Manuscript: egusphere-2023-129

Object: answer to Anonymous Referee #2, comment posted on 27 Mar 2023

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Dear Reviewer,

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

Thank you for your encouragements!

The authors

Summary

The inversion of geophysical data is non-unique. This non-uniqueness is often tackled by spatial regularization promoting simple models, where simplicity is often formulated in terms of spatial smoothness and fails to honor geological realism. The authors present a novel framework to honor constraints derived from implicit geological modeling during the deterministic inversion of geophysical data and demonstrate its advantages using different synthetic geological models and synthetically-generated gravity data. The paper is well-written and accompanied by 17 figures of good quality. I recommend the publication of this manuscript subject to minor revisions. Aside from some specific comments below, I have several suggestions for improvement:

- The authors demonstrate their method on a number of synthetic case studies. In all of these, the starting models is relatively close to the true reference model used to create the synthetic data. A more detailed analysis on how the proposed method depends on the starting model would be insightful.

  A similar comment was made by the other reviewers, and we refer to the Appendices mentioned in our general answer and to the text and figure we added at the beginning of Section 5.3 with a starting model that is geologically unrealistic but which fits the gravity data. What we refer to as a “degenerate starting model” is obtained by rotating the original starting model by 180 degrees around the vertical axis.

  In addition, we already ran one test with a starting model that is geologically unrealistic. This is shown in case (5) of the second synthetic model. To make this more complete, we performed a similar exercise with the first synthetic model where we start inversion with geological correction applied to the results of the uncorrected case. We added this in Section 5.3.:

“To simulate this, we first perform inversion with geological correction applied, starting from the uncorrected case in the synthetic example presented in 5.1. The inverted model obtained in this fashion is shown in Figure 15a. The starting model is shown in Figure 15b. The application of geological correction results in the removal of a number of unrealistic features from the uncorrected inversion results used as a starting model. Here, results obtained by application of geological correction to unrealistic inversion results seem to present an intermediate case between the scenario with application of geological correction from the onset of inversion (Figure 15c) and the uncorrected case (Figure 15b). 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 15b and Figure 15a by application of geological correction, all models are geophysical equivalent in that they present similar geophysical data misfit values. This shows that, for this dataset, there exists a continuum of models with discrete density values 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.”

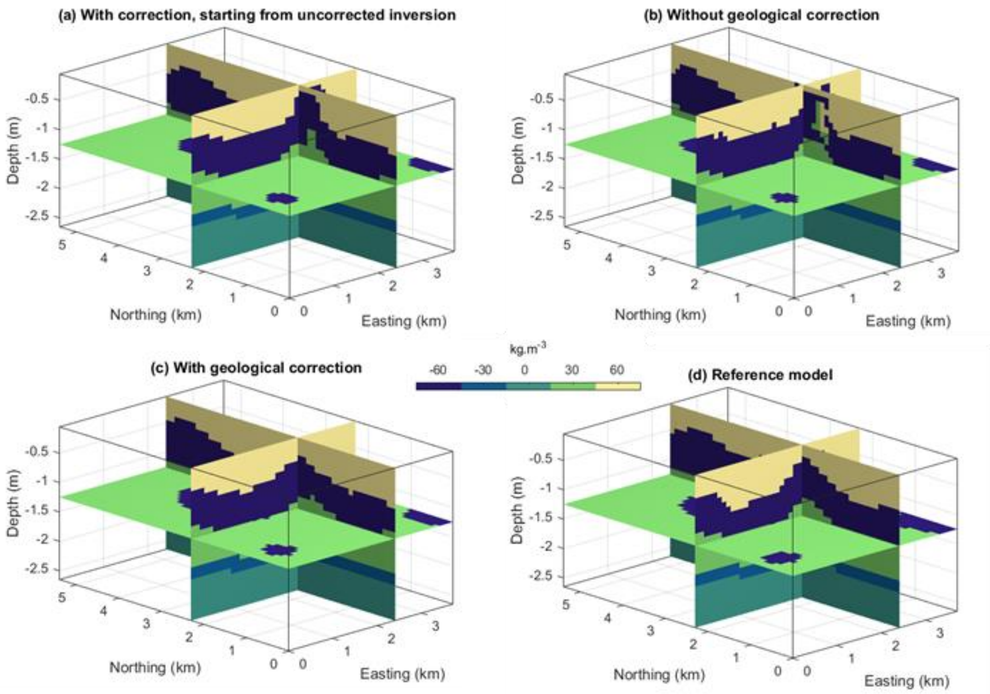

Figure 1. Comparison of inversion results with (a) geological correction starting from inverted model obtain without geological correction, as shown in (b); results with geological correction (c) and reference model (d).

