Supervised learning

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

Departamento de Automática

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`

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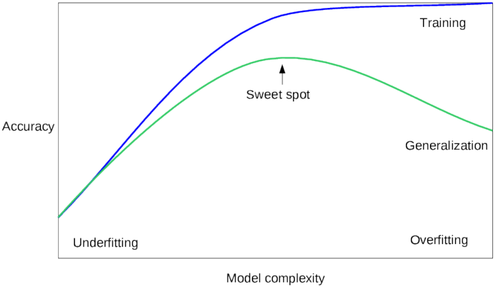
Generalization, overfitting and underfitting

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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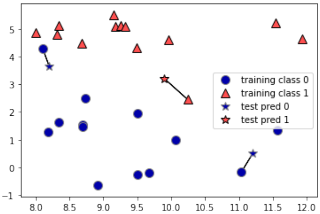
k-Nearest Neighbors

k-NN classification (I)

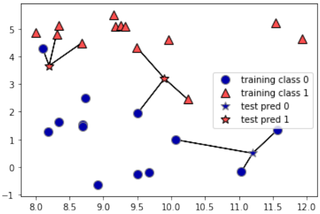
k-NN (k-Nearest Neighbors): Likely, the simplest classifier

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

1-NN



3-NN



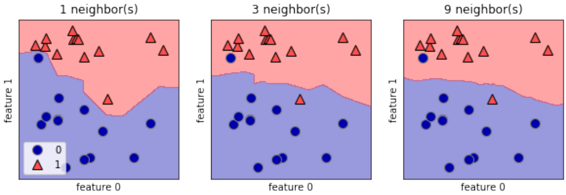
k-NN does not generate a model

- 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)



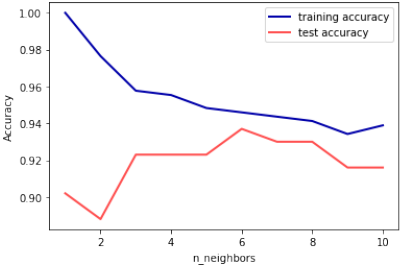
k determines the model complexity

- 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)

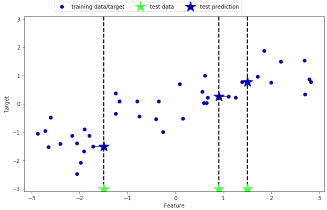
k-NN regression

Given a data point

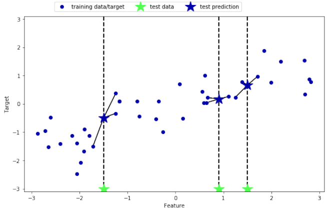
1. Take the k closest data points
2. Predict same target value (1-NN) or averate target value (k-NN)

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

1-NN

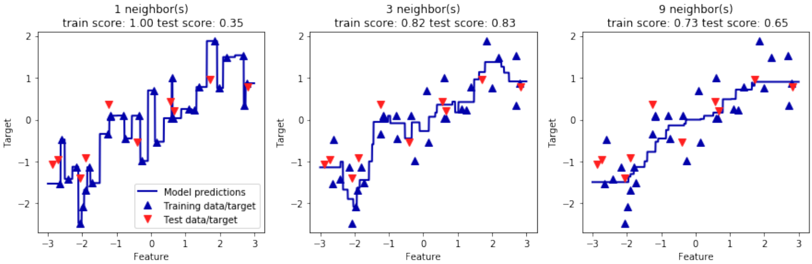


3-NN



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

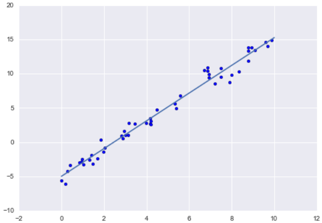
Linear model (I)

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

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

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)
$\alpha \sum_j^n \lvert\beta_j\rvert$

