Machine Learning for Social Sciences
Part 1: Regularisation

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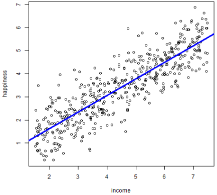
Regression

Linear regression minimizes the in-sample sum of squared residuals (“deviance”).

That is, it finds a $\hat{\beta}$ that maximizes in-sample R^2.

$$\text{dev}_{IS}(\hat{\beta}) \propto \sum_{i=1}^{n} (y_i - X_i'\hat{\beta})^2 \tag{1}$$



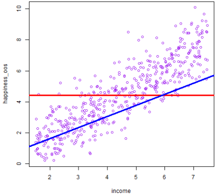
Regression

All that matters for prediction is the out-of-sample (OOS) deviance.

For OOS R^2, $\hat{\beta}$ is still the same (still fit with observations 1...n), but deviance is now calculated over new observations:

$$\text{dev}_{OOS}(\hat{\beta}) \propto \sum_{i=n+1}^{n+m} (y_i - X_i' \hat{\beta})^2 \tag{2}$$

OOS R2 will be positive if it performs better than the null model (simple average).



Exercise 1

How do we assess ou-of-sample (OOS) fit?

Let's cover different types of cross validation using the code here based on this article.

K-Fold Out-Of-Sample (OOS) Cross Validation (CV)

Given a dataset of n observations, $\{[X_i, y_i]\}_{i=1}^{n}$:

- Split the data into K evenly random subsets (*folds*).
- For $k = 1 ... K$:
    - Fit the coefficients $\hat{\beta}$ using all but the kth fold of data
    - Record R^2 on the left-out kth fold.

This will yield a sample of K OOS R^2 values. This sample is an *estimate* of the distribution of your model's predictive performance on new data.

Information criteria (AIC, BIC, AICc) are analytic approximations for these estimates. However, CV is the better choice.

Exercise 2

Let's try to predict survival of people on board of the titanic.

- The data titanic_sample.csv is a sample of people on board and provides some (historically true) individual information.
- The R code here predicts survival based on characteristics with linear and logistic regression, and perform k-fold OOS validation. Note that it uses manual coding for many steps to improve understanding (we will later use wrapper packages for many of these).

Regression

Poor prediction properties of OLS

- **Overfitting:** analysis corresponds too closely to data
- **Multiplicity:** false discovery rate (FDR)[1] might be high if small share of covariates is irrelevant
- **Added noise:** too many irrelevant controls reduce quality of relevant predictors

[1] FDR = expectation of false positives among significant tests.

Regularisation

How do we decide which model to build?

- Regression setting with p potential covariates have 2^p different possible models (with 20 covariates already > 1M).

Regularization: Penalizing model complexity to come up with with promising candidate models.

Approaches to be avoided:

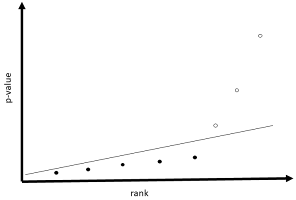
- *Backward stepwise regression:* Looking at full model fit and cutting down, e.g. using p-values with Benjamin Hochberg algorithm.
- *Forward stepwise regression:* Adding covariates stepwise that most increase OOS R^2.

Controlling expected false discovery rate (FDR)

Benjamin-Hochberg (BH) FDR control algorithm:

For N tests, with p-values $p_1 ... p_n$ and target FDR q:

- Order your p-values from smalles to largest as $p_1 ... p_n$.
- Set the p-value cutoff as $p^\star = q\frac{k}{N}$
- Select those features as significant with p-values above $p^\star$



Regularisation

Minimize a *penalized* deviance:

- **OLS:** $L_{OLS}(\hat{\beta}) = \sum_{i=1}^{n}(y_i - x_i'\hat{\beta})^2$
- **Ridge:** $L_{Ridge}(\hat{\beta}) = \sum_{i=1}^{n}(y_i - x_i'\hat{\beta})^2 + \lambda \sum_{j=1}^{m} \hat{\beta}_j^{\,2}$
- **Lasso:** $L_{Lasso}(\hat{\beta}) = \sum_{i=1}^{n}(y_i - x_i'\hat{\beta})^2 + \lambda \sum_{j=1}^{m} |\hat{\beta}_j|$
- **Elastic Net:** $L_{ElasticNet}(\hat{\beta}) = \frac{\sum_{i=1}^{n}(y_i - x_i'\hat{\beta})^2}{2n} + \lambda(\frac{1-\alpha}{2} \sum_{j=1}^{m} \hat{\beta}_j^{\,2} + \alpha \sum_{j=1}^{m} |\hat{\beta}_j|)$

where

- α is mixing parameter between ridge and lasso.
- λ is the penalty strength and a *tuning parameter*

Regularisation

Lasso is a fantastic default because

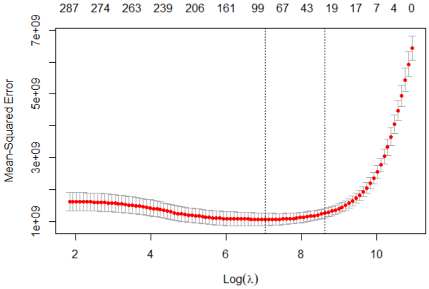
- it gives least possible amount of bias while preserving stability
- it yields automatic variable screening (some of the solved $\hat{\beta}$ are exactly zero)

Ridge penalty $\hat{\beta}_j^2$ places heavy penalty on large vales of β. Use only if you think that all covariates have small effects and there are no big dominating effects.

Regularisation

Lasso alone cannot do model selection, but *enumerates* a number of possible candidate models for different λ.

- → Use k-fold cross validation for each candidate model.
- → Choose the model with the smallest OOS sum of squared residuals ("mean squared prediction error").



Regularisation

Practical Hints

- Factor reference level matters under penalisation: get rid of reference level and create separate dummies for each factor level
- Size of coefficient matters: standardize covariates or standardise βs in the cost function by multiplying coefficients with standard deviation of corresponding covariates
- Note that you might still want to avoid standardisation if you have indicator covariates (penalty would mechanically be higher on common categories)

Preparation

Dealing with missing data

- **Categorical variables:** Treat "missing" as separate category: use *naref()* function provided here
- **Numerical variables:** Replace depending on sparsity: If variable has many zeros, replace with zero. Otherwise replace with mean. Use *mzimpute()* function provided here

Bias-Variance Trade-Off

Consider a model $y_i = f(x_i) + \epsilon_i$

where

- $\text{Var}(\epsilon_i) = \sigma^2$
- $\text{E}(\epsilon_i) = 0$
- ϵ_i independent across i
- ϵ_i and x_i independent

Bias-Variance Trade-Off

Suppose we fit a mapping $\hat{f}$ from sample D and use it to predict a value for y_0 at some x_0

Mean Square Error of Prediction = $E[(y_0 - \hat{f}(x_0))^2]$

$\text{MSE} = \sigma^2 + \text{Var}(\hat{f}(x_0)) + \text{Bias}(\hat{f}(x_0))^2$

- Adding relevant variables to a regression reduces bias.
- Adding any variable to a regression increases variance of each estimated coefficient.

→ with many covariates, OLS is unbiased but has highvariance

→ idea behind regularisation is to introduce (small) bias into coefficient estimates and to reduce variance.

Exercise 3

Let's use some meta-packages to implement lasso and elastic net:

- Here is a coding example using *glmnet*.
- Here is a coding example using *caret*.
- Here is a coding example for elastic net, also using *caret*.

Classification

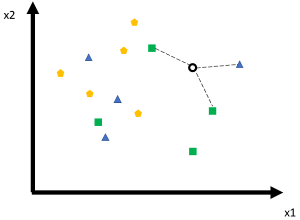
Classification: Predicting response variable y that represents membership in one of many categories.

Let's cover

- K Nearest Neighbours
- Logistic regression (again)
- Performance metrics
- Distributed Multinomial Regression

Classification

K nearest neighbours: predicted class is most common class in the set of k nearest neighbours.



Good idea for intuition, but too crude to be useful in practice.

Classification

Logistic Regression: Estimate probability p for binary response variable to be 1.

