Shrinkage and variable selection

Data Mining - CdL CLAMSES

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Homepage

- This unit will cover the following **topics**:
  - Best subset regression
  - Principal component regression
  - Ridge regression
  - Lasso, LARS, elastic-net
- The common themes are called **variable selection** and **shrinkage estimation**.
- The issue we face is the presence of a high number p of covariates that are **potentially irrelevant**.
- This problem is quite challenging when the **ratio** p/n is **large**.
- In the **extreme case** $p > n$, is there any hope of fitting a meaningful model?

A biostatistical motivation

The prostate dataset

- The prostate cancer data investigates the relationship between the prostate-specific **antigen** and a number of clinical measures in men about to receive a prostatectomy.
- This dataset has been used in the **original paper** by Tibshirani (1996) to present the lasso. A description is given in **Section 3.2.1** of HTF (2009).
- We want to **predict** the logarithm of a **prostate-specific antigen** (lpsa) as a function of:
  - logarithm of the cancer volume (lcavol);
  - logarithm of the prostate weight (lweight);
  - age each man (age);
  - logarithm of the benign prostatic hyperplasia amount (lbph);
  - seminal vesicle invasion (svi), a binary variable;
  - logarithm of the capsular penetration (lcp);
  - Gleason score (gleason), an ordered categorical variable;
  - Percentage of Gleason scores 4 and 5 (pgg45).

A glimpse of the prostate dataset

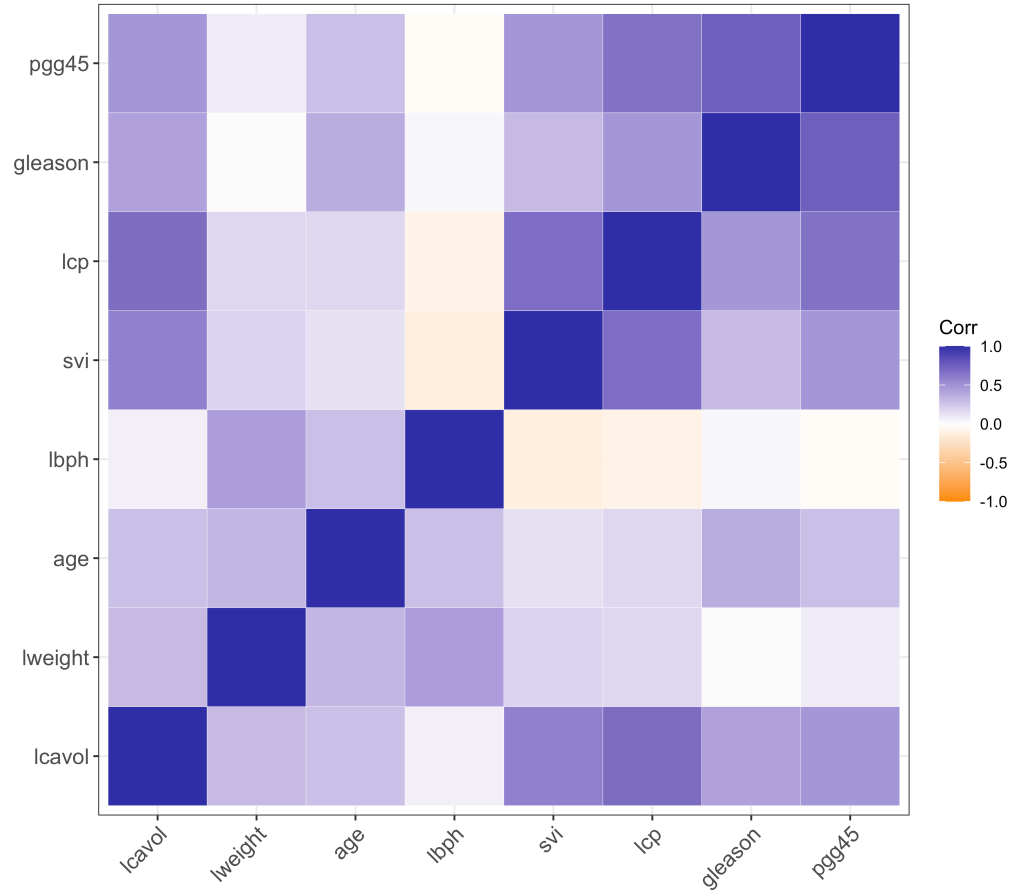
- Summarizing, there are in total 8 **variables** that can be used to predict the antigen `lpsa`.
- We **centered** and **standardized** all the covariates before the training/test split.
- There are $n = 67$ observations in the **training** set and 30 in the **test** set.

Original dataset | Standardized dataset

```
Rows: 97
Columns: 10
$ lcavol  <dbl> -0.5798185, -0.9942523, -0.5108256, -1.2039728, 0.7514161, -1.…
$ lweight <dbl> 2.769459, 3.319626, 2.691243, 3.282789, 3.432373, 3.228826, 3.…
$ age     <int> 50, 58, 74, 58, 62, 50, 64, 58, 47, 63, 65, 63, 63, 67, 57, 66…
$ lbph    <dbl> -1.3862944, -1.3862944, -1.3862944, -1.3862944, -1.3862944, -1…
$ svi     <int> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,…
$ lcp     <dbl> -1.3862944, -1.3862944, -1.3862944, -1.3862944, -1.3862944, -1…
$ gleason <int> 6, 6, 7, 6, 6, 6, 6, 6, 6, 6, 6, 6, 7, 7, 7, 6, 7, 6, 6, 6, 6,…
$ pgg45   <int> 0, 0, 20, 0, 0, 0, 0, 0, 0, 0, 0, 0, 30, 5, 5, 0, 30, 0, 0, 0,…
$ lpsa    <dbl> -0.4307829, -0.1625189, -0.1625189, -0.1625189, 0.3715636, 0.7…
$ train   <lgl> TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, FALSE, TRUE, FALSE, FALSE,…
```

Home page

Correlation matrix of prostate



Home page

The regression framework

- In this unit, we will assume that the response variables Y_i (`lpsa`) are obtained as

$$Y_i = f(\boldsymbol{x}_i) + \epsilon_i,$$

  where ϵ_i are **iid** random variables with $\mathbb{E}(\epsilon_i) = 0$ and $\text{var}(\epsilon_i) = \sigma^2$.

- Unless specifically stated, we will **not** assume the **Gaussianity** of the errors ϵ_i nor make any specific assumption about $f(\boldsymbol{x})$, which could be **non-linear**.

- In practice, we **approximate** the true $f(\boldsymbol{x})$ using a **linear model**, e.g., by considering the following function

$$f(\boldsymbol{x}_i; \beta_0, \beta) = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = \beta_0 + \boldsymbol{x}_i^T \beta,$$

  in which the regression coefficients must be estimated.

- In this unit, the **intercept** β_0 will often play a special role therefore we use a slightly different notation compared to Unit A.

The variable selection problem

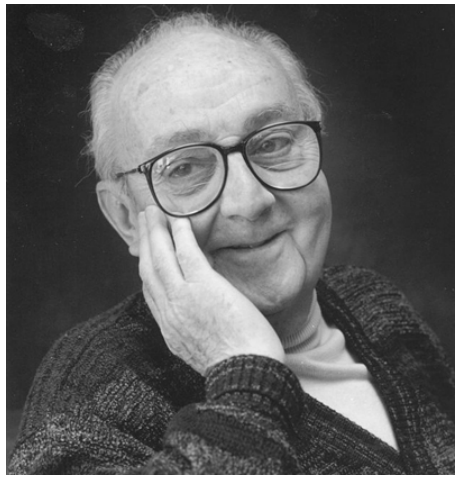
- Including a lot of covariates in the model is not necessarily a good thing!
- Indeed, some variables are likely to be **irrelevant**:
  - they might be **correlated** with other covariates and therefore **redundant**;
  - they could be uncorrelated with the response `lpsa`.
- If we use all the $p = 8$ available covariates, the estimated $f(\boldsymbol{x}; \hat{\beta}_0, \hat{\beta})$ might have a **high variance**, without an important gain in terms of bias, i.e., a **large mean squared error**.
- We are looking for a **simpler model** having, hopefully, a lower mean squared error.
- These considerations are particularly relevant in cases in which $p > n$!

A naïve approach: (ab)using p-values

	(Intercept)	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45
estimate	2.46	0.68	0.26	-0.14	0.21	0.31	-0.29	-0.02	0.27
std.error	0.09	0.13	0.10	0.10	0.10	0.12	0.15	0.15	0.15
statistic	27.60	5.37	2.75	-1.40	2.06	2.47	-1.87	-0.15	1.74
p.value	0.00	0.00	0.01	0.17	0.04	0.02	0.07	0.88	0.09

- It is common practice to use the **p-values** to perform **model selection** in a stepwise fashion.
- However, what if the true $f(\boldsymbol{x})$ were not linear?
- In many data mining problems, a **linear model** is simply an approximation of the unknown $f(\boldsymbol{x})$ and hypothesis testing procedures are ill-posed.
- Even if the true function were linear, using p-values would **not be a good idea**, at least if done without appropriate **multiplicity corrections**.
- The above p-values are meant to be used in the context of a single hypothesis testing problem, **not** to make **iterative choices**.

The predictive culture



George E. P. Box

- "*All models are approximations. Essentially, all models are wrong, but some are useful.*"

  George E. P. Box
- If the **focus** is on **prediction**, we do not necessarily care about selecting the "true" set of parameters.
- In many data mining problems, the focus is on **minimizing** the **prediction errors**.
- Hence, often we may **accept some bias** (i.e., we use a "wrong" but useful model), if this leads to a **reduction in variance**.

Overview of this unit

- In this unit, we will discuss two "discrete" methods:
  - Best subset selection and its greedy approximations: forward / backward regression;
  - Principal components regression (PCR).
- Best subset selection perform **variable selection**, whereas principal components regression **reduces the variance** of the coefficients.
- These "discrete" methods can be seen as the naïve counterpart of more advanced and **continuous** ideas that are presented in the second part of the Unit.

	Shrinkage	**Variable selection**
Discrete	Principal component regression	Best subset selection, stepwise
Continuous	Ridge regression	Relaxed Lasso

- Finally, the **lasso** and the **elastic-net** perform both shrinkage and variable selection.

Overview of the final results

	Least squares	Best subset	PCR	Ridge	Lasso
(Intercept)	2.465	2.477	2.455	2.467	2.468
lcavol	0.680	0.740	0.287	0.588	0.532
lweight	0.263	0.316	0.339	0.258	0.169
age	-0.141	.	0.056	-0.113	.
lbph	0.210	.	0.102	0.201	.
svi	0.305	.	0.261	0.283	0.092
lcp	-0.288	.	0.219	-0.172	.
gleason	-0.021	.	-0.016	0.010	.
pgg45	0.267	.	0.062	0.204	.

Best subset selection

Best subset selection

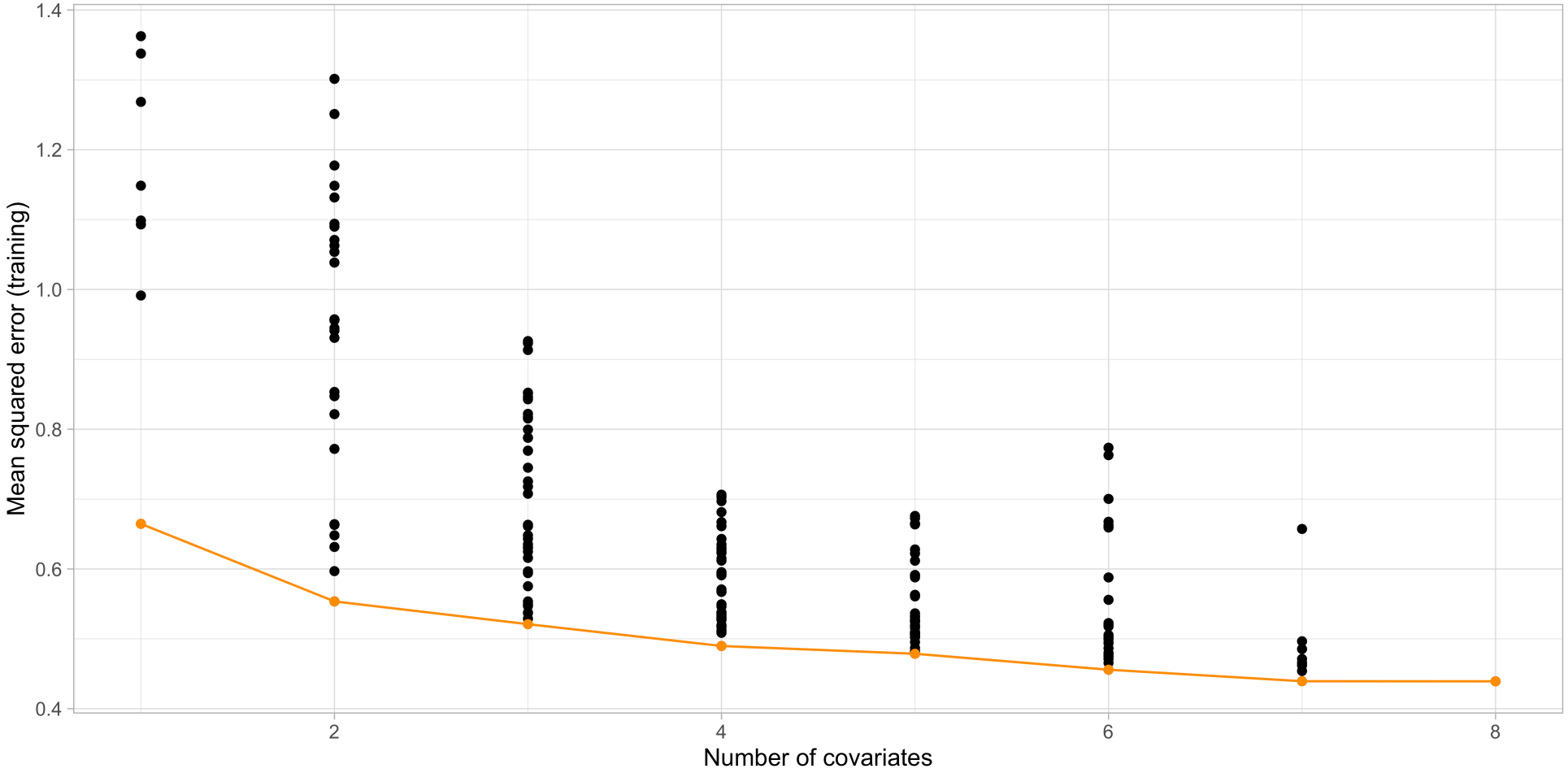
- Let us return to our **variable selection problem**.
- In principle, we could perform an **exhaustive search** considering all the 2^p possible models and then selecting the one having the best out-of-sample predictive performance.

