

Discussion on referee 1's comments: Miniaturised visible and near-infrared spectrometers for assessing soil health indicators in mine site rehabilitation by Shen et al.

We thank the referee for the review and comments. Below we clarify and discuss those comments (in blue text and preceded by **Authors:**). We denote 'manuscript' as 'MS', 'page' as 'P', 'line' as 'L', when referring to locations in the manuscript.

Comment 1: The paper number soil-2021-138 of Zefang Shen and co-authors regards the repeatability of the spectrometers and the accuracy of the spectroscopic models built with seven statistical and machine learning algorithms. The authors found that miniaturised spectrometers and combinations predicted 24 of the 29 soil properties with moderate or greater accuracy. The repeatability of the miniaturised NIR spectrometers was similar to that of the full-range, portable spectrometer. The manuscript is potentially a contribution of interest for remote sensing application and it is within its specific scopes but in my opinion the manuscript don't fit in the scope of this journal.

Authors: Thank you, the general summary of the paper is correct. However, it is incorrect to suggest that our manuscript pertains to a 'remote sensing application'. Soil visible and near-infrared (vis-NIR) spectroscopy is an analytical technique that is used in the laboratory or in the field. When used in the field, the method is referred to as proximal soil sensing (Viscarra Rossel et al., 2011). Measurements in this same spectral range can be made with remote sensors, from airborne or satellite platforms, but usually with lower spectral resolution and measuring only the very surface of the soil, when it isn't covered by vegetation cover, buildings, etc.(Campbell and Wynne, 2011). The soil samples that we used in our analysis originate from two depths, 0–20 cm and 50–70 cm.

The manuscript fits well in the scope of SOIL, e.g. under "soil protection and remediation" and "soil and methods"

(https://www.soil-journal.net/about/aims_and_scope.html), and there are examples of other soil spectroscopic research published in the journal (Baumann et al., 2021; Ng et al., 2020; Yang et al., 2022; England and Viscarra Rossel, 2018). Therefore, we strongly believe our research fits in the scope of SOIL, which includes all topics that fall within the study of soil science as a discipline.

Comment 2: In my opinion the work lacks of a clear application of soil, same part of the ms. are very difficult to understand and don't permit to comprehend the originality of the paper.

Authors: We are perplexed by the comments that the manuscript lacks a clear soil science application, and that our manuscript lacks originality, but we agree that the description of our experiments are, by the very nature of the technology and analyses, complicated, making parts of the manuscript dense reading.

The 'soil application' pertains to the development of a rapid and cost-effective soil analytical method for the assessment of mining soil and for the purpose of post-mining soil rehabilitation. The conclusions also extend to other soil science applications (i.e. beyond post-mining rehabilitation) where cost-effective measurements of soil properties are required. We feel that this is clearly articulated in the manuscript, particularly in the introduction and discussion.

The originality of our research is summarised in the submitted manuscript (MS P4 L91-93). Of course, if that isn't clear, we can emphasise that in a revision: Our study is the first to evaluate portable, miniaturised vis-NIR spectrometers for assessments of soil in post-mining soil rehabilitation; We compared a diverse set of soil physical, chemical, and biological properties (29 in total) to cover a wide range of soils in different mining contexts; We evaluated miniaturised spectrometers alone and in combinations, which is important as different spectral ranges contain different and potentially unique information; We compared seven different algorithms to demonstrate the robustness of the spectroscopic method; We validated the models using two methods to prevent overly promising results; We considered both the

accuracy and repeatability of the miniaturised spectrometers and their combinations.

We understand that parts of the manuscript are difficult to follow, because our experimental design was complicated by the different comparisons that we made. However, we feel a robust assessment of the method necessitates these comparisons. Thus, in a revision, we propose to improve the readability of the manuscript by including a diagram to summarise the experimental design and experiments conducted. For instance, we could include a diagram like that shown in Figure 1.