A *classification rule*, or cutoff, is the probability p at which you predict

- $\hat{y}_f = 0$ for $p_j <= p$
- $\hat{y}_f = 1$ for $p_j > p$.

Such a rule involves two types of errors (false positive, and false negatives), which can be converted into rates. Note that these statistics are normalized by classification.

- **False Positive Rate** $= \frac{\text{expected \# false positives}}{\text{\#classified positive}}$
- **False Negative Rate** $= \frac{\text{expected \# false negatives}}{\text{\#classified negative}}$

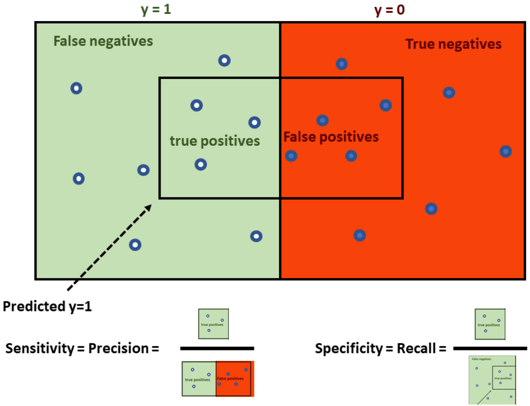
Classification

Another measure for classification errors normalizes by true examples in each class:

- **Sensitvity ("Precision"):** proportion of true $y = 1$ classified as such
- **Specificity ("Recall"):** proportion of true $y = 0$ classified as such

Classification

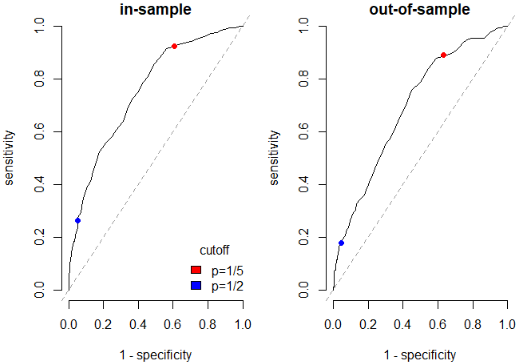
The **F1 Score** combines the precision and recall of a classifier into a single metric by taking their harmonic mean: $\text{F1 Score} = 2 * \frac{\text{Precision} * \text{Recall}}{\text{Precision} + \text{Recall}}$



Classification

A nice visual summary of potential classification rules is the ROC curve that plots sensitivity against 1 - specificity.[2].

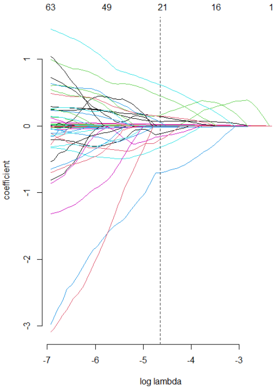
The area under the curve of the out-sample ROC plot is often used as performance measure for a classification model.

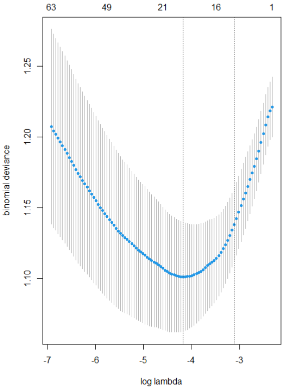


[2] ROC = receiver operating characteristic

Classification

You can plot the regularisation path and CV results:





Exercise 4

Let's build a model to predict default on loans using a real dataset on loans and credit from a set of local lenders in Germany.

- The data can be downloaded here.
- Here is a coding example for classification, using Matt Taddy's *gamlr* package.

Classification

What if our outcome is not binary, but has multiple classes (one of K categories)?

- We can use *multinomial logistic regression*.
- But multinomial regressions can be slow...

Solution: Distributed multinomial regression (DML)

- Trick: multinomial logistic regression coefficients will be – for all practical purposes – similar to those we can get through *independent* poisson estimation for each of the log-linear equations $E[y_{ik}|\mathbf{x}_i] = exp(\mathbf{x}_i'\beta_k)$.

Exercise 5

Let's try to predict glass type from glass features.

- This coding example implements multinomial logistic regression with parallel computing.

References

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