Data Driven Modeling 2: Classification

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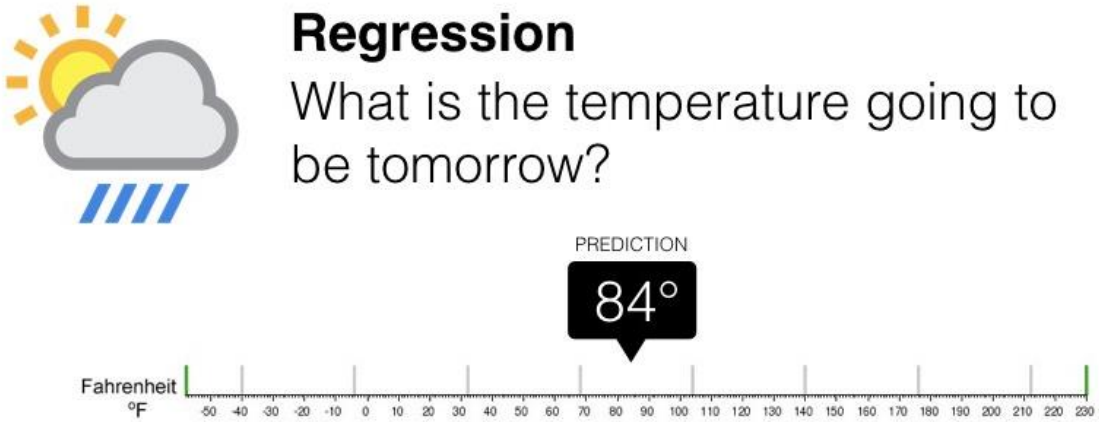
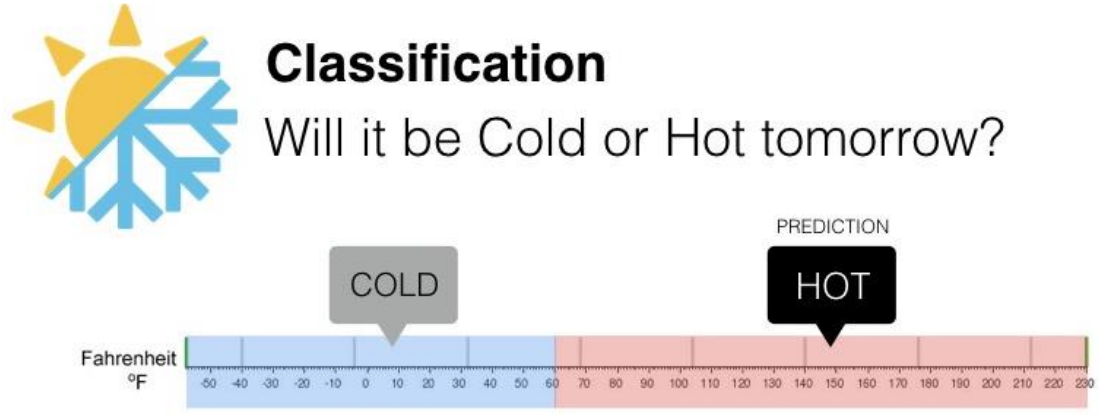
"To be or not to be..."

Rapid Advancement in Process Intensification Deployment

Classification





- Classification is the machine learning task where you want to predict a categorical output, called a 'class'

Examples

Is a catalyst good, bad or average?

