Machine Learning analysis with the ERA Database

A) Summarize and subset the Dataset

The most recent version of the ERA dataset contains 107952 instances and 142 attributes. I will carry out the experiment on this whole data but for now, let's focus on the LER outcomes. The new subset has 808 instances and 142 attributes. For this case, we will focalize on the most important attributes (factors) leading to this. Let's first see the type of attributes we have:

Type of Attributes

We can have some examples from the first 6 attributes listed below

```
Index Code Author Date Journal DOI "integer" "character" "character" "integer" "character" "character"
```

The 3 types of attributes we have here are:

```
"integer" "character" "numeric"
```

The 8 most important factors are

- -MeanC
- -MeanT
- -Yield
- -Mean annual precipitation (MAT)
- -Total seasonal precipitation (TSP)
- -Soil organic carbon at start of experiment (SOC)
- -Soil pH
- -Duration

First, our target here will be the product we get out of this. In total, we have 59 type of products and this is a **multi-class or a multinomial classification problem.**

B) Create a Validation Dataset

We need to know that the model we created is any good.

Later, we will use statistical methods to estimate the accuracy of the models that we create on unseen data. We will split the loaded dataset into two, 80% of which we will use to train our models and 20% that we will hold back as a validation dataset.

This doesn't seem to be interesting since some classes have a single record. Let's carry out our analysis in the other direction and target the possible outcomes. In this case let's target the full dataset with the attributes listed above. We get 86 types of outcomes.

A view of the class distribution gives us the following where we have their frequencies (number of instances of each class) and percentage

	freq	percentage
Aboveground Biomass	32	0.029642804
Animal Mortality	89	0.082444049
Animal Survival	186	0.172298799
Belowground Biomass	24	0.022232103
Beneficial Organisms	675	0.625277901
Benefit Cost Ratio (GRTC)	233	0.215836668
Benefit Cost Ratio (GRVC)	242	0.224173707
Benefit Cost Ratio (NRTC)	59	0.054653920
Benefit Cost Ratio (NRVC)	105	0.097265451

C) Statistical Summary

We can take a look at a summary of each attribute. We can also see the amount of each NA value

MAT	TSP	SOC	Soil.pH	yi	MeanC	MeanT
Length:107952	Min. : 0.0	Min. : 0.00	Min. : 3.20	Min. : -Inf	Min. : -270380	Min. : -46415
Class :character	1st Qu.: 321.4	1st Qu.: 0.74	1st Qu.: 4.90	1st Qu.:-0.069	1st Qu.: 1	1st Qu.: 1
Mode :character	Median : 472.0	Median : 1.70	Median : 5.60	Median : 0.141	Median: 3	Median: 4
	Mean : 548.0	Mean : 8.45	Mean : 5.67	Mean : NaN	Mean : 2825	Mean : 4751
	3rd Qu.: 736.0	3rd Qu.: 6.20	3rd Qu.: 6.20	3rd Qu.: 0.483	3rd Qu.: 25	3rd Qu.: 27
	Max. :1935.0	Max. :21200.00	Max. :57.50	Max. : Inf	Max. :16380000	Max. :139713846
	NA's :96950	NA's :72163	NA's :59338	NA's :3191	NA's :2004	
Duration	Out.SubInd					
Min. : 0.000	Length:107952					
1st Qu.: 1.000	Class :character					
Median : 1.000	Mode :character					
Mean : 2.437						
3rd Qu.: 3.000						
Max. :78.000						
NA's :3358						

D) Visualize Dataset

We now have a basic idea about the data. We need to extend that with some visualizations.

We are going to look at two types of plots:

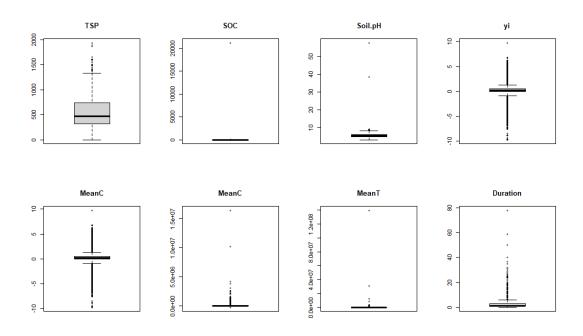
Univariate plots to better understand each attribute. **Multivariate** plots to better understand the relationships between attributes.

Univariate Plots

We start with some univariate plots, that is, plots of each individual variable.

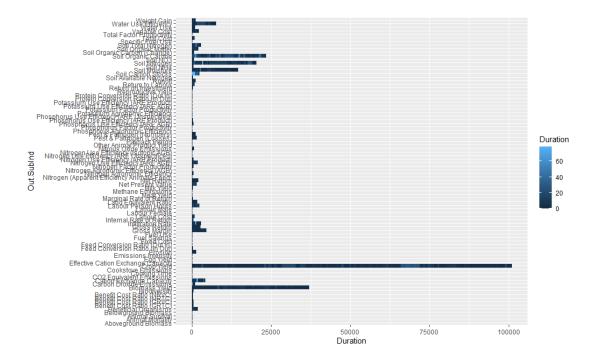
It is helpful with visualization to have a way to refer to just the input attributes and just the output attributes. Let's set that up and call the inputs attributes x and the output attribute (or class) y.

This gives us a much clearer idea of the distribution of the input attributes:



Box and Whisker Plots in R

We can also create a barplot of the outcomes class variable



Multivariate Plots

Now we can look at the interactions between the variables.

