Author Response RC3 - Multiphysics property prediction from hyperspectral drill core data

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We thank the reviewers for their constructive feedback. Please find a full set of responses, including a revised manuscript and record of the corresponding changes with the changed line numbers in the attached pdf file.

Sincerely,
Akshay Kamath and authors

Reviewer Comment 3

Dear Reviewer,

We thank you for your time and effort reviewing the submitted manuscript, and are pleased that you appreciated our results. We have incorporated your suggestions into the revised manuscript, as detailed in the following pages. Please note that to facilitate the evaluation of our revision, the page and line numbers of the reviewers' comments refer to the originally submitted manuscript while page and line numbers of our responses refer to our revised manuscript.

Kindest regards,
Akshay Kamath, Samuel Thiele, Moritz Kirsch and Richard Gloaguen

Q) Does the paper address relevant scientific questions within the scope of SE?

Yes, the research aligns well with the scope of SE, especially in the areas of geophysics, spectroscopy and applications of machine learning techniques in geosciences.

Q) Does the paper present novel concepts, ideas, tools, or data?

Yes. The idea of using deep learning to predict the petrophysical properties from high resolution hyperspectral data can be considered as a novel approach in upscaling workflows. Also, application of the Shapely method for analysing the impact of different spectral bands on the model's predictions is an innovative addition.

Q) Are substantial conclusions reached?

Largely, yes. Conclusions are well supported by the key results, however some additional work on uncertainty quantification would be very beneficial.

Could the authors quantify the uncertainty of predictions using techniques such as Monte Carlo dropout, Bayesian inference or confidence intervals?

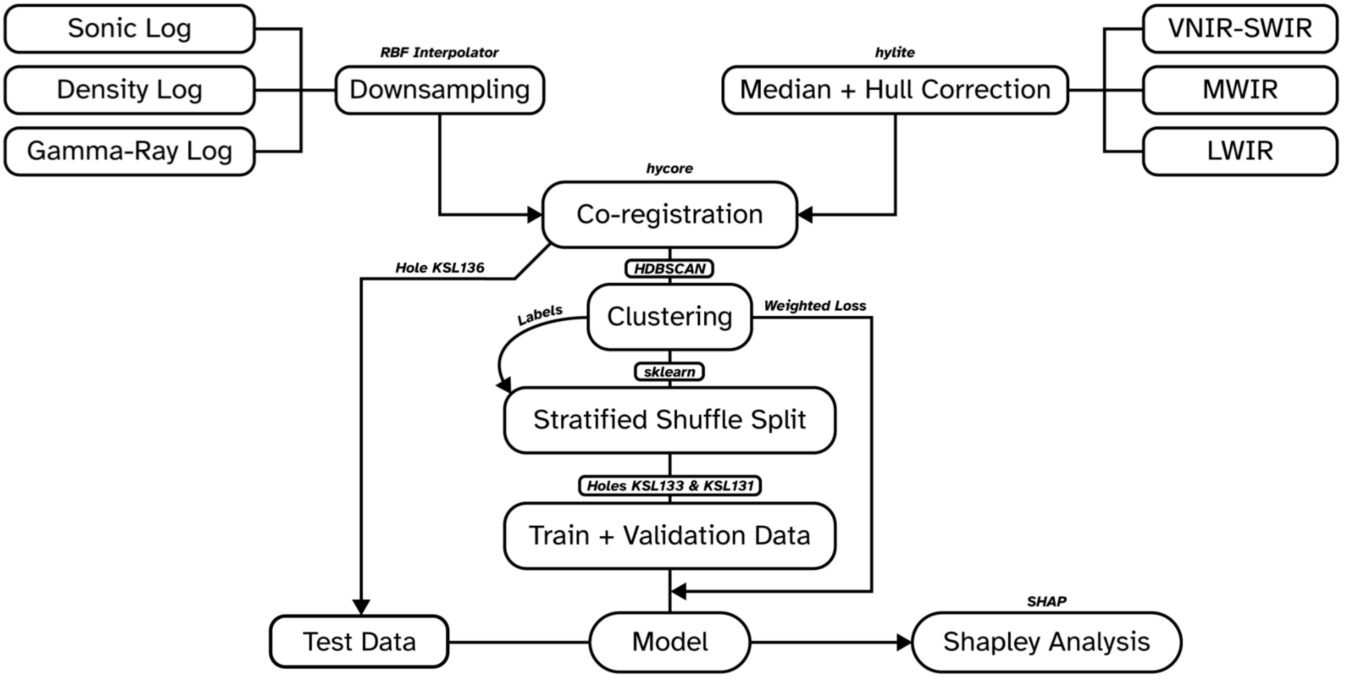
We agree that uncertainty predictions would be an interesting next step (e.g., using an ensemble model), but we consider this to be beyond the scope of the current work and suggest that this would be better addressed as a follow-up publication rather than adding extra complexity to our current manuscript. While feasible, this would require to develop an entire framework and would not add value to this submission. We argue that the XAI analysis demonstrates the robustness of the methods and that a qualitative assessment is sufficient at this stage.

