

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

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# Integrating Scientific Knowledge into Machine Learning using Interactive Decision Trees

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## Abstract

Decision Trees (DT) is a machine learning method that has been widely used in the environmental sciences to automatically extract patterns from complex and high dimensional data. However, like any data-based method, 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 data. We created a toolbox that contains methods and visualization techniques that allow users to interact with the DT. Users can create new composite variables, manually change the variable and threshold to split, manually prune and group variables based on physical meaning. We demonstrate with three case studies that iDT help experts incorporate their knowledge in the DT models achieving higher interpretability and realism in a physical sense.

**Keywords:** Interactive Decision Trees; Machine Learning; Human-in-the-Loop; Interpretability; Open-source toolbox

# 1. Introduction

In the past few decades, geosciences and environmental sciences have seen a deluge of data produced by new observational possibilities (such as remote sensing) and by simulation models with rapidly increasing scale and resolution. Our ability to collect, store and access large volumes of data has increased in unprecedented rates due to improved monitoring techniques and sensors (Hart and Martinez, 2006; Butler, 2007; Karpatne et al., 2017; Zhou et al., 2017). Simulation models add to this deluge because they are often used to produce large and complex datasets. 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). At the same time, we are experiencing a remarkable increase in computational power (Washington et al., 2009) which has paved the way for the systematic processing and analysis of the available data often using Machine Learning or other data driven and statistical methods (Reichstein et al., 2019; Karpatne et al., 2019).

Machine Learning (ML) has emerged as a widely adopted and quickly growing collection of data-based tools to aid the human effort of discovering patterns hidden in such complex datasets (Bzdok et al., 2017; Reichstein et al., 2019). Machine learning, a term defined by (Samuel, 1959), is a branch of artificial intelligence (AI) and computer science which focuses on the use of data and algorithms to imitate the way that humans learn, gradually improving its accuracy (IBM, 2020). Thus, the main purpose of ML is to explore and construct algorithms that can learn from historical data and perform tasks (e.g. predictions, classification) on new input data. The capability of ML methods to automatically extract patterns from large volumes of complex and high dimensional data and to optimize their learning behaviour to improve performance (Bergen et al., 2019) (see advantages of ML methods in **Table 1**) have made them an important part in many research driven applications in our field. There are many classes of ML methods with the two most common being (Flach, 2012):

- Supervised: The ML model is fed with a set of input and well labelled output data and the model learns to map the input with the correct output.
- Unsupervised: The ML model is fed only with a set of input data. Not having labeled output data the ML model will try to look for interesting relationships and patterns in the input dataset.

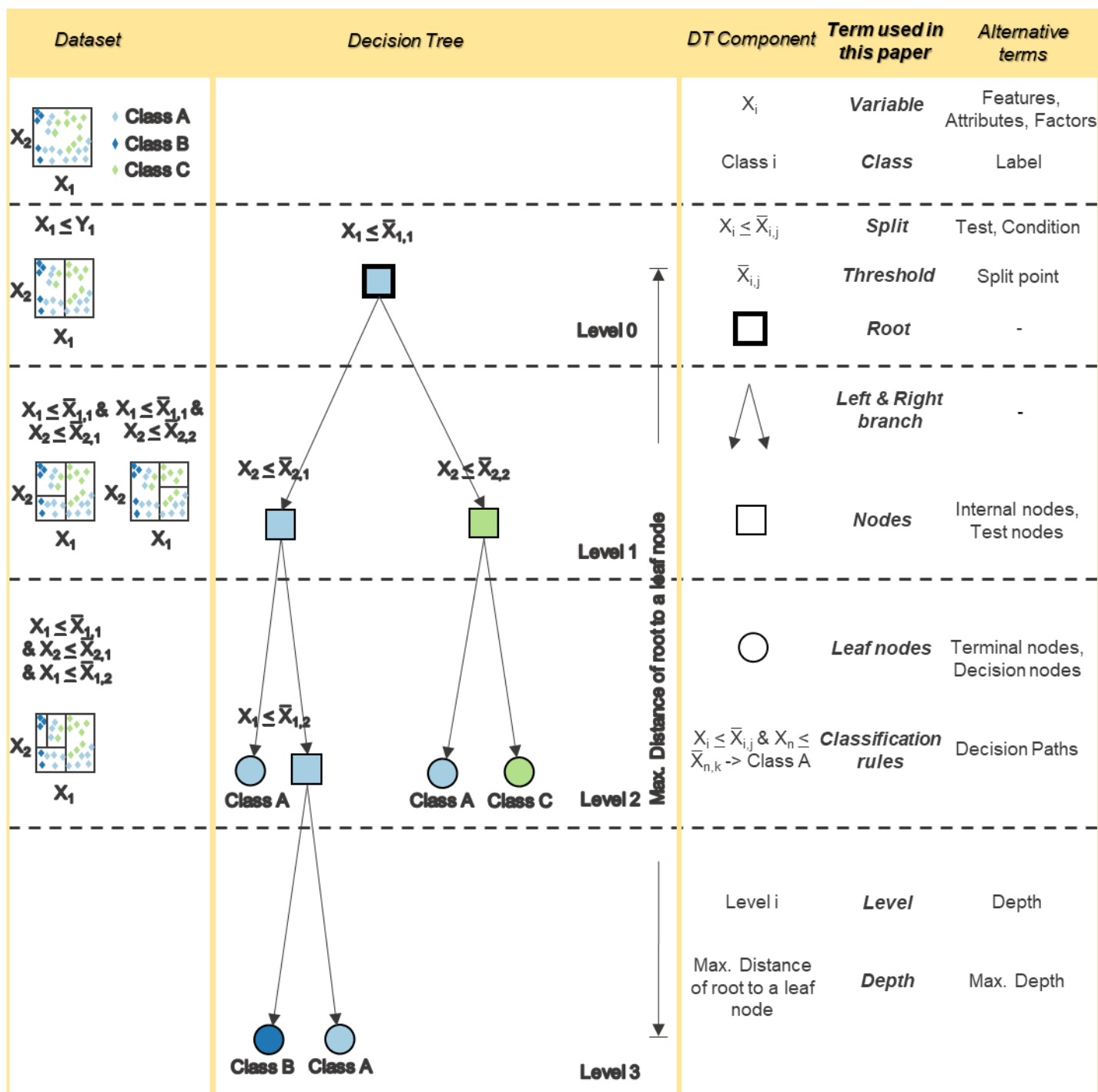
In this paper we focus on Decision Trees (DT) (Breiman et al., 1984), a supervised ML method that is widely used in geosciences and environmental sciences (In the rest of this paper for simplicity we use the term environmental sciences to refer to both geosciences and environmental sciences). A DT is a ML model which is based on an algorithm that recursively

partitions the data space of input variables into subspaces using a set of hierarchical decisions on the input variables. 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 of nodes and branches. Each node is associated with a logical expression, i.e. a “split” which consists of the variable and threshold to split. A split could be of the form e.g. variable  $X_i$  lies below  $\bar{X}_{i,j}$ . The threshold  $\bar{X}_{i,j}$  lies in the range of the available data points. Each node will lead to two (if binary) branches that correspond to the different possible outcomes of the split. The terminal nodes are called leaves and represent a class. The paths from root to leaf represent classification (or regression) rules. An ensemble of DT is called Random Forest (RF). DT have been commonly used for (Flach, 2012):

- Classification: The model is trained on data that are categorized under different classes according to various variables and then predicts classes for unseen data. In environmental applications the different classes may also represent continuous variables which have been previously grouped into classes.
- Regression: In contrast to classification, the model predicts the numeric data (continuous values) instead of classes (discrete values or categories).

