Title: Integrating Scientific Knowledge into Machine Learning using Interactive Decision Trees

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Highlights

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- We propose a framework for building Decision Trees that put humans in the loop.
- The framework compensates for dataset issues encountered in standard Decision Trees.
- Interactive Decision Trees enhance interpretability and physical consistency.
- We developed an open-source toolbox for constructing Interactive Decision Trees

Integrating Scientific Knowledge into Machine Learning using Interactive Decision Trees

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Georgios Sarailidis: Georgios Sarailidis developed the proposed method & toolbox and prepared the manuscript; Thorsten Wagener: Thorsten Wagener supervised the method development and testing and revised the manuscript. Francesca Pianosi: Francesca Pianosi supervised the method development and testing and revised the manuscript.

ABSTRACT

Decision Trees (DT) is a machine learning method that has been widely used in the geosciences to automatically extract patterns from complex and high dimensional data. However, like any data-based method, the application of DT is hindered by data limitations and potentially physically unrealistic results. We develop interactive DT (iDT) that put the human in the loop and integrate the power of experts' scientific knowledge with the power of the algorithms to automatically learn patterns from large datasets. We created an open-source Python toolbox that implements the iDT framework. Users can create new composite variables, manually change the variable and threshold to split, manually prune and group variables based on their physical meaning. We demonstrate with three case studies that iDT help experts incorporate their knowledge in the DT development achieving higher interpretability.

1. Introduction

In the past few decades, our ability to collect, store and access large volumes of earth systems data has increased at unprecedent rates thanks to improved monitoring and sensing techniques (Hart and Martinez, 2006; Butler, 2007; Karpatne et al., 2017; Zhou et al., 2017), ever growing computational power (Washington et al., 2009), and the development of simulation models that produce large datasets at increasing scale and resolution. An example is the CMIP-5 dataset of the Climate Model Intercomparison Project, which has been used extensively for scientific groundwork towards periodic climate assessments (Reichstein et al., 2019). This 'data deluge' has paved the way for the systematic processing and analysis of observational and simulation data, often using Machine Learning or other statistical methods (Reichstein et al., 2019; Karpatne et al., 2019; Sun et al., 2022).

Machine Learning (ML), a term defined by Samuel (1959), is a branch of artificial intelligence (AI) and computer science which focuses on discovering patterns hidden in complex datasets (Bzdok et al., 2017; Reichstein et al., 2019) by imitating the way that humans learn (IBM, 2020). The main purpose of ML is to develop algorithms that can learn from historical data and perform tasks (e.g. predictions and classification) on new input data. The capability of ML methods to automatically extract patterns from large volumes of complex and high-dimensional (Table 1) data have made them an important part of research in many fields, including geosciences (Bergen et al., 2019, Sun et al., 2022).

In this paper we focus on Decision Trees (DT) (Breiman et al., 1984), a supervised ML method that is widely used in the geosciences. A DT model is developed through an automatic algorithm that recursively partitions the space of input variables into subspaces using a set of hierarchical decisions. In Figure 1, we show a DT with a schematic representation of the recursive partitioning of the dataset along with basic terms used in this paper. A DT model is a hierarchical tree structure that comprises nodes and branches. Each node is associated with a logical expression, i.e. a "split", which consists of the variable and threshold to split, e.g. "X_i smaller $\overline{X}_{i,j}$". Each node will lead to two branches that correspond to the different possible outcomes of the split. The terminal nodes are called leaves and are associated to either a class or a specific value for the output. The paths from root to leaf thus represent a set of classification (or regression) rules for the output. DT are commonly used for (Flach, 2012):

- Classification: The DT is trained on output data that are categorized under different classes (discrete values or non-numerical categories) and then predicts classes for unseen data. In geosciences applications, the output classes are sometimes obtained by previously grouping continuous variables.

- Regression: The DT is trained on continuous output variables, and it predicts continuous values instead of classes.

Different variants of the DT method have been used in geosciences for a variety of purposes, including catchment classification (Sawicz et al., 2014; Kuentz et al., 2017), land cover classification (Gislason et al., 2006), studying uncertain factors of simulation models (Almeida et al., 2017; Sarazin, 2018), analyzing rainfall-runoff relationships (Iorgulescu and Beven, 2004; Singh et al., 2014), empirical streamflow simulation (Shortridge et al., 2016), soil mapping (Grimm et al., 2008; Hengl et al., 2017), characterizing hydrological signatures (Addor et al., 2018).

DTs are quite appealing in geosciences because geophysical processes often reveal a hierarchical structure of controlling variables, and the hierarchical structure of DT with nodes, branches and splits is a straightforward way to capture those significant controlling variables and how they are organized to lead to different outputs. In the context of geosciences applications, DT are particularly appealing for the purpose of organizing spatially distributed entities, such as catchments or other landscape units, and showing how large-scale (e.g. climatic) controls interact with small-scale (e.g. land use or geology) controls.

Despite these advantages, there are three main challenges in the application of DTs in geosciences that are important to our discussion:

1) Like any statistical tool, DT methods rely on data and consequently their credibility is dependent on the quantity and quality of data available. DT require large amounts of data for training which are not always available (Kirchner et al., 2020). When available, data in geosciences can be complex, uncertain, noisy, heterogeneous and continuously changing (e.g. due to changes in the instruments or the data processing algorithms) (Solomatine and Ostfeld, 2008; Faghmous and Kumar, 2014; Beven et al., 2018; Karpatne et al., 2019). Therefore, the accuracy of DTs deteriorates with decreasing size or quality of the training dataset (Pal and Mather, 2003).
2) DT development relies on statistical metrics and algorithmic decisions aimed at statistical optimality, usually measured in terms of classification rate or regression accuracy. However, this development process does not guarantee that the outcome is physically consistent (Roscher et al., 2020). By physical consistency we mean that a DT should not violate scientific principles or overlook important physical characteristics of the system investigated. For example, some input variables may have physically meaningful threshold values that may be missed by the DT because other threshold values might produce

a statistically better result for the (noisy) dataset used for training. Moreover, most DT algorithms use split rules based on a single variable at each node, whereas combinations of multiple variables may play a significant role in partitioning the data space (Loh, 2014; Almeida et al., 2017).

