Lecture 9: Feature selection and regularised regression

Felix Held, Mathematical Sciences

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CHALMERS UNIVERSITY OF TECHNOLOGY | UNIVERSITY OF GOTHENBURG

Goals of modelling

1. **Predictive strength:** How well can we reconstruct the observed data? Has been most important so far.
2. **Model/variable selection:** Which variables are **part of the true model**? This is about uncovering structure to allow for mechanistic understanding.

Feature Selection

Remember ordinary least-squares (OLS)

Consider the model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

where

- $\mathbf{y} \in \mathbb{R}^n$ is the **outcome**, $\mathbf{X} \in \mathbb{R}^{n \times (p+1)}$ is the **design matrix**, $\boldsymbol{\beta} \in \mathbb{R}^{p+1}$ are the **regression coefficients**, and $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ is the **additive error**
- **Five basic assumptions** have to be checked

  Underlying relationship is linear (1)

  Zero mean (2), uncorrelated (3) errors with constant variance (4) which are (roughly) normally distributed (5)
- **Centring** ($\frac{1}{n} \sum_{l=1}^{n} x_{lj} = 0$) and **standardisation** ($\frac{1}{n} \sum_{l=1}^{n} x_{lj}^2 = 1$) of predictors simplifies interpretation
- **Centring** the outcome ($\frac{1}{n} \sum_{l=1}^{n} y_l = 0$) and features removes the need to estimate the intercept

Feature selection as motivation

Analytical solution exists when $\mathbf{X}^\top\mathbf{X}$ is invertible

$$\hat{\boldsymbol{\beta}}_{\mathrm{OLS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$$

The solution can be unstable or impossible to compute if

- there is **high correlation** between predictors, or
- if $p > n$.

Solutions: **Regularisation** or **feature selection**

Filtering for feature selection

- Choose features through pre-processing
  - Features with maximum variance
  - Use only the first k PCA components
- Examples of other useful measures
  - Use a univariate criterion, e.g. **F-score:** Features that correlate most with the response
  - **Mutual Information:** Reduction in uncertainty about $\mathbf{x}$ after observing y
  - **Variable importance:** Determine variable importance with random forests
- **Summary**
  - **Pro:** Fast and easy
  - **Con:** Filtering mostly operates on single features and is not geared towards a certain method
  - Care with cross-validation and multiple testing necessary
- Filtering is often more of a pre-processing step and less of a proper feature selection step

Wrapping for feature selection

- **Idea:** Determine the best set of features by fitting models of different complexity and comparing their performance
- **Best subset selection:** Try all possible (**exponentially many**) subsets of features and compare model performance with e.g. cross-validation
- **Forward selection:** Start with just an intercept and add in each step the variable that improves fit the most (**greedy algorithm**)
- **Backward selection:** Start with all variables included and then remove sequentially the one with the least impact (**greedy algorithm**)
- As discreet procedures, all of these methods **exhibit high variance** (small changes could lead to different predictors being selected, resulting in a potentially very different model)

Embedding for feature selection

- **Embed/include** the feature selection into the model estimation procedure
- Ideally, penalization on the number of included features

  $$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda \sum_{j=1}^{p} \mathbb{1}(\beta_j \neq 0)$$

  However, **discrete optimization problems** are hard to solve
- **Softer regularisation methods** can help

  $$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda ||\boldsymbol{\beta}||_q^q$$

  where λ is a tuning parameter and $q \geq 1$ or $q = \infty$.

Feature selection

Feature selection can be addressed in multiple ways

- **Filtering:** Remove variables before the actual model for the data is built
  - Often crude but fast
  - Typically only pays attention to one or two features at a time (e.g. F-Score, MIC) or does not take the outcome variable into consideration (e.g. PCA)
- **Wrapping:** Consider the selected features as an additional hyper-parameter
  - computationally very heavy
  - most approximations are greedy algorithms
- **Embedding:** Include feature selection into parameter estimation through penalisation of the model coefficients
  - Naive form is equally computationally heavy as wrapping
  - **Soft-constraints** create biased but useful approximations

Regularised regression

Constrained and regularised regression

The optimization problem

$$\arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 \quad \text{subject to} \quad ||\boldsymbol{\beta}||_q^q \leq t$$

for $q > 0$ is equivalent to

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda||\boldsymbol{\beta}||_q^q$$

when $q \geq 1$. This is the **Lagrangian** of the constrained problem.

Note: Constraints are convex for all $q \geq 1$ but not differentiable in $\boldsymbol{\beta} = \mathbf{0}$ for $q = 1$.