DT (in different variations) have been used for 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/parameters (Iorgulescu and Beven, 2004; Singh et al., 2014), soil mapping (Grimm et al., 2008; Hengl et al., 2017), characterizing hydrological signatures (Addor et al., 2018).

DTs are quite appealing in environmental sciences because entities in this field regularly reveal a hierarchical structure of controlling variables and we often look to derive a predictive model that also provides insight into which variables control the prediction, i.e. the model is interpretable (Molnar, 2019). DTs are potentially interpretable because unlike some other models, such as neural networks, experts can see how the model arrives at specific classes. The hierarchical tree structure of DT with nodes, branches and splits is a straightforward way to visualize the significant controlling variables across the data space and how these are organised to lead to different classes. In the context of environmental science applications, DT are particularly appealing for the purpose of organizing spatially distributed entities (e.g. catchments or other landscape units). Through their structure, DTs can reveal a hierarchy of controlling variables by showing how larger scale (e.g. climatic) controls interact with smaller scale variability (e.g. land use or geology).



**Figure 1** Left frame: A schematic representation of the recursive partitioning of the data space from a tree algorithm. Middle frame: A typical decision tree. Right Frame: A table showing the terms used in this paper as well as alternative terms for basic decision tree components.

Despite their common use for classification and regression, there are three main challenges in their application to environmental sciences that are important to our discussion:

- 1) Like any statistical tool, DT rely on data and consequently their credibility is dependent on the quantity and quality of data available. Environmental data can be complex, uncertain, noisy, heterogeneous and they continuously change (e.g. change in the instruments or the data processing algorithms) (Faghmous and Kumar, 2014; Beven

et al., 2018; Karpatne et al., 2019), thus putting into question the quality of the DT model results. DT require large amounts of data for training which are not always available (Kirchner et al., 2020). Therefore, in data rich cases DT could work very well but their accuracy gets worse with decreasing size or quality of training data (Pal and Mather, 2003).

- 2) DT rely on statistical metrics and algorithmic decisions to derive DT at statistical optimality in an automated manner (usually in terms of classification or regression accuracy). However, this process (like any regression) does not guarantee an outcome that is scientifically or physically consistent (Roscher et al., 2020). By physical consistency we mean that a DT should not violate scientific principles or miss important physical characteristics of the case study an expert investigates. For example, some processes or phenomena studied may have physically meaningful values (or thresholds) that serve a specific purpose. DT may miss physically meaningful values or subsets because other values might produce a statistically better result for the dataset used. Moreover, most (if not all) tree algorithms split the dataset into two sub-datasets according to a single variable and threshold at each node, thus potentially ignoring combinations of variables that may play a significant role in partitioning the data space (Loh, 2014; Almeida et al., 2017)
- 3) DT complexity and/or existing tree visualization tools may decrease DT interpretability and consequently limit their usefulness in environmental applications. By interpretability we mean the ability to make sense of the obtained model (Molnar, 2009) that is experts 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, 2009; Lipton, 2018). Visualization could 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 instances/samples), 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 environmental applications (Almeida et al., 2017).

Scientific experts - through their domain knowledge, their cognitive abilities and their ability to formulate hypotheses and theories – have the potential to overcome some of the challenges we just listed. **Table 1** summarizes how humans can contribute in overcoming these challenges. Domain knowledge can help reduce the complexity of the phenomena under study or generate physically consistent results. For example, experts can eliminate variables they know are not relevant and can discard model results that are physically unrealistic. Or they

can combine variables that they believe interact in controlling DT classes, if the DT does not automatically allow for the detection and utilization of such interactions. Experts have good knowledge of the area or the phenomena they are studying. In cases where models are missing important variables of the study case, experts can contribute with their knowledge to make them more consistent. Moreover, experts can learn from few examples because they have a certain expectation of relevant causal relationships. This could be an advantage for overcoming the inherent limitations of environmental data (e.g. limited sample size is a caveat for capturing the full complexity of environmental processes, high dimensionality) and guide the algorithm to learn from smaller amounts of data. Finally, experts could use their cognitive abilities to fit DT in their specific scientific context. They can inspect the new patterns discovered from the algorithm, find the physical meaning behind them and think of ways to feed this new information back to the algorithm. In this way, experts could develop DT models that are optimal in physical sense and fit their needs. Therefore, we believe that the combination of empirical analysis tools like DT with scientific theory and knowledge from experts might be a good combination for achieving scientific progress (Read et al., 2019). However, traditionally DT are designed to work automatically and leave little (or no) space for the expert to interact with them.

**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)	1. Has domain knowledge of the area and data under investigation
	2. Can reach optimal solutions by optimizing its learning behavior (satisfy certain criteria/metrics at each step)	2. Can learn and draw conclusions by small amount of data
	3. Can achieve the above automatically and in reasonable amount of time (in comparison with humans)	3. Can inspect the results and consider causal relationships

In this paper, we develop interactive decision trees (iDT) that put human experts in the development loop. Our iDT establish a two way interaction between the tree and the expert. In this way, experts integrate scientific knowledge with the power of algorithms and design interpretive ML models that fit an experts' knowledge framework and scientific application context while still allowing for surprising new patterns to be discovered (Gil et al., 2019). We

define iDT as a group of methods or visualization techniques that are developed to involve the human element in all (or some) parts of the tree building process. Thus, we develop methods and visualization techniques (e.g. create new composite variables, new node visualization, manually changing nodes' variables and thresholds to split) that allow the experts to interact with the data and the DT based on their knowledge. We argue that iDTs are meaningful not only as predictive tools for classification and regression but also as informative tools that help experts achieve meaningful interpretations of their case studies or ensure physical consistency of their models and results. To show that, we interact with the DT or the data in three case studies by:

- Applying a new nodes visualization (based on expert based-color coded groups of input variables) and creating new composite variables (1<sup>st</sup> case study).
- Manually changing nodes' thresholds to split (2<sup>nd</sup> case study).
- And manually changing nodes' variables and thresholds to split and classes in leaves nodes (3<sup>rd</sup> case study).