Best subset procedure

1. Let $\mathcal{M}_0$ be the **null model**, which contains no predictors, i.e. set $\hat{y}_i = \hat{\beta}_0 = \bar{y}$.
2. For $k = 1, \ldots, p$, do:
   i. Estimate **all** the $\binom{p}{k}$ models that contain exactly k covariates;
   ii. Identify the "best" model with k covariates having the smallest $\text{MSE}_{k,\text{train}}$; call it $\mathcal{M}_k$.

- A model with more variables has lower **training** error, namely $\text{MSE}_{k+1,\text{train}} \leq \text{MSE}_{k,\text{train}}$ by construction. Hence, the optimal subset size k must be chosen e.g., via **cross-validation**.

Step 1. and 2. of best subset selection



Home page

The "best" models $\mathcal{M}_1, \ldots, \mathcal{M}_p$

- The output of the **best subset selection**, on the training set is:

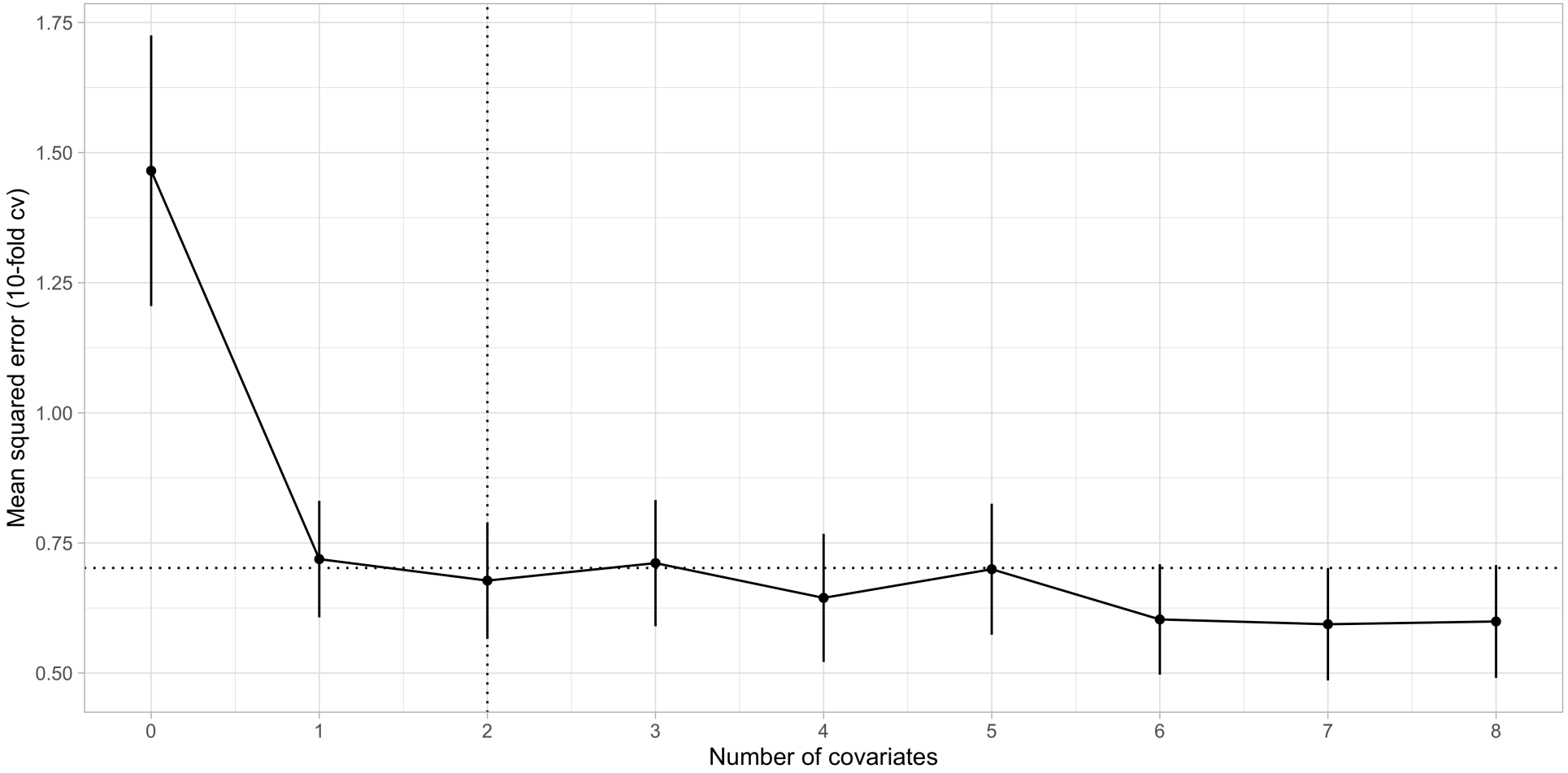
```
          lcavol lweight age lbph svi lcp gleason pgg45
1  ( 1 ) "*"    " "     " " " "  " " " " " " "     " "
2  ( 1 ) "*"    "*"     " " " "  " " " " " " "     " "
3  ( 1 ) "*"    "*"     " " " "  "*" " " " " "     " "
4  ( 1 ) "*"    "*"     " " "*"  "*" " " " " "     " "
5  ( 1 ) "*"    "*"     " " "*"  "*" " " " " "     "*"
6  ( 1 ) "*"    "*"     " " "*"  "*" "*" " " "     "*"
7  ( 1 ) "*"    "*"     "*" "*"  "*" "*" " " "     "*"
8  ( 1 ) "*"    "*"     "*" "*"  "*" "*" "*"     "*"
```

- The above table means that the best model with $k = 1$ uses the variable `lcavol`, whereas when $k = 2$ the selected variables are `lcavol` and `lweight`, and so on.
- Note that, in general, these models are **not** necessarily **nested**, i.e. a variable selected at step k is not necessarily included at step $k + 1$. Here they are, but it is a coincidence.
- What is the **optimal subset size** k in terms of out-of-sample mean squared error?

The wrong way of doing cross-validation

- Consider a regression problem with a **large number of predictors** (relative to n) such as the `prostate` dataset.
- A typical strategy for analysis might be as follows:
  1. Screen the predictors: find a subset of "good" predictors that show a reasonably strong correlation with the response;
  2. Using this subset of predictors (e.g., `lcavol`, `lweight` and `svi`), build a regression model;
  3. Use cross-validation to estimate the prediction error of the model of the step 2.
- Is this a correct application of cross-validation?
- If your reaction was "**this is absolutely wrong!**", it means you correctly understood the principles of cross-validation.
- If you thought this was an ok-ish idea, you may want to read **Section 7.10.2** of HTF (2009), called "the wrong way of doing cross-validation".

Step 3. of best subset selection via cross-validation



- By applying the "1 standard error rule", we select $k = 2$, i.e. `lcavol` and `lweight`.

Home page

Comments and computations

- The correct way of doing cross-validation requires that the **best subset selection** is performed on **every fold**, possibly obtaining different "best" models with the same size.
- Best subset selection is conceptually appealing, but it has a **major limitation**. There are

$$\sum_{k=1}^{p} \binom{p}{k} = 2^p$$

  models to consider, which is **computationally prohibitive**!
- There exist algorithms (i.e. **leaps and bounds**) that make this feasible for $p \approx 30$.
- Recently, Bertsimas et al., 2016 proposed the usage of a mixed integer optimization formulation, allowing p to be in the order of hundreds.
- Despite these advances, this problem remains **computationally very expensive**. See also the recent paper Hastie et al. (2020) for additional considerations and comparisons.

Forward regression

- Forward regression is **greedy approximation** of best subset selection that produces a sequence of **nested** models. It is computationally feasible and can be applied when $p > n$.

Forward regression

1. Let $\mathcal{M}_0$ be the **null model**, which contains no predictors, i.e. set $\hat{y}_i = \hat{\beta}_0 = \bar{y}$.
2. For $k = 0, \ldots, \min(n-1, p-1)$, do:
   i. Consider the $p - k$ models that augment the predictors in $\mathcal{M}_k$ with **one additional covariate**.
   ii. Identify the "best" model among the above $p - k$ competitors having the smallest $\text{MSE}_{k,\text{train}}$ and call it $\mathcal{M}_k$.

- It can be shown that the identification of the **optimal new predictor** can be efficiently computed e.g. using the **QR decomposition**.

Backward regression

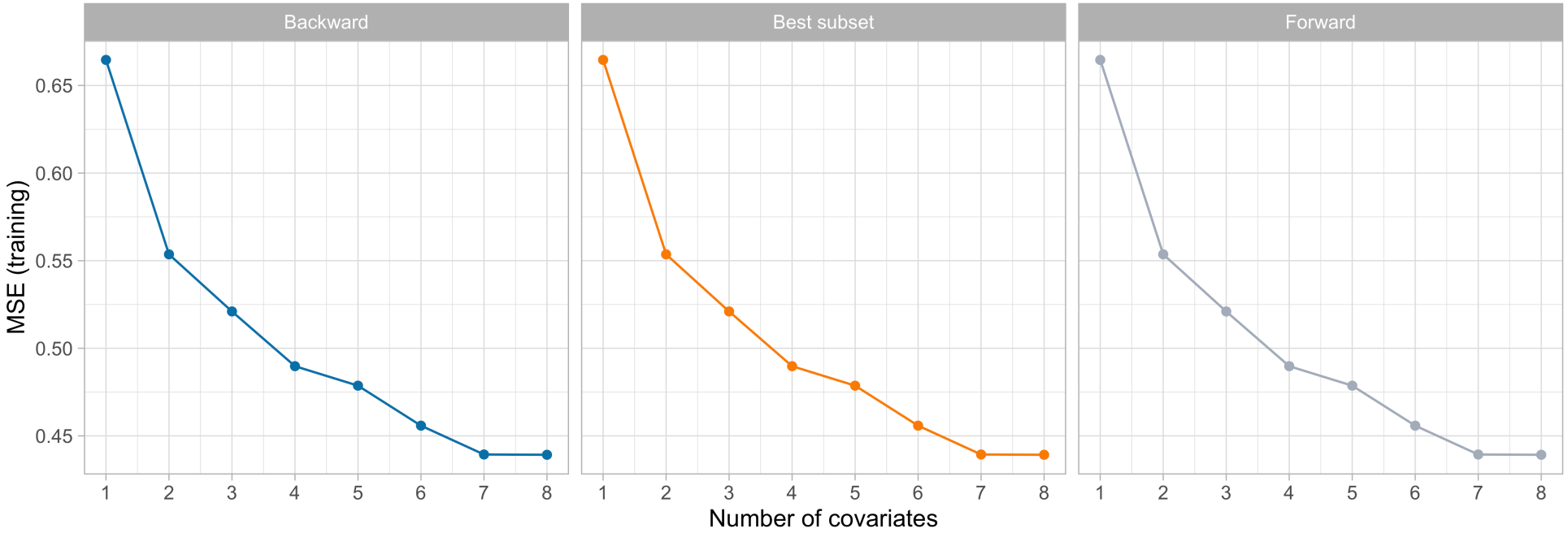
- When $p < n$, an alternative greedy approach is **backward regression**, which also produces a sequence of **nested** models.

Backward regression

1. Let $\mathcal{M}_p$ be the **full model**, which contains all the predictors.
2. For $k = p, p-1, \ldots, 1$, do:
   i. Consider the k models that contain **all but one** of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
   ii. Identify the "best" model $\mathcal{M}_k$ among these k models having the smallest $\mathrm{MSE}_{k,\mathrm{train}}$.

- It can be shown that the **dropped predictor** is the one with the lowest absolute Z-score or, equivalently, the **highest p-value**.

Forward, backward and best subset



- In the `prostate` dataset, forward, backward and best subset selection all gave precisely the **same path of solutions** on the full training set.

Pros and cons of subset selection strategies

Pros

- Best subset selection is appealing because of its **conceptual simplicity**.
- Best subset and forward regression can be used, if computationally feasible, even when $p > n$.

Cons

- Subset strategies tend to select models that are "**too simple**", especially in presence of correlated variables.
- Despite the recent advances, when p is large best subset selection is **computationally unfeasible**.
- Leaps and bounds computational strategies can not be easily generalized to GLMs.

Principal components regression

Data compression

- At this point, we established that **many covariates = many problems**.
- Instead of selecting the "best" variables, let us consider a different perspective.
- We consider a **compressed** version of the covariates that has smaller dimension k but retains most information.
- Intuitively, we want to **reduce the variance** by finding a good compression without sacrificing too much bias.
- The main statistical tool, unsurprisingly, will be the celebrated **principal components analysis** (PCA).
- We will compress the covariate information $\boldsymbol{X}$ using a smaller set of variables $\boldsymbol{Z}$, i.e. the principal components.

