JOM RESEARCH

Introduction to classification model

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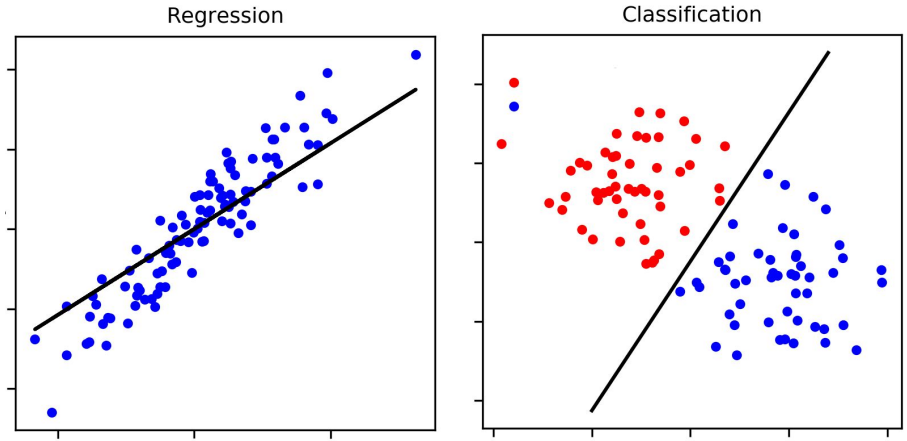
Classification

- A supervised ML task in which the model predict the categorical outcome
- Classification task can be further divided into:
  - Binary or two class classification
  - Multiclass classification

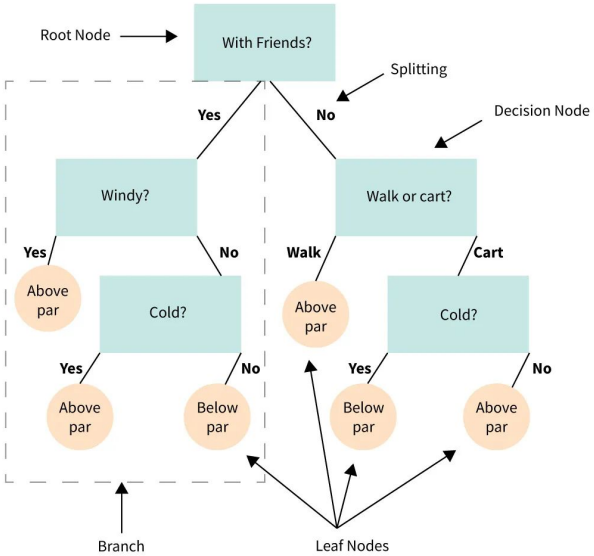


Classification algorithms

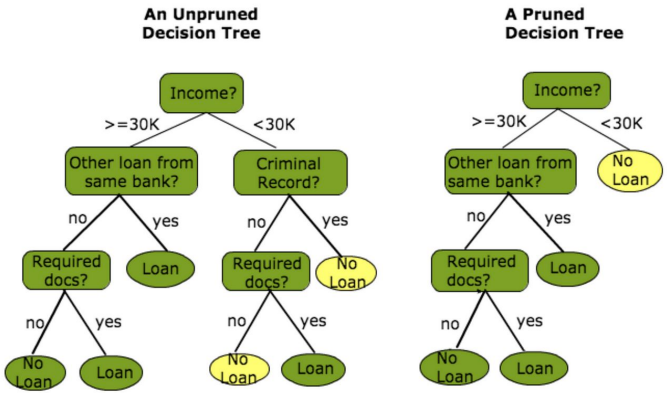
- Just to list a few:
  - Logistic Regression
  - Decision Trees
  - Random Forest
  - Support Vector Machines (SVM)
  - k-Nearest Neighbors (kNN)
  - Naive Bayes
  - Artificial Neural Networks (ANN)
- Full list of algorithms in parsnip package

Decision tree

- Can be used for regression and classification - classification and regression trees (CART) models
- The order of the variable to be splitted is determined by the purity:
  - Gini impurity
  - Entropy and information gain
- Purity - how well separated the points are at the nodes

