Machine Learning and Programming in Python

Lecture for Master and PhD students

Chair of Data Science in Economics

Ruhr University Bochum

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Lecture 5

Linear Regression

Linear Regression

- Linear regression is a simple approach to **Supervised Learning**. It assumes that the dependence of Y on $X_1, X_2, ..., X_p$ is linear
- Although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically
- Starting point for many more advanced methods in Data Science
- If the linear functional relationship is not the true one between X and y, then the performance/prediction accuracy will be bad

Questions that might be asked:

- Is there a relationship between y und X ?
- How strong is the relationship between y und X ?
- Which variables in X contribute to y?
- How well can the strength of the relationship between a variable in X and y be estimated?
- What will be our prediction for y? How accurately can we predict y?
- Is the relationship between X and y (the f) linear?
- Is there synergy among the variables in X (interaction terms)?

- We assume a model

  $$Y = \beta_0 + \beta_1 * X + \epsilon$$

  where β_0 and β_1 are two unknown constants that represent the intercept and slope, also known as coefficients or parameters, and ϵ is the error term.

- Given some estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients, we predict y using

  $$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 * x$$

  where $\hat{y}$ indicates a prediction of Y on the basis of X = x. The hat symbol denotes an estimated value

- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 * x_i$ be the prediction for Y based on the ith value of X.
  Then $e_i = y_i - \hat{y}_i$ represents the ith residual

- We define the residual sum of squares (RSS) as

  $$RSS = e_1^2 + e_2^2 + ... + e_n^2,$$

  or equivalently as

  $$RSS = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 * x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 * x_2)^2 + ... + (y_n - \hat{\beta}_0 - \hat{\beta}_1 * x_n)^2$$

- The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS.

  The minimizing values can be shown to be

  $\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$

  $\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$

  where $\overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$ and $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ are the sample means.

- The OLS (ordinary least squares) estimator chooses the βs (for p X-variables and the intercept), in order to minimise the RSS:

$$\begin{aligned} \min\ RSS &= \textstyle\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \textstyle\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 * x_{i1} - \hat{\beta}_2 * x_{i2} - \ldots - \hat{\beta}_p * x_{ip})^2 \end{aligned}$$

- The OLS estimator works well, when $n >> p$ and when Y is approximatively linearly related to X:
    - Small Bias and small Variance
    - Easy to interpret
    - Usable for inference

Regularisation

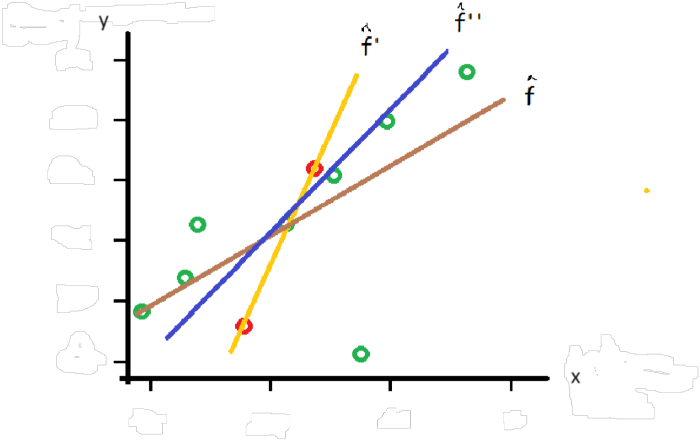
Regularisation

- If n only a bit larger than p, OLS models have high variance, overfitting and making poor predictions.
- If $n <= p$, no unique solution. (see explanations during the lecture)
- Regularisation: Systematic shrinkage of OLS coefficients:
  - Can get a big reduction in variance at the cost of some bias.
  - Improves OLS, improves the prediction
  - Like imposing a cost on complexity to reduce overfitting.
  - For example: Ridge (L2 regularisation), Lasso (L1 regularisation).
- What are these methods and why do they work?

