Introduction to Data Science with Python Lecture 2: Supervised Learning

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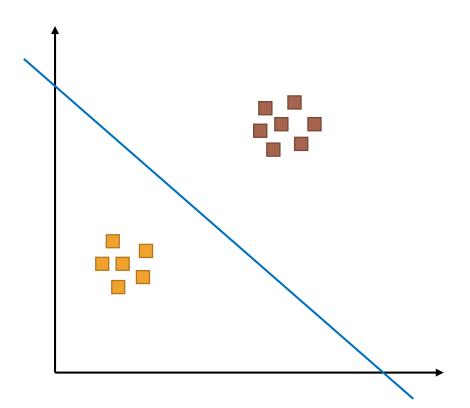
Signify Research (formerly known as Philips Lighting)

Outline

- Supervised Learning
 - Regression and Classification
 - Linear Regression (Ridge, Lasso)
 - Logistic Regression
 - CART (Classification and regression trees)
 - k-nearest neighbors algorithm
- Evaluation metrics
 - Confusion Matrix
 - Accuracy
 - Precision, Recall
 - F-beta Score
- Concepts
 - Overfitting/Underfitting
 - Cross validation

Supervised Learning

- The core idea of supervised learning is using given set of points that associated to set of outcomes to build a classifier that learns how to **predict outputs from inputs**.
- Type of predictions: continuous (regression) and class (classification)
- Linear models
- Non-parametric approaches
 - Tree-based models
 - Nearest Neighbours methods



Linear Regression

The main assumption is that predicted value is expected to be a **linear** combination of the input variables.

- Simple Linear Regression
 - Minimization the sum of squared residuals
 - Highly sensitive to random errors
- Ridge regression
 - Introducing L2 penalty for weights
 - Alpha parameters helps to control shrinkage
- Lasso regression
 - Introducing L1 penalty for weights
 - Effectively reducing the number of variables

$$\min_{w} ||Xw - y||_2^2$$

$$\min_{w} ||Xw - y||_2^2 + \alpha ||w||_2^2$$

$$\min_{w} \frac{1}{2n_{samples}} ||Xw - y||_{2}^{2} + \alpha ||w||_{1}$$

Logistic Regression

- Used for classification, actually non-linearity over a linear classifier
- Predict the probability of categorical dependent variable
- Types: binary(sigmoid activation), multi-class(softmax activation)
- Loss function: cross-entropy

$$J(\mathbf{w}) \ = \ rac{1}{N} \sum_{n=1}^N H(p_n,q_n) \ = \ - rac{1}{N} \sum_{n=1}^N \ \left[y_n \log \hat{y}_n + (1-y_n) \log (1-\hat{y}_n)
ight]$$

Trees (CART)

• Decision Tree



 Decision tree builds classification or regression models in the form of a tree structure. It breaks down a dataset into smaller and smaller subsets while at the same time an associated decision tree is incrementally developed.

Random Forest

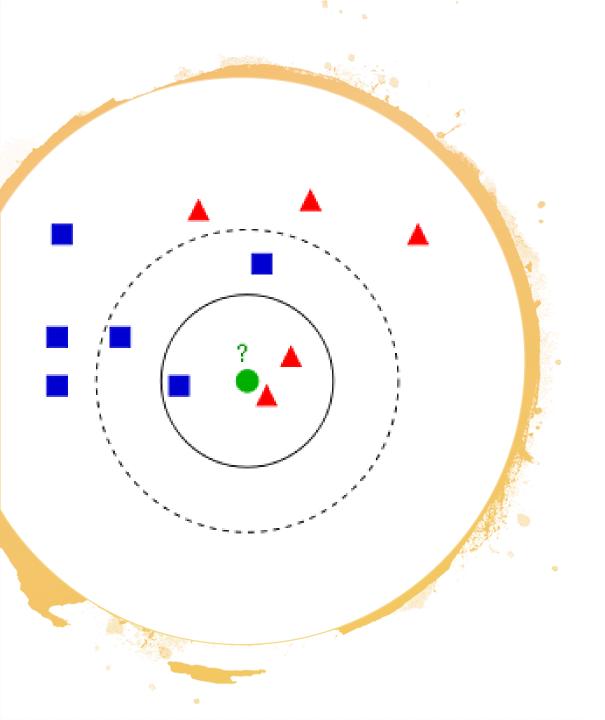


 Random forest builds multiple decision trees and merges them together to get a more accurate and stable prediction.



