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Introduction to classification model

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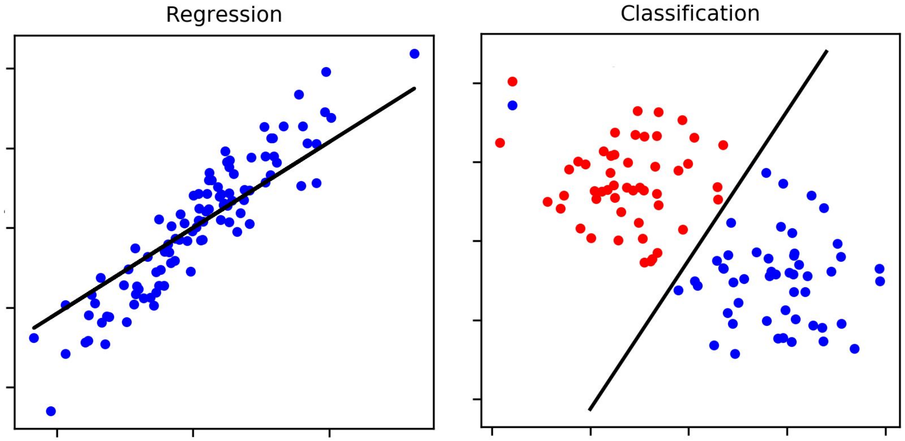
Contents

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

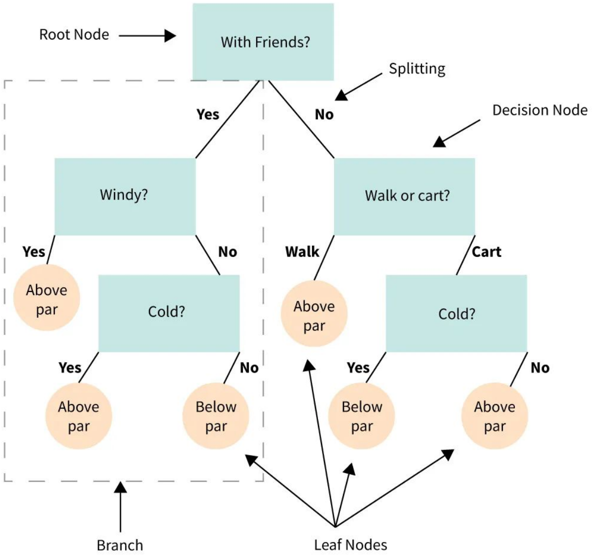


Classification algorithms

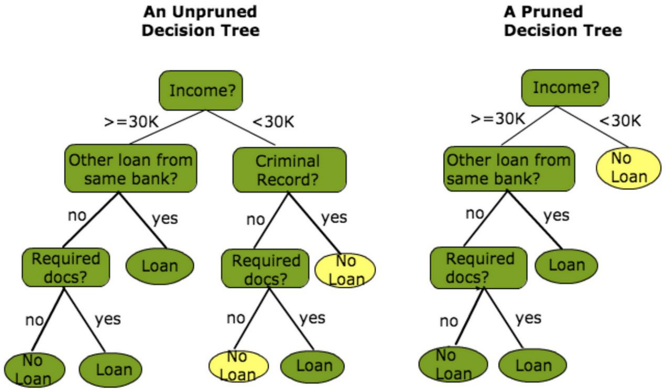
- Just to list a few:
    - Logistic Regression
    - Decision Trees
    - Random Forest
    - Support Vector Machines (SVM)
    - k-Nearest Neighbors (kNN)
    - Naive Bayes
    - Artificial Neural Networks (ANN)
- Full list of algorithms in parsnip package