In addition, we have added the following to the manuscript, in the discussion section:

‘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"'

- Inversion models should not under- or overfit the measured data. The very important topic of measurement error and data weights during the inversion should deserve more attention in this manuscript. Was the synthetic data noisified before inversion? If yes, which type of noise was used (e.g., Gaussian White Noise)? How were measurement errors treated in the inversion? Currently, this seems a bit arbitrary (e.g., no data weights in the formulas, inversion stops at 0.5 mGal.).

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 acceptable values for legacy data (Barnes et al., 2011). The gravity data simulated for the reference and starting models are shown in Figure 9. We consider the data produced by the reference model as the field measurements corresponding to the model we try to recover. We assume zero error to test the ability of the method to recover the reference in a perfect data settings (See Appendix 3: Robustness to noise and Appendix 4: Robustness to a degenerate starting model for a more realistic case including data errors)."

In the methodology section, we have added the following after the description of the cost function (eq. 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 be 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."

Although we agree that data noise can have an impact in practical studies, we did not add noise to the data, so the data is noise-free. One reason is to test the ability of this new method to recover sensible results in an ideal case. Also, in the tests that JG ran when developing the method, he observed that it was robust to Gaussian random noise. A possible explanation is that Gaussian 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 it is generally the case for many inversion schemes.

We investigate the impact of noise with the simulation of contaminated data in Appendix 3 and 5, which we refer to for more information, as mentioned in our general answer.

- Discussion of existing literature with similiar motivations: While it is true that the majority of literature either attempts to invert geophysical data using smoothness-constraints or simple geometrical definitions such layer-based parameterizations, there are a few recent examples where a geological modeling engine was used in the inversion of geophysical data. Putting these into context is in my view much more valuable for the readers (and the impact of the presented method) than pointing out differences to conventional approaches such as Thikonov regularization.
  - Güdük, N., de la Varga, M., Kaukolinna, J., & Wellmann, F. (2021). Model-Based Probabilistic Inversion Using Magnetic Data: A Case Study on the Kevitsa Deposit. In Geosciences (Vol. 11, Issue 4, p. 150). MDPI AG. https://doi.org/10.3390/geosciences11040150
  - Liang, Z., Wellmann, F., & Ghattas, O. (2022). Uncertainty quantification of geologic model parameters in 3D gravity inversion by Hessian-informed Markov chain Monte Carlo. In GEOPHYSICS (Vol. 88, Issue 1, pp. G1–G18). Society of Exploration Geophysicists. https://doi.org/10.1190/geo2021-0728.1

Thanks for the references. We have added a citation of Liang et al. (2023) in the introduction:

"To mitigate this, several solutions may be devised. One possibility, explored recently by Güdük et al. (2021) and Liang et al. (2023), consists in computing the geophysical response directly on geological models".

We have added the following to the Discussion (section 6.1):

"Finally, the approach presented here belongs to a family of inversion approaches that could be referred to as 'geometry driven'. That is, the main driver for fitting the geophysical data is the geometry of the subsurface model. One of our working assumptions is that geological data used to derive structural geological models are complemented by geophysical data, with the possibility to alter the shape of geological models. Another 'geometry driven' approach, consists in sampling points controlling the interpolated geological models within uncertainty and to integrate their forward geophysical response to the calculation of a posterior distribution (Güdük et al., 2021, Liang et al., 2023). This method is very elegant as it uses a unique geological level set parameterization, but it does not explicitly address the integration of spatial geological data as provided by drillholes or reflection seismic data. In contrast, our method can honour (up to discretization errors) spatial data. The mapping between the geophysical level set $\boldsymbol{\phi}$ and geological level sets $\boldsymbol{\phi}$ makes it challenging to derive sensitivities directly as in Liang et al. (2023), but it probably makes it possible to explore a larger model space by possibly departing from geological acceptable solutions during the non-linear iterations. Although further tests and comparisons between the two approaches are probably needed, this feature could be useful to prevent the optimization from converging to local minima and possibly in the future for stochastic inversions"

