Dear Mr. Vanderborght,

Thank you for receiving our revised manuscript. Please find the replies to your comments and to the reviewer comments below. Replies are displayed in blue and include the relevant changes made in the manuscript. Line numbers in the replies refer to the revised manuscript with tracked changes. Line numbers in the reviewer comments refer to the first manuscript version. Please find the marked-up manuscript version at the end of this .pdf file.

Kind regards
Anika Gebauer

Editor comments to the author

I agree with your responses to the reviewer comments on your paper. Your paper is mainly about a methodology to determine a pedotransfer function using a boosted regression tree and how the parameters of this model could be derived (using grid search or a differential evolution algorithm). In view of this, I think it is very important to address the comments by Alexandre Wadoux and include your responses in your paper.
The comments of Alexandre Wadoux were addressed and our responses were included in the paper (please see the replies to the comments of Alexandre Wadoux included in this .pdf file).

I would propose to put less focus on the derived pedotransfer functions themselves but more on the procedure on how to derive pedotransfer functions. The title of your paper puts the focus on these pedotransfer functions for tropical mountain soilscapes.
Our paper had two equally important aims (lines 80 ff.): developing water retention pedotransfer functions for two tropical soil-landscapes and comparing the differential evolution algorithm to grid search for parameter tuning. The title essentially refers to these two aspects.

But, would your pedotransfer functions be applicable for any other tropical mountain soilscape than the two that you considered? Since you developed two different pedotransfer functions, one for each landscape, I really doubt this. In the paper, these transfer functions are rather black boxes and it is far from clear whether they have any predictive power for other sites, land uses, …, than the sites where they were developed for. They do not provide insights in which input variables are most important to explain the output variables (at least, that was not reported in the paper) and it is not clear how they could be applied to datasets with different input data.
Pedotransfer functions were developed for each soilscape separately, as both areas are characterized by soils with very different properties. We made these differences more explicit in the abstract (lines 11ff). Please also compare text sections in lines 94 ff. and 247 ff.:

- lines 11 ff.: "(…) two remote tropical mountain regions of rather different soil-landscapes, dominated by (1) peat soils and soils under volcanic influence with high organic matter contents, and (2) tropical mineral soils."
- lines 94 ff.: "Quinuas (…) the mean annual temperature ranges between 5.3 and 8.7 °C (…) mean annual precipitation varies between 900 and 1600 mm (…). The Quinuas catchment can be allocated to the Páramo ecosystem (…). The Laipuna dry forest region (…) mean annual temperature varies between 16 and 23 °C and mean annual precipitation between 540 and 630 mm (…)."
- lines 243 ff.: "BD values in Quinuas range from 64 to 807 kg m^{-3}, while SOC values vary between 8.8 and 46.4 wt.%. … water retention ranges from 0.25 (pF 2.5) to 0.94 cm^3 cm^{-3} (pF

0). (…) For Laipuna, BD ranges between 1157 and 1727 kg m^{-3}(…) SOC content (…) varies between 0.4 and 3.8 wt. %. (…) Water retention values are ranging between 0.25 (pF 2.5) and 0.61 cm^3 cm^{-3} (pF 0). (…) Quinuas soils go along with the low density, porous soils, rich in organic material…Comparatively high water retention values can be attributed to the porous structure of Páramo soils (...)".

We are well aware that the collected dataset used for PTF development is rather small. Accordingly, applicability of the PTFs to other tropical soilscapes is not necessarily given but has to be tested. However, currently, there is a lack of PTFs for tropical soilscapes (compare lines 36-49, 223-233). For tropical peat soils under volcanic influence, there is probably none at all (lines 82 f.).

You are going to make the pedotransferfunctions that you developed available. It is however also necessary to make the dataset with input and output data available. This is important for the further improvement and generalization of pedotransfer functions.

The dataset used for PTF development comprising response (output) variables and predictor (input) variables will be uploaded to the Open Science Framework (OSF) upon acceptance (added to lines 488 ff.).

Short comment of Alexandre Wadoux

I agree with the authors that a grid-search process is by far the most used method for parameter tuning in Pedometrics, but claiming that (L. 64) differential evolution has been applied for the first time in Gebauer et al. (2019) is not correct. Differential evolution is routinely used in Pedometrics since several years, in particular to find optimal values of parameters, see for example https://doi.org/10.1016/j.geoderma.2018.03.010 or https://doi.org/10.1016/j.catena.2016.02.016 .
Thank you for pointing out these interesting manuscripts to us. Further applications of the differential evolution algorithm in soil-related research questions were added to lines 70 ff.. Nevertheless, we would like to emphasize that applications for parameter tuning in machine learning in pedometrics are scarce.

For parameter tuning in ML applied to soil mapping,Wu et al. (2016) (10.1007/s11368-016-1374-9) compared a genetic algorithm, Particle Swarm optimization and a grid search process to find optimal ML tuning parameters.
Without any surprise an optimization algorithm leads to more optimal parameter values than a grid-search process. This is obvious because a global optimization algorithm searches for any possible value within pre-defined boundaries while a grid-search is limited to a user-defined number of values.
The results of Wu et al. (2016) are contradictory. Please compare Lines 318 ff.: "In pedometrics, studies with direct comparison of grid search and mathematical optimization applied to parameter tuning in machine learning are scarce. Wu et al. (2016) compared both tuning strategies to train support vector machine (SVM) models for the prediction of soil contamination in the Jiangxi Province (China). However, their results are contradictory: In tuning only two real-valued SVM parameters, grid search outperformed the tested optimization algorithms, while tuning three parameters led to the opposite result. This shows that a lucky selection of predefined parameter vectors can result in grid search outperforming optimization algorithms – in particular, if the number of optimization iterations is small. Overall, the more values are tested during parameter tuning (grid search or optimization), the higher the probability of finding the global optimum. Wu et al. (2016) did not mention the number of iterations of the optimization algorithms, but we assume that increasing the number of iterations would have led to results that are at least as good as those achieved by grid search. Even though the benefits of optimization algorithms towards grid search are obvious, further direct comparisons of mathematical optimization algorithms and grid search applied for machine learning parameter tuning in soil related research questions are necessary."

It should be noted that grid-search parameter tuning is by far the most used because the user knows in advance the number of iterations that will be needed.
This is impossible to estimate with differential evolution, even though user-defined values in differential evolution can make the optimization to converge faster. This is a major limitation and the main reason why differential evolution (or any global optimization algorithm such as SA or PSO) are not routinely used for ML tuning parameter optimization.
Parameter tuning of ML models is computationally expensive and in most cases differential evolution will be too slow. In my experience differential evolution can need several hundreds to several thousands of iterations to find a global optimum.
We agree that it is beneficial to know the number of tuning iterations in advance. However, the differential evolution algorithm allows defining a stopping criterion. In this case, we stopped the differential evolution optimization either after 10 iterations without improvement or a maximum number of 200 iterations (lines 186 f.).
Regardless of the chosen parameter tuning technique, restricting the number of parameter values to be tested reduces the probability of finding the global optimum. Please see lines 447 ff.: "For both parameter tuning techniques, increasing the number of parameter values to be tested enhances the probability of finding the global optimum. (…) However, for tuning real-valued parameters, it is impossible to know the necessary number of iterations in advance. Accordingly, a trade-off between computing time and the probability of finding the global optimum has to be made for any parameter

tuning technique."
We agree that parameter tuning of machine learning models requires computing power. But with computers becoming more efficient and the possibility of parallelization, a parameter tuning technique should be judged based on the predictive power of the resulting machine learning model and not on the required computing resources.
We assume that it requires more computational resources to find the global optimum of real-valued parameters by testing every possible parameter combination during grid search instead of converging towards the optimum using a well-adjusted optimization algorithm. Making the wrong decisions in predefining the parameter values to be tested might even prohibit grid search from ever reaching the global optimum in tuning real-valued parameters (lines 55 ff.).

For this reason, when ML parameters need to be tuned, other more efficient algorithms are used in the ML literature. Bayesian optimization is one of them. Bayesian optimization has been designed for parameter tuning of ML models but is much faster than other global optimization algorithms. Bayesian optimization finds the optimal tuning parameter values in very few iterations. Another advantage is that the algorithm does not need specific pre-defined boundaries. I personally applied it for ML parameters tuning in https://doi.org/10.5194/soil-5-107-2019 .
Thank you for recommending Bayesian optimization. We see the advantages of the proposed parameter tuning technique, but want to mention that the differential evolution algorithm is able to outperform it in certain applications.
Please see lines 67 ff.:"It is also able to outperform bayesian approaches in certain applications. Comparisons of both algorithms led to contradictory results: while some studies found Bayesian approaches to be superior (e.g. Carr et al., 2016) others reported the opposite result (e.g. Schmidt et al., 2019)."
Further comparisons of other optimization algorithms including bayesian approaches and differential evolution in machine learning parameter tuning applications are necessary (added to lines 362 ff.).

Can the authors make a plot with in the x axis the number of iterations and in the y axis the value of the tuning parameters? This would be useful to see how the algorithm converges.
In accordance with comment C42 of the anonymous referee #1, the number of differential evolution iterations was added to lines 413 ff. We refrain from adding a plot, as a figure showing the converging algorithm for each tuning parameter and each cross validation fold would be rather confusing.

Referee comment 1 (a number was added to each comment)

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.
Thank you for your general comments. Our answers can be found below, next to the corresponding specific comments.

Specific comments

C1: L1-2: please specify in the title somehow that you derived PTFs to predict soil hydrological properties.
We changed the title to "Development of pedotransfer functions for water retention in tropical mountain soilscapes: Spotlight on parameter tuning in machine learning"

C2: L15: please add name of the country.
The name of the country was added (line 16).

C3: 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?
Due to monetary short cuts in the project grants we do not have all the required laboratory data in order to classify the soil profiles according to WRB. This is why we refrain from mentioning specific soil reference groups.

C4: L98-99: please give number of soil profiles and soil samples, instead of number of sites

and sampling depth.
Lines 118 ff. were adapted.

C5: 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?
The suction applied in hPa was added to lines 121 f.. Water retention at pF 4.2 was not determined because of high soil organic matter contents in Quinuas (added to lines 124 f.). To be able to compare the model input of both research areas, water retention was measured at the same pF values.

C6: L100: please add reference for the determination of soil water retention and BD.
References were added in lines 122 f. and 126.

C7: L101-103: please add if it is the standard method in Germany for the determination of PSD.
There are several methods to determine soil texture. We refrain from calling one of them a standard method. The applied methodology is given in lines 129 ff.

C8: 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.
Please refer to lines 132 f. and lines 98 f.

C9: L105: please add reference to CaCO3 determination.
Adapted accordingly in lines 127 f.

C10: L126: it would be helpful to shortly summarize what happens in 1) grid search and 2) with the differential evolution algorithm.
Lines 167 ff. were adapted accordingly. The differential evolution algorithm is explained in lines 172 ff.

C11: L129: … were compared in grid search… Please add the name of R package you used to apply the grid search for tuning the parameters.
We did not use an R package for grid search and programmed it on our own.

C12: L134: please define here the meaning of v. Is the meaning of v = 100 the same in L139?
Yes, adapted accordingly in line 177.

C13: 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.
Soil variables that were used as predictors were explained in Section 2.2 (added to lines 125 f.).

C14: L177: please add that the description is in the text e.g.: … to the modelling steps described in text …
The caption of Fig. 3 was adapted accordingly.

C15: L182: what do you mean that number of samples was 51 and 46? Please rephrase the sentence accordingly.
The sentences in lines 240 ff. were rephrased.

C16: L186-191: please add unscaled RMSE value with unit as well already here, because

readers are familiar with that.
Lines 186-191 (now lines 245 ff.) describe the dataset shown in Figure 4 and 5. No RMSE values are shown.
The BRT models were trained on scaled values, which is why we provided scaled RMSE values in Section 3.2. A text section to explain this aspect was added in lines 138 ff..

C17: L199-201: The two sentence could be concatenated: the one starting with “Measured BD …” and the other starting with “The water …”.
The two sentences are separated as both refer to different literature references.

C18: L203: please explain what you mean by “correspond to soil samples with a higher proportion of mineral components or andic properties”.
The sentence in lines 264 ff. was rephrased.

C19: L208: you could highlight here why it is an interesting dataset for deriving a new hydraulic pedotransfer function.
Please see lines 35 ff. and lines 80 ff.

C20: 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.
The violin plots of both sides were not included into one plot because BD and SOC ranges are rather different for Laipuna and Quinuas.
The cumulative PSD distribution was used instead of separate texture triangle diagrams, as it allows to show mean values and standard deviations per texture class (added to the caption of Fig. 4). The caption of Fig. 4 was adapted to explain why PSD was not measured for Quinuas and to add the number of samples.