3) DT complexity may decrease their interpretability and consequently limit their usefulness in geosciences applications. By interpretability we mean the ability by a human expert of making sense of the obtained model (Molnar, 2020), understand how the model works and reaches a specific decision. Decision trees are easier to interpret if they are small. The greater the number of terminal nodes, the deeper the tree and the more difficult it becomes to interpret. (Molnar, 2020; Lipton, 2018). Visualization could also help increase the interpretability of DT. However, existing visualization techniques focus on displaying information related to the statistical properties of the DT (e.g. impurity, node data points), whereas they do not support the display of information related to the physical properties of the variables – something that would potentially be more useful for geosciences applications (Almeida et al., 2017).

Integration of human experts in the DT development process – and hence of their domain knowledge and their cognitive ability to formulate hypotheses and theories – may help overcome some of these challenges (Table 1). For example, experts can discard DT branches that are physically unrealistic, or define thresholds values for splitting rules that are physically meaningful. They can define combinations of input variables that they believe interact in controlling outputs, where current algorithms would not allow for the detection of such combinations. Moreover, experts can learn patterns from few data examples because they have a certain expectation of relevant causal relationships, so they could guide the algorithm to learn from smaller amounts of data, or dataset where a particular output class is under-represented ("imbalanced dataset" (García and Herrera, 2009)). Incorporating scientific knowledge into Machine Learning models to improve their physical realism and interpretability has been highlighted as a major challenge and opportunity for ML applications in the geosciences (Read et al., 2019; Sun et al., 2022). Inclusion of domain knowledge in the model building process can also increase trust in the modelling results (Solomatine and Ostfeld, 2008).

In this paper, we propose a framework to develop "interactive Decision Trees" (iDTs) that put human experts in the development loop of Decision Trees. Our iDT framework establish a two-way interaction between the automatic DT development algorithm and the expert, allowing the expert to manually create new composite variables, changing variables and thresholds values at splitting node, manually pruning leaf nodes, and visualizing DTs in physically meaningful ways. Previous attempts at demonstrating the value of some of these functionalities include Ankerst et al. (2000), Han and Cercone (2001), Teoh and Ma (2003), Do (2006), Solomatine and Siek 2004 and van den Elzen and van Wijk, 2011, although to our knowledge none of these authors publicly shared the code to run their analyses, which was then not followed up by others. Outside the scientific literature we found two commercial software products that allow users to interact with the DT development algorithm, Dataiku (https://www.dataiku.com/) and IBM SPSS (https://www.ibm.com/analytics/spss-statistics-software). The former is freely available for academic purpose, but the latter is not, and neither of them is open-source. In this study we thus develop an open-source Python package to implement the iDT framework and demonstrate it on three case studies representatives of typical challenges encountered in geoscience applications. In the first one, we show how color-coding the tree nodes based on their physical meaning produce a more meaningful visualization, and how the expert can create new composite variables to add to the tree; in the second case study, we show how the expert can manually change the splitting threshold values of the tree nodes, based on other sources of knowledge, to increase interpretability; and in case study three, how manually changing the node variables and threshold values can be used by the expert to include under-represented classes in an imbalanced datasets.

2. Methodology

In this section we describe our framework for establishing interactions between the expert and an automatic DT training algorithm to integrate scientific knowledge in DT development. Moreover, we describe the Python package and the Jupyter Lab Graphical User Interface we developed to implement the framework. Finally, we present our ideas on how to evaluate DT predictive and interpretive performance.

2.1 A framework for interactive construction and analysis of decision trees

Figure 2 shows our framework for interactive construction and analysis of DTs and compares it to the classical approach of automatic development. In the classical approach, the analyst prepares the dataset to feed to the ML algorithm, specifies the algorithm's tuning parameters, executes it, and obtains the classification/regression model. In the interactive framework, the analyst (expert) can input their prior knowledge and/or feedback to the automatic algorithm additional knowledge discovered after inspecting the DT first generated by the algorithm, Specifically, the expert can:

1) organize and (pre-)process the input datasets, by assigning input variables to physically meaningful groups (such as climate variables, land surface properties, soil properties, etc.) and colour code the tree nodes based on this grouping, or by creating new composite variables to be added to the input dataset.
2) directly manipulate the structure of the DT model, by changing the nodes' variables and threshold values to split, or manually pruning the DT or changing leaf node class. This can be useful when the expert is aware of physically meaningful threshold values for certain variables (for example thresholds for climate variables that are commonly used to classify different climate zones) and would like to see them in the splitting nodes so to improve the DT's physical interpretability. Another case when the expert may want to manipulate the DT structure is that of an imbalanced dataset, where a certain class is under-represented in the dataset and thus an automatic algorithm may not represent that class in the DT. Different tactics have been proposed to overcome this problem, such as resampling (García and Herrera, 2009), synthetic generation (Chawla et al., 2002) or penalized models, although they often are time consuming (Zhou et al., 2017). iDT may offer an easier way to overcome the problem by allowing the expert to force the tree to include the under-represented class by manually changing nodes' variable and thresholds to split and/or leaves nodes classes.

2.2 A Python package and Graphical User Interface in Jupyter Lab for interactive construction and analysis of decision trees

In order to maximise the reusability, replicability and reproducibility of our proposed approach (Gil et al., 2016; Hutton et al., 2016) we developed and shared an open-source Python package and a GUI in Jupyter Lab for implementing the IDTs framework. The code is available at https://github.com/Sarailidis/Interactive-Decision-Trees (https://doi.org/10.5281/zenodo.5011487). We used the sklearn library of scikit-learn package in Python (Pedregosa et al., 2011) that contains the implementation of the tree algorithm (for more details see Supplementary material) to use as a basis for developing our interactive tools. We created a new package, called "InteractiveDT", which consists of (1) an "iDT" module containing the functions that enable the expert to interact with the DT or the dataset, and (2) an "iDTGUIfun" module which incorporates these functions into widgets, which are then used in the Jupyter Lab script called "InteractiveDecisionTrees" to create the user interface. Further details about this GUI are also provided in the Supplementary material.

2.3 Evaluating DT predictive and interpretive performance

Decision trees are generally used as predictive tools for either classification or regression, and therefore their evaluation is typically based on statistical metrics of their prediction ability (Lipton, 2018). Examples of such metrics include classification accuracy, confusion matrices, precision, recall, accuracy rate, root mean square, and mean error (Pedregosa et al., 2011). However, in geosciences applications we often would like the DT to be not only a good predictor, but also to be interpretable (Lipton, 2018). Differently from predictive performance, interpretability is a less well defined concept and metrics to measure interpretability are not well established (Doshi-Velez and Been, 2017). A widely used proxy for interpretability is the complexity of the tree, as it can be reasonably assumed that a less complex tree is easier to interpret (Molnar, 2020; Lipton, 2018). The complexity of a DT can be easily quantified through the number of leaf nodes and/or the depth of the tree (Molnar, 2020). We will adopt these simple metrics to evaluate DT interpretability in our first case study.

