

Referee's comments on soil-2020-93

Title: Predicting soil carbon by efficiently using variation in a mid-IR soil spectral library

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The topic addressed by the paper is interesting and definitely in the scope of the journal. The article deals with the use of mid-IR spectroscopy in conjunction with chemometrics by means of PLS regression to predict soil carbon content of organic soils collected from two peatland regions of Switzerland. More specifically, the authors propose a statistical and rational approach based on three datasets: i) local dataset from the two peatland regions, ii) national soil spectral library (SSL) spiked with local samples, and iii) subsets containing local and representative SSL samples.

The results of this research work are of interest for the scientific community, particularly those involved in the use of IR spectroscopy for the study and characterization of soils. The proposed approach allows promoting the use of SSL (national or regional) for local predictions while minimizing the number of local reference analyses required. Having said that there are several points that need to be fixed by the authors.

General comments

The authors do not satisfactorily explain the relevance of their choice to work on the calibration of total carbon prediction models rather than organic and/or inorganic carbon separately. In most research work, the organic form is given much more attention because of its central role in the functioning of soils.

The approach for the calibration of local models, by considering calibration set with data (15, 20, 25, 30 ...) less or equal to that of the validation set, is statistically questionable. Moreover, how robust are these calibration models? What would happen if we made 5 random draws instead of the KS algorithm? The classical approach consists in splitting a data set, taking 2/3 for calibration and 1/3 for validation. So why the authors did not go so far as to test this classical subdivision?

The authors used the following statistical criteria R^2 , bias and RMSE to evaluate the prediction performance of spectral models in both calibration and validation. Most of the scientist involved in the field of soil spectroscopy also use RPD or even RPIQ (recommended when the distribution is not normal) criterion. I think the authors should provide them so that they are available to readers who would like to compare their results.

Specific comments

Title: Maybe it should refer to peatlands to make it a bit more explicit.

L. 116-119: The BDM database is made up of soil samples collected from topsoil (0-20 cm), is it the same for NABO samples?

L. 120: The organic soils are not sufficiently represented in the SSL. It would nevertheless be interesting to know their amount (or fraction) and their range of variation in SC content.

L. 122-123: the local HAFL consists of samples collected from 0 up to 2 m depth. I assume these are soil cores that were collected. In that case, what was the thickness of the soils taken for the reference analyses and what were the depths considered?

L. 168-169: No need to talk about Cubist models since the results are not included in this article.

L. 218-219: There is an ambiguity in this sentence: "where soils with a low carbon content had higher absorbance than soils with a high carbon content". According to the pre-processing carried out by the authors, Figure 3(b) shows the 1st derivative of the absorbance. Therefore, this figure shows the spectral variation of absorbance and not absorbance.

L. 218: There is an extra "the" to delete.

L. 224: Delete one of the two words "location"

L. 234-235: The RS-LOCAL subset contains 122 soil samples, of which 20 are the local HAFL samples. This subset is also shown in Figure 5. As a result, there is something I do not understand anymore. Figure 2 shows, in case of RS-LOCAL calibration subset, more than 300 samples. Where does this difference come from?

Figure 5. Why, in this case, did the authors prefer to perform PCA analysis on the unscaled and uncentered data?

L. 284: How the color affect the mid-IR spectral absorbance?

L. 300-301: I do not understand this sentence very well, it suggests that mid-IR-FTIR can only be used to analyse transmitted light and not the reflected one, which is not true. There is a need to clarify this.

A general comment on the section 5.1. Although it is interesting to know the different interactions between IR radiations and molecular bonds, I do not see the interest of this section with regard to the aim of this paper.

L. 324-329: Sounds good idea! The authors have, a priori, a dataset that would have allowed them to study the evolution of the RMSE by increments of 10% SC as suggested. Therefore, the question arises as to why this was not done.