Supervised learning

Aprendizaje Automático para la Robótica
Máster Universitario en Ingeniería Industrial

Departamento de Automática

Universidad de Alcalá   ISG

Objectives

1. Extend supervised learning algorithms
2. Apply supervised learning to real-world problems
3. Introduce Scikit-Learn API for supervised algorithms

Bibliography

- Müller, Andreas C., Guido, Sarah. *Introduction to Machine Learning with Python*. O'Reilly. 2016
- Géron, Aurélien. *Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow*. 2nd Edition. O'Reilly. 2019

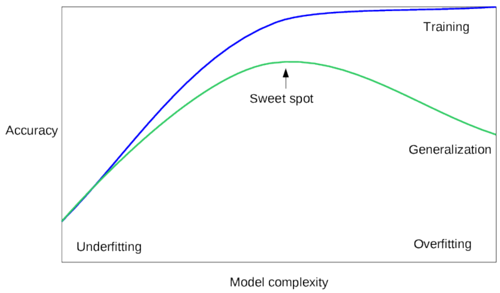
Most figures have been taken from (A. Müller) and (A. Géron)

Table of Contents

Generalization, overfitting and underfitting

Generalization: accurate predictions on unseen data

- i.e. there is no overfitting neither underfitting
- Depends on model complexity and data variability



(Source)

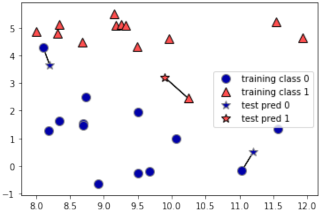
k-Nearest Neighbors

k-NN classification (I)

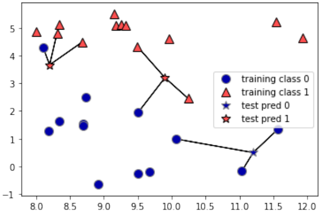
k-NN (`k-Nearest Neighbors`): Likely, the simplest learner

- Given a data point, it takes its *k* closests neighbors
- Same prediction than the majority of its neighbors
- *k* uses to be an odd number (1-NN, 3-NN, 5-NN, ...)

1-NN



3-NN

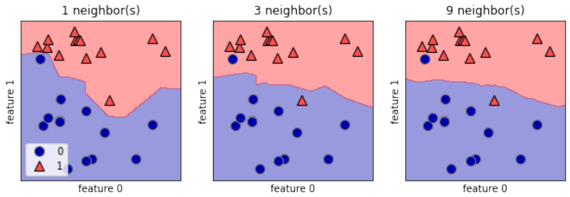


k-NN does not generate a model

- The whole dataset must be stored

k-Nearest Neighbors

k-NN classification (II)



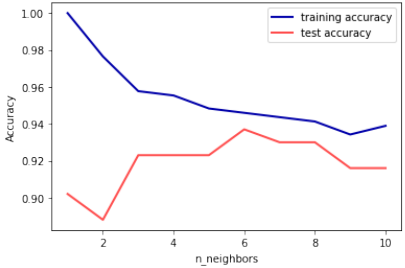
k determines the model complexity

- Smoother boundaries in larger k values
- Model complexity decreases with k

How to figure out the best k?

k-Nearest Neighbors

k-NN classification (III)



k-Nearest Neighbors classifier
Scikit-learn

`sklearn.neighbors.KNeighborsClassifier`

Constructor arguments:

- `n_neighbors`: int, default=5
- `metric`: string, default='minkowski'
- `p`: int, default=2 ($p = 1$ Manhatan distance, $p = 2$ euclidean distance)

Attributes:

- `classes_`: ndarray (n_samples)

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

k-Nearest Neighbors

kNN regression (I)

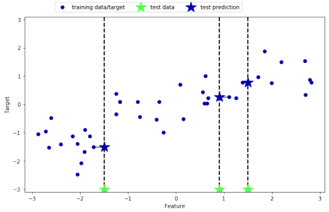
k-NN regression

Given a data point

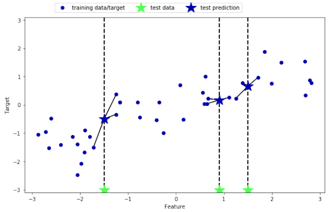
1. Take the k closest data points
2. Predict same target value (1-NN) or averaged target value (k-NN)