The intercept term

- In principal component regression and other related methods (ridge, lasso, and elastic-net), we do **not** wish to **compress** the **intercept** term β_0. We would like to "remove it".
- Let us consider a **reparametrization** of the linear model, in which $\alpha = \beta_0 + \bar{\boldsymbol{x}}^T\beta$. This is equivalent to a linear model with **centered predictors**:

$$f(\boldsymbol{x}_i; \alpha, \beta) = \beta_0 + \boldsymbol{x}_i^T\beta = \alpha - \bar{\boldsymbol{x}}^T\beta + \boldsymbol{x}_i^T\beta = \alpha + (\boldsymbol{x}_i - \bar{\boldsymbol{x}})^T\beta.$$

- The estimates for (α, β) can be now computed separately and **in two steps**.
- The **estimate** of the **intercept** with centered predictors is $\hat{\alpha} = \bar{y}$. In fact:

$$\hat{\alpha} = \arg\min_{\alpha\in\mathbb{R}} \sum_{i=1}^{n} \{y_i - \alpha - (\boldsymbol{x}_i - \bar{\boldsymbol{x}})^T\beta\}^2 = \frac{1}{n}\sum_{i=1}^{n} \{y_i - (\boldsymbol{x}_i - \bar{\boldsymbol{x}})^T\beta\} = \frac{1}{n}\sum_{i=1}^{n} y_i.$$

- Then, the **estimate of** β can be obtained considering a linear model **without intercept**:

$$f(\boldsymbol{x}_i; \beta) = (\boldsymbol{x}_i - \bar{\boldsymbol{x}})^T\beta,$$

employed to predict the **centered responses** $y_i - \bar{y}$.

Centering the predictors I

- In principal components regression, we replace **original data** $Y_i = f(\boldsymbol{x}_i) + \epsilon_i$ with their **centered** version:

$$x_{ij} - \bar{x}_j, \qquad y_i - \bar{y}, \qquad i = 1, \ldots, n; \;\; j = 1, \ldots, p.$$

- In the end, we will make predictions in the **original scale**, which requires a simple **final adjustment**. One need to compute the intercept term

$$\hat{\beta}_0 = \bar{y} - \bar{\boldsymbol{x}}\hat{\beta},$$

and then compute the predictions via the formula $\hat{\beta}_0 + \boldsymbol{x}_i^T\hat{\beta} = \hat{\alpha} + \boldsymbol{x}_i^T\hat{\beta}$.

- **Remark**. The centering operation is a mathematical trick that facilitate the exposition but is unconsequential from an estimation point of view.

Centering the predictors II

Centering assumption

In principal components regression, we assume the data have been previously **centered**:

$$\frac{1}{n}\sum_{i=1}^{n} y_i = 0, \qquad \frac{1}{n}\sum_{i=1}^{n} x_{ij} = 0, \qquad j = 1, \ldots, p.$$

- Using centered predictors means that we can focus on linear models **without intercept**:

$$f(\boldsymbol{x}_i; \beta) = x_{i1}\beta_1 + \cdots + x_{ip}\beta_p = \boldsymbol{x}_i^T \beta.$$

- Under the centering assumption, the **covariance matrix** of the data is simply

$$S = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X}.$$

Singular value decomposition (SVD)

- Let $\boldsymbol{X}$ be a $n \times p$ matrix. Then, its full form **singular value decomposition** is:

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T = \sum_{j=1}^{m} d_j \tilde{\boldsymbol{u}}_j \tilde{\boldsymbol{v}}_j^T,$$

  with $m = \min\{n, p\}$ and where:

  - the $n \times n$ matrix $\boldsymbol{U} = (\tilde{\boldsymbol{u}}_1, \ldots, \tilde{\boldsymbol{u}}_n)$ is **orthogonal**, namely: $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{U}\boldsymbol{U}^T = I_n$;
  - the $p \times p$ matrix $\boldsymbol{V} = (\tilde{\boldsymbol{v}}_1, \ldots, \tilde{\boldsymbol{v}}_p)$ is **orthogonal**, namely: $\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{V}\boldsymbol{V}^T = I_p$;
  - the $n \times p$ matrix $\boldsymbol{D}$ has **diagonal** entries $[\boldsymbol{D}]_{jj} = d_j$, for $j = 1, \ldots, m$, and zero entries elsewhere;

- The real numbers $d_1 \geq d_2 \geq \cdots \geq d_m \geq 0$ are called **singular values**.
- If one or more $d_j = 0$, then the matrix $\boldsymbol{X}$ is singular.

Principal component analysis I

- Le us assume that $p < n$ and that $\mathrm{rk}(\boldsymbol{X}) = p$, recalling that $\boldsymbol{X}$ is a **centered** matrix.
- Using SVD, the matrix $\boldsymbol{X}^T\boldsymbol{X}$ can be expressed as

$$\boldsymbol{X}^T\boldsymbol{X} = (\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T)^T\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{D}^T\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{\Delta}^2\boldsymbol{V}^T,$$

  where $\boldsymbol{\Delta}^2 = \boldsymbol{D}^T\boldsymbol{D}$ is a $p \times p$ **diagonal** matrix with entries $d_1^2, \ldots, d_p^2$.
- This equation is at the heart of **principal component analysis** (PCA). Define the matrix

$$\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{V} = \boldsymbol{U}\boldsymbol{D},$$

  whose columns $\tilde{\boldsymbol{z}}_1, \ldots, \tilde{\boldsymbol{z}}_p$ are called **principal components**.
- The matrix $\boldsymbol{Z}$ is orthogonal, because $\boldsymbol{Z}^T\boldsymbol{Z} = \boldsymbol{D}^T\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{D} = \boldsymbol{\Delta}^2$, which is diagonal.
- Moreover, by definition the entries of $\boldsymbol{Z}$ are linear combination of the original variables:

$$z_{ij} = x_{i1}v_{i1} + \cdots + x_{ip}v_{ip} = \boldsymbol{x}_i^T\tilde{\boldsymbol{v}}_j.$$

  The columns $\tilde{\boldsymbol{v}}_1, \ldots, \tilde{\boldsymbol{v}}_p$ of $\boldsymbol{V}$ are sometimes called **loadings**.

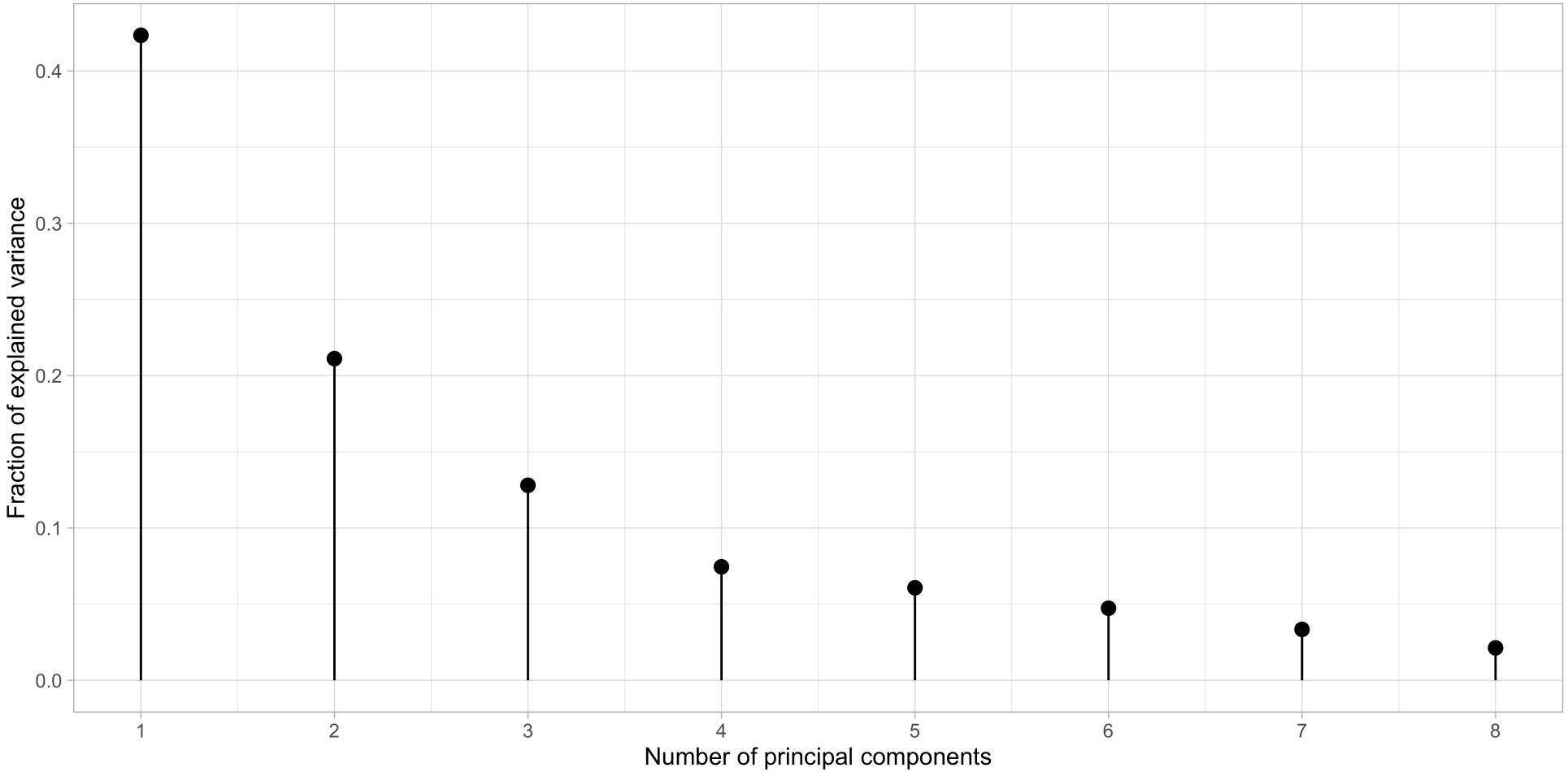
Principal component analysis II

- Principal components form an orthogonal basis of $\boldsymbol{X}$, but they are not a "random" choice, and they do **not** coincide with them **Gram-Schmidt** basis of Unit A.
- Indeed, the **first principal component** is the linear combination having **maximal variance**:

$$\tilde{\boldsymbol{v}}_1 = \arg\max_{\boldsymbol{v}\in\mathbb{R}^p} \mathrm{var}(\boldsymbol{X}\boldsymbol{v}) = \arg\max_{\boldsymbol{v}\in\mathbb{R}^p} \frac{1}{n}\boldsymbol{v}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{v}, \quad \text{subject to} \quad \boldsymbol{v}^T\boldsymbol{v} = 1.$$

- The **second principal component** maximizes the variance under the additional constraint of being **orthogonal** to the former. And so on.
- The values $d_1^2 \geq d_2^2 \geq \cdots \geq d_p^2 > 0$ are the **eigenvalues** of $\boldsymbol{X}^T\boldsymbol{X}$ and correspond to the rescaled **variances** of each principal component, that is $\mathrm{var}(\tilde{\boldsymbol{z}}_j) = \tilde{\boldsymbol{z}}_j^T\tilde{\boldsymbol{z}}_j/n = d_j^2/n$.
- Hence, the quantity $d_j^2 / \sum_{j'=1}^{p} d_{j'}^2$ measures the amount of total variance captured by principal components.

Principal component analysis: prostate data



Home page

Principal components regression (PCR)

- We use the first $k \leq p$ **principal components** to predict the responses y_i via

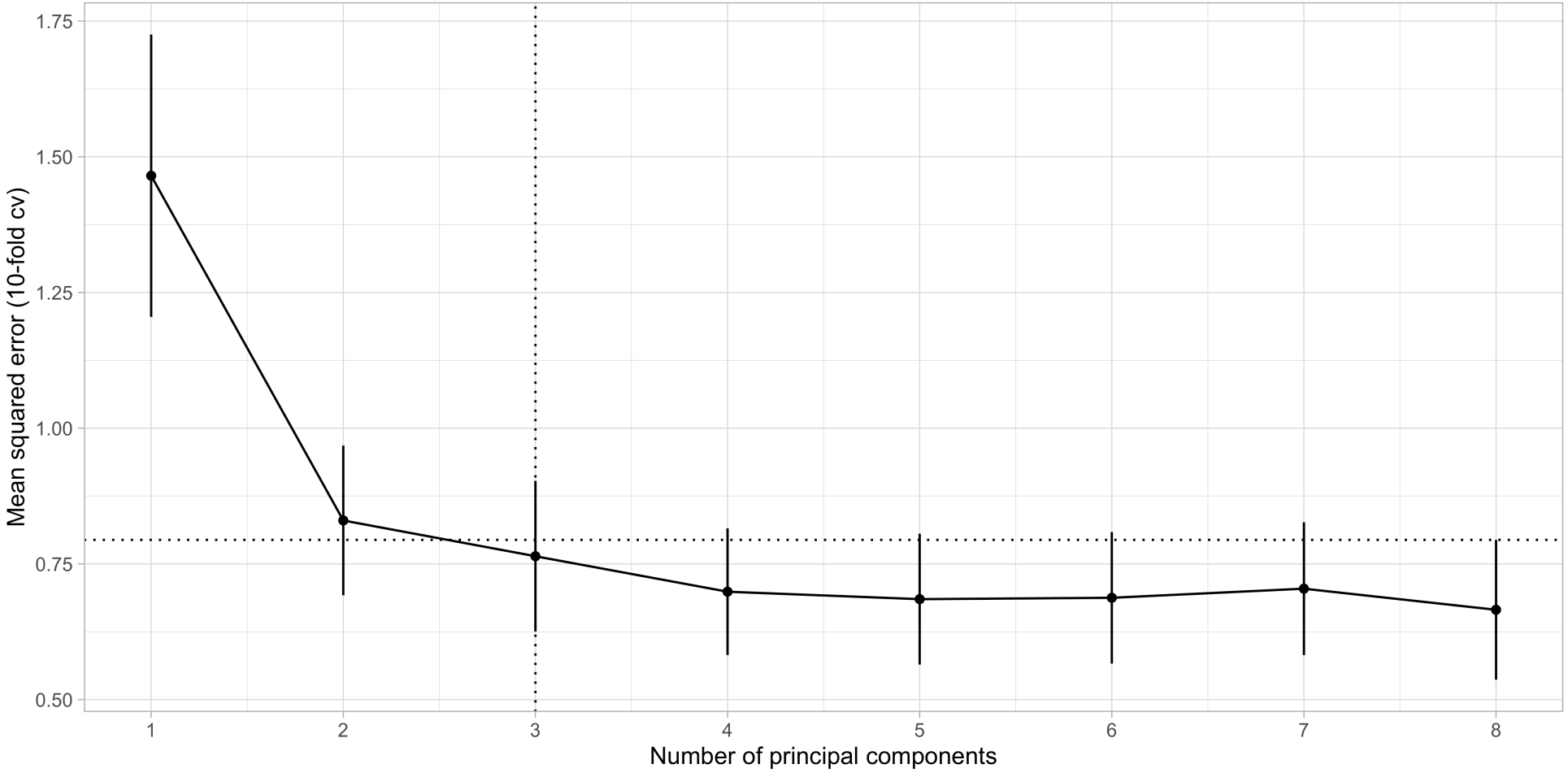
$$f(\boldsymbol{z}_i; \gamma) = \gamma_1 z_{i1} + \cdots + \gamma_k z_{ik}, \qquad i = 1, \ldots, n,$$

- Because of orthogonality, the least squares solution is straightforward to compute:

$$\hat{\gamma}_j = \frac{\tilde{\boldsymbol{z}}_j^T \boldsymbol{y}}{\tilde{\boldsymbol{z}}_j^T \tilde{\boldsymbol{z}}_j} = \frac{1}{d_j^2} \tilde{\boldsymbol{z}}_j^T \boldsymbol{y}, \qquad j = 1, \ldots, k.$$

- The principal components are in **order of importance** and effectively **compressing the information** contained in $\boldsymbol{X}$ using only $k \leq p$ variables.
- When $k = p$, we are simply rotating the original matrix $\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{V}$, i.e. performing **no compression**. The predicted values coincide with OLS.
- The number k is a **complexity parameter** which should be chosen via information criteria or cross-validation.