C21: L213: Figure 5: - please add number of samples to the figure, e.g: in title or caption.
The number of samples was added to the caption of Fig. 5.

C22: 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.
Please see comment C16.

C23: L219-223: please add unscaled RMSE value with unit as well.
Please see comment C16.

C24: L232: … models, regarding $RMSE_E$ and R_E values …
The sentence relates to the difference between the scatterplots in Fig. 8 and 9.

C25: L234: please consider to delete “However,”.
“However” was deleted (line 295).

C26: 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.
The result of every tuning method (i.e. the parameter values) indirectly depends on the dataset, as parameter tuning means adjusting a model to the specific modelling problem / dataset (lines 52 f.). As discussed in e.g. lines 315 ff. or lines 339 ff. the number of samples and the number of predictors (and their information content) influence the performance of the BRT models. In general, a larger dataset of high quality results in more explicit relationships between response and predictor variables that can be detected and reproduced more easily by a model. This might reduce the required differential optimum iterations and the probability of getting stuck into a local optimum (added to lines 460 ff.).

Concerning the general questions:
The optimization methods should be chosen based on the type of model algorithm. Models with real valued parameters require a different tuning technique than those with discrete valued parameters (lines 55 ff.). The selection of the tuning technique does not depend on the number of parameters to be tuned. Grid search and optimization algorithms allow the tuning of only one parameter as well as the tuning of several parameters.
The computation capacity is still a limiting factor when it comes to optimization. But with computers becoming more efficient and the possibility of parallelization, a parameter tuning technique should be judged based on the predictive power of the resulting machine learning model and not on the required computing resources.

C27: L242-243: please mention under materials and methods the mean stone content of the Laipuna samples, if stoniness is characteristic for those.
The stone content was not determined for all samples.

C28: 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.
Soil variables used as predictors are mentioned in lines 125 f. (please see comment C13). Reasons, why PSD measurements were not possible for Quinuas, are explained in lines 132 f. (please see comment C8). The sentences in lines 315 ff. were adapted.

C29: 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.
We detected an error in Fig. 7 that was corrected: R^2 values of the differential evolution pF 0 Laipuna models range from 0.64 to 0.78 and are similar to those achieved in Quinuas. No significant difference between models of both research areas can be detected based on the R^2 values and the scatter plots shown in Fig. 8 and 9.
It was discussed how to improve model performance in different sections of the paper (please see comment C36).

C30: 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.
A new Section (3.3) was added under Results and discussion.

C31: L253: please add number of samples of the Laipuna dataset. Did you use the test set for the comparision?
Please see comment C37.

C32: L254: … PTFs from the literature were selected … Or add something similar.
"from the literature" was added to line 226.

C33: L254-256: please move it under Materials and methods.
The selection of existing PTFs to be applied on the Quinuas and Laipuna datasets was explained in a new Section (2.6) under Materials and methods.

C34: L256: it might be more precise to write that silt and sand content was converted to 2-50 _m and 50-2000 _m fractions by spline interpolation to calculate the USDA texture classes.
The sentences in lines 229 ff. were adapted.

C35: L263: add unit of RMSE.
Please see comment C37.

C36: L266-267: please mention other factors as well which could increase the performance of the PTFs.
The predictive performance of a model is affected by three factors: 1) The adjustment of the algorithm to the modelling problem by parameter tuning, which is discussed in Section 3.4. 2) The quality and size of the dataset forming the model input, which is discussed in lines 315 ff., 339 ff. and 460 f.. And 3) the chosen model algorithm, which was added to lines 342 f..

C37: 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.
The same test sets were used to evaluate the performance of the newly developed PTFs and the existing PTFs. Using cross validation each sample was used for testing (please see Section 2.5). In Table 2 the numbers of response – predictor variable data pairs were added and "Theta" was changed to "pF". The RMSE values are shown without the unit (please see comment C16).

C38: L275-278: for easier comparison Figures 6 and 7 could be concatenated by using grouped boxplots.
The boxplots of Fig. 6 and Fig.7 were not concatenated as models built on datasets of two research areas with very different properties cannot be compared directly.

C39: 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.
Fig. 8 and 9 show scaled values, which was added to the figure captions. As predicted and observed values were scaled in the same way, the not scaled scatterplots would look like the scaled ones – except for the axis labels. Scaled values were used to be able to use the same axis (between 0 and 1) for each plot. It enhances comparability without losing information.

C40: 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?
As mentioned in lines 430 ff. there is a difference in bag fraction, which cannot be explained (lines 446 f.). There might not even be an optimum for bag fraction (lines 444 f.).
We made an assumption about the parameter importance in lines 443 f.. A sensitivity analysis could be used to estimate the importance of each parameter. As the model performance depends on the

interaction of all parameter values (added to lines 442 f.), we recommend tuning the number of trees, shrinkage, interaction depth and bag fraction simultaneously.

C41: L318: … for the final differential evolution models derived for Laipuna site (Fig. 9) …
The sentence in lines 441 f. was adapted.

C41: L334, 339: In the caption of Figure 10 and 11: add number of tested parameter vectors for both method.
The number parameter vectors tested by grid search is mentioned in lines 170 f.. In accordance with the review of Mr. Wadoux the number of differential evolution iterations was added to lines 413 ff.. One iteration compared 100 parameter vectors (line 182).

C42: 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.
Please see lines 35 ff.. The comparison to other existing PTFs that were developed under conditions as similar as possible (lines 225 f.) is important to legitimate the developed BRT PTF and should be mentioned in the conclusions.

C43: 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.
The conclusion was divided into two new paragraphs to highlight the two achievements. The last two sentences were concatenated (lines 484 f.)

C44: L354: please consider to provide availability of derived PTFs – which you recommend to use – for users.
The developed PTFs, as well as the underlying datasets, will be uploaded to the Open Science Framework (OSF) upon acceptance (added to lines 488 ff.).

Technical comments

TC1: L67: Please add the country after Páramo.
”Ecuador” was added after “Páramo” (line 82).

TC2: L151: The acronym of BRT is not included in the flowchart.
“BRT = boosted regression trees” was removed from line 195.

TC3: L343: … readily available …
„ready“ was changed to „readily“ (line 475).

Referee comment 2

The objective of the study is to develop pedotransfer function for water contents at four pressure heads (PF 0, PF 0.5, PF 1.5, PF 2.5) for two tropical mountain regions with high soil organic carbon content. Boosted regression tree technique was used to fit the models for both areas considering two tuning procedures to determine the regression tree-model parameters (n.tree, shrinkage, interation depth, bag fraction): grid search and differential evolution, the latter showing better results on the water retention estimates for the both areas. The work also compared the performance of the proposed PTFs with other PTFs from literature confirming the better performance of the proposed models. I congratulate the authors for the effort in collecting physico-chemical and hydrological data in such atypical soils and for using innovative techniques, such as the differential evolution, in order to get better results on the models fits. I also congratulate them for developing PTFs for organic soils which are not so common in the literature. The work in well written and structured and the subject is well posed. Some general and specific comments are summarized below:

a) Line 45: In organic Finnland soils?
Yes, in Finish peat soils. The sentence in line 47 was adapted.

b) It was not clear in the text why you have chosen the boosted regression tree models (Lines 72-73);
The reasons for using boosted regression tree models were added to lines 86 ff..

c) The sentence in line 97-98 should be reformulated ("It allows representing a research…to the accessible area"). The way it was written was unclear to me.
The description of the sampling site selection algorithm was extended (lines 115 ff.)

d) Line 105. Sometimes outliers should carry important information from the studied area. You should detail the reason of removing them.
The sentences in lines 134 ff. were adapted and extended to explain why it was decided to remove outliers.

e) The description of the boosted regression tree should be improved by describing clearer its fitting procedure (Lines 110-115).
The BRT fitting procedure was described more detailed (lines 152 ff.)

f) Line 144: What the word "respectively" is related to?
The sentence in lines 186 f. was adapted.

g) Line 182: After explaining the reasons for excluding the outliers it would be interesting to inform the range of their values for each soil property;
As only data pairs of response and predictor variables that were identified as multivariate outliers were removed (lines 135 f.), it is not useful to inform about the range for each soil property. The complete dataset, including data pairs identified as multivariate outliers, will be available upon acceptance (please see comment r).

h) Lines 182-190: What is right and left- skewed distribution? It is not clear.
The terms "right- and left- skew" were changed to the more common terms "negative- and positive-skew" (Section 3.1). Negative skew: the mean is smaller than the median. Positive skew: the median is smaller than the mean.

i) Line 199: I suggest to correct this sentence: "..organic matter being characterized by a high water holding capacity" to *organic matter which is associated with soils with a high water holding capacity*
The sentence was corrected (lines 258 ff.).

j) Line 218: How the scaled water retention value was defined? This needs to be clarified;
Water retention values were scaled to the range [0, 1] using Eq. 1 (added to lines 138 ff.).

k) Line 230: Change Fig.11 and 12 to Fig 8 and 9;
Fig.11 and 12 were changed to Fig. 8 and 9 (lines 302 f.).

l) Line 240: Change Section 3.2 to Section 3.3;
Section 3.2 was changed to Section 3.3 (line 312).

m) Line 245: "PSD measurements were not included..in this area". This sentence should go to Section 3.1 when you call Fig.4 in the text.
The sentence in line 332 was deleted. Following the comments of the anonymous referee #1 , it was explained why PSD measurements were not possible for Quinuas (section 2.2, lines 124 ff.). The caption of Fig. 4 was adapted.

n) Line 234: Change Fig.9 a-d and 10 a-d to Fig.8 a-d to Fig.9 a-d;
Fig.9 and 10 were changed to Fig. 8 and 9 (lines 295 f.).

o) Lines 253-263: Did you apply the PTFs from the literature to the Laipura soils considering their range values applicability?
The test Laipura soils were included in the calibration of the proposed PTFs (BRT PTF – Table 2)? This need to be clarified.
Reliable PTFs, that were developed under conditions as similar as possible to the Laipuna dataset were selected (lines 225 f.). Selected PTFs are more general (line 16) as they were developed on larger datasets. The number of response – predictor variable data pairs was added to Table 2. However, the selected PTFs were not specifically developed for soils of Ecuadorian dry forest ecosystems and therefore response and predictors variable do not always match concerning their range.
The same test sets were used to evaluate the performance of the BRT PTFs and the existing PTFs. Using cross validation each sample was used for testing (please see Section 2.5).

p) Avoid vague sentences: ex: "these values are.."(Line 268), "in this case"(Line 320), "this might.." (line 320), "This might also result" (lines 325-326);
The sentences in lines 438-445 were adapted.

q) The code of the proposed models should be presented;
The developed PTFs, as well as the underlying datasets, will be uploaded to the Open Science Framework (OSF) upon acceptance (added to lines 489 ff.).

r) Is it possible to provide the study database to the readers?
Please see comment q.

Manuscript with tracked changes

Development of pedotransfer functions for water retention in tropical mountain soilscapes: Spotlight on parameter tuning in machine learning

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Abstract. Machine learning algorithms are good in computing non-linear problems and fitting complex composite functions, which makes them an adequate tool to address multiple environmental research questions. One important application is the development of pedotransfer functions (PTF). This study aims to develop water retention PTFs for two remote tropical mountain regions of rather different soil-landscapes, dominated by (1) ~~organic~~ peat soils and soils under volcanic influence with high organic matter contents, and (2) tropical mineral soils. Two tuning procedures were compared to fit boosted regression tree models: (1) tuning by grid search, which is the standard approach in pedometrics, and (2) tuning by differential evolution optimization. A nested cross-validation approach was applied to generate robust models. The developed area-specific PTFs outrival other more general PTFs. Furthermore, the first PTF for typical soils of Páramo landscapes (Ecuador), i.e. organic soils under volcanic influence, is presented. Overall, results confirmed the differential evolution algorithm's high potential for tuning machine learning models. While models based on tuning by grid search roughly predicted the response variables' mean for both areas, models applying the differential evolution algorithm for parameter tuning explained up to ~~22~~ 25 times more of the response variables' variance.

1 Introduction

Machine learning algorithms are good at fitting highly complex non-linear functions (Witten et al., 2011). Major application fields in soil science investigate the soils' spatial variability (Heung et al., 2016), relate data from soil sensing to soil properties (Viscarra Rossel et al., 2016), or develop pedotransfer functions (PTFs, Botula et al., 2014; Van Looy et al., 2017). McBratney et al. (2019) give a timeline on developments in pedometrics, that refer to machine learning in multiple applications.