Performace is measured with a regression metric

1-NN

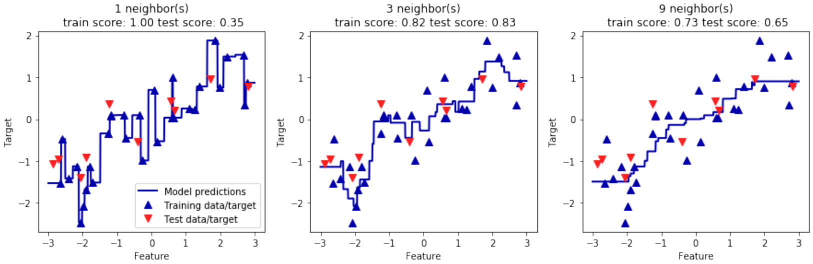


3-NN



k-Nearest Neighbors

kNN regression (II)



k determines the boundary smoothness

- With large k values, fit is smoother

k-Nearest Neighbors regressor

Scikit-learn

`sklearn.neighbors.KNeighborsRegressor`

Constructor arguments:

- `n_neighbors`: int, default=5
- `metric`: string, default='minkowski'
- `p`: int, default=2 ($p = 1$ Manhatan distance, $p = 2$ euclidean distance)

Attributes:

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

k-Nearest Neighbors

Summary

Hyperparameters	Advantages	Disadvantages
k	Simple	Slow with large datasets
Distance	Baseline	Bad performance with hundreds or more attributes
		No model
		Dataset must be stored in memory

Linear models

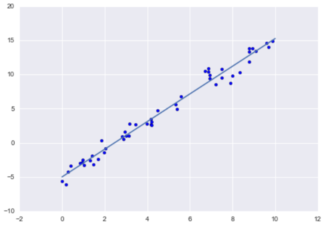
Linear model (I)

Linear model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n$$

for a single feature $y = \beta_0 + \beta_1 x_1$, where

- β_0 is the intercept
- β_1 is the slope



Lineal models assume a linear relationship among variables

- This limitation can be easely overcomed
- Surprisingly good results in high dimensional spaces

Intepretable model

Linear models

Linear regression

Different linear models for regression

- The difference lies in how β_i parameters are learned

Ordinary Least Squares (OLS): Minimizes mean squared error

- OLS does not have any hyperparameter
- No complexity control

$$\text{MSE} = \frac{1}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2$$

where m is the number of instances

Linear models

Regularized linear models

Regularization: Term that penalizes complexity

- Added to the cost function
- Lineal models remain the same
- Train to minimize cost function and penalty
- Intercepts are not part of regularization

Three regularizations

- L1 (Lasso regression), L2 (Ridge regression) and ElasticNet (L1 and L2)

Lasso (L1)

$\alpha \sum_{j=1}^{n} |\beta_j|$

Ridge (L2)

$\alpha \sum_{j=1}^{n} \beta_j^2$

ElasticNet

$\alpha \left(r \sum_{j=1}^{n} |\beta_j| + (1-r) \sum_{j=1}^{n} \beta_j^2 \right)$

Linear models

Ridge regression

Ridge regression (or L2 regularization) adds a new term to cost function

$$\text{MSE} + \alpha \sum_{i=1}^{n} \beta_i^2$$

α controls the penalty

- If $\alpha = 0$ Ridge becomes a regular linear regression
- Optimal α depends on the problem

Ridge by default

Linear models

Lasso regression (I)

Lasso regression (or L1 regularization) adds a new term to cost function

$$\mathrm{MSE} + \alpha \frac{1}{2} \sum_{i=1}^{n} |\beta_i|$$

α controls the penalty (and model complexity)

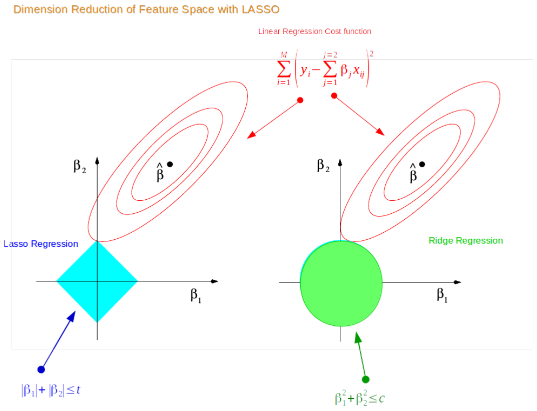
- If $\alpha = 0$ Lasso becomes a regular linear regression
- Optimal α depends on the problem