## 2. Methods

In this section we describe our framework for establishing interactions between the expert and DT to integrate scientific knowledge. Moreover, we provide information about the Python package and the Jupyter Lab Graphical User Interface we developed for interactive construction and analysis of DT. 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

We believe that the human element can add value when using DT in the environmental sciences and that interaction with experts should be an integral part of the model building process. How can we achieve this interaction? In **Figure 2** we present our idea of interactive DT analysis in a schematic flowchart, and we compare it to the classical approach. The figure highlights the differences between the classical and the interactive approach, the available options for the expert to input scientific knowledge and it distinguishes the role of the expert and the role of the algorithm in the process.





Domain Expert



Machine Learning  
Decision Trees

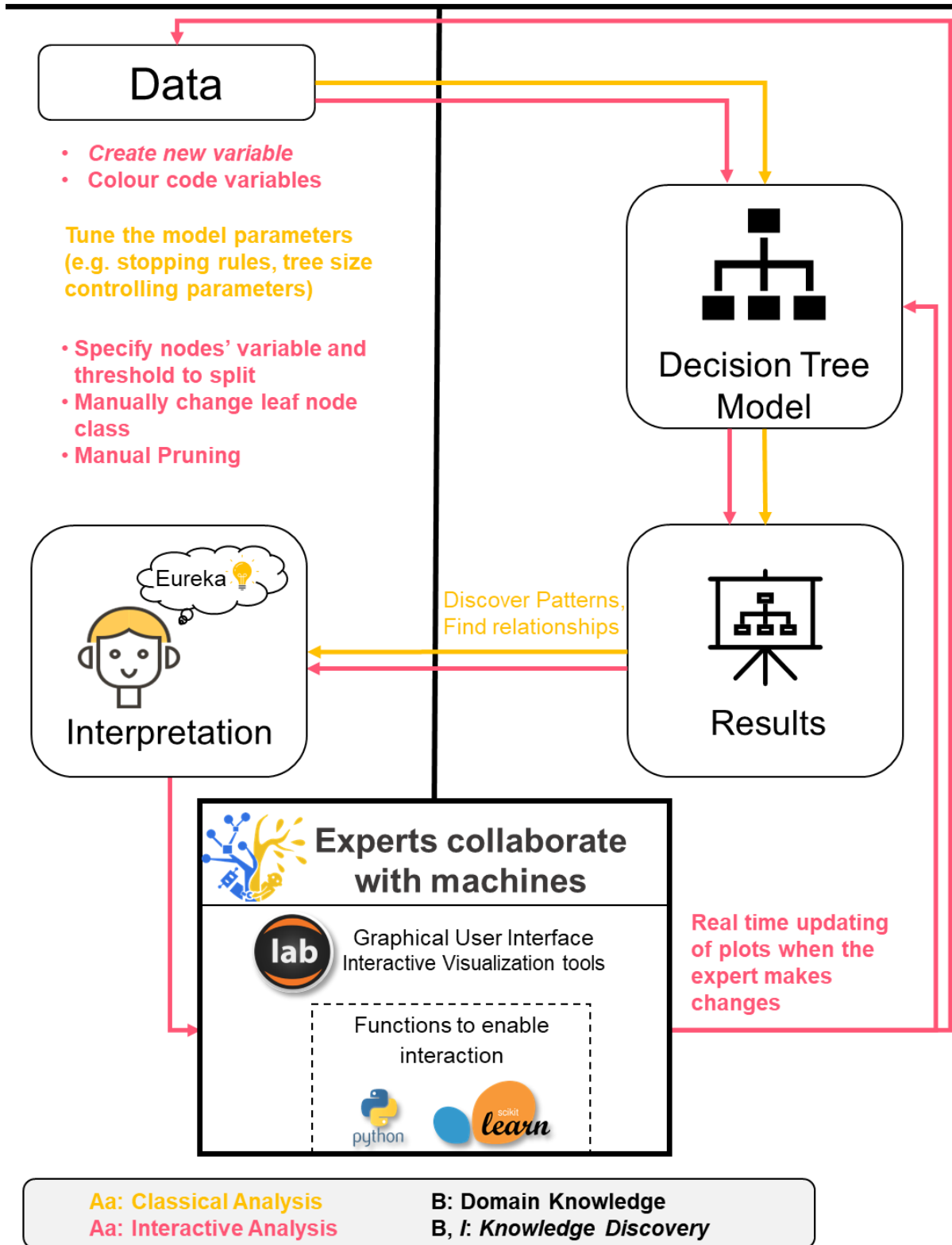


Figure 2 Flowcharts of Classical and Interactive analysis

In classical ML approach the expert is required to prepare data to feed to the ML algorithm, then specify tuning parameters and execute the algorithm to get a result, i.e. the classification/regression model (in our case a DT), which she then has to interpret. On the other hand, in the interactive analysis case, the experts can input their prior knowledge and/or feed back additional knowledge to the model discovered during the analysis, by:

- 1) organizing and (pre-)processing the dataset (e.g. group variables and colour code the groups or create new composite variables). For example, in many cases in environmental sciences the input variables represent different properties and/or processes (climatic controls, soil properties etc.). Experts might be interested to understand what properties dominate the DT. But currently standard DT provide no intuitive way to visualize that. Through iDT this information can be provided using an alternative nodes colouring that can be achieved easily by enabling the experts to group the variables and colour code the groups.
- 2) directly manipulating the structure of the DT model (e.g. specify nodes' variable and threshold to split, manually prune the DT or change leaf node class). For example, in cases of an imbalanced dataset, when a certain class is under-represented, the DT may not represent this class because it is not statistically relevant enough to influence the DT performance, though we might know that physically is quite important. There are different tactics proposed to combat this issue like, resampling the dataset (García and Herrera, 2009), generate synthetic samples (a well-known technique is SMOTE, Chawla et al., 2002), penalized models (penalties that bias the model to give more attention to the minority class) or collect more data. Even though the above methods are useful in overcoming this problem, some of them may require additional computation steps or data processing (resampling, synthetic samples, penalized models) and consequently are time consuming (Zhou et al., 2017). While others (like collect more data) may not even be feasible. iDT offer an easier and straight forward way to overcome this issue by manually forcing the model to include the under-represented class by manually changing nodes' variable and threshold to split and leaves nodes classes based on expert's knowledge.

