Title:	Regression
Course:	Machine Learning
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Master:	Data Science and Business Analytics
Master:	Artificial Intelligence and Innovation
Master:	Finance and Financial Technologies
Academic Year:	2023/2024

Regression – Forecasting continuous values

- Supervised task
- The target variable is numeric
- Minimize the error of the prediction with respect to the target

This topic was already included in the Statistics and Data Analysis module, it is included here only for completeness

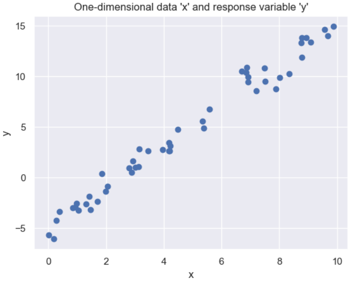
Linear Regression

- data set $\mathcal{X}$ with N rows and D columns
  - x_i is a D dimensional data element
- response vector $\overline{y}$ with N values y_i
- w is a D-dimensional vector of coefficients that needs to be learned
- we model the dependence of each response value y_i from the corresponding independent variables x_i as

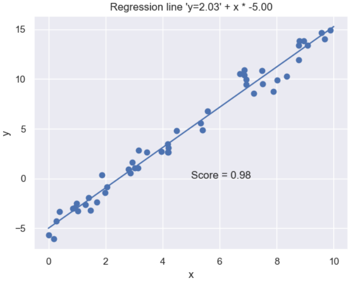
$$y_i \approx w^T \cdot x_i \quad \forall i \in [1 \dots N]$$

- such that the error of modelling is minimised
- Classical statistic method (1805)

Data and regression line



One–dimensional data and response variable



Regression and score - Score range $(-\inf : 1)$

Objective function and minimisation OPTIONAL I

$$\mathcal{O} = \sum_{i=1}^{N}(w^T \cdot x_i - y_i)^2 = ||Xw^T - y||^2$$
$$= (Xw^T - y)^T.(Xw^T - y)$$

Gradient of $\mathcal{O}$ with respect to w

$$2X^T(Xw^T - y)$$

Constraining the gradient to 0 we obtain the optimisation condition

$$X^TXw^T = X^Ty$$

Objective function and minimisation OPTIONAL II

If the symmetric matrix $X^T X$ is *invertible* the solution can be derived as

$$w = (X^T X)^{-1} X^T y$$

and the forecast is given by

$$y^f = X \cdot w^T$$

Matrix calculus

OPTIONAL

- Issues related to matrix calculus if $\overline{x}^T\overline{x}$ is not invertible
- *Moore–Penrose pseudoinverse*
- *Tikonov regularisation* (also known as *ridge regression*)
- *Lasso regularisation*

Quality of the fitting - R^2

Mean of the observed data $y^{avg} = \frac{1}{N} \sum_i y_i$

Sum of squared residuals $SS_{res} = \sum_i (y_i - y_i^f)^2$

Total sum of squares $SS_{tot} = \sum_i (y_i - y^{avg})^2$

Coefficient of determination $\mathbf{R^2 = 1 - \frac{SS_{res}}{SS_{tot}}}$

Intuition about R^2

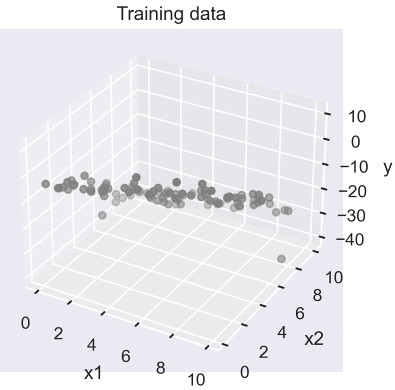
- It compares the fit of the chosen model with that of a horizontal straight line
- With perfect fitting the numerator of the second term is zero and $R^2 = 1$
- If the model does not follow the trend of the data the numerator of the second term can reach or exceed the denominator, and R^2 can also be negative
- Despite the name, R^2 isn't the square of anything

