one local minimum of the geophysical data cost function and ends up to another one, less geologically unfavourable, that is different from the case where geological correction is applied from the beginning. We note that some unrealistic thickness variations for Unit 3 (dark blue unit). On this premise, if large unrealistic features appear, we recommend to run geological correction from the beginning of inversion.

We have added the following prose to describe and interpret this example:

"To with the level set method without geological correction as obtained in Section 5.1 (Figure 16a), and run inversion with geological correction applied. The inverted model obtained in this fashion is shown in Figure 16b. The application of geological correction manages to remove a number of unrealistic features present in the starting model. However, the effect of the geological correction seems visually smaller than in the application of geological correction from the onset of inversion (Figure 16c). On this premise, if large unrealistic features appear, we recommend to run geological correction from the beginning of inversion instead of as an ad-hoc process. We note that in the transition between Figure 16a and Figure 16b by application of geological correction, all models are geophysically equivalent or nearly equivalent in that they present similar geophysical data misfit values. This suggests that, for this dataset, a continuum of models exists fitting the geophysical data to a similar level while presenting different degrees of geological realism. In what follows, we investigate this possibility further using the synthetic dataset presented in Sect. 5.2."

"Then, an argument could be made that the cumulative geological corrections applied at each iteration could be summed into one single geological correction applied at the end of the geophysical inversion. Or perhaps a geological correction is not necessary at every iteration."

This would be the ideal case and might work in theory but it is unfortunately not so. The geological correction is non linear and the geological modelling problem is also non unique. At any iteration in the inversion, geological correction calculates the geological image of the current model. It uses it to adjust the search direction of geophysical inversion so that the model evolves along a path made up of a series of geologically realistic models (or, at least, more realistic than without correction). Consequently, it is possible that without geological correction, the inversion converges to a model for whose geological image differs from that obtained with geological correction applied throughout the inversion. In such case, applying geological correction to the inverse model would result in a model that might be relatively close, yet different, from the model obtained with correction applied from the beginning.

We note that the paragraph above holds also for the use of a prior geological modelling term.

"A plot showing the evolution of the geological correction with every iteration would be appropriate here"

We agree that showing the evolution can be useful, but we decided not to add it to the paper for length reasons. The GIF image we added as supplementary material gives an qualitative indication of the importance of the evolution of the geological correction at each iteration.

Following are a few specific/technical comments.

L 38: Presumably “units” refer to rock units. Either add “rock” in front of “units”, or define what “units” are in this context

We have added “rock” before “units”.

L 45: When the parenthetical phrase is removed, the sentence reads “representing equal to zero.” I suggest changing “equal” to “equality”

We have change the phrasing to “In the implicit boundary representation, the units’ boundaries correspond to the zero iso-value of the implicit functions representing the signed distance to interfaces.”

L 46: Change “inverts” to “invert”

Thanks.

L 51 – 53: The sentence “In comparison … potential field data.” makes it sound like petrophysical inversions are not geologically meaningful. Suggest rephrasing or clarify what is meant by geologically meaningful

We replaced meaningful by “In comparison to the direct inversion of physical properties (i.e., density, electrical resistivity, seismic velocities, etc.), these geometrical inversions present a direct pathway to obtaining geologically realistic outcomes from the inversion of potential field data.”

We replaced ‘meaningful’ by ‘realistic’ in that a model can be readily applicable geologically or directly fed back to a geological modelling engine.

L 103: It is unclear what “is” refers to. Presumably it’s the “tau” parameter

Yes this is correct. We have corrected it.

L 149: Add “a” between “as” and “prior”

Done.

L 220: I question the value of including Figure 1. Adding illustrations would add value to Figure 1, and would also elucidate the proposed workflow. I would even suggest a possibility of combining with Figure 2. But as it stands, Figure 1 only contains text and adds little value to the manuscript

Thank you for the suggestion. We took this opportunity to shorten the manuscript and deleted Figure 1. We moved Figure 2 (now Figure 1 in the manuscript) higher up in the text in 3.2.1.

L 316: Is it “qualitative” or “quantitative”?

It is quantitative.

L 362: The sentence “Figure 5a and Figure 5b … starting data misfit” is awkward. Is Figure 5 meant as a reference to the sentence? What is meant by a “strong” data misfit?