## 2.2 Free and Open-Source modules in Python and Graphical User Interface in Jupyter Lab for Interactive construction and analysis of decision trees

Implementing the above framework as free and open-source codes or tools, contributes to the advancement of iDT for several reasons. Firstly, having access to the source codes of a tool will help people identify its strengths and weaknesses, understand if it is useful for their needs and whether and how it can be improved to fit to their case studies. At the same time, experts in our field would start using iDT in their research projects (or adjust it to their needs) more

quickly because they would not have to build their own from scratch. Furthermore, sharing software or codes helps in reproducibility of the results of a research project an issue that concerns environmental scientists (Gil et al., 2016; Hutton et al., 2016).

We looked for available software that could contain an implementation of the above described generic framework. We only found a limited number of papers in the scientific literature focusing on constructing DT interactively (Ankerst et al., 2000; Han and Cercone, 2001; Teoh and Ma, 2003; Do, 2006, van den Elzen and van Wijk, 2011), and two commercial softwares Dataiku (which is not open, but available to download for free <https://www.dataiku.com/>) and IBM SPSS (which is neither open nor free to download) that include an interactive tree plugin. The cited tools include many interesting functionalities e.g., expand nodes, manually change nodes' split, manual pruning. However, we did not use them as a baseline for our development for the following reasons:

- 1) They lack some of the functionalities we considered necessary for our study cases (see section 2.3). For example, the tool from (van den Elzen and van Wijk, 2011) did not include options for creating composite variables or grouping variables and colour coding the groups, and it could not handle the size of the datasets we used.
- 2) We could not gain access to the software for some of the tools we found in the literature.
- 3) Regarding the commercial softwares Dataiku and IBM SPSS, in addition to reason 1, their source codes are closed. This discouraged us from using it since we would not be able to edit, modify and build on and adjust it to our needs.

Therefore, to the best of our knowledge currently there are no available free and open-source codes or tools to interactively build a DT. Therefore, we created modules in Python and a Graphical User Interface (GUI) in Jupyter Lab for interactive construction and analysis of DT. The source codes are 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 "iDT" module which contains the functions that enable the expert to interact with the DT or the dataset and "iDTGUIfun" module which incorporates these functions into widgets that are used to create user interfaces for the implementation of expert DT interactions. Then, this is used in a Jupyter Lab script called "InteractiveDecisionTrees" which is essentially, the Graphical User Interface (GUI) that we created to support the user in the model building process. The presentation of the GUI is provided in the Supplementary material but bits of the GUI we have used in the cases studies of this paper are shown in the results section.

## 2.3 Evaluating DT predictive and interpretive performance

DT (and ML in general) are generally used as powerful predictive tools for classification and regression and therefore their evaluation was based on statistical metrics on how well prediction or classification has been achieved (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). Each metric may be more appropriate for certain situations, and we include typical metrics in our case studies below. However, in environmental sciences applications we would like DT to not only be good classifiers but also to be interpretable (Lipton, 2018). Consequently, we argue that evaluating models based only on prediction or classification accuracy is not sufficient in this context.

The second aspect we therefore want to consider in the evaluation of DT is their interpretive performance. Differently from predictive performance, interpretability is less established concept and metrics are not well established. A widely used proxy for DT interpretability is the complexity of the tree (Molnar, 2009; Lipton, 2018). Thus, DT interpretability could be quantified through the number of leaf nodes and/or the depth of the tree (Molnar, 2009). We adopt these simple metrics to quantify and evaluate DT interpretability in our first case study. We argue that visualization could play a significant role in interpreting the DT. Thus, we proposed a new nodes visualization based on physical meaning. The use of colours may provide useful insights (e.g. reveal the dominant physical characteristics of the DT) in the interpretation of the DT. Even though this is not a criterion to assess interpretability it is a qualitative way that makes the interpretation process easier for the expert. (Doshi-Velez and Been, 2017) suggests that one of the desired properties of interpretability is to assist scientific understanding and ensure physical consistency. However, sometimes DT interpretability for scientific understanding can be defined only in an application specific context. Therefore, we define specific interpretability criteria for case studies two and three, which we discuss in the next section.

## 3. Case Study Results

### 3.1 Case Study 1 – Increasing interpretability by colour-coding groups of variables and constructing new composite variables

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 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

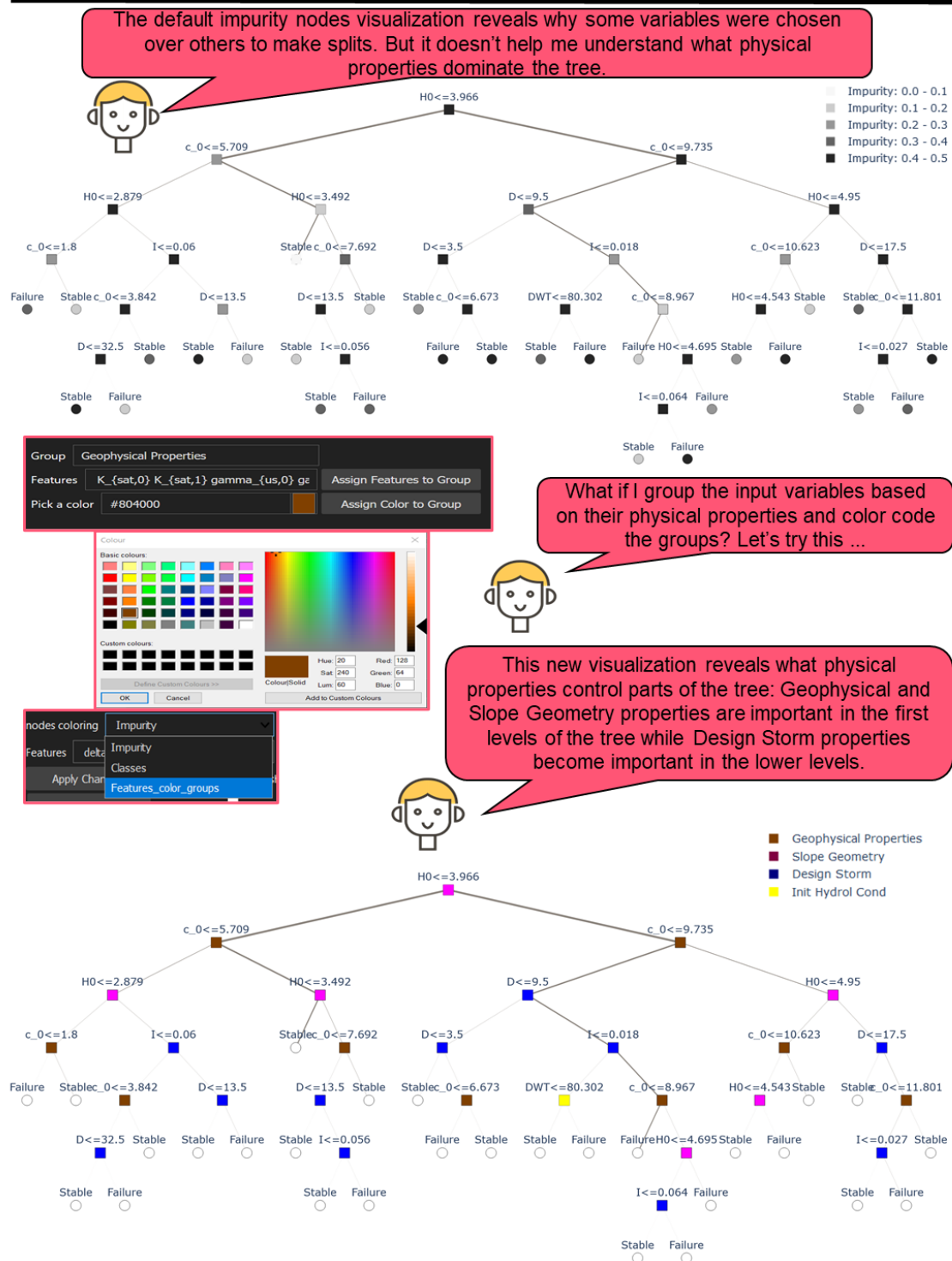
and Machine Learning toolbox) was used to identify dominant drivers of slope instability. We will apply our iDT procedure to the same dataset to demonstrate two functionalities of our iDT toolbox: how to increase the visual interpretability of the DT by colour coding variables based on their physical meaning (i.e. slope geometry, soil property, rainfall property); and how to capture interactions between variables by creating new composite variables. Using the composite variables enables the identification of a much smaller DT, which also contributes to increased interpretability.