Selection of k: cross-validation



Shrinkage effect of principal components I

- A closer look at the PCR solution reveals some interesting aspects. Recall that:

$$\tilde{\boldsymbol{z}}_j = \boldsymbol{X}\tilde{\boldsymbol{v}}_j = d_j\tilde{\boldsymbol{u}}_j, \qquad j = 1, \ldots, p.$$

- The **predicted values** for the **centered responses** $\boldsymbol{y}$ of the PCR with k components are:

$$\sum_{j=1}^{k} \tilde{\boldsymbol{z}}_j\hat{\gamma}_j = \boldsymbol{X}\sum_{j=1}^{k} \tilde{\boldsymbol{v}}_j\hat{\gamma}_j = \boldsymbol{X}\hat{\beta}_{\text{pcr}}, \qquad \text{where} \qquad \hat{\beta}_{\text{pcr}} = \sum_{j=1}^{k} \tilde{\boldsymbol{v}}_j\hat{\gamma}_j.$$

- This representation highlights two important aspects:
  - It is possible to express the PCR solution in the original scale, for better **interpretability**;
  - The vector $\hat{\beta}_{\text{pcr}}$ is a **constrained solution**, being a combination of $k \leq p$ coefficients, therefore **reducing** the **complexity** of the model and **shrinking** the coefficients.
- When $k = 1$, then the $\hat{\beta}_{\text{pcr}}$ estimate coincide with the scaled loading vector $\hat{\beta}_{\text{pcr}} = \hat{\gamma}_1\tilde{\boldsymbol{v}}_1$;
- When $k = p$ then the $\hat{\beta}_{\text{pcr}}$ coincides with **ordinary least squares** (see Exercises).

Shrinkage effect of principal components II

- The **variance** of $\hat{\beta}_{\text{pcr}}$, assuming iid errors ϵ_i in the **original data**, is:

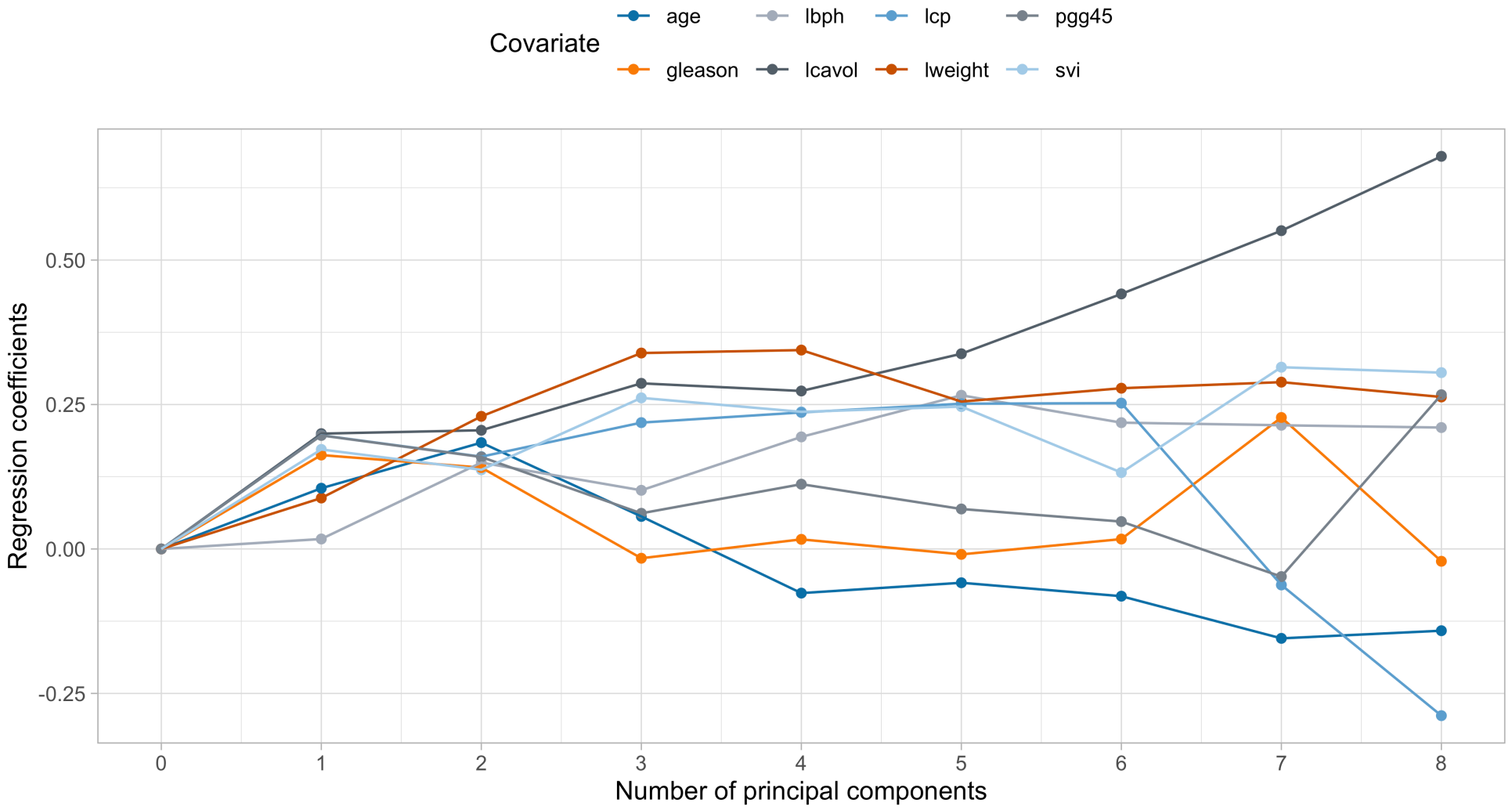
$$\text{var}(\hat{\beta}_{\text{pcr}}) = \sigma^2 \sum_{j=1}^{k} \frac{1}{d_j^2} \tilde{\boldsymbol{v}}_j \tilde{\boldsymbol{v}}_j^T.$$

- In case of **multicollinearity**, then the **last** principal components will have a small variance, i.e., a small d_j^2. Its removal, therefore, drastically **reduces** the **variance** of $\hat{\beta}_{\text{pcr}}$.
- Furthermore, the predicted values for the **centered data** can be expressed as

$$\boldsymbol{X}\hat{\beta}_{\text{pcr}} = \sum_{j=1}^{k} \tilde{\boldsymbol{z}}_j \hat{\gamma}_j = \sum_{j=1}^{k} \tilde{\boldsymbol{z}}_j \frac{\tilde{\boldsymbol{z}}_j^T \boldsymbol{y}}{\tilde{\boldsymbol{z}}_j^T \tilde{\boldsymbol{z}}_j} = \sum_{j=1}^{k} d_j \tilde{\boldsymbol{u}}_j \frac{d_j}{d_j^2} \frac{\tilde{\boldsymbol{u}}_j^T \boldsymbol{y}}{\tilde{\boldsymbol{u}}_j^T \tilde{\boldsymbol{u}}_j} = \sum_{j=1}^{k} \tilde{\boldsymbol{u}}_j \tilde{\boldsymbol{u}}_j^T \boldsymbol{y}.$$

- The columns of $\boldsymbol{U}$, namely the vectors $\tilde{\boldsymbol{u}}_j$ are the **normalized principal components**.
- Hence, we are shrinking the predictions towards the main **principal directions**.

Shrinkage effect of principal components III



Home page

Pros and cons of PCR

Pros

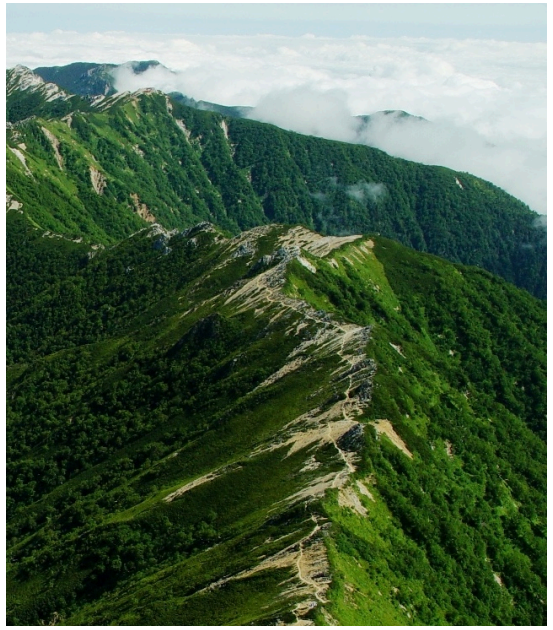
- Principal components are a natural tool to **reduce the complexity** of the data, especially in the presence of **highly correlated** variables.
- If you transform back the coefficients, there is a **clean interpretation** of the impact of the covariates on the response.
- Principal components might be interesting in their own right, as they describe the **dependence structure** among covariates.

Cons

- **All the variables** are used for predictions, which could be computationally demanding.
- The shrinkage effect on the regression coefficients is somewhat indirect and not smooth.

Ridge regression

Shrinkage methods



- Shrinkage methods are popular tools for handling the issue of multiple variables.
- Shrinkage **regularizes** the estimates, **constraining** the **size** of the regression coefficients.
- This leads to **biased estimator** with, hopefully, lower variance.
- As a byproduct, the induced regularization procedure enables estimation even when $p > n$.
- The first method that has been proposed is called **ridge regression**. The lasso and the elastic-net are other examples.

The ridge regularization method

- The ridge estimator is the most common **shrinkage method** and is the **minimizer** of

$$\sum_{i=1}^{n}(y_i - \beta_0 - \boldsymbol{x}_i^T\beta)^2 \qquad \text{subject to} \qquad \sum_{j=1}^{p}\beta_j^2 \leq s.$$

- When the **complexity parameter** s is small, the coefficients are explicitly **shrinked**, i.e. biased, **towards zero**.
- On the other hand, if s is large enough, then the ridge estimator coincides with ordinary least squares.
- In ridge regression, the **variability** of the estimator is explicitly **bounded**, although this comes with some **bias**. The parameter s controls the bias-variance trade-off.
- The intercept term β_0 is **not penalized** because there are no strong reasons to believe that the mean of y_i equals zero. However, as before, we want to "remove the intercept".

Centering and scaling the predictors I

- The ridge solutions are **not equivariant** under **scalings of the input**, so one normally **standardizes** the input to have unit variance if they are not on the same scale.
- Moreover, as for PCR, we can estimate the intercept using a **two-step procedure**:
  - The reparametrization $\alpha = \beta_0 + \bar{\boldsymbol{x}}^T \beta$ is equivalent to centering the predictors;
  - The estimate for the centered intercept is $\hat{\alpha} = \bar{y}$;
  - The ridge estimate can be obtained by considering a model without intercept, using centered responses and predictors.
- Hence, in ridge regression, we replace **original data** $Y_i = f(\boldsymbol{x}_i) + \epsilon_i$ with their **standardized** version:

$$\frac{x_{ij} - \bar{x}_j}{s_j}, \qquad y_i - \bar{y}, \qquad i = 1, \dots, n; \;\; j = 1, \dots, p.$$

where $s_j^2 = n^{-1} \sum_{i=1}^{n} (x_{ij} - \bar{x}_j)^2$ is the **sample variance**.

Centering and scaling the predictors II

- It is easy to show (see Exercises) that the **coefficients** expressed in the **original scale** are

$$\hat{\beta}_0 = \bar{y} - \bar{\boldsymbol{x}}\hat{\beta}_{\text{scaled-ridge}}, \qquad \hat{\beta}_{\text{scaled-ridge}} = \text{diag}(1/s_1, \ldots, 1/s_p)\hat{\beta}_{\text{ridge}}.$$

  Thus, the **predictions** on the **original scale** are $\hat{\beta}_0 + \boldsymbol{x}_i^T \hat{\beta}_{\text{scaled-ridge}} = \bar{y} + \boldsymbol{x}_i^T \hat{\beta}_{\text{ridge}}$.

For ridge problems, we will assume the data have been previously **standardized**, namely

$$\frac{1}{n}\sum_{i=1}^{n} y_i = 0, \qquad \frac{1}{n}\sum_{i=1}^{n} x_{ij} = 0, \qquad \frac{1}{n}\sum_{i=1}^{n} x_i^2 = 1 \qquad j = 1, \ldots, p.$$

- We will say that the **ridge estimator** $\hat{\beta}_{\text{ridge}}$ is the **minimizer** of following system

$$\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\beta)^2 \qquad \text{subject to} \qquad \sum_{j=1}^{p}\beta_j^2 \leq s.$$

Lagrange multipliers and ridge solution

- The ridge regression problem can be **equivalently expressed** in its Lagrangian form, which greatly facilitates computations. The ridge estimator $\hat{\beta}_{\text{ridge}}$ is the **minimizer** of

$$\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\beta)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 = \underbrace{||\boldsymbol{y} - \boldsymbol{X}\beta||^2}_{\text{least squares}} + \underbrace{\lambda||\beta||^2}_{\text{ridge penalty}},$$

  where $\lambda > 0$ is a **complexity parameter** controlling the **penalty**. It holds that $s = ||\hat{\beta}_{\text{ridge}}||^2$.