Some coefficiets may be exactly zero

- Implicit feature selection
- Easier interpretation
- Better with large number of attributes

Linear models

Lasso regression (II)


Dimension Reduction of Feature Space with LASSO
Linear Regression Cost function
$\sum_{i=1}^{M}\left(y_i - \sum_{j=1}^{j=2}\beta_j x_{ij}\right)^2$
β_2
$\hat{\beta}$
β_1
Lasso Regression
$|\beta_1| + |\beta_2| \leq t$
β_2
$\hat{\beta}$
β_1
Ridge Regression
$\beta_1^2 + \beta_2^2 \leq c$

(Source)

Linear models

ElasticNet

Lasso and Ridge can be combined

$$\text{MSE} + \alpha \left(r \sum_{i=1}^{n} |\beta_i| + (1-r) \sum_{i=1}^{n} \beta_i^2 \right)$$

Two hyperparameters

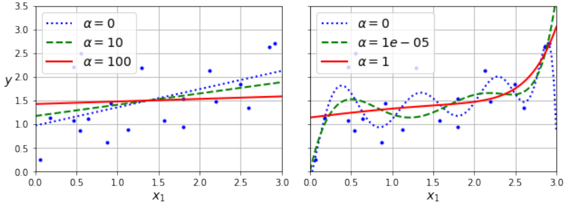
- α controls the model complexity
- r balances between L1 and L2

ElasticNet is not a neural network!

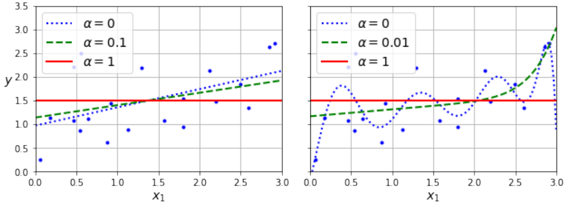
Linear models

Regularized linear models comparison

Ridge - L2



Lasso - L1



Linear models

Scikit-learn (I)

`sklearn.linear_model.LinearRegression`

Constructor arguments:

- `fit_intercept`: boolean, default=True

Attributes:

- `coef_`: ndarray (n_features,)
- `intercept_`: float, ndarray (n_targets,)

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

Linear models

Scikit-learn (II)

`sklearn.linear_model.Ridge`

Constructor arguments:

- `fit_intercept`: boolean, default=True
- `alpha`: float, default=1.0

Attributes:

- `coef_`: ndarray (n_features,)
- `intercept_`: float, ndarray (n_targets,)

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

Linear models

Scikit-learn (III)

`sklearn.linear_model.Lasso`

Constructor arguments:

- `fit_intercept`: boolean, default=True
- `alpha`: float, default=1.0

Attributes:

- `coef_`: ndarray (n_features,)
- `intercept_`: float, ndarray (n_targets,)
- `n_features_in_`: int

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

Linear models

Scikit-learn (IV)

`sklearn.linear_model.ElasticNet`

Constructor arguments:

- `fit_intercept`: boolean, default=True
- `alpha`: float, default=1.0
- `l1_ratio`: float, default=0.5

Attributes:

- `coef_`: ndarray (n_features,)
- `intercept_`: float, ndarray (n_targets,)

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

Linear models

Linear models for classification (I)

A linear regression can be used as classifier

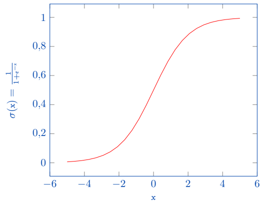
- Just compare the prediction with a threshold (0, for instance)
  - If $\hat{y} > 0$, assign C_1; if $\hat{y} \leq 0$, assign C_2
- The decision boundary is a line, plane or hyperplane

A logistic regression is a generalization of a linear regression

- Probabilistic binary classifier

$$\hat{p} = \sigma\left(\beta_0 + \sum_{i=1}^{n} \beta_i x_i\right), \hat{y} = \begin{cases} C_1, & \text{if } \hat{p} < 0{,}5 \\ C_2, & \text{if } \hat{p} \geq 0{,}5 \end{cases}$$

where $\sigma(t)$ is the logistic function, defined as $\sigma(t) = \frac{1}{1+e^{-t}}$