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



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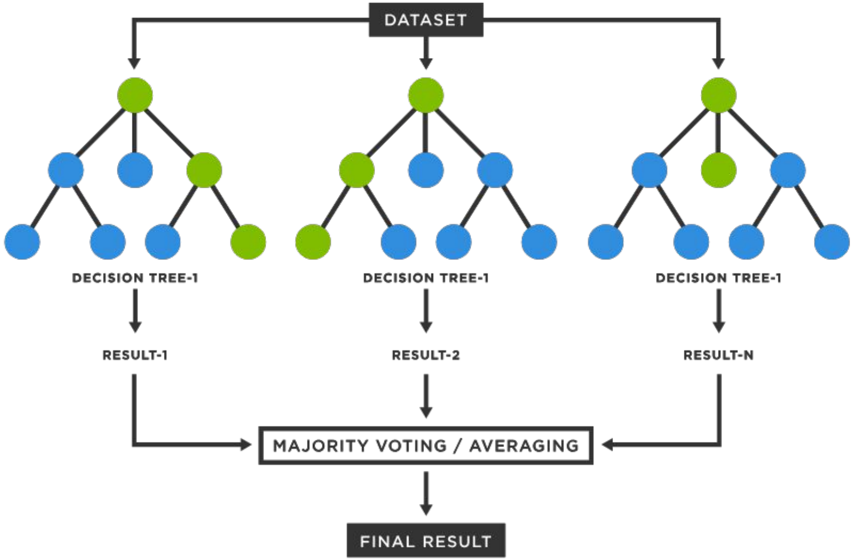
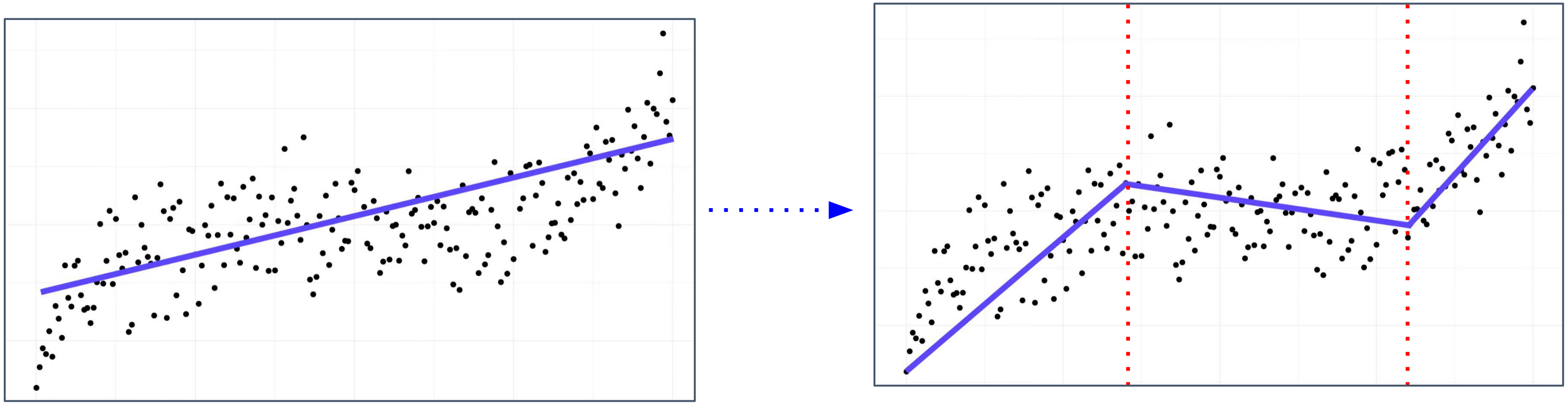
Random forest

