Supervised learning

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster en Ciencia y Tecnología desde el Espacio

Departamento de Automática

Universidad de Alcalá

ISG

Objectives

1. Extend supervised learning algorithms
2. Apply supervised learning to real-world problems

Bibliography

- Müller, Andreas C., Guido, Sarah. *Introduction to Machine Learning with Python.* O'Reilly. 2016

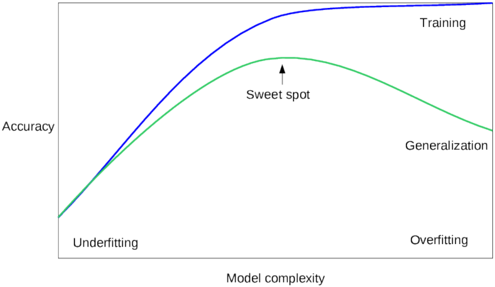
All figures have been taken from
`https://github.com/amueller/introduction_to_ml_with_python/blob/master/02-supervised-learning.ipynb`

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



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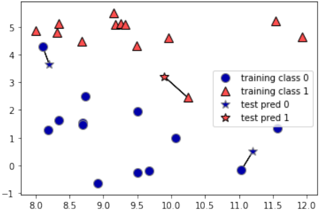
k-Nearest Neighbors

k-NN classification (I)

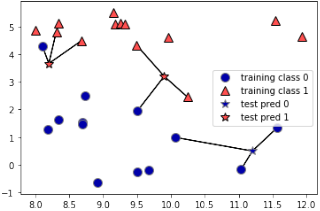
k-NN (k-Nearest Neighbors): Likely, the simplest classifier

- Given a data point, it takes its k closests neighbors
- Same prediction than its neighbors

1-NN



3-NN



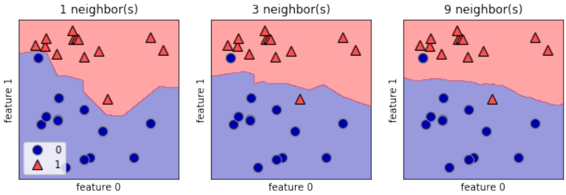
k-NN does not generate a model

- The whole dataset must be stored

k uses to be an odd number (1-NN, 3-NN, 5-NN, ...)

k-Nearest Neighbors

k-NN classification (II)



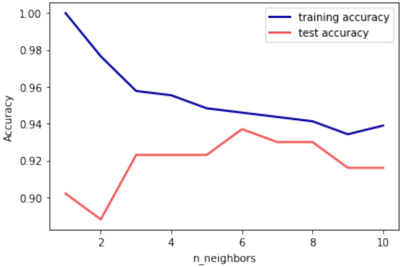
k determines the model complexity

- Smoother boundaries in larger k values
- Model complexity decreases with k
- If k equals the number of samples, k-NN always predicts the most frequent class

How to figure out the best k?

k-Nearest Neighbors

k-NN classification (III)



k-Nearest Neighbors

kNN regression (I)

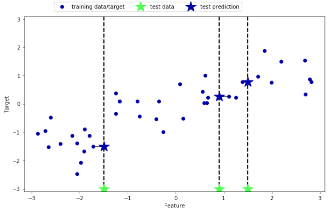
k-NN regression

Given a data point

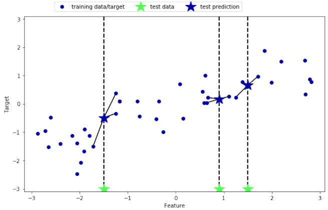
1. Take the k closest data points
2. Predict same target value (1-NN) or averate target value (k-NN)