Classes

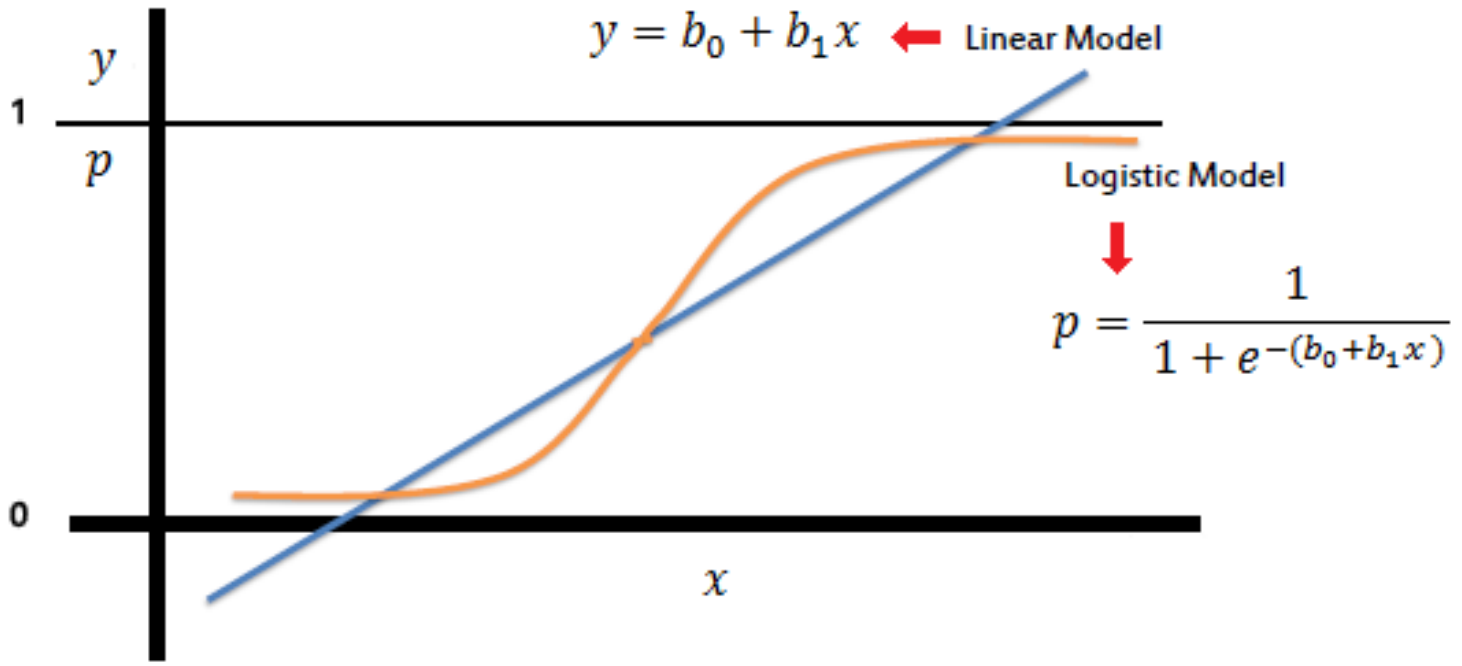
Good Average Bad

Is the flow laminar or turbulent?