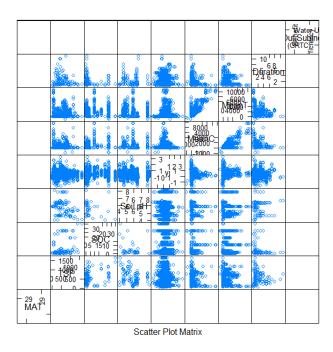
Let's first study the missing data or null values

Our data contain a lot of missing values and NA values. The column with missing data are

"MAT" "TSP" "SOC" "Soil.pH" "yi" "MeanC" "Duration"

The new dataset contains 2366 rows compared to 107952 with the original dataset.

First let's look at **scatterplots** of all pairs of attributes and color the points by class. In addition, because the scatterplots show that points for each class are generally separate, we can draw ellipses around them.



E) Evaluate Some Algorithms

Let's create some models of the data and estimate their accuracy on unseen data.

Here is what we are going to cover in this step:

- 1. Set-up the test harness to use 10-fold cross validation.
- 2. Build 5 different models to predict outcomes from these agroforestry attributes.
- 3. Select the best model.

We will use the cleaned data with 2366 instances and 9 attributes

1 Test

We will use 10-fold cross validation to estimate accuracy.

This will split our dataset into 10 parts, train in 9 and test on 1 and release for all combinations of train-test splits. We will also repeat the process 3 times for each algorithm with different splits of the data into 10 groups, in an effort to get a more accurate estimate.

2 Build Model

Here we will evaluate 5 different algorithms:

- Linear Discriminant Analysis (LDA)
- Classification and Regression Trees (CART).
- K-Nearest Neighbors (kNN).
- Support Vector Machines (SVM) with a linear kernel.
- Random Forest (RF)

Let's build our five models

```
# a) linear algorithms
set.seed(7)
fit.lda <- train(Out.SubInd~., data=Mdat_drop, method="lda", metric=metric, trControl=control)
# b) nonlinear algorithms
# CART
set.seed(7)
fit.cart <- train(Out.SubInd~., data=Mdat_drop, method="rpart", metric=metric, trControl=control)
# kNN
set.seed(7)
fit.knn <- train(Out.SubInd~., data=Mdat_drop, method="knn", metric=metric, trControl=control)
# c) advanced algorithms
set.seed(7)
fit.svm <- train(Out.SubInd~., data=Mdat_drop, method="svmRadial", metric=metric, trControl=control)
# Random Forest
set.seed(7)
fit.rf <- train(Out.SubInd~., data=Mdat_drop, method="rf", metric=metric, trControl=control)
```

3 Select Best Model

Unfortunately we can't compare because only one model works with our data Classification and Regression Trees (CART). We will have to figure this out later.

Here is the summary of the model and we can see the model doesn't perform well

```
> fit.cart
CART
2366 samples
   8 predictor
25 classes: 'Benefit Cost Ratio (GRTC)', 'Benefit Cost Ratio (GRVC)', 'Benefit Cost Ratio (NRVC)', 'Biomass Yield', 'Carbon Dioxide Emissions', 'Cation Exchange Capacity', 'C O2 Equivalent Emissions', 'Crop Yield', 'Erosion', 'Gross Margin', 'Gross Return', 'Labo
ur Cost', 'Land Equivalent Ratio', 'Methane Emissions', 'Net Return', 'Nitrogen Use Effi
ciency (ARE AGB)', 'Nitrous Oxide Emissions', 'Soil Moisture', 'Soil Nitrogen', 'Soil Organic Carbon', 'Soil Total Nitrogen', 'Total Cost', 'Variable Cost', 'Water Use', 'Water
 Use Efficiency'
No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 2129, 2128, 2130, 2128, 2133, 2130, ...
Resampling results across tuning parameters:
                    Accuracy
                                   Kappa
   0.02271114 0.5228390 0.3166095
  0.02555004 0.4991828 0.2666937
0.04802460 0.4435037 0.1147268
Accuracy was used to select the optimal model using the largest value.
The final value used for the model was cp = 0.02271114.
```

F) Make Predictions

Now we want to get an idea of the accuracy of the model on our validation set.

We can run the Classification and Regression Trees model directly on the validation set and summarize the results in a **confusion matrix**

```
Overall Statistics
      Accuracy : 0.5129
95% CI : (0.4664, 0.5593)
No Information Rate : 0.4116
P-Value [Acc > NIR] : 6.781e-06
                               Kappa : 0.2711
 Mcnemar's Test P-Value : NA
Statistics by Class:
                               Class: Benefit Cost Ratio (GRTC) Class: Benefit Cost Ratio (GRVC) Class: Benefit Cost Ratio (NRVC)
0.000000 0.000000 0.00000
1.000000 1.000000 1.00000
NaN NaN NaN NaN NaN 0.997845 0.98276 0.99569
                                                                                                      0.00000
1.00000
NaN
0.98276
Sensitivity
Specificity
Pos Pred Value
Neg Pred Value
Prevalence
Detection Rate
Detection Prevalence
Balanced Accuracy
                                                                                                                                          0.98276
0.01724
0.00000
0.00000
0.50000
                                                                               0.002155
0.000000
0.000000
                                                                                                                                                                                                     0.00431
                                                                                                                                                                                                     0.00000
                                                                               0.500000
                                                                                                                                                                                                     0.50000
```

G) Let's carry out the experiment without dropping the NA values