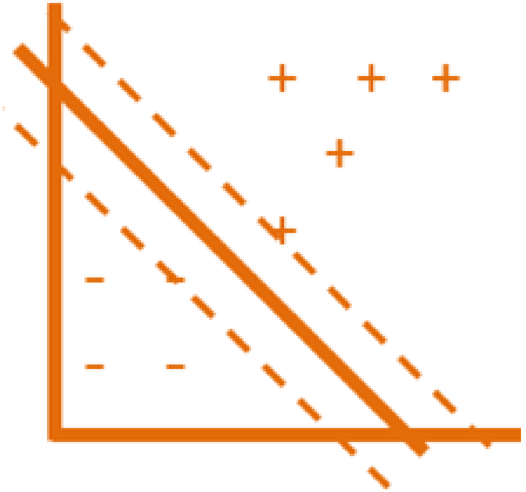
Support Vector Machines

Simple algorithm with a clever trick



Yordan Darakchiev
Technical Trainer
iordan93@gmail.com

sli.do

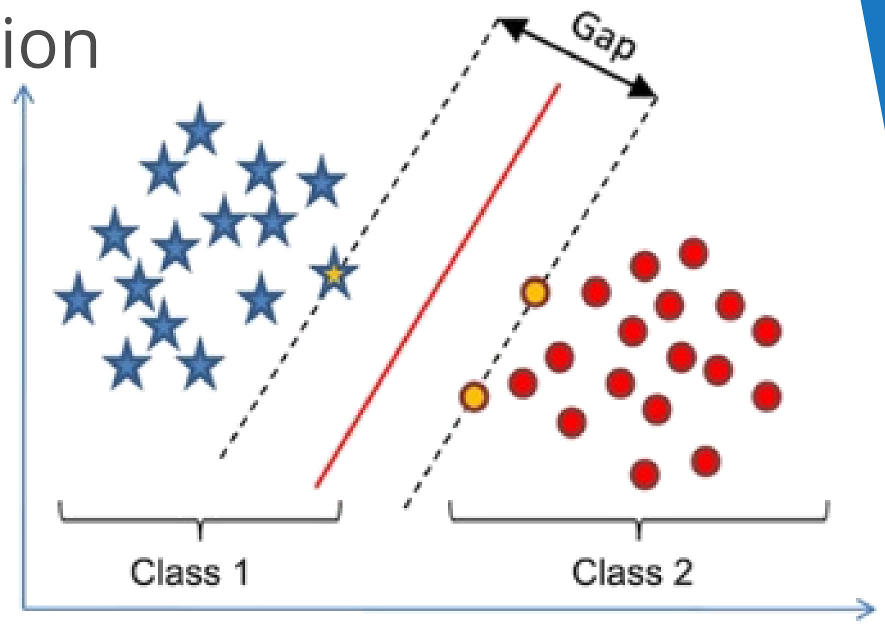
#MachineLearning

Table of Contents

- Support vector machines
  - Kernel trick
- k-nearest neighbors
- Anomaly detection and outlier detection

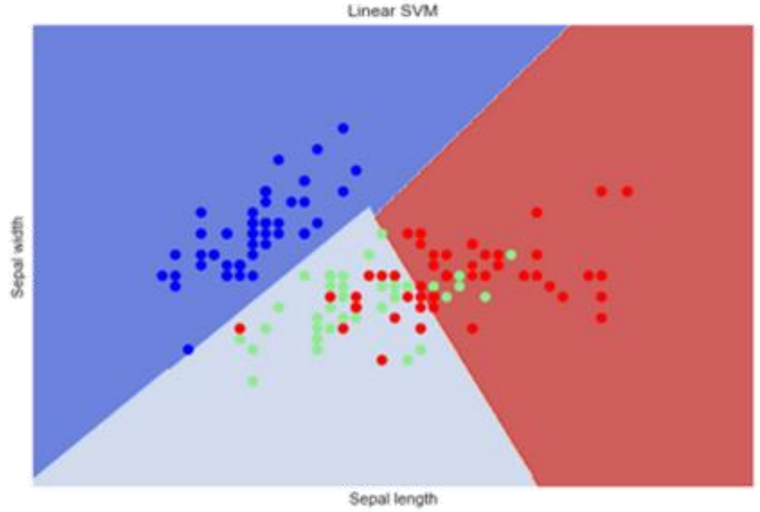
Support Vector Machines

- Extreme(ly easy) case
  - Two linearly separable classes
    - Decision boundary: simple line (plane in many dimensions)
- Goal
  - Choose the line that best separates the classes
  - Maximum margin
  - The math formula for the objective function is a little complex because it involves matrix algebra
- Applications:
  - Mainly for classification
    - `sklearn.svm.SVC`, `LinearSVC`
  - Regression: `sklearn.svm.SVR`



