

## Responses to Reviewer 1

This manuscript proposed to create a digital soil map of Australia based on a series of environmental covariates acquired at distinct spatial resolutions. Modeling was achieved with a machine learning algorithm trained on a large available soil geochemistry dataset and evaluated in another independent soil dataset. While the premise of the work seems very interesting and the results provided can be a major contribution to mineral exploration in Australia, I have some concerns regarding the representability of the input data after resampling as well of the external validation dataset. The correlation between input and predicted variables is also not very convincing. Some key literature works could help to give another dimension to the work, especially in the discussion. I would also like to see some general comments on the possibility of conducting similar approaches in other regions of the globe. I will try to explain each of these issues in more detail, hoping to help the authors to improve their work.

*Despite the low prediction accuracy, this paper demonstrates a step forward in the development of machine learning in generating predictive geochemical maps, not limited to Li. Similar approach can be implemented globally provided the availability of national database of the geochemical data along with relevant environmental covariates.*

### Specific comments

Main comments

1. It should be clear from the beginning of the abstract which other types of input data (besides geochemical data) were used for modeling.

*We did mention that we utilised both data from geochemical survey and environmental covariates to predict and map the spatial distribution of Lithium. We further clarify in the text that the environmental covariates that affect soil formation are utilised.*

### Add input data

2. One of my main concerns is related to model validation since the authors claim the success of the method proposed based on the external validation dataset. Is NAGS representative of all of Australia? In my view, soil characteristics and the Li content of the soils will vary throughout the country, and model performance will vary accordingly. Moreover, the NGSA and NAGS correspond to different sampling campaigns, with different collection dates and sampling densities. Despite the leveling employed by the authors, how can you confirm that the NAGS is suitable for the validation of the model trained in another dataset? Are the results obtained with the NAGS comparable to the out-of-the-bag validation using the NGSA data?

*We agree that the model performance would be different for different sites and understand that NAGS may not be representative of all Australia. It is the best available data that we can obtain to evaluate the model performance. We believe it is more suitable for evaluation, instead of simply dividing the NGSA dataset as calibration and validation. NAGS is suitable for the validation of the model trained in another dataset because the distribution of the data is similar based on the Kolmogorov-Smirnov test. The validation results from NAGS ( $R^2 = 0.32$ ) are higher than those for NGSA TOS ( $R^2 = 0.20$ ).*

3. Resampling of the data: the authors have resampled data acquired at 30 m or 90 m spatial resolution to a final resolution of 3 km. How can you ensure important information is not being lost with the resampling?

*A bilinear resampling method is implemented. As this is a continental evaluation, we are aiming to provide a continental trend rather than local trend.*

4. Remote sensing has limited penetration depth (0-10cm). How can you correlate the remote sensing variables with the BOS dataset?

Rao, K.S., Chandra, G. & Narasimha Rao, P.V. Study on penetration depth and its dependence on frequency, soil moisture, texture and temperature in the context of microwave remote sensing. J Indian Soc Remote Sens 16, 7–19 (1988).

<https://doi.org/10.1007/BF03014300>

*We agree that the remote sensing (Landsat) has limited penetration depth. In this study, we trained a prediction model for each depth, and developed the correlation of remote sensing data and the elemental concentration from each depth separately. We did not solely use Landsat data, we also used climate, subsoil clay content and topographical data. In addition, the BOS data is highly correlated with TOS ( $r = 0.75$ ,  $p < 0.0001$ .) and thus we can still infer BOS from climate, soil, topography and Landsat information.*

1. Figure 3: all variables show correlations below 0.3, which is considered by many authors as a negligible correlation. Taking this into account, how can you create a reliable model and consequently digital soil map?

*We did mention in the text that the correlation of an individual variable to Lithium concentration is relatively low. We did not claim that we developed reliable model. This manuscript demonstrates a case study on utilisation of machine learning to develop predictive geochemical maps.*

2. Which is the advantage of this method compared with traditional interpolation approaches (IDW, kriging)? I am aware that a comparison with other methods is beyond the scope of this manuscript, but the authors could comment on the advantages/disadvantages compared to previous works (if available), considering the NGSA dataset.