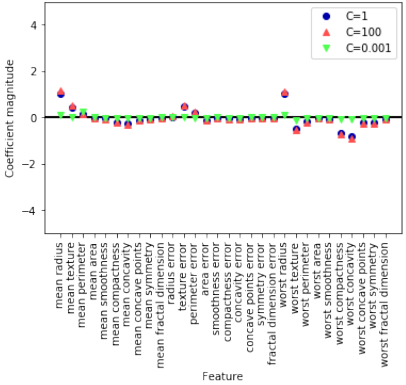


Linear models

Linear models for classification (II)

Regularization with L1, L2 and ElasticNet

- In Scikit-Learn, regularization strength is given by C
- C is the inverse of regularization strength
- Smaller values of C correspond to stronger regularization



Linear models

Scikit-learn

`sklearn.linear_model.LogisticRegression`

Constructor arguments:

- `penalty`: ‘l1’, ‘l2’, ‘elasticnet’, ‘none’, default=’l2’
- `fit_intercept`: boolean, default=True
- `C`: float, default=1.0
- `l1_ratio`: float, default=0.5

Attributes:

- `coef_`: ndarray (n_features,)
- `intercept_`: ndarray (n_targets,)

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

Linear models

Summary

Hyperparameters	Advantages	Disadvantages
	Fast train and predict	Limited in low dimensional spaces
α (L1, L2, ElasticNet)	Scales well to large datasets	Limited generalization
$l1\_ratio$ (ElasticNet)	Better in high dimensional spaces	
	Few hyperparameters	
	Interpretable	

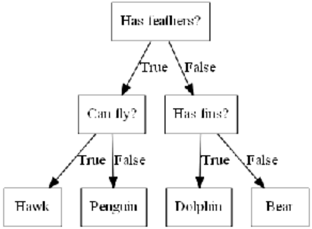
Decision Trees

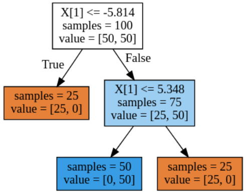
Decision trees are a family of algorithms

- Classification, regression and anomaly detection
- They learn a tree data strucure
- Hierarchy of if/else questions (test, or node)
- Decision (terminal node or leaf)

Usually, datasets does not contain binary attributes

- Continous features
- Is feature i larger than value a?





Decision Trees

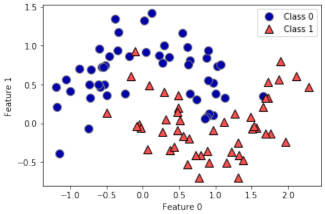
Building decision trees (I)

Tree learning algorithm

1. Begin with the root node
2. Searches all possible tests (according to a purity measure)
3. The most informative test is taken
4. Repeat recursively

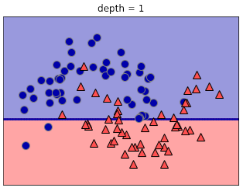
Prediction of a new data point

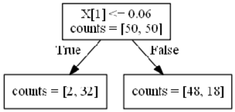
- Classification: Majority class in the partition
- Regression: Average value of target values in the partition

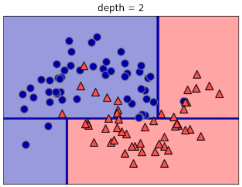


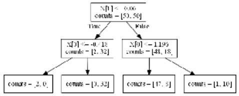
Decision Trees

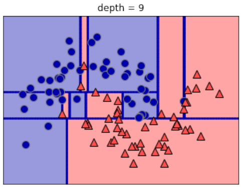
Building decision trees (II)

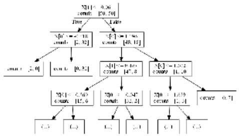












Decision Trees

Building decision trees (III)

We need a measure of 'impurity'