To add more context about other techniques pursuing the same goal, we have also added the following in the introduction:

"More recently, surface-based inversion has become practical for seismic and for potential field inversion by using either an explicit formulation for the interface between rock units (Galley et al., 2020) or using the level-sets in the inversion (e.g., Dahlke et al., 2020; Giraud et al., 2021a; Li et al., 2017, 2020; Rashidifard et al., 2021; Zheglova et al., 2018)"

Specific comments

- L52: In near-surface geophysics, "petrophysical (joint) inversion" is a widespread term implying the use of petrophysical relations for parameter transformation (e.g., electrical conductivity to water content) within the parameter estimation.

  We have rephrased the sentence that we thought was ambiguous to:

  "In comparison to the direct inversion of ~~petrophysical parameters~~ <u>physical properties (i.e., density, electrical resistivity, seismic velocities, etc.)</u>, these geometrical inversions …"

- L119 / L120: "regularization" vs. "regularisation". Check the entire mansucript for the consistent user of either British or American English.

  Thanks for picking on this. We have corrected the case of regularization vs regularisation and other such words.

- L132: Is the opening bracket before "see" intended? If yes, make sure it closes.

  Yes it was intended; problem corrected.

- Eq. 6: This seems to be redundant. Maybe psi^prior could be already introduced in equation 4?

  We agree that this is redundant. We have removed the equation. As psi^prior is not referred to later in the text, we just removed it.

- L181: Remove the comma after data

  Done, thanks.

- L199: Mentioning a few alternative geological modeling engines which could be used seems useful here.

  We have added references to GeoModeller and GemPy, SKUA-GOCAD, Petrel and Leapfrog. The modified text is as follows:

  "…be carried out with other implicit geological modelling engines, such as through GeoModeller's application programming interface Calcagno et al. (2008); Guillen et al. (2008), GemPy De La Varga et al. (2019), SKUA-GOCAD (Jayr et al. (2008)), Petrel Souche et al. (2015), or Leapfrog Cowan and Beatson (2002)"

- Eq. 16: Measurement errors seem to be neglected here. Was noise use to make the synthetic experiments more realistic? If yes, a data error estimate should also be used in the inversion. This needs to be clarified.

  We provide an answer to this question in our reply to your general comment above.

- L382: "... the data misfit visible in Fig. 5a and Fig. 5b" is misleading here, since no data misfits are shown. I recommend to rephrase to "... the corresponding data misfit of the inversion results shown in Fig. 5a and Fig. 5b".

  We have rewritten part of the sentence as:

  "… the requirement to reduce the data misfit component of Eq. (4) (the evolution of which is shown in Figure 3a and Figure 3b) leads the inversion to produce …"

- L459: Why 0.5 mGal? Was the data noisified and would this value mean the data was descirbed within its error bounds? The very important topic of data error/weights should deserve a bit more attention in this manuscript.

  We provided an answer to this issue when addressing your general comment above (second bullet point).

- L660: Is the code related to the method presented in this paper part of LoopStructural or is it made available with this manuscript in a separate repository?

  The inversion code is not yet available. We clarity this with the following text:

  "The inversion used here is a prototype under development that will be released in the future." in the data and code availability section.

- L738: The link to the pdf refers to a local filesystem.

  Thanks for spotting this. Corrected.

- L797: The editor's last name is Schmelzbach (last letter h not k), the publisher is Elsevier, and the name of the book series ("Advances in Geophysics", https://www.sciencedirect.com/bookseries/advances-in-geophysics) may be added.

  Thanks for spotting this; we have added the name of the book series.

References

Barnes, G. J., Lumley, J. M., Houghton, P. I., and Gleave, R. J.: Comparing gravity and gravity gradient surveys, Geophys. Prospect., 59, 176–187, https://doi.org/10.1111/j.1365-2478.2010.00900.x, (2011).