Pedotransfer functions derive laborious and complex soil parameters (response variables) from more readily available soil properties (predictor variables). Most PTFs are developed to predict soil hydraulic properties. ~~A review~~Reviews on the involved ~~methodology~~ methodologies ~~is~~ are provided by Pachepsky and Rawls~~,~~ (2004), ~~Shein and Arkhangel'skaya (2006),~~ Shein and Arkhangel'skaya (2006) and Vereecken et al. (2010). Machine learning algorithms applied for PTF development include e.g. support vector machines (Lamorski et al., 2008), artificial neural networks (Haghverdi et al., 2012) and regression trees (Tóth et al., 2015). According to ~~the review by~~ Van Looy et al. (2017), most PTFs are developed for mineral soils, while PTFs applicable to organic soils or ~~to~~ soils with specific properties like volcanic ash soils are highly underrepresented. Patil and Singh (2016) and Botula et al. (2014) provide reviews of hydrological PTFs for mineral soils of certain tropical and temperate regions. With particle size distribution (PSD) being the basic input parameter to derive soil hydrologic properties, most PTFs also use bulk density (BD) and soil organic carbon content (SOC) as predictors. As summarized ~~in the review of~~by Patil and Singh (2016), the application of existing hydrological PTFs is often restricted ~~by~~ because of two reasons: (1) The majority of PTFs are developed on soils that developed under certain conditions. Often these PTFs cannot be applied ~~sufficiently~~ in other regions as the site-specific soil-forming conditions can cause considerable differences in physical and chemical soil properties. This is for example demonstrated by ~~the studies of~~ Botula et al. (2012) and Moreira et al. (2004) who were able to show that, when applied to independent tropical soil data, existing temperate PTFs perform worse than existing tropical PTFs. (2) ~~On the other hand, t~~The applicability of existing PTFs is further restricted by the required input data. As stated by Morris et al. (2019) hydraulic PTFs developed on mineral soils are often inapplicable to organic soils. The measurement of the predictor variable PSD may be hampered by high organic matter contents, and~~other~~ organic soils may not include sufficient mineral soil material to justify PSD analysis at all. Overall, there is ~~In general,~~ only a small number of ~~very few~~ PTFs that were developed for organic soils and most of them are based on data from specific temperate regions and rely on very specific predictor variables. Korus et al. (2007) for example related the water retention of polish peat soils to the predictors ash content, specific surface area, BD, pH, and iron content. In Finish peat~~Finnland~~ soils semi-empirical water retention PTFs were developed on different predictors including BD, sampling depth and botanical residues (Weiss et al., 1998). Even though it was never intended to be used for predictions, Rocha Campos et al. (2011) provide the only regression model known to us, which relates the soil hydrologic parameters of tropical organic soils to independent variables (fiber content, mineral material, BD and~~,~~ organic matter fraction~~sated into humin as well as fulvic and humic acids~~).

~~Finally, t~~The application of machine learning algorithms requires them to be adjusted to the specific model~~l~~ing problem by parameter tuning. Tuning parameter values cannot be calculated analytically, so in soil science applications~~,~~ grid search is often used as a standard technique (e.g. Babangida et al., 2016; Khlosi et al., 2016; Twarakavi et al., 2009). It works by testing a number of predefined parameter values or combinations of parameter values to finally choose the best. Accordingly, the predominant part of the multivariate parameter space cannot be searched in the case of real-valued parameters and the optimum might not be found. To overcome this limitation, mathematical ~~optimisation~~ optimization is a promising alternative. Commonly applied ~~optimisation~~ optimization algorithms include artificial bee colony, simulated annealing, particle swarm ~~optimisation~~optimization, the nelder-mead method, bayesian optimization or evolutionary and genetic strategies. Their applications range from pattern recognition (e.g. Jayanth et al., 2015; Liu and Huang, 1998), through solving combinatorial problems (e.g. Kang-Ping Wang et al., 2003; Reeves, 1993) to parameter tuning in machine learning (e.g. Imbault and Lebart, 2004; Ozaki et al., 2017). We would like to particularly emphasize the differential evolution algorithm. Price et al. (2005), who ~~C~~compared it to various~~the other~~other optimization algorithms, were able to show that ~~mentioned above,~~ it usually leads to better results and ~~a~~ comparatively low computing times~~ (Price et al., 2005)~~. This has been confirmed by the results of ~~(~~Chen et al.~~,~~ (2017) who compared differential evolution to particle swarm optimization and a genetic algorithm in landslide modeling, and ~~(~~Yin et al. ~~,~~ (2018) who compared differential evolution to simulated annealing, particle swarm optimization, artificial bee colony and genetic algorithms in geotechnical engineering. It is also able to outperform bayesian approaches in certain applications. Comparisons of both algorithms led to contradictory results: while some studies found bayesian approaches to be superior (e.g. Carr et al., 2016) others reported the opposite result (e.g. Schmidt et al., 2019).

The differential evolution algorithm was~~It has been~~ applied to diverse ~~optimisation~~ optimization problems including the prediction of stable metallic clusters (Yang et al., 2018), the navigation of robots (Martinez-Soltero and Hernandez-Barragan, 2018), the classification of microRNA targets (Bhadra et al., 2012), parity-P problems (~~Slowik and Bialko, 2008),~~ Slowik and Bialko, 2008) or the parameter tuning of machine learning models trained to e.g. predict landslides (Tien Bui et al., 2017). In soil-related research questions it was applied e.g. to optimize parameters of geostatistical models (Brus et al., 2016; Wadoux et al., 2018) or to optimize parameters defining the shape of well-known soil water retention curves (Maggi, 2017; Ou, 2015). However, in pedometrics, applications for parameter tuning in machine learning are scarce (e.g.~~, and last but not least the first successful application in pedometrics (~~ Gebauer et al., 2019).

~~Compared to the other algorithms mentioned above, it usually leads to better results and a comparatively low computing time (Price et al., 2005).~~

This study first of all aims to develop water retention PTFs for two tropical soil-landscapes dominated by (1) peat~~organic~~ soils and soils under volcanic influence with high organic matter contents, like they are commonly occurring in Páramo regions (Ecuador), and (2) tropical soils of a dry climate. Currently, PTFs suitable for the soils of these regions are at best very few, if any, at all. ~~As we assume~~ T~~t~~he parameter tuning technique is assumed ~~technique~~ to affect the performance of the machine learning based PTFs. This is why ~~,~~ our second and equally important aim is to ~~test the power of~~compare the differential evolution ~~optimization~~ algorithm ~~for tuning by comparing it~~ to ~~the~~ grid search. ~~approach usually applied in pedometrics.~~ On average, different machine learning algorithms perform equally well (Wolpert, 2001). We have chosen to fit boosted regression tree models, because ~~W~~we assume that the pre-eminence of optimization for parameter tuning in machine learning will particularly show when applying it to a machine learning algorithm that requires not only the fitting of discrete-valued parameters, but also the fitting of numerous real-valued parameters. ~~This is why we have chosen to fit boosted regression tree models. According to our knowledge, this is the first time both parameter tuning techniques are directly compared for a machine learning application in soil science.~~

2 Material and methods

2.1 Research areas

The two investigated soil-landscapes are situated in southern Ecuador (Fig. 1). The Quinuas ~~Catchment~~ catchment encompasses an area of about 93 km^2, including parts of the Cajas National Park (Fig. 1c). Being located between 3000 and 4400 m above sea level (a.s.l.), the mean annual temperature ranges between 5.3 and 8.7 °C with no seasonality (Carrillo-Rojas et al., 2016). With peaks in March/May and October (Celleri et al., 2007) mean annual precipitation varies between 900 and 1600 mm (Crespo et al., 2011). Due to volcanic ash deposits and the cold and wet climate, soils with a low bulk density and high SOC contents are typical (Buytaert et al., 2007). The Quinuas ~~Catchment~~ catchment can be allocated to the Páramo ecosystem (Guio Blanco et al., 2018), which plays a major role in the water supply of the inter-Andean region ~~(Buytaert et al., 2006a, 2006b, 2007).~~ (Buytaert et al., 2006a, 2006b, 2007).

The Laipuna dry forest region is part of the "Laipuna Conservation and Development Area" and covers approximately 16 km^2 (Fig. 1d). Its temperature profile shows little seasonal variability, while there is a rain period from January to May. Depending on the altitude ranging between 400 and 1500 m a.s.l., the mean annual temperature varies between 16 and 23 °C and mean annual precipitation between 540 ~~mm~~ and 630 mm (Peters and Richter, 2011b, 2011a). Additionally, the El Niño-Southern Oscillation influences the area (Bendix et al., 2003, 2011). Laipuna is part of an ecosystem with high biodiversity and many endemic species (Best and Kessler, 1995; Linares-Palomino et al., 2009), which are strongly adapted to the ecosystem and may be threatened by possible climate-induced changes of the water supply.

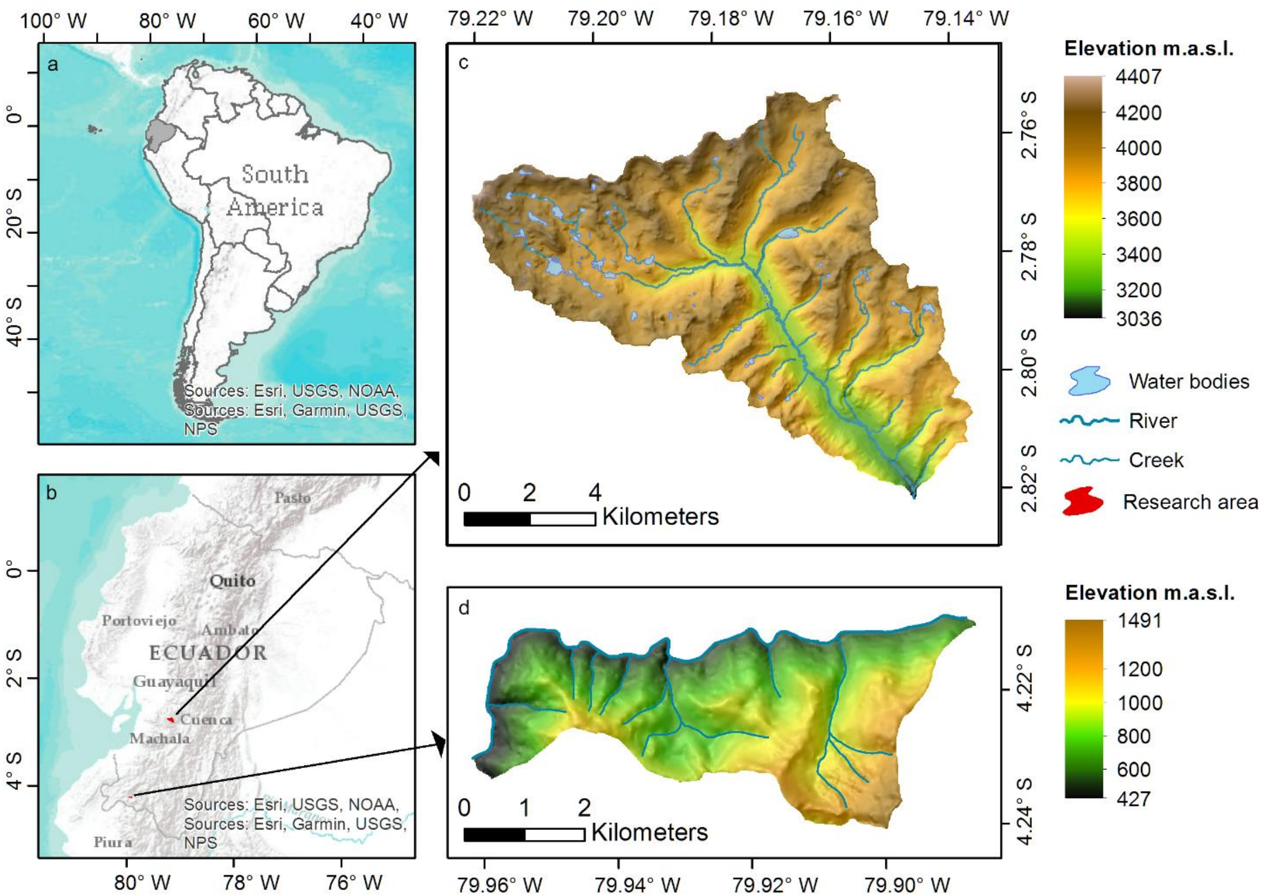


Fig. 1. Research areas. a) Ecuador within South America~~;~~, b) Research areas within Ecuador~~;~~, c) Quinuas~~.~~, d) Laipuna (overlaid hillshading with a light source from north). Adapted from Ließ (2015). Topographical data was used with permission from the Ecuadorian Geographical Institute (2013, national base, scale 1:50.000), further GIS data was provided by NCI and ETAPA.

