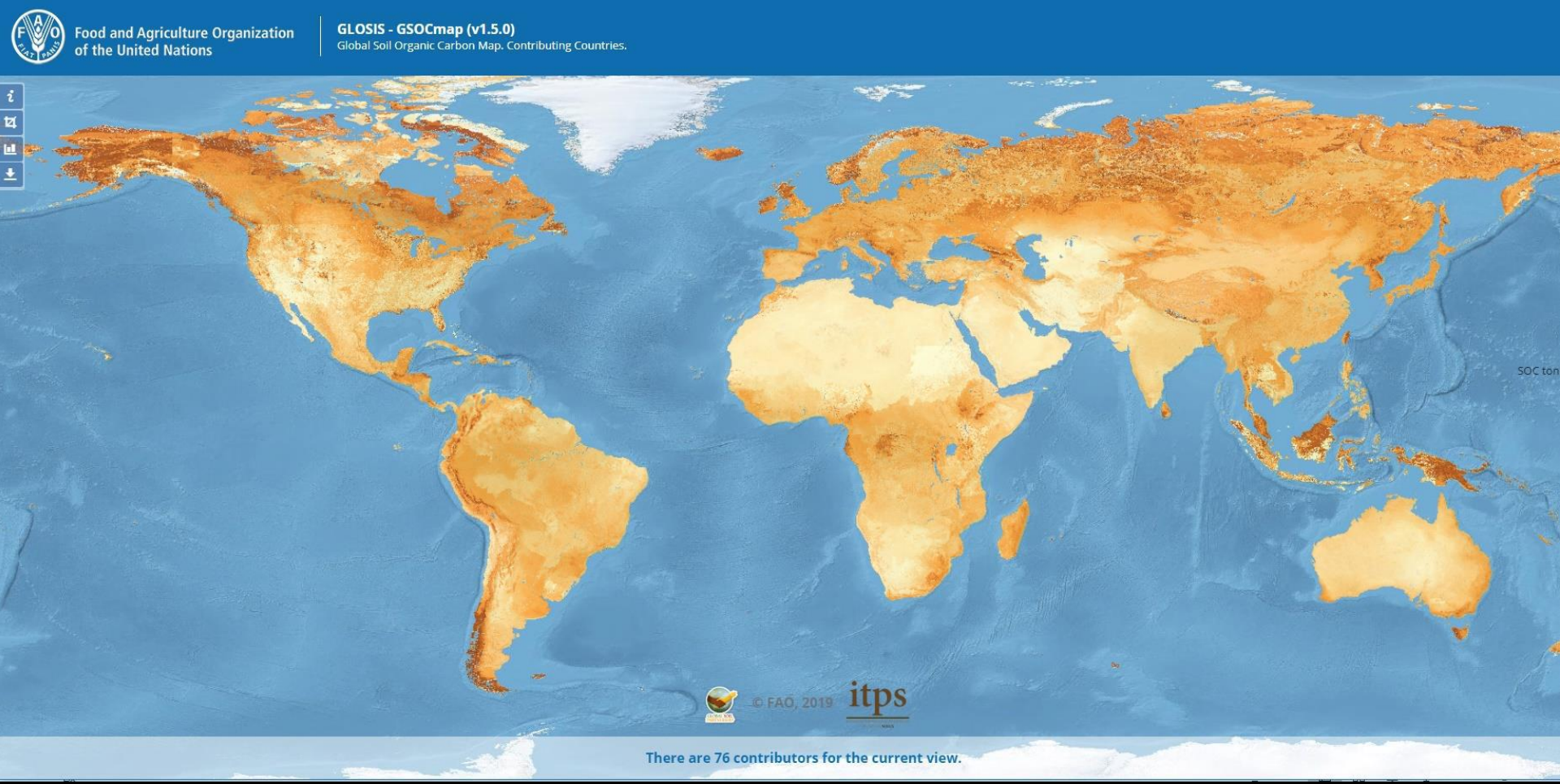

Machine Learning for Digital Soil Mapping-Part 1

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Content

- **Part 1**
  - **Digital Soil Mapping**
  - **Machine Learning**
    - **Decision Tree**
    - **Random Forest**
- **Part 2**
  - **Lets practice!**

SCORPAN model

$$S = f\ (s, c, o, r, p, a, n) + \varepsilon$$

S : Soil, at a specific point in space and time: soil classes, Sc or soil attributes, Sa

From Jenny's Equation

c : climate, climate properties of the environment;
o : organisms, vegetation;
r : topography, landscape attributes;
p : parent material, lithology;
a : age or time factor;

Additions:

s : soil, prior knowledge of the soil at a point;
n : space, relative spatial position;
ε : auto-correlated random spatial variation.

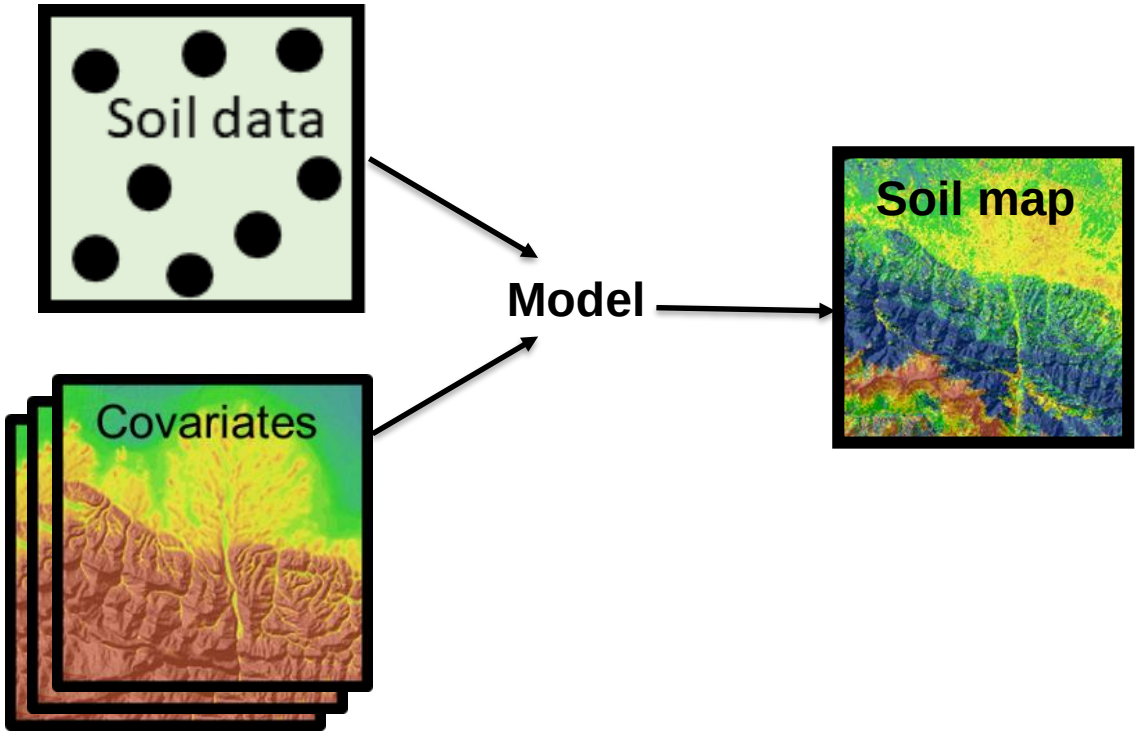
f() : Quantitative function *f* linking S to ***scorpan*** factors

McBratney et al., 2003

SCORPAN model

$$S = f(s, c, o, r, p, a, n) + \varepsilon$$

- S: Soil data
- f: Model
- (s, c, o, r, p, a, n): Covariates
- ε: spatially dependent residuals



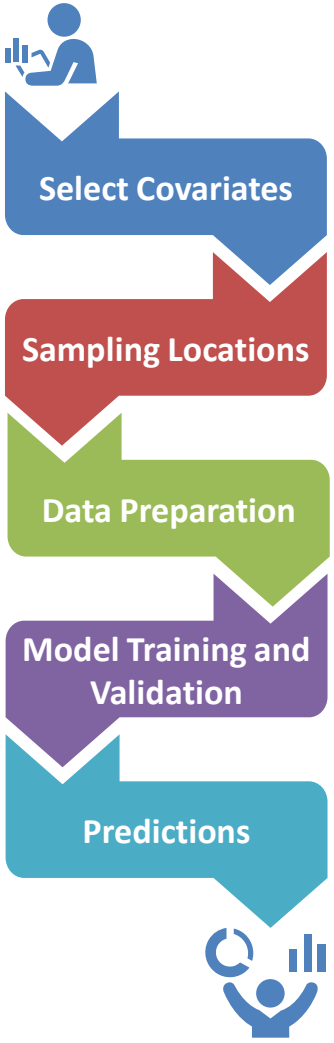
SCORPAN Model

$$S = f(s,c,o,r,p,a,n) + \varepsilon$$

Machine learning

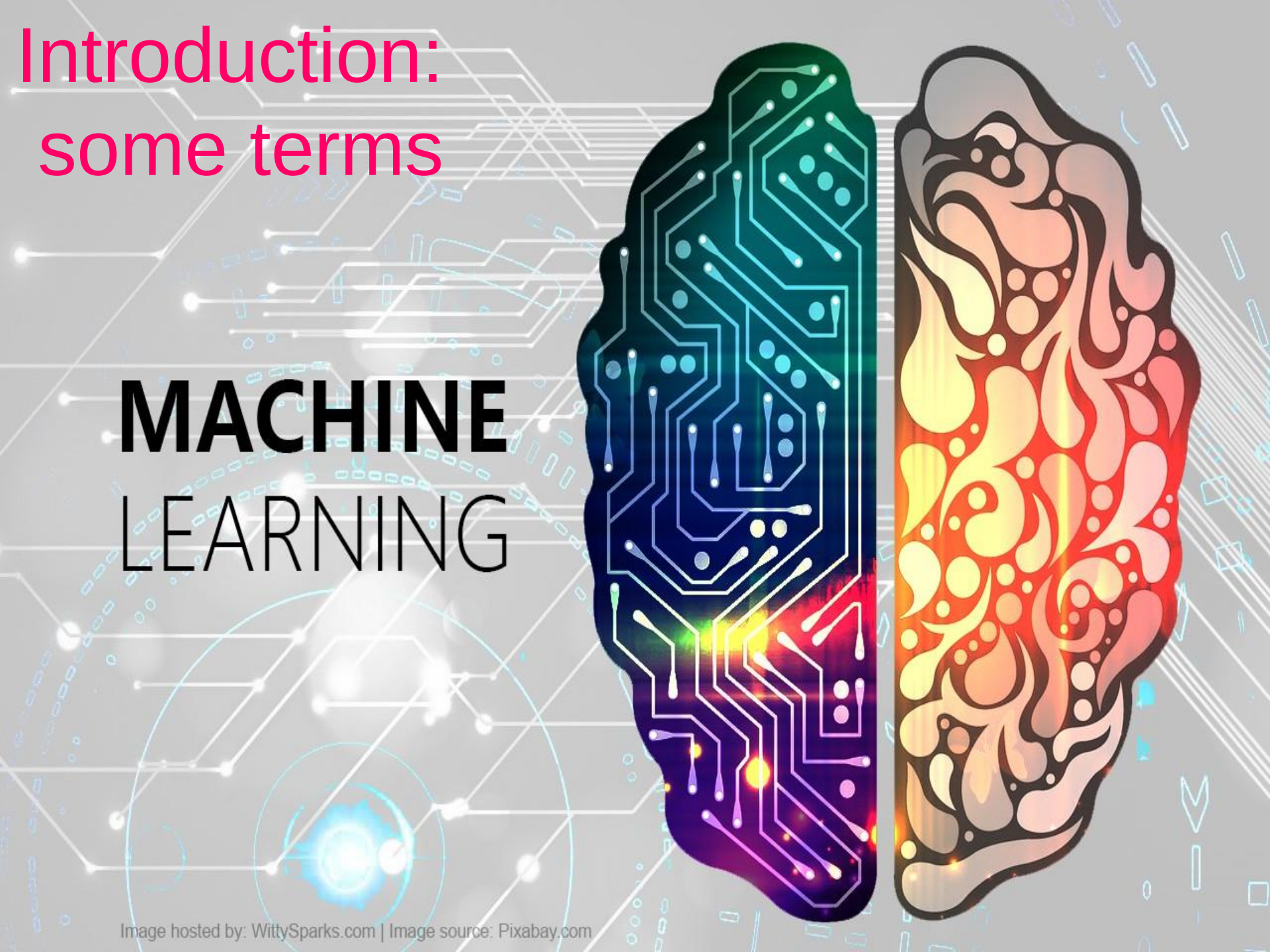
f() : Quantitative function *f* linking S to ***scorpan*** factors

Sequence of DSM Steps

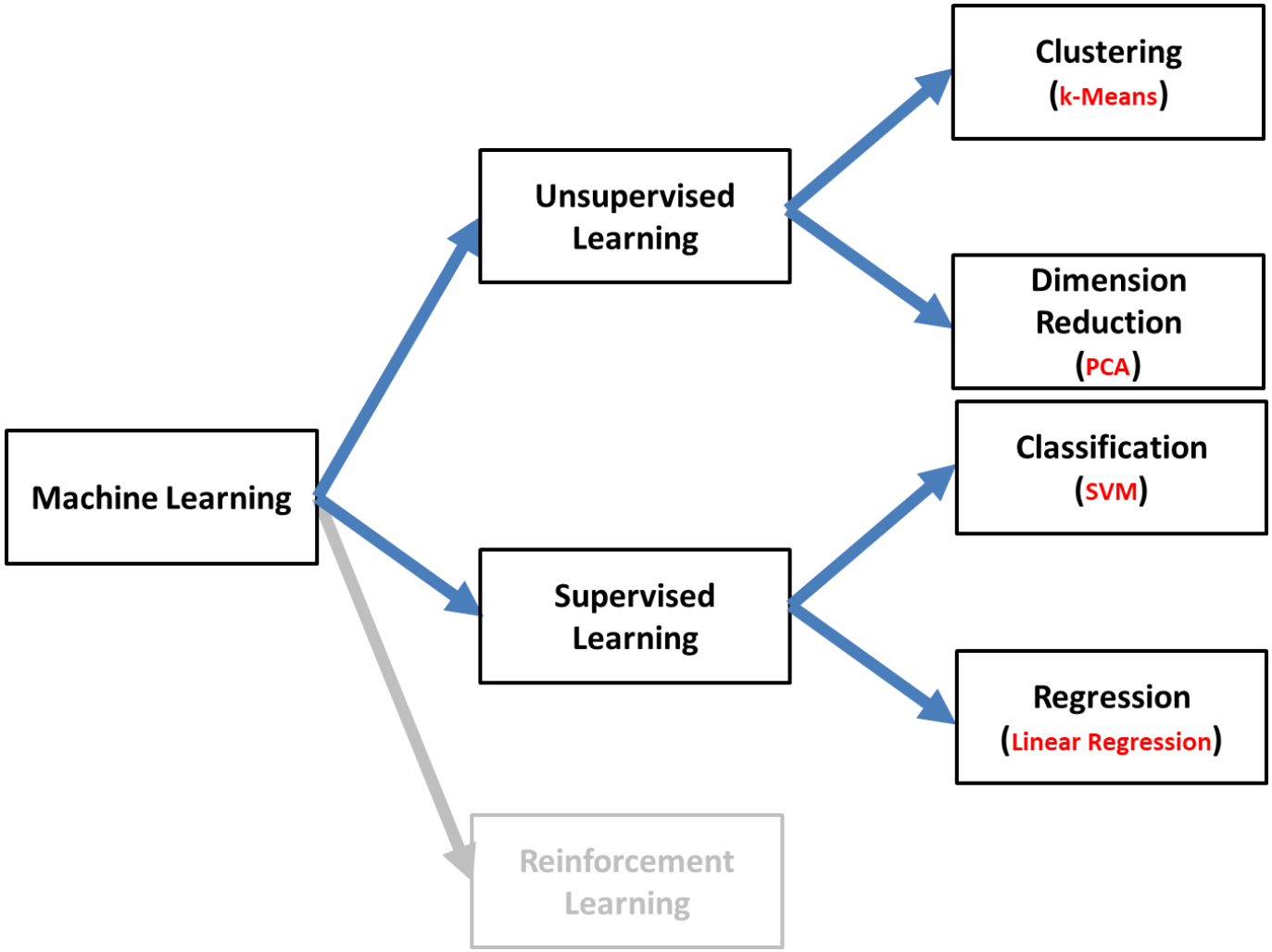


1. Environmental covariates, relevant as predictors of soil property/class, are derived from remote sensing, digital elevation, climatic datasets, …
2. Soil samples are collected at the specified locations (e.g., Latin hypercube sampling) and soil property is measured in the laboratory.
3. Intersecting the covariates with the soil point observations.
4. Machine learning models (e.g., random forest) are trained using training data, and accuracy assessment is carried out using the test data set.
5. The ML models are applied to the entire study area in order to produce a soil property/class map.