The need for interpretability is often linked to the use of models to assist scientific understanding (Doshi-Velez and Been (2017). The evaluation of interpretability for scientific understanding though is context specific. In case study 2, we will give an example of a case-specific definition of interpretability, based on the consistency of the DT partitioning of the input space with an independent classification system of some of the input variables (climate in our case).

3.0 Results

3.1 Case Study 1 – Color-coding groups of variables and constructing new composite variables to reduce the DT complexity and increase interpretability

We used a dataset from Almeida et al. (2017). It includes 10,000 combinations of 28 input variables of a slope stability model (the list is given in Table S.1 in the supplementary material). These variables are model parameters characterising the slope geometry, soil and design storm properties and initial hydrological conditions. The model output is the slope factor of safety (FoS). This leads to defining two classes: “stable”, when FoS is above 1, and “failure” otherwise. In Almeida et al. (2017) a conventional CART algorithm (implemented in the Matlab Statistics and Machine Learning toolbox) was used to identify dominant drivers of slope instability. We will apply our iDT procedure to the same dataset to demonstrate two functionalities of our iDT toolbox: how to increase the visual interpretability of the DT by colour coding variables based on their physical meaning, and how to capture interactions between variables by creating new composite variables.

In Figure 3 we show the statistically optimal DT initially delivered by the automatic DT algorithm. Nodes are coloured based on Impurity, a default choice in many software. Figure 3 also shows the graphical interface of the InteractiveDT tool, which allows to define groups of input variables and colour code the nodes accordingly. The resulting tree with nodes colour-coded based on their meaning is shown below. With this visualization, it is evident that the first three levels of the tree are dominated by "geophysical properties" and "slope geometry variables", while levels 4 and 5 are mainly dominated by "design storm properties". Furthermore, the colour coding helps spotting a repetition of two variables, cohesion (c_0) and thickness of topsoil (H0), in the first levels of the tree, which indicates that these two factors interact with each other. This pushes the expert to create a composite variable, called Soil Ratio, given by the ratio of cohesion and thickness of topsoil (Soil Ratio=c_0/H0). A second composite variable is created based on domain knowledge that rainfall intensity and duration interact in the context of slope stability, as also confirmed by node repetitions in levels 4 and 5 of the DT. The second composite variable is called Storm Ratio and is the ratio of the logarithms of rainfall intensity and duration (Storm Ratio=-log10(D)/log10(I)). Figure 4 shows the interface of the InteractiveDT tool used to create these two composite variables and the new tree delivered by the DT algorithm when fed by a training dataset including the two new variables. The new tree is overlaid on the initial tree, shown in light grey. The changes made by the algorithm in response to the expert changes are shown with Bold and Italic letters followed by an asterisk. Overall, the new DT is "better" than the original one because it is much smaller (11 leaves nodes instead of 29, and a depth of 5 layers instead of 8) and thus more interpretable, for about the same classification accuracy (also shown in Figure 4).

3.2 Case Study 2 – Increasing interpretability by changing splitting threshold values based on other relevant knowledge sources

Here, we used a revised version of the dataset created by Sarazin (2018) which includes 17,000,000 simulations of 34 input variables of a hydrological model. These variables are model parameters characterizing climate properties, land cover and soil characteristics of karst systems across Europe under current and future climate. The model outputs are values of annual groundwater recharge, which are the classified into four classes, namely, C1 (<20 mm/yr), C2 (20 – 100 mm/yr), C3 (100 – 300 mm/yr) and C4 (>300 mm/yr). Here, a DT is built to reveal the key controls of groundwater recharge. In order to increase the interpretability of the tree, we use our iDT framework to manually change some of the nodes' thresholds consistently with a simplified version of the Holdridge life zones classification scheme. The Holdridge scheme provides a classification of land areas based on annual precipitation and aridity index (i.e. the ratio between potential evaporation and precipitation; Figure S.2 in the Supplementary material shows the original and our simplified scheme). By imposing that the threshold values for Precipitation (Pm) and Aridity index (AI) in the DT be the same as in the Holdridge chart thresholds, we aim to obtain a more physically meaningful tree. We then want to explore whether a tree so constructed leads to leaf nodes that are more interpretable, i.e. they map into fewer Holdridge life zones, and whether this gain in interpretability comes with a significant loss in classification accuracy.

To answer these questions, we generated 15 datasets of 1000 samples each by random sampling from the original dataset (of 17,000,000 samples). For each dataset we derived a statistically optimal (SO) and an interactive (iDT) decision tree. To derive the SO decision tree, we tried different combinations of the algorithm tuning parameters (splitting criterion based on "Gini impurity" or "entropy", maximum number of leaf nodes varied from 15 to 25, maximum impurity decrease of 10^{-5}, 10^{-6}, 10^{-7}) and retained the best SO tree based on 10-fold Cross Validation strategy. To derive the corresponding iDT, we used the iDT framework to manually change all the splitting thresholds for Pm and AI to the closest Holdridge chart threshold values.

Figure 5 shows an example of a statistically optimal DT (top) and the corresponding iDT (middle). Below the leaf nodes, we reported the number of Holdridge life zones (HLZs) each leaf is mapped to. The bottom panel in Figure 5 shows the average number of HLZs for each leaf across the four recharge classes and in total. Overall, the Figure shows that when moving from the statistically optimal DT to the iDT, the number of HLZs associated to each leaf node tend to decrease. This may increase the interpretability of the iDTs, as the leaf nodes not only provide a prediction of the output class (amount of groundwater recharge) but also have a clearer mapping into climate zones. Figure S.3 in the Supplementary material shows the performance of the statistically optimal DTs and the iDTs on the training and test set. Generally, the differences are not pronounced, which means the changes made by the expert to the trees did not lead to a significant change in performance. As expected, the statistically optimal DTs always show a slightly higher classification accuracy in the training sets. Interestingly though, the iDTs outperform the statistically optimal trees in most cases (9 out of 15) in the test sets. In conclusion, this example shows that incorporating knowledge in the DT development by manually changing the split thresholds led to a more concise and meaningful mapping with limited effect on classification accuracy (and even a small improvement on the test dataset).