Q) Are the scientific methods and assumptions valid and clearly outlined?

Authors have outlined each step of data processing in detail; however, inclusion of a workflow flowchart would greatly enhance clarity. A visual representation of the step-by-step process, including data acquisition, data preprocessing, clustering, deep learning, evaluation, Shapely analysis, and final outputs would be very helpful for readers.

We agree with the reviewer in that a flowchart would be helpful. Due to the high number of figures already present in the manuscript, we have added the following flowchart as a supplementary figure, as referred to on L3.14:

“Hyperspectral data were acquired and coregistered with downhole petrophysical logging data, and then used to train machine learning regression models. The various steps needed to preprocess our training data and build the deep-learning models (see Supplementary Figure for an overview) are described in detail below.”



Q) Are the results sufficient to support the interpretations and conclusions?

The performance metrics used (R^2 and RMSE) support the claim that hyperspectral data can predict the petrophysical properties accurately.

Nevertheless, the model struggles with unseen lithologies, more cross validation on other datasets can help generalise the conclusions.

We agree with the reviewer on the conditions for generalisability, and have highlighted them in the Discussion, at L10.15 (after including the additions suggested by RC1):

"A common challenge for deep learning models based on CNNs is whether or not they can be generalised. In this study, training and applying the model to three drill cores from the same geological sequence does not mean that similar results could be attained in different geological sequences. However, given the results from our Shapley value analysis, we suggest that it is unlikely that the model is "just" learning to distinguish different lithologies and returning appropriate (average) predictions. Instead, it appears to generate predictions based on the mineralogical and textural information captured by the spectra. This is key to its demonstrated ability to identify intra-lithology variations in each of the petrophysical properties (Fig. 7), and possibly explains why it produced broadly reasonable predictions for the unseen basement lithology. The model appears to be sensitive to the fundamental mechanical and petrophysical properties of the rock, which suggests that it could be generalised on more diverse data."

We also agree that testing on unseen lithologies would be helpful, which is why the high R^2 scores in density and gamma-ray predictions for the argillaceous basement (which has not been seen by the model) has been highlighted in L8.13:

"R^2 scores for this test hole were 0.86 and 0.9 for the density and gamma-ray logs, respectively, indicating very reasonable accuracy on unseen data, which even included a basement lithology that was not sampled by the other training drill cores (highlighted by the grey box labelled Tonschiefer i.e., argillaceous basement). The slowness prediction in KSL136 showed a relatively lower R^2 score of 0.7, with most of the erroneous predictions lying within the unseen lithology. The measured sonic log here shows significant fluctuations, whereas our model prediction remains steady (suggesting the lithology is spectrally quite uniform)."

As for the reviewer's comment on external validation, we agree that validation on different datasets would make the model more robust. However, we do not (currently) have access to additional datasets with hyperspectral and petrophysical data. This could thus represent an interesting follow-up work.