- When $\lambda = 0$ then $\hat{\beta}_{\text{ridge}} = \hat{\beta}_{\text{ols}}$ whereas when $\lambda \to \infty$ we get $\hat{\beta}_{\text{ridge}} = 0$.

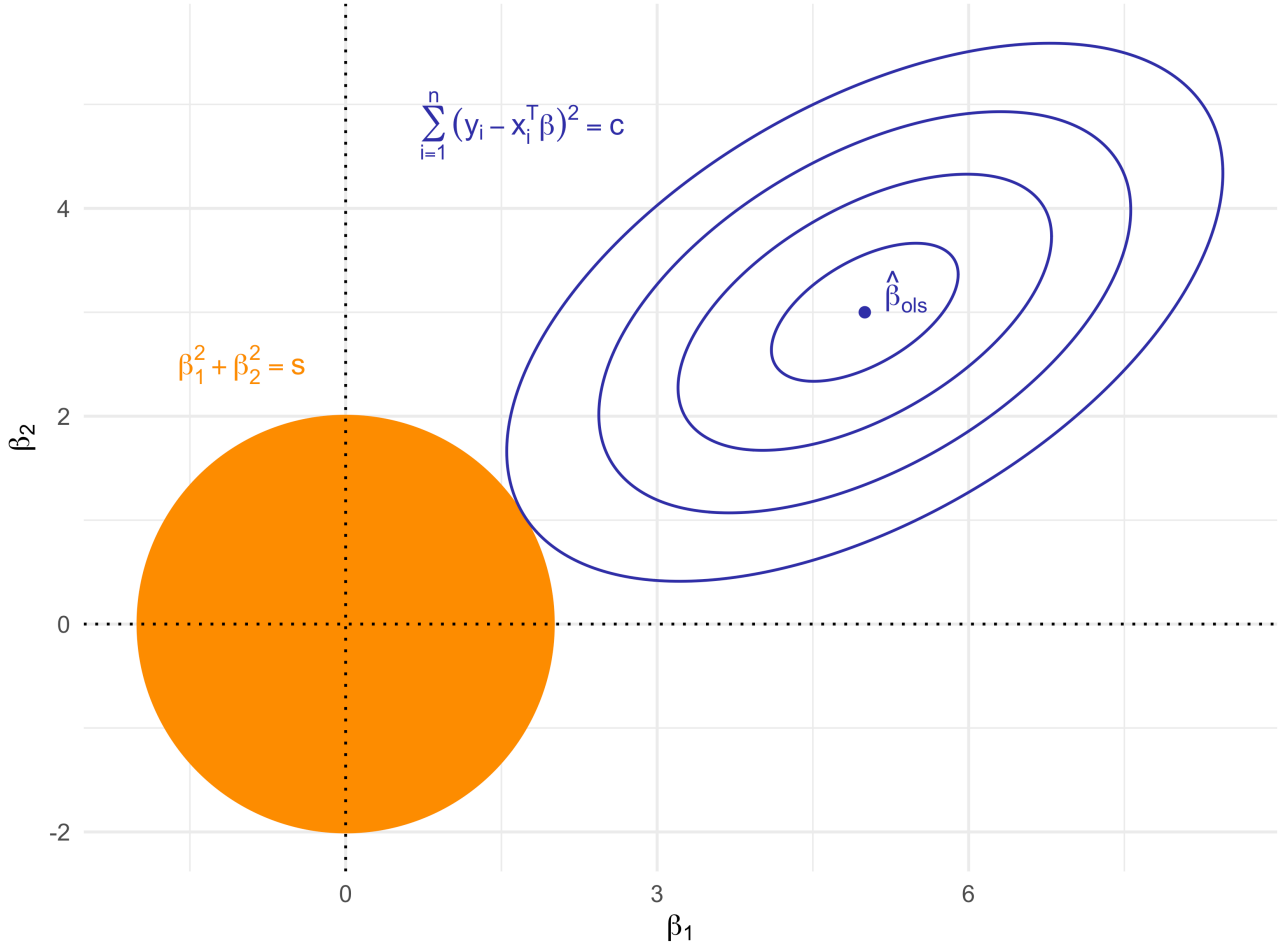
Ridge regression estimator

For any $n \times p$ design matrix $\boldsymbol{X}$, not necessarily of full-rank, the ridge estimator is

$$\hat{\beta}_{\text{ridge}} = (\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

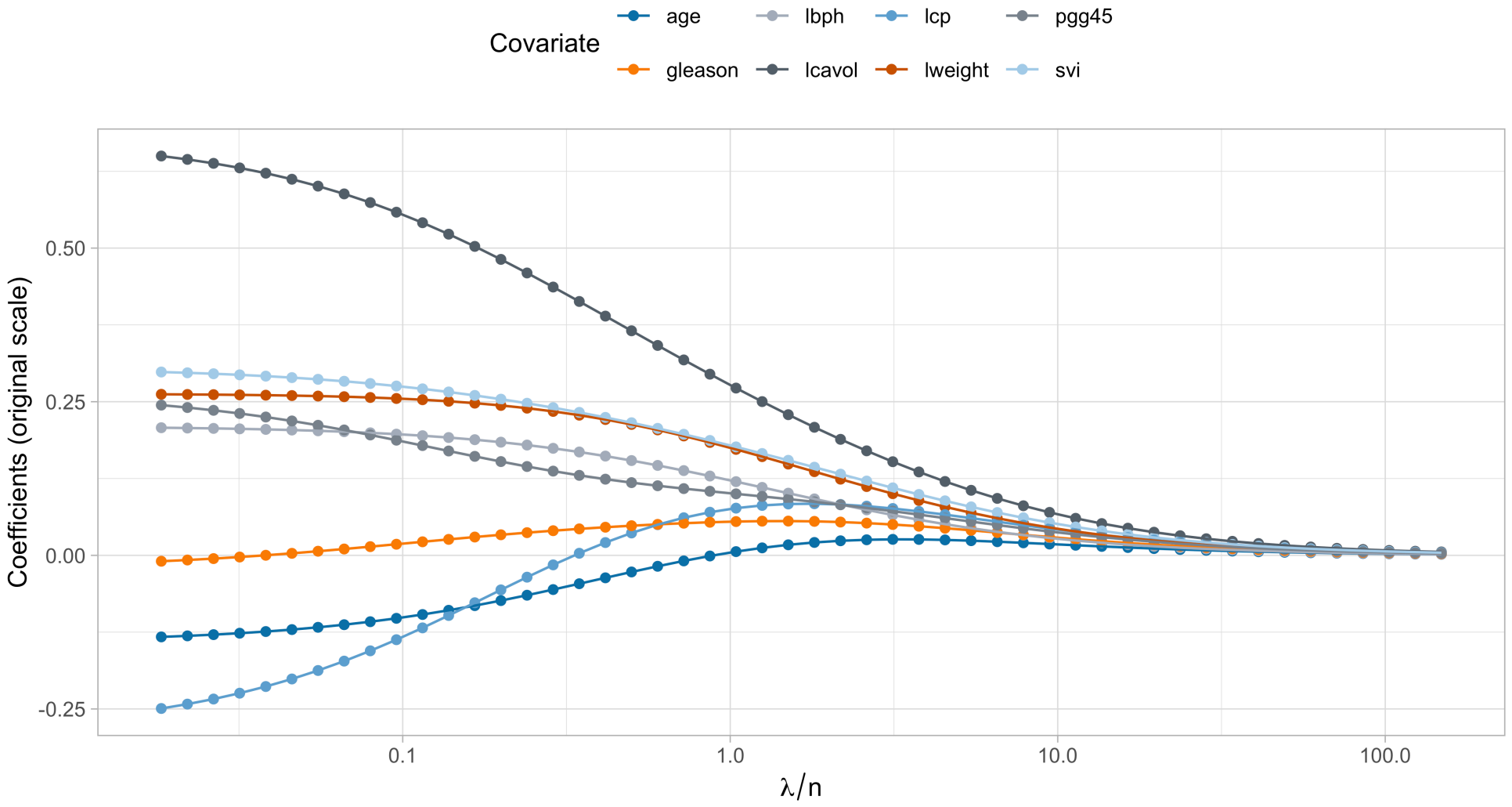
Such an estimator **always exists** and is **unique** (even when $p > n$).

The geometry of the ridge solution



Home page

The ridge path



Home page

Comments on the ridge path

- The values of λ are in somewhat **arbitrary scale**. The ridge penalty has a concrete effect starting from $\lambda/n > 0.1$ or so.
- The variable `lcavol` is arguably the most important, followed by `lweight` and `svi`, which are those receiving less shrinkage compared to the others.
- The coefficient of `age`, `gleason`, and `lcp`, is negative at the beginning and then becomes positive for large values of λ.
- This indicate that their negative value in $\hat{\beta}_{\text{ols}}$ was probably a consequence of their **correlation** with other variables.
- There is an interesting similarity between this plot and the one of principal component regression... is it a coincidence?

Shrinkage effect of ridge regression I

- Considering, once again, the **singular value decomposition**, we get:

$$\begin{aligned}
\boldsymbol{X}\hat{\beta}_{\text{ridge}} &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)^{-1}\boldsymbol{X}^T\boldsymbol{y} \\
&= \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T[\boldsymbol{V}(\boldsymbol{D}^T\boldsymbol{D} + \lambda I_p)\boldsymbol{V}^T]^{-1}(\boldsymbol{U}\boldsymbol{D}\boldsymbol{V})^T\boldsymbol{y} \\
&= \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T\boldsymbol{V}(\boldsymbol{D}^T\boldsymbol{D} + \lambda I_p)^{-1}\boldsymbol{V}^T\boldsymbol{V}\boldsymbol{D}^T\boldsymbol{U}^T\boldsymbol{y} \\
&= \boldsymbol{U}\boldsymbol{D}(\boldsymbol{D}^T\boldsymbol{D} + \lambda I_p)^{-1}\boldsymbol{D}^T\boldsymbol{U}^T\boldsymbol{y} \\
&= \boldsymbol{H}_{\text{ridge}}\boldsymbol{y} = \sum_{j=1}^{p} \tilde{\boldsymbol{u}}_j \frac{d_j^2}{d_j^2 + \lambda}\tilde{\boldsymbol{u}}_j^T\boldsymbol{y},
\end{aligned}$$

  where $\boldsymbol{H}_{\text{ridge}} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)^{-1}\boldsymbol{X}^T$ is the so-called **hat matrix** of ridge regression.

- This means that ridge regression **shrinks** the **principal directions** by an amount that depends on the **eigenvalues** d_j^2.
- In other words, it **smoothly reduces** the impact of the **redundant** information.

Shrinkage effect of ridge regression II

- A sharp **connection** with **principal components regression** is therefore revealed.
- Compare the previous formula for $\boldsymbol{X}\hat{\beta}_{\text{ridge}}$ with the one we previously obtained for $\boldsymbol{X}\hat{\beta}_{\text{pcr}}$.
- More explicitly, for **ridge regression** we will have that

$$\hat{\beta}_{\text{ridge}} = \boldsymbol{V}\text{diag}\left(\frac{d_1}{d_1^2+\lambda}, \ldots, \frac{d_p}{d_p^2+\lambda}\right)\boldsymbol{U}^T\boldsymbol{y}.$$

  whereas for **principal components regression** with k components we get

$$\hat{\beta}_{\text{pcr}} = \boldsymbol{V}\text{diag}\left(\frac{1}{d_1}, \ldots, \frac{1}{d_k}, 0, \ldots, 0\right)\boldsymbol{U}^T\boldsymbol{y}.$$

- Both operate on the singular values, but where principal component regression **thresholds** the singular values, **ridge regression** shrinks them.

Bias-variance trade-off

- The ridge regression **add some bias** to the estimates, but it **reduces** their **variance**.
- The **variance** of $\hat{\beta}_{\text{ridge}}$, assuming iid errors ϵ_i in the **original scale** with variance σ^2, results:

$$\text{var}(\hat{\beta}_{\text{ridge}}) = \sigma^2 \sum_{j=1}^{p} \frac{d_j^2}{(d_j^2 + \lambda)^2} \tilde{\boldsymbol{v}}_j \tilde{\boldsymbol{v}}_j^T,$$

  whose diagonal elements are always smaller than those of $\text{var}(\hat{\beta}_{\text{ols}})$.

- The above formula highlights that ridge will be very **effective** in presence highly **correlated variables**, as they will be "shrunk" away by the penalty.
- What typically happens is that such a reduction in variance **compensate** the increase in bias, especially when p is large relative to n.

A historical perspective I

- The ridge regression estimator was originally proposed by Hoerl and Kennard (1970) with a quite different motivation in mind.
- In linear models, the estimate of β is obtained by solving the **normal equations**

$$(\boldsymbol{X}^T\boldsymbol{X})\beta = \boldsymbol{X}^T\boldsymbol{y},$$

  which could be **ill-conditioned**.
- In other words, the **condition number**

$$\kappa(\boldsymbol{X}^T\boldsymbol{X}) = \frac{d_1^2}{d_p^2},$$

  might be very large, leading to **numerical inaccuracies**, since the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is **numerically singular** and therefore not invertible in practice.