Ridge regression

For $q = 2$ the constrained problem is **ridge regression** (Tikhonov regularisation)

$$\hat{\boldsymbol{\beta}}_{\text{ridge}}(\lambda) = \arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda||\boldsymbol{\beta}||_2^2$$

where $||\boldsymbol{\beta}||_2^2 = \sum_{j=1}^{p} \beta_j^2$.

An **analytical solution** exists if $\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p$ is invertible

$$\hat{\boldsymbol{\beta}}_{\text{ridge}}(\lambda) = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\mathbf{y}$$

If $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$, then

$$\hat{\boldsymbol{\beta}}_{\text{ridge}}(\lambda) = \frac{\hat{\boldsymbol{\beta}}_{\text{OLS}}}{1 + \lambda},$$

i.e. $\hat{\boldsymbol{\beta}}_{\text{ridge}}(\lambda)$ is **biased** but has **lower variance**.

SVD and ridge regression

Recall: The SVD of a matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ was

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$$

The analytical solution for ridge regression becomes ($n \geq p$)

$$\begin{aligned}
\hat{\boldsymbol{\beta}}_{\mathrm{ridge}}(\lambda) &= (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\mathbf{y} \\
&= (\mathbf{V}\mathbf{D}^2\mathbf{V}^\top + \lambda\mathbf{I}_p)^{-1}\mathbf{V}\mathbf{D}\mathbf{U}^\top\mathbf{y} \\
&= \mathbf{V}(\mathbf{D}^2 + \lambda\mathbf{I}_p)^{-1}\mathbf{D}\mathbf{U}^\top\mathbf{y} \\
&= \sum_{j=1}^{p} \frac{d_j}{d_j^2 + \lambda}\mathbf{v}_j\mathbf{u}_j^\top\mathbf{y}
\end{aligned}$$

Ridge regression **acts strongest** on principal components with **lower eigenvalues**, e.g. in presence of correlation between features.

Effective degrees of freedom

Recall the **hat matrix** $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$ in OLS. The trace of $\mathbf{H}$

$$\operatorname{tr}(H) = \operatorname{tr}(\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top) = \operatorname{tr}(\mathbf{X}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}) = \operatorname{tr}(\mathbf{I}_p) = p$$

is equal to the trace of $\widehat{\boldsymbol{\Sigma}}$ and the **degrees of freedom** for the regression coefficients.

In analogy define for ridge regression

$$\mathbf{H}(\lambda) := \mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top$$

and

$$\operatorname{df}(\lambda) := \operatorname{tr}(\mathbf{H}(\lambda)) = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda},$$

the **effective degrees of freedom**.

Lasso regression

For $q = 1$ the constrained problem is known as the **lasso**

$$\hat{\boldsymbol{\beta}}_{\text{lasso}}(\lambda) = \arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda||\boldsymbol{\beta}||_1$$

- Smallest q in penalty such that constraint is still convex
- Produces **sparse solutions** (many coefficients exactly equal to zero) and therefore performs **feature selection**

Intuition for the penalties (I)

Assume the OLS solution $\boldsymbol{\beta}_{\text{OLS}}$ exists and set

$$\mathbf{r} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}_{\text{OLS}}$$

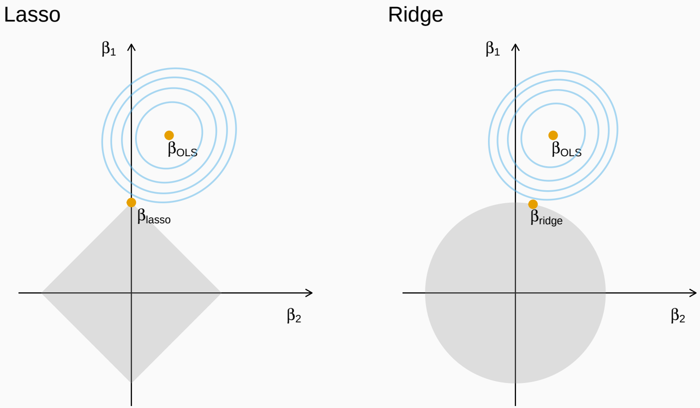
it follows for the **residual sum of squares (RSS)** that

$$\begin{aligned} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 &= ||(\mathbf{X}\boldsymbol{\beta}_{\text{OLS}} + \mathbf{r}) - \mathbf{X}\boldsymbol{\beta}||_2^2 \\ &= ||(\mathbf{X}(\boldsymbol{\beta} - \boldsymbol{\beta}_{\text{OLS}}) - \mathbf{r}||_2^2 \\ &= (\boldsymbol{\beta} - \boldsymbol{\beta}_{\text{OLS}})^\top \mathbf{X}^\top \mathbf{X}(\boldsymbol{\beta} - \boldsymbol{\beta}_{\text{OLS}}) - 2\mathbf{r}^\top \mathbf{X}(\boldsymbol{\beta} - \boldsymbol{\beta}_{\text{OLS}}) + \mathbf{r}^\top \mathbf{r} \end{aligned}$$

which is an **ellipse** (at least in 2D) centred on $\boldsymbol{\beta}_{\text{OLS}}$.