3.3 Case Study 3 Manually changing nodes' variables and threshold values to include under-represented classes in imbalanced datasets and ensure physical consistency.

This case study is an example of application of iDT in cases where certain classes are under-represented in a dataset, a situation known as “imbalanced datasets”. We use again the dataset from Sarazin (2018) as in Sec. 3.2, and randomly generated 5 subsample datasets of increasing sizes (1000, 5000, 10000, 50000 and 100000 samples). We then split each subsample dataset into a training and a test set (75% and 25% of the dataset size respectively) and randomly remove data points that belong to class C2 from the training dataset. Therefore, the training sets contain only few data points of class C2 (<2%). Similarly, to Sec. 3.2, for each dataset we train a Statistically Optimal (SO) decision tree and then derive an iDT by manually changing the nodes’ variables and thresholds until the iDT included the unrepresented class C2 in some of its leaf nodes. In some cases, we also manually changed the class of a leaf node to class C2. For example, in Figure 6a on the left we show a part of the SO tree obtained for sample dataset 2. We know from Sarrazin (2018) that low recharge class C2 should appear for low precipitation values, but the algorithm fails to include the C2 class in the SO tree as the class is under-represented in the training dataset. Hence, we manually change the threshold in the split node *“Pm<=639.075”* and the node variable in the split *Vr<=201.14”*, so to create a branch in the tree that specifically explore low precipitation cases. In response to these manual changes, the algorithm creates a leaf node for class C2 in the iDT (top right of Fig. 6). The change induces a loss of classification accuracy in the training dataset (see Figure 6b, case ‘dat2’) but an increase in performance on the test dataset against unseen data. A similar trend is found for all other datasets: as expected, SO trees perform better in the training sets but iDTs outperform SO trees in in test set, particularly for smaller datasets.

4 Conclusions

This work proposes a framework for the construction and analysis of interactive decision trees (iDTs) for application in the geosciences. We created an open-source implementation of iDT in Python and Jupyter Lab, which we hope will encourage the use of iDT in future research applications. We demonstrated the iDT approach in three case studies that represent typical challenges encountered in applications of decisions trees in the geosciences. We found that our proposed iDT framework supports the development of decision trees that are easier to visualise and interpret in a physical sense. Perhaps surprisingly, in our second case study we find that manual adjustment of splitting thresholds can lead to developing a more physically meaningful tree with almost no loss in classification performance. In the third example, we show how experts can build physically consistent DT in cases of imbalanced datasets that can generalize better on unseen data. Even though manually changing the nodes’ variables and threshold values based on domain knowledge to include the under-represented class deteriorated the classification accuracy in training sets, it improved it in test sets.

One direction for future research could look at how to achieve closer interaction between human experts and machine algorithms by including domain knowledge in algorithmic form (Solomatine and Ostfeld, 2008). For example, experts could force the algorithm to search for thresholds in a specific range of values for selected variables, or they could define constraints on variable selection to eliminate unrealistic sequence of variables to split. Another area for future improvement would be to expand the range of visualisation techniques (e.g. partial dependence plots, accumulated local effects, feature interaction; see for example application in Shortridge et al. (2016) that could be used in parallel to the main visualization of the DT to further enhance interpretability.

We hope that this paper will contribute to foster the development and use of interactive decision trees and, more broadly, of methods to better integrate domain knowledge in ML, which can be particularly relevant for geoscience applications.

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Code availability section

Name of the code/library: InteractiveDT, (GPL-3.0 License)

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Hardware requirements: The presented toolbox has been tested on a computer with the following characteristics:

- Processor: Intel(R) Core (TM) i7-8700 CPU @ 3.20GHz 3.19 GHz
- RAM: 16.0 GB (15.8 GB usable)
- System Type: 64-bit operating system, x64-based processor

Program language: Python

Software required: python, jupyter lab, anaconda navigator

Program size: 4658 KB

Access to the code, datasets and workflows to reproduce the results presented in this paper:
https://github.com/Sarailidis/Interactive-Decision-Trees