2.2 Soil data

To ~~select~~ ensure representative datasets for ~~the two~~both -areas, ~~random stratified sampling was applied~~ sampling sites were selected using the algorithm “QC-arLUS” (Ließ, 2015). ~~It allows representing a research area`s complete landscape structure~~The algorithm divides a research area into strata, which represent characteristic landscape structures. Actual sampling site selection per stratum is limited to the accessible area. For Quinuas and Laipuna ~~in sampling site selection while actual site selection is limited to the accessible area. Two~~ two sampling sites were ~~sampled~~ chosen per landscape stratum, resulting in 46 sites for Quinuas and 55 for Laipuna. Soil profiles were excavated at these sites. However, due to laboratory constraints, samples for the determination of soil water retention were taken from the topsoil, only. Water retention at pF 0 (-10^{0} hPa), 0.5 ($-10^{0.5}$ hPa), 1.5 ($-10^{1.5}$ hPa) and 2.5 ($-10^{2.5}$ hPa) was measured in three replicate samples according to ~~(~~DIN EN ISO 11274:2014-07~~, 2014)~~: ~~applying~~ hanging water columns of increasing length were applied to undisturbed steel core samples of 100 cm³. The high amount of organic matter in the Quinuas soil samples prevented water retention measurements at higher pF values. BD and SOC content were used as predictors for both research areas to develop the water retention PTFs, PSD only for Laipuna. For BD measurements according to DIN EN ISO 11272:2017-07, undisturbed ~~the~~ samples (three replicates) were oven-dried at 105 °C for three days. Disturbed samples (three replicates), were tested for carbonates with 10% hydrochloric acid, sieved to 2 mm, and ground before SOC content determination using dry combustion (DIN EN 15936:2012-11~~, 2012~~). ~~For Laipuna, d~~Disturbed samples from Laipuna were oven-dried at 40 °C, sieved to 2 mm and PSD was determined according to DIN ISO 11277:2002-08 in two (sand fractions) and three (clay and silt fractions) replicate samples. Measurements distinguish the following particle size classes: clay (< 2 µm), fine silt (2 – 6.3 µm), medium silt (6.3 – 20 µm), coarse silt (20 – 62 µm), fine sand (62 – 200 µm), medium sand (200 – 630 µm) and coarse sand (630 – 2000 µm). The high soil organic matter contents prevented PSD measurements in Quinuas. ~~Sieved samples were ground and tested for carbonates prior to the SOC determination using dry combustion.~~ As suggested by ~~(~~Guio Blanco et al.~~,~~ (2018), models built on the Quinuas dataset could be improved by treating samples from mineral soils as outliers and removing them. For both research areas, it was decided to remove only data pairs of response and predictor variables that were identified as multivariate outliers. Tests for multivariate outliers ~~Multivariate outlier~~were done by building hierarchical clusters ~~removal was carried out~~ using the "hclust" function from R-package "fastcluster" (Müller, 2018), version 3.4.4. To enhance comparability, models were trained on response variables scaled to the range [0, 1] following Eq (1):

$$x_j[0,1] = \frac{x_j - \min(x)}{\max(x) - \min(x)}, \qquad (1)$$

where x is the vector of the response variables of length *j*.

2.3 Boosted regression trees

The BRT algorithm combines the machine learning techniques regression trees and boosting. Tree models use decision rules, which involve the predictor variables, to recursively partition the response variable data into increasingly similar subgroups until terminal nodes are reached (Kuhn and Johnson, 2013). For each subgroup, ~~T~~the response variable values of the terminal regression tree nodes are averaged to be used for the prediction (James et al., 2017). The boosting machine learning technique improves the overall model accuracy by combining a number of simple models (Witten and Frank, 2005). To develop the PTFs, BRT models were trained using the "gbm" R-package, version 2.1.3 (Ridgeway, 2017), which is based on Friedman's (2002) stochastic gradient boosting. This boosting technique iteratively fits a number of simple regression tree models to random training data subsets. In each iteration a new regression tree is added to the model until many simple regression trees form a linear combination: the final BRT model. Each tree that is added, improves the overall model performance. The first tree improves model performance the most. The further regression trees are fitted with emphasis on observations that are predicted poorly by the existing model. ~~to finally make them form a linear combination. Thereby, each new regression tree is fitted to explain most of the previous model's residuals.~~ To apply a BRT model, usually up to four parameters are tuned:

number of trees (n.trees), shrinkage, interaction depth, and bag fraction (e.g. Ottoy et al., 2017; Wang et al., 2017; Yang et al., 2016). Elith et al. (2008) provide a detailed analysis of their function: The n.trees parameter describes the number of regression tree models to be iteratively fitted. Shrinkage defines the model's learning rate by scaling the outcome of each simple regression tree, thereby controlling ~~their~~ its contribution to the final ~~prediction~~model. The interaction depth parameter controls the number of splits in each tree to divide the response variable data into subgroups. The bag fraction parameter determines the size of the randomly selected data subsets. This is able to reduce the risk of overfitting (Friedman, 2002), but may lower the model robustness (Elith et al., 2008). To develop PTFs for Quinuas and Laipuna, these four parameters were tuned following the steps described in Section 2.4 and 2.5.

2.4 Parameter tuning

Parameter tuning was done in two different ways: (1) by grid search and (2) by optimization applying the differential evolution algorithm. Grid search compares a certain number of predefined k dimensional parameter vectors. In order to reduce computing time, the number of predefined values of the $k = 4$ parameters ~~to be compared by grid search~~ was limited to five for each ~~for each of the k parameters~~. The selected values were based on the recommendations of Elith et al. (2008) and Ridgeway (2012). They are ~~summarised~~ summarized in Table 1. Finally, ~~k^5~~ 5^k different combinations of tuning parameter values, i.e. 625, ~~four-dimensional vectors~~ were compared.

In contrast to this, the ~~mathematical optimization algorithm "~~differential evolution optimization algorithm, developed ~~"~~ by Storn and Price (1995), is able to search the multivariate space between defined upper and lower parameter limits. The parameter values are optimized by minimizing an objective function, which defines their suitability. The objective function is allowed to be stochastic and noisy and does not need to be differentiable or continuous (Mullen et al., 2011). Following the evolutionary theory, this is done by repeating three steps for i iterations: mutation, crossover, and selection (Fig. 2). At first, an initial parent population of a number (v) of k-dimensional parameter vectors is generated randomly. With each iteration i, these vectors are changed by mutation and randomly mixed by crossover to generate a new population. Selection compares the objective function values belonging to the parent and the new vector to decide whether a new vector replaces its parent vector. Differential evolution was applied using the R-package "DEoptim", version 2.2.4 (Ardia et al., 2016). For each tuning parameter, optimization limits correspond to the maximum and minimum ~~smallest and largest~~ grid search values (Table 1). The number of vectors of size $k = 4$ tuning parameters was set to $v = 100$. The R-package's default mutation strategy was used, which changes each parent vector by adding two summands: (1) the difference between two random parent vectors and (2) the difference between the vector to be perturbed and the best vector found in the parent population. Summands were scaled by the factor 0.8. ~~During~~ For crossover, the probability of randomly mixing the parent and the mutated vectors' elements was set to 50%. To reduce computing time, the ~~optimisation~~ optimization process was stopped either after i_{max} = 10 iterations without improving the objective function or a maximum number of 200 iterations~~, respectively~~. ~~Prior to~~two- the selection step, the discrete tuning parameter values (n.trees, interaction depth) were rounded, as the differential evolution algorithm treats all values as real numbers during mutation and crossover. To select the final tuning parameter values, grid search and differential evolution both ~~minimised~~ minimized the cross validated $RMSE_T$ as objective function. $RMSE_T$ calculation is explained in Section 2.5.

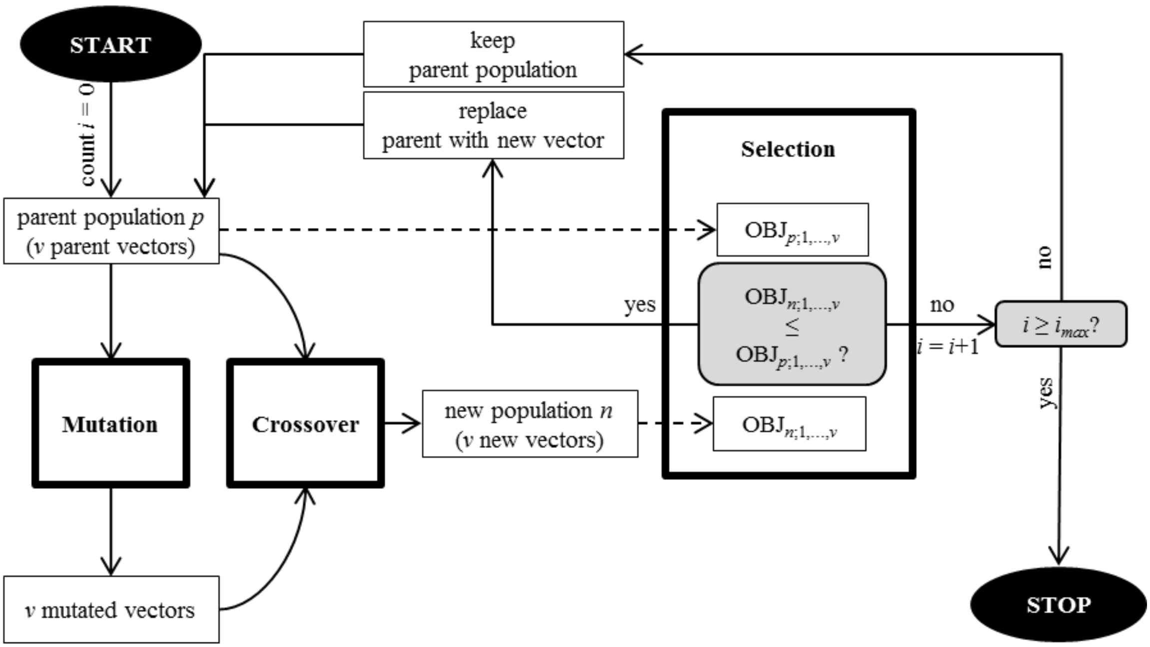


Fig. 2. Flowchart of the differential evolution algorithm. OBJ = objective function, p = parent population, n = new population, i = iteration, i_{max} = maximum number of iterations, v = number of vectors~~., BRT = boosted regression trees.~~ Adapted from Gebauer et al. (2019).

Table 1. Tuning parameter values to be tested by grid search and optimization limits required by the differential evolution algorithm.

Tuning parameter	Grid search values	L~~ower and upper~~D ~~d~~ifferential evolution limits	
n.trees	100; 1000; 2000; 3000; 4000	100	4000
shrinkage	0.001; 0.005; 0.01; 0.05; 0.1	0.001	0.1
interaction depth	1; 2; 3; 4; 5	1	5
bag fraction	0.5; 0.6; 0.7; 0.8; 0.9	0.5	0.9

2.5 Performance evaluation

In order to build robust models, we followed a nested cross-validation (CV) approach. Stratified five-fold ~~cross-validation~~ ~~(~~CV~~)~~ was applied for two purposes: (1) to conduct robust parameter tuning on resampled data subsets by either grid search or the differential evolution algorithm, and (2) to evaluate the final performance of models built on tuned parameter values. CV provides error metrics with good bias and variance properties, is beneficial for small datasets and avoids overfitting (Arlot and Celisse, 2009; James et al., 2017). Following the steps shown in Fig. 3, the stratified five-fold CV was implemented with five repetitions for model evaluation and one repetition for parameter tuning. In Step 1, the complete dataset (n = 100%) was split into five folds with each of them (n = 20%) once used as the test set, leaving the remaining folds as the model training set. For resampling in parameter tuning (Step 2), each model training set was again subdivided, similar to Step 1. Each tuning parameter vector in grid search and the differential evolution algorithm was evaluated by the cross-validated $RMSE_T$ (Step 3, Step 4). By comparing the $RMSE_T$, the best vector of tuning parameter values for each model evaluation training set was selected and applied (Step 5, Step 6). To assess model performance, the coefficient of determination (R^2_E) and the root mean squared error ($RMSE_E$) of model evaluation were calculated by predicting the associated test set data (Step 7). To divide the datasets into folds, the function "partition_cv_strat" from R-package "sperrorest", version 2.0.0 (Brenning et al., 2017) was applied, with three equal probability strata of the response variable's density function.