- 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



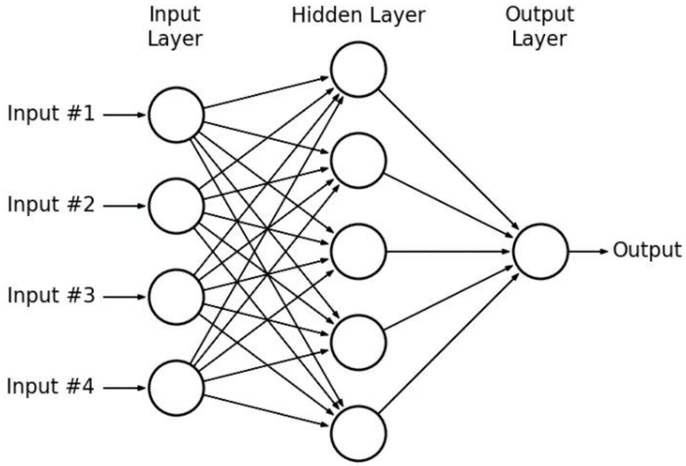
MARS

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

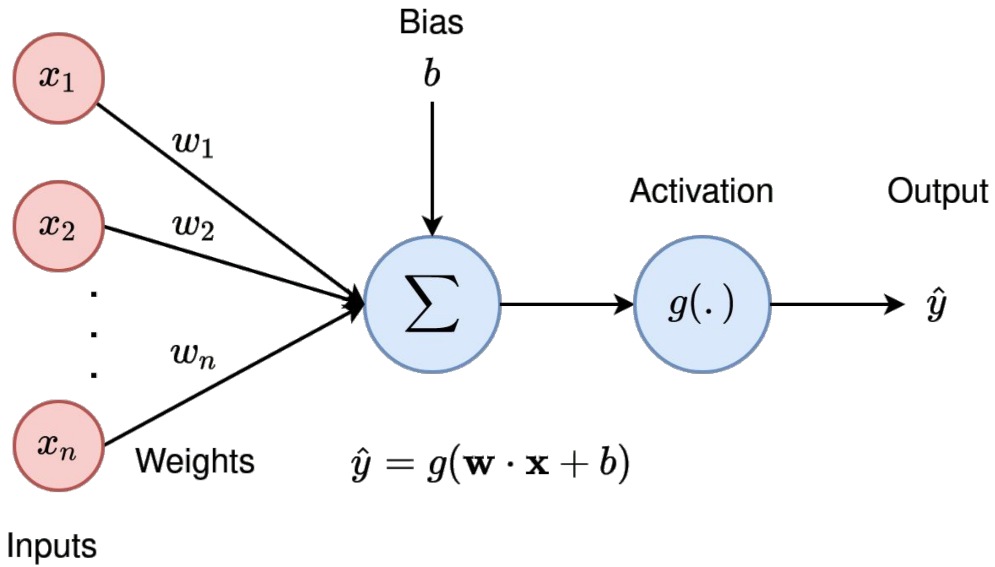


Artificial Neural Network (ANN)

- 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:

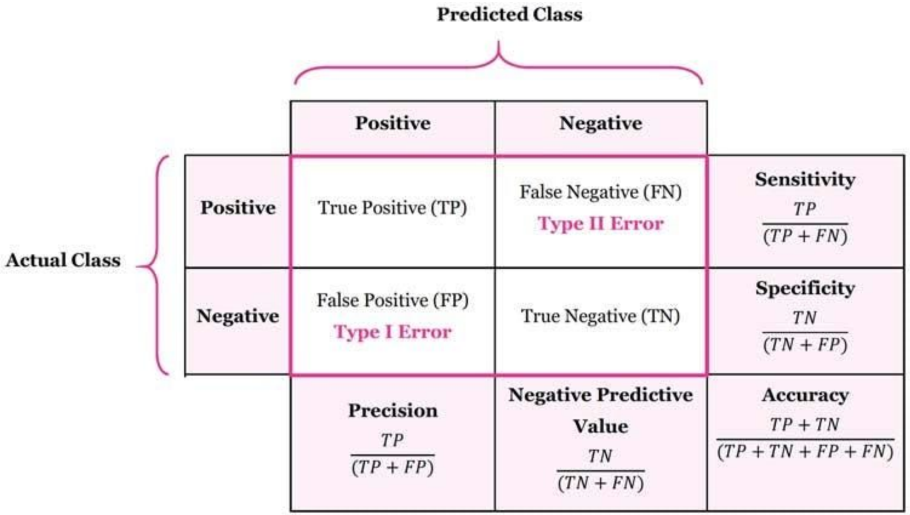


$$\hat{y} = g(\mathbf{w} \cdot \mathbf{x} + b)$$

Performance metrics

Confusion matrix

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



		Predicted Class		
		Positive	Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) Type II Error	Sensitivity $\frac{TP}{(TP+FN)}$
	Negative	False Positive (FP) Type I Error	True Negative (TN)	Specificity $\frac{TN}{(TN+FP)}$
		Precision $\frac{TP}{(TP+FP)}$	Negative Predictive Value $\frac{TN}{(TN+FN)}$	Accuracy $\frac{TP+TN}{(TP+TN+FP+FN)}$