R^2 and *Mean Squared Error*

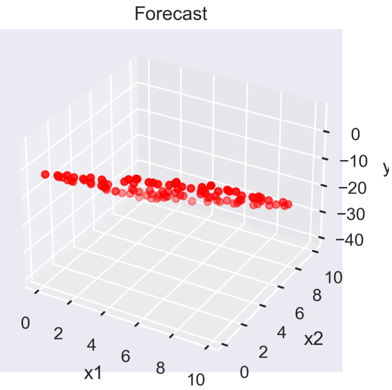
- Both refer to the error of the predictions
- R^2 is a standardised index,
- *RMSE* measures the mean error, this it is influenced by the order of magnitude of the data,
- Both *RMSE* and R^2 quantifies how well a linear regression model fits a dataset
- The RMSE tells how well a regression model can predict the value of a response variable in absolute terms
- R^2 tells how well the predictor variables can *explain the variation in the response variable*
- For comparing the accuracy among different linear regression models, RMSE is a better choice than R Squared
- R^2 is not meaningful for non–linear or non–algebraic regression models

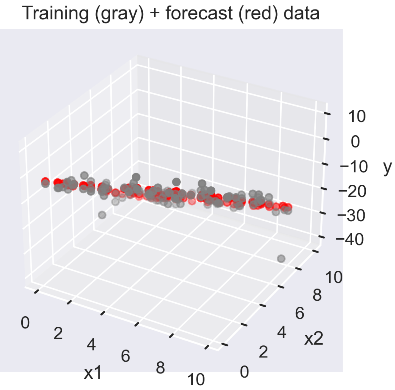
Multiple regression

- The response variable depends by more than one features
- The regression technique is quite similar to that of simple regression
- In `scikit-learn` the estimator is the same



Multiple regression - forecast



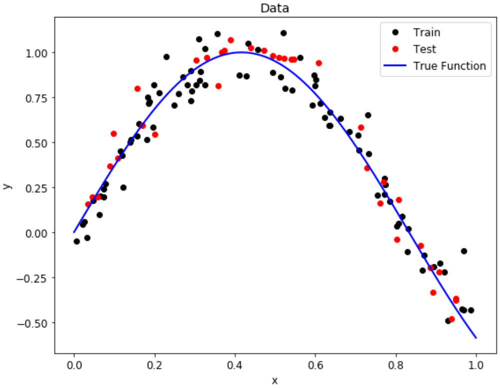


Overfitting and Regularisation

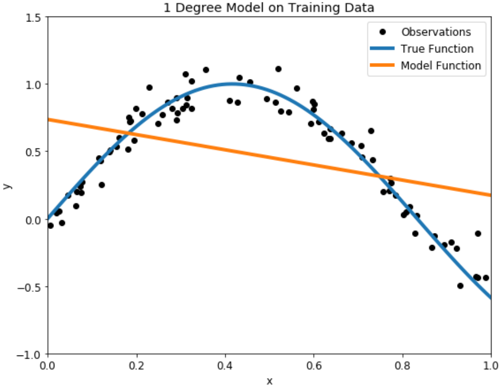
- In presence of high number of features overfitting is possible
  - performance on test data becomes much worse
- Regularisation reduces the influence of less interesting attributes and therefore reduces overfitting

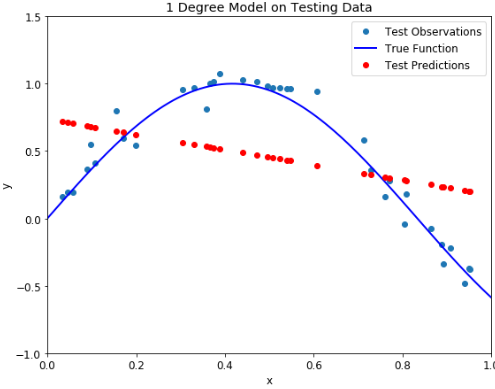
Polynomial regression

- Target is influenced by a single feature
- The relationship cannot be described by a straight line