Performace is measured with a regression metric, by default, R^2

1-NN

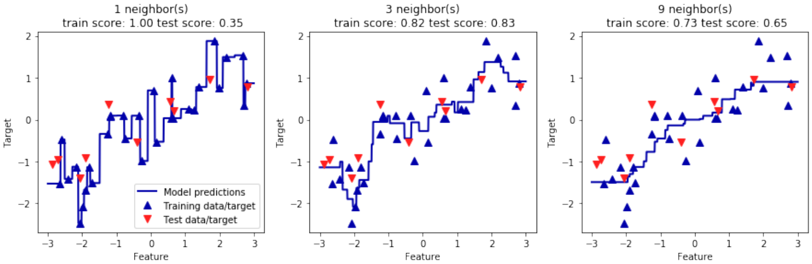


3-NN



k-Nearest Neighbors

kNN regression (II)



k determines boundary smoothness

1. With $k = 1$, prediction visits all data points
2. With large k values, fit is worse

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

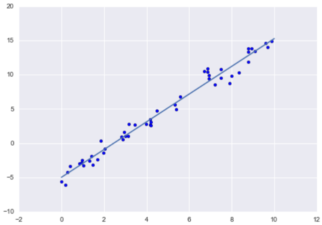
Linear model (I)

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
- Intepretable model



Lineal models assume a linear relationship among variables

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

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

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2$$

Linear regression can be used to fit non-linear models

- Just adding new attributes

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 coefficients
- Intercepts are not part of regularization

Three regularizations

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

Lasso (L1)

$\alpha \sum_j^n |\beta_j|$

Ridge (L2)

$\frac{\alpha}{2} \sum_j^n \beta_j^2$

ElasticNet

$\alpha \left(\frac{\lambda}{2} \sum_j^n \beta_j^2 + (1 - \lambda) \sum_j^n |\beta_j| \right)$

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 model complexity

- 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

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

α controls the model complexity

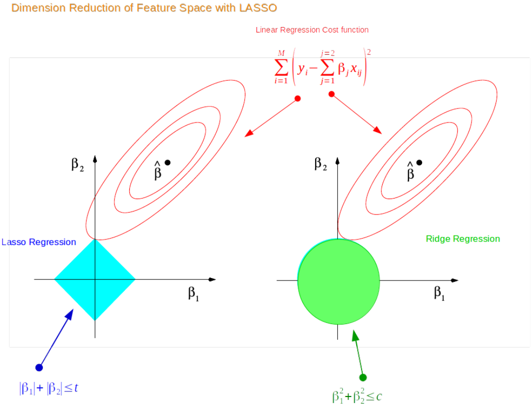
- If $\alpha = 0$ Ridge becomes a regular linear regression
- Optimal α depends on the problem

Some coefficiets may be exactly zero

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

Linear models

Lasso regression (II)



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Linear models

ElasticNet

Lasso and Ridge can be combined

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

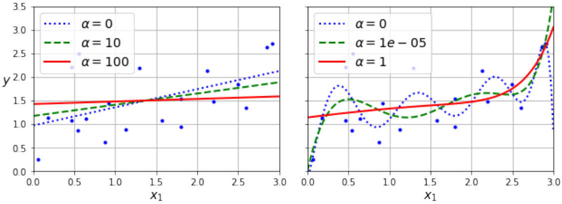
Two hyperparameters

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

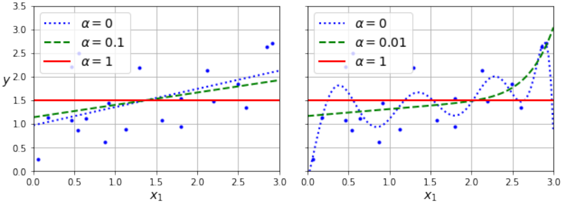
Linear models

Regularized linear models comparison

Ridge - L2



Lasso - L1



Linear models

Linear models for classification (I)

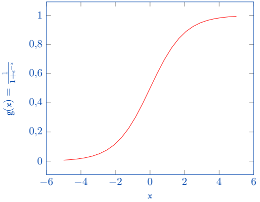
A linear regression can be used as classifier

- Just compare the prediction with a threshold (0, for instance)
  - If $\hat{y} > 0$, assign class 1
  - If $\hat{y} <= 0$, assign class -1
- The decision boundary for any binary linal classifier is a line, plane or hyperplane