Support Vector Machines (2)

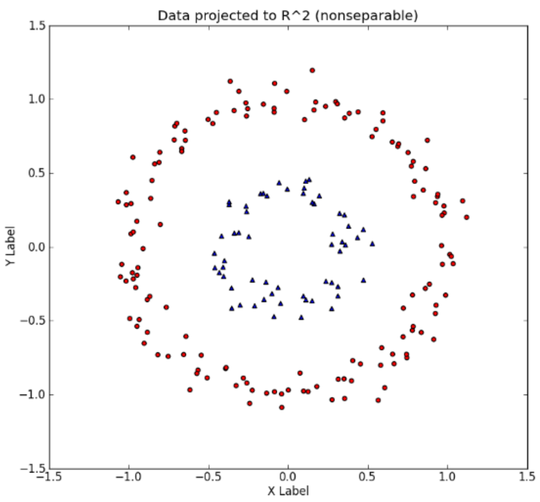
- Difficult to separate classes ⇒ use regularization
  - C – penalty for misclassification (L2, $C = 1/\lambda$)
    - Smaller value = stricter (more regularization)
- Many classes
  - `scikit-learn` uses the "one-vs-one" approach
    - Trains $c(c-1)/2$ classifiers
      (c – number of classes)

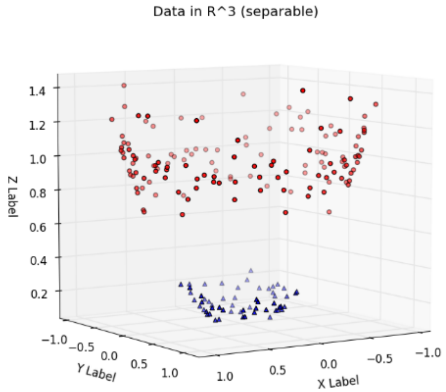


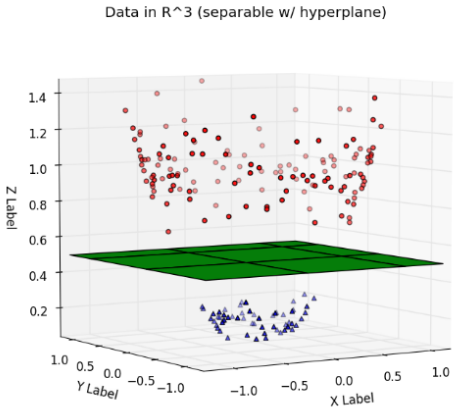
- Considerations
  - Few datasets are linearly separable
  - High complexity: between $O(m.n^2)$ and $O(m.n^3)$
    - m – number of features, n – number of samples
    - Feasible for max $\sim 10^5$ samples

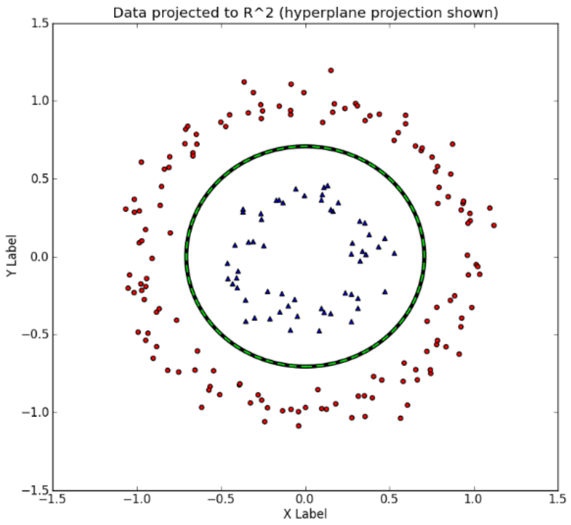
"Kernel Trick"