Overall, the iDT derived in this case study is “better” to the standard one because it is more interpretable (in terms of visualization and complexity) and with slightly better classification accuracy on unseen data. In **Figure 3** we show the initial statistically optimal DT (nodes are coloured based on Impurity, a default choice in many softwares), the interface of the tools used to group the variables and colour code the groups, and the resulting tree with the alternative nodes colouring visualization. Using this node colouring visualization, it is evident that the first 2-3 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, it helps spotting a repeating combination of two variables in the first levels of the tree. Therefore, this first type of expert interaction with the tree facilitated spotting the type of variables dominating the tree and the existing interactions among input variables enhancing in that way the DT interpretability.

In **Figure 4** the initial DT, the interface of the tool used to create the new composite variables and the iDT tree is shown. The need to create the first variable is “revealed” to us from the DT model itself. The repeating combination of cohesion and thickness of topsoil in the first levels of the tree indicates that these two factors interact with each other. The first new variable that we created is called Soil Ratio and is the ratio of cohesion and thickness of topsoil ( $\text{Soil Ratio} = c_0/H_0$ ). The reason for creating the second variable is based on our domain knowledge. It is already known from the existing scientific literature that rainfall intensity and duration interact in the context of slope stability. This is also confirmed in levels 4 and 5 of our DT. The second new variable is called Storm Ratio and is the ratio of the logarithms of rainfall intensity and duration ( $\text{Storm Ratio} = -\log_{10}(D)/\log_{10}(I)$ ). In **Figure 4** the modified tree is overlaid on the initial tree which is 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. The figure shows how this second expert-DT interaction enabled the identification of a much smaller and thus more interpretable tree. More specifically, we significantly reduced the number of leaves nodes from 29 to 11, and the depth of the tree from 8 to 5. Moreover, classification accuracy on the training set remained the same and it was slightly improved on the test set as shown in **Figure 4**.



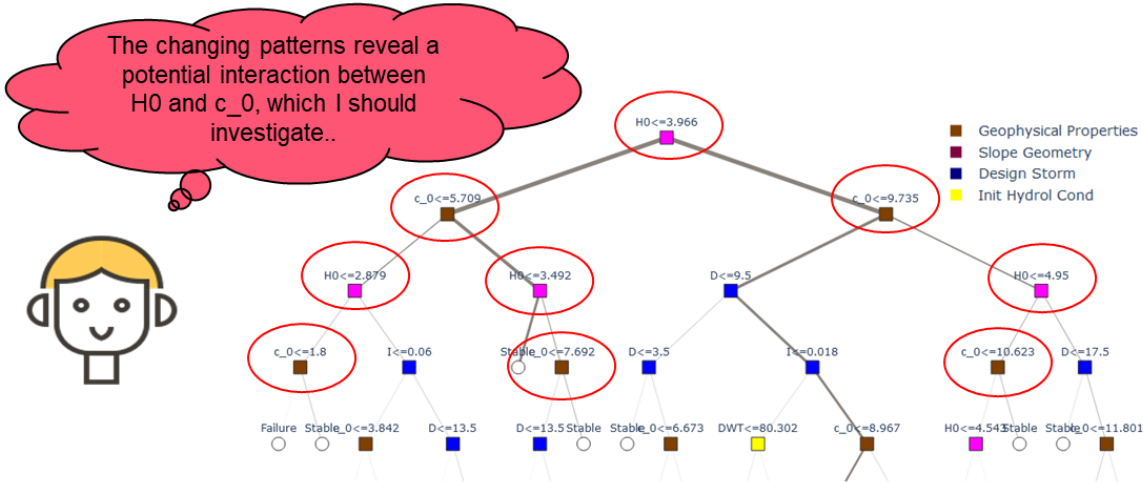
## Enhance DT interpretability through physically meaningful nodes visualization of expert based-color coded groups of input variables



**Figure 3** The tree in the top shows the default impurity nodes colouring and the bottom tree shows the proposed alternative nodes colouring visualization based on expert created colour coded groups. Using this node colouring 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 visualisation.