A logistic regression is a generalization of a linear regression

- It is a binary classifier
- Its output is a probability

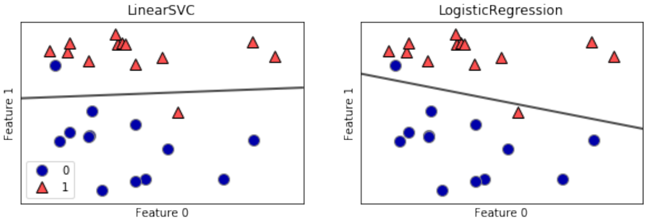
$$p = \sigma\left(\beta_0 + \sum_{i=1}^{n} \beta_i x_i\right),$$



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

Linear models

Linear models for classification (II)

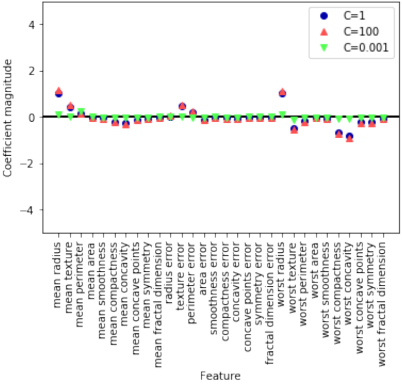


Linear models

Linear models for classification (III)

The model can be regularized with L1, L2 and ElasticNet

- In Scikit-Learn, regularization strength is given by C
- Lower values of C correspond to smaller regularization strength



Linear models

Summary

Hyperparameters	Advantages	Disadvantages
-	Fast train and predict	No complexity tuning
α (L1, L2, ElasticNet)	Scales well to large datasets	Limited in low dimensional spaces
l1_ratio (ElasticNet)	Better in high dimensional spaces	
	Few hyperparameters	
	Interpretable	

Better when the number of features is large compared to the number of samples

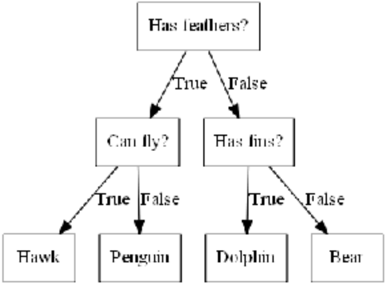
Decision Trees

Decision trees are a family of algorithms for classification and regression

- 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

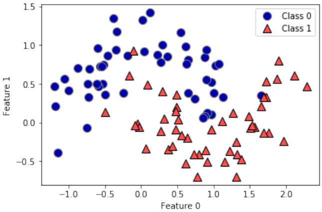
Building decision trees (I)

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

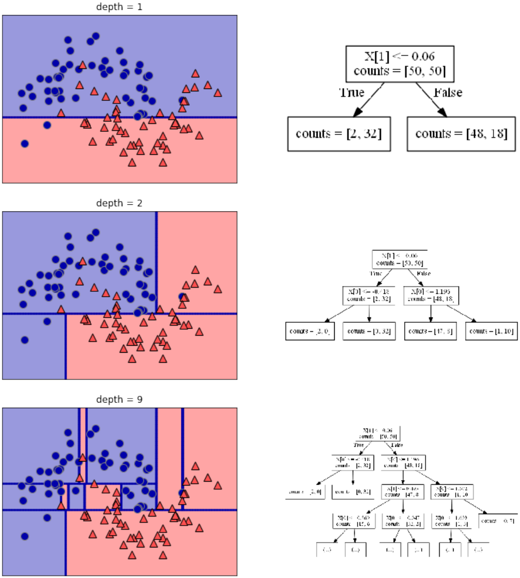
Prediction of a new data point

- 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)