*Both IDW (Inverse Distance Weight) and kriging are interpolation method that utilise known values at certain location to predict values at unknown points without the use of covariates. The DSM method predicts the unknown values from the trained chemometrics model that relate the environmental covariates with the known values at each depth using machine learning models.*

3. Similarly, which is the advantage of the produced maps (Figure 6) when compared with the maps of Figure 1? Are any regions highlighted by the proposed method that were not highlighted in Figure 1? This information would be important for the readers to assess with the method you proposed is of interest.

*Figure 1 represents the Li concentration at a particular location, while Figure 6 represents the predictive Li concentration across the map. We point out locations that have anomalous Li concentration that can be investigated. Their shape and extent are defined using the higher spatial resolution model than the original sparse point-data.*

Minor comments

#### *Introduction*

- Lines 56-60: the authors explain that Li extraction from brines is in the form of Li-chloride. However, it would also be important to clarify that Li-carbonate is not directly extracted from Li-minerals, but the Li metal instead.

*Thank you for the comment. We added this into the revised version of the manuscript.*

- Lines 61-76: a brief description of the behavior of Li in soils is presented and previous works on soil geochemistry are presented. Other works related to this topic are also worth mentioning:

Luecke, W. (1984). Soil Geochemistry above a Lithium Pegmatite Dyke at Aclare, Southeast Ireland. *Irish Journal of Earth Sciences*, 6(2), 205–211.  
<http://www.jstor.org/stable/30002472>

Steiner, B. (2018). Using Tellus stream sediment geochemistry to fingerprint regional geology and mineralisation systems in Southeast Ireland. *Irish Journal of Earth Sciences*, 36, 45-61. doi: 10.3318/ijes.2018.36.45.

*We have included the additional references as suggested.*

- Lines 82-89: a summary of mineral prospectivity mapping is made, but other recent prospectivity mapping studies are missing:

Parsa, M. (2021). A data augmentation approach to XGboost-based mineral potential mapping: An example of carbonate-hosted ZnPb mineral systems of Western Iran. *Journal of geochemical exploration*, 228, 106811. doi: <https://doi.org/10.1016/j.gexplo.2021.106811>.

von der Heyden, B. P., Todd, C., Mayne, M. J., & Doggart, S. (2023). Zipf rank analysis highlights the exploration potential for Lithium-Caesium-Tantalum -type pegmatites in the Northern Cape, South Africa. *Journal of African Earth Sciences*, 197, 104769. doi: <https://doi.org/10.1016/j.jafrearsci.2022.104769>.

*We added more recent references as suggested.*

- Lines 92-96: a short literature review on the use of remote sensing for Li pegmatite identification is presented. Some of these works could be replaced by more recent studies:

Cardoso-Fernandes, J., Teodoro, A. C., Lima, A., & Roda-Robles, E. (2020). Semi-Automatization of Support Vector Machines to Map Lithium (Li) Bearing Pegmatites. *Remote Sensing*, 12(14), 2319. doi: 10.3390/rs12142319.

Morsli, Y., Zerhouni, Y., Maimouni, S., Alikouss, S., Kadir, H., & Baroudi, Z. (2021). Pegmatite mapping using spectroradiometry and ASTER data (Zenaga, Central Anti-Atlas, Morocco). *Journal of African Earth Sciences*, 177, 104153. doi: <https://doi.org/10.1016/j.jafrearsci.2021.104153>.