# Improve DT interpretability by reducing its complexity through the creation of new composite variables

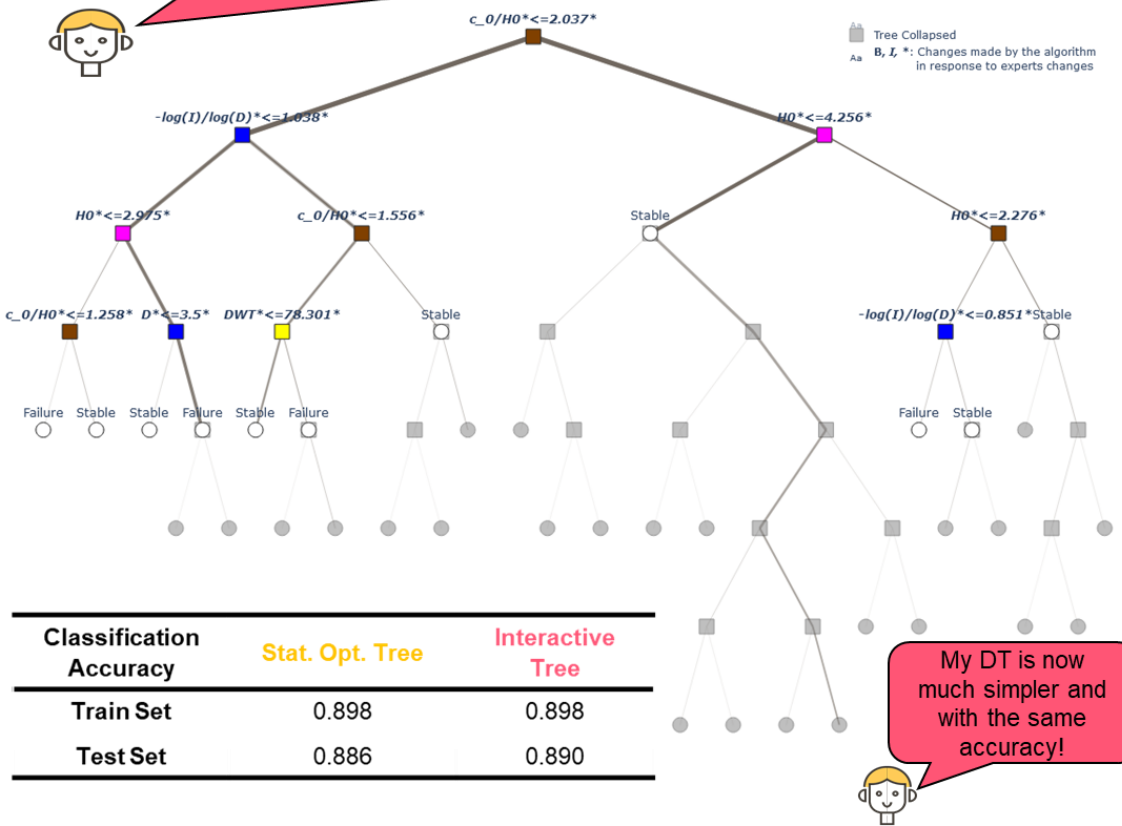


Indeed, the scatter plot confirms the interaction. But CART make splits only on a single axis. How can I benefit? Let's create a composite variable:  $c_0/H_0$

Variable Name:  $c_0/H_0$  Group Name: Geophysical Properties Equation:  $c_0/H_0$  Create Feature

I also notice that  $I$  and  $D$  appear multiple times and I know from the literature that they interact in the context of landslide stability. Let's create another composite variable:  $-\log_{10}(I)/\log_{10}(D)$

Variable Name:  $-\log_{10}(I)/\log_{10}(D)$  Group Name: Design Storm Equation:  $-\log_{10}(I)/\log_{10}(D)$  Create Feature



**Figure 4** 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 which 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.

### 3.2 Case Study 2 – Improve DT interpretability by finding physically meaningful connections of the DT classes with other relevant scientific 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 and land cover types. The model outputs are recharge values which are classified into four classes, namely, C1 (<20 mm/yr), C2 (20 – 100 mm/yr), C3 (100 – 300 mm/yr) and C4 (>300 mm/yr). Applying any tree algorithm will produce a DT which shows how the different input variables are combined to produce more or less recharge. We apply our iDT procedure to show that experts can achieve physically meaningful interpretations of the DT classes more consistently than standard algorithms. To demonstrate that, we manually change nodes' thresholds to map the recharge classes (leaves nodes) of the DT to climatic zones. For this purpose, we use a simplified version of the Holdridge life zones classification scheme. It is a triangle chart for classifying land areas based on precipitation and aridity index (ratio between potential evaporation and precipitation). **Figure S.2** in the Supplementary material shows the original and our simplified scheme.

We derived statistically optimal (SO) and interactive (iDT) DT for 15 different random samples of limited size: dimensions are [1000, 34]. To derive the SO DT, we set up the following parameter space:

- Criterion: [gini, entropy]
- Max\_leaf\_nodes: [15:26 or 30, step=1]
- Min\_impurity\_decrease: [ $10^{-5}$ ,  $10^{-6}$ ,  $10^{-7}$ ]

All the possible combinations of parameter values were evaluated based on 10-fold Cross Validation strategy, and the best combination was retained. To derive the iDT we manually change the Precipitation and Aridity Index thresholds based on the Holdridge chart thresholds. The thresholds appearing in the SO DT are the optimal values, but these are not necessarily physically meaningful ones. On the contrary, we argue that the thresholds appearing in the Holdridge chart represent the accumulated, scientific knowledge and are physically meaningful values.

The results of this case study indicate that iDT are better models than the standard ones because they enabled a more meaningful connection of the DT classes with other scientific information that was relevant to us, thus improving DT interpretability without significant loss of classification performance. Classification performance results showed that statistically optimal DT perform always better in the training sets as expected. But iDT outperform statistically optimal trees in most cases in the test sets (9 out of 15). The differences in the accuracies in both sets are not pronounced which is a good indication that the changes made



by the expert did not lead to a significant loss of performance. Moreover, incorporating scientific knowledge to DT by manually changing statistically optimal thresholds to scientifically meaningful ones decreased the number of diamonds some leaves nodes can be mapped to, leading to more concise mapping of two out of four recharge classes of the DT to land area types. Indicatively, we selected one of the 15 pairs of DT and plotted them in **Figure 5 (a and b)**. The number below the leaves nodes of each DT denotes the number of diamonds the leaf is mapped to. The most significant reduction in the number of diamonds is seen in the middle part of the tree. Moreover, for selected nodes we plotted the Holdridge scheme and highlighted the diamonds the leaves are mapped to. In **Figure 5c** we plotted the average decrease in the number of diamonds for each recharge class and for the whole DT. The biggest reduction is observed for classes C2 (20-100 mm/yr) and C3 (100-300 mm/yr).

Enhance DT interpretability by manually changing nodes' thresholds.