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

Gini

$$G(Q_m) = \sum_k p_{mk}(1 - p_{ml})$$

Log Loss or Entropy

$$H(Q_m) = -\sum_k p_{mk} log(p_{ml})$$

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

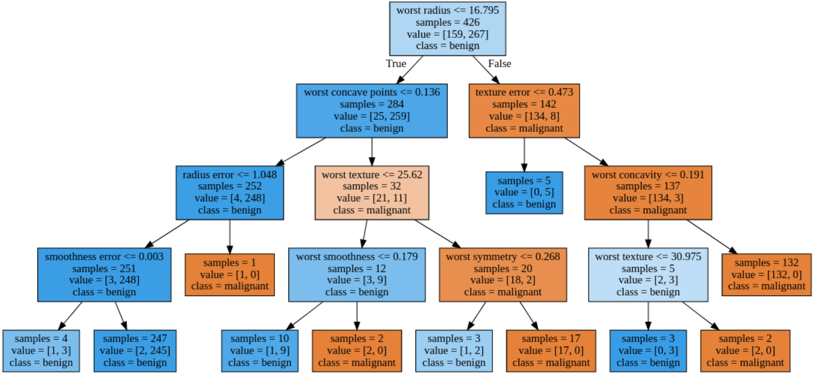
- Pre-prunning: Stop the creation of the tree early accorgind to some criteria
  - Maximum depth, number of leaves, minimum number of points in a node, ...
  - Implemented in Sciki-Learn
- Post-prunning: Build the tree and then remove nodes with little information

Decision Trees

Analyzing decision trees

Decision trees is easily explained to nonexperts

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

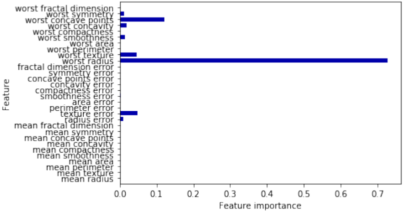


Decision Trees

Analyzing decision trees

Feature importace 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

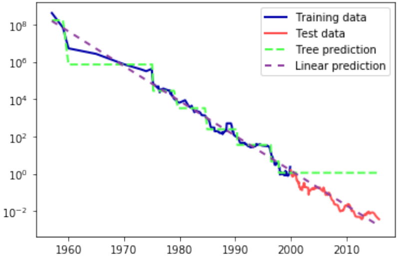
- It does not inform about the relationship between attribute and target
- It quantifies the importance in the tree
  - Correlated attributes may score low importance

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

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

TODO

Ensembles of Decision Trees

Summary

Hyperparameters	Advantages	Disadvantages

Support Vector Machines

TODO

Support Vector Machines

Kernelized Support Vector Machines

TODO

Support Vector Machines

Summary

Hyperparameters	Advantages	Disadvantages

A

B

TODO

A

B: Summary

Hyperparameters	Advantages	Disadvantages

Algorithms

ARIMA (I)

AR: Autoregressive model

- Current observation depends on the last p observations
- Long term memory

MA: Moving Average model

- Current observation linearly depends on the last q innovations
- Short term memory

AR(p)

$$X_t = c + \sum_{i=1}^{p} \phi_i X_{t-1} + \epsilon_t$$

MA(q)

$$X_t = \mu + \epsilon_t + \theta_1 \epsilon_{t-1} + \ldots + \theta_q \epsilon_{t-q}$$

ARMA model = AR + MA

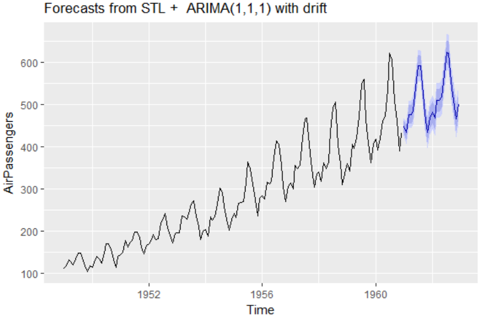
- ARMA(p, q): Two hyperparameters, p and q

Algorithms

ARIMA (II)

ARIMA = AR + i + MA (AR integrated MA)

- ARIMA(p, d, q)
- Three integer parameters: p, q and d (in practice, low order models)



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autoarima: search over p, q and d