- Used when data is not linearly separable
- Algorithm
  - Create non-linear combinations of the features using a mapping function (kernel)
    - This projects them to a higher-dimensional space
- Most widely used: Radial Basis Function (Gaussian) kernel
  - Hyperparameter γ – needs to be optimized (e.g. via grid search)



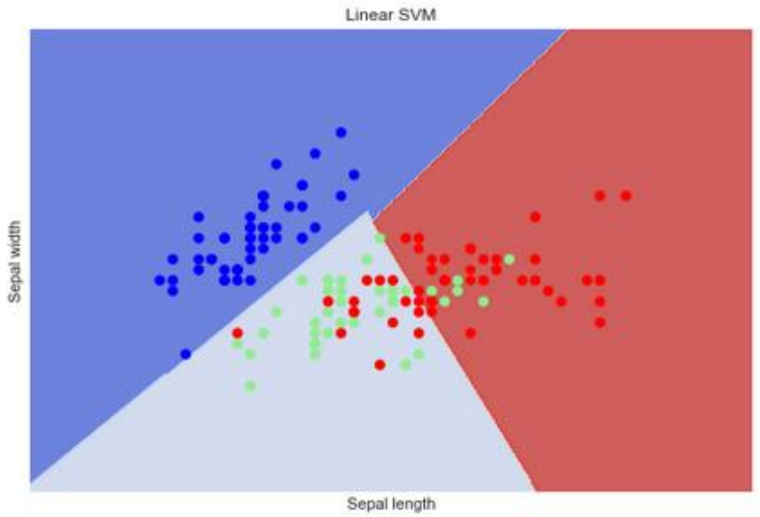


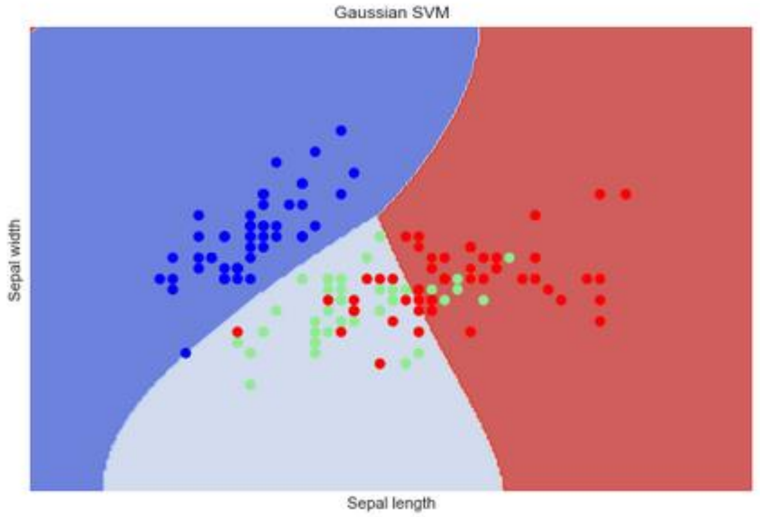




Example: Kernel SVM

- Use a Gaussian SVM to predict Iris classes
  - Try to fine-tune the parameters (C, γ)
    - Using cross-validation
  - Print out-of-sample test scores for the model
  - Plot the decision regions
  - Plot a ROC curve
  - Perform model selection
    - Linear vs. RBF (Gaussian) kernel
- Some other explanations of the "kernel trick"
  - Quora
  - Reddit
  - Medium (a little more math)



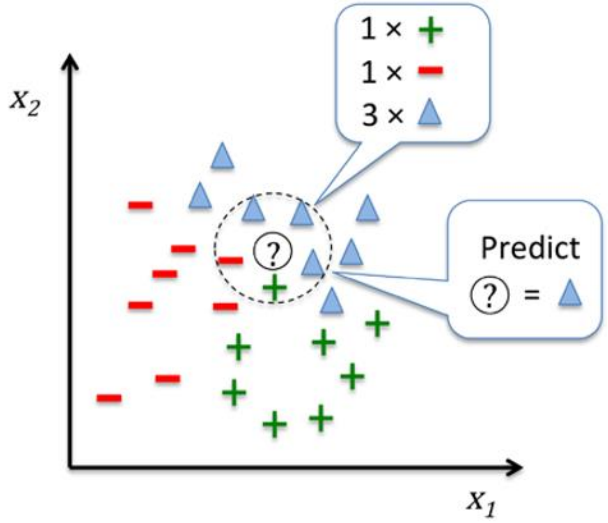


k-Nearest Neighbors

"Lazy learning"

k-Nearest Neighbors (kNN)