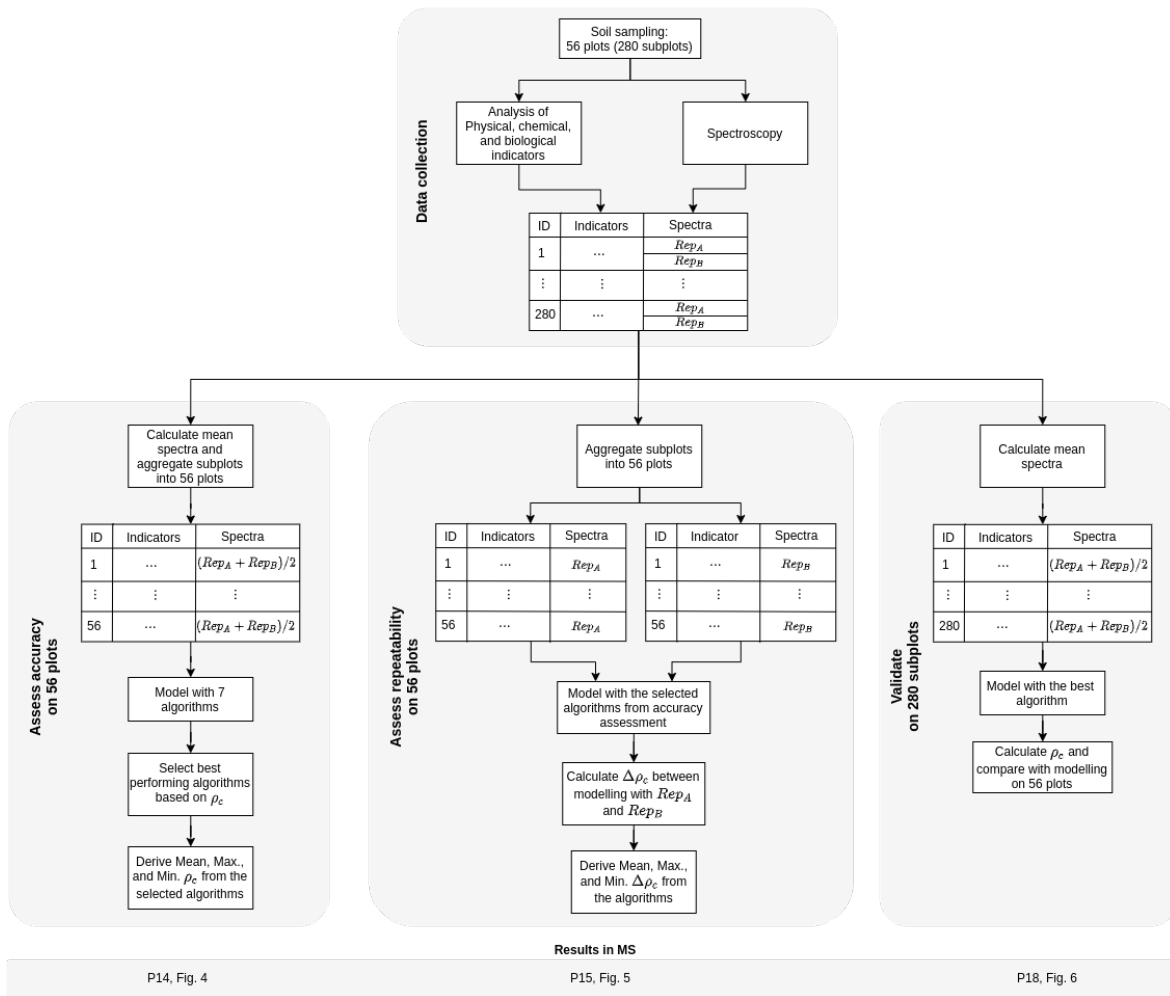


Figure 1: Study design

Comment 3: As is written do not explain the main results and should be connected with the aim of the research. Instead, the aim (L85-90, pg. 4)) focus only in several approach of multivariate procedure, seems just a mere exercise of multivariate

statistics applied to remote sensing equipment's. .

Authors: We assume that the reviewer missed the connection between our aims and results because parts of the manuscript are complex. As we state in our previous discussion point, we propose to improve this in a revision. To clarify, our aim was to assess the repeatability and the accuracy of spectrometers, and their ability to estimate a wide range of soil properties that are considered key indicators of soil health in mine site soil rehabilitation and restoration (MS P3-4, L87-88). To 'connect' our aims and results we used sub-headings in the Results section that directly relate to the aims: Section 3.2 (Assessment of the spectroscopic modelling with the spectrometers, P13) assesses the accuracy of the spectrometers; Section 3.3 (Effect of repeatability on the spectroscopic modelling, P14) assesses the repeatability of the spectrometers via modelling with two spectral replicates respectively; Section 3.4 (overall assessment of the spectrometers, P15) reports the performance of each spectrometer/combination considering both accuracy and repeatability for each of the 29 soil properties. We note also, that we used a similar structure of sub-headings in the Methods for clarity and ease of reference.