Calcagno, P., Chilès, J. P., Courrioux, G., and Guillen, A.: Geological modelling from field data and geological knowledge. Part I. Modelling method coupling 3D potential-field interpolation and geological rules, Phys. Earth Planet. Inter., 171, 147–157, https://doi.org/10.1016/j.pepi.2008.06.013, (2008).

Cowan, J. and Beatson, R.: Rapid Geological Modelling, in: Australian Institute of Geoscientists Bulletin 36, (2002).

Dahlke, T., Biondi, B., and Clapp, R.: Applied 3D salt body reconstruction using shape optimization with level sets, Geophysics, 85, R437–R446, https://doi.org/10.1190/geo2019-0352.1, (2020).

Galley, C. G., Lelièvre, P. G., and Farquharson, C. G.: Geophysical inversion for 3D contact surface geometry, GEOPHYSICS, 85, K27–K45, https://doi.org/10.1190/geo2019-0614.1, (2020).

Giraud, J., Lindsay, M., and Jessell, M.: Generalization of level-set inversion to an arbitrary number of geologic units in a regularized least-squares framework, GEOPHYSICS, 86, R623–R637, https://doi.org/10.1190/geo2020-0263.1, (2021).

Güdük, N., De La Varga, M., Kaukolinna, J., and Wellmann, F.: Model-based probabilistic inversion using magnetic data: A case study on the kevitsa deposit, Geosci., 11, 1–19, https://doi.org/10.3390/geosciences11040150, (2021).

Guillen, A., Calcagno, P., Courrioux, G., Joly, A., and Ledru, P.: Geological modelling from field data and geological knowledge. Part II. Modelling validation using gravity and magnetic data inversion, Phys. Earth Planet. Inter., 171, 158–169, https://doi.org/10.1016/j.pepi.2008.06.014, (2008).

Jayr, S., Gringarten, E., Tertois, A. L., Mallet, J. L., and Dulac, J. C.: The need for a correct geological modelling support: the advent of the UVT-transform, First Break, 26, https://doi.org/10.3997/1365-2397.26.10.28558, (2008).

De La Varga, M., Schaaf, A., and Wellmann, F.: GemPy 1.0: Open-source stochastic geological modeling and inversion, Geosci. Model Dev., 12, 1–32, https://doi.org/10.5194/gmd-12-1-2019, (2019).

Li, W., Lu, W., Qian, J., and Li, Y.: A multiple level-set method for 3D inversion of magnetic data, GEOPHYSICS, 82, J61–J81, https://doi.org/10.1190/geo2016-0530.1, (2017).

Li, W., Qian, J., and Li, Y.: Joint inversion of surface and borehole magnetic data: A level-set approach, GEOPHYSICS, 85, J15–J32, https://doi.org/10.1190/geo2019-0139.1, (2020).

Liang, Z., Wellmann, F., and Ghattas, O.: Uncertainty quantification of geologic model parameters in 3D gravity inversion by Hessian-informed Markov chain Monte Carlo, Geophysics, 88, G1–G18, https://doi.org/10.1190/geo2021-0728.1, (2023).

Rashidifard, M., Giraud, J., Lindsay, M., Jessell, M., and Ogarko, V.: Constraining 3D geometric gravity inversion with a 2D reflection seismic profile using a generalized level set approach: application to the eastern Yilgarn Craton, Solid Earth, 12, 2387–2406, https://doi.org/10.5194/se-12-2387-2021, (2021).

Souche, L., Lepage, F., Laverne, T., and Buchholz, C.: Depositional Space: Construction and Applications to Facies and Petrophysical Property Simulations, in: Day 2 Mon, December 07, 2015, https://doi.org/10.2523/IPTC-18339-MS, (2015).

Wellmann, J. F., de la Varga, M., Murdie, R. E., Gessner, K., and Jessell, M.:

Uncertainty estimation for a geological model of the Sandstone greenstone belt, Western Australia – insights from integrated geological and geophysical inversion in a Bayesian inference framework, Geol. Soc. London, Spec. Publ., SP453.12, https://doi.org/10.1144/SP453.12, (2017).

Zheglova, P., Lelièvre, P. G., and Farquharson, C. G.: Multiple level-set joint inversion of traveltime and gravity data with application to ore delineation: A synthetic study, GEOPHYSICS, 83, R13–R30, https://doi.org/10.1190/geo2016-0675.1, (2018).