- "Lazy learner"
  - Doesn't learn a fitting function but memorizes the training data
- Algorithm
  - Choose a number k and a distance metric (e.g. Euclidean)
    - This choice provides bias / variance balance
    - Minkowski distance: generalized Euclidean distance
  - Find the k nearest neighbors of the current sample
  - Use majority vote to classify
- Advantage: easily adapts to new data
- Downside: computational complexity grows linearly with new samples
  - Efficient implementation: k-d trees

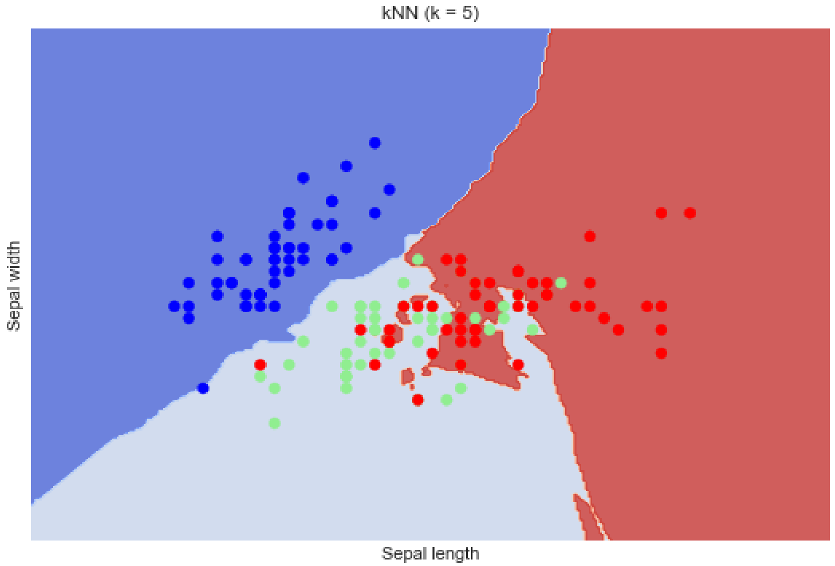


Example: k-Nearest Neighbors

- Perform kNN on Iris data
  - It can also be used for regression
    - We need to be extremely careful, especially in the case of extrapolation
- Display the decision regions

```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors = 5)
knn.fit(iris.data, iris.target)
```



- Voronoi tiling (tessellation)
  - Very useful in image processing and working with graphs

```
knn = KNeighborsClassifier(n_neighbors = 1)
```

- Can also be used for regression
  - [Docs](#) (scikit-learn)

Anomaly Detection

Using SVMs to find unusual data

One-Class SVM

- Anomaly / novelty detection
  - Given a dataset **free of outliers**, detect anomalies in new observations
- Outlier detection
  - Given a "polluted" dataset, filter out the outliers
    - We already know about RANSAC – this is one of many methods
- We can use a one-class SVM as an anomaly detector
  - [Docs and example]()
  - Kernel: usually RBF
  - Parameters:
    - γ – kernel coefficient
    - ν – probability of finding a regular observation far from the others
      - $0 \leq \nu \leq 1$, $0{,}5$ by default
  - Works for outlier detection too, but not on all datasets

Example: Outlier Detection

- Use a one-class SVM to detect anomalies in the Boston housing dataset
  - Plot the anomalous observations
- * Optionally, compare different outlier detectors
  - E.g., RANSAC vs. one-class SVM
  - Follow the tutorial in the `scikit-learn` docs
    - Apply it to the Boston data
- Notes
  - Be extremely careful with the testing data
    - It must be properly stratified
  - You'll see that these algorithms don't accept a y parameter
    - Unsupervised learning

Summary

- Support vector machines
  - Kernel trick
  - A mathematically rigorous tutorial (Microsoft)
- k-nearest neighbors
- Anomaly detection and outlier detection

Questions?