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)

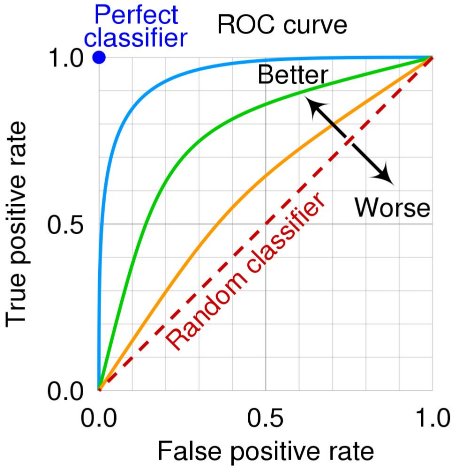
- Indicates proportion of subjects with a predicted positive who truly positive
- High precision - low false positive

Negative predictive value (NPV)

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

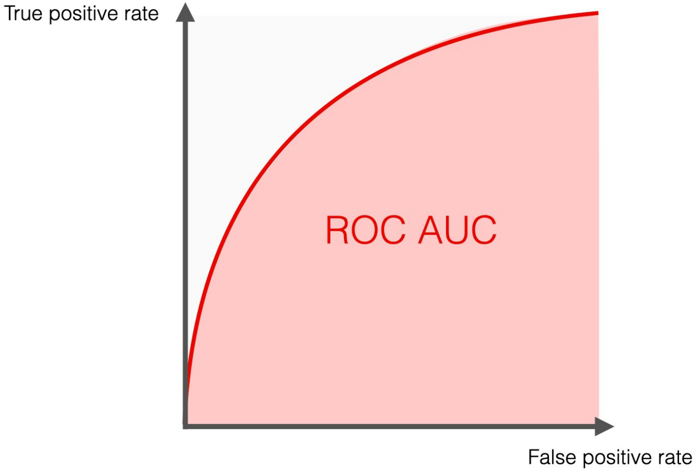
Receiver operating characteristic (ROC) curve

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



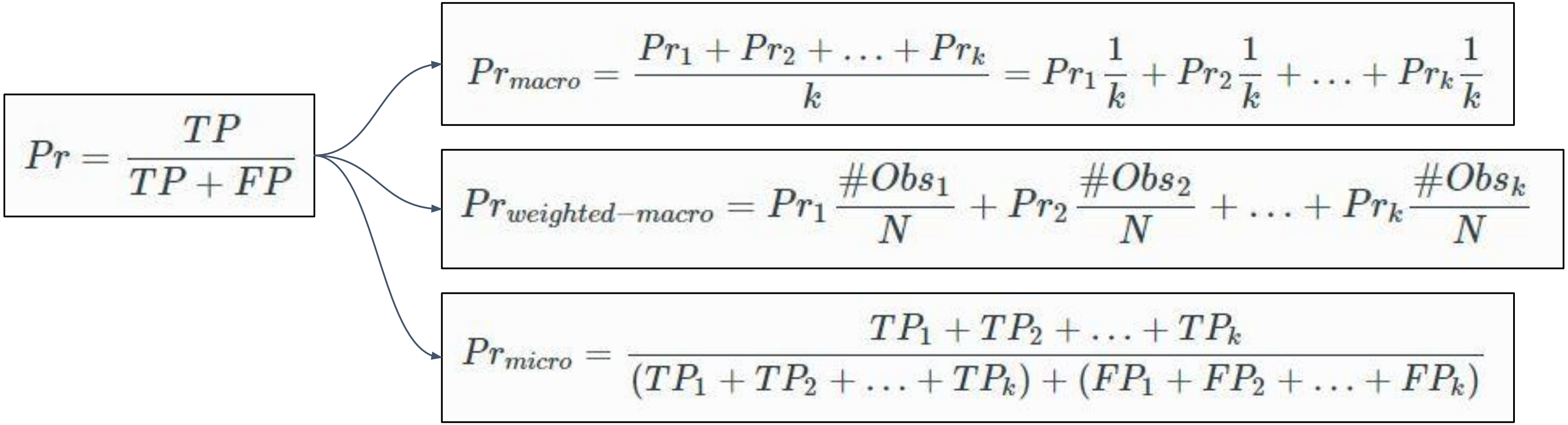
ROC-Area under the curve (ROC-AUC)