Introduction: some terms



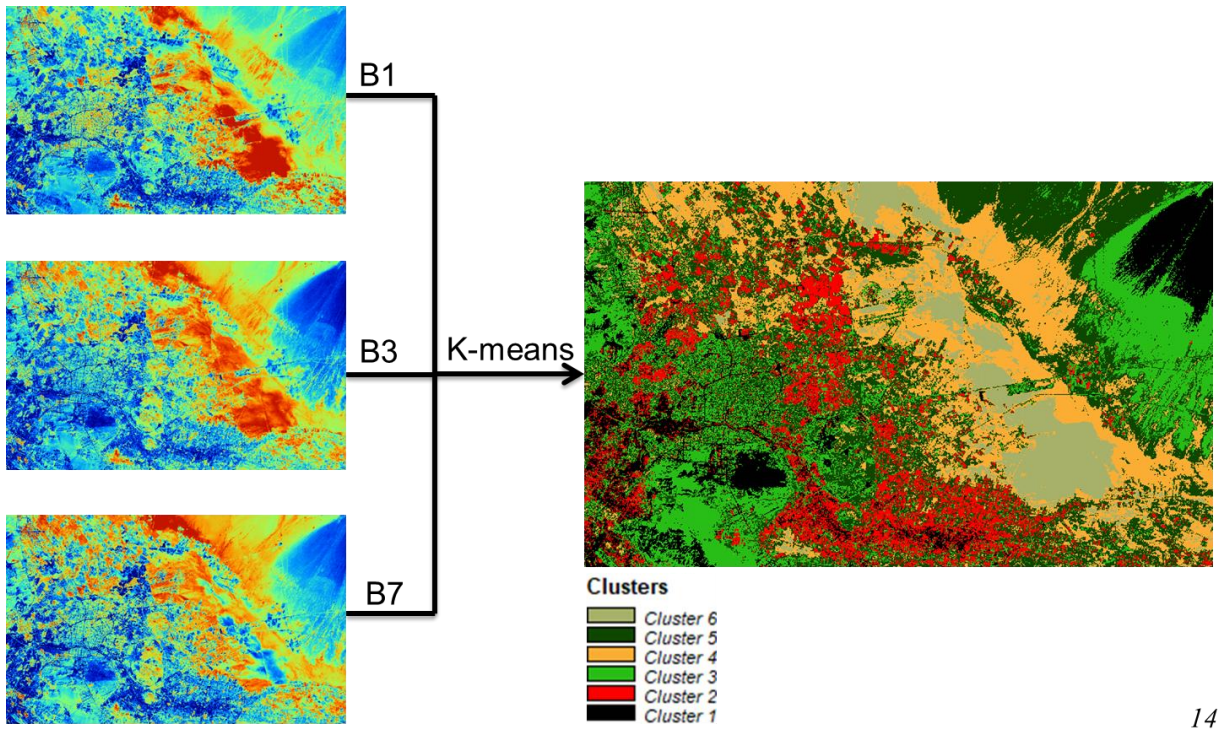
Types of Machine Learning



Unsupervised Learning

Unsupervised learning

- No response, **just** "*covariates*", (x_i)
- Algorithm identifies clusters
- No training data required
- e.g., clustering of satellite image by similar values



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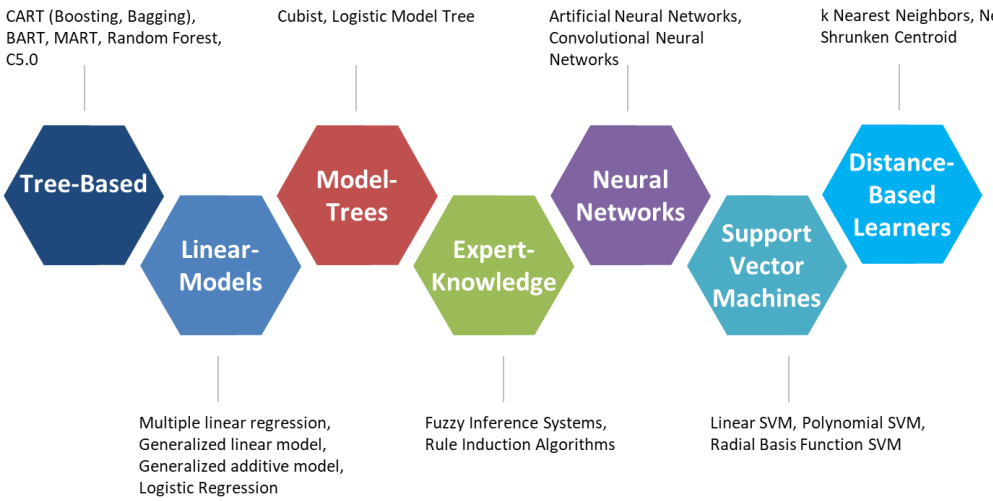
Supervised Learning

Supervised learning

- For each covariate value $\mathbf{x}_i$ there is also a response value $\mathbf{y}_i$
- → e.g. random forest
- ⟶ what we usually do for soil mapping

Supervised learning

- – Regression: continuous responses, e.g. soil clay content, rainfall
- – Classification: categorical responses (binary or multinomial), e.g. soil type



Things to Keep in Mind

- Each model predicts one realization of a DSM

- Effectiveness of the model are dependent on:
  → Study Area (Extent and Resolution)
  → Target Variable
  → Environmental Covariates
  → Model Structure (e.g. Linear vs. Hierarchical)

- Each model has its own set of hyperparameters (i.e. model settings) that need to be optimized.

- Some models are more computationally efficient than others.

- Each model may produce drastically different results given the same inputs.

- Some models tend to overfit.

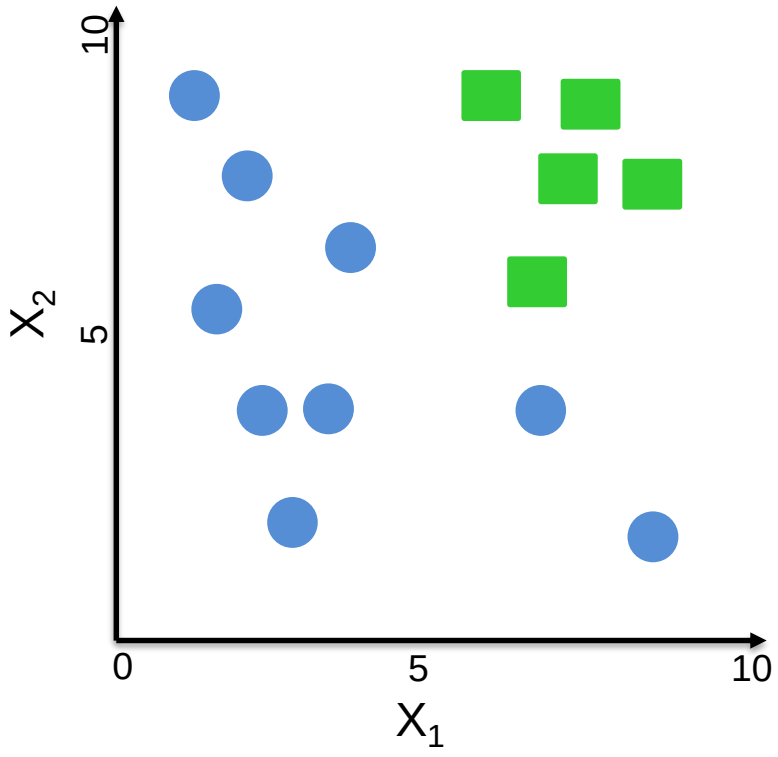
From Available Models

Decision Tree

Decision Tree: Definition

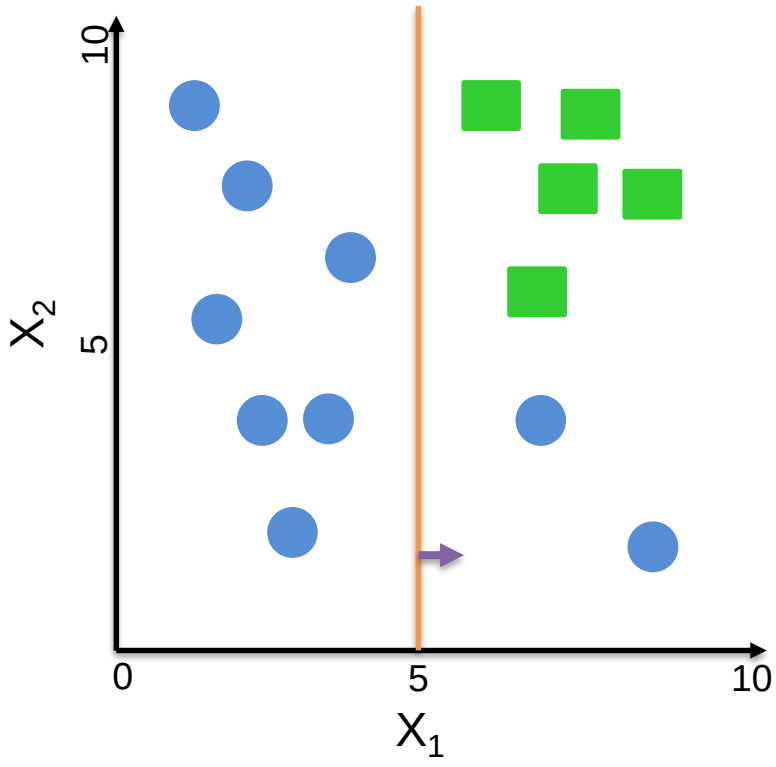
- Decision Tree is a supervised learning approach.
- It can be used for solving regression (e.g., clay content) and classification (e.g., soil types) problems.
- It partitions the data into subsets.
- The partitioning process starts with a binary split (Yes-No) and continues until no further splits can be made.
- It predicts the outcome by asking a set of if-else questions.
- It resembles a tree-like graph, easy to understand

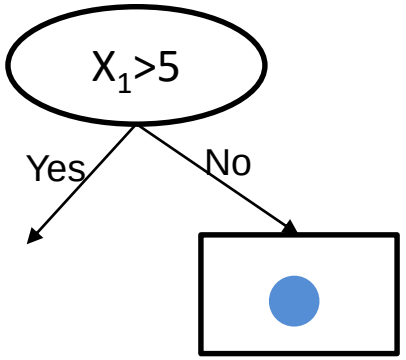
Decision Tree: example I



Example of a dataset and the corresponding decision tree. (Alpaydin, 2010)

Decision Tree: example I





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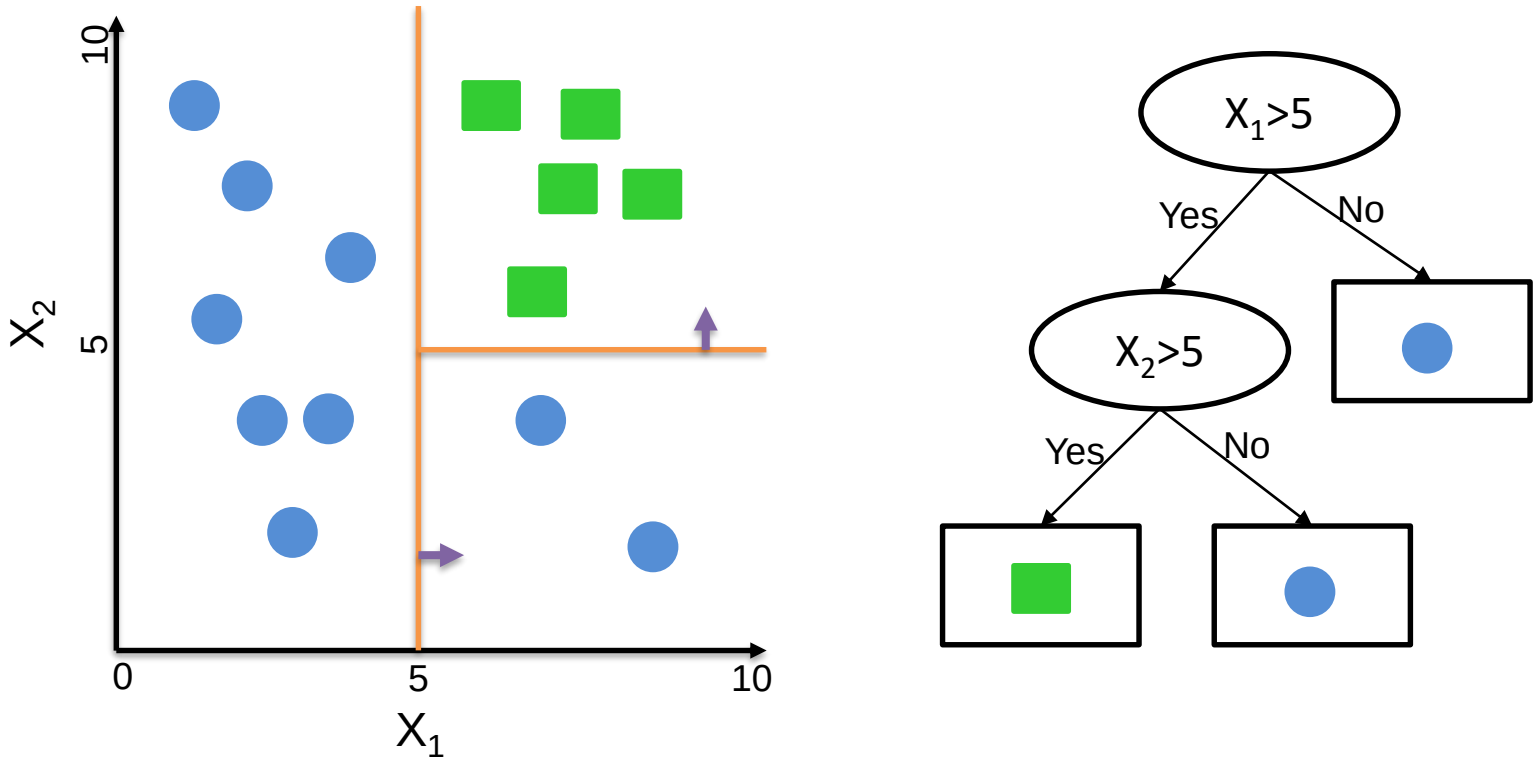

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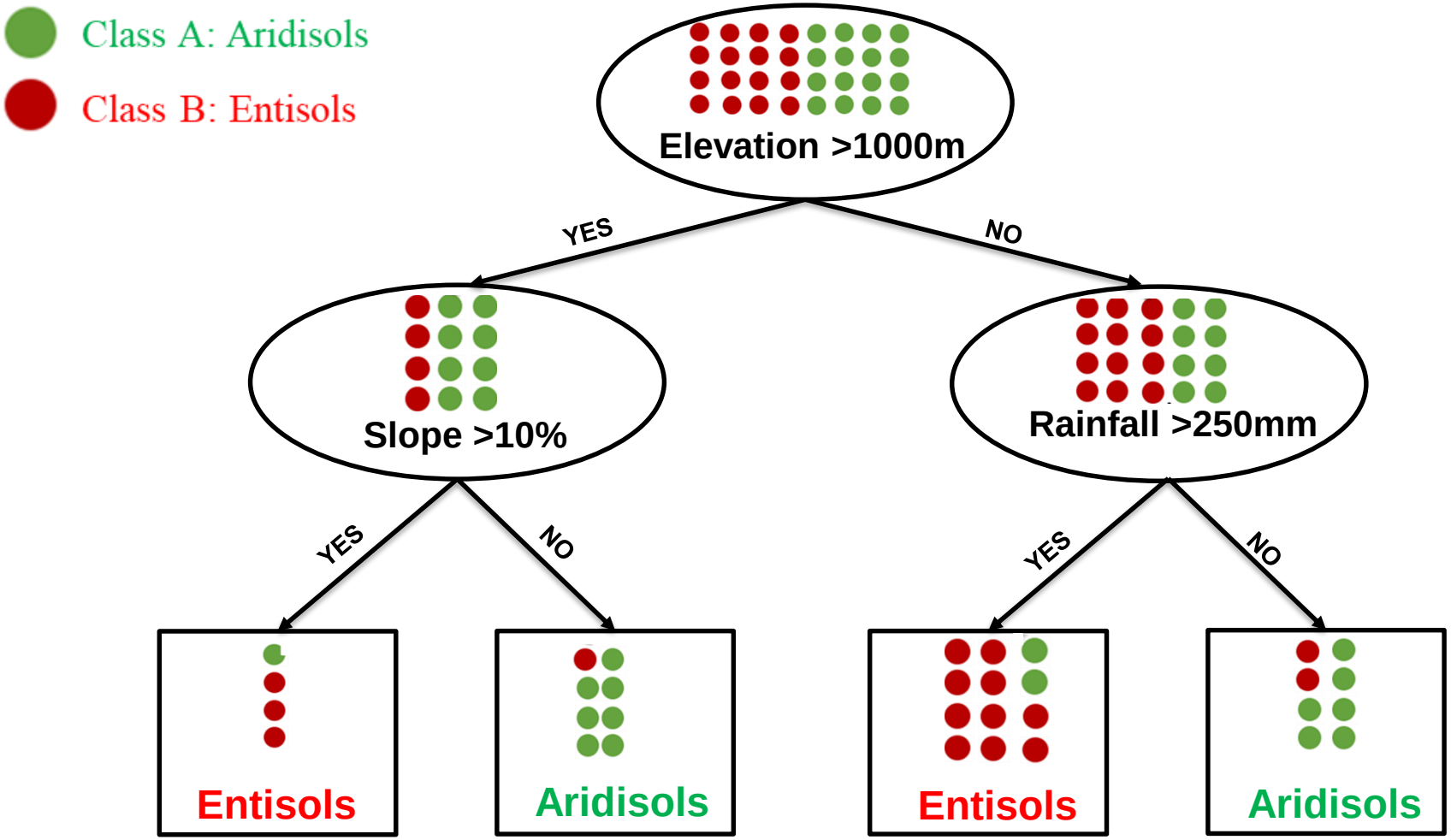
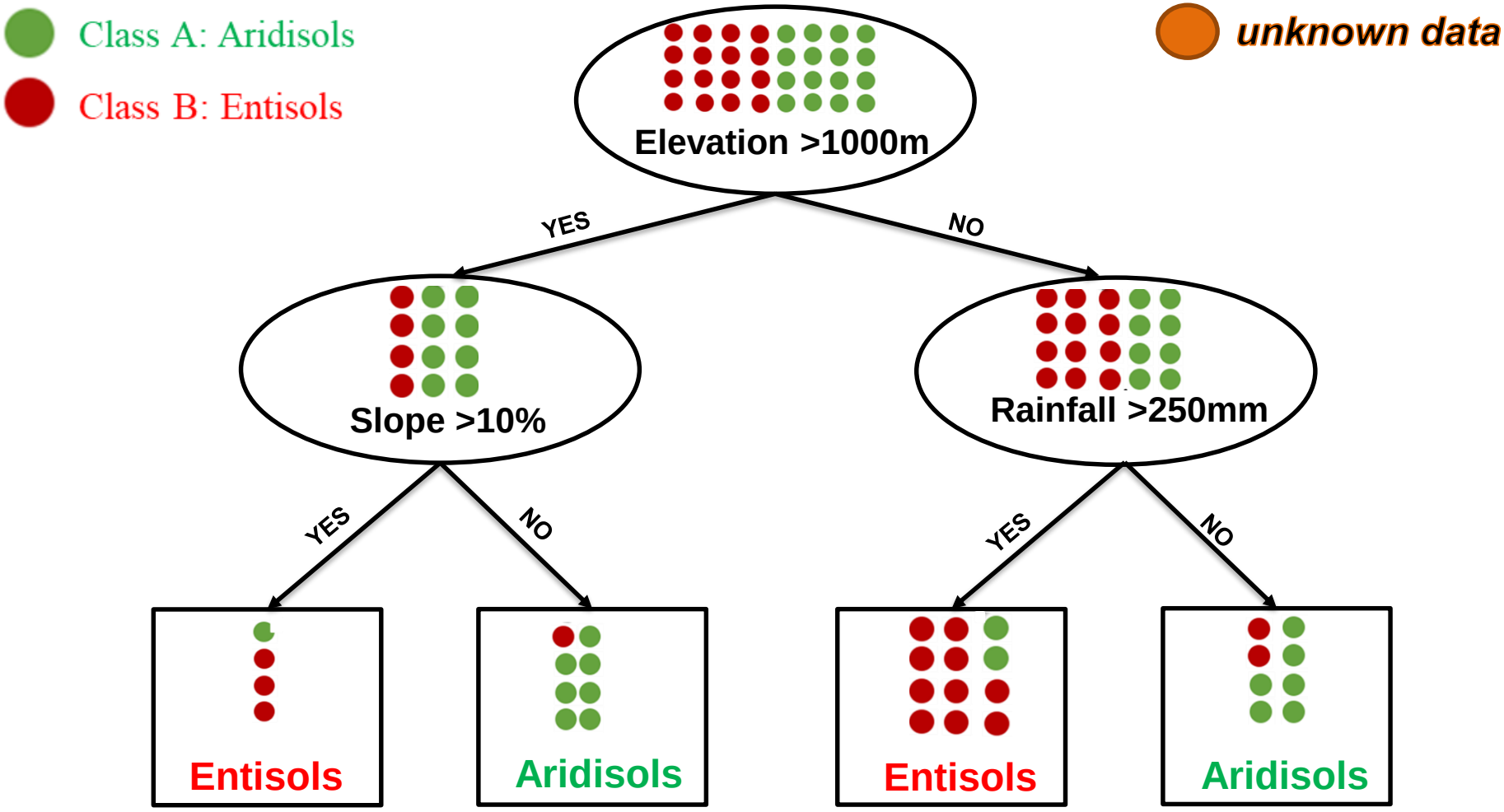
Decision Tree: example II