A historical perspective II

- Ridge provides a **remedy** for **ill-conditioning**, by adding a "ridge" to the diagonal of $\boldsymbol{X}^T\boldsymbol{X}$, obtaining the modified normal equations

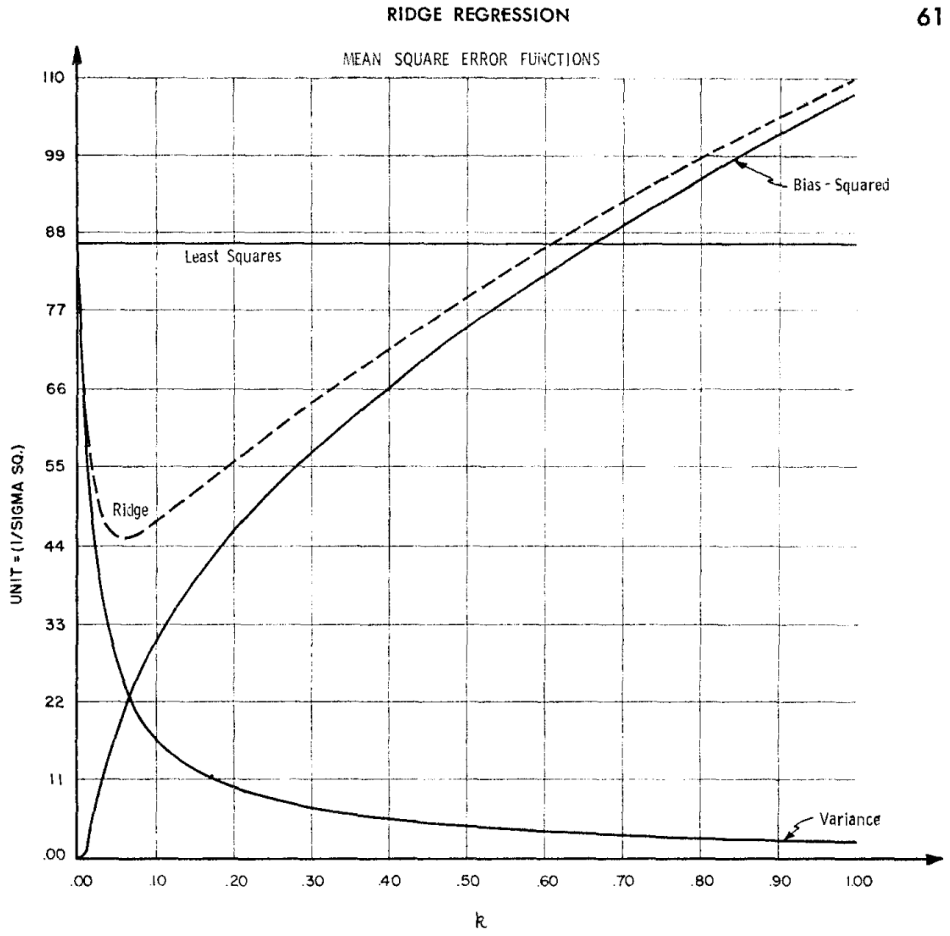
$$(\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)\beta = \boldsymbol{X}^T\boldsymbol{y}.$$

- The **condition number** of the modified $(\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)$ matrix becomes

$$\kappa(\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p) = \frac{\lambda + d_1^2}{\lambda + d_p^2}.$$

- Notice that even if $d_p = 0$, i.e. the matrix $\boldsymbol{X}$ is **singular**, then the condition number will be finite as long as $\lambda > 0$.
- This technique is known as **Tikhonov regularization**, after the Russian mathematician Andrey Tikhonov.

A historical perspective III



- Figure 1 of the **original paper** by Hoerl and Kennard (1970), displaying the bias-variance **trade-off**.

Home page

On the choice of λ

- The **penalty parameter** λ determines the amount of bias and variance of $\hat{\beta}_{\text{ridge}}$ and therefore it must be carefully **estimated**.
- **Minimizing** the loss $||\boldsymbol{y} - \boldsymbol{X}\hat{\beta}_{\text{ridge}}||^2$ over λ is a **bad idea**, because it would always lead to $\lambda = 0$, corresponding to $\hat{\beta}_{\text{ridge}} = \hat{\beta}_{\text{ols}}$.
- Indeed, λ is a **complexity** parameter and, like the number of covariates, should be selected using **information criteria** or training/test and **cross-validation**.
- Suppose we wish to use an **information criteria** such as the AIC or BIC, of the form

$$\text{IC}(p) = -2\ell(\hat{\beta}_{\text{ridge}}) + \text{penalty}(\text{“degrees of freedom”}).$$

  We need a careful definition of **degrees of freedom** that is appropriate in this context.
- The current definition of degrees of freedom, i.e., the number of **non-zero coefficients**, is **not appropriate** for ridge regression because it would be equal to p for any value of λ.

Effective degrees of freedom I

- Let us recall that the original data are $Y_i = f(\boldsymbol{x}_i) + \epsilon_i$ and that the **optimism** for a generic estimator $\hat{f}(\boldsymbol{x})$ is defined as the following average of covariances

$$\text{Opt} = \frac{2}{n} \sum_{i=1}^{n} \text{cov}(Y_i, \hat{f}(\boldsymbol{x}_i)),$$

  which is equal to $\text{Opt}_{\text{ols}} = (2\sigma^2 p)/n$ in **ordinary least squares**.

Effective degrees of freedom

Let $\hat{f}(\boldsymbol{x})$ be an estimate for the regression function $f(\boldsymbol{x})$ based on the data $Y_1, \ldots, Y_n$. The **effective degrees of freedom** are defined as

$$\text{df} = \frac{1}{\sigma^2} \sum_{i=1}^{n} \text{cov}(Y_i, \hat{f}(\boldsymbol{x}_i)).$$

Effective degrees of freedom II

- The effective degrees of freedom of **ordinary least squares** and **principal component regression** are

$$\mathrm{df}_{\mathrm{ols}} = p + 1, \qquad \mathrm{df}_{\mathrm{pcr}} = k + 1,$$

  where the additional term corresponds to the **intercept**.

- After some algebra, one finds that the effective degrees of freedom of **ridge regression** are

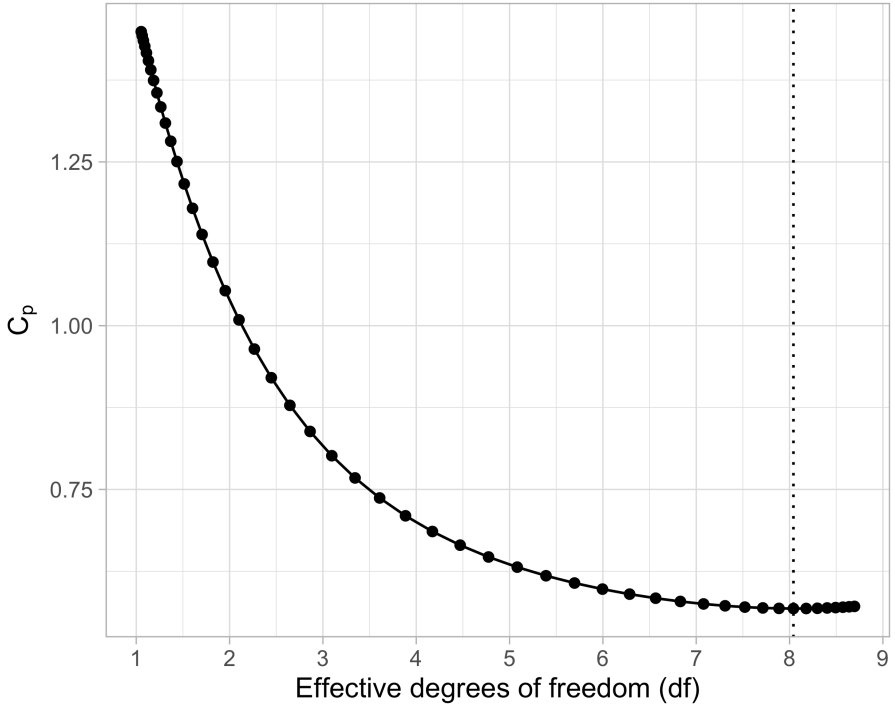
$$\mathrm{df}_{\mathrm{ridge}} = 1 + \mathrm{tr}(\boldsymbol{H}_{\mathrm{ridge}}) = 1 + \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda}.$$

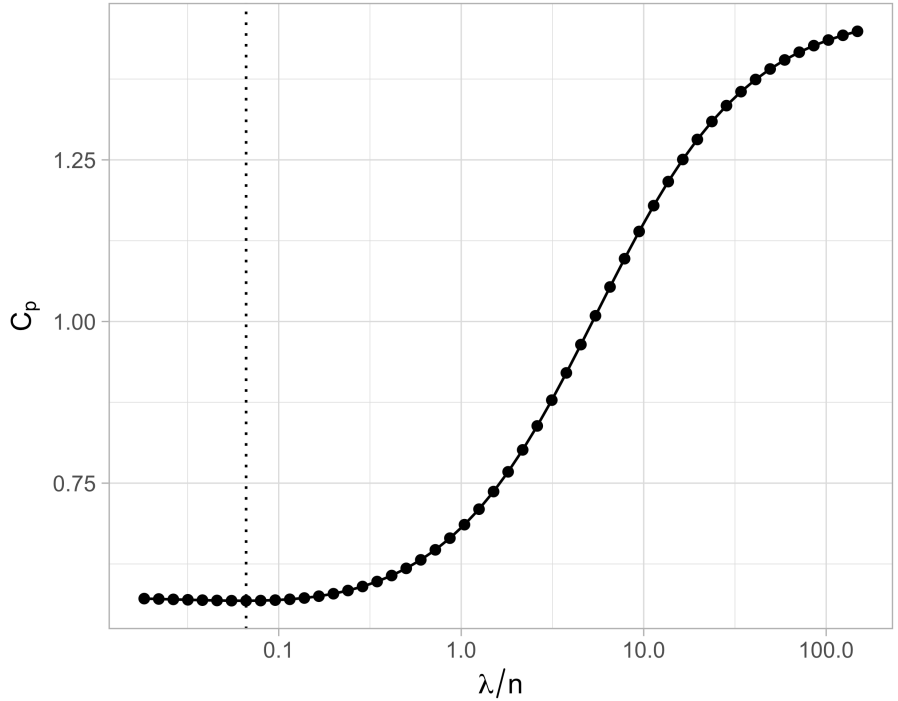
- Using the above result, we can **plug-in** $\mathrm{df}_{\mathrm{ridge}}$ into the formula of the C_p **of Mallows**:

$$\widehat{\mathrm{ErrF}} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \boldsymbol{x}_i^T \hat{\beta}_{\text{scaled-ridge}})^2 + \frac{2\hat{\sigma}^2}{n} \mathrm{df}_{\mathrm{ridge}}.$$

  where the residual variance is estimated as $\hat{\sigma}^2 = (n - \mathrm{df}_{\mathrm{ridge}})^{-1} \sum_{i=1}^{n} (y_i - \boldsymbol{x}_i^T \hat{\beta}_{\text{scaled-ridge}})^2$.

Effective degrees of freedom III





Cross-validation for ridge regression I

- Training/test strategies and **cross-validation** are also valid tools for selecting λ.
- Most statistical software packages use a slightly **different parametrization** for λ, as they minimize

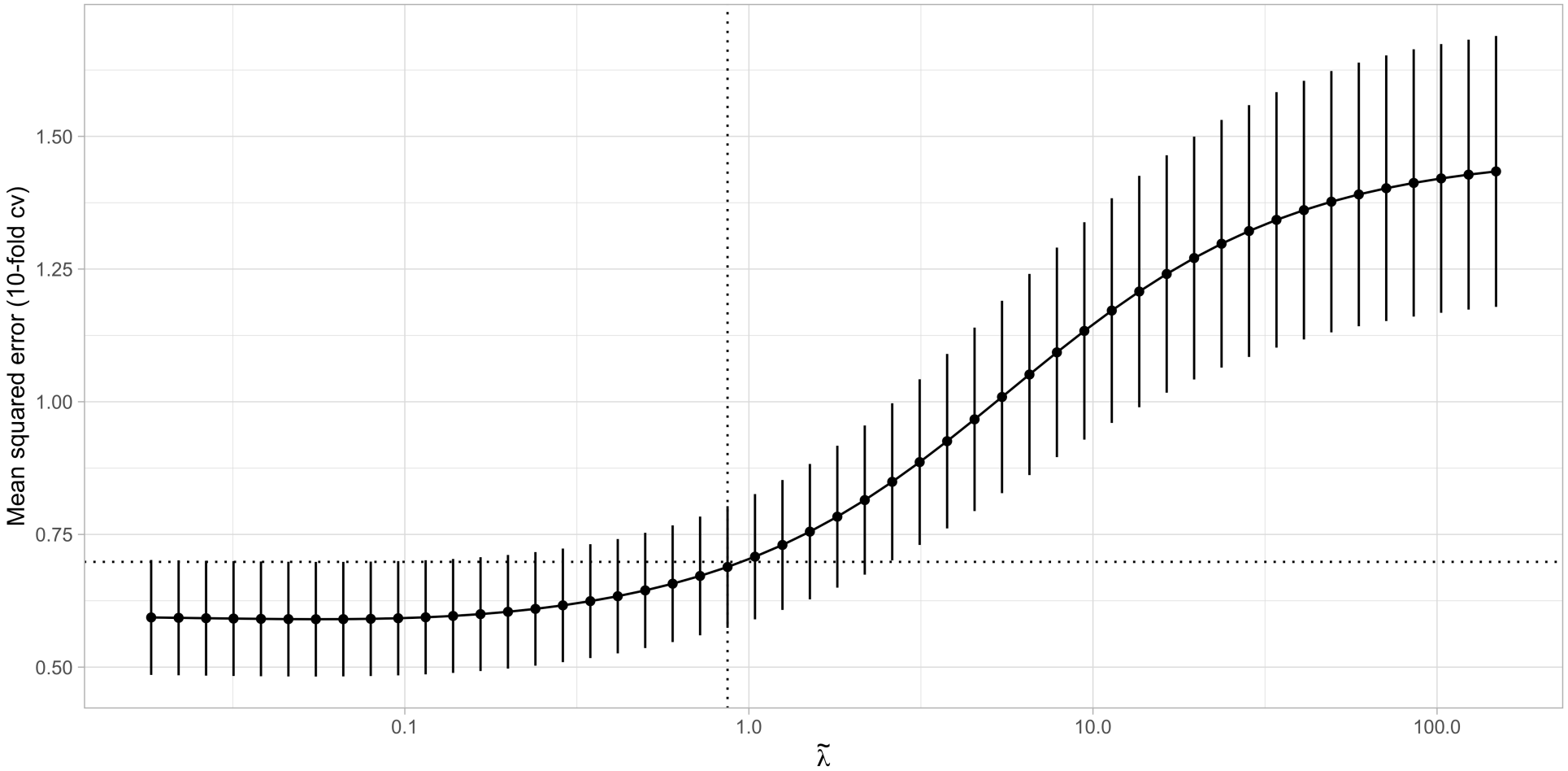
$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\beta)^2 + \tilde{\lambda}\sum_{j=1}^{p}\beta_j^2,$$

  where the penalty parameter $\tilde{\lambda} = \lambda/n$.