- Gini: $G(Q_m) = \sum_k p_{mk}(1 - p_{ml})$
- Entropy: $H(Q_m) = -\sum_k p_{mk} \log(p_{ml})$

where p_{mk} is the propotion of class k in node m, and Q_m the data in node m

Decision Trees

Controlling complexity of decision trees

Trees tend to grow until all leaves are pure

- Very big trees in real problems
- Big trees use to be overfitted models

Two strategies to prevent overfitting

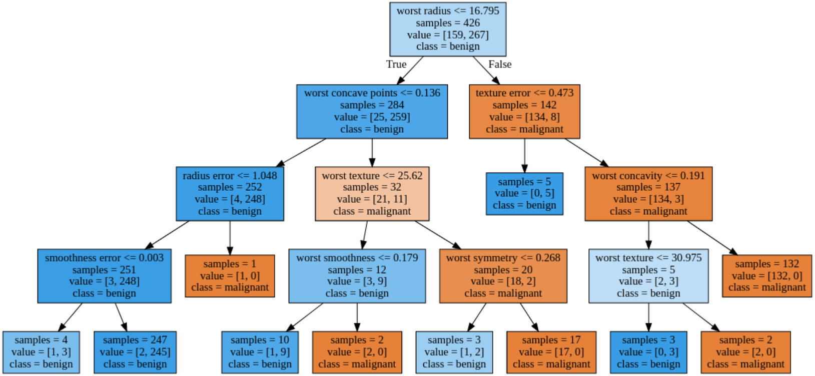
- Pre-prunning: Stop the creation of the tree early according to some criteria
  - Maximum depth, number of leaves, minimum number of points in a node, ...
  - Implemented in Scikit-Learn
- Post-prunning: Build the tree and then remove nodes with little information

Decision Trees

Analyzing decision trees

Decision trees are easily explained to nonexperts

- Interpretable models
- Deep trees are overwhelming
- Trick: Observe the path with most data

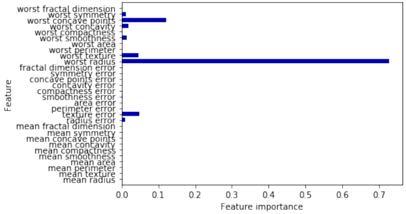


Decision Trees

Analyzing decision trees: Feature importance

Feature importance is a metric that summarizes features

- Number between 0 (not used at all) and 1 (perfect prediction)
- Feature importances sum to one
- Useful for feature selection and model interpretation



Some considerations

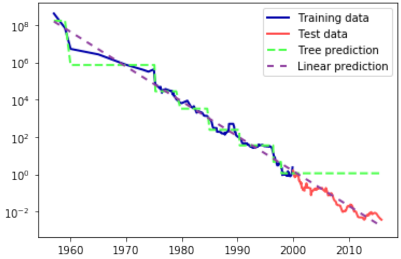
- It does not inform about the relationship between attribute and target
- It quantifies the importance in *the tree*

Decision Trees

Decision trees in regression

Decision trees are not able to extrapolate

- i. e. to predict outside of the range of the training data
- It is specially important in regression problems



Decision Trees

Scikit-learn

`sklearn.tree.DecisionTreeClassifier`

Constructor arguments:

- `criterion`: 'gini', 'entropy', 'log_loss', default='gini'
- `max_depth`: int, default=None
- `max_leaf_nodes`: int, default=None
- `min_samples_leaf`: int or float, default=1

Attributes:

- `classes_`: ndarray (n_classes,)
- `feature_importances_`: ndarray (n_features,)
- `tree_`: Tree instance

Methods: `fit()`, `predict()`, `decision_path()`, `get_depth()`, `get_n_leaves()`

(Scikit-Learn reference)

(See also DecisionTreeRegressor)

Decision Trees

Summary

Hyperparameters	Advantages	Disadvantages
`max_depth`	Visualization	Tend to overfit
`max_leaf_nodes`	Interpretable by non-experts	Poor generalization
`min_samples_leaf`	Invariant to scale	
`criterion`	Mix of categorial and numerical data	

Ensembles of Decision Trees

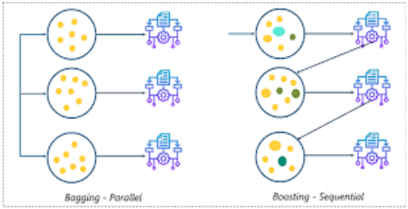
Ensembles

Ensembles, in ML, refers to the combination of several models

- For instance, an ensemble of three classifers voting

Two common aproaches to build ensembles

- Bagging (or *bootstrap*) samples the dataset with replacement
    - The ensemble make prediction by aggregating its predictors
- Boosting trains models to correct previous models



(Source)

Ensembles of Decision Trees

Random forests

A tree is good doing his job, but does not generalize well

- Different trees could overfit in different ways
- Idea: Use many trees and aggregate their results