Classes

Laminar Turbulent

Logistic Regression



Descriptors

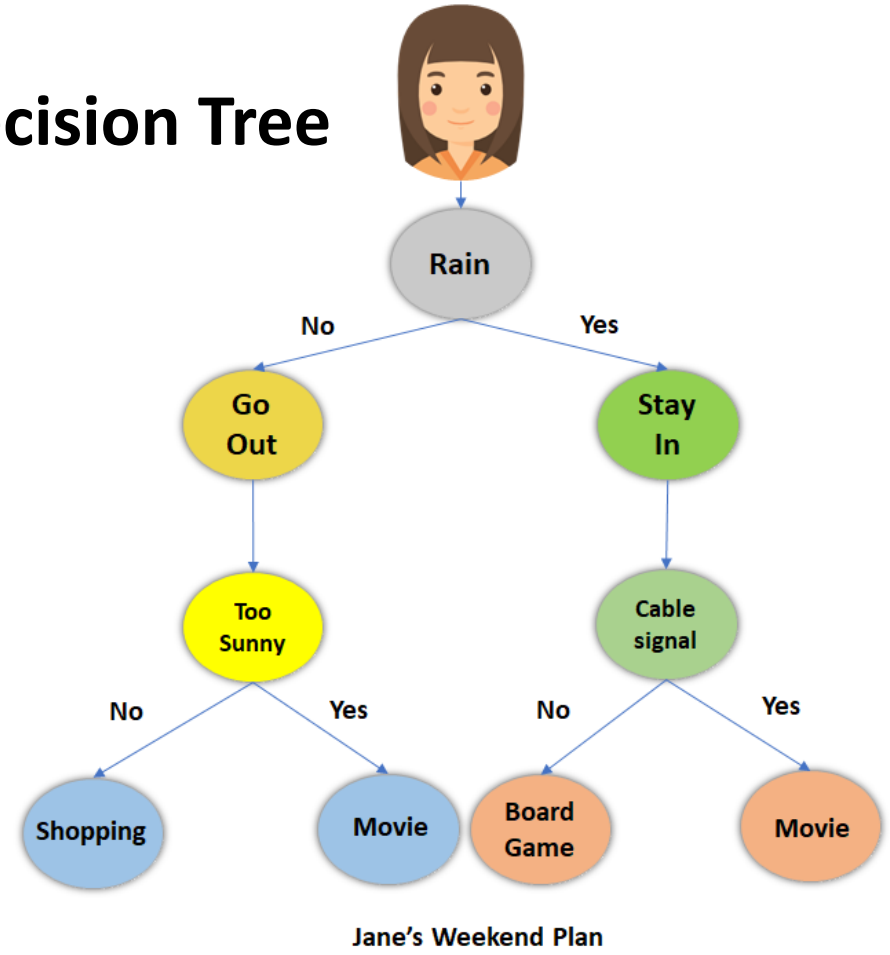
B0, B1

Class Membership

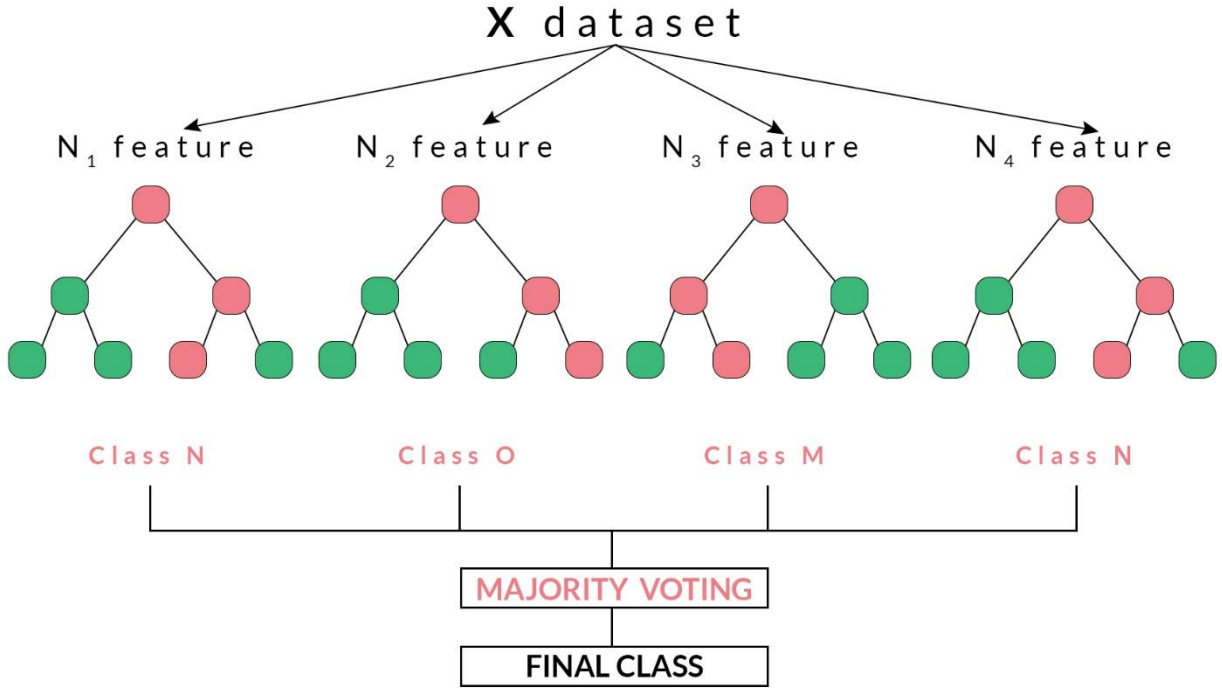
- Logistic regression is a linear model for **binary classification**