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List of Figures

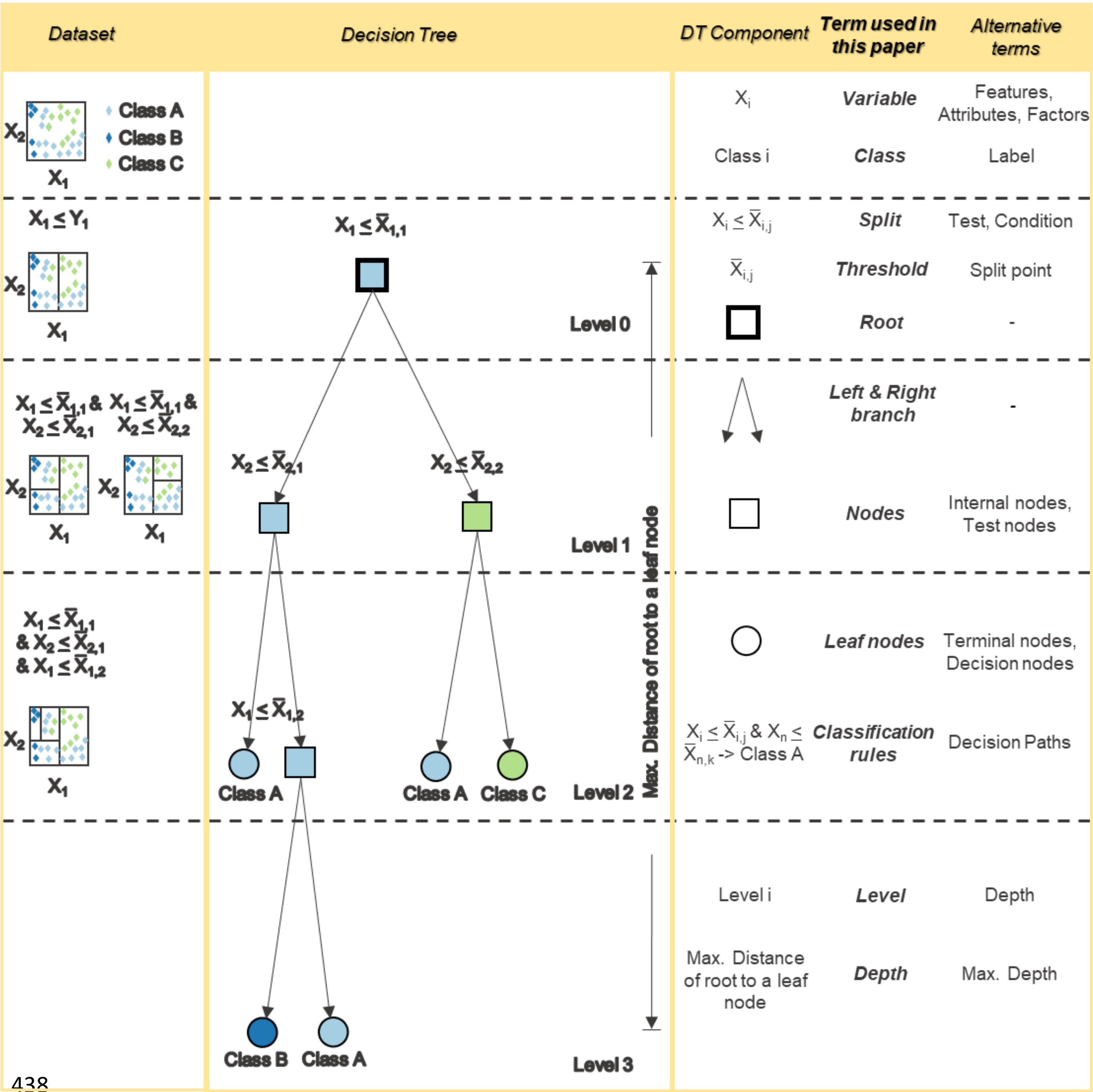
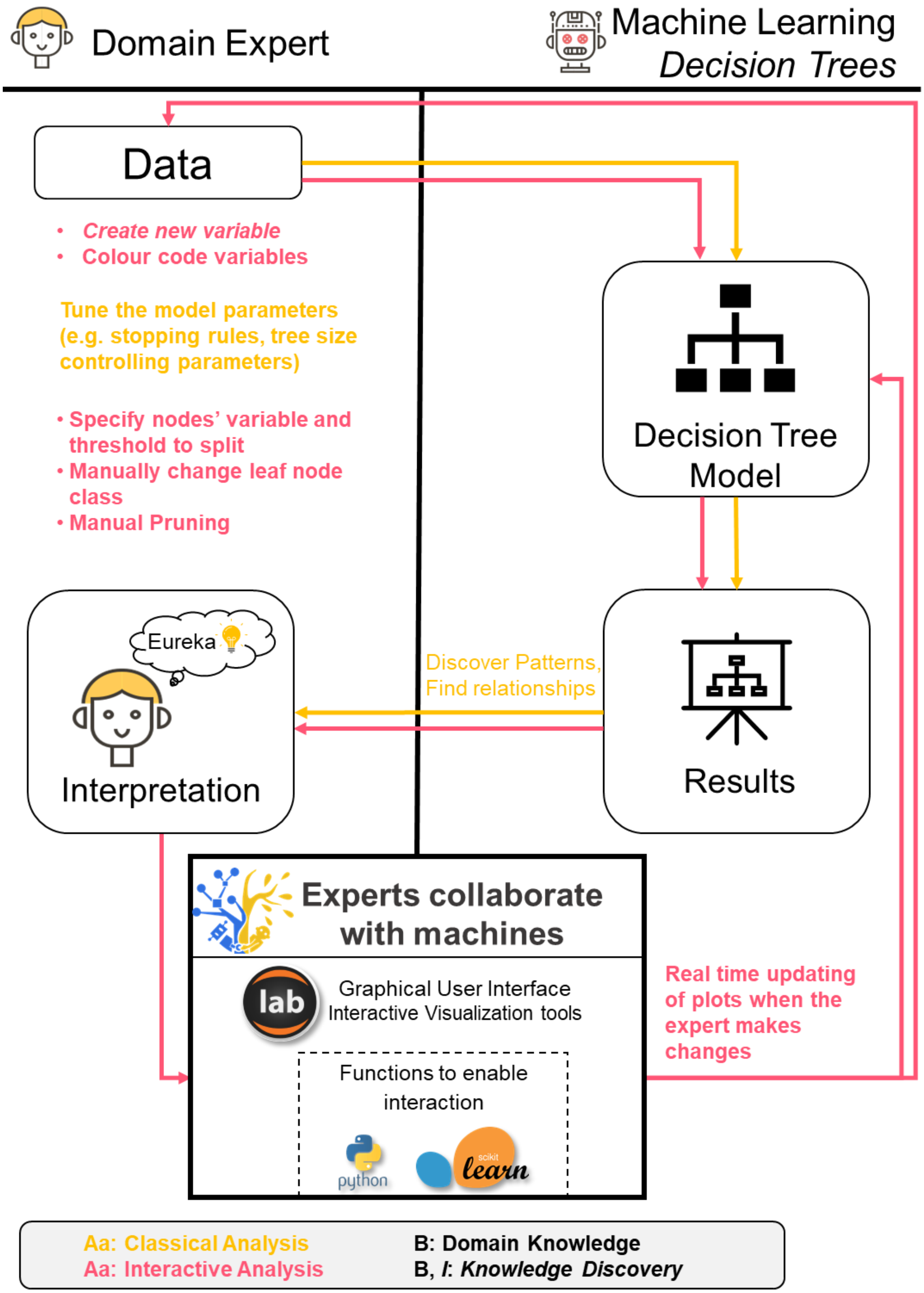


Figure 1 Left: A schematic representation of the recursive partitioning of the data space performed by a Decision Tree development algorithm. Middle: A typical Decision Tree. Right: Terminology.