A decision tree model to predict Entisols and Aridisols

Decision Tree: example II



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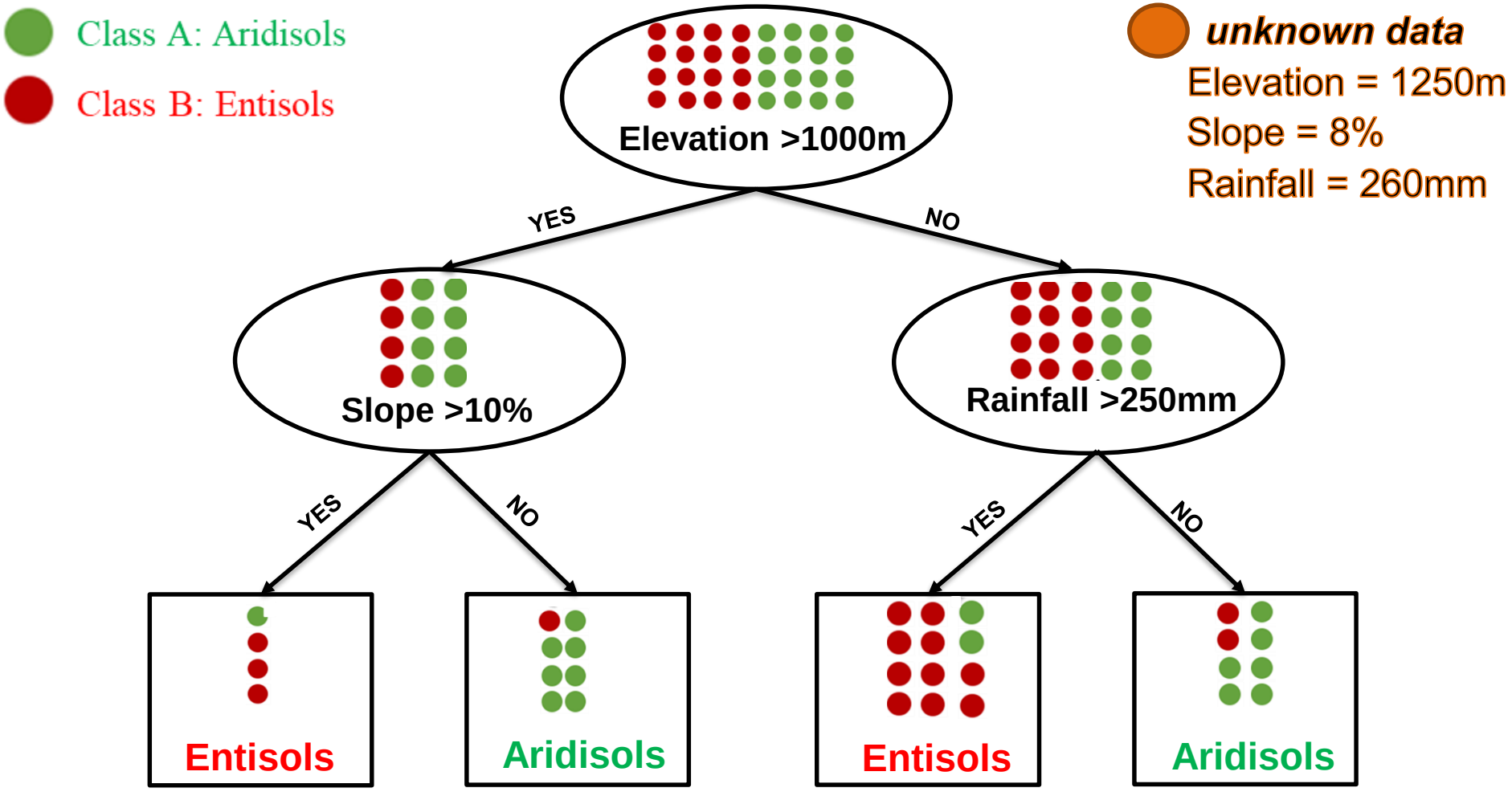

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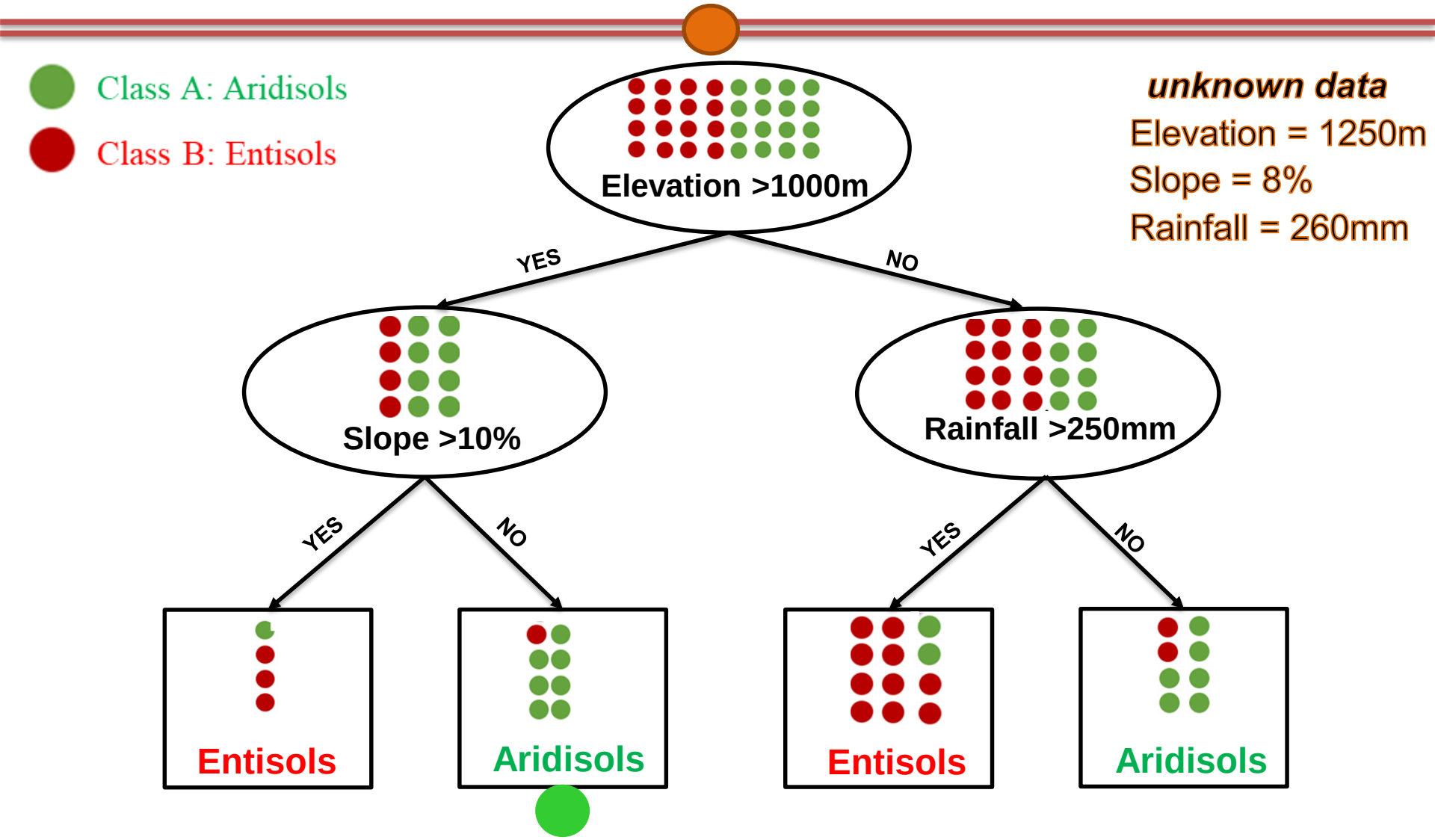
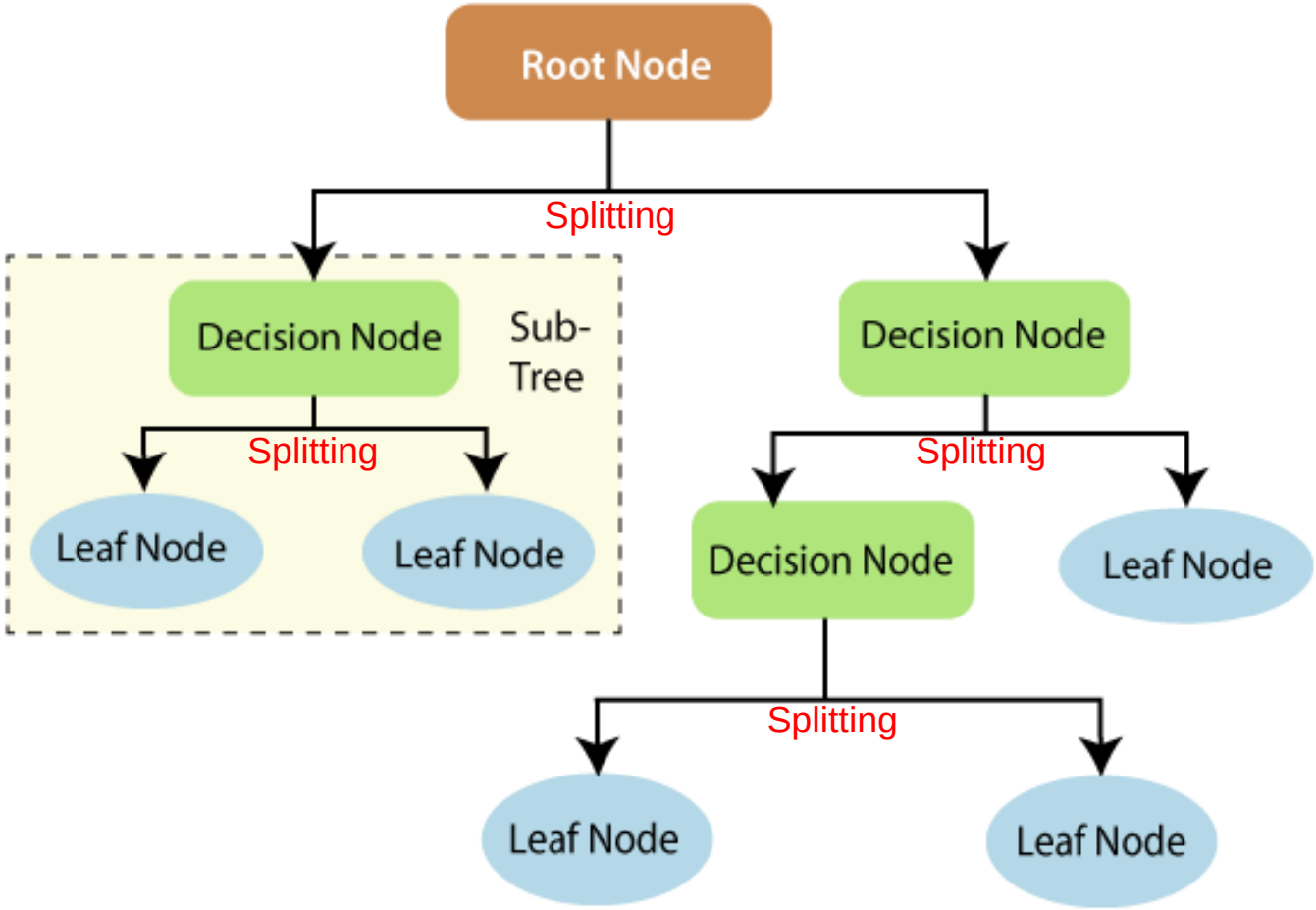


A decision tree model to predict Entisols and Aridisols

Decision Tree: graphic



https://www.kdnuggets.com/

Decision Tree: Terminology

- Root Node: It represents the entire population or sample and this further gets divided into two or more homogeneous sets.
- Decision Node: When a sub-node splits into further sub-nodes, then it is called the decision node.
- Leaf/Terminal Node: Nodes do not split is called Leaf or Terminal node.
- Parent and Child Node: A node, which is divided into sub-nodes is called a parent node of sub-nodes whereas sub-nodes are the child of a parent node.
- Splitting: It is a process of dividing a node into two or more sub-nodes.
- Pruning: When we remove sub-nodes of a decision node, this process is called pruning. You can say the opposite process of splitting.
- Branch/Sub-Tree: A subsection of the entire tree is called branch or sub-tree.

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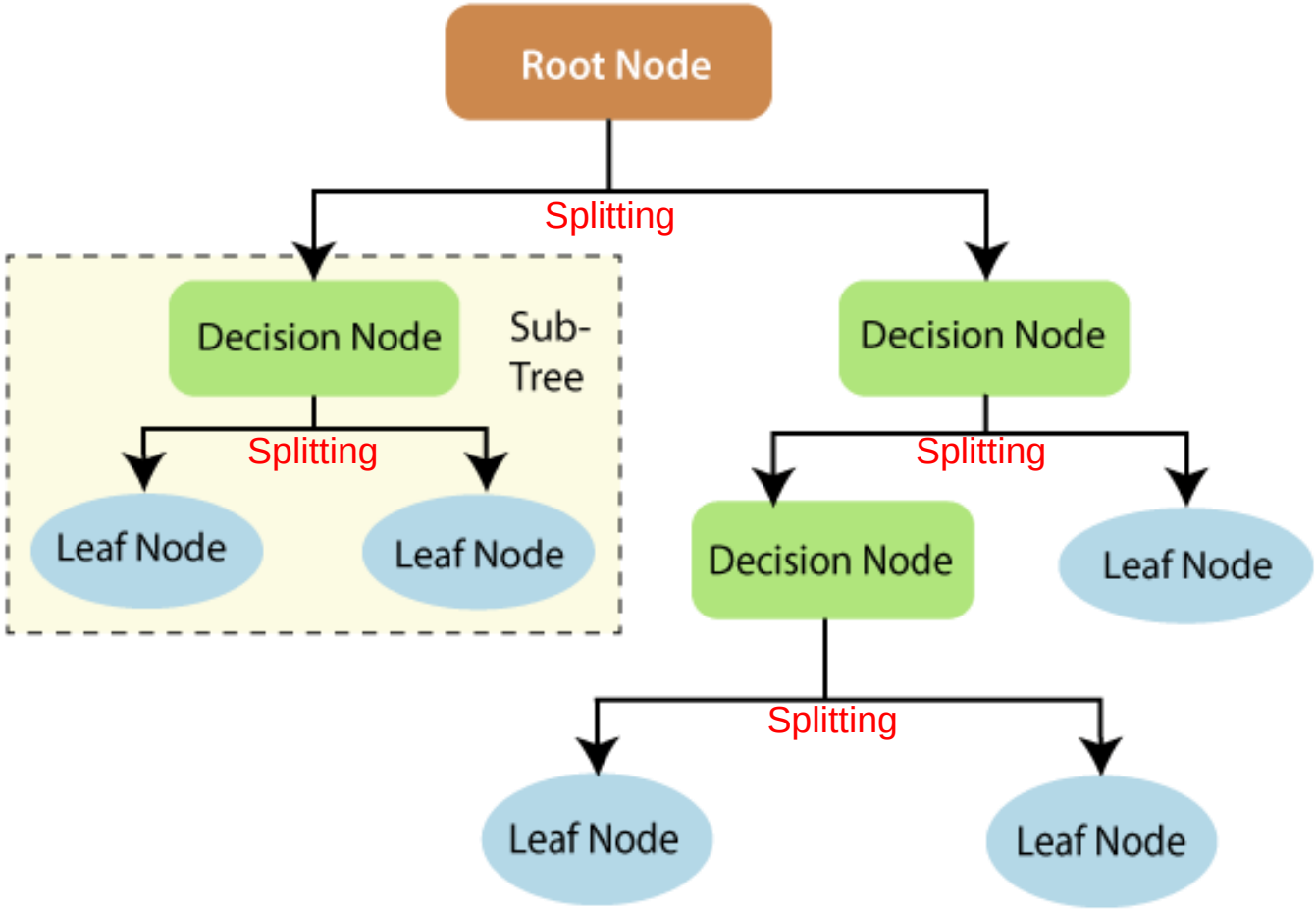
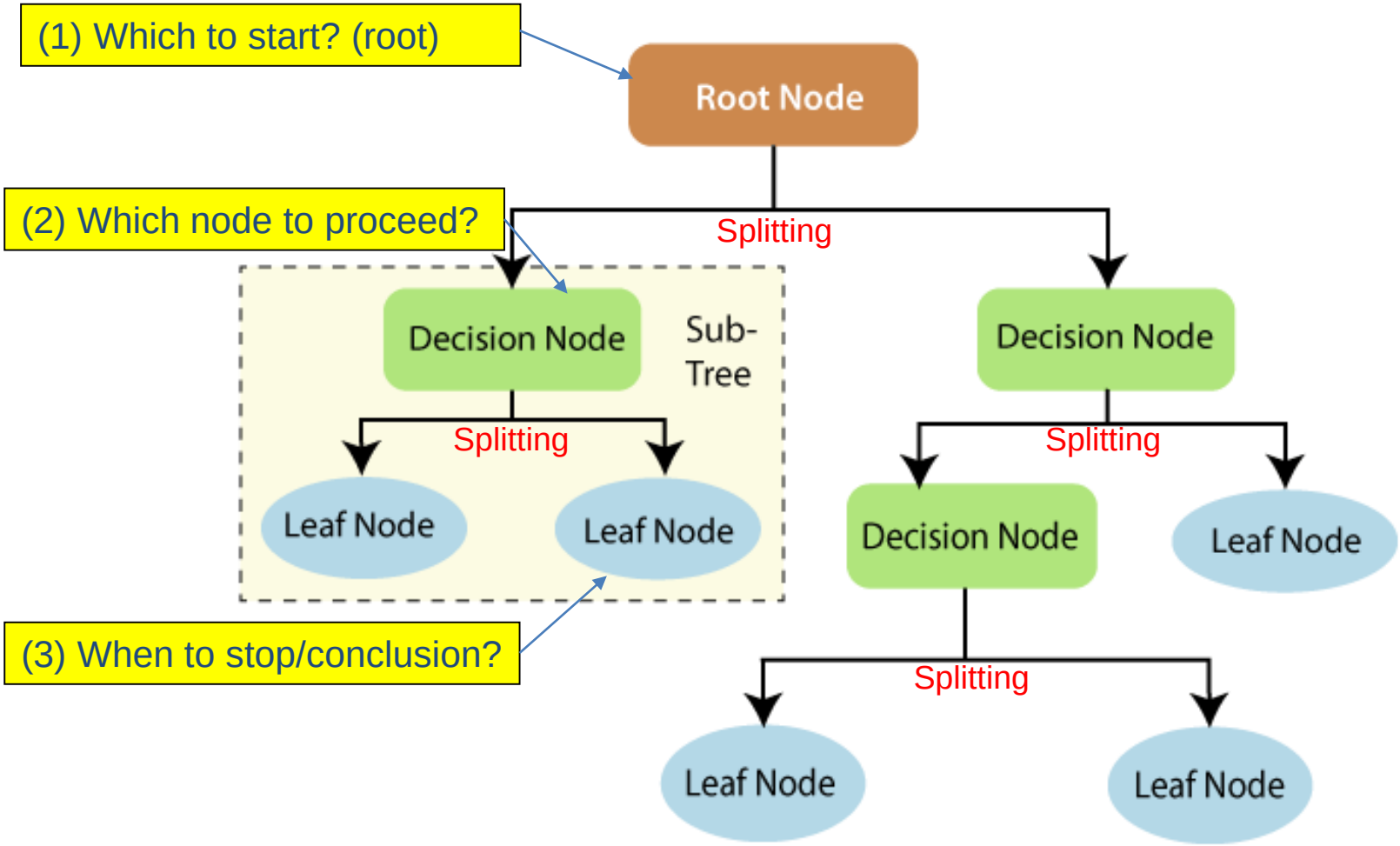
Splitting Issues