Random forest is a popular algorithm based on ensembles of trees

- Classification and regression
- Limits overfitting found in trees

It encourages tree diversity through training set and feature selection

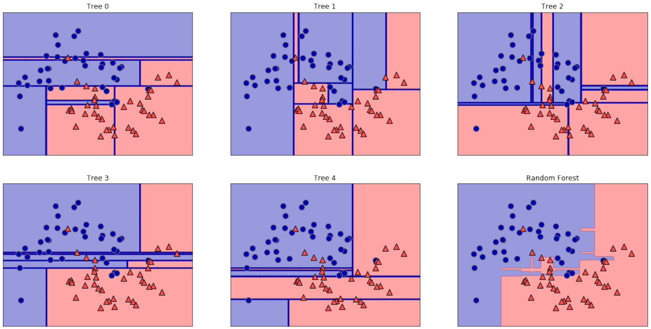
- Selecting data: Bootstrap
- Selecting features in each test
    - It does not look for the best test
    - It looks for the best test involving a random subset of features
    - The size of the features subset is a critical hyperparameter

Same hyperparameters than decision trees

Ensembles of Decision Trees

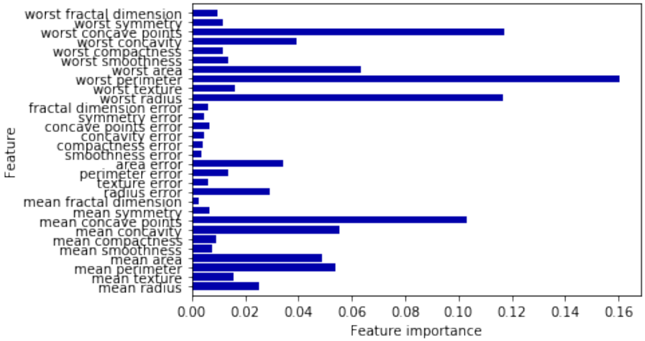
Analyzing random forests (I)

Random forest with five trees



Ensembles of Decision Trees

Analyzing random forests (II)



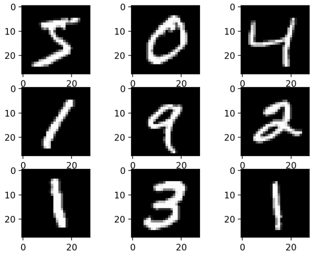
Feature importance can be aggregated

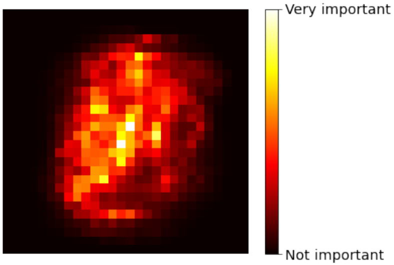
- More informative than single trees
- The algorithm must consider many possible explanations

Ensembles of Decision Trees

Analyzing random forests (III)

Random forest classifier with MNIST dataset





Ensembles of Decision Trees

Ensembles of Decision Trees : Scikit-learn

`sklearn.ensemble.RandomForestClassifier`

Same than RandomForestClassifier

Constructor arguments:

- `n_estimators`: int, default=100
- `max_features`: “sqrt”, “log2”, None, int or float, default=”sqrt”
- `bootstrap`: bool, default=True
- `max_samples`: int or float, default=None

Methods: `fit()`, `fit_predict()`

Attributes:

- `feature_importances_`: ndarray (n_features,)
- `estimators_`: List of DecisionTreeClassifier

(Scikit-Learn reference)

(See also RandomForestRegressor)

Ensembles of Decision Trees

Summary: Random forest

Hyperparameters	Advantages	Disadvantages
Same than trees	Same than trees	Interpretation
Number of trees	High performance	High dimensional data
Number of features	Robust	Sparse data
	Widely used	Memory and CPU
	Parallelized	

Ensembles of Decision Trees

Gradient boosted regression trees (I)

Gradient boosting trees is an ensemble of trees

- Based on boosting, builds trees in a serial manner
- One tree corrects the mistakes of the previous one

A set of *weak learners* is used

- Shallow trees (by default, 3 in Sklearn)
- No data randomization, strong pre-pruning

A new hyperparameter: *learning rate*

- How strongly each tree tries to correct
- High learning rate makes stronger corrections: More complex models
- More trees also adds more complexity