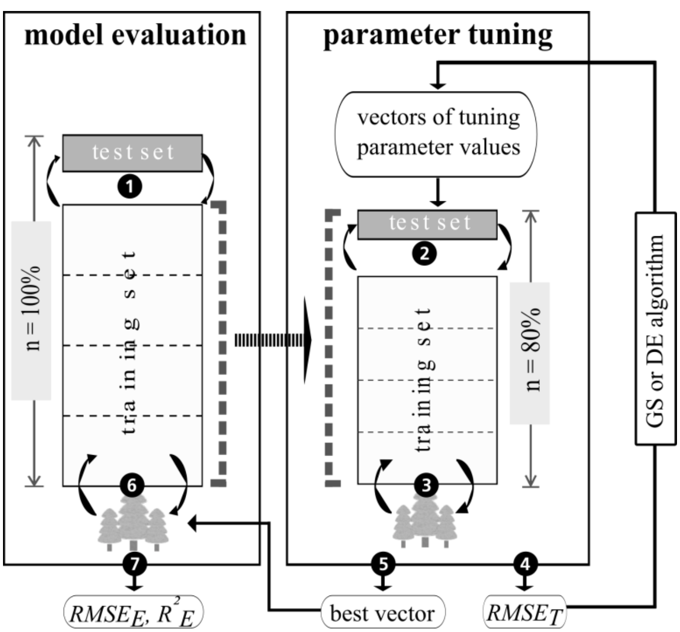


Fig. 3. Nested cross-validation approach comprising model evaluation and parameter tuning. Adapted from Guio Blanco et al. (2018). The tree icons symbolize BRT models, which are repeatedly (circular arrows) trained and tested on different data sets. The numbers within black circles belong to the ~~modeling~~ steps~~,~~ ~~description~~described in Section 2.5. $RMSE_T$ = root mean squared error of parameter tuning, $RMSE_E$ = root mean squared error of model evaluation, R^2_E = coefficient of determination of model evaluation, GS = grid search, DE = differential evolution.

2.6 Comparison to existing PTFs

To further assess the developed BRT PTFs, it was decided to compare their results to predictions resulting from the application of existing PTFs. PTFs that were developed on different datasets, but under conditions as similar as possible to those of Quinuas and Laipuna, were selected from the literature. If more than one PTF was provided per study, the one with the best reported performance was applied. For Laipuna, seven PTFs (Table 2) were chosen based on four criteria: (1) developed for tropical soils, (2) similar predictor variables, (3) regression equation provided and (4) included in the peer-reviewed Clarivate Analytics' Web of Science database. To be able to apply the readily available equations with predictors of the Laipuna dataset, it was necessary to convert the determined soil texture classes to the respective USDA classes. Following the approach of Shang (2013), texture conversion was done using spline interpolation. Because of different predictor variables, it is difficult to find organic PTFs applicable to the Quinuas dataset. An exhaustive literature search revealed only the PTF of Boelter (1969), who related water retention at pF 0 to BD for temperate peat soils in northern Minnesota.

~~Because of differences in the predictors, it is difficult to find organic PTFs applicable to the Quinuas dataset. An exhaustive literature search revealed only the PTF of Boelter (1969), who related water retention at pF 0 to BD for temperate peat soils in northern Minnesota.~~

3 Results and discussion

3.1 Model input

For Laipuna, data pairs of four sampling sites were identified as multivariate outliers. After removing ~~multivariate~~them ~~outliers~~, the datasets contained predictor and response variables of 51 and 46 ~~values~~ sampling sites for Laipuna and Quinuas, respectively. A summary of the remaining unscaled data is shown in Fig. 4 and 5. As expected both areas show huge differences regarding the values of response and predictor variables. ~~-~~BD values in Quinuas range from 64 to 807 kg m^{-3}, while SOC values vary between 8.8 and 46.4 wt.~~-~~%. SOC values are normally distributed, while BD data display a positive ~~is~~ skew~~ed~~ ~~right~~. Averagely decreasing by 22%, water retention ranges from 0.25 ~~cm^3 cm^{-3}~~ (pF 2.5) to 0.94 cm^3 cm^{-3} (pF 0). While the data ~~is skewed to the right~~displays a positive skew for pF 0, the data distribution for the other pF values ~~is~~ shows a negative skew~~left-skewed~~. For Laipuna, BD ranges between 1157 and 1727 kg m^{-3}, displaying a ~~right-skewed~~ distribution with a positive skew. The SOC content is normally distributed and varies between 0.4 and 3.8 wt. %. Clay content ranges between 17 and 48 %, silt between 24 and 45 % and sand between 14 and 50 %. Especially fine and medium silt show ~~a~~ skewed distributions. Water retention values are ranging between 0.25 ~~cm^3 cm^{-3}~~ (pF 2.5) and 0.61 cm^3 cm^{-3} (pF 0). On average, they decrease by 37 ~~± 0.09~~ % with increasing water tension. Data is skewed ~~right~~ positively for pF 0 and ~~skewed~~ negatively~~left~~ for pF 0.5.

Quinuas soils go along with the low density, porous soils, rich in organic material, that are found throughout the Paute river basin (Buytaert et al., 2007; Poulenard et al., 2003). Loosely bedded volcanic ash deposits ~~further~~ explain the low bulk density values (Buytaert et al., 2007). High SOC contents are caused by low redox potentials and the presence of organometallic complexes inhibiting degradation processes (Buytaert et al., 2006a). Comparatively high water retention values can be attributed to the porous structure of Páramo soils being able to retain a lot of water (Buytaert et al., 2007). ~~The relatively small decrease in water retention with increasing water tension is assumed to be caused by the high~~ High ~~amounts~~ contents of soil organic matter are ~~matter~~ associated with soils~~being~~ characterized by a high water holding capacity (Buytaert et al., 2007), which explains ~~(Buytaert et al., 2007).~~ the relatively small decrease in water retention with increasing water tension. Measured BD and SOC contents are in accordance with data observed for other Páramo regions (e.g. Buytaert et al., 2007, 2006b). ~~t~~The water retention values are ~~also~~ comparable to data obtained in other Páramo areas (Buytaert et al., 2005) and soils with high organic matter contents (Schwärzel et al., 2002, 2006). Extreme values in BD and water retention (Fig. 4 and Fig. 5) correspond to less frequent mineral soils with much lower SOC contents ~~soil samples with a higher proportion of mineral components or andic properties~~ (Guio Blanco et al., 2018). Expecting these values to be reliable, they were not removed from the model input. The BD and SOC ~~data~~ values measured ~~for the~~in Laipuna ~~soil samples~~ correspond to other dry forest ecosystems (e.g. Conti et al., 2014; de Araújo Filho et al., 2017; Singh et al., 2015), whereas the PSD shows higher clay contents compared to the dry forest soils investigated by Cotler and Ortega-Larrocea (2006), Jha et al. (1996) and Sagar et al. (2003). Measured water retention values are higher than those obtained in a tropical dry forest in Brazil (Vasques et al., 2016), probably caused by the higher clay content enhancing the water holding capacity.

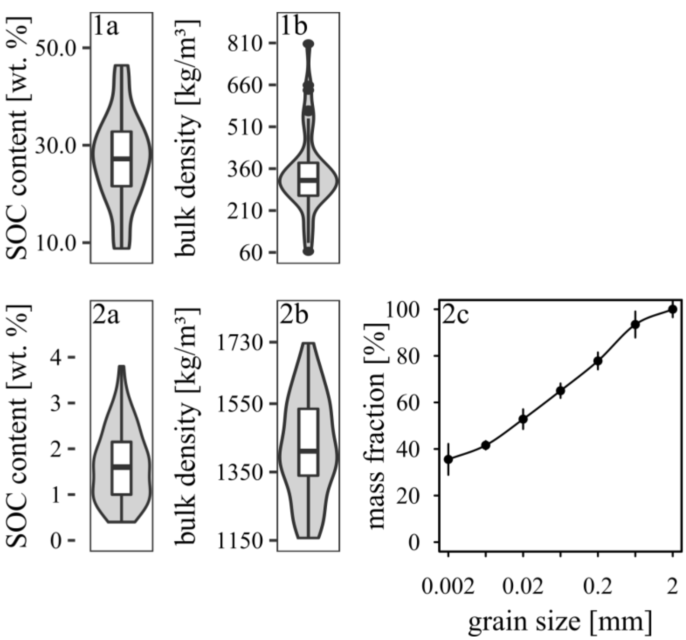


Fig. 4. Predictor variables. 4.1 Quinuas (46 samples), 4.2 Laipuna (51 samples), a) SOC content, b) bulk density, c) particle size distribution displayed as a cumulative distribution function (mean values with standard deviation). High organic matter contents prevented measurements of the particle size distribution in Quinuas.

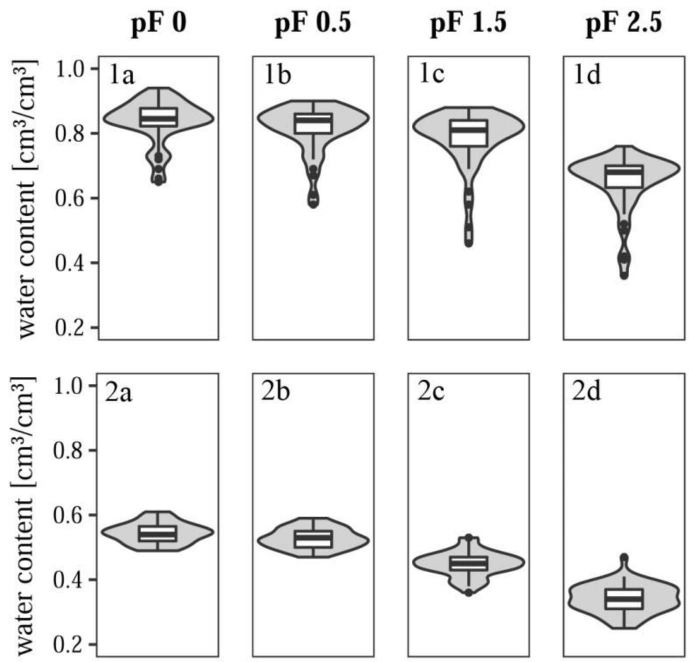


Fig. 5. Response variables. 5.1 Quinuas (46 samples), 5.2 Laipuna (51 samples), water retention at a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5.

3.2 Model performance

The performance of the final models built on parameters selected by grid search and the differential evolution algorithm is demonstrated by the error metrics R^2_E and $RMSE_E$ in Fig. 6 (Quinuas) and 7 (Laipuna) as well as by scatterplots comparing observed and predicted water retention values in Fig. 8 (Quinuas) and 9 (Laipuna). Error metrics as well as scatterplots are based on response variables scaled to the range [0, 1]. ~~Models optimized by the differential evolution algorithm show a better predictive performance than models tuned by grid search. Based on scaled water retention values, a~~All grid search models resulted in very similar mean $RMSE_E$ values between 0.20 (pF 1.5) and 0.22 (pF 0~~mean 0.20 ± 0.01~~) for Quinuas, and between 0.19 (pF 2.5) and 0.25 (pF 0, pF 0.5) ~~while~~ for Laipuna. ~~mean $RMSE_E$ range between 0.19 ± 0.00 (pF 2.5) and 0.25 ± 0.00 (pF 0 and pF 0.5). Looking at both error metrics, the performance of the differential evolution based Quinuas models worsens with increasing pF values, whereas for Laipuna model performance improves: final models with parameter tuning by d~~Differential evolution models trained on the Quinuas datasets correspond to mean $RMSE_E$ values ranging from ~~-~~0.11 ~~11 ± 0.01~~ (pF 0) to 0.~~17~~ 17 ~~± 0.01~~ (pF 2.5). The Laipuna differential evolution models resulted in the same mean $RMSE_E$ values ranging from 0.15 (pF 2.5) to 0.28 (pF 0) ~~for Quinuas and from 0.15 ± 0.01 (pF 2.5) to 0.26 ± 0.01 (pF 0) for Laipuna.~~ Mean R^2_E values resulting from grid search, are varying between 0.~~04~~ 03 ~~± 0.03~~ (pF 0) and 0.09 ~~± 0.07~~ (pF 1.5) for Quinuas and between 0.03 ~~± 0.04~~ (pF 0.5, pF 2.5) and 0.05 ~~± 0.05~~ (pF 1.5) for Laipuna. The differential evolution algorithm resulted in mean R^2_E values ~~ranging~~ increasing from 0.58 ~~± 0.09~~ (pF 2.5) to 0.79 ~~± 0.04~~ (pF 0) for Quinuas and from 0.~~27~~ 35 ~~± 0.08~~ (pF 0.5) to 0.~~61~~ 68 ~~± 0.04~~ (pF ~~2.5~~0) for Laipuna. As demonstrated by the scatterplots, the grid search models roughly reproduce the mean water retention values, while the models with parameter tuning by differential evolution are able to explain more of the observations' variance. The five grid search predictions for each observation (Fig. 8.1 and 9.1), cover a smaller range than the differential evolution predictions (Fig. 8.2 and 9.2). Especially the differential evolution results of the Laipuna pF 0 and pF 0.5 models are characterized by comparatively high variance. Caused by the better adjustment to the modeling problem, the differential evolution models show a higher predictive performance than the models tuned by grid search: ~~In comparison to grid search, models tuned by differential evolution show a higher predictive performance for all Quinuas models and the Laipuna models for pF 1.5 and pF 2.5:~~ mean R^2_E values are up to ~~22~~ 25 (Quinuas, pF 0) and ~~18~~ 19 (Laipuna, pF 2.5) times higher, while scaled $RMSE_E$ values are up to ~~1~~2.~~9~~1 (Quinuas, pF 0) and 1.3 (Laipuna, pF 2.5) times lower than those obtained by grid search. This corresponds to the scatterplots (Fig. ~~11~~ 8 and ~~12~~9): the largest difference between grid search and differential evolution can be recognized for the pF 0 (Quinuas) and pF 2.5 (Laipuna) models. ~~Additionally, as demonstrated by the scatterplots, the grid search models roughly predict the water retention values' mean, while the models with parameter tuning by differential evolution are able to explain more of the observations' variance. However, the five grid search predictions for each observation (Fig. 9 a-d and 10 a-d), cover a smaller range than the differential evolution predictions. Especially the differential evolution results of the Laipuna pF 0 and pF 0.5 models are characterized by comparatively high variance.~~