Splitting Issues



https://www.kdnuggets.com/

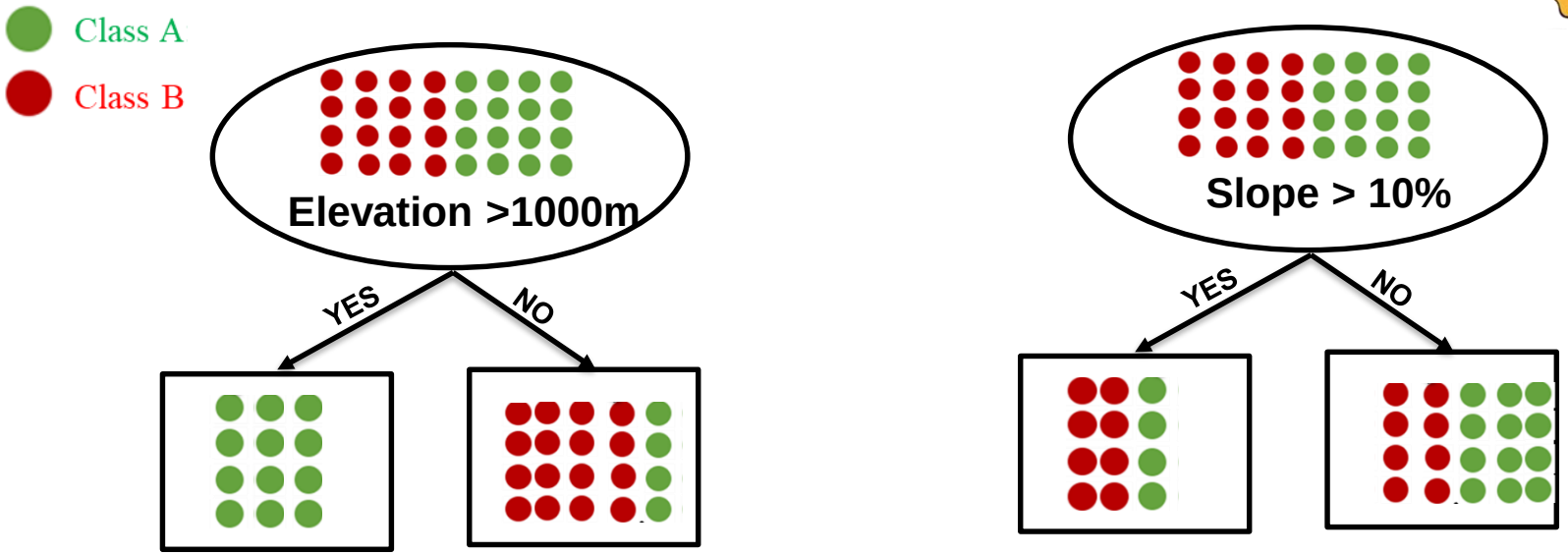
Splitting Issues

Issues

- How to determine the Best Split
- Determine when to stop splitting

How to determine the Best Split

- at each step, we look for the best split (Greedy Strategy).

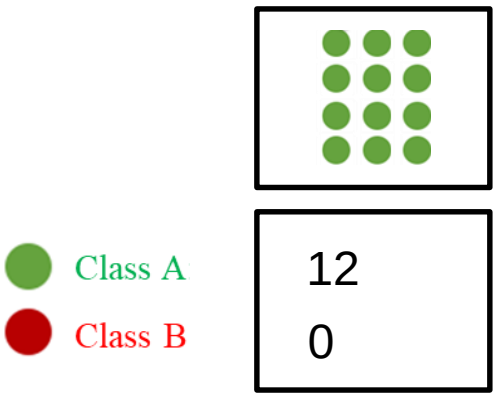


Which test split is the best?

How to determine the Best Split

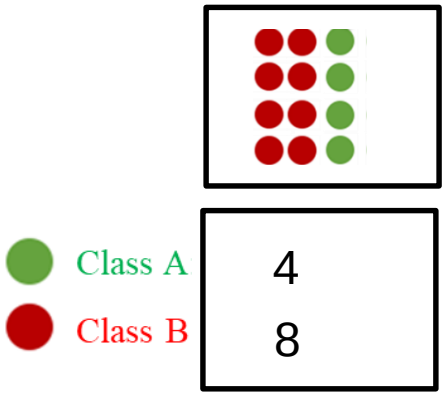
- Nodes with homogeneous class distribution are preferred

- Need a measure of node impurity:



Homogeneous,

Low degree of impurity



Non-homogeneous,

High degree of impurity

Measures of Node Impurity

- Gini Index or Gini ratio
- This measure provides a ranking to the attributes for splitting the data.

- It stores sum of squared probabilities of each class. We can formulate it as illustrated below.

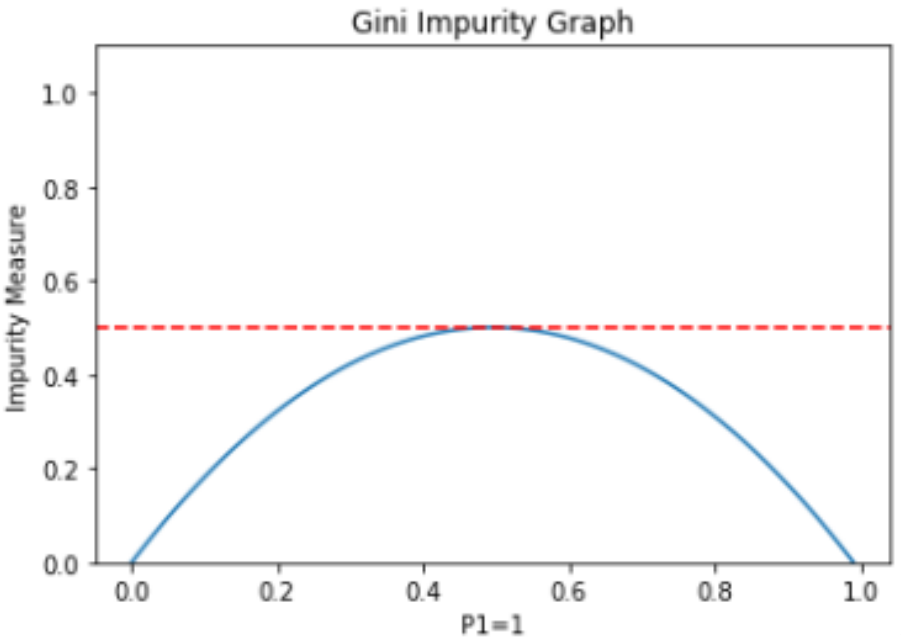
$$Gini = 1 - \sum(P_i)^2$$

i =1 to number of classes

P = probabilities of each class

A Gini Impurity of **0** is the lowest.

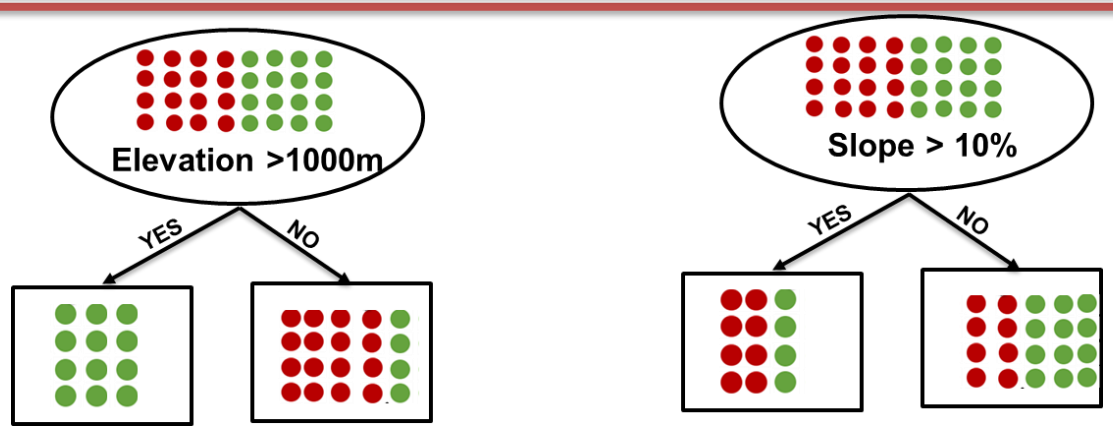
It can only be achieved when everything is the same class



$Gini = 1 - \sum(P_i)^2$ Gini Index

Class A

Class B



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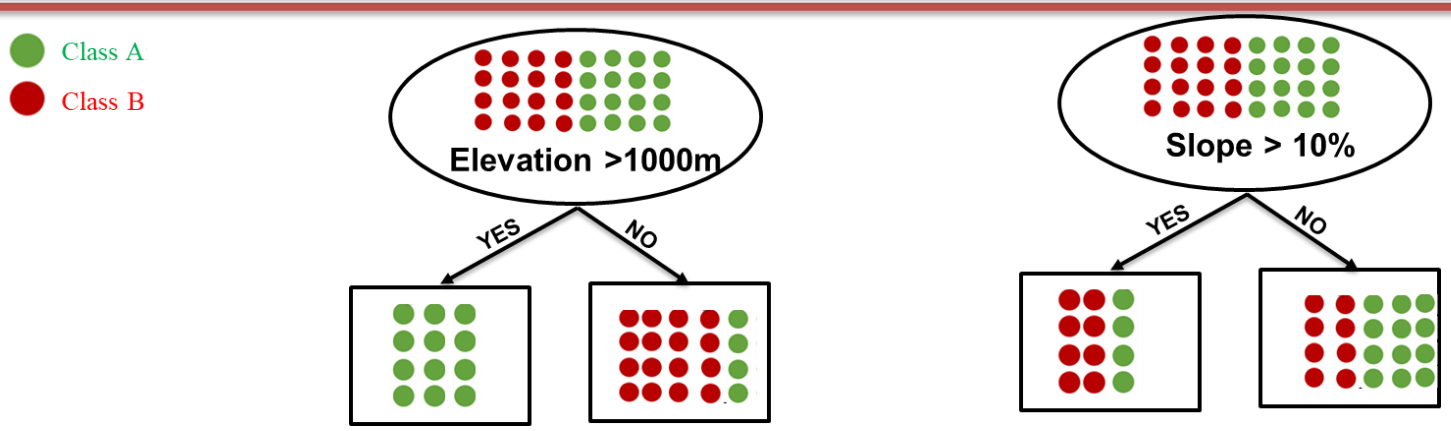
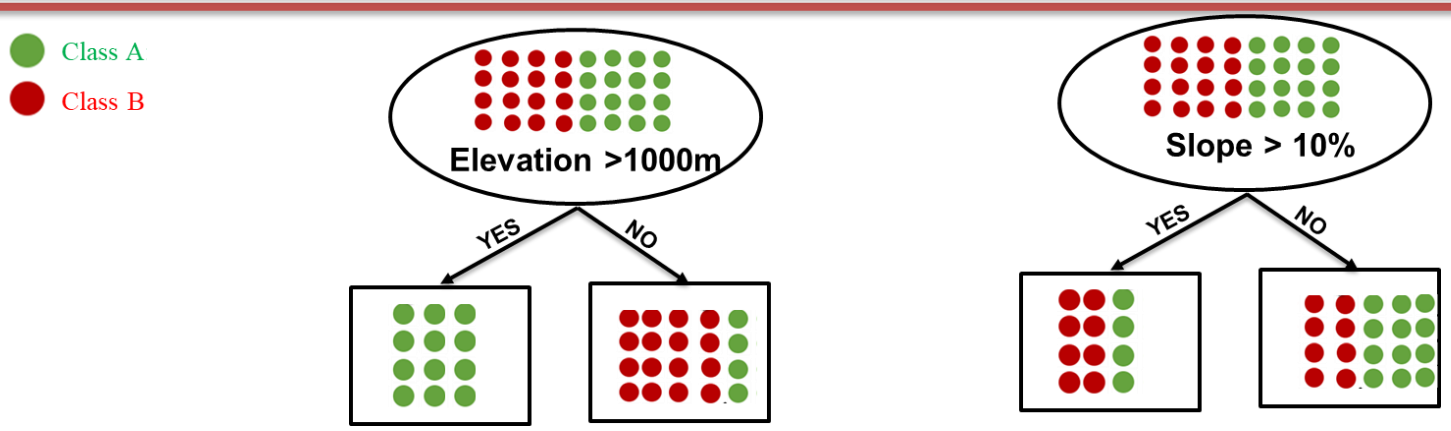


Elevation	A	B	P (A)	P (B)	Gini
>1000 m	12	0	12÷12=1	0÷12=0	$1-[(1)^2+(0)^2]=0$
<1000 m	4	16	4÷20=0.2	16÷20=0.8	$1-[(0.2)^2+(0.8)^2]=0.32$

$Gini = 1 - \sum(P_i)^2$ Gini Index



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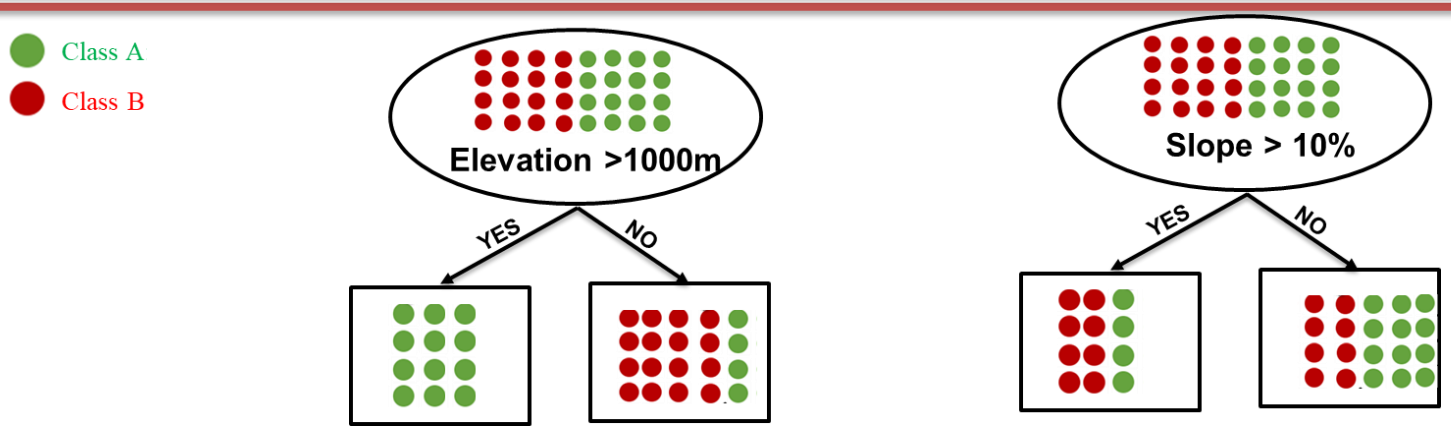
$$Gini(Elevation) = \left(\frac{12}{32}\right) \times 0 + \left(\frac{20}{32}\right) \times 0.32 = 0.20$$

$Gini = 1 - \sum(P_i)^2$ Gini Index



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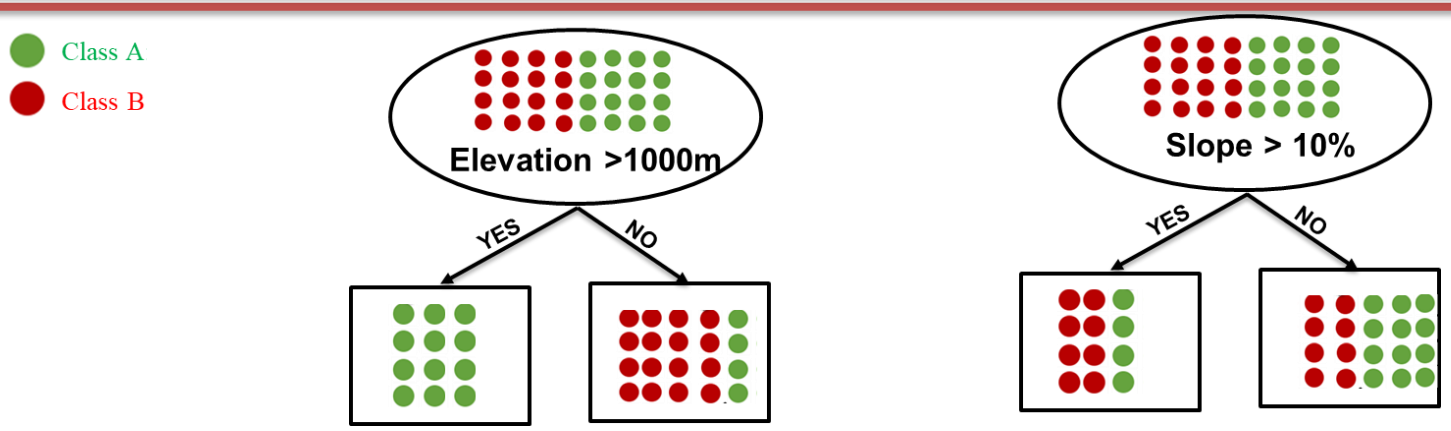
>10 %	4	8	4÷12=1	8÷12=0	$1-[(0.22)^2+(0.66)^2]=0.44$
<10 %	12	8	12÷20=0.2	8÷20=0.8	$1-[(0.6)^2+(0.4)^2]=0.48$

$$Gini(Slope) = \left(\frac{12}{32}\right) \times 0.44 + \left(\frac{20}{32}\right) \times 0.48 = 0.46$$

$Gini = 1 - \sum(P_i)^2$ Gini Index



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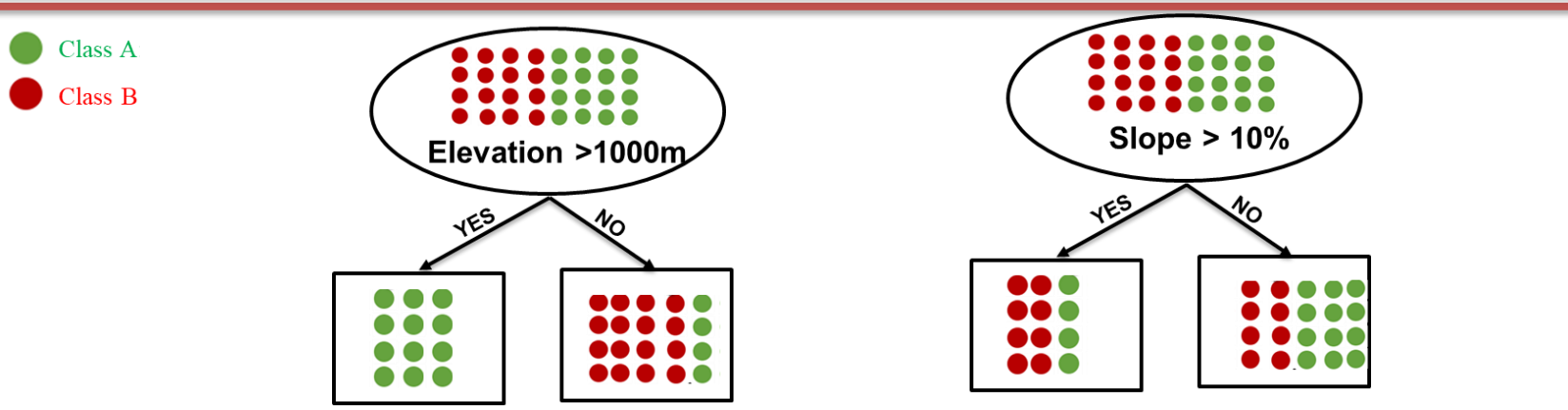

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Splitting Issues

Issues

- How to determine the Best Split
- Determine when to stop splitting

Determine when to stop splitting

- Stopping Rule
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of instances is less than some user-specified threshold
    - Stop if class distribution of instances are independent of the available features
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini index).