Ridge Regression

- Consider the following example:

  Y, X and f(X)
  Whole sample: green and red dots
  True relationship f(X) is the brown-coloured line
  Small training data sample: red dots
  OLS fit from training data sample is the yellow-coloured curve
  Ridge regression fit: blue line


y
$\hat{f}'$
$\hat{f}''$
$\hat{f}$
x

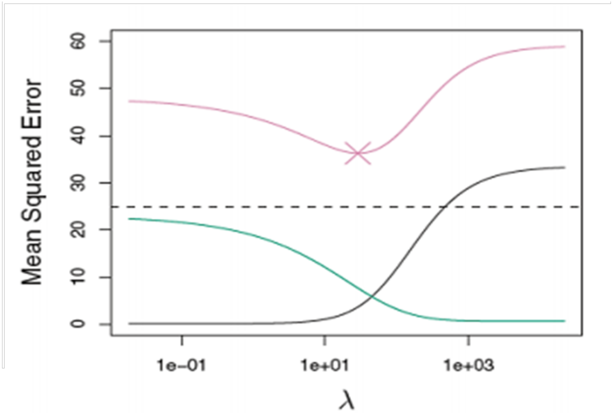
- OLS: Estimate βs in order to minimise:
  $RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

- Ridge: Estimate βs in order to minimise:
  $RSS + \lambda \sum_{j=1}^{p} {\beta_j}^2$

- $\lambda \sum_{j=1}^{p} {\beta_j}^2$ is the penalty term

- λ is a model tuning parameter, cost of complexity
- $\lambda \sum_{j=1}^{p} {\beta_j}^2$ shrinks βs to zero (only the slope coefficients but not the intercept β_0)
- $\lambda = 0$ yields the standard OLS solution
- $\lambda \Rightarrow \infty$ makes βs approach 0 asymptotically
  - y will be less sensitive to changes of X, the larger gets λ
  - Ridge penalizes large $|\beta|$
- different λ imply different sets of $\hat{\beta}$

- Ridge regression on simulated data for n=50, p=45
- Squared bias (black), variance (green), test MSE (purple).
- For $\lambda = 0$, no bias but high variance.
- As λ rises, variance falls fast with small increase in bias
- Aim: to minimise the MSE



- OLS coefficients are scale equivariant
  - If X_j scales by a constant c, $\hat{\beta}_j$ scales by $\frac{1}{c}$.
  - E.g. if X_j is weight in kg, and is rescaled to pounds, the original $\hat{\beta}_j$ is divided by 2.2.
  - $\hat{\beta}_j X_j$ remains constant.
- Ridge regression coefficients are **not** scale equivariant
  - $\hat{\beta}_j^R X_j$ depends on λ and the scale of X_j.
- Solution: standardise the predictors:

$$\tilde{X}_j = \frac{X_j}{\sigma_{X_j}}$$

- All Xs are in the same scale (1 unit change = 1 standard deviation)
- Then Ridge regression fit does not depend on scale of X.

Lasso Regression

- The Lasso is an alternative to Ridge regression.
- It picks βs to minimise $\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$
- The Lasso also shrinks the βs towards zero.
- But unlike the Ridge regression, the Lasso forces some βs to be exactly 0 for large enough λ.
- Lasso yields sparser models - fewer coefficients - easier to interpret.

- The Ridge regression solves the following problem:

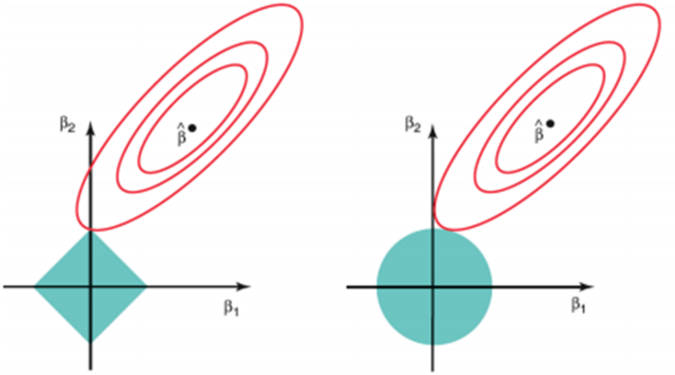
$$\min_{\beta} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \text{ subject to } \sum_{j=1}^{p} \beta^2_j \leq c$$

- The Lasso solves:

$$\min_{\beta} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \text{ subject to } \sum_{j=1}^{p} |\beta_j| \leq c$$