~~Probably caused by the better adjustment to the modeling problem, differential evolution models are able to explain more of the water retention's variance than the models tuned by grid search.~~ The higher variability of the differential evolution predictions corresponds to the differential evolution tuning parameter values covering a wider range than those achieved by applying grid search (Section 3.~~2~~3). ~~For Laipuna, the improvement of the differential evolution models with increasing pF values is assumed to be caused by the used predictors. With increasing pF values the influence of PSD on water retention increases. At the same time the influence of BD decreases, which improves model performance as BD measurements were not corrected for stone content and are, therefore, not as good a predictor as they could be.~~ For Quinuas, the decreasing predictive performance with increasing pF values can probably be attributed to the lack of further predictors. While the predictors BD and SOC content are able to explain most of the water retention values at pF 0 to pF 1.5, the lack of predictors related to the soil matrix, e.g. ~~-~~PSD information, prevents further improvement for pF 2.5. In pedometrics, studies with a direct comparison of grid search and mathematical optimization applied for parameter tuning in machine learning are scarce. In fact we are only aware of one application: Wu et al. (2016) compared both tuning strategies to train support vector machine (SVM) models for the prediction of soil contamination in the Jiangxi Province (China). Their results are contradictory: Overall, using optimization to tune three SVM parameters led to the best model performance. Unfortunately, the comparison with grid search was only applied to a reduced two-parameter tuning problem. Surprisingly, here, grid search outperformed the tested optimization algorithms. Unfortunately, the tuning of a different number of SVM parameters is hampering the direct comparison. Still, the results of Wu et al. (2016) show that a lucky selection of predefined parameter vectors can result in grid search outperforming optimization algorithms – in particular, if the number of optimization iterations is small. Overall, the more values are tested during parameter tuning (grid search or optimization), the higher the probability of finding the global optimum. Wu et al. (2016) did not mention the number of iterations of the optimization algorithms, but we assume that increasing the number of iterations would have led to results that are at least as good as those achieved by grid search. Even though the benefits of optimization algorithms towards grid search are obvious, further direct comparisons of mathematical optimization algorithms and grid search applied for machine learning parameter tuning in soil related research questions are necessary.

~~measurements were not conducted due to the prevalence of soils with organic properties in this area.~~ Overall, the predictive power of all differential evolution based Quinuas models and the Laipuna pF 0 and 2.5 models are comparable to other studies. Botula et al. (2013) for example obtained R^2 values ranging from 0.32 to 0.68 (pF 0) and from 0.60 to 0.68 (pF 1.5) by using the k-nearest neighbor algorithm for soil data originating from the Lower Congo. Keshavarzi et al. (2010) used an artificial neural network to predict water retention at different pF values for soils from the Qazvin province in Iran. Haghverdi et al. (2012) used the same machine learning technique on soils from northeastern and northern Iran. While Keshavarzi et al. (2010) gained R^2 values of 0.77 (pF 2.5) and 0.72 (pF 4.2), Haghverdi et al. (2012) reached R^2 values ranging from 0.81 to 0.95. In general, we expect ~~BRT~~ model performance to improve ~~further~~ by removing extreme values in the model input or by using larger datasets. Even though they were not identified as multivariate outliers, the ~~Especially for Quinuas,~~ low water retention values are underrepresented in the Quinuas dataset. According to Guio Blanco et al. (2018), these values are primarily observed in the lower part of the river valley and include measurements from mineral soils. Furthermore, it needs to be tested if different model algorithms are able to improve PTFs for both research areas.

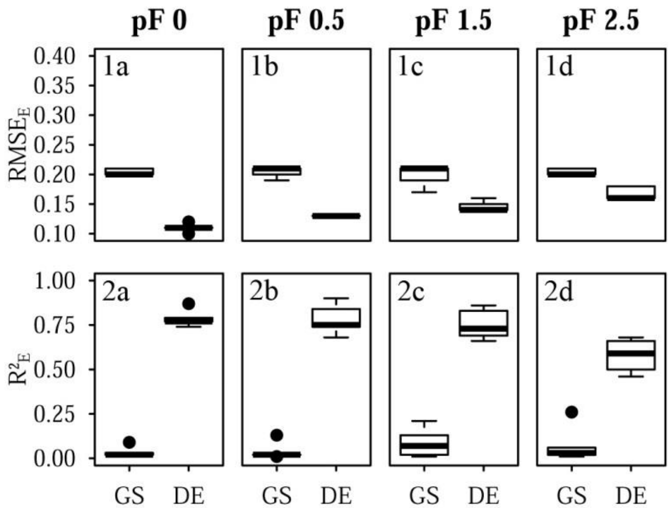
~~Applying existing PTFs on the Laipuna dataset confirmed the good performance of the differential evolution BRT models.~~ l~~PTFs were selected based on four criteria: (1) developed for tropical soils, (2) similar predictor variables, (3) regression equation provided and (4) included in the peer-reviewed Clarivate Analytics' Web of Science database. Following the approach of Shang (2013), soil texture was previously converted to the USDA classification system by spline interpolation. Mean~~ ~~$RMSE_E$ values of the differential evolution tuned BRT models were between 1.5 times (pF 2.5, Minasny and Hartemink (2011) and Tomasella et al. (2000)) and 8.8 times (pF 1.5, Barros et al. (2013) better (Table 2). Because of differences in the predictors, it is difficult to find organic PTFs applicable to the Quinuas dataset. An exhaustive literature search revealed only the PTF of Boelter (1969), who related water retention at pF 0 to BD for temperate peat soils in northern Minnesota. Water retention values predicted by the existing PTF differed a lot from measured values. For BD higher than 370 kg~~ ~~m^{-3}~~ ~~predictions became even negative. While applying differential evolution BRT models resulted in a mean~~ ~~$RMSE_E$~~ ~~of 0.032 (unscaled), applying the Minnesota PTF resulted only in an RMSE of 1.860. The high RMSE value is assumed to be caused by large differences between the Minnesota and Quinuas soils and underlines the necessity of developing water retention PTFs specifically for tropical organic soils.~~

~~In general, we expect BRT model performance to improve further by removing extreme values in the model input or by using larger datasets. Especially for Quinuas, low water retention values are underrepresented in the dataset. According to Guio Blanco et al. (2018), these values are primarily observed in the lower part of the river valley and include measurements from mineral soils.~~

~~Table 2. Unscaled root mean squared errors for the tested PTFs.~~ ~~**The best results for each matric potential are underlined. BRT PTF results are averaged.**~~

~~PTF [data origin]~~	~~Theta 0~~	~~Theta 0.5~~	~~Theta 1.5~~	~~Theta 2.5~~
~~BRT PTF [Laipuna]~~	~~0.031~~	~~0.029~~	~~0.032~~	~~0.030~~
~~Barros et al. (2013) [Brazil] *~~	~~0.176~~	~~0.118~~	~~0.280~~	~~0.071~~
~~Gaiser et al. (2000) [Brazil and Niger]~~	~~-~~	~~-~~	~~-~~	~~0.062~~
~~Minasny and Hartemink (2011) [various tropical regions]~~	~~-~~	~~-~~	~~-~~	~~0.044~~
~~Nguyen et al. (2014) [Vietnam]~~	~~-~~	~~-~~	~~0.047~~	~~0.070~~
~~Obalum and Obi (2012) [Nigeria]~~	~~-~~	~~-~~	~~-~~	~~0.150~~
~~Pollacco (2008) [USA]~~	~~-~~	~~-~~	~~-~~	~~0.068~~
~~[Brazil] *~~	~~0.080~~	~~0.071~~	~~0.053~~	~~0.044~~

~~* applied to predict parameters of the Van Genuchten equation first.~~



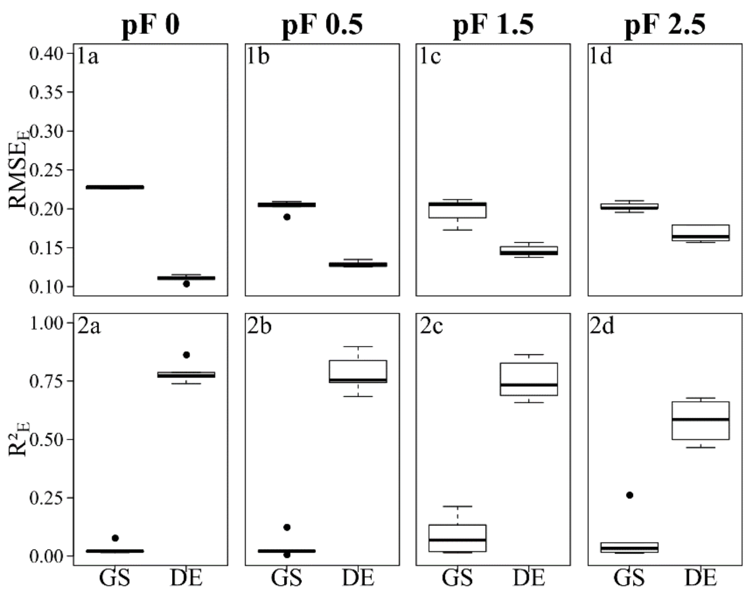
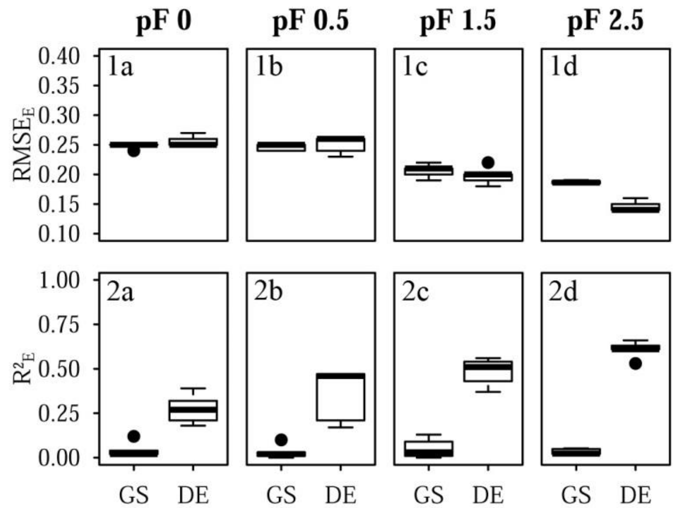


Fig. 6. Error metrics of the Quinuas BRT models. 6.1 RMSE$_E$, 6.2 R^2_E, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on five values resulting from five CV repetitions. GS = grid search, DE = differential evolution algorithm. Error metrics were calculated based on response variables scaled to the range [0, 1]



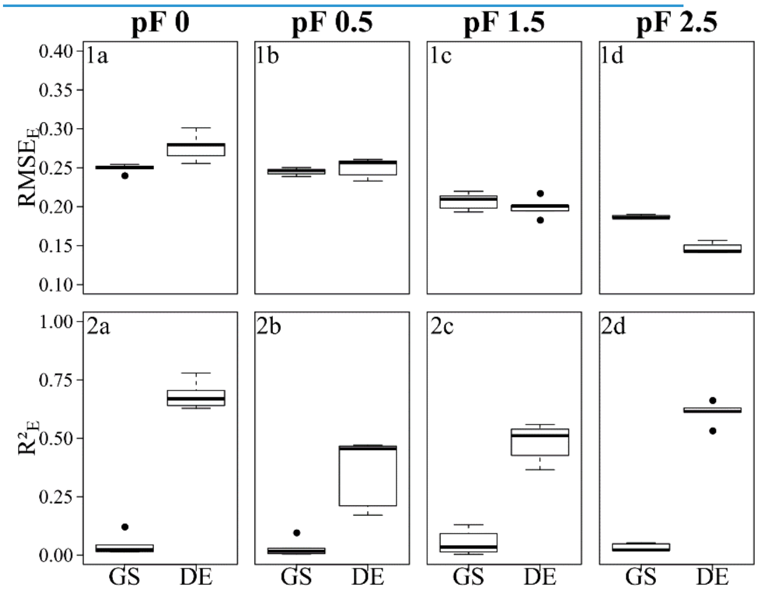


Fig. 7. Error metrics of the Laipuna BRT models. 7.1 RMSE$_E$, 7.2 R^2_E, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on five values resulting from five CV repetitions. GS = grid search, DE = differential evolution algorithm. Error metrics were calculated based on response variables scaled to the range [0, 1].