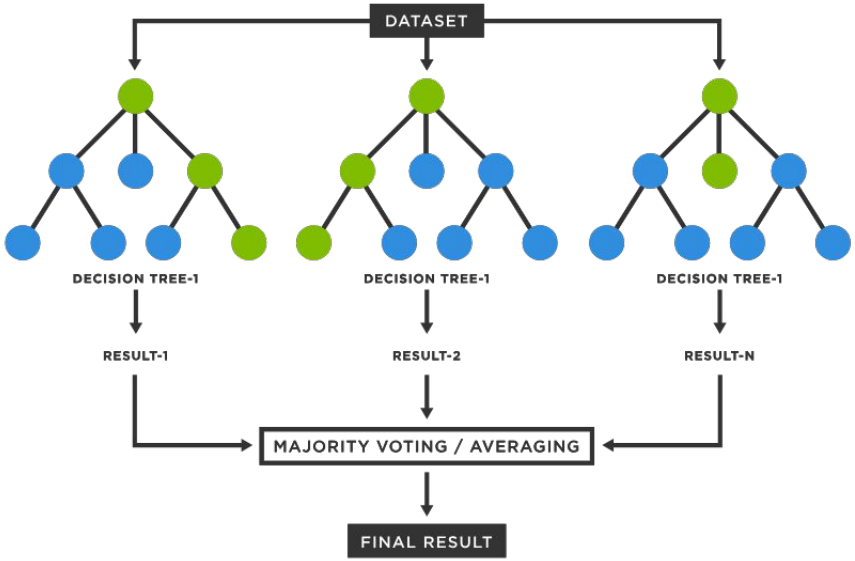


- Pros:
  - Easy to understand
  - Fast computation
  - Able to handle missing data and outliers
- Cons:
  - Tree overfitting - can be overcome with a pruning or CV methods



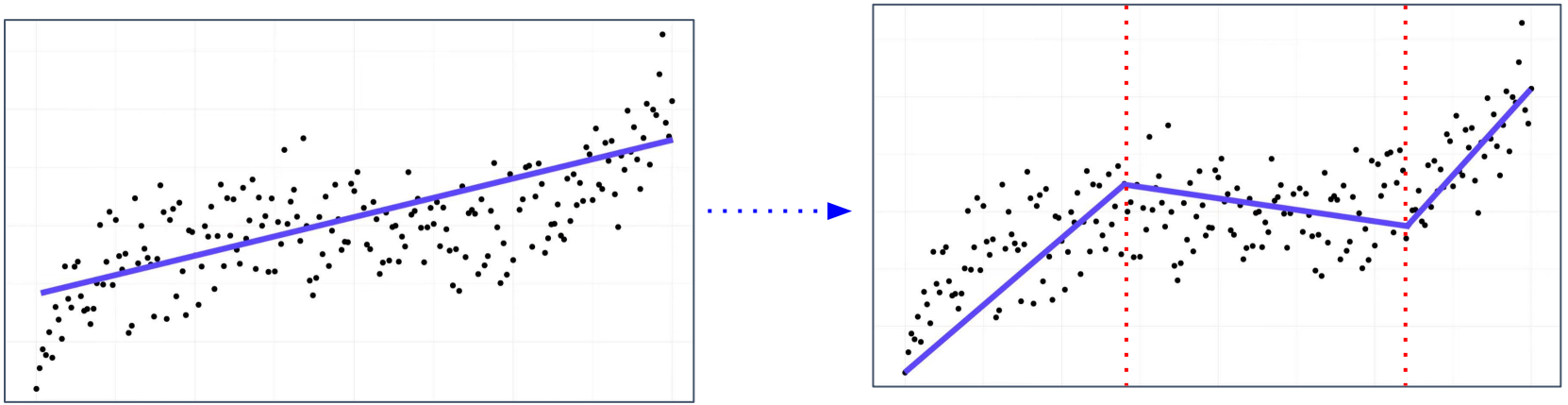
Random forest

- Basically, a collection of decision tree
- Pros:
  - Low risk of overfitting
  - Usually more accurate
  - Able to handle missing data and outliers
- Cons:
  - Relatively slow computation
  - Low interpretability