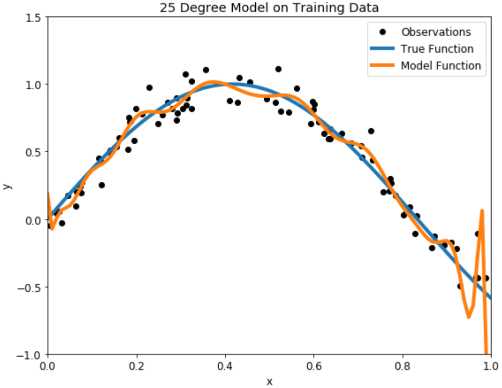


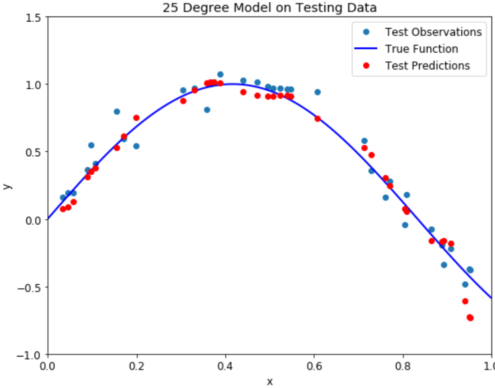
Underfitting



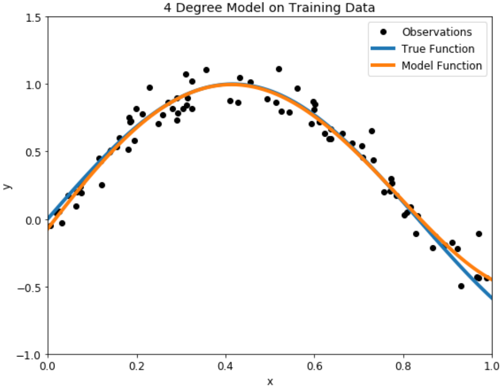


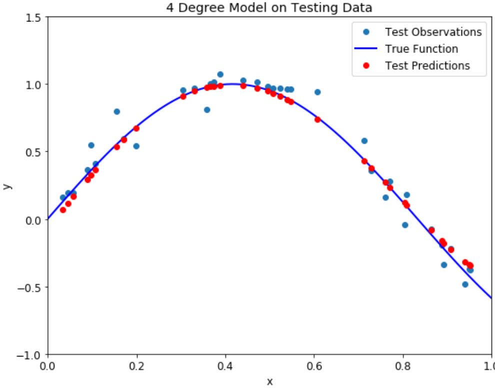
Overfitting



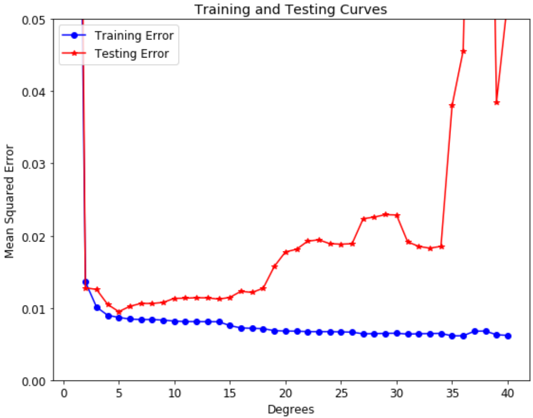


Good fitting





Model complexity vs fitting



Selection of Regression Models

Method	*Library*	*Model Name*
Linear Regression	sklearn.linear_model	LinearRegression
Elastic Net Regression	sklearn.linear_model	ElasticNet
Stochastic Gradient Descent Regression	sklearn.linear_model	SGDRegressor
Bayesian Ridge Regression	sklearn.linear_model	BayesianRidge
Lasso Regression	sklearn.linear_model	Lasso
Support Vector Machine	sklearn.svm	SVR
Kernel Ridge Regression	sklearn.kernel_ridge	KernelRidge
Gradient Boosting Regression	sklearn.ensemble	GradientBoostingRegressor
XGBoost Regressor	xgboost	XGBRegressor
CatBoost Regressor	catboost	CatBoostRegressor
LGBM Regressor	lightgbm	LGBMRegressor