Domain Expert
Machine Learning
Decision Trees
Data
Create new variable
Colour code variables
Tune the model parameters (e.g. stopping rules, tree size controlling parameters)
Specify nodes' variable and threshold to split
Manually change leaf node class
Manual Pruning
Decision Tree Model
Results
Discover Patterns, Find relationships
Eureka
Interpretation
Experts collaborate with machines
lab
Graphical User Interface
Interactive Visualization tools
Functions to enable interaction
python
scikit learn
Real time updating of plots when the expert makes changes
Aa: Classical Analysis
Aa: Interactive Analysis
B: Domain Knowledge
B, I: Knowledge Discovery

Figure 2 Flowcharts of the steps performed to develop a Decision Tree in a “Classical” analysis and with our proposed Interactive analysis

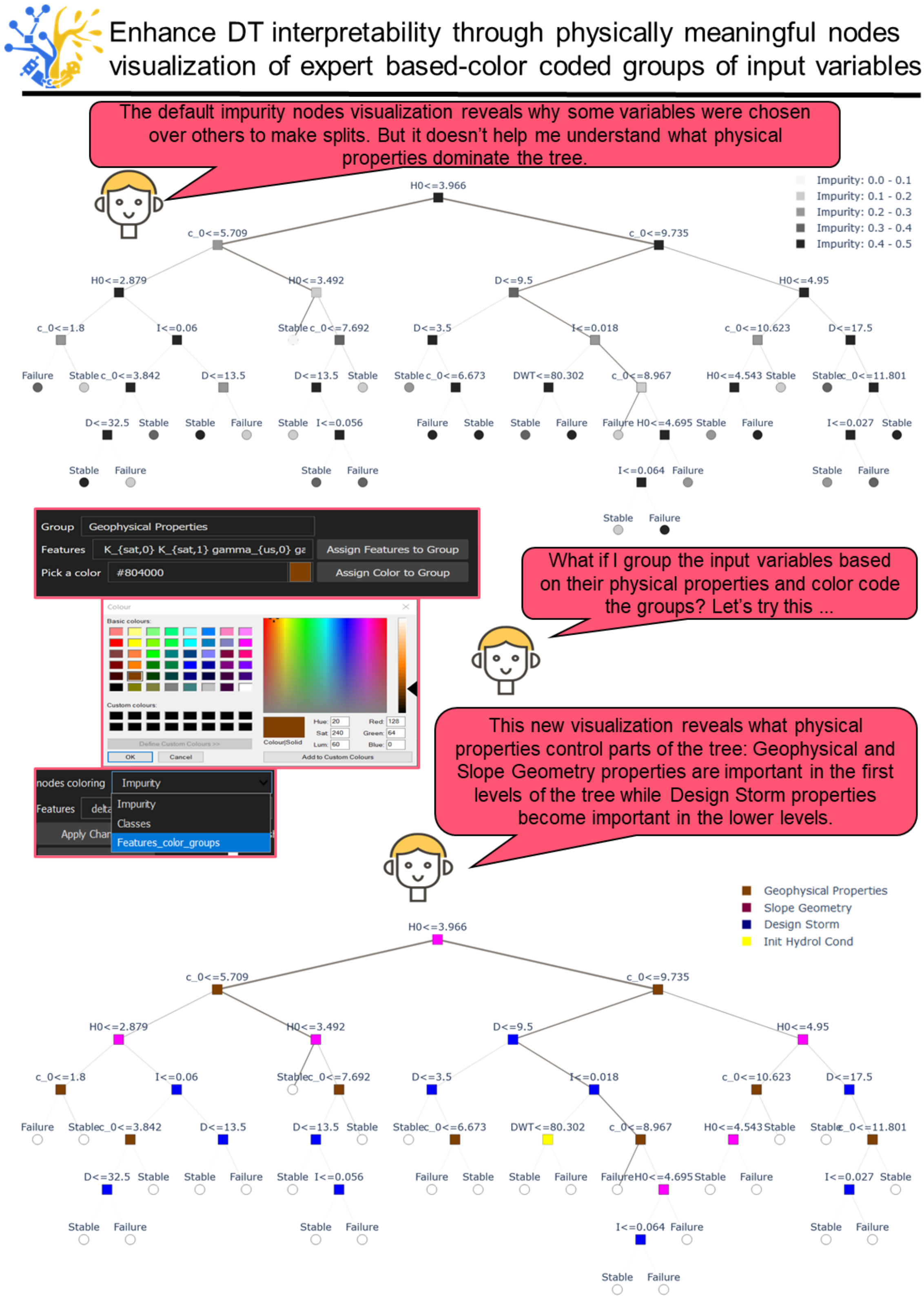
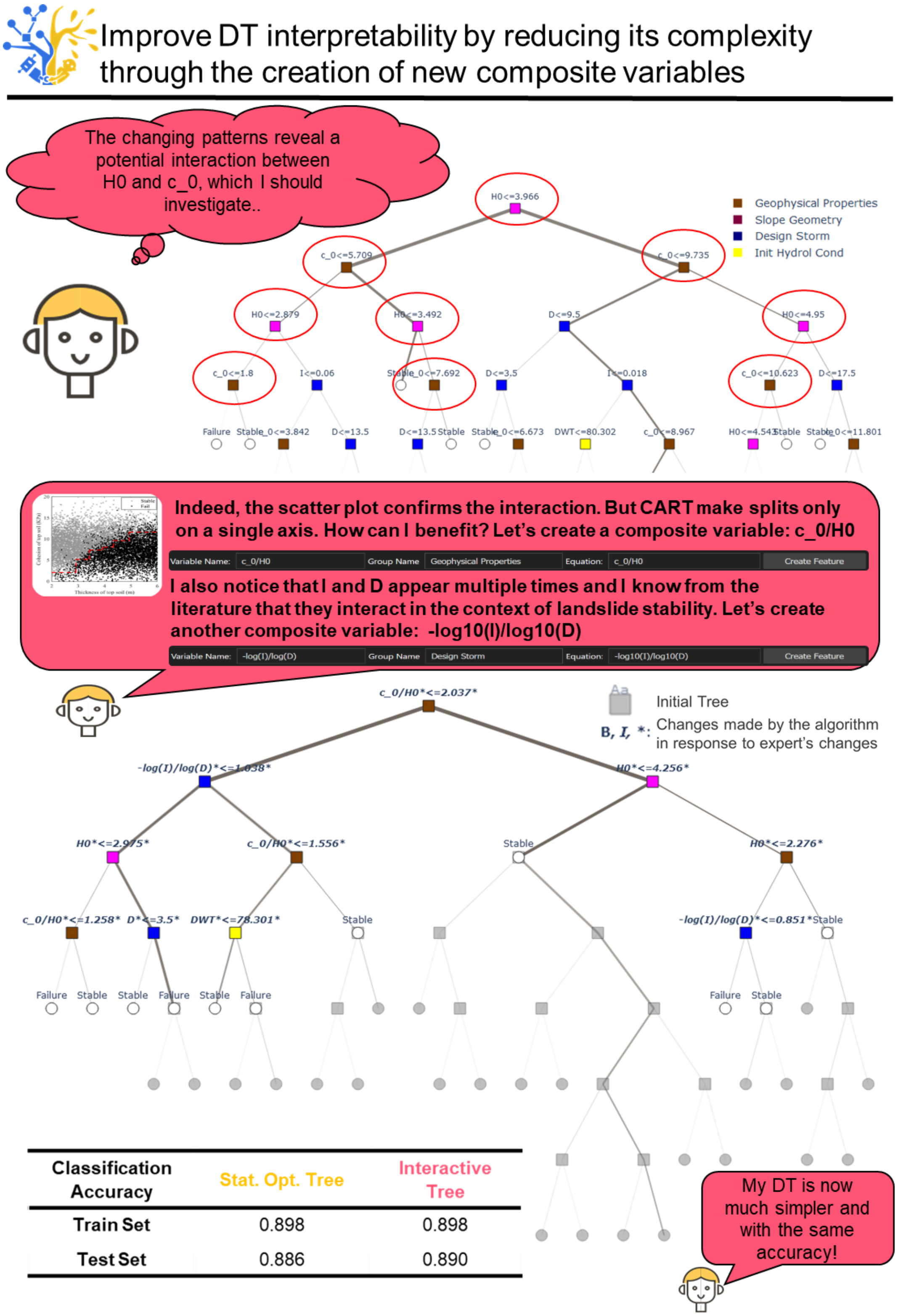