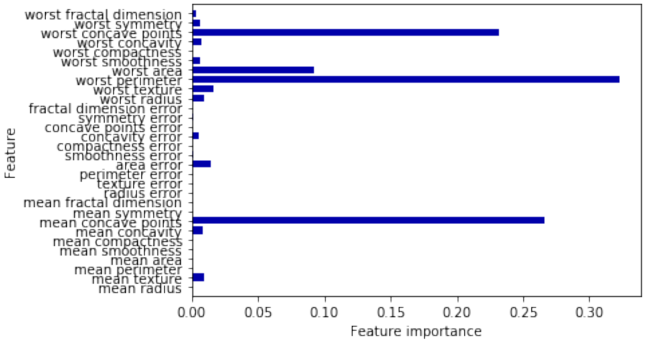
State of the art results

- Widely adopted by industry
- Comparable in performance with deep neural networks

Ensembles of Decision Trees

Gradient boosted regression trees (II)

Feature importances with cancer dataset



The (XGBoost) package provides a high performance implementation of gradient boosted trees

Ensembles of Decision Trees

Ensembles of Decision Trees : Scikit-learn

sklearn.ensemble.GradientBoostingClassifier

Constructor arguments:

- `n_estimators`: int, default=100
- `learning_rate`: float, default=0.1
  Same than DecisionTreeClassifier

Attributes:

- `feature_importances_`: ndarray (n_features,)

Methods: `fit()`, `predict()`

(Scikit-Learn reference)
(See also GradientBoostingRegressor)

Ensembles of Decision Trees

Summary: Gradient boosting

Hyperparameters	Advantages	Disadvantages
Same than trees	Very high performance	Slow
Number of trees	Invariant to scale	High dimensional data
Learning rate	Mix of categorial and numerical data	Tricky hyperparameter tuning
		Overfitting

Support Vector Machines

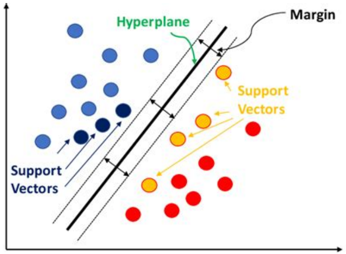
Linear SVM (I)

SVM, or *Support Vector Machines*, is a popular and flexible learning model

- Classification, regression and outlayer detection
- Linear and non-linear models
- Quite popular with small and medium datasets

Learning SVMs

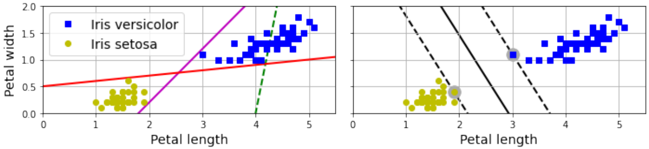
1. It localizes data points in the boundary of the classes
   - They are named *support vectors*
2. Determine an hyperplane that splits them maxizing *margin*



(Source)

Support Vector Machines

Linear SVM (II)

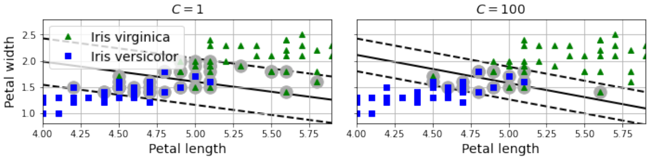


Two big problems with hard margins

- Most datasets are not linearly separable and outlaiers

We look for a balance between good fit and margin violations: C

- C sets the tolerance to margin violations
- Low C $\longrightarrow$ High tolerance

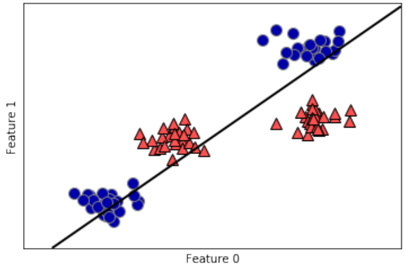


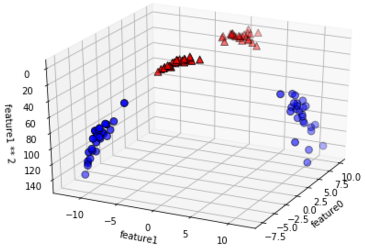
Support Vector Machines

Linear models and nonlinear features (I)

Plain SVMs are limited in low-dimensional spaces

- Lines, planes and hyperplanes
- Adding new features is a way to overcome this limitation