Thanks. This sentence does not bring much information so we have removed it.

L 370: In Figure 5, the gravity anomaly maps on the top make it difficult to see the reference and starting models. I would suggest presenting the gravity anomaly maps as a separate figure

We have modified the Figure so that the model is more visible and the data less transparent (Figure 2):

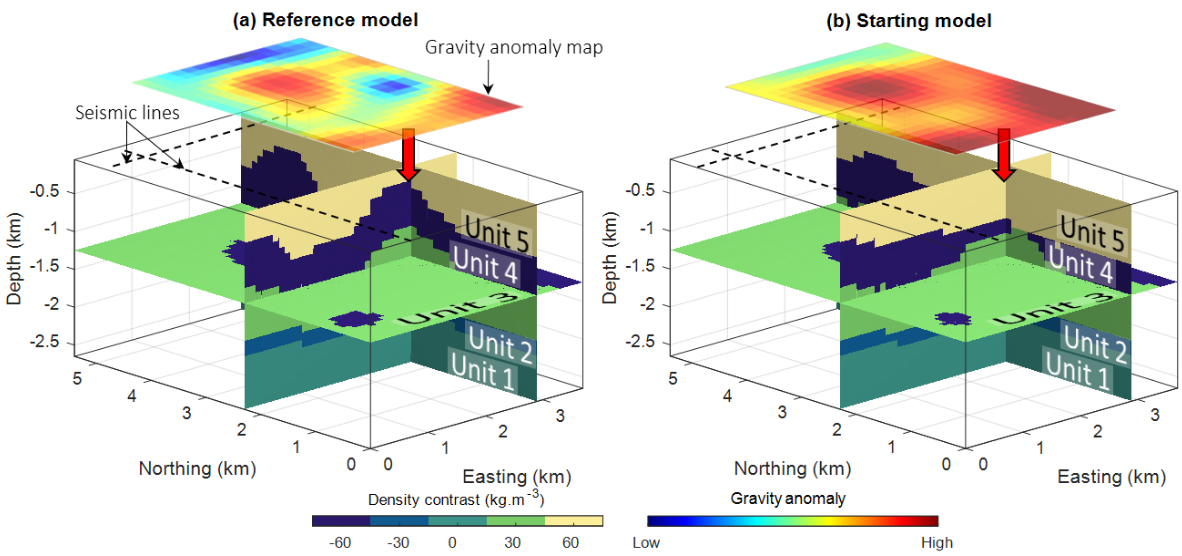

Figure 2.

L 412, 515, 655: Either define ‘geologify’ or rephrase to something along the lines of “ensuring geological realism”

We have added the underlined text: “to use geological correction a posteriori <u>to ensure geological realism</u> (to ‘geologify’)”

L 426: Similar to above comment, define “younging” or rephrase to something like “direction towards younger strata”

We have defined “younging” and added the following in 5.2.1.: “indicating the direction towards younger strata (later referred to as the ‘younging’ direction)”

L 431: Add “are” between “area” and “shown”

Done.

L 509: What is the sentence “This indicate.” referring to?

'This' refers to our analysis of adjacency matrices. We replace "this indicates" by "The comparison of adjacency matrices indicates"

L 511: Why is 'improves' in quotations?

We used quotations because saying that a model is improved is somewhat suggestive. We have replaced this by "greatly increases the geological realism of the final model".

L 534: Is reference to Figure 3 missing, or what is flow (1) referring to?

Yes the reference to Figure 3 was missing. Thanks, we have corrected it.

L 539: Did you mean "increase" in OC?

Yes, together with a reduction of the model misfit. We have corrected the sentence as:
"… which shows an overall increase in OC and a decrease in model misfit"

L 562 – 563: Sentence "As geophysical inversion … solution space." is not clear. Are you saying that geophysical inversions can be used to explore different regions of the solution space?

Yes. We have rephrased the sentence as:
"As geophysical inversion may be sensitive to features geological modelling has little to no sensitivity to, geophysical inversion can be used to explore different regions of the solution space"

L 603: Change "scenarii" to "scenarios"

Done

L 627: Add "of" after "birth"

Done

L 641: Remove "to" between "remediate" and "some"

Done