- This parametrization does not alter the estimate of $\hat{\beta}_{\text{ridge}}$ but is more amenable for **cross-validation** as the values of $\tilde{\lambda}$ can be compared across datasets with **different sample sizes**.

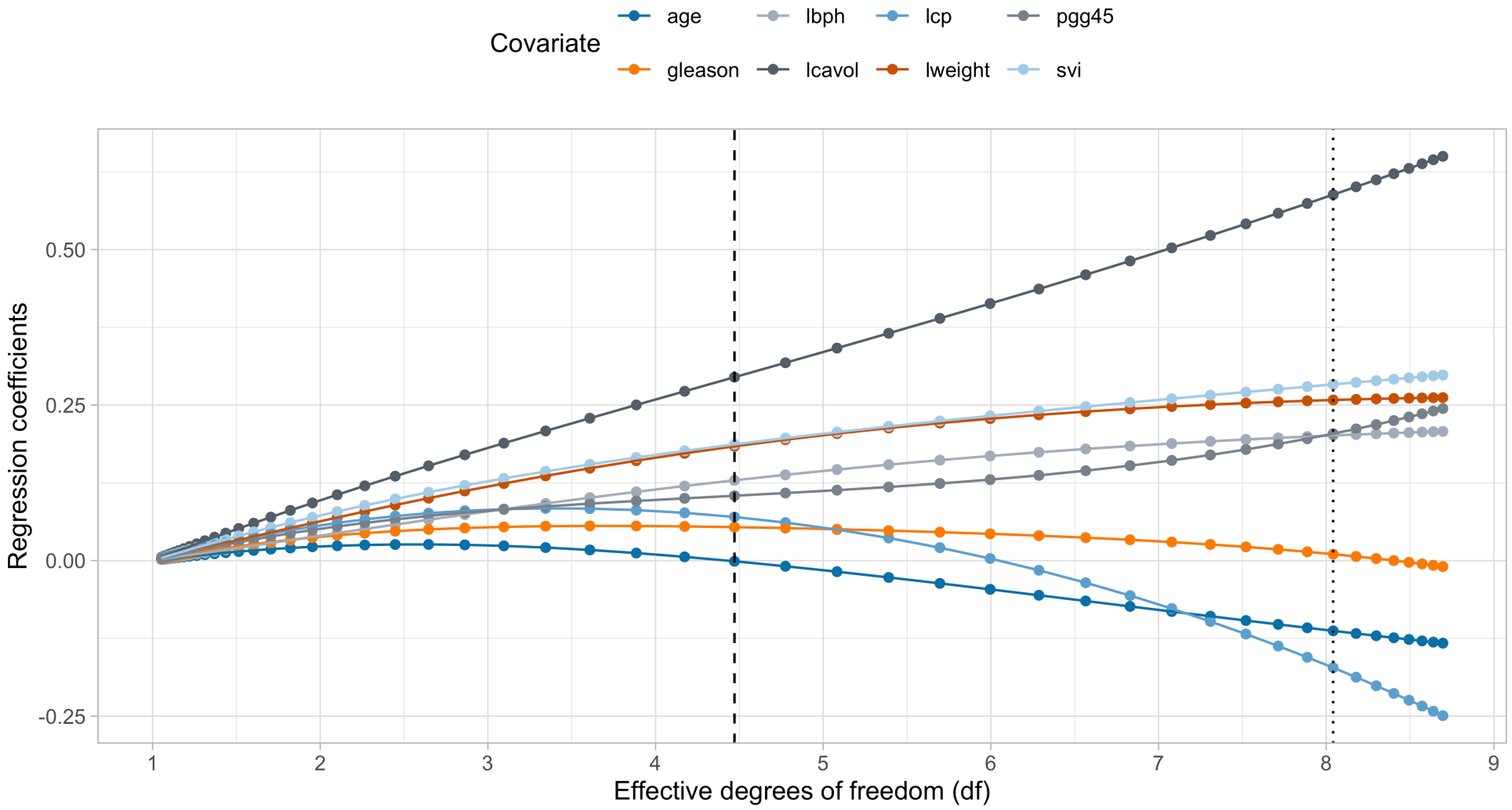
- Different R packages have **different defaults** about other aspects too.
- For instance, the R package `glmnet` uses $\tilde{\lambda}$ and also **standardizes the response $\boldsymbol{y}$** and then **transforms back** the estimated coefficients into the **original scale**.

Cross-validation for ridge regression II



Home page

The ridge estimate



Home page

Further properties of ridge regression

- Ridge regression has a transparent **Bayesian interpretation**, since the penalty can be interpreted as a Gaussian prior on β.
- If two variables are identical copies $\tilde{\boldsymbol{x}}_j = \tilde{\boldsymbol{x}}_\ell$, so are the corresponding ridge coefficients $\hat{\beta}_{j,\text{ridge}} = \hat{\beta}_{\ell,\text{ridge}}$.
- Adding p **fake observations** all equal to 0 to the response and then fitting ordinary least squares leads to the ridge estimator. This procedure is called **data augmentation**.
- A computationally convenient formula for **LOO cross-validation** is available, which requires the model to be estimated only once, as in least squares.
- In the $p > n$ **case** there are specific **computational strategies** that can be employed; see Section 18.3.5 of Hastie, Tibshirani and Friedman (2011).

Pros and cons of ridge regression

Pros

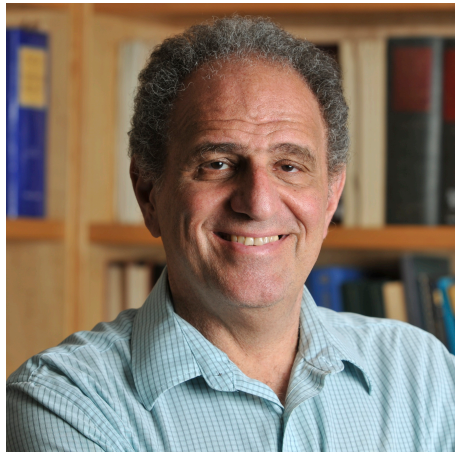
- Ridge regression trades some **bias** in exchange of a **lower variance**, often resulting in more accurate predictions.
- The ridge solution **always exists** and is **unique**, even when $p > n$ or in presence of perfect **collinearity**.
- For fixed values of λ, **efficient computations** are available using QR and Cholesky decompositions.

Cons

- In ridge regression, **all variables** are used. This is in contrast with best subset selection.

The lasso

Looking for sparsity



Robert Tibshirani

- Signal **sparsity** is the assumption that only a small number of predictors have an effect, i.e.,

$$\beta_j = 0, \qquad \text{for most} \qquad j \in \{1, \dots, p\}.$$

- In this case we would like our estimator $\hat{\beta}$ to be **sparse**, meaning that $\hat{\beta}_j = 0$ for many $j \in \{1, \dots, p\}$.
- Sparse estimators are desirable because:
  - perform **variable selection** and improve the **interpretability** of the results;
  - Speed up the **computations** of the predictions because fewer variables are needed.
- Best subset selection is sparse (but computationally unfeasible), the ridge estimator is not.

The least absolute selection and shrinkage operator

- The **lasso** appeared in the highly influential paper of Tibshirani (1996). It is a method that performs both **shrinkage** and **variable selection**
- The lasso estimator is the **minimizer** of the following system

$$\sum_{i=1}^{n}(y_i - \beta_0 - \boldsymbol{x}_i^T\beta)^2 \qquad \text{subject to} \qquad \sum_{j=1}^{p}|\beta_j| \leq s.$$

  therefore when the **complexity parameter** s is small, the coefficients of $\hat{\beta}_{\text{lasso}}$ are **shrinked** and when s is large enough $\hat{\beta}_{\text{lasso}} = \hat{\beta}_{\text{ols}}$, as in ridge regression.

- The lasso is **deceptively similar** to ridge. However, the change from a quadratic penalty to an absolute value has a crucial **sparsity** implication.
- The intercept term β_0 is **not penalized**, as for ridge, because we can remove it by centering the predictors.

Centering and scaling the predictors

- Thus, as for ridge regression, we will center and scale predictors and response.
- It is easy to show that the **coefficients** expressed in the **original scale** are

$$\hat{\beta}_0 = \bar{y} - \bar{\boldsymbol{x}}\hat{\beta}_{\text{lasso}}, \qquad \hat{\beta}_{\text{scaled-lasso}} = \text{diag}(1/s_1, \ldots, 1/s_p)\hat{\beta}_{\text{lasso}}.$$

  Thus, the **predictions** on the **original scale** are $\hat{\beta}_0 + \boldsymbol{x}_i^T \hat{\beta}_{\text{scaled-lasso}} = \bar{y} + \boldsymbol{x}_i^T \hat{\beta}_{\text{lasso}}$.

For lasso problems, we will assume the data have been previously **standardized**, namely

$$\frac{1}{n}\sum_{i=1}^{n} y_i = 0, \qquad \frac{1}{n}\sum_{i=1}^{n} x_{ij} = 0, \qquad \frac{1}{n}\sum_{i=1}^{n} x_i^2 = 1 \qquad j = 1, \ldots, p.$$

- We will say that the **lasso estimator** $\hat{\beta}_{\text{lasso}}$ is the **minimizer** of following system

$$\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\beta)^2 \qquad \text{subject to} \qquad \sum_{j=1}^{p}|\beta_j| \leq s.$$

Lagrange multipliers and lasso solution

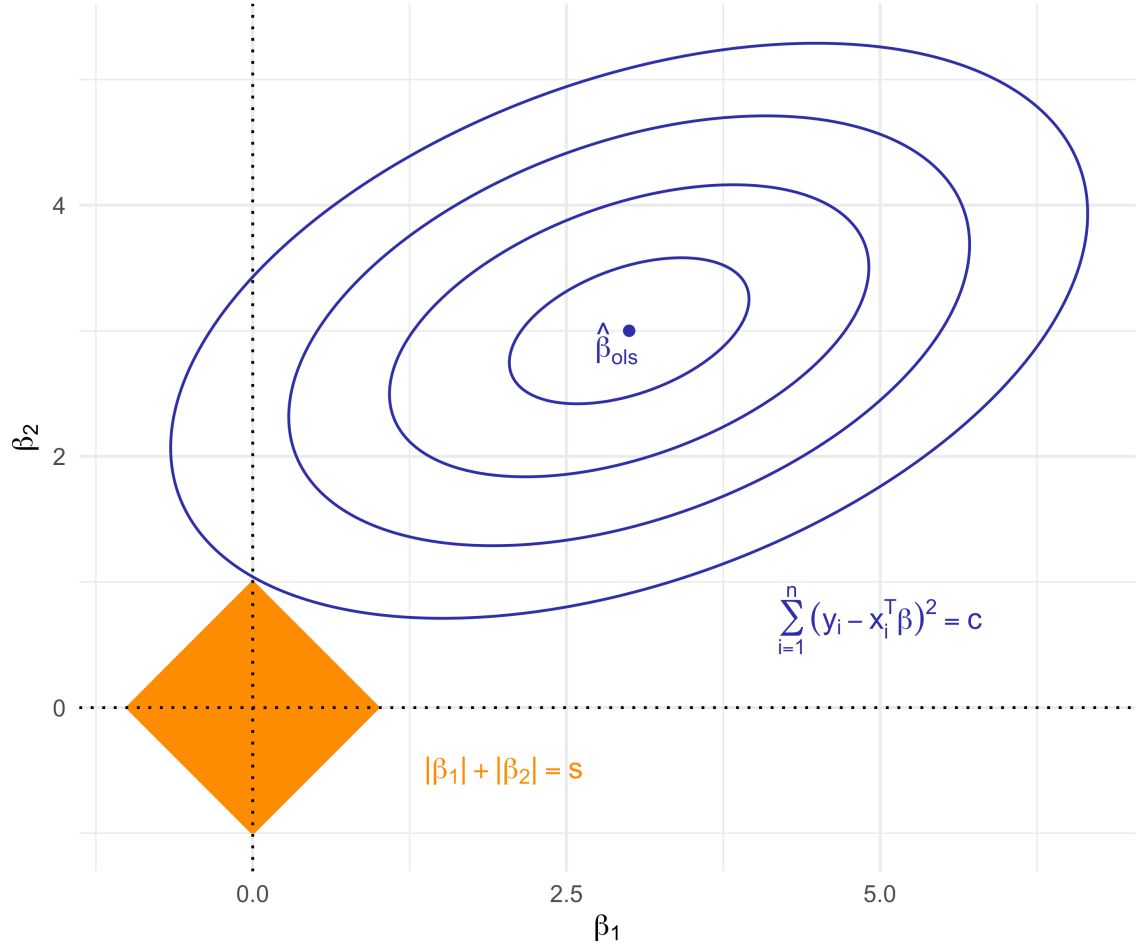
- The lasso problem can be **equivalently expressed** in its Lagrangian form, which is more amenable for computations.
- Having removed the intercept, the lasso estimator $\hat{\beta}_{\text{lasso}}$ is the **minimizer** of

$$\underbrace{\frac{1}{2n}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\beta)^2}_{\text{least squares}} + \underbrace{\lambda\sum_{j=1}^{p}|\beta_j|}_{\text{lasso penalty}}$$

  where $\lambda > 0$ is a **complexity parameter** controlling the **penalty**.

- When $\lambda = 0$ the penalty term disappears and $\hat{\beta}_{\text{lasso}} = \hat{\beta}_{\text{ols}}$. On the other hand, there exists a finite value of $\lambda_0 < \infty$ such that $\hat{\beta}_{\text{lasso}} = 0$.
- For any intermediate value $0 < \lambda < \lambda_0$ we get a combination of **shrinked** but positive coefficients, and a set of coefficients whose value is **exactly zero**.
- Unfortunately, there is **no closed-form expression** for the lasso solution.