Intuition for the penalties (II)

The least squares RSS is minimized for $\boldsymbol{\beta}_{\text{OLS}}$. If a constraint is added ($||\boldsymbol{\beta}||_q^q \leq t$) then the RSS is minimized by the closest $\boldsymbol{\beta}$ possible that fulfills the constraint.



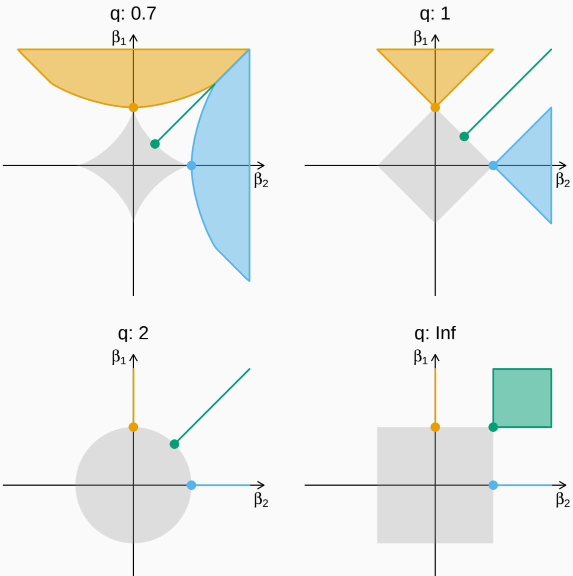
The blue lines are the contour lines for the RSS.

Intuition for the penalties (III)

Depending on q the different constraints lead to different solutions. If $\boldsymbol{\beta}_{\mathrm{OLS}}$ is in one of the coloured areas or on a line, the constrained solution will be at the corresponding dot.

Sparsity only for $q \leq 1$

Convexity only for $q \geq 1$



Computational aspects of the Lasso (I)

What estimates does the lasso produce?

Target function

$$\arg\min_{\boldsymbol{\beta}} \frac{1}{2}||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda||\boldsymbol{\beta}||_1$$

Special case: $\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$. Then

$$\frac{1}{2}||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda||\boldsymbol{\beta}||_1 = \frac{1}{2}\mathbf{y}^\top\mathbf{y} - \underbrace{\mathbf{y}^\top\mathbf{X}}_{=\boldsymbol{\beta}_{\mathrm{OLS}}^\top}\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\beta}^\top\boldsymbol{\beta} + \lambda||\boldsymbol{\beta}||_1 = \mathrm{g}(\boldsymbol{\beta})$$

How do we find the solution $\hat{\boldsymbol{\beta}}$ in presence of the **non-differentiable** penalisation $||\boldsymbol{\beta}||_1$?

Computational aspects of the Lasso (II)

For $\mathbf{X}^\top \mathbf{X} = \mathbf{I}_p$ the target function can be written as

$$\arg\min_{\boldsymbol{\beta}} \sum_{j=1}^{p} -\beta_{\mathrm{OLS},j}\beta_j + \frac{1}{2}\beta_j^2 + \lambda|\beta_j|$$

This results in p **uncoupled** optimization problems.

- **If** $\beta_{\mathrm{OLS},j} > 0$, then $\beta_j > 0$ to minimize the target
- **If** $\beta_{\mathrm{OLS},j} \leq 0$, then $\beta_j \leq 0$

Each case results in

$$\widehat{\beta}_{\mathrm{lasso},j} = \mathrm{sign}(\beta_{\mathrm{OLS},j})(|\beta_{\mathrm{OLS},j}| - \lambda)_+ = \mathrm{ST}(\beta_{\mathrm{OLS},j}, \lambda),$$

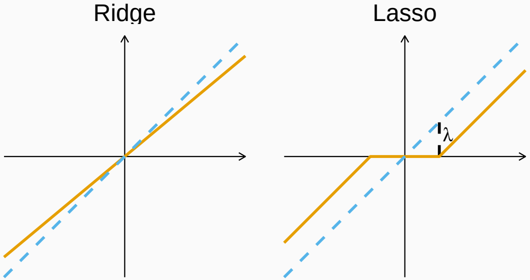
where

- $x_+ = x$ if $x > 0$ or 0 otherwise,
- and ST is called the **soft-thresholding operator**

Relation to OLS estimates

Both ridge regression and the lasso estimates can be written as functions of $\boldsymbol{\beta}_{\mathrm{OLS}}$ if $\mathbf{X}^{\top}\mathbf{X} = \mathbf{I}_p$.

$$\beta_{\mathrm{ridge},j} = \frac{\beta_{\mathrm{OLS},j}}{1+\lambda} \quad \text{and} \quad \widehat{\beta}_{\mathrm{lasso},j} = \mathrm{sign}(\beta_{\mathrm{OLS},j})(|\beta_{\mathrm{OLS},j}| - \lambda)_+$$



Visualisation of the transformations applied to the OLS estimates.