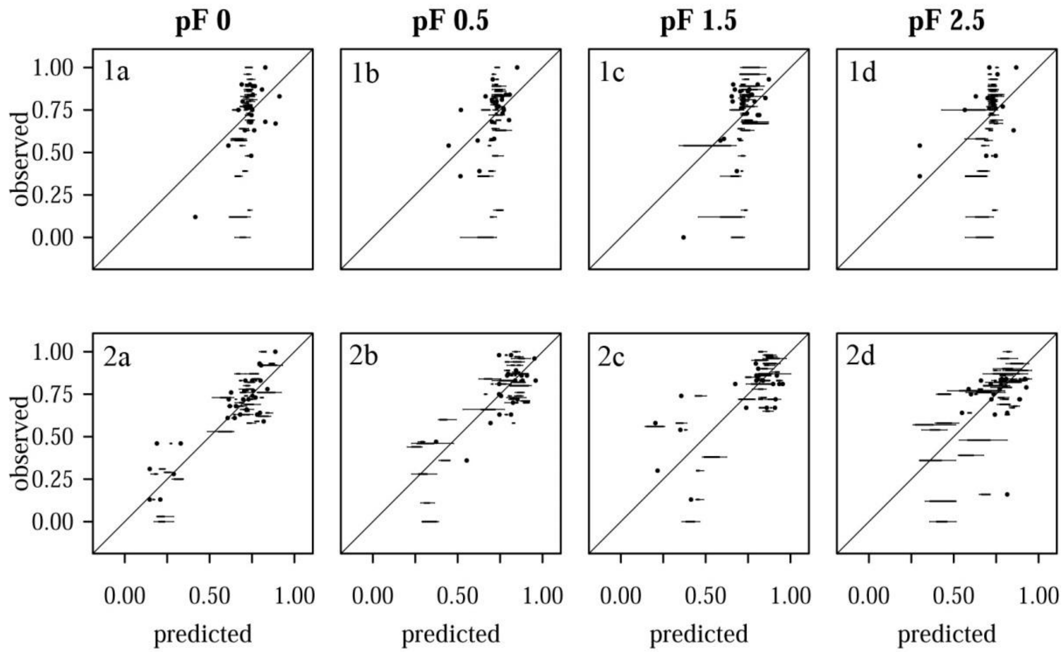


Fig. 8. Comparison of predicted and observed water retention values for Quinuas. 8.1 Models with tuning by grid search, 8.2 Models with parameter tuning by differential evolution, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on five values resulting from five CV repetitions. Predicted and observed values were scaled to the range [0, 1].

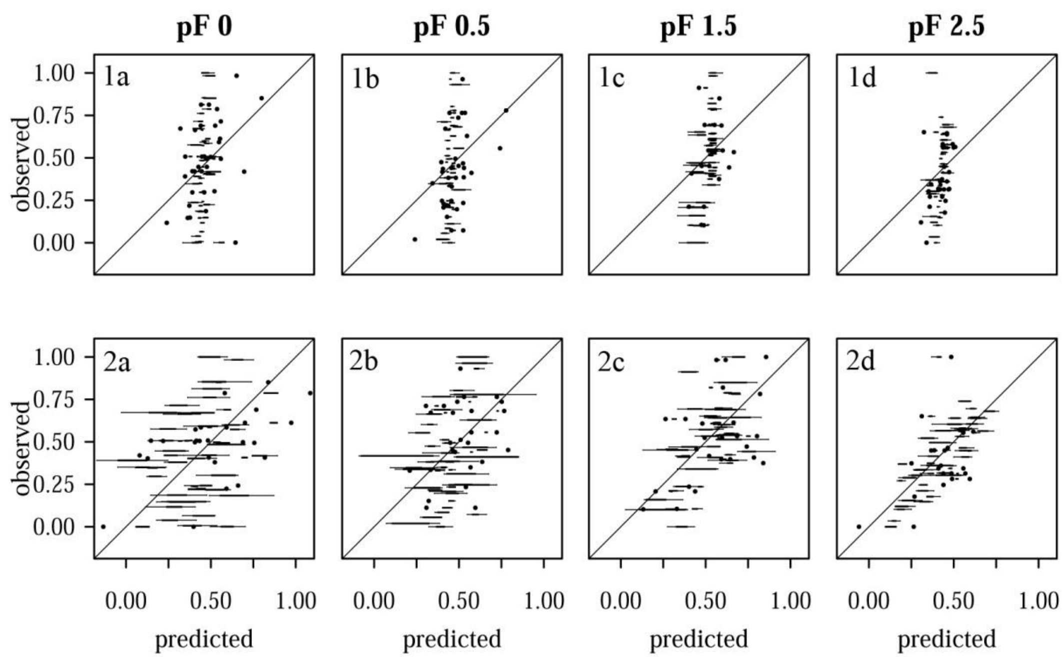


Fig. 9. Comparison of predicted and observed water retention values for Laipuna. 9.1 Models with tuning by grid search, 9.2 Models with parameter tuning by differential evolution, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on five values resulting from five CV repetitions. Predicted and observed values were scaled to the range [0, 1].

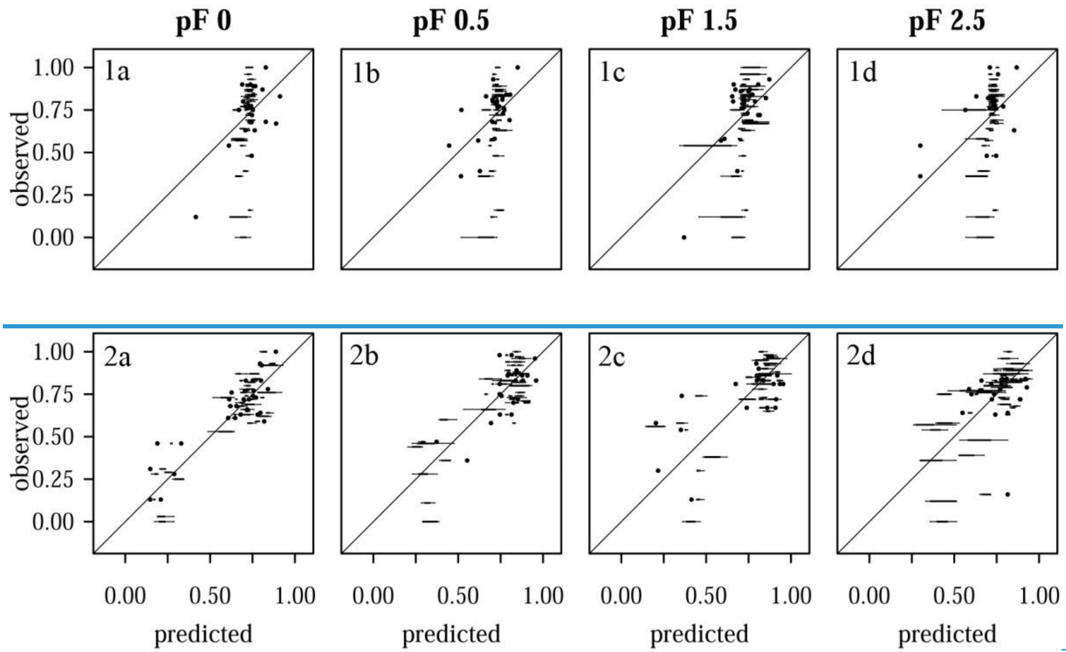
3.3 Comparison to existing PTFs

Applying the existing PTFs with predictor variables sampled in Quinuas and Laipuna confirmed the good performance of the differential evolution BRT models. RMSE values of the respective PTFs are shown in Table 2. They were calculated by comparing the unscaled measured water retention of each soil profile to the water retention values calculated by applying the readily available PTFs. For Laipuna, mean $RMSE_E$ values of the differential evolution tuned BRT models were between 1.3 times (pF 2.5, Minasny and Hartemink (2011) and Tomasella et al. (2000)) and 9.3 times (pF 1.5, Barros et al. (2013)) better (Table 2). For Quinuas, the application of the differential evolution BRT models resulted in a mean $RMSE_E$ of 0.03, while applying the PTF of Boelter (1969) resulted only in an RMSE of 1.86. For BD higher than 370 kg m^{-3} predictions became even negative. The high RMSE value is assumed to be caused by large differences between the temperate organic soils in Minnesota and the soils in Quinuas. This underlines the necessity of developing water retention PTFs specifically for tropical organic soils.

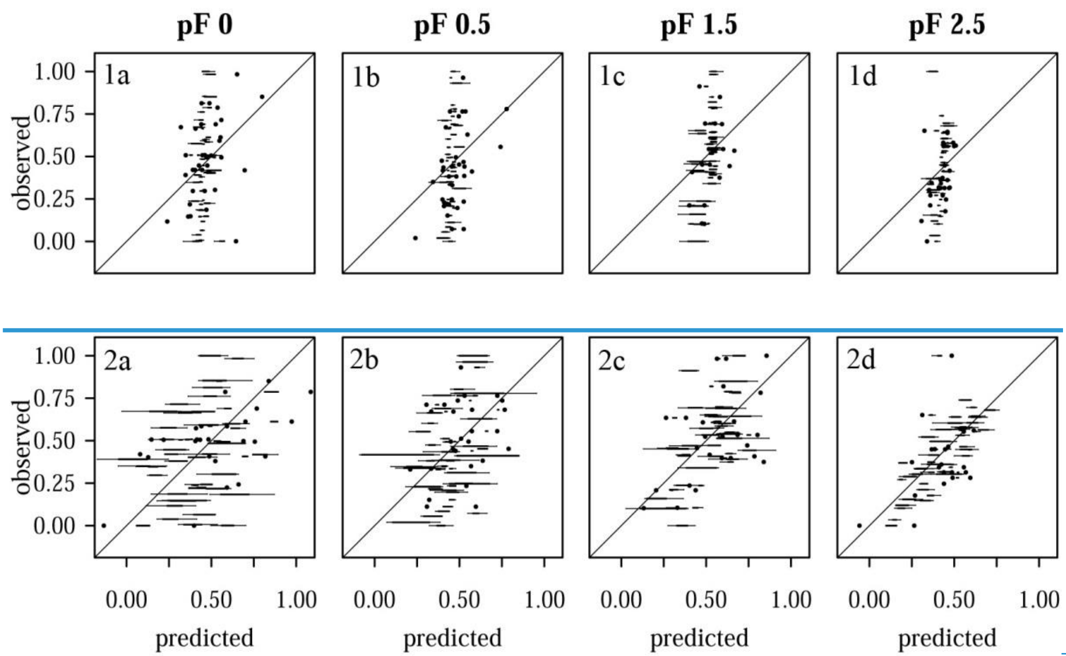
Table 2. Unscaled root mean squared errors for the tested PTFs. The best results for each matric potential are underlined. BRT PTF results are averaged.

PTF [data origin, size of the dataset]	pF 0	pF 0.5	pF 1.5	pF 2.5
BRT PTF [Laipuna, 51]	0.03	0.03	0.03	0.03
Barros et al. (2013) [Brazil, 668] *	0.18	0.12	0.28	0.07
Gaiser et al. (2000) [Brazil and Niger, 627]	-	-	-	0.06
Minasny and Hartemink (2011) [various tropical regions, 652]	-	-	-	0.04
Nguyen et al. (2014) [Vietnam, 160]	-	-	0.05	0.07
Obalum and Obi (2012) [Nigeria, 54]	-	-	-	0.15
Pollacco (2008) [USA, 18552]	-	-	-	0.07
Tomasella et al. (2000) [Brazil, 630] *	0.08	0.07	0.05	0.04

* applied to predict parameters of the Van Genuchten equation first.



