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Interactive comment on "Development of pedotransfer functions for tropical mountain soilscapes: Spotlight on parameter tuning in machine learning" *by* Anika Gebauer et al.

Anonymous Referee #1

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Summary

In the manuscript by Gebauer et al. new pedotransfer functions are derived to predict the soil water retention at pF 0, 0.5, 1.5 and 2.5 for organic soils with volcanic influence and tropical mineral soils. The soil samples were collected in two tropical mountain regions in Ecuador. The authors use boosted regression trees method to predict the soil water retention from easily available soil properties. They analyse the performance of two parameter tuning methods: 1. the widely used grid search and 2. differential evolution optimization. The performance of the newly derived PTFs are compared to existing tropical PTFs on one studied site. The authors found that 1. the differential

evolution method outperformed the grid search, 2. the newly derived PTFs were more accurate than the readily available ones.

General comments

The authors derived pedotransfer functions also for soils which rarely have information on soil hydraulic properties: organic soils under volcanic influence with low bulk density and high organic carbon content. Soil hydraulic behaviour of these soils are unique, pedotransfer functions derived on mineral, non volcanic soils cannot be successfully applied for them. The presented study fills a gap related to describing soil hydraulic properties of an underrepresented soil system. For those, who are non-experts in the topic of the manuscript, it would be important to explain why separate pedotransfer functions were developed for the two studied sites.

The manuscript is well structured, the methods used to derive and optimize the predictions are adequate. Machine learning methods are common tools to predict soil properties. The selection of method to optimize the parameters of a particular machine learning method depends on the size of the dataset (number of samples in the training dataset), number of predictors, type of algorithm (how many parameters have to be optimized) and computation capacity. It would be important to mention and discuss these factors when performance of grid search and differential evolution algorithm is compared.

It is very positive that the newly derived PTFs are compared with existing PTFs – derived for tropical soils and available from the literature –, but it is not clear how many samples of the Laipuna site were used for it. The number of samples used for the analysis are generally not clear in the text, suggestions for clarification are included in the specific comments below.

It would be more informative to show results based on unscaled values, i.e.: Figures 6-8 and lines 186-191 and 219-223. It would enhance comparison of the results with the literature.

Authors could put more focus on soil physical interpretation of the results. Prediction of soil hydraulic properties of such specific soils as presented in the study is particular and very useful. The novelty of the paper could be connected to this.

It is not mentioned how the derived pedotransfer functions can be accessed.

Specific comments

L1-2: please specify in the title somehow that you derived PTFs to predict soil hydrological properties.

L15: please add name of the country.

L82, 88: could you please add the WRB (IUSS Working Group WRB: World Reference Base for Soil Resources 2014. International soil classification system for naming soils and creating legends for soil maps, Rome, 121 pp., 2014.) name of the most typical soils occurring in the studied sites?

L98-99: please give number of soil profiles and soil samples, instead of number of sites and sampling depth.

L99: Please add e.g. suction applied in hPa or matric potential head in cm. Why did you choose to measure water retention at pF 0, 0.5, 1.5 and 2.5? What is the reason for not determining water retention at pF 4.2?

L100: please add reference for the determination of soil water retention and BD.

L101-103: please add if it is the standard method in Germany for the determination of PSD.

L104: if I have understood it well, you didn't measure PSD for the Quinuas site because of the high SOC content. Please mention it here and shortly describe the reason for it.

L105: please add reference to CaCO3 determination.

L126: it would be helpful to shortly summarize what happens in 1) grid search and 2)

with the differential evolution algorithm.

L129: . . . were compared in grid search. . . Please add the name of R package you used to apply the grid search for tuning the parameters.

L134: please define here the meaning of v. Is the meaning of v = 100 the same in L139?

L147: add somewhere in the materials and methods section which soil variables you use as predictors by sites. In the present manuscript reader gets information about it only from Fig. 4. under Results and discussion section.

L177: please add that the description is in the text e.g.: . . . to the modelling steps described in text . . .

L182: what do you mean that number of samples was 51 and 46? Please rephrase the sentence accordingly.

L186-191: please add unscaled RMSE value with unit as well already here, because readers are familiar with that.