Stop the algorithm before it becomes a fully-grown tree (Pre-Pruning)

Overfitting In Decision Trees

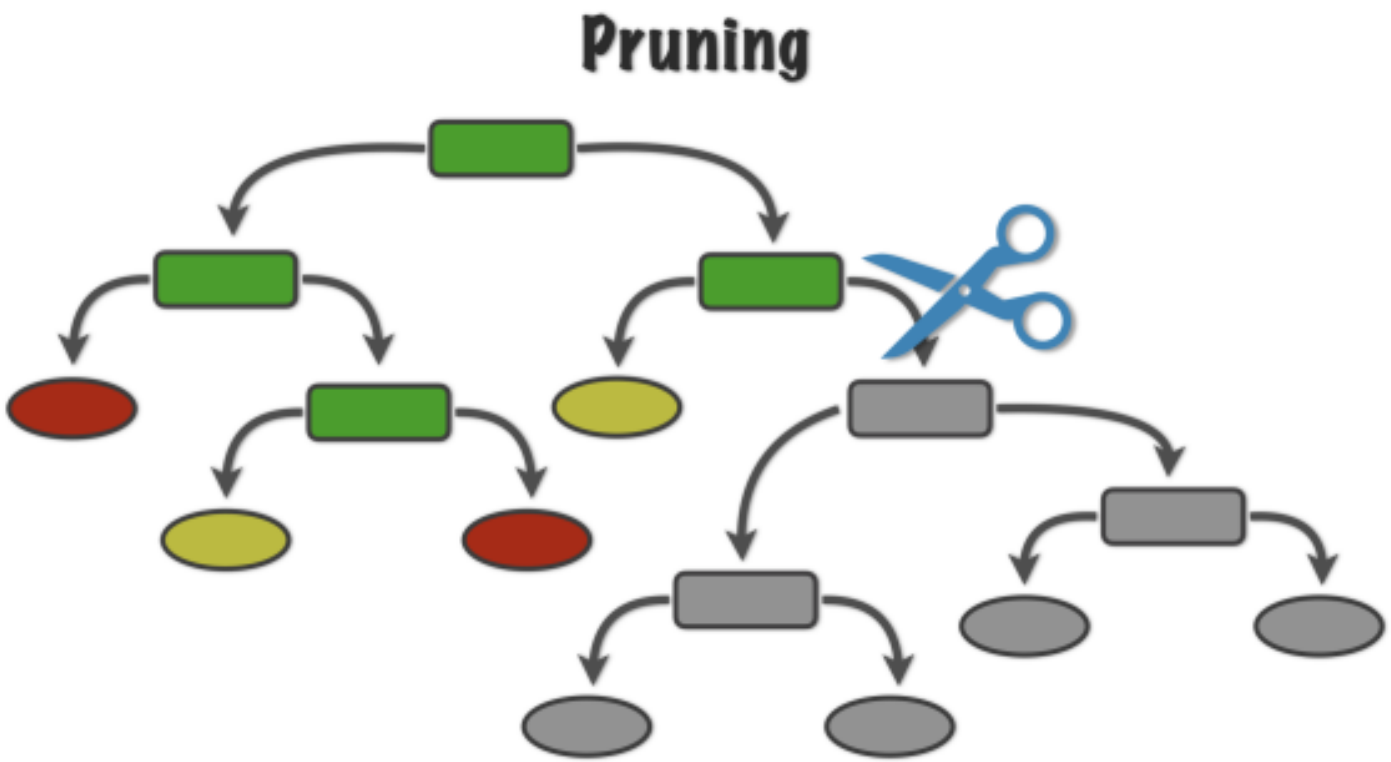
Overfitting happens when a decision tree tries to be as perfect as possible by increasing the depth of tests and thereby reduces the error.

- Post-pruning
  - Grow decision tree to its entirety
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node.
  - Class label of leaf node is determined from majority class of instances in the sub-tree

Pruning

Comparing pre-pruning and post-pruning,

- Pre-pruning is faster but
- Post-pruning generally leads to more accurate trees.



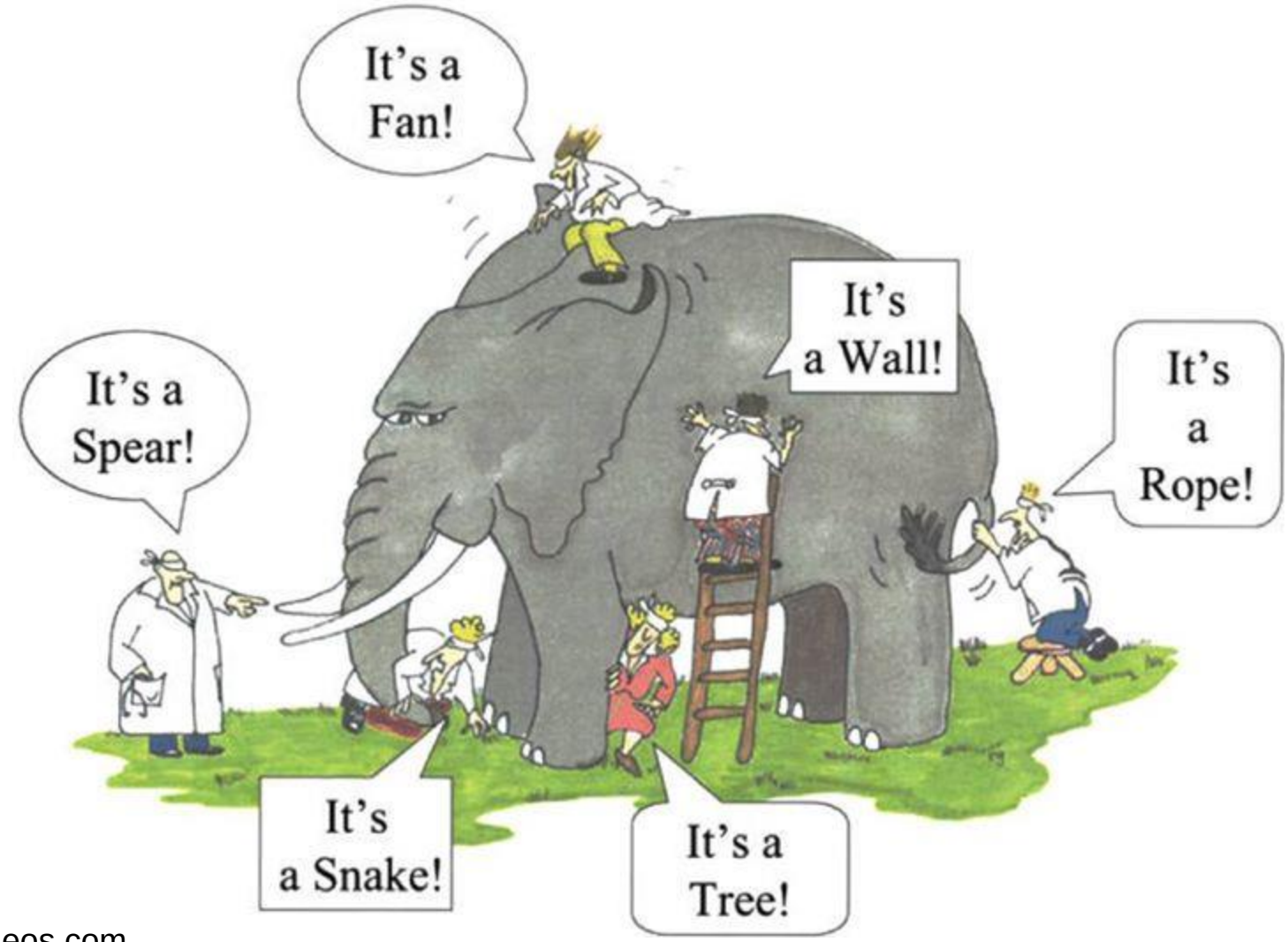
https://alanjeffares.wordpress.com/tutorials/decision-tree/

Advantages and Disadvantages

- Advantages:
  - Extremely fast at classifying unknown records.
  - Simple to understand and to interpret for small-sized trees
  - Trees can be visualized.
  - Excludes unimportant features.

- Disadvantages:
  - Easy to overfit.
  - Decision trees can be unstable because small variations in the data might result in a completely different tree being generated. This problem is mitigated by using decision trees within an **ensemble**.

Ensemble Methods



Source: Patheos.com

Bagging

- Bagging or Bootstrap aggregating (Breiman 1994):

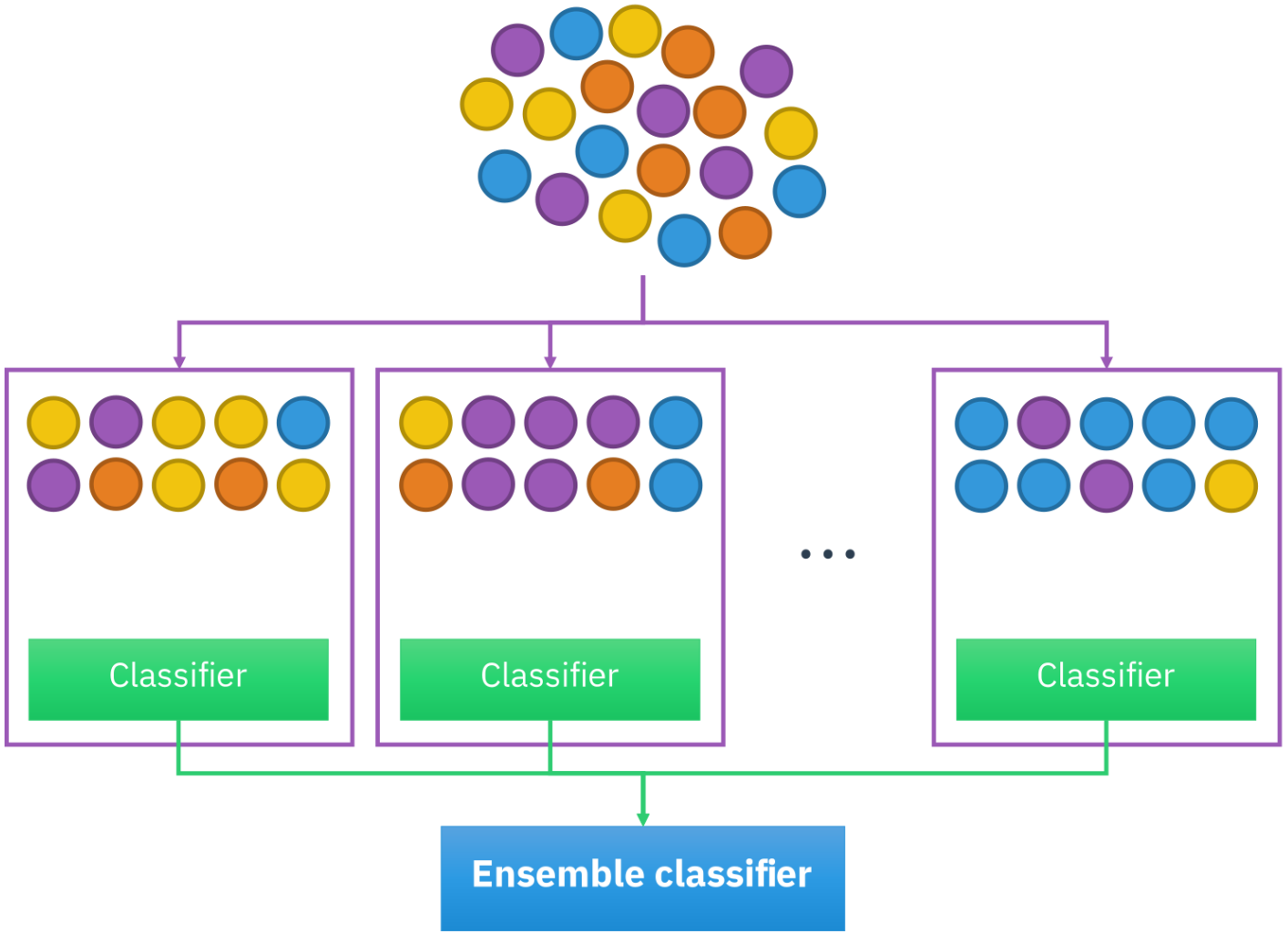
- First, we **create multiple bootstrap samples** so that each new bootstrap sample will act as another (almost) independent dataset drawn from true distribution.

- Then, we can fit a weak learner (**decision tree**) for each of these samples

- Finally **aggregate them** (simple average for regression or simple majority vote for classification)

Bootstrap: a statistical technique, for generating samples of **size B** (called bootstrap samples) from an initial dataset of **size N** by randomly drawing with replacement B observations.