Figure 3 The tree in the top shows the default impurity nodes coloring and the bottom tree shows the proposed alternative nodes coloring visualization based on expert created color coded groups. Using this node coloring option,

it is evident what kind of variables dominate the tree. The figure shows the tool that was developed and used by the expert to achieve this alternative visualization.



Classification Accuracy	Stat. Opt. Tree	Interactive Tree
Train Set	0.898	0.898
Test Set	0.886	0.890

Figure 3 The tree in the top shows the starting tree in which an interaction between two variables emerged. In the middle the interface of our tool to create new composite variables is shown. The DT in the bottom is the new

"modified" DT and is plotted on top of the initial tree which is shown in light grey. The new "modified" DT is dominated by the new composite variables (Soil Ratio and Storm Ratio), it is less complex and with same accuracy for the training set and slightly improved for the test set.

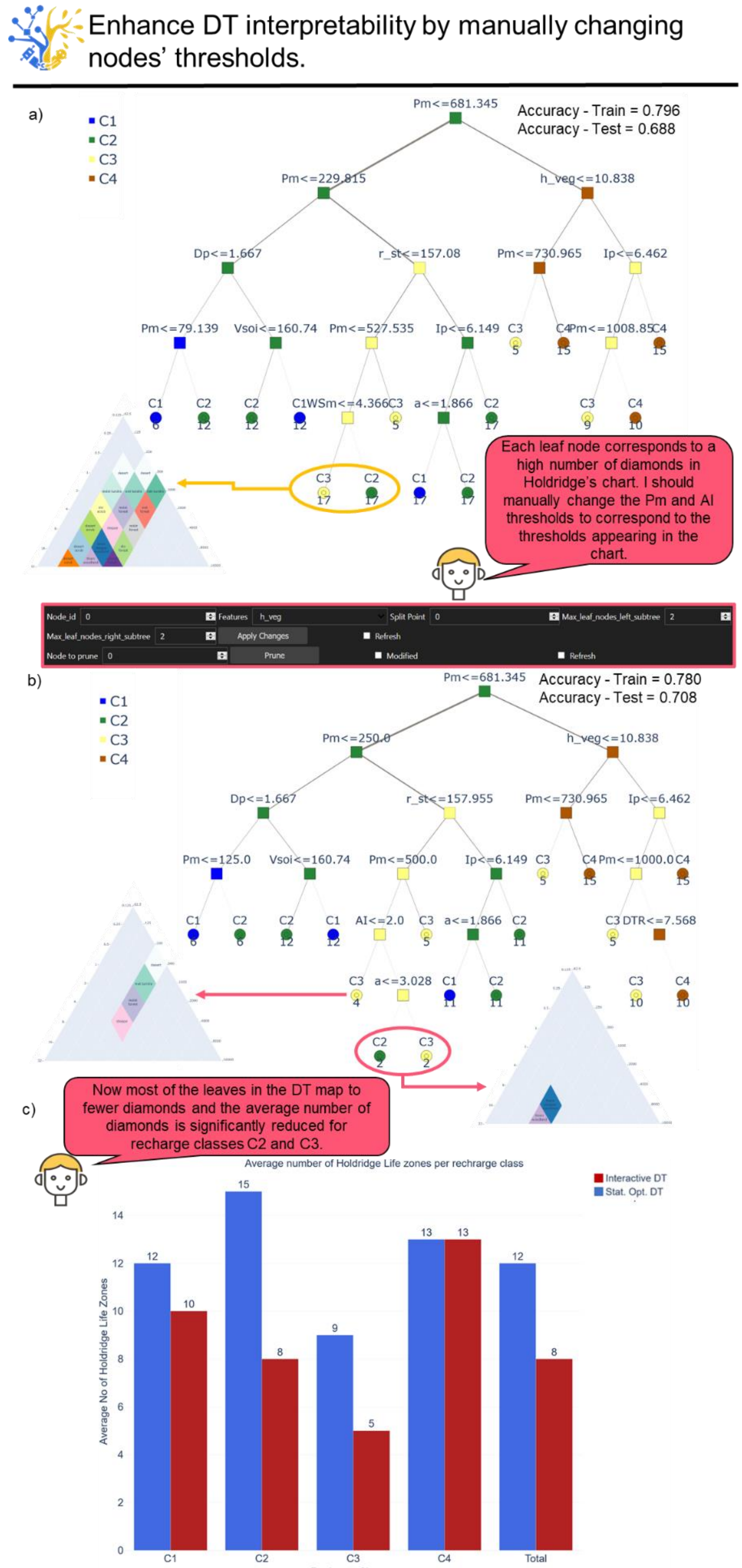

Enhance DT interpretability by manually changing nodes' thresholds.
a)
C1
C2
C3
C4
Accuracy - Train = 0.796
Accuracy - Test = 0.688
Pm<=681.345
Pm<=229.815
h_veg<=10.838
Dp<=1.667
r_st<=157.08
Pm<=730.965
Ip<=6.462
Pm<=79.139
Vsoi<=160.74
Pm<=527.535
Ip<=6.149
Pm<=1008.85
WSm<=4.366
a<=1.866
Each leaf node corresponds to a high number of diamonds in Holdridge's chart. I should manually change the Pm and AI thresholds to correspond to the thresholds appearing in the chart.
Node_id
Features
h_veg
Split Point
Max_leaf_nodes_left_subtree
Max_leaf_nodes_right_subtree
Apply Changes
Refresh
Node to prune
Prune
Modified
Refresh
b)
C1
C2
C3
C4
Accuracy - Train = 0.780
Accuracy - Test = 0.708
Pm<=681.345
Pm<=250.0
h_veg<=10.838
Dp<=1.667
r_st<=157.955
Pm<=730.965
Ip<=6.462
Pm<=125.0
Vsoi<=160.74
Pm<=500.0
Ip<=6.149
Pm<=1000.0
AI<=2.0
a<=1.866
DTR<=7.568
a<=3.028
c)
Now most of the leaves in the DT map to fewer diamonds and the average number of diamonds is significantly reduced for recharge classes C2 and C3.