L199-201: The two sentence could be concatenated: the one starting with "Measured BD . . ." and the other starting with "The water . . .".

L203: please explain what you mean by "correspond to soil samples with a higher proportion of mineral components or andic properties".

L208: you could highlight here why it is an interesting dataset for deriving a new hydraulic pedotransfer function.

L210: Figure 4: - it would help comparison of Quinuas and Laipuna data if the min. and max. values of y-axis would be the same, you could include violin plot of both sites in one plot: one plot for OC and another for BD, - add in caption that PSD of Quinuas was not measured, and shortly add reason for it, - instead of showing the cumulative distribution of the PSD (Fig 4. c)) texture triangle diagrams separately would be more informative, - please add number of samples to the figure, e.g: in title or caption.

L213: Figure 5: - please add number of samples to the figure, e.g: in title or caption.

L218: you didn't mention in Materials and methods that you use scaled water retention values in the algorithm, please add it there and the reason for it there.

L219-223: please add unscaled RMSE value with unit as well.

L232: . . . models, regarding RMSEE and RE values . . .

L234: please consider to delete “However,”.

L237-238: please consider if number of samples can influence the performance of parameter tuning in sentence starting with “Probably”. Maybe it could be discussed how performance of tuning methods would change if you could include other predictors as well, e.g.: pH, CEC, etc.

L242-243: please mention under materials and methods the mean stone content of the Laipuna samples, if stoniness is characteristic for those.

L245: It is not clear what predictors were used to predict water retention of Quinuas. Please add it as mentioned before. It could be explained which suction heads can be covered by the predictors you have for Quinuas. Sentence starting with “PSD” should be moved under Materials and methods section, please see previous comments.

L246: Why performance of Laipuna PTFs for pF0, pF 0.5 and pF 1.5 is lower that that of Quinuas? Please discuss how those could be improved.

L253-273: Please add title to that section, to highlight that you applied existing PTFs on the sites to compare the performance of the newly derived PTFs to those.

L253: please add number of samples of the Laipuna dataset. Did you use the test set for the comparision?

L254: . . . PTFs from the literature were selected . . . Or add something similar.

L254-256: please move it under Materials and methods.

L256: it might be more precise to write that silt and sand content was converted to 2-50 μm and 50-2000 μm fractions by spline interpolation to calculate the USDA texture classes.

L263: add unit of RMSE.

L266-267: please mention other factors as well which could increase the performance of the PTFs.

L271: Table 2: - add number of samples – by pF values – used to test the newly derived and existing PTFs, did you use the test set of Laipuna dataset? - please use also here pF 0, 0.5, 1.5 and 2.5 instead of Theta 0, 0.5, 1.5 and 2.5., - add unit of the RMSE.

L275-278: for easier comparison Figures 6 and 7 could be concatenated by using grouped boxplots.

L280-285: based on Figure 5 observed pF values of Quinuas site is greater then 0.30 cm3/cm3, for Laipuna those are greater than 0.20 cm3/cm3. Please check in calculations why you have observed pF values close to 0 cm3/cm3 on Figures 8 and 9. Or are those scaled observed and scaled predicted variables? It would be more informative to show the scatterplot for not scaled observed and predicted values. Please revise Figures 8 and 9.

L293-294: Sentence starting with “Difference”: there is difference between GS and DE in case of the bag fraction as well. Is it possible to show which parameter – among number of trees, shrinkage, interaction depth, bag fraction – has the most dominant influence on the performance of BRT?

L318: . . . for the final differential evolution models derived for Laipuna site (Fig. 9) . . .

L334, 339: In the caption of Figure 10 and 11: add number of tested parameter vectors for both method.

L343-344: please note that in most of the cases local PTFs perform better than PTFs trained on dataset originating from elsewhere with different soil forming factors. Please revise the sentence.

L351-354: please consider to concatenate the last two sentence of the conclusions to better balance highlight both on the newly derived PTFs and results of comparing parameter tuning methods.

L354: please consider to provide availability of derived PTFs – which you recommend to use – for users.

Technical comments

L67: Please add the country after Páramo.

L151: The acronym of BRT is not included in the flowchart.

L343: . . . readily available . . .

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