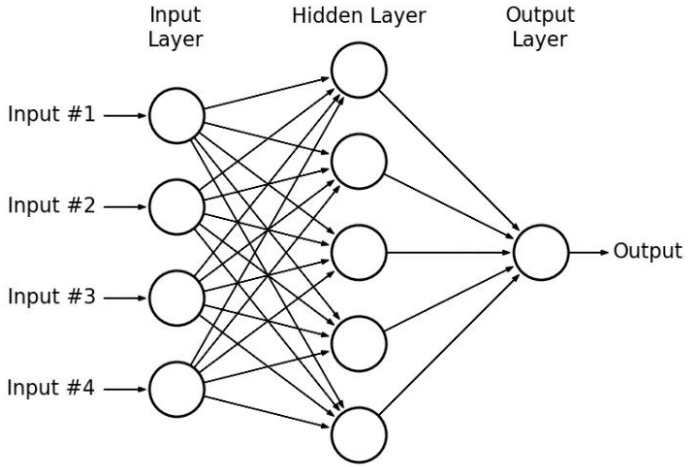
MARS

- Multivariate adaptive regression splines - MARS
- Non-parametric regression technique
- Introduced in 1991 by Friedman
- Main idea - cut the regression line into several cut points

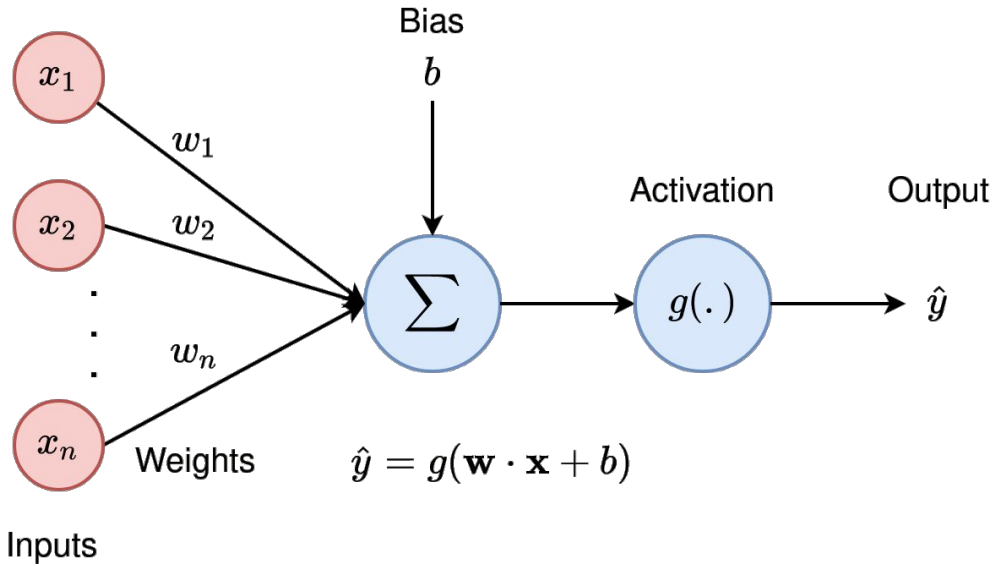


Artificial Neural Network (ANN)

- Neural network is the basis of deep learning
- ANN can be used for regression and classification
- Simple ANN is a single layer, feed-forward neural network, which also known as multilayer perceptron (MLP)
- ANN is formed of:
  - Input layer
  - Hidden layer
  - Output layer



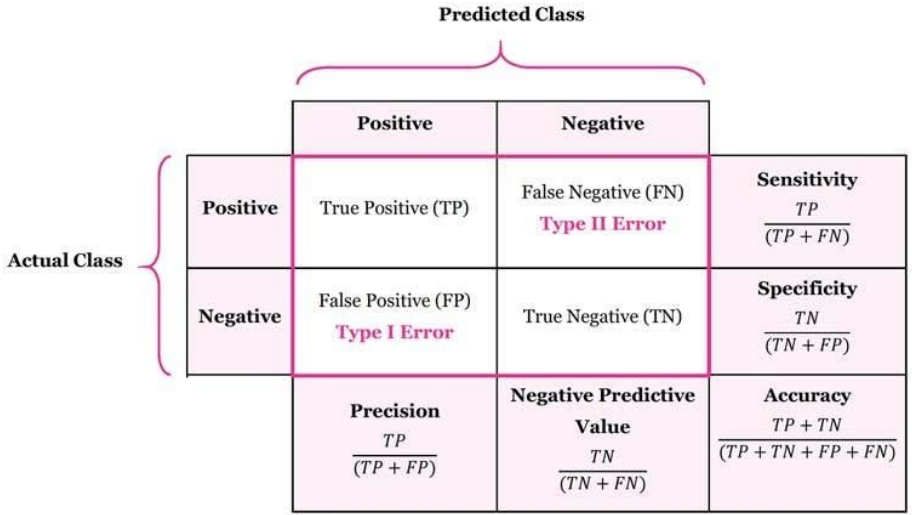
- Breakdown of ANN:



Performance metrics - binary

Confusion matrix

- It is a table comparing the predicted and the actual classes
- Best confusion matrix is at a wiki page



Accuracy

- Proportion of correctly classified cases out of the total cases

Sensitivity/recall

- High sensitivity means effective at detecting the true positive cases
- High sensitivity means low false negative

Specificity

- High specificity means effective at detecting the true negative cases
- High specificity means low false positive

Precision/positive predictive value (PPV)

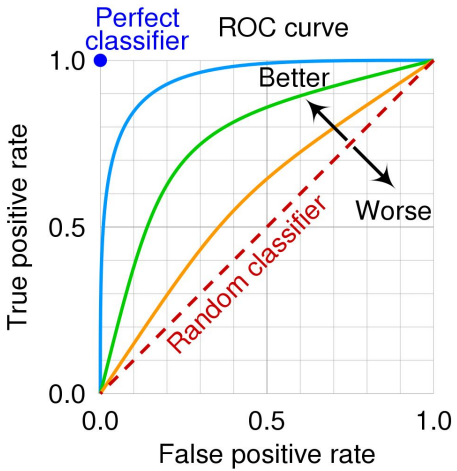
- Indicates proportion of subjects with a predicted positive who truly positive
- High precision - low false positive

Negative predictive value (NPV)

- Indicates proportion of subjects with a predicted negative who truly negative
- High NPV - low false negative

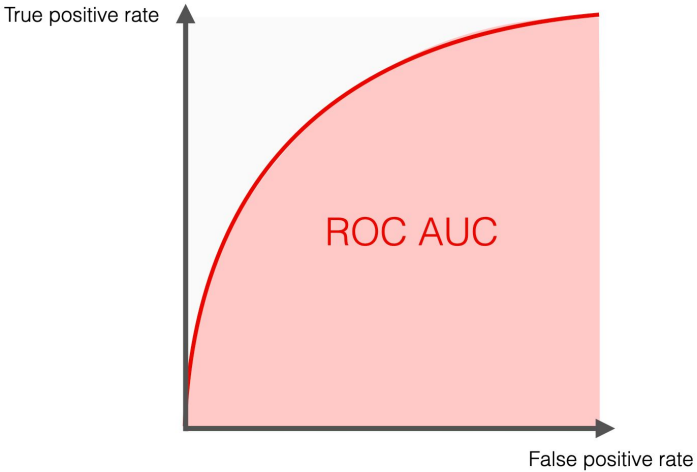
Receiver operating characteristic (ROC) curve

- Reflects a performance of classification models at certain threshold (usually 0.5)
- Can be used to compare different classification ML models



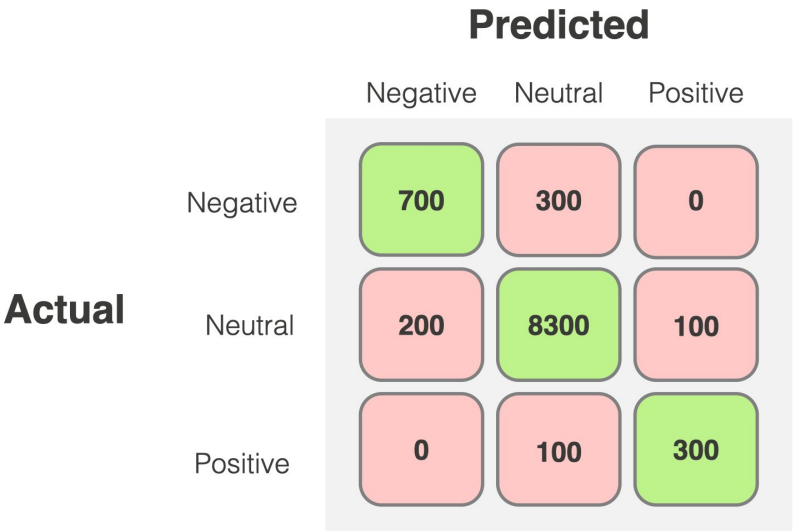
ROC-Area under the curve (ROC-AUC)

- It provides an aggregate measure of the model's performance
- AUC of 0.5 = no discriminant ability, while AUC of 1 = perfect classification
- Can be used to compare different classification ML models