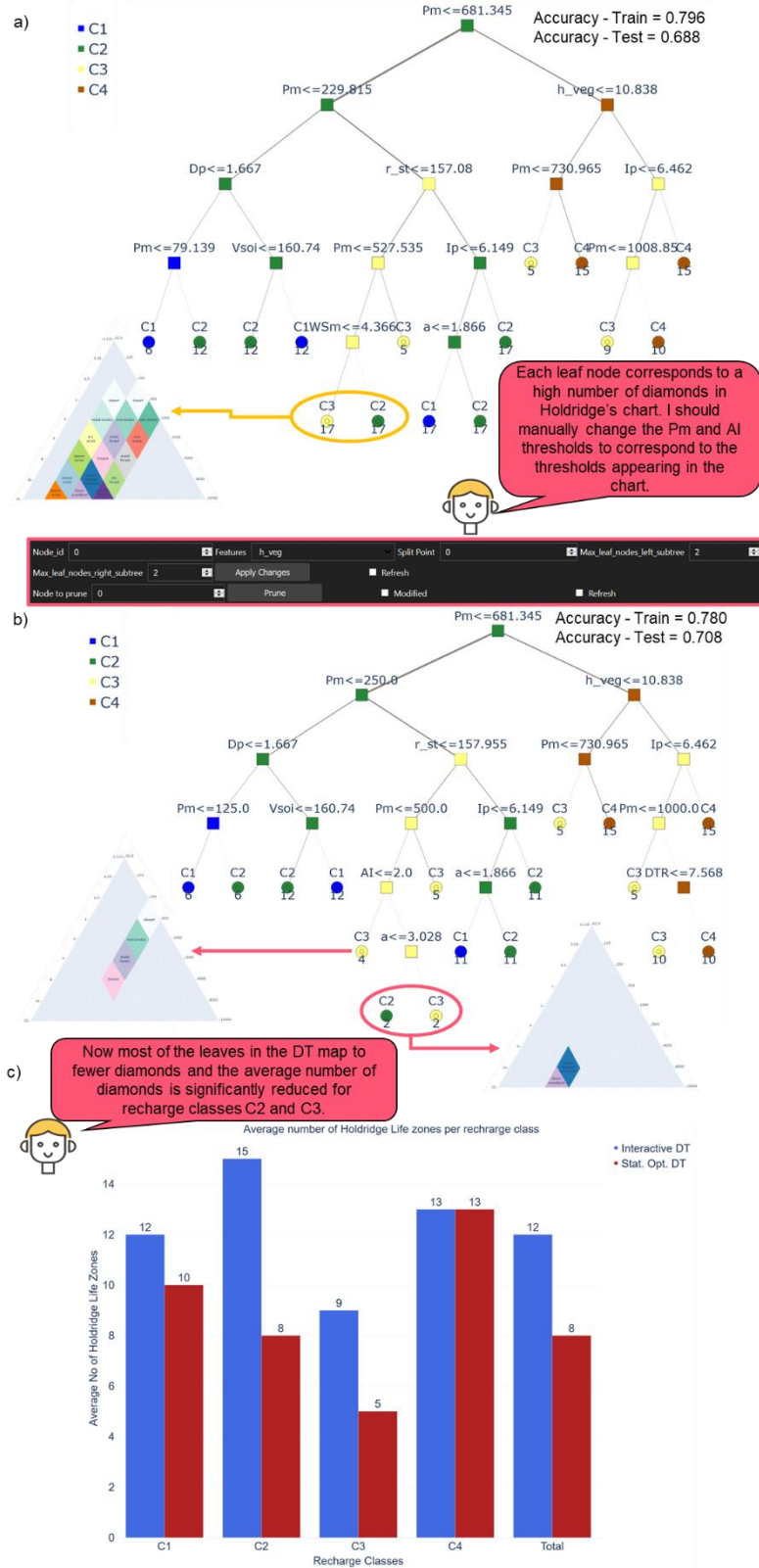


Figure 5 a) Statistically optimal DT, b) iDT (the UI of the tool used to manually change nodes' thresholds is shown on the top of the DT), c) Average number of Holdridge Life Zones per recharge class and for the DT in total. Below the leaves nodes of each DT there is a number denoting the number of diamonds 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.*

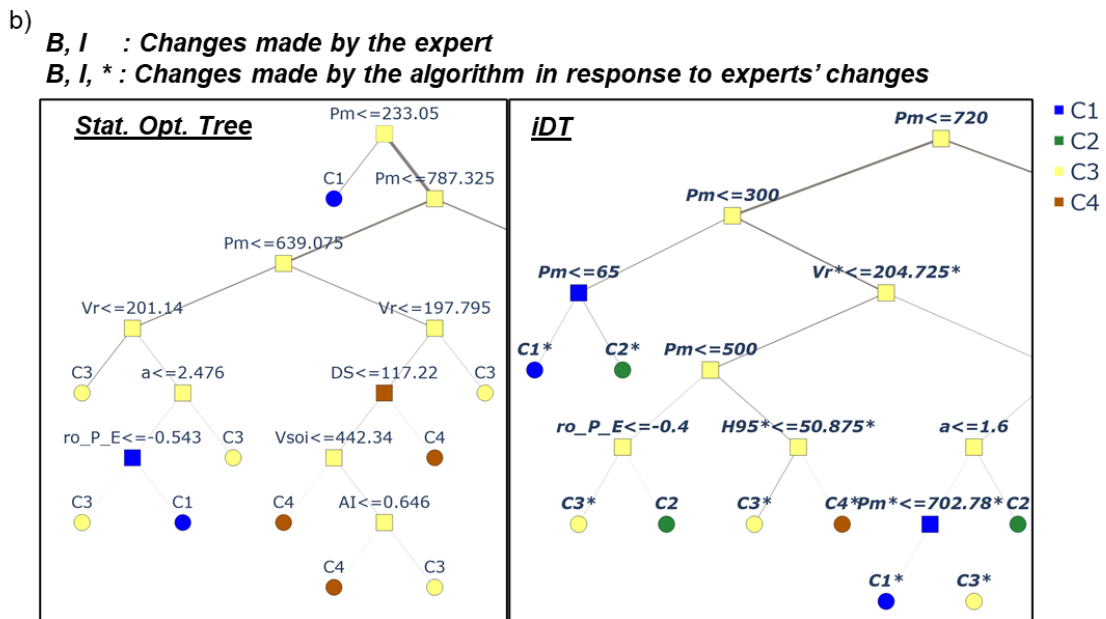
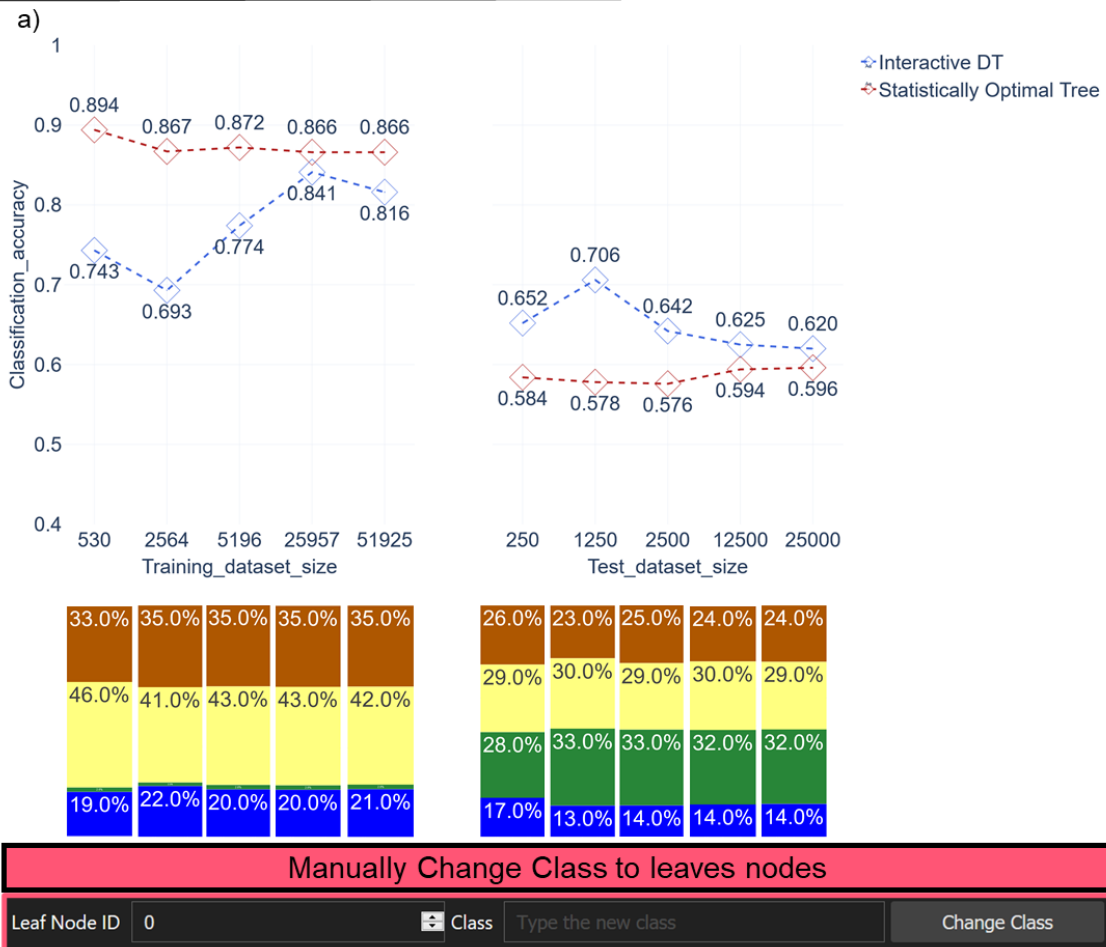
### 3.3 Case Study 3 - Ensure physical consistency of the DT by manually changing nodes' variables and thresholds to split and leaves nodes classes