~~**Fig. 8. Comparison of predicted and observed water retention values for Quinuas.** 8.1 Models with tuning by grid search, 8.2 Models with parameter tuning by differential evolution, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on five values resulting from five CV repetitions.~~

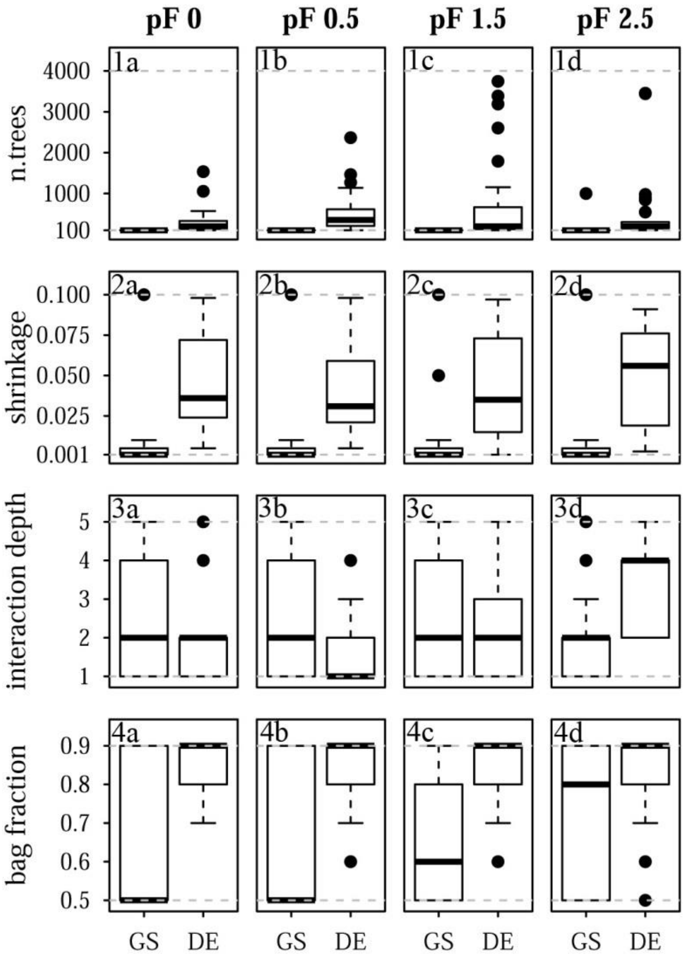


~~**Fig. 9. Comparison of predicted and observed water retention values for Laipuna.** 9.1 Models with tuning by grid search, 9.2 Models with parameter tuning by differential evolution, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on five values resulting from five CV repetitions.~~

3.~~3~~ 4 Model parameters

~~T~~he final tuning parameter values obtained by grid search and the differential evolution algorithm are ~~summarised~~ summarized in Fig. 10 (Quinuas) and 11 (Laipuna). ~~The displayed boxplots show the selected 25 tuning parameter values corresponding to the models built by five-fold CV with five repetitions. Grid search compared~~ 625 previously defined parameter vectors were compared by grid search. ~~, while~~On average ~~the differential evolution algorithm~~ 31 (pF 0, 0.5), 33 (pF 1.5) and 28 (pF 2.5) iterations of the differential evolution algorithm were necessary to find the optimal tuning parameter values for the Quinuas models. For Laipuna 32 (pF 0), 28 (pF 0.5), 25 (pF 1.5) and 22 (pF 2.5) iterations were needed. ~~tested at least 1000 parameter vectors in the defined ranges of the four-dimensional parameter space.~~ Differences between the ~~two~~ parameter tuning techniques are most distinct for n.trees and shrinkage ~~for both research areas~~. Neglecting outliers, values obtained by the differential evolution algorithm cover a wider range than those resulting from grid search: while n.trees was in most cases set to the lowest tested value (100) by grid search, the differential evolution algorithm resulted in mean n.trees values (± standard deviation) ranging from 310 ± 321 (pF 0) to 810 ± 1132 (pF 1.5) for Quinuas and from 727 ± 851 (pF 0) to 1688 ± 1345 (pF 2.5) for Laipuna. Thereby, the mean n.trees values obtained by differential evolution parameter tuning are more than five (Quinuas) and more than ten times (Laipuna) higher than the mean grid search values. Neglecting extreme values, the shrinkage values resulting from the differential evolution algorithm also cover a wider range than the values obtained by the grid search tuning technique. For both areas, the shrinkage values were usually set to 0.001 or 0.01 by grid search, while applying the differential evolution algorithm resulted in mean shrinkage values ranging from 0.040 ± 0.028 (pF 0.5) to 0.047 ± 0.030 (pF 2.5) for Quinuas and from 0.034 ± 0.03 (pF 0) to 0.062 ± 0.027 (pF 2.5) for Laipuna. On average, the differential evolution shrinkage values are approximately 14 (Quinuas) and 17 (Laipuna) times higher than those obtained by grid search. The observed pattern is more complex for the other two tuning parameters: interaction depth and bag fraction. Although the selected parameter ranges differ for most pF values, the median interaction depth values are the same for half of the cases for grid search and tuning by the differential evolution algorithm. The median of the selected bag fraction is at the upper limit for the Quinuas models that were tuned by the differential evolution algorithm, while grid search resulted in median bag fraction values at the lower limit in two cases. Laipuna bag fraction values do not show this pronounced difference between grid search and tuning by the differential evolution algorithm.

The selected tuning parameter values correspond to the differential evolution based models having more predictive power than those adapted by the common grid search approach. Usually higher n.trees values, as received from the differential evolution algorithm, are known to improve model performance (Elith et al., 2008). However, according to the results of Elith et al. (2008), by using more trees the shrinkage parameter gets smaller. The comparatively high differential evolution shrinkage values ~~might~~ are ~~be~~ an indication of the n.trees values still being too small. For both areas, the differential evolution values for n.trees and shrinkage, covering a wider range than the grid search results, ~~might~~ are assumed to be caused ~~be explained~~ by an incomplete ~~by the differential evolution~~ optimization caused by not using enough iterations or the algorithm ~~not being completed or~~ being stuck in a local optimum. This corresponds to the high prediction variability of the final differential evolution models derived for Laipuna (~~Section 3.2~~Fig. 9). It should be noted that model performance depends on the combination of parameter values. However, ~~A~~as n.trees and shrinkage control how precisely the model learns the input data~~'s~~ structure, these parameters are assumed to be more important than interaction depth and bag fraction. In this case, there ~~might~~ would not even be an optimum for the latter two parameters. Especially for Laipuna, this ~~might~~ explains the interaction depth and bag fraction values of both tuning techniques covering the whole range of possible values. ~~For Laipuna t~~The bag fraction differences between differential evolution and grid search tuning remain unexplained. For both parameter tuning techniques, increasing the number of parameter values to be tested enhances the probability of finding the global optimum~~. The results of both tuning techniques might be improved by testing more parameter values~~. For grid search, this can be realized by increasing the number of values to be compared for each tuning parameter. Increasing the number of iterations and starting with larger and thereby more heterogeneous initial populations is expected to do the same for differential evolution. This ~~might~~ is assumed to~~also~~ result in less variable differential evolution results. However, for tuning real-valued parameters, it is impossible to know the necessary number of iterations in advance. Accordingly, a trade-off between computing time and the probability of finding the global optimum has to be made for any parameter tuning technique. Besides increasing the number of iterations and the number of initial vectors, the risk of the differential evolution algorithm getting stuck in a local optimum can also be reduced by changing the parameters "crossover probability" and the "mutation scaling factor" as well as applying another mutation strategy (Das and Suganthan, 2011). To overcome the problem of choosing the right control parameters as well as the mutation strategy, self-adaptive differential evolution algorithms (e.g. Nahvi et al., 2016; Pierezan et al., 2017; Qin et al., 2009), which are able to automatically adjust their settings during the ~~optimisation~~ optimization process, could be applied in future studies. Furthermore, a larger model input of high quality would result in more explicit relationships between response and predictor variables that can be detected and reproduced more easily by the BRT models. This is assumed to reduce the probability of the differential evolution algorithm getting stuck into a local optimum as well as the number of required iterations. ~~-~~In general, the superiority of differential evolution needs to be verified by applying it to further machine learning algorithms and applications, and by comparing it to further parameter tuning techniques.



465 **Fig. 10. Selected tuning parameter values for Quinuas.** 10.1 n.trees, 10.2 shrinkage, 10.3 interaction depth, 10.4 bag fraction, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on 25 values corresponding to the five-fold CV with five repetitions. Dashed grey lines are indicating the chosen optimization limits. GS = grid search, DE = differential evolution algorithm.

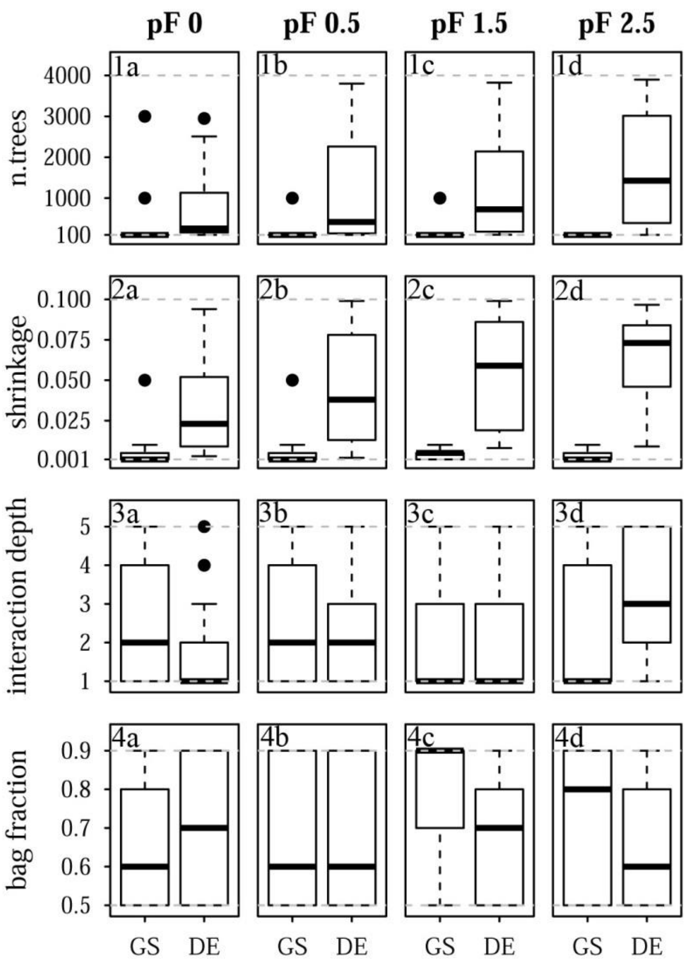


Fig. 11. Selected tuning parameter values for Laipuna. 11.1 n.trees, 11.2 shrinkage, 11.3 interaction depth, 11.4 bag fraction, a) pF 0, b) pF 0.5, c) pF 1.5, d) pF 2.5. Each boxplot is based on 25 values corresponding to the five-fold CV with five repetitions. Dashed grey lines are indicating the chosen optimization limits. GS = grid search, DE = differential evolution algorithm.

4 Conclusions

~~W~~e successfully developed new PTFs for two tropical mountain regions. The comparison with ~~ready~~ readily available PTFs showed their high performance to predict soil water retention for the soils in these areas. This is of particular importance for soil ~~process and~~ hydrological modeling. Whether the two PTFs may also be applied to other areas of similar soils still has to be tested. The developed PTF for the Páramo area provides a novelty since PTFs for tropical organic soils under volcanic influence were unavailable until now.

Furthermore, our study presents the first successful application of parameter tuning by differential evolution in PTF development. The comparison with the standard grid search technique revealed the superiority of the differential evolution algorithm and emphasizes the importance of parameter tuning for the successful application of machine learning models. Of course, this finding has to be confirmed by further applications in pedometrics including different machine learning algorithms. Especially for parameter tuning of real-valued machine learning algorithms, ~~W~~ we ~~, therefore,~~ hope to promote the implementation of optimization algorithms ~~for parameter tuning~~ within the pedometrics community ~~by this study~~. ~~To sum up, especially for parameter tuning of real-valued machine learning algorithms future applications of the differential evolution algorithm are highly recommended.~~

Data availability

The developed PTFs, as well as the underlying datasets, will be uploaded to the Open Science Framework (OSF) upon acceptance.

Competing interests

The authors declare that they have no conflict of interest.

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