Performance metrics - multiclass

- For metrics such as as accuracy, confusion matrix, etc, multiclass does not affect them



$$\text{Accuracy} = \frac{\text{Correct predictions}}{\text{All predictions}}$$

- Methods for metrics such as sensitivity, specificity, precision, PR-AUC, etc:
  - Macro averaging (default in tidymodels)
  - Weighted macro averaging
  - Micro averaging

$$Pr = \frac{TP}{TP + FP}$$

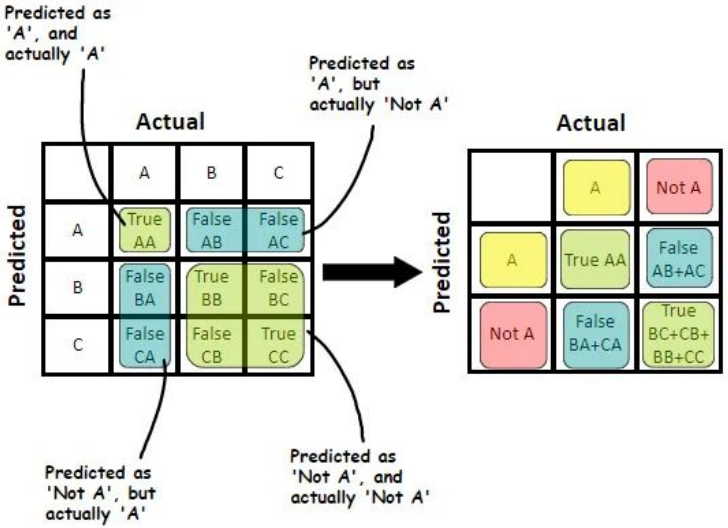
$$Pr_{macro} = \frac{Pr_1 + Pr_2 + \ldots + Pr_k}{k} = Pr_1 \frac{1}{k} + Pr_2 \frac{1}{k} + \ldots + Pr_k \frac{1}{k}$$

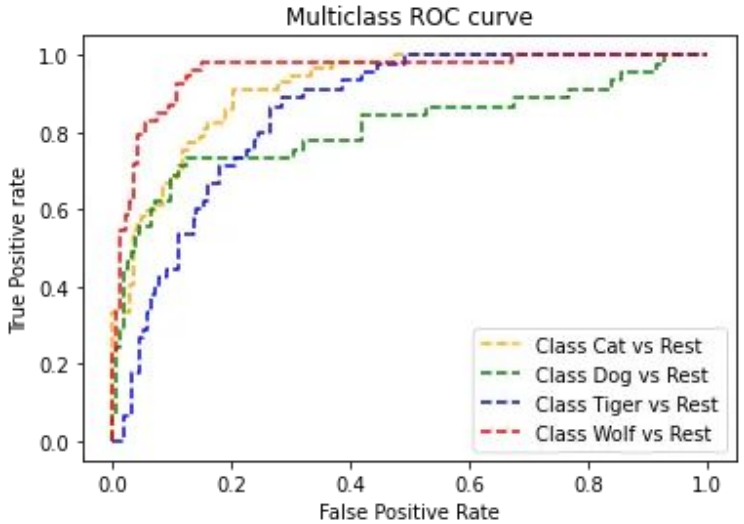
$$Pr_{weighted-macro} = Pr_1 \frac{\#Obs_1}{N} + Pr_2 \frac{\#Obs_2}{N} + \ldots + Pr_k \frac{\#Obs_k}{N}$$

$$Pr_{micro} = \frac{TP_1 + TP_2 + \ldots + TP_k}{(TP_1 + TP_2 + \ldots + TP_k) + (FP_1 + FP_2 + \ldots + FP_k)}$$

- Methods for ROC-AUC:
  - Macro averaging
  - Weighted macro averaging
  - Hand Till (default in tidymodels)
    - Computes the AUC for every pair of classes using a one-vs-one approach and then averages the results
    - Insensitive to class distribution - thus, more robust for class imbalance

- For metrics such as ROC and precision-recall curve, one versus all method is usually utilised





Suggested readings/references

- Kuhn, M., & Silge, J. (2022). Tidy Modeling with R: A Framework for Modeling in the Tidyverse. O'Reilly Media.
- Burger, S. V. (2018). Introduction to machine learning with R: Rigorous mathematical analysis (First edition). O'Reilly Media.

Any question?

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