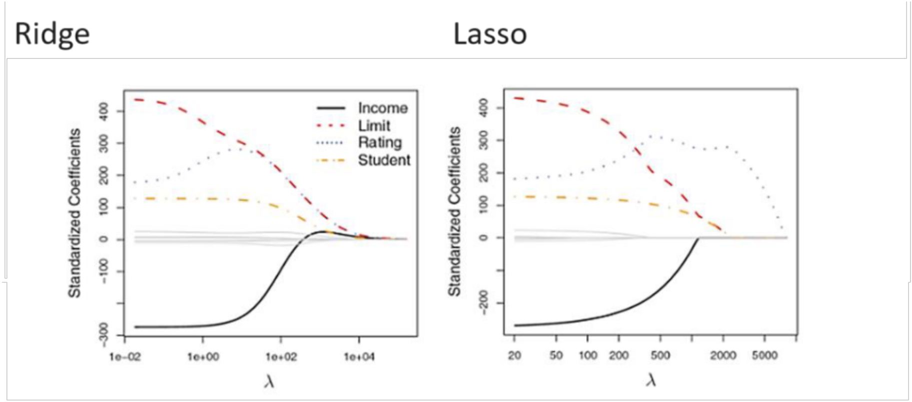
In the following graph:

- the ellipses are $\hat{\beta}$ values that form "iso-RSS" contours
- the ellipses are centered on the standard OLS minimum of $\hat{\beta}$s and RSS increases from inwards to outwards
- the shaded diamond and circle are the Lasso and Ridge constraints
- the Lasso constraint has corners on the axes: The ellipse will sooner intersect at a corner (than for Ridge), hence yield a zero coefficient



β_2
$\hat{\beta}$
β_1
β_2
$\hat{\beta}$
β_1

Example: Data set with several X-variables to explain credit default
The following Figures show the β coefficients
We have the OLS coefficients when $\lambda = 0$
Change of Ridge and Lasso coefficients, when tuning parameter $\lambda = 0$ changes



Elastic net

- Elastic net is based both on Ridge and Lasso regression
- Estimate βs in order to minimise:
  $\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda_1 \sum_{j=1}^{p} {\beta_j}^2 + \lambda_2 \sum_{j=1}^{p} |\beta_j|$
- If $\lambda_2 = 0$, then we have Ridge regression. If $\lambda_1 = 0$ we have Lasso
- May use cross-validation to determine the best ratio between L1 and L2 penalty strength
- It is important to first standardize our data before feeding it into our regularised model

Summary

- The Lasso:
  - Yields a simpler model.
  - Will perform better if only a subset of the X have non-trivial coefficients; forces the remaining X with small coefficients to be zero.
- Ridge regression does better if most or all of the X matter and have roughly similar-sized coefficients.
- But...ex ante often not known how Y is related to different predictors; use cross-validation to pick the best model.

- Elastic net uses both the L1 and L2 penalty

Scikit-learn in Python

Scikit-learn in Python

- So far we focussed on processing data $\Rightarrow$ use Numpy and Pandas to handle and import data
- Scikit-Learn provides a range of Supervised and Unsupervised Learning algorithms

  https://scikit-learn.org/stable/

- Comes with some data sets for learning (Iris, Digits, formerly: Boston house prices, etc.)

  https://scikit-learn.org/stable/datasets/toy_dataset.html
  https://scikit-learn.org/stable/datasets/real_world.html

Scikit-learn facilitates:

- Data processing and normalisation
- Creating training and test data samples
- Cross-validation
- Model evaluation

How to implement a ML model in scikit-learn in Python

- 1. Import the model that one intends to use
  - All scikit-learn ML models are implemented as Python classes
  - For example:

    from sklearn.linearmodel import LinearRegression
  - https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression

- 2. Set up the specific model - instantiate the class
  - For example:

    model1 = LinearRegression()

- 3. Fit the model to the training data and store the parameter estimates
  - The data will include the X variables and the Y (outcome or classes)
  - For example:

    ```
    model1.fit(X_train, Y_train)
    ```

- 4. Predict Y for the test data
    - For example:

      predictions1 = model1.predict(X_test)

Data Project

Data Project

- 1. Beer consumption, worldwide
- https://worldpopulationreview.com/country-rankings/beer-consumption-by-country
- Use Numpy and Pandas in Python
  - analyse the data set

- 2. Boston house prices
- formerly built-in data set in scikit-learn
- Use scikit-learn in Python
  - analyse the data set
  - estimate Linear regression, Lasso and Ridge regression

Literature

Literature:

James, Witten, Hastie, Tibshirani, Taylor (2023), An Introduction to Statistical Learning, Springer, Chapter 3, pp. 69 - 99; Chapter 6, pp. 240-253.