We have already clarified the comments around the aims and that this research isn't about 'remote sensing', but here, we must stress that this research isn't only a statistical exercise. Multivariate modelling is fundamental for assessing the soil spectroscopic method. Without the multivariate modelling of the soil properties we could not compare the performance of the spectrometers. We used seven algorithms that account for linear responses (PLSR) to more complex, non-linear responses (e.g. SVM), that also operate and are categorised differently: statistical (PLSR), tree-based (CUBIST, RF, XGBoost), Gaussian process-based (GPRL and GPRR), and support vector methods (SVM). All these algorithms have been employed in literature for soil spectroscopy modelling (Rossel and Behrens, 2010; Liu et al., 2016; Yang et al., 2019; Martínez-España et al., 2019). For a thorough and reliable assessment and comparison, we needed to test these different algorithms. This type of modelling,

and particularly machine learning, is largely dependent on the data set used and there isn't a single 'best' method for all applications. Using only one algorithm could lead to inaccurate conclusions. In a revision, we could of course emphasise the rationale of using the different algorithms, e.g. in section 2.4 Spectroscopic modelling (MS P7).

Comment 4: The novelty is not explained as well as the gap in our knowledge that the manuscript with its objectives should fill. For example if the novelty are studies on 1) hyperspectral quantitative analysis (L155 to provide comparison data for the 29 soil chemical, physical and biological soil properties to be assessed using spectroscopic methods) 2) compare Spectral range, resolution, price, weight, and dimensions of miniaturised and portable spectrometers used in this study. (?), 3) to assess the spectroscopic modelling with different statistical and machine learning algorithms, as well as 4) the accuracy of the spectrometers estimates and their repeatability, 5) assessment of the spectroscopic modelling algorithms (L160) with data from plots or (finally!) a model analysis of physicochemical indicators of polluted soil (?). The gap that results from a state-of-the-art topic should be clarify form the beginning .

Authors: Once again, we can only assume that the presentation has made the research difficult to follow and masked the clarity of the knowledge gap our research addresses. In the above discussion points, we have proposed that in a revision, we would improve the clarity of our presentation and description of the experimental design and we have also addressed comments around the aims and originality/novelty of our work. Here, we stress that to robustly assess the use of the miniaturised vis-NIR spectrometers for estimating soil health indicators in mine site rehabilitation, we needed to perform all of the tests and comparisons that we report (most of these are listed by the reviewer in his/her comment points 1-5).

Of course, we can emphasise the knowledge gap that our work addresses. However, we note that in the submitted manuscript (MS, L20-46) we describe context and the knowledge gap by explaining that mine site rehabilitation is guided by the measurement of a range of soil physical, chemical, and biological health indicators

because soil health assessment is key for returning functioning ecosystems, as the soil supports both above- and below-ground biodiversity. Conventional measurement of these indicators is expensive (MS, L52-54). Soil vis–NIR spectroscopy offers a cost-efficient solution for such assessments, and there is growing interest in using miniaturised spectrometers (Kademi et al., 2019; Alcalà et al., 2013; Catelli et al., 2020; Shariffar et al., 2019; Ng et al., 2020; Tang et al., 2020).

Comment 5: In my opinion the authors have to clarify in the state of art: 1) why they use these soil health indicators in mine site rehabilitation 2) if the procedure adopted is able to predict the level of contamination or soil health, 3) what are the limits of their predictive model, 4) if the model can be used for other places, because the authors do not compare their results with similar studies.

Authors: We believe that the submitted manuscript addresses point 1), and we refer the reviewer to the Introduction and cited references that explain the need of a comprehensive set of soil physical, chemical and biological properties (or indicators) for assessments of soil health in mining (Rayment and Lyons, 2010; Munoz-Rojas et al., 2016; Hart et al., 2020).