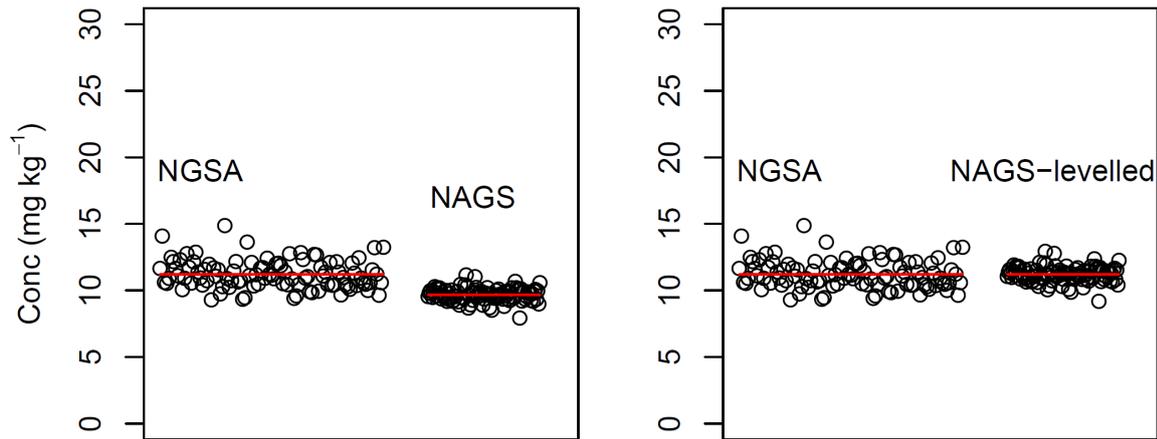
Booyesen, R., Lorenz, S., Thiele, S. T., Fuchsloch, W. C., Marais, T., Nex, P. A. M., & Gloaguen, R. (2022). Accurate hyperspectral imaging of mineralised outcrops: An example from lithium-bearing pegmatites at Uis, Namibia. *Remote Sensing of Environment*, 269, 112790. doi: <https://doi.org/10.1016/j.rse.2021.112790>.

*We added more recent references as suggested.*

#### *Materials and methods*

- Lines 143-145: "levelling method were utilized using the standards Certified Reference Materials (Main and Champion, 2022). In short, a correction factor based on the CRM measurements from the two datasets is calculated and applied as multiplier to relevel the data". Can we see a figure showing this leveling process?

*The following figure is for illustrative purpose only as no actual data was made available. Only the average of CRM-TILL 1 measurement was provided for each dataset.*



*The figure on the left showed the spread of TILL-1 CRM from both NGSA and NAGS dataset. It can be clearly seen that the concentration of TILL-1 CRM on NAGS dataset is slightly lower than those from NGSA. The correction factor is developed by calculating the ratio of mean concentration from NGSA dataset against the NAGS dataset. The NAGS is then levelled using the correction factor for better representation. This is very important because NGSA dataset was utilised for the prediction on the NAGS dataset.*

- Table 1: Spatial resolution of Landsat data is 30 m and not 25 m.

*We are not utilising raw Landsat data. The Landsat data we used was produced from another study (Wilford and Roberts, 2019) that pre-processed the Landsat data to expose Australia on its barest land.*

#### *Results and discussion*

- Line 239: “concentrations ranging from 0.1 – 67.4 and 0.1 – 56 mg kg<sup>-1</sup>, for TOS and BOS respectively”. These values do not seem to match Figure 2. Please revise.

*The bin width was too large in the original figure. We have corrected this.*

- Line 242: “mean Li concentration”. Which is the mean for the TOS and BOS datasets? Right now, you are comparing the median and the mean.

*We have corrected this.*

- Lines 261-262: “Despite other studies (Robinson et al., 2018; Kashin, 2019) reporting strong correlations between Li and Mg, and other elements elsewhere”. Extensive work on Li correlations with other elements for both stream sediment samples and a large pegmatite dataset for the Iberian Peninsula. Please consider comparing your results with other works.

Cardoso-Fernandes, J., Lima, J., Lima, A., Roda-Robles, E., Köhler, M., Schaefer, S., Barth, A., Knobloch, A., Gonçalves, M. A., Gonçalves, F., & Teodoro, A. C. (2022).