Q) Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?

Mostly, yes. As mentioned before, all processing steps have been well documented. However, model hyperparameters could be better detailed for traceability of the results.

We have now included the jupyter notebook used to train our models, as now mentioned in the

Data and Code Availability section (can be found here). These document the model hyperparameters we have used and ensure reproducibility.

Q) Do the authors give proper credit to related work and clearly indicate their own new/original contribution?

Yes.

Q) Does the title clearly reflect the contents of the paper?

Yes.

Q) Does the abstract provide a concise and complete summary?

Partially. Authors need to clearly state the problem and motivation upfront. They should start the abstract by emphasising why upscaling petrophysical measurements using hyperspectral data is important. This would draw the attention of the readers. Since automating petrophysical property predictions could lead to major cost and efficiency benefits, this should be explicitly stated in the abstract.

We agree with the reviewer and have highlighted the possibility of speeding up petrophysical data acquisition by changing the abstract as follows:

"Hyperspectral data provides rich ~~quantitative~~ information on both the mineralogical and fine-scale textural properties of rocks which also ~~, in turn, largely~~ control their petrophysical characteristics. We propose that some physical rock properties can be predicted directly from hyperspectral data, improving petrophysical characterisation and reducing the need for often laborious measurements. In this contribution we explore correlations between hyperspectral and petrophysical data using a deep convolutional neural network. ~~We therefore developed a deep learning model to predict petrophysical properties directly from hyperspectral drill core data.~~ Our model learns relevant features from high-dimensional hyperspectral data ~~and co-registered sonic, gamma-gamma density and gamma-ray logs~~ to predict ~~infer~~ slowness, density, and gamma-ray values using training and testing data from .~~We demonstrated the performance of this approach on data acquired in the~~ Spremberg ~~region of,~~ Germany. Our results show ~~demonstrate~~ that, with careful ~~meticulous~~ pre-processing ~~steps~~ and thorough data cleaning, ~~one can overcome the~~ differences in capturing ~~resolution~~ can be overcome to ~~and~~ learn the relationship between hyperspectral data and petrophysics. Using a test dataset from a spatially independent borehole, we generated ~~generate~~ a pixel-resolution (≈ 1 mm^2) model of the petrophysical properties and resampled ~~resample~~ it to match the measured logs. This test indicated ~~indicates~~ substantial accuracy, with R^2 scores and root-mean-squared errors (RMSE) of 0.7 and 16.55 $\mu s.m^{-1}$, 0.86 and 0.06 $g.cm^{-3}$ and 0.90 and 15.29 API for the slowness, density and gamma-ray predictions readings respectively. We also analysed the Shapley values of our model to gain deeper insights into its predictions. These ~~Overall,~~ our findings lay the groundwork for building deep learning models that can learn to predict physical and mechanical rock properties from hyperspectral data. Such models could provide the high-resolution but large-extent data needed to bridge the different scales of mechanical and petrophysical characterisation."

Q) Is the overall presentation well structured and clear?

Yes.

Q) Is the language fluent and precise?

Yes.

Q) Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

Yes.

Q) Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?

The legend of Figure 7 contains German geological terms for lithologies (e.g., Salzton, Werra Anhydrit, Kupferschiefer). Authors should translate such terms into English (e.g., Salt Clay, Werra Anhydrite, Copper Shale).

Other figures are well presented.

We have translated lithological descriptions to English (e.g., Karbonat to Carbonate), as suggested by the reviewer in Figure 7. However, we have refrained from changing commonly used stratigraphic terms (e.g., Kupferschiefer). We have, however, added the translation for Kupferschiefer in Section 2, at L2.27:

> "...("Copper-Shale")..."

The corresponding occurrences for the other german terms within the text (entirely within section 4) have been changed to match the legend.

Q) Are the number and quality of references appropriate?

Yes.

Q) Is the amount and quality of supplementary material appropriate?

Yes.