Bagging



Original Data

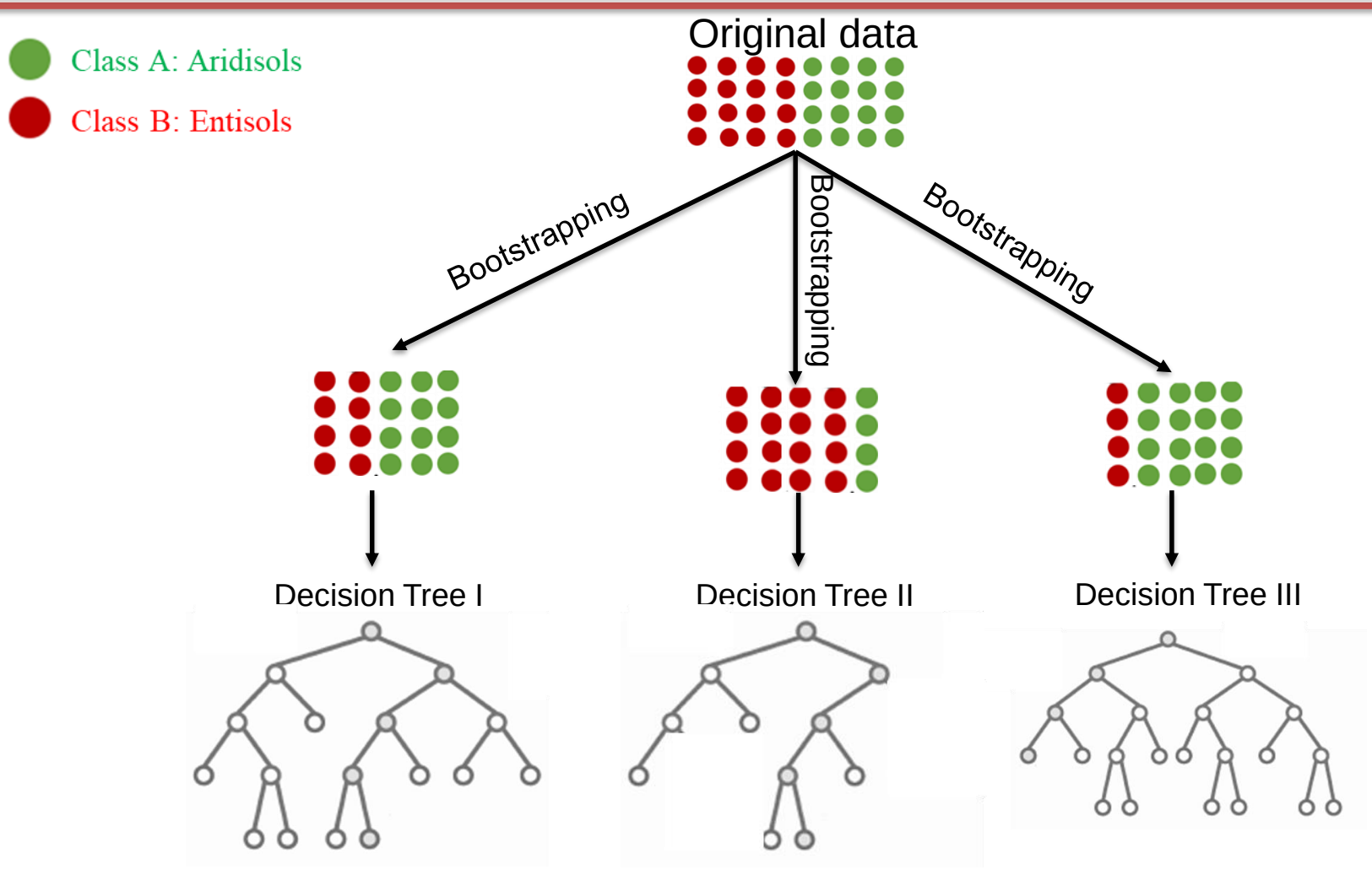
Bootstrapping

Aggregating

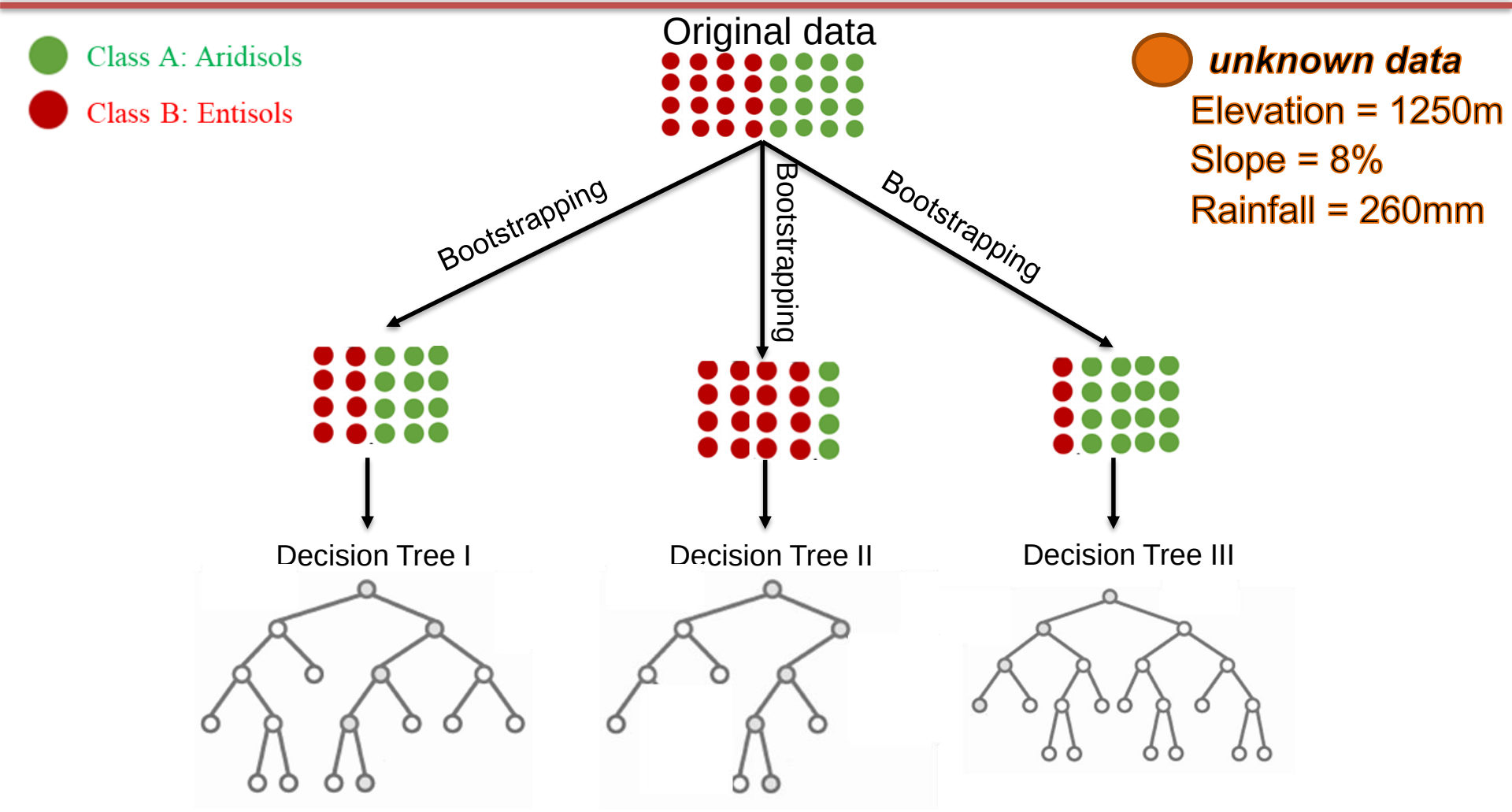
Bagging

https://www.pluralsight.com/guides/ensemble-methods:-bagging-versus-boosting

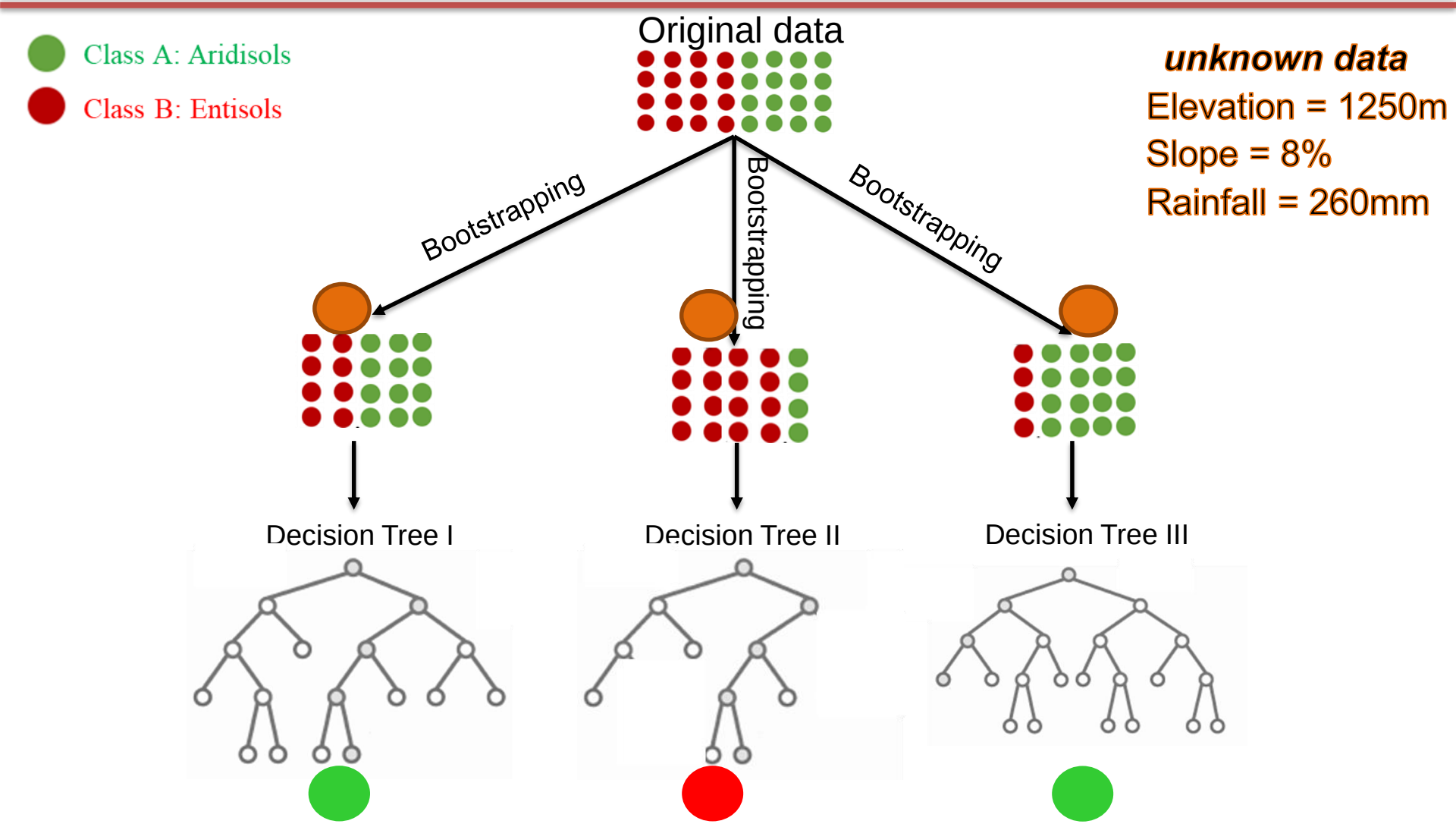
Bagging: example I



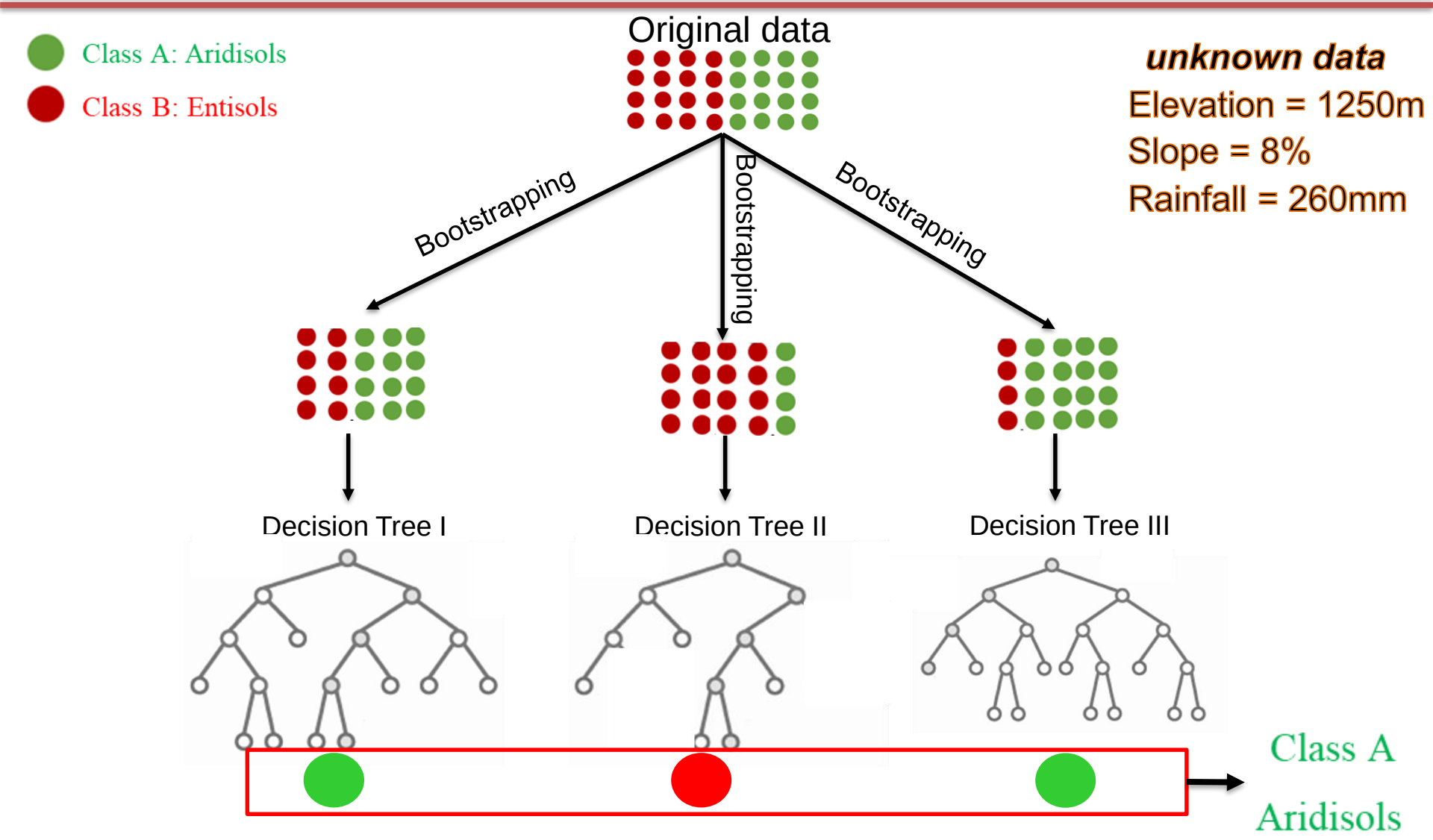
Bagging: example I



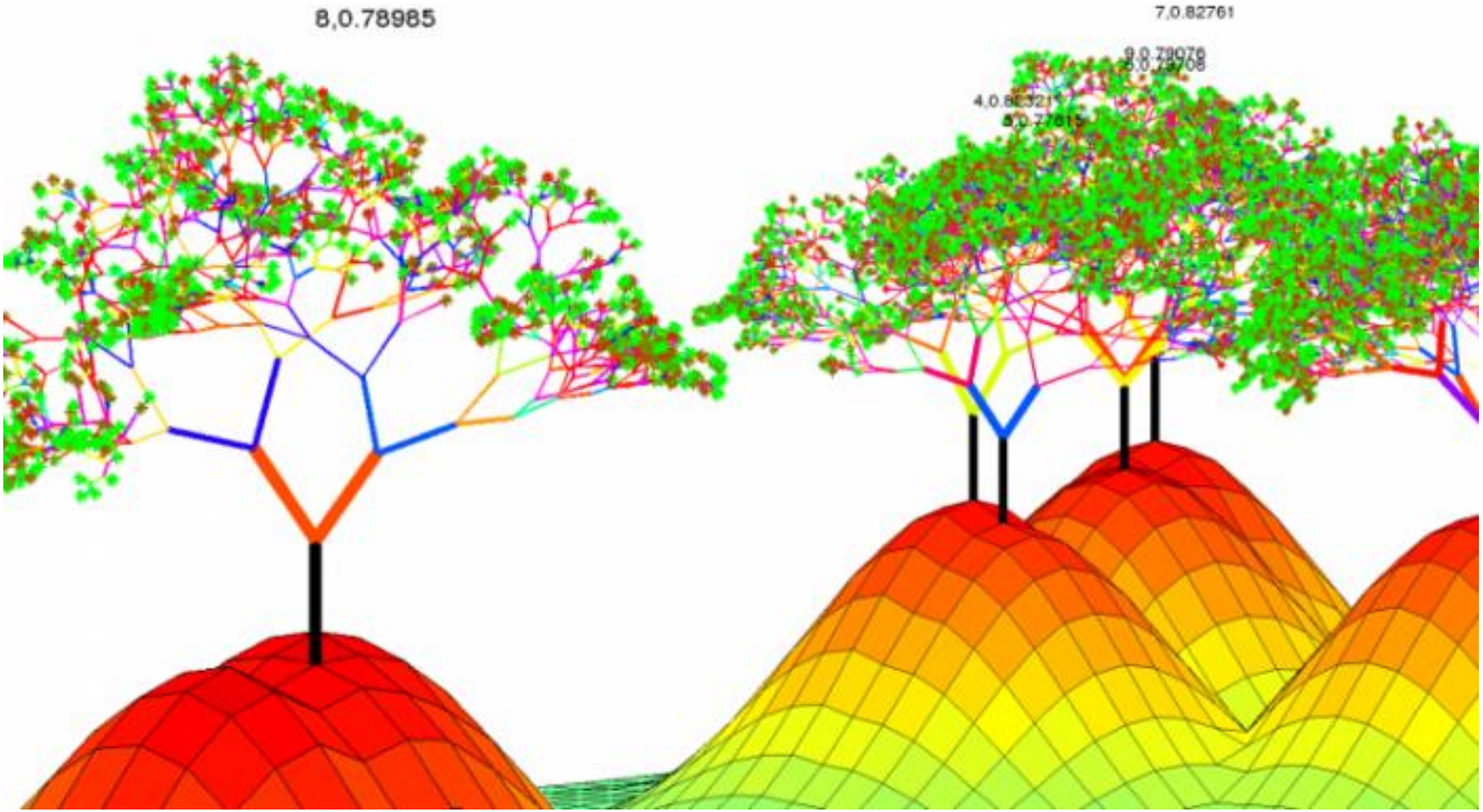
Bagging: example I



Bagging: example I



Random Forest



https://towardsdatascience.com/random-forest-learning-essential-understanding-1ca856a963cb

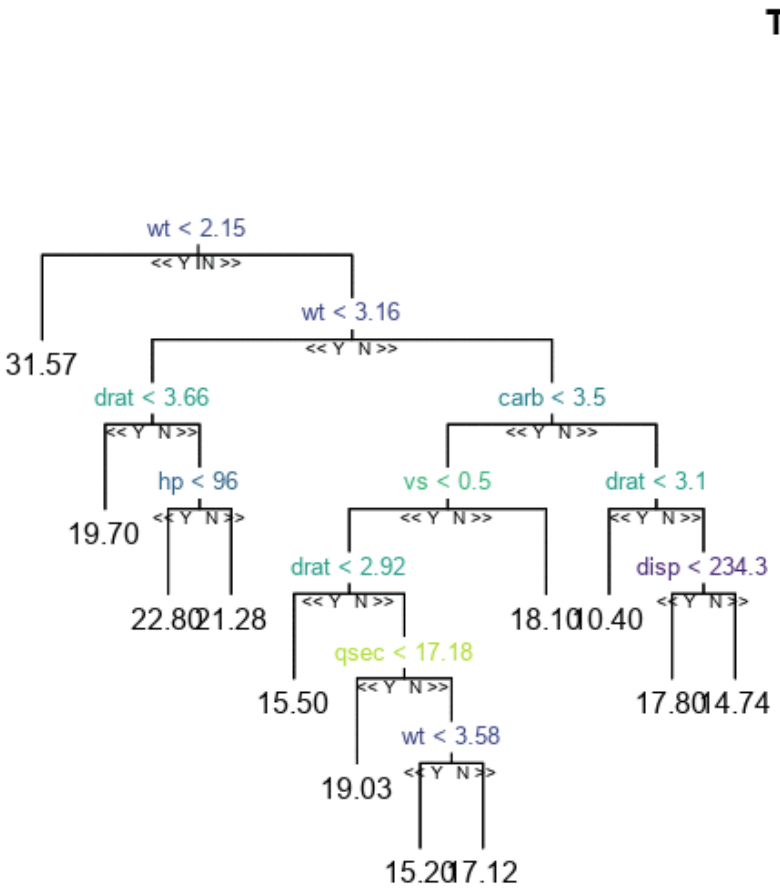
Random Forest

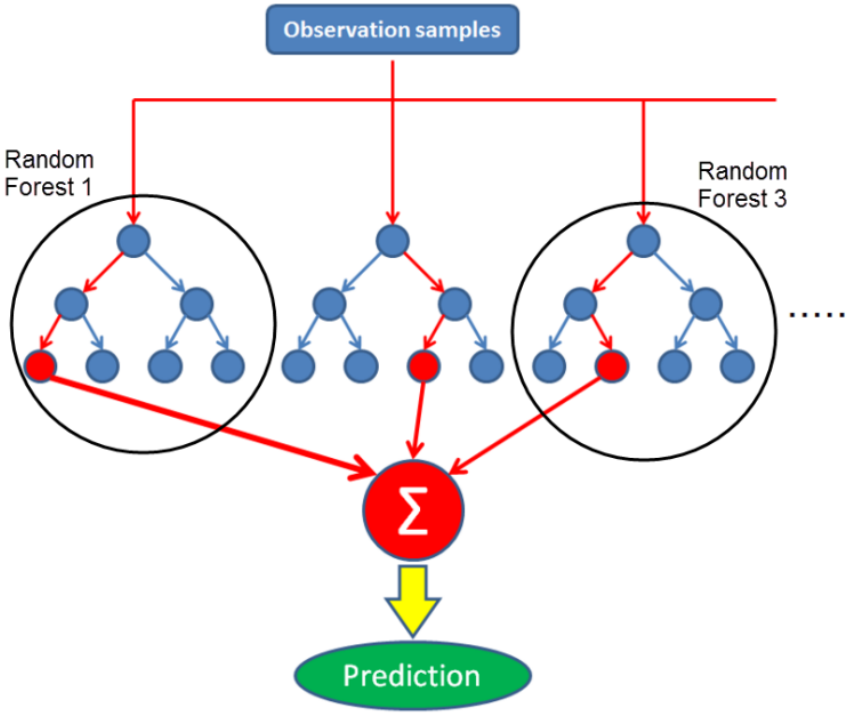
- Random Forest:
  - The random forest approach is a **bagging method** for classification and regression that operate by constructing multiple decision trees at training phase and outputting the class that is the mode of the classes or mean/average prediction of the individual trees.
  - Random forests also use another trick to make the multiple decision trees a bit less correlated with each others:
  - when growing each tree, instead of **only** sampling over the observations in the dataset to generate a bootstrap sample, we also sample over **covariates** and keep only a random subset of them to build the tree.