Stream sediment analysis for Lithium (Li) exploration in the Douro region (Portugal): A comparative study of the spatial interpolation and catchment basin approaches. Journal of geochemical exploration, 236, 106978. doi: <https://doi.org/10.1016/j.gexplo.2022.106978>.

*We have provided the comparison of our results to different studies.*

- Section 3.1.1: Please explain which threshold was used to consider a strong/moderate correlation.

*We have added the definition of threshold for correlation analysis.*

- Lines 267-271: Please consider key works on the alteration of Li minerals to clays: London, D., & Burt, D. M. (1982). Chemical models for lithium aluminosilicate stabilities in pegmatites and granites. American Mineralogist, 67(5-6), 494-509.

Quensel, P. (1937). Minerals of the Varuträsk Pegmatite. Geologiska Föreningen i Stockholm Förhandlingar, 59(2), 150-156. doi: 10.1080/11035893709444939.

Quensel, P. (1938). Minerals of the Varuträsk Pegmatite. Geologiska Föreningen i Stockholm Förhandlingar, 60(2), 201-215. doi: 10.1080/11035893809444995.

*We have added additional references as suggested.*

- Line 283: "Landsat bands 3, 5 and 6 had stronger negative correlations ( $r = -0.14$  to  $-0.16$ )". Please notice that  $-0.15$  and  $-0.17$  represent stronger negative correlations than  $-0.14$  and  $-0.16$ . Moreover, the graph scale is not the same for TOS and BOS in Figure 3. That is why the bars seem bigger for the BOS data when the values are smaller in module.

*We have rescaled the x axis to be the same, and reworded the sentence.*

- Lines 306-307: there are some studies on the spectral behavior of Li minerals and in some cases cross-analysis with the Li content:

Cardoso-Fernandes, J., Silva, J., Perrotta, M. M., Lima, A., Teodoro, A. C., Ribeiro, M. A., Dias, F., Barrès, O., Cauzid, J., & Roda-Robles, E. (2021). Interpretation of the Reflectance Spectra of Lithium (Li) Minerals and Pegmatites: A Case Study for Mineralogical and Lithological Identification in the Fregeneda–Almendra Area. Remote Sensing, 13(18), 3688. doi: 10.3390/rs13183688.

*I am missing the point here. The study refers to the use of reflectance spectroscopy to identify types of mineral deposits; this is more towards proximal sensing instead of mapping despite the authors claiming similar concept can be applied to the reflectance spectroscopy data obtained from satellite data (which most likely will be noisier).*

- Lines 334-335: “the model separates out prediction values based on its spectral response of vegetation”. I do not understand. Didn't you use the bare soil dataset where the vegetation influence was removed? Please comment.

*The bare soil dataset does not remove data for annual vegetation. It mainly removed seasonal vegetation influence. We double checked the representation of model, and noted a mistake was made, and have corrected the figure.*

- Line 343: “Landsat bands 2 and 6, and temperature range also affect model conditions”. Again, remote sensing data has low penetration depth, therefore the correlation with the BOS dataset should be low. How do you explain these results?

*Not applicable. We double checked the representation of model, and noted a mistake was made, and have corrected the figure. Please see the reply above on the correlation between TOS and BOS.*

- Lines 356-357: “the model developed here to have a higher concentration of soil Li, especially for the BOS model”. However, this is the model with a higher standard deviation. Please comment.

*We simply claim that the predictive map yielded results that make sense. There is higher Li concentration on areas where the existing Li mines were located.*

- Figure 7 is just a zoom of Figure 6, not bringing new information. I would prefer a comparison between the predicted contents in the validation area with both NGS and NAGS measured values.