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 the dataset from Sarazin (2018) (described above) and created sample datasets of 5 different sizes ([1000,34], [5000,34], [10000,34], [50000,34], [100000,34]). We then split each sample dataset into train and test sets (75% and 25% of the sample dataset size respectively). Finally, from the training sets we randomly remove data points that belong to C2 class. Therefore, the training sets contain only few instances of class C2 (<2%) while the test sets have a more balanced representation of the classes. The objective here is to ensure that important classes will appear in the DT even if they are under-represented. To achieve that we manually change nodes' variables and thresholds to split and classes in leaf nodes.

Results of this case study suggest that iDT are more suitable to use in cases of imbalanced datasets because they are physically consistent (they include C2 class even though there are only few data points of this class in the sample datasets) and with better classification performance on unseen data. In Figure 6a we show that statistically optimal trees perform always better in the training sets as expected. However, iDT outperform statistically optimal trees in all cases in the test sets. The differences in the accuracy are more pronounced for small sample datasets and they decrease while the dataset sizes get bigger. Moreover, in Figure 6b we show the initial and the iDT with the expert's modifications for one of the cases. By making amendments only to the left part of the tree and even though C2 class has only few data points in the training dataset, the difference in the performance for the two DT on unseen data, is significant in this case.



## Ensure physical consistency of the DT by manually changing split points/features to split and leaves nodes classes



**Figure 6 a)** Classification accuracies for statistical optimal (left) and interactive (right) 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 **b)** Statistical optimal (left) and interactive (right) DT for the case with the biggest difference in classification performance (the UI of the tool used to manually change nodes variables and thresholds to split is shown on the top of the DTs).

## 4. Conclusions and outlook

This work is probably the first effort in environmental sciences to propose an interactive framework for the construction and analysis of DT. In our framework, experts can interact with the DT by modifying the underlying data or the tree structure by creating new composite variables, grouping variables and colour coding the groups, manually changing nodes' variables and thresholds to split, manually changing leaf node classes and manual pruning. We created an open-source implementation of iDT in Python and Jupyter Lab and we hope this will encourage the use of iDT in more research applications in environmental sciences. Our application of iDT to three different case studies - representing typical situations that we encounter in the environmental sciences - shows an interactive approach can address a range of typical challenges. The integration of classical automated strategies and human involvement can increase DT interpretability, ensure physical consistency, and achieve meaningful interpretations of the models they build. Finally, we hope that this paper is a first step in building the foundations for integrating scientific knowledge through the development of interactive ML methods and encourages follow-on work in this direction.

The methodology and results of the case studies show that DT have the potential to become even more meaningful for experts; besides being used only for predictions they can also be used as interpretive tools. This could be achieved if more future efforts focus on defining DT interpretability more coherently and find ways to properly measure and/or assess it. We believe we contributed to this evolution with the development of interactive DT. Even though there is need to define more generic ways to measure or assess interpretability, the proposed framework and implementation of iDT provides a flexible new tool for experts. Enabling the construction of DT that are meaningful within an expert's own knowledge framework and application context.

The framework presented in this paper is a first attempt for expert DT interaction in an environmental sciences context and there is a lot of space for further improvement. It would be interesting to achieve closer expert interaction with the algorithm that produces the DT. For example, experts could force the algorithm to search for thresholds in a specific range of values for selected variables. In this way avoiding physically inconsistent splits in the DT. Or they could define constraints on variable selection to eliminate unrealistic sequence of variables to split. Expert DT interaction is essential to increase DT interpretability. This interaction should be supported with plots that are helpful for tree interpretation. What if it is not obvious how the variables of a dataset are related? (Molnar 2009) discusses key concepts about interpretability of ML methods and there are many plots (e.g. partial dependence plots,

accumulated local effects, feature interaction) that could be used in parallel to the main visualization of the DT to enhance its interpretability.

## 5. Software and Data availability

The Python package “InteractiveDT” and the Jupyter Lab InteractiveDecisionTrees notebook, are widely available on the GitHub repository <https://github.com/Sarailidis/Interactive-Decision-Trees> (<https://doi.org/10.5281/zenodo.5011487>). In the same repository the datasets used in the case studies presented in this paper are provided. In addition, the repository includes workflows to reproduce the results of the case studies presented in this paper.

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