Random Forest

Decision Tree

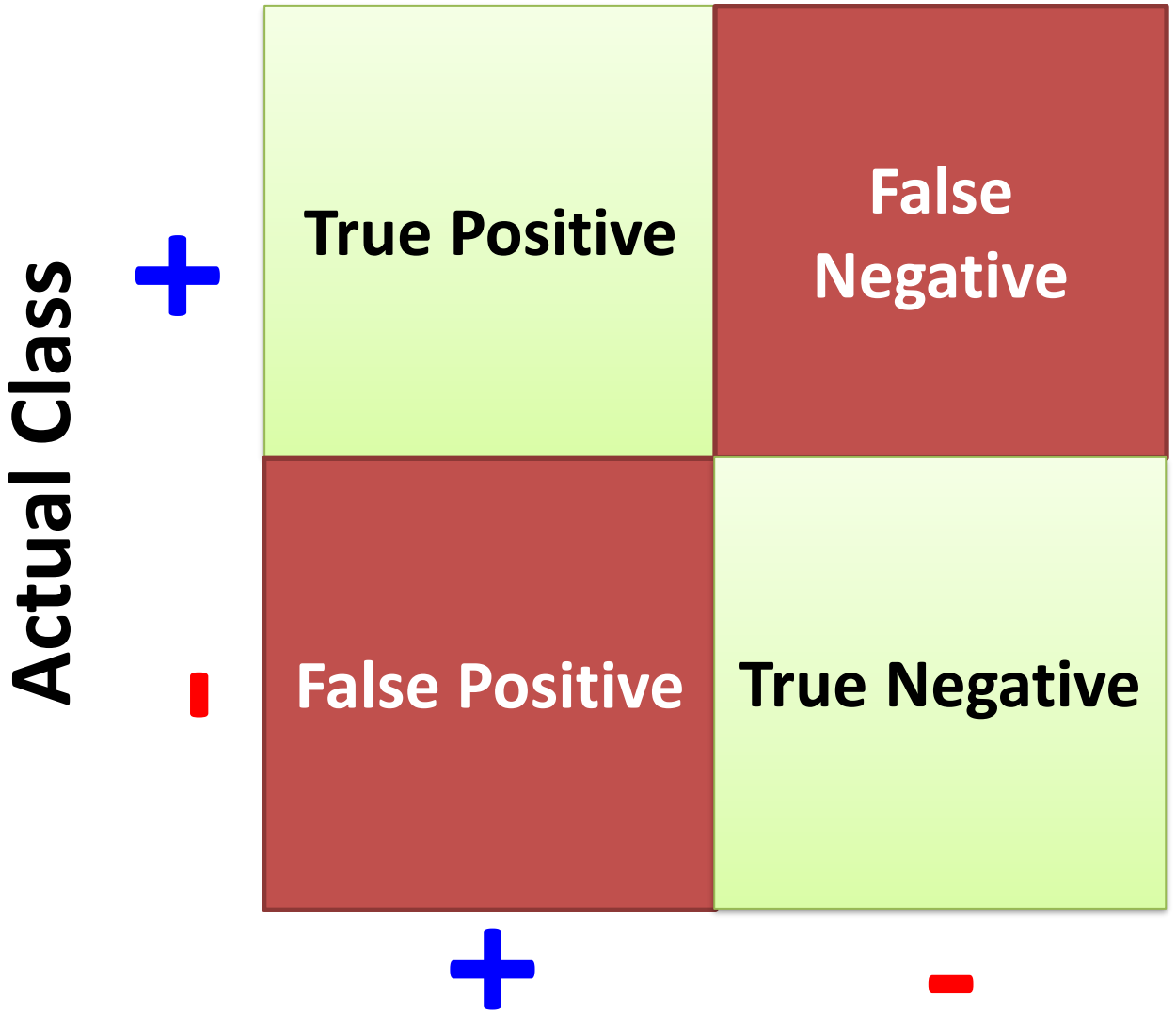


A Random Forest



- Random forest uses a collection of decision trees to classify a sample
- **Can be used for multiclass classification**