How Does It Work?

- Random Forest:
  - Bagging
    - Draw a bootstrap sample:
      - Random selection of 2/3 of the training data; repeat *n* times.
      - Grow an unpruned tree to each bootstrap sample
    - Random predictor selection: for each split in each tree a random subset is selected from the predictor variables. The best split is chosen from among the selected predictors.
    - Predict new data by aggregating the predictions of the n trees.
      - Average for continuous variables
      - Majority vote for categorical variables

Random Forest





Out Of Bag Accuracy Assessment

- Random Forest:
  - Random Forest comes with an internal accuracy assessment (based on cross validation).
  - Bootstrap sampling: the algorithm sets aside ~36% of the training data for each tree grown: out of bag data (OOB).
  - OOB data can be used to asses prediction accuracy:
    - Predict the data not in the bootstrap sample for each tree
    - Aggregate the OOB predictions: mean (continuous data), majority vote (categorical data).

Variable Importance

- Random Forest:
  - Ensembles of trees are not easy to interpret.
  - Ensemble can reflect the potentially (complex) effect of a variable on the response
  - Variable importance plot: shows how much prediction error increases when the values of one predictor are permuted (break association with response) while all others are left unchanged.
  - Permuted variable is used together with other variables to predict the response, prediction accuracy will decrease.

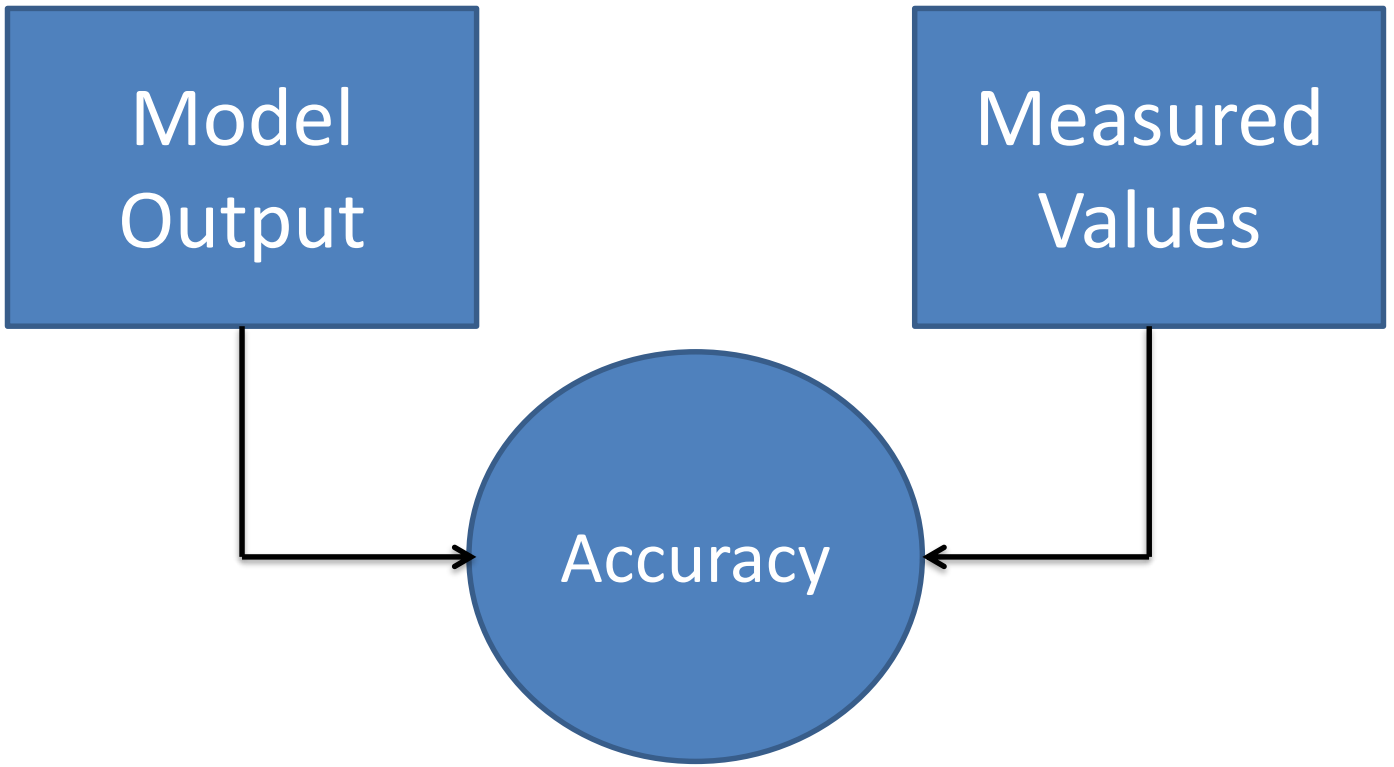
Advantages and Disadvantages

- Advantages:
  - Quite fast
  - Models interactions in the data / non linear relationships
  - Very good predictive power expected
  - Yields covariate importance, makes covariate selection possible

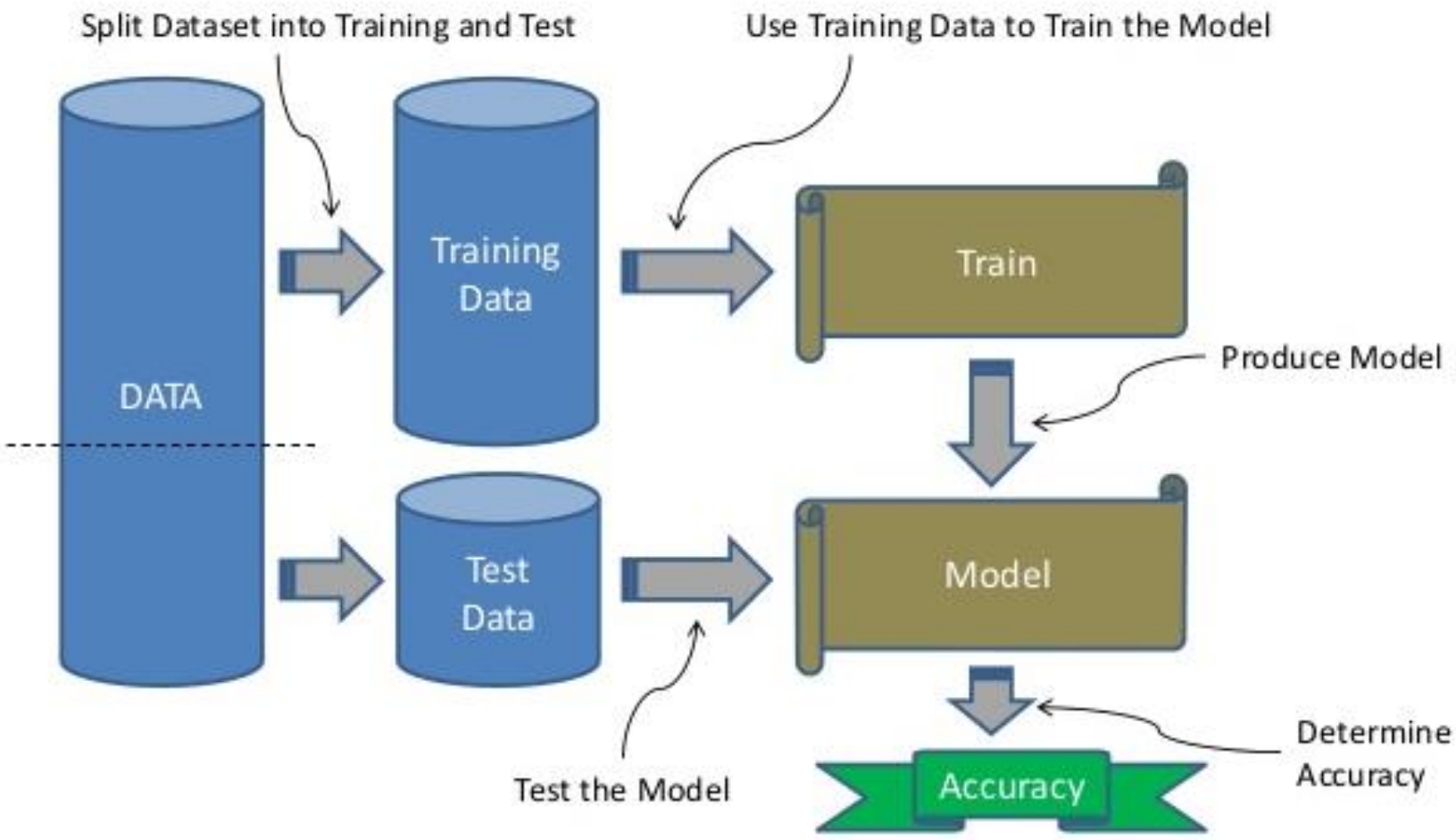
- Disadvantages:
  - Difficult to interpret

Accuracy Assessment of Models

- Assess accuracy of a model output is one of the most important steps in digital soil mapping

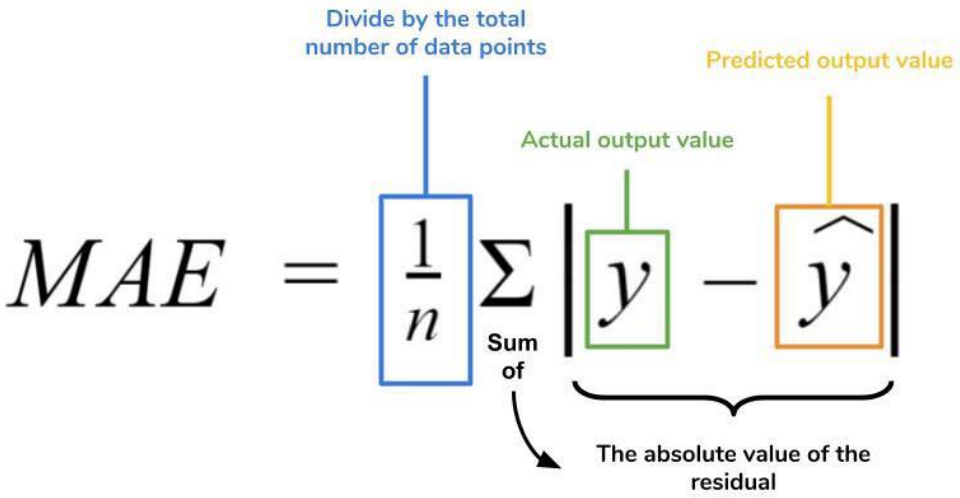


Training and Testing the Models



Performance Metrics for Regression

- Mean Absolute Error:



- Root Mean Square Error:

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

Practice

Import covariates

Import point data

Overlay point data on covariates

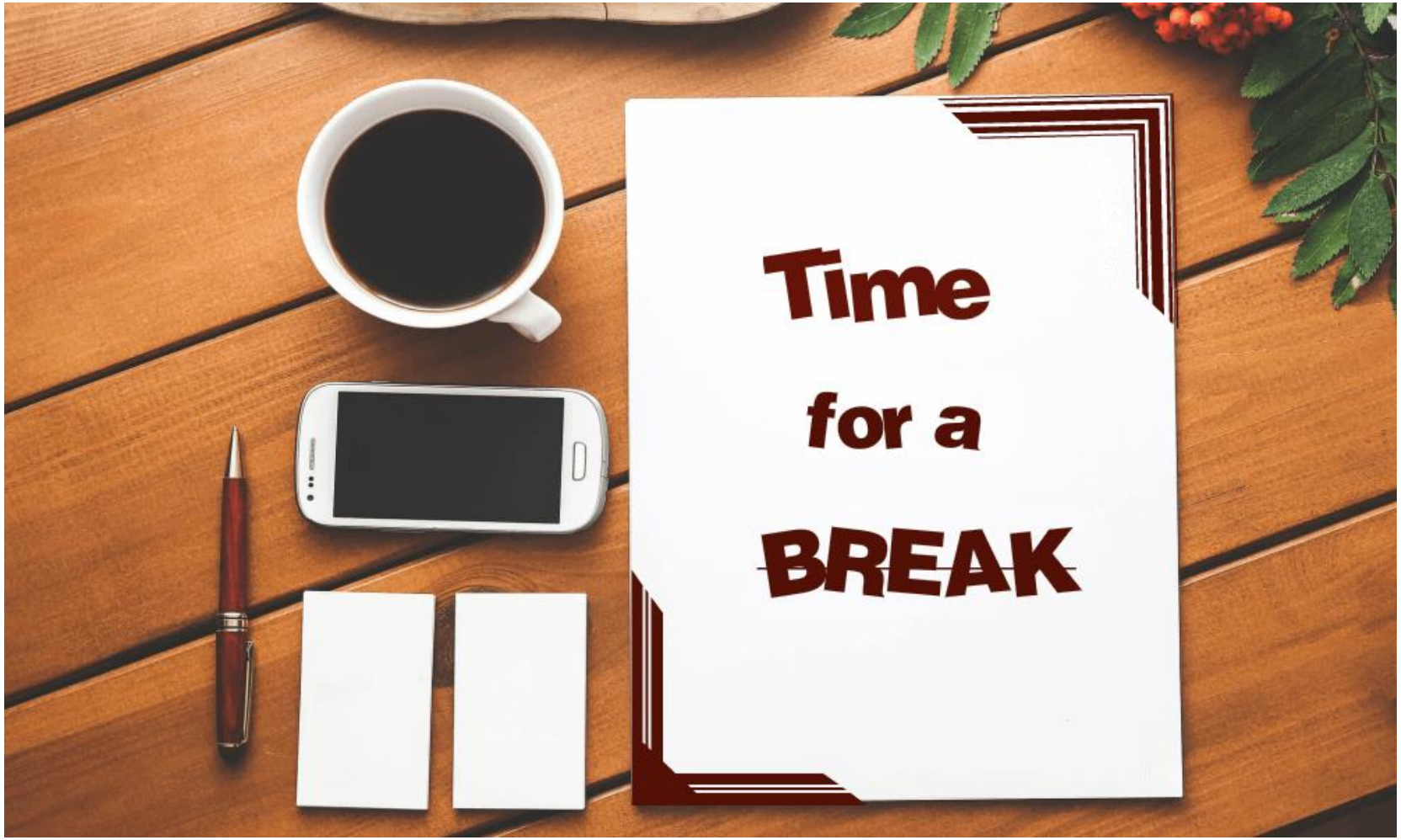
Make a geodatabase

Split the geodatabase to training and testing sets

Train machine learning models

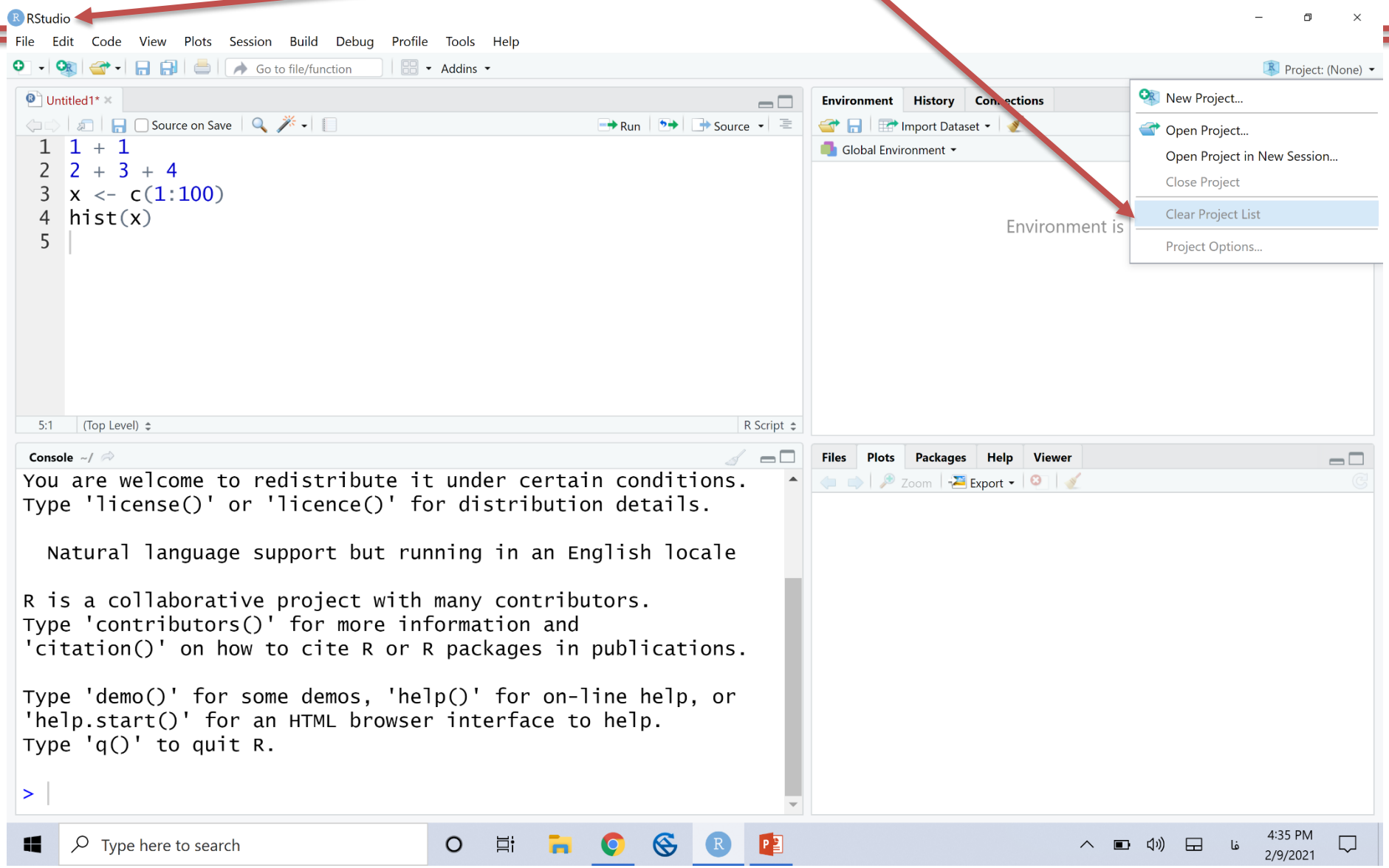
Test machine learning models

Predict soil maps

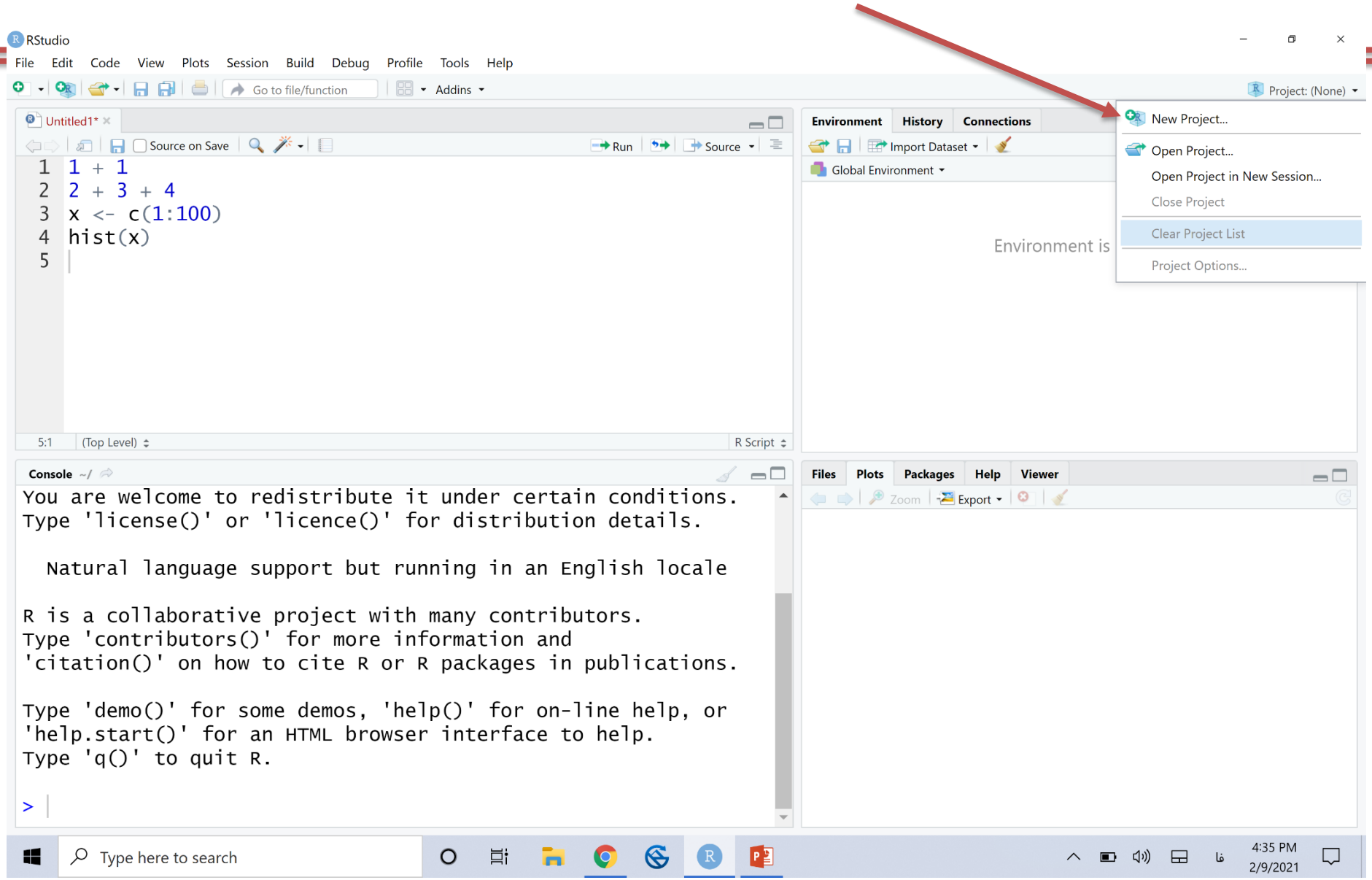

Time
for a
BREAK

1. Open Rstudio

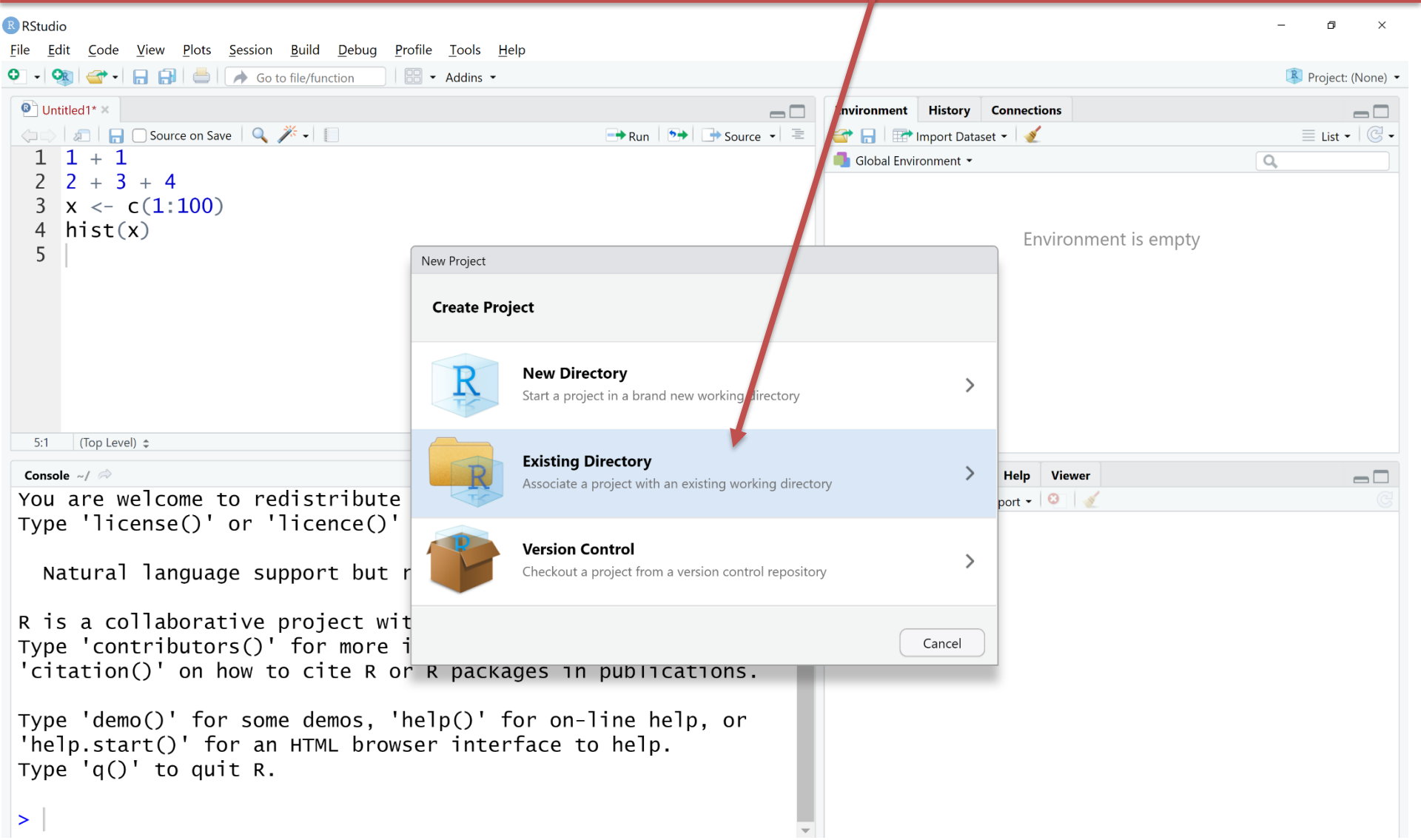
2. Clear Project List



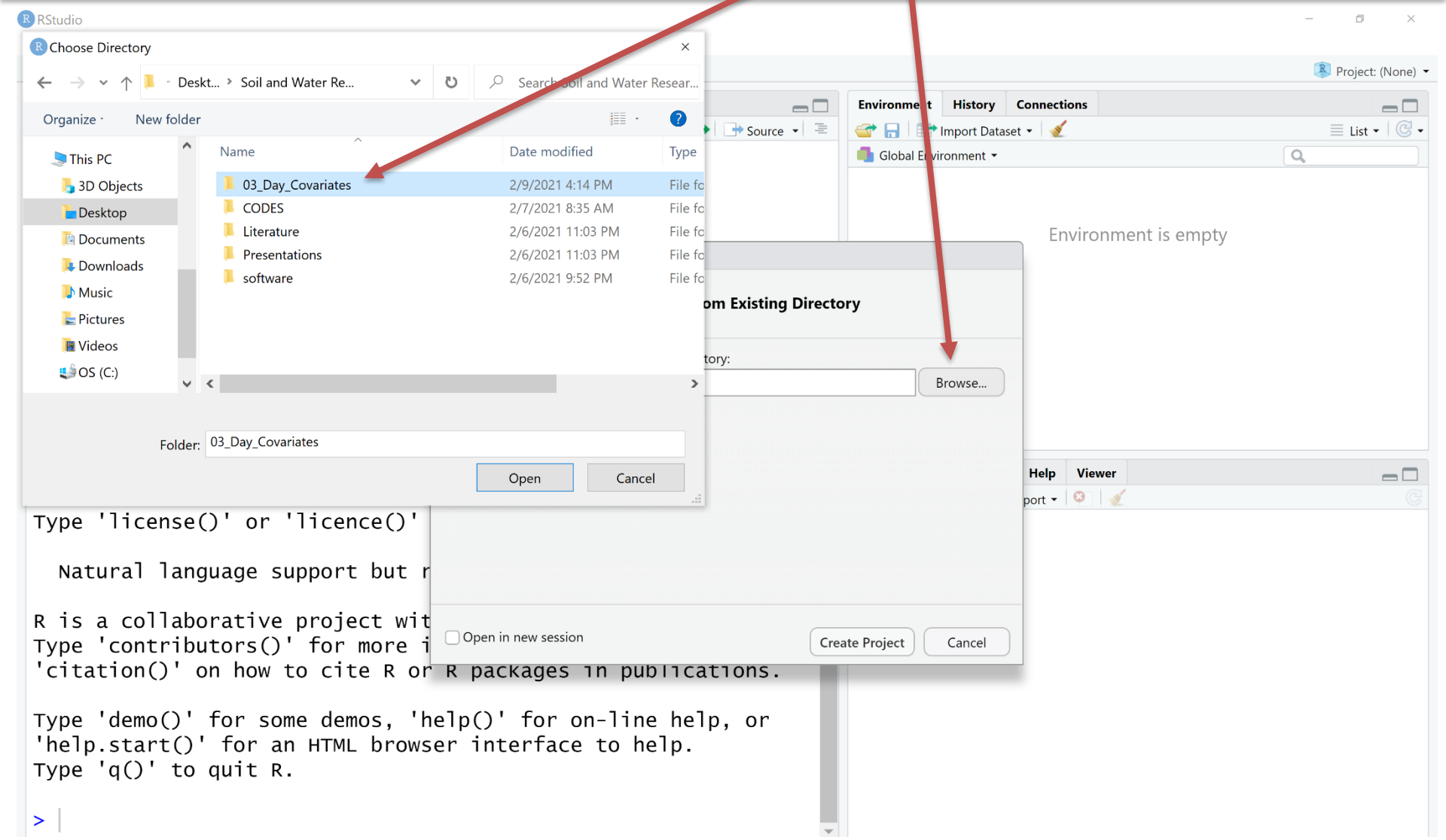
3. New Project



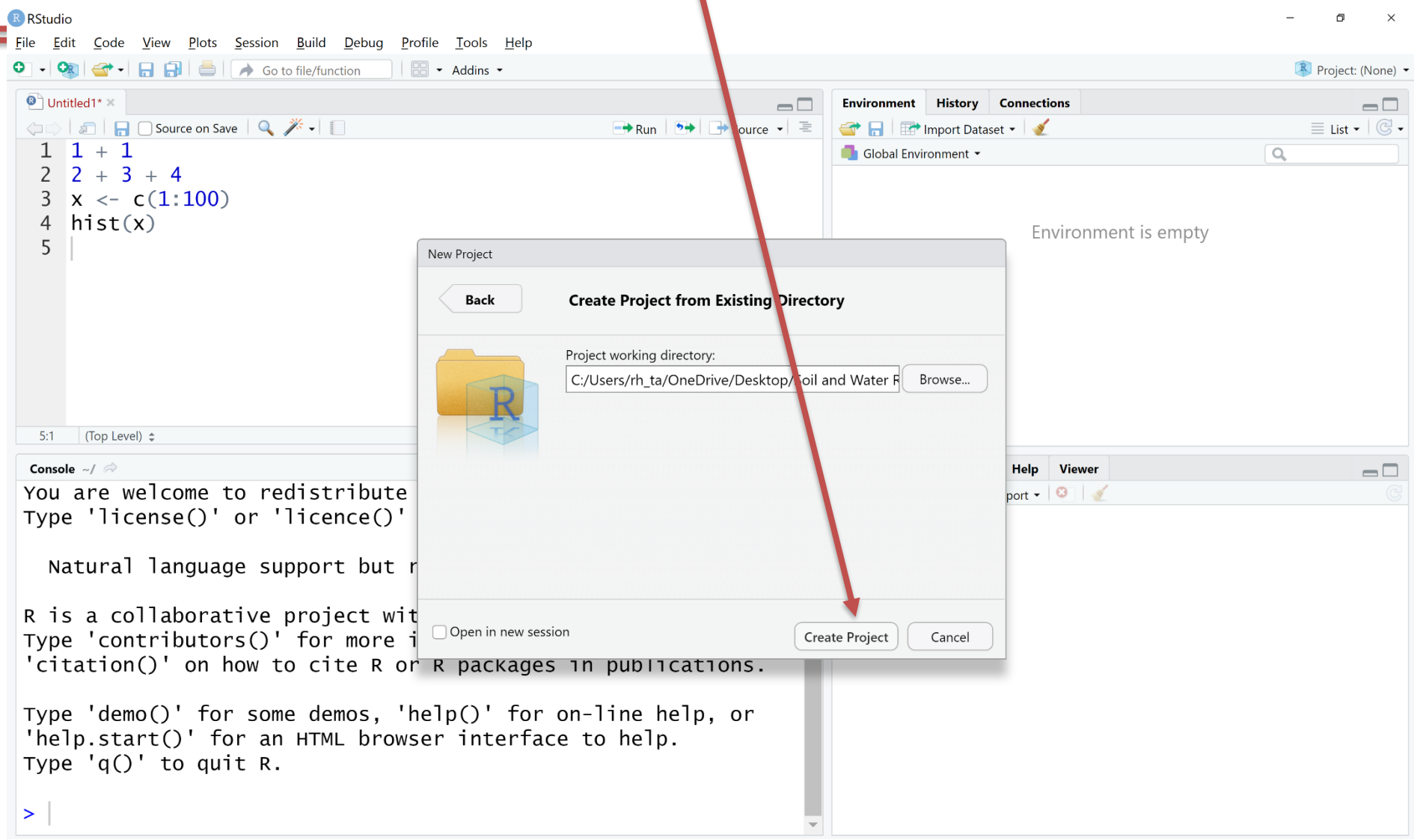
4. Existing Directory



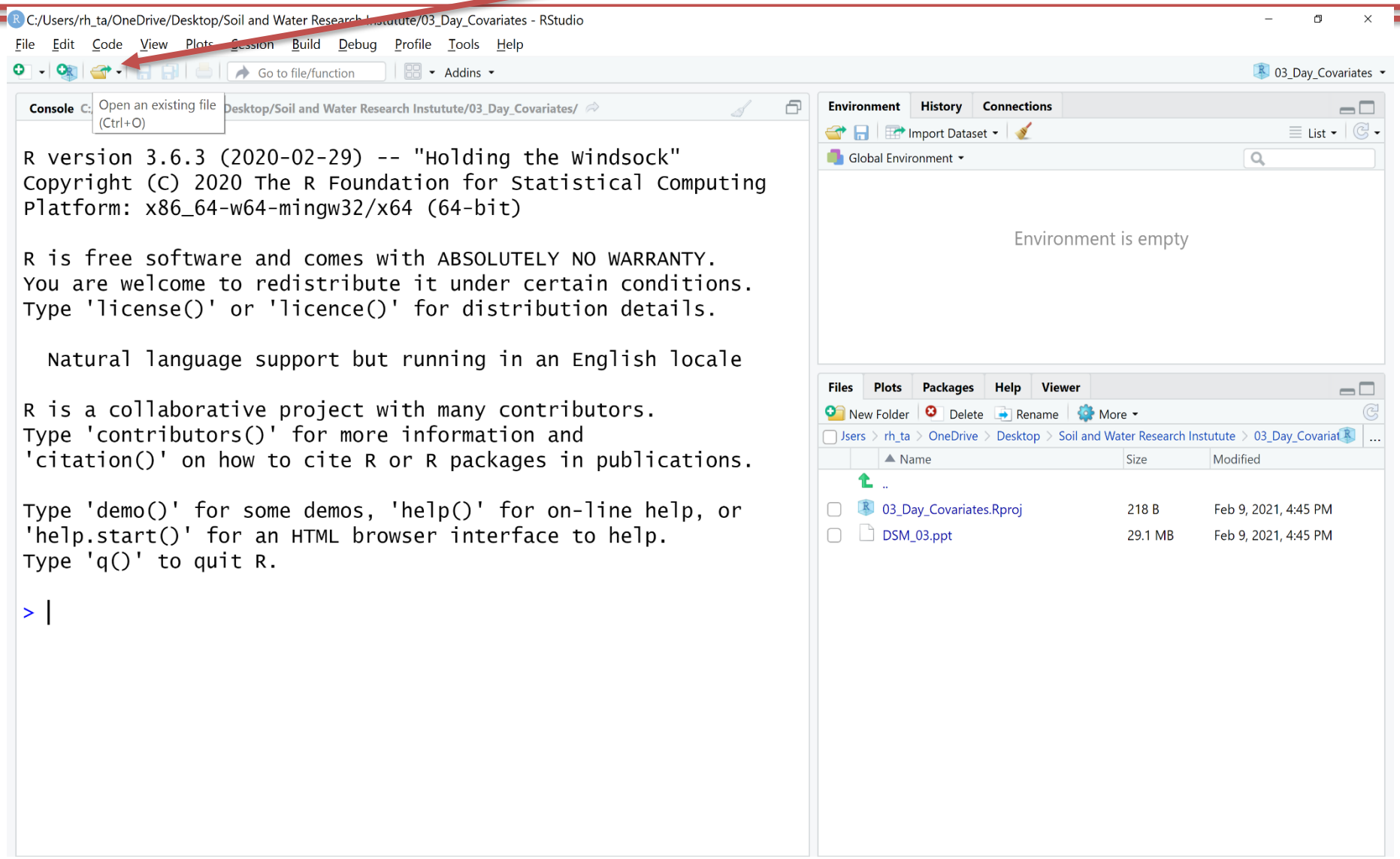
5. Find the folder and find **Day_04_Machine Learning-P1** and open



6. Create project



7. Open an existing file and find **04_R_Cov.R**



8. Open 04_R_Cov.R