Shrinkage and effective degrees of freedom

When λ is fixed, the **shrinkage** of the lasso estimate $\boldsymbol{\beta}_{\text{lasso}}(\lambda)$ compared to the OLS estimate $\boldsymbol{\beta}_{\text{OLS}}$ is defined as

$$s(\lambda) = \frac{||\boldsymbol{\beta}_{\text{lasso}}(\lambda)||_1}{||\boldsymbol{\beta}_{\text{OLS}}||_1}$$

Note: $s(\lambda) \in [0, 1]$ with $s(\lambda) \to 0$ for increasing λ and $s(\lambda) = 1$ if $\lambda = 0$

Recall: For ridge regression define

$$\mathbf{H}(\lambda) := \mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top$$

and

$$\text{df}(\lambda) := \text{tr}(\mathbf{H}(\lambda)) = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda},$$

the **effective degrees of freedom**.

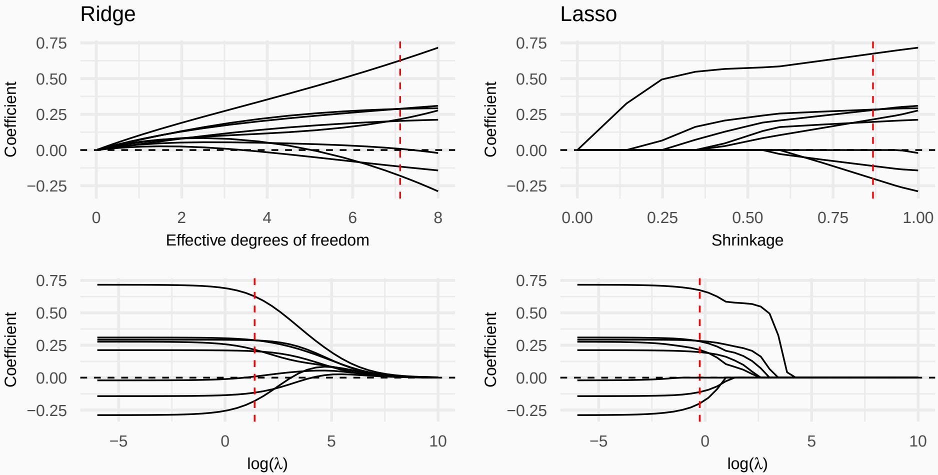
Prostate cancer dataset

Data to examine the correlation between the level of a prostate cancer-specific substance and a number of clinical measurements in men who just before partial or full removal of the prostate in patients.

- $n = 67$ samples
- A continuous response on the log-scale
- $p = 8$ features
  - e.g. log cancer volume, log prostate weight or age of patient

Regularisation paths for varying λ

Red dashed lines indicate the λ selected by cross-validation



Notes on the lasso

- In the general case, i.e. $\mathbf{X}^\top\mathbf{X} \neq \mathbf{I}_p$, there is no explicit solution.
- Numerical solution possible, e.g. with **coordinate descent** where each β_j is updated separately with the remaining β_i with $i \neq j$ fixed
- As for ridge regression, **estimates are biased**
- **Degrees of freedom** are equal to the number of non-zero coefficients

Potential caveats of the lasso (I)

- **Sparsity of the true model:**
  - The lasso only works if the data is generated from a sparse process.
  - However, a dense process with many variables and not enough data or high correlation between predictors can be unidentifiable either way
- **Correlations:** Many non-relevant variables correlated with relevant variables can lead to the selection of the wrong model, even for large n
- **Irrepresentable condition:** Split $\mathbf{X}$ such that $\mathbf{X}_1$ contains all **relevant variables** and $\mathbf{X}_2$ contains all **irrelevant variables**. If

$$|(\mathbf{X}_2^\top \mathbf{X}_1)(\mathbf{X}_1^\top \mathbf{X}_1)^{-1}| < 1 - \eta$$

for some $\eta > 0$ then the lasso is (almost) guaranteed to pick the true model

Potential caveats of the lasso (II)

In practice, both the **sparsity of the true model** and the **irrepresentable condition** cannot be checked.

- Assumptions and domain knowledge have to be used

Take-home message

- Filtering and wrapping methods useful for feature selection in practice but can be unprincipled or have high variance
- Regularised regression can help in numerically unstable situations (such as in ridge regression)
- The lasso can in addition perform variable selection