Confusion Matrix



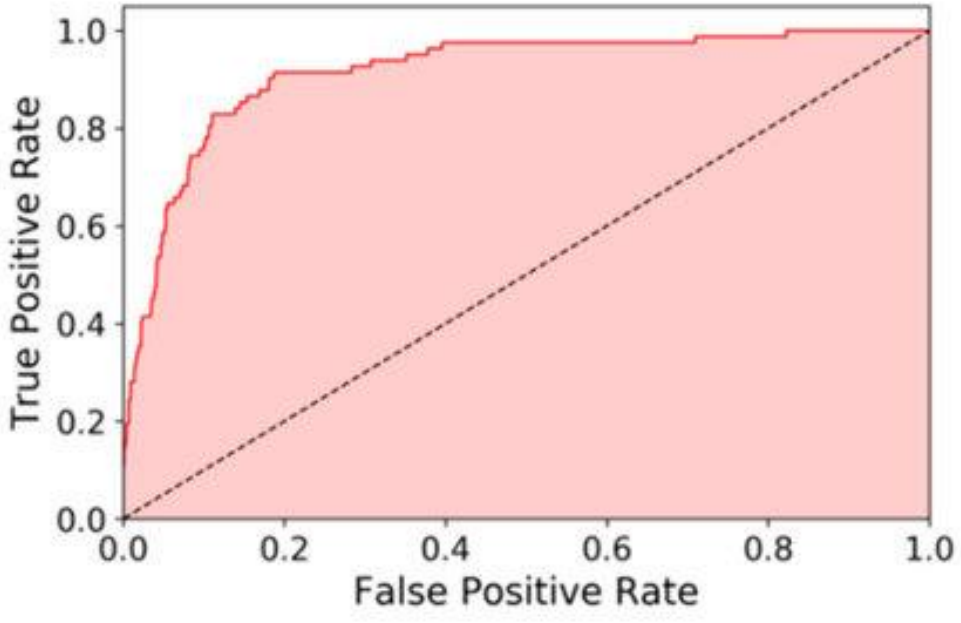
Measures and Metrics

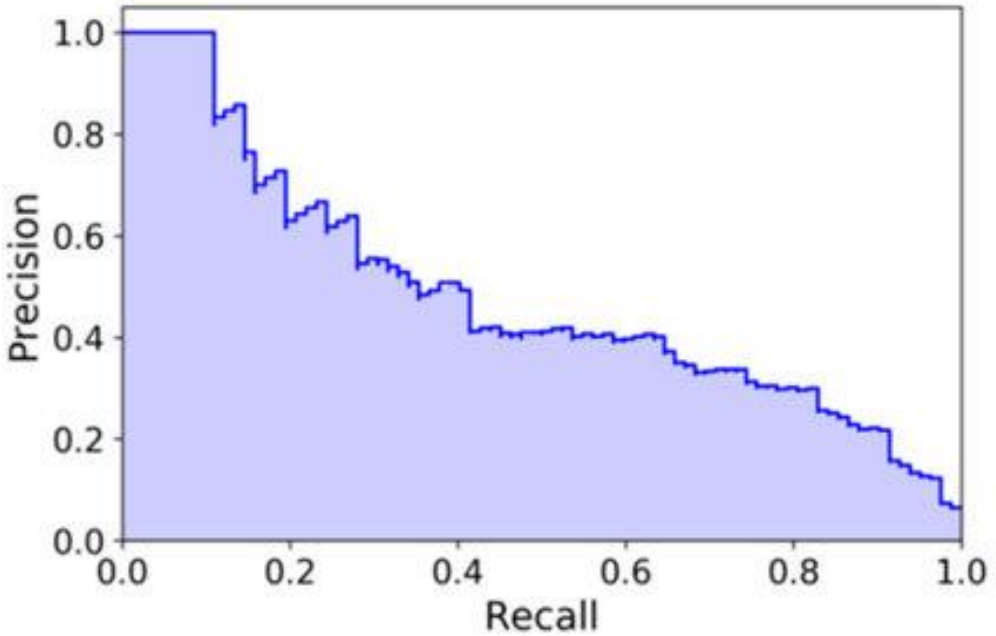
Accuracy: $\frac{Correct\ Predictions}{Total\ Predictions}$

Precision and Recall curve are good measures for imbalanced datasets with lot of negatives

Recall: $\frac{True\ Positive}{True\ Positive + False\ Negative}$

Precision: $\frac{True\ Positive}{True\ Positive + False\ Positive}$





Problem Set-up

- We will look at the California dataset and instead of predicting exact house price (regression), we will predict if a house has a high or low price (classification) based on some cutoff value.