Average number of Holdridge Life zones per rechrarge class
Interactive DT
Stat. Opt. DT
Average No of Holdridge Life Zones
Recharge Classes
C1
C2
C3
C4
Total

Figure 4 a) Statistically optimal DT, b) iDT (the UI of the tool used to manually change nodes' thresholds is shown on the top of the DT), c) Average number of Holdridge Life Zones per recharge class and for the DT in total. Below the leaves nodes of each DT there is a number denoting the number of diamonds the leaf is mapped to. Indicatively, we plotted the Holdridge scheme and highlighted only the diamonds that the leaves can be mapped to, for the leaves nodes with the biggest reduction.

Manually changing nodes' splitting variables and threshold values to include under-represented class in imbalanced datasets and ensure physical consistency

a)

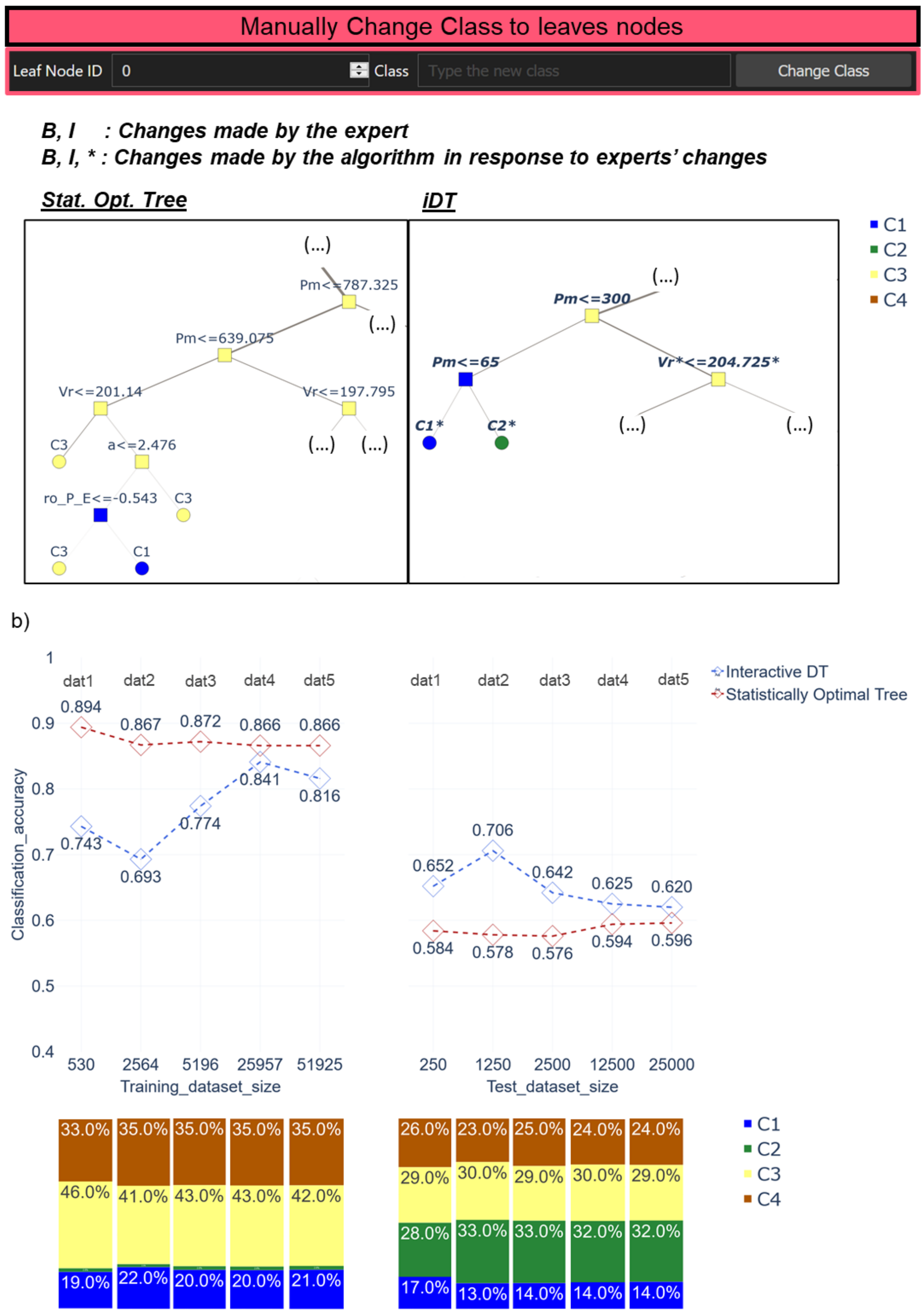


Figure 5 a) Statistical optimal (left) and interactive (right) DT for sample dataset "dat2" (the UI of the tool used to manually change nodes variables and thresholds to split is shown on the top of the DTs). b) Classification accuracies for statistical optimal (red) and interactive (blue) DT on the training (left) and test (right) sets. At the bottom of the graphs the distribution of each class for each dataset is shown

List of Tables

Table 1 Strengths and Limitations of Machines Learning Algorithms and Experts.

	Machine (Algorithm)	Expert
Strengths	1. Extracts patterns hidden in large/high dimensional datasets by performing complex computations (applying rules) 2. Can reach optimal solutions by optimizing its learning behavior (satisfy certain criteria/metrics at each step) 3. Can achieve the above automatically and in reasonable amount of time (in comparison with humans)	1. Has domain knowledge of the area and data under investigation 2. Can learn and draw conclusions by small amount of data 3. Can inspect the results and consider causal relationships