Regarding point 2), the research presented in this paper focuses on accurately predicting various soil properties that are indicators of soil health. We do not make an assessment of soil health because this is out of scope in this manuscript. With the measured indicators one can derive assessments of soil health, for example, using methods that are proposed in literature (Rinot et al., 2019). We plan to tackle that problem in a following study. Soil health is a complex concept and how it can be accurately estimated is a topic of significant current debate in the literature; its estimation here would only further complicate this research and deviate from the research question, i.e. can we accurately estimate soil health indicators with miniaturised vis–NIR spectrometers to support post-mining soil rehabilitation?

In terms of point 3), we agree that the current Discussion can be enriched by reference to the limitations of the spectroscopic method. Of course, there are

limitations and in a revision, we can elaborate on those.

Regarding point 4), we do not compare our results to similar studies because we have not found any other published research on the use of vis-NIR spectroscopy for mining soil assessments for rehabilitation, or actually on the use of vis-NIR for assessing a diverse range of soil physical, chemical and biological properties. Our results suggest that the miniaturised spectrometers with machine learning can be used to estimate 24 out of 29 soil physical, chemical, and biological properties from different soil types and mining contexts (P4, Table 1). Practitioners can use our results and conclusions to also develop their own models following the sensors and methods we proposed.

Comment 6: The second problem of this work is in the preprocessing method that is very confused. The Materials and Methods section (L160-185) does not provide sufficient detail to follow the progress of the manuscript. Regarding methods, there is a use of PLSR, RF, SVM, GBXBoost, CUBIST, SVM, GPRL, GPRP an incredible set of algorithms without explaining the criteria or limits or even if they are designed for these tools. So the reader is assuming or just have to imagine if the spectra were preprocessed. So the row data were filtered with Savitzky-Goaly (SGR) may be with multiplicative scatter correction MSC, or standard normal variate SNV, if they are treated with linear baseline correction LBC, peak normalization N, mean center MC. All this pre-processing are without explanation, whereas all the rest of the methods are only to be found in the results and conclusion discussion section. It is not explained why these methods were used and not others, how they are related to each other, nor is there sufficient detail to understand what was done and how these methods achieved the objectives of the manuscript.

Authors: This is a confusing comment. The comment that the ‘preprocessing method is very confused’ cannot be further from the truth. We described the preprocessing that we used in section ‘2.3 Soil spectroscopy’ (P7, L149-150) and what we did is very simple: ‘The reflectance (R) spectra of the soil samples recorded with

each instrument were transformed to apparent absorbance using $\log_{10}(1/R)$, and interpolated to 10 nm intervals to attain a consistent wavelength interval.’ In our opinion there is nothing confusing about that. We do not use any other preprocessing method. As the reviewer must know, preprocessing methods are data specific and used to correct for errors in the measurements (e.g. either from random noise, or additive, or multiplicative errors). In this case we found no reason to use them. We are perplexed by the reviewer’s comment ‘...All this pre-processing are without explanation, whereas all the rest of the methods are only to be found in the results and conclusion discussion section...’ etc. – these and the remaining text in Comment 6 are all obviously incorrect.

Regarding the comment that we do not adequately describe the different algorithms that we used—in a previous discussion point, above, we have already commented on the rationale for using the seven algorithms. Of course, we can provide detail on the algorithms in a revision, however, other authors have described these methods in some detail and have shown how they are suitably used with soil vis-NIR spectra. The manuscript provides references that the interested reader can find to learn more about them. We do not think it necessary to describe the algorithms in this manuscript because others have done so in published papers elsewhere and doing so would unnecessarily lengthen and complicate the manuscript further.

Comment 7: I am sorry for the Authors but no revision can at this point improve this work. Many other comments would be possible both for the sections ‘Materials and methods’ and ‘Results and discussion’, but it is useless because the comments made are more than sufficient to recommend the rejection of the manuscript.

Authors: We hope that our discussion points above clarify and show that the reviewer misunderstood our research and manuscript. We acknowledge that the reporting and presentation of our experiments could be improved, and we have proposed how we might do that in a revision. Finally, we are very concerned about the recommendation to reject our manuscript because as we have shown, the

recommendation is based on significant misunderstandings, misinterpretations and in some instances on comments that appear not to relate to this manuscript.

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