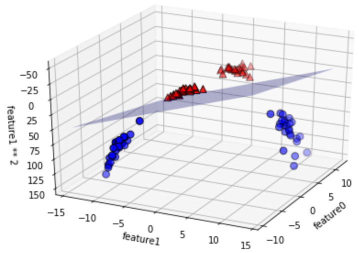


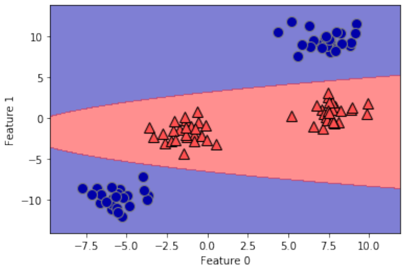


$$feature\_2 = feature\_1^2$$

Support Vector Machines

Linear models and nonlinear features (II)





Support Vector Machines

The kernel trick

Adding nonlinear attributes makes linear models much more powerful

- Which features should we add?
- How we compute interations in a 100-dimensional feature space?

Some mathematical magic: The *kernel trick*

- It computes data distances for expanded feature representation ...
- ... without computing the expansion!

It applies a function named kernel

- Polynomial kernel, up to a certain degree
- Radial basis function (RBF) kernel (Gaussian kernel)
- Linear kernel, no expansion is done

The kernel trick can be used in other techniques like PCA

Support Vector Machines

Understanding SVMs (I)

To predict a new point, the distance to each of the support vector is computed

- Distance is measured by the Gaussian kernel
- Decision is taken based on the distance and learned importance

$$k_{rbf}(x_1, x_2) = \exp(-\gamma||x_1 - x_2||^2)$$

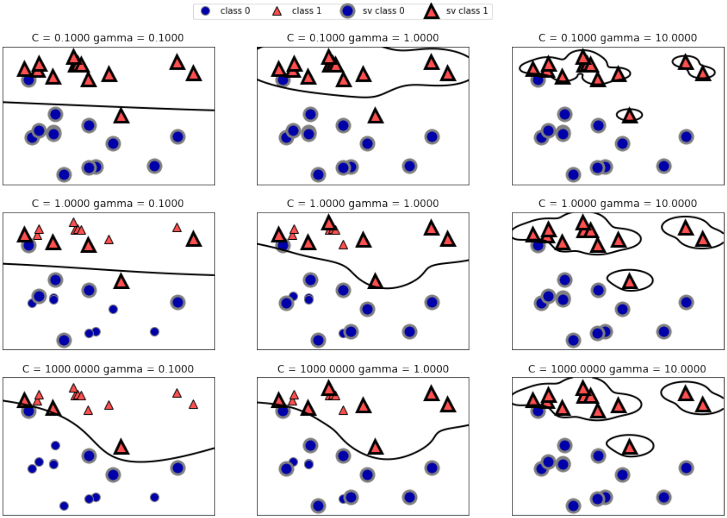
where $||\cdot||$ denotes Euclidean distance and γ is an hyperparameter

- γ determines how far the influence of a single point reaches
- Low γ, lower complexity

Remember, C is a regularization parameter

Support Vector Machines

Understanding SVMs (II)

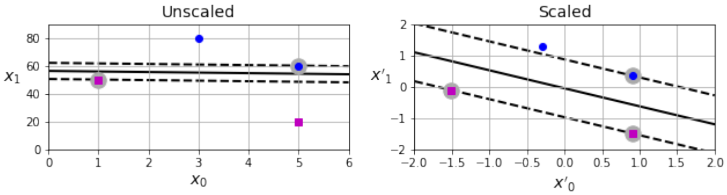


Support Vector Machines

Understanding SVMs (III)

SVM is very sensitive to scale

- Always use standarized or normalized data



Support Vector Machines

Scikit-learn

sklearn.svm.SVC

Constructor arguments:

- `C`: float, default=1.0
- `kernel`: 'linear', 'poly', 'rbf', default='rbf'
- `degree`: int, default=3
- `gamma`: 'scale', 'auto' or float, default='scale'

Attributes:

Methods: `fit()`, `predict()`

(Scikit-Learn reference)

(See also SVR) (See also LinearSVC)

Support Vector Machines

Summary

Hyperparameters	Advantages	Disadvantages
C	Powerful	Memory and CPU
γ	Low and high dimensional	Number of samples
Kernel	Flexible	Scaling
		No interpretable