Gradient-Boosted Tree

• Classifier is trained on data, taking into account the previous classifiers' success. After each training step, the weights are redistributed. Misclassified data increases its weights to emphasize the most difficult cases. In this way, subsequent learners will focus on them during their training.

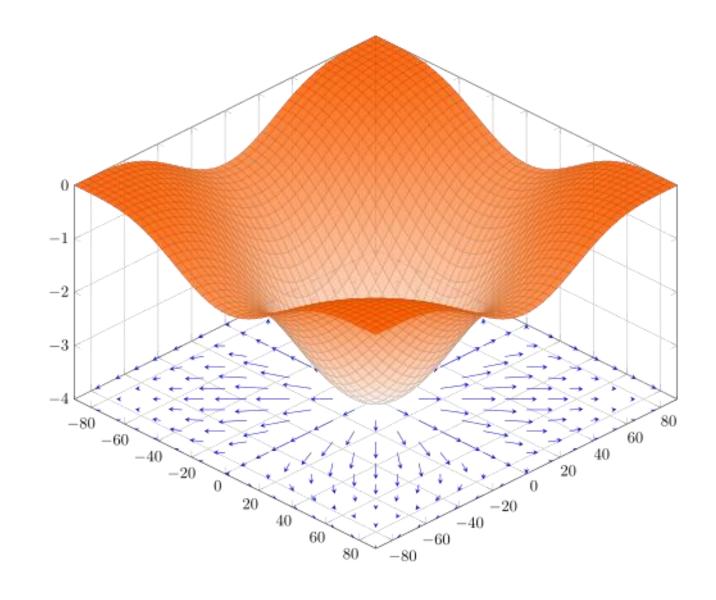


Nearest-Neighbor Methods

- Idea: find some amount of closest points (with classes that we know) and then average their responses
 - Metric: Euclidian Distance
 - Classification: Majority Vote
 - Regression: Average of values
- Sensitive to local structure of the data

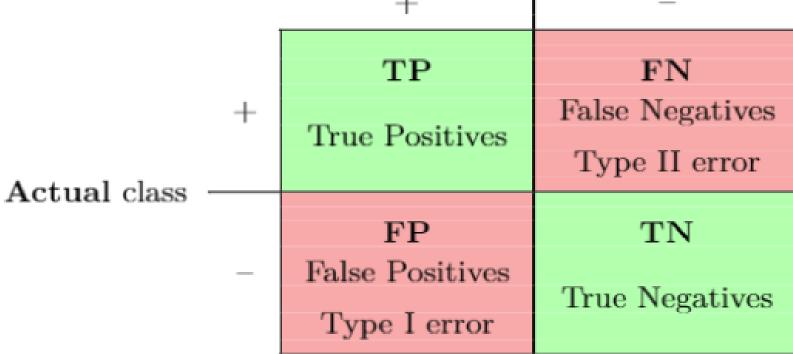
Stochastic Gradient Descent

- Gradient points in the direction of the greatest rate of increase of the function
- Descending the gradient = moves to anti-gradient direction



Evaluation Metrics (Classification)

Predicted class



Evaluation Metrics (Classification)

| Metric | Formula | Interpretation | |
|-----------------------|---|---|--|
| Accuracy | $\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}}$ | Overall performance of model | |
| Precision | $\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$ | How accurate the positive predictions are | |
| Recall Sensitivity | $\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$ | Coverage of actual positive sample | |
| Specificity | $\frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}}$ | Coverage of actual negative sample | |
| F1 score | $\frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$ | Hybrid metric useful for unbalanced classes | |

Evaluation Metrics (Regression)

- Mean Absolute Error
- Mean Squared Error
- Root Mean Squared Error
- Root Mean Squared Logarithmic Error
- Coefficient of determination (R2 score)

Cross-validation





Bias/variance tradeoff

| | Underfitting | Just right | Overfitting |
|------------|--|---|--|
| Symptoms | - High training error - Training error close to test error - High bias | - Training error slightly lower than test error | - Low training error - Training error much lower than test error - High variance |
| Regression | | | My |



Practice

- http://scikitlearn.org/stable/user_guide.html
- http://scikitlearn.org/stable/supervised learning.html
- http://scikitlearn.org/stable/auto_examples/index.html

Assignment 2



Titanic: Machine Learning from Disaster

Start here! Predict survival on the Titanic and get familiar with ML basics

Getting Started · Ongoing · • tutorial, tabular data, binary classification



House Prices: Advanced Regression Techniques

Predict sales prices and practice feature engineering, RFs, and gradient boosting Getting Started ⋅ Ongoing ⋅ ♠ tabular data, regression