*Figure 7 is indeed a zoom of Figure 6. It might be of interest to observe the variation within an area.*

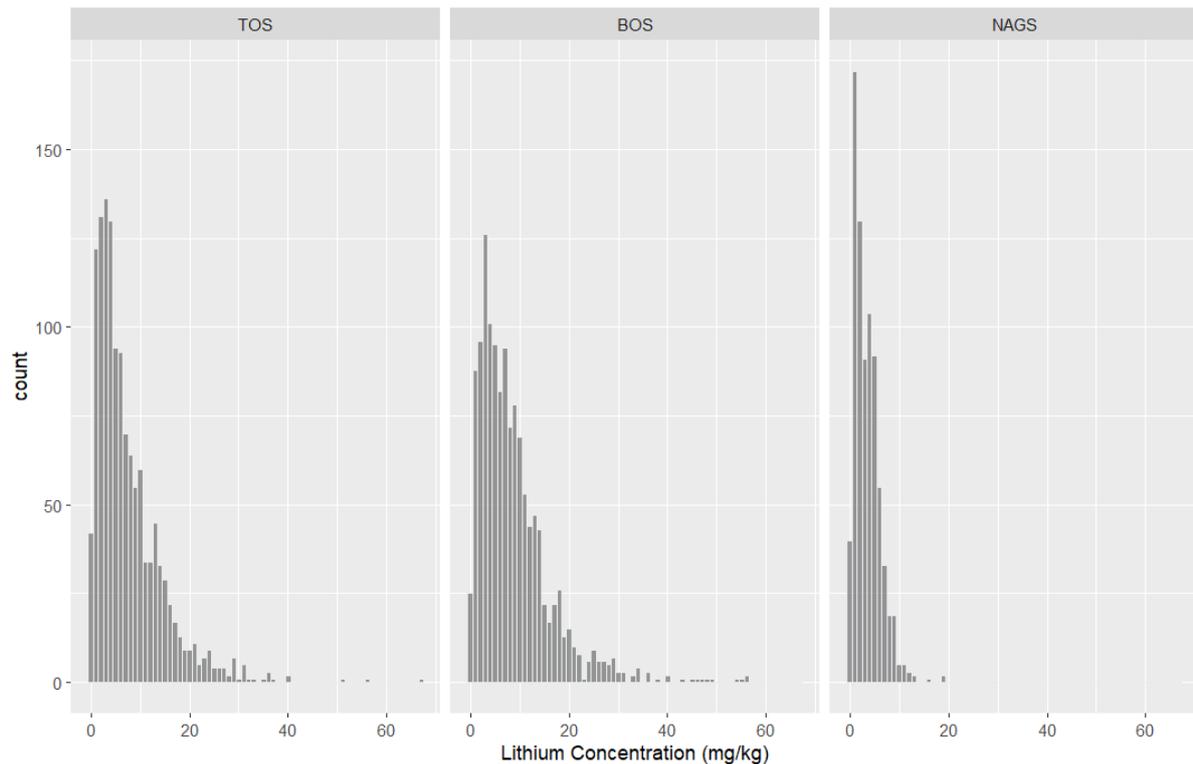
### **Technical corrections**

- Figure 1: Can you improve the quality of Figure 1? Is it possible to display the Li concentration with a ramp color to aid visualization? Can you separate the two maps into subfigures A (TOS) and B (BOS)?

*We have improved the quality of the figure for review. It is possible to do Lithium concentration with ramp color. However, we believed it would make the map too noisy. Hence, we kept the previous way of plotting. We would like to keep both figures as a set for cohesion purpose.*

- Figure 2: in the histogram of the left we don't see values > 40 mg/kg. Also, can we see the histogram for the NAGS dataset?

*We have included the histogram for all dataset*



- Figure 3: the graph bars go further than the X-axis. Please correct this issue.

*We have updated the plot.*

- Line 301: "Higher accuracy was observed in TOS". Higher, but still low. Please consider revising the sentence.

*We have corrected the sentence.*

- Table 2: the metric values presented for the external validation do not match the values mentioned in the text. Please revise.

*We have revised the values.*

- Figure 8: there are no units on the Y-axis.

*We have added units on the Y-axis.*

- Please revise the use of acronyms throughout the manuscript.

*We have revised the use of acronyms throughout the manuscript.*

Please see the **attached pdf file** (edited version of the original file) with some minor corrections/suggestions and yellow highlights that need to be addressed carefully.