- 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



Multiclass performance metrics

- There are at least 3 methods:
  - Macro averaging
  - Weighted macro averaging
  - Micro averaging



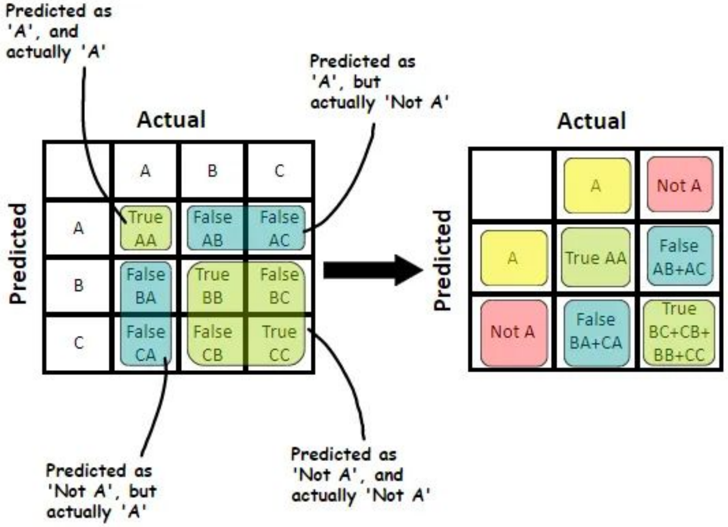
$$Pr = \frac{TP}{TP + FP}$$

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

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

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

- For metrics such as ROC and ROC-AUC, one versus all method can be used



Predicted as 'A', and actually 'A'

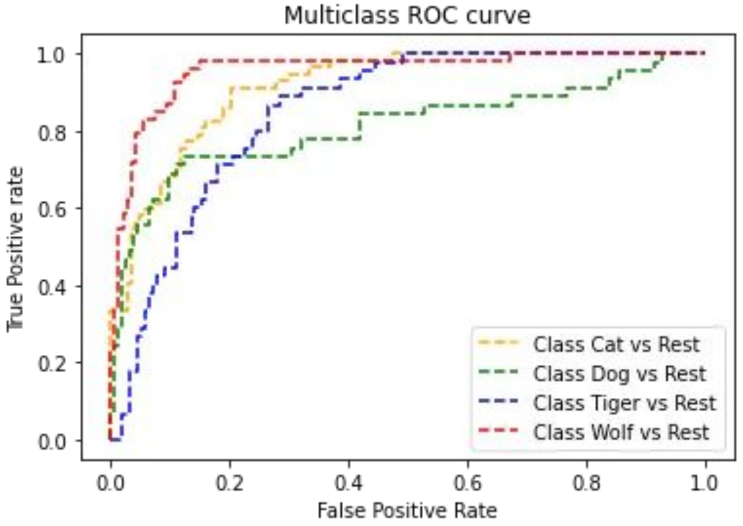
Predicted as 'A', but actually 'Not A'

Predicted as 'Not A', but actually 'A'

Predicted as 'Not A', and actually 'Not A'

Predicted \ Actual	A	B	C
A	True AA	False AB	False AC
B	False BA	True BB	False BC
C	False CA	False CB	True CC

Predicted \ Actual	A	Not A
A	True AA	False AB+AC
Not A	False BA+CA	True BC+CB+BB+CC



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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