Ridge (L2)
$\frac{\alpha}{2} \sum_j^n \beta_j^2$

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

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

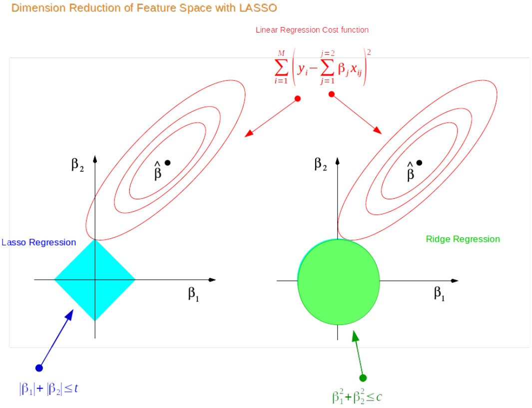
- If $\alpha = 0$ Ridge becomes a regular linear regression
- Optimal α depends on the problem

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

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

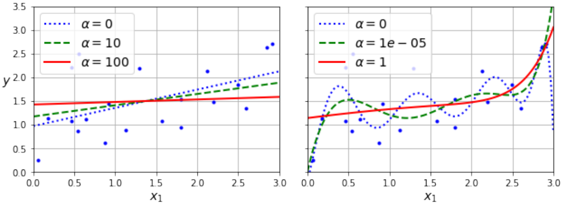
Two hyperparameters

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

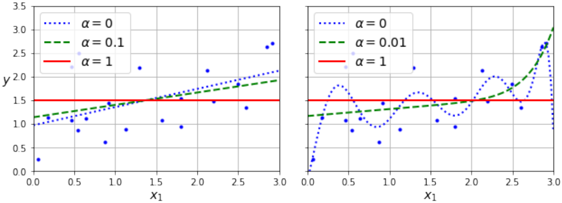
Linear models

Regularized linear models comparison

Ridge - L2



Lasso - L1



Linear models

Linear models for classification (I)

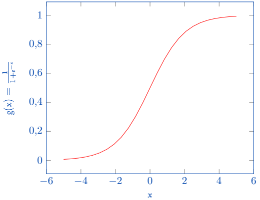
A linear regression can be used as classifier

- 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

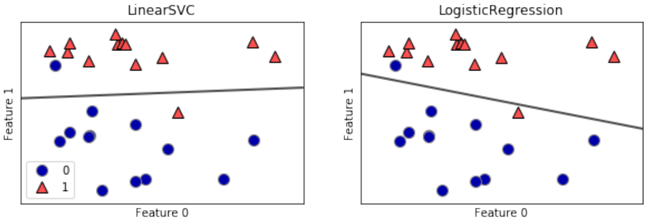
$$p = \sigma\left(\beta_0 + \sum_{i=1}^{n} \beta_i x_i\right),$$



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

Linear models

Linear models for classification (II)

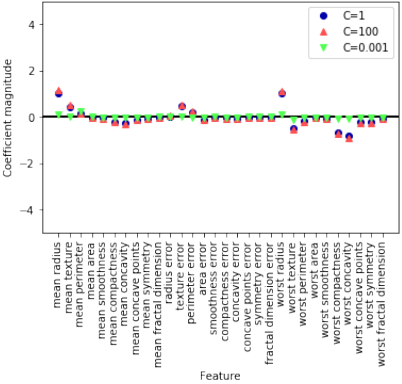


Linear models

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

Decission Trees

TODO

Decission Trees

Summary

Hyperparameters	Advantages	Disadvantages

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

AR(p)

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

MA: Moving Average model

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

MA(q)

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

ARMA model = AR + MA

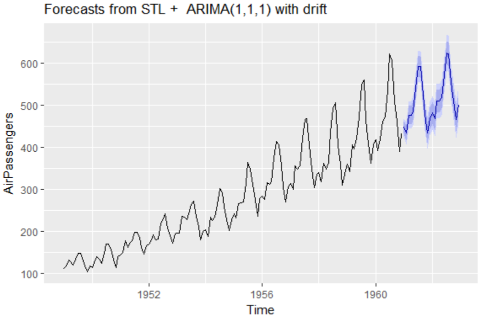
- ARMA(p, q): Two hyperparameters, p and q

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