The geometry of the lasso solution



Home page

Lasso with a single predictor I

- To gain some understanding, let us consider the **single-predictor** scenario, in which

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} \frac{1}{2n} \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda|\beta|.$$

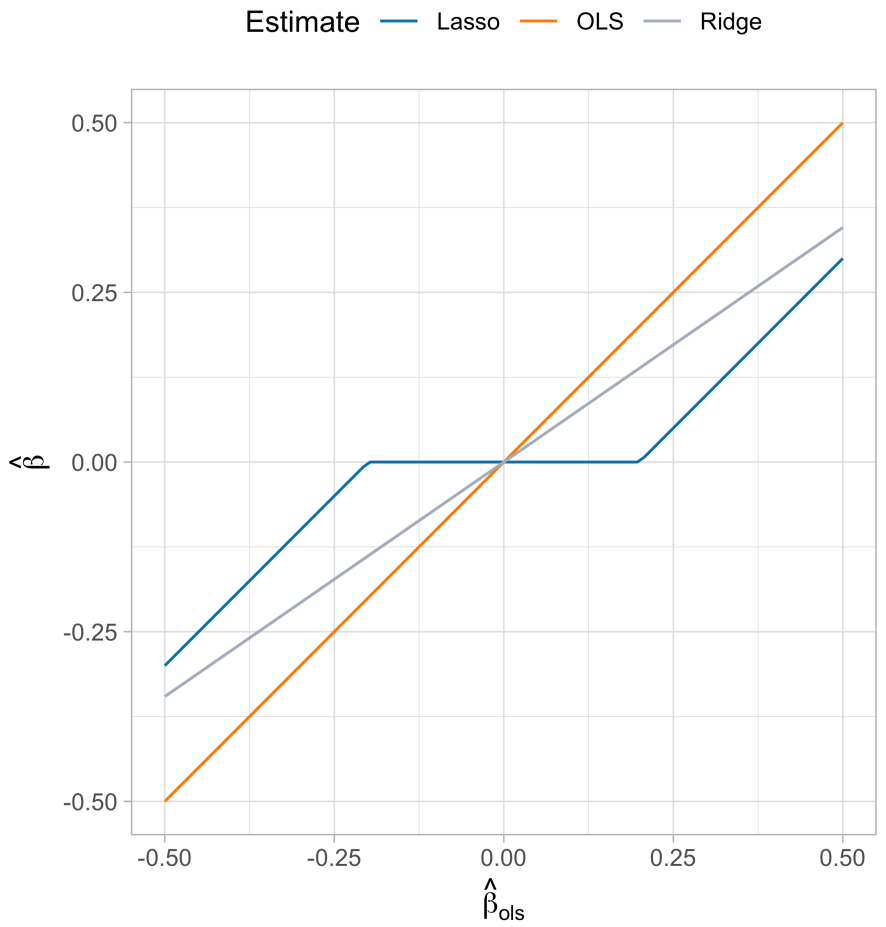
- This simple problem admits an **explicit expression** (see Exercises), which is

$$\hat{\beta}_{\text{lasso}} = \begin{cases} \text{cov}(x,y) - \lambda, & \text{if} \quad \text{cov}(x,y) > \lambda \\ 0 & \text{if} \quad |\text{cov}(x,y)| \leq \lambda \\ \text{cov}(x,y) + \lambda, & \text{if} \quad \text{cov}(x,y) < -\lambda \end{cases}$$

- The above solution can be written as $\hat{\beta}_{\text{lasso}} = \mathcal{S}_\lambda(\hat{\beta}_{\text{ols}})$, where $\mathcal{S}_\lambda(x) = \text{sign}(x)(|x| - \lambda)_+$ is the **soft-thresholding** operator and $(\cdot)_+$ is the **positive part** of a number (`pmax(0, x)`).
- For **ridge regression** (including a n^{-1} factor in the least squares penalty; see here) we get:

$$\hat{\beta}_{\text{ridge}} = \frac{1}{\lambda + 1}\text{cov}(x,y) = \frac{1}{\lambda + 1}\hat{\beta}_{\text{ols}} = \frac{1}{\lambda + 1}\frac{1}{n}\sum_{i=1}^{n} x_i y_i.$$

Lasso with a single predictor II

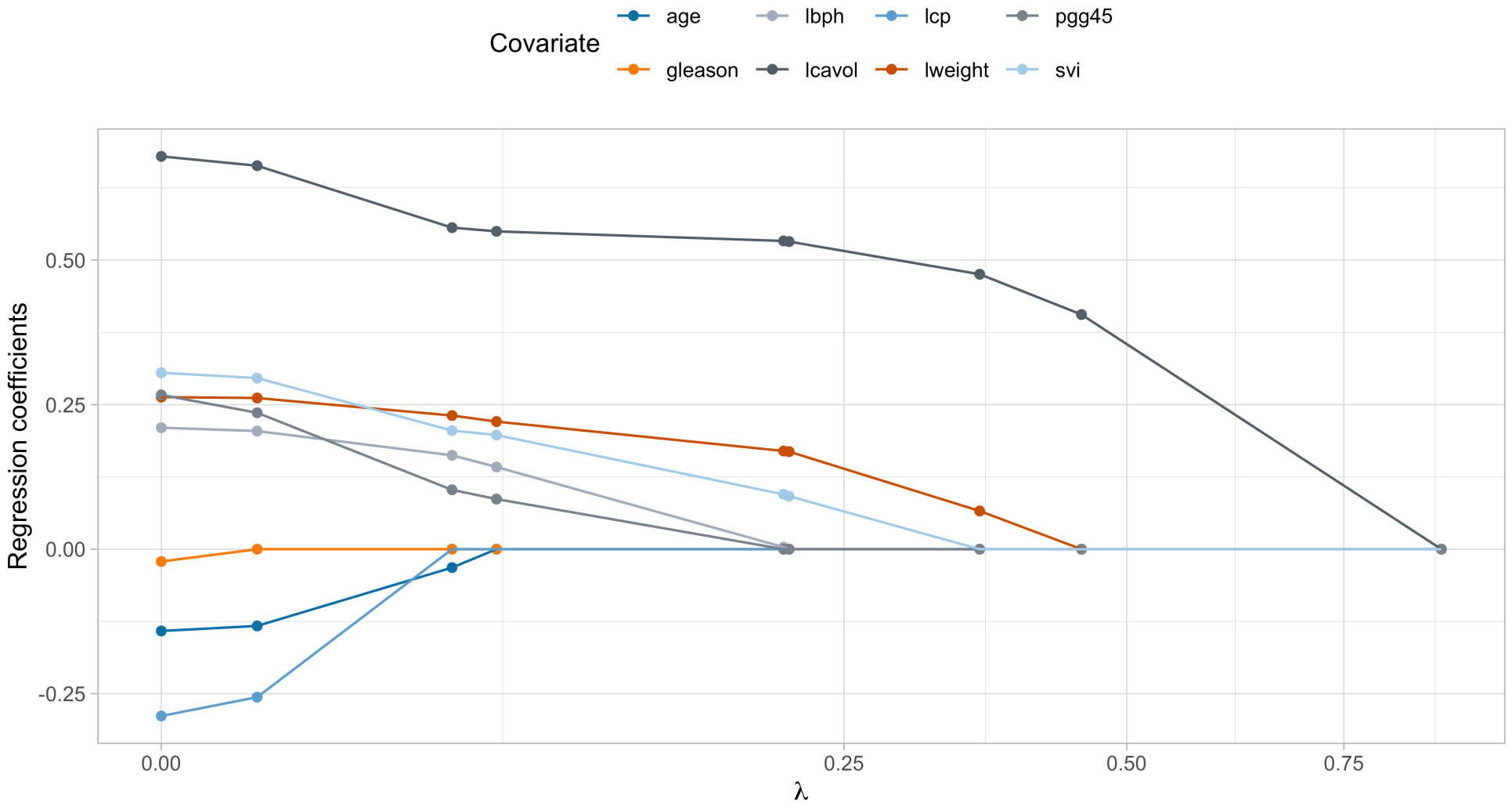


Home page

Soft-thresholding and lasso solution

- The single predictor special case provides further intuition of why the lasso perform **variable selection** and **shrinkage**.
- Ridge regression induces shrinkage in a **multiplicative** fashion, and the regression coefficients reach zero as $\lambda \to \infty$.
- Conversely, the lasso shrinks the ordinary least squares in an **additive** manner, **truncating** them at **zero** after a certain threshold.
- Even though we do not have a closed-form expression for the lasso solution $\hat{\beta}_{\text{lasso}}$ when the covariates $p > 1$, the main intuition is preserved: lasso induces **sparsity**!

The lasso path



Home page

Least angle regression I

- Least angle regression (LAR) is a "**democratic**" version of **forward stepwise regression**.
- Forward stepwise builds a model **sequentially**, adding one variable at a time. At each step, the best variable is included in the **active set** and then the least square fit is updated.
- LAR uses a similar strategy, but any new variable contributes to the predictions only "as much" as it deserves.

Main result of LAR

- The LAR algorithm provides a way to **compute** the entire **lasso path** efficiently at the cost of a full least-squares fit.
- LAR sheds light on important **statistical aspects** of the lasso. A nice **LAR - lasso - boosting** relationship is established, which is computationally and conceptually sound.

Least angle regression algorithm (LAR)

1. After centering and standardization, define the residuals $\boldsymbol{r}_0 = \boldsymbol{y}$ and let $\hat{\beta}^{(0)} = 0$.
2. Find the predictor $\tilde{\boldsymbol{x}}_j$ **most correlated** with the residuals $\boldsymbol{r}_0$, i.e. having the largest value for $\text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{r}_0) = \text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{y})$. Call this value λ_0 and let $\mathcal{A} = \{j\}$ be the **active set**.
   i. **Move** $\beta_j(\lambda)$ from $\hat{\beta}_j^{(0)} = 0$ **towards** its **least squares solution** by decreasing λ, i.e.

$$\beta_j(\lambda) = \frac{\lambda_0 - \lambda}{\lambda_0} \text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{y}), \qquad 0 < \lambda \leq \lambda_0,$$

   keeping track of the residuals $\boldsymbol{r}(\lambda) = \boldsymbol{y} - \tilde{\boldsymbol{x}}_j \beta_j(\lambda)$. It can be shown that

$$|\text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{r}(\lambda))| = \lambda.$$

   ii. Identify the value $\lambda > 0$ such that **another variable** $\boldsymbol{x}_\ell$ has **as much correlation** with the residuals as $\boldsymbol{x}_j$. Call this value λ_1, obtaining: $|\text{cov}(\tilde{\boldsymbol{x}}_\ell, \boldsymbol{r}(\lambda_1))| = \lambda_1$.
   iii. Obtain the **estimate** $\hat{\beta}^{(1)} = (0, \ldots, \beta_j(\lambda_1), \ldots, 0)$ and set $\boldsymbol{r}_1 = \boldsymbol{r}(\lambda_1)$. Define the new **active set** $\mathcal{A} = \{j, \ell\}$ and let $\boldsymbol{X}_\mathcal{A}$ be the corresponding matrix.

Least angle regression algorithm (LAR)

3. For $k = 2, \ldots, K = \min(n-1, p)$, do:

   i. **Move** the coefficients $\beta_{\mathcal{A}}(\lambda)$ from $\hat{\beta}_{\mathcal{A}}^{(k-1)}$ **towards** their **least squares solution**:

   $$\beta_{\mathcal{A}}(\lambda) = \hat{\beta}_{\mathcal{A}}^{(k-1)} + \frac{\lambda_{k-1} - \lambda}{\lambda_{k-1}} (\boldsymbol{X}_{\mathcal{A}}^T \boldsymbol{X}_{\mathcal{A}})^{-1} \boldsymbol{X}_{\mathcal{A}}^T \boldsymbol{r}_{k-1}, \qquad 0 < \lambda \leq \lambda_{k-1},$$

   keeping track of $\boldsymbol{r}(\lambda) = \boldsymbol{y} - \boldsymbol{X}_{\mathcal{A}} \beta_{\mathcal{A}}(\lambda)$. The covariances with the residuals are **tied**:

   $$|\text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{r}(\lambda))| = \lambda, \qquad j \in \mathcal{A}.$$

   ii. Identify the largest value $\lambda > 0$ such that **another variable** $\boldsymbol{x}_\ell$ has **as much correlation** with the residuals. Call this value λ_k, so that $|\text{cov}(\tilde{\boldsymbol{x}}_\ell, \boldsymbol{r}(\lambda_k))| = \lambda_k$.

   iii. Set the **estimate** $\hat{\beta}^{(k)}$ with entries $\hat{\beta}_{\mathcal{A}}^{(k)} = \beta_{\mathcal{A}}(\lambda_k)$ and zero otherwise. Let $\boldsymbol{r}_k = \boldsymbol{r}(\lambda_k)$. Define the new **active set** $\mathcal{A} \leftarrow \mathcal{A} \cup \{\ell\}$ and design matrix $\boldsymbol{X}_{\mathcal{A}}$.

4. Return the pairs $\{\lambda_k, \hat{\beta}^{(k)}\}_0^K$.

Least angle regression: remarks

- The coefficients in LAR change in a **piecewise** fashion, with knots in λ_k. The LAR path coincides **almost always** with the lasso. Otherwise, a simple modification is required:

LAR: lasso modification

3.ii+. If a nonzero coefficient crosses zero before the next variable enters, drop it from $\mathcal{A}$ and recompute the joint least-squares direction using the reduced set.

Practical details

- In **Step 3.ii**, we do **not** take small steps and then recheck the covariances. Instead, the new variable $\boldsymbol{x}_\ell$ "catching up" and the value λ_k can be identified with some algebra.
- The LAR algorithm is **extremely efficient**, requiring the same order of computation of least squares. The main bottleneck is **Step 3.i**, but **QR decomposition** can be exploited.

☠️ - Lasso and LAR relationship

- What follows is **heuristic intuition** for why LAR and lasso are so similar. By construction, at any stage of the LAR algorithm, we have that:

$$\text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{r}(\lambda)) = \frac{1}{n}\sum_{i=1}^{n} x_{ij}\{y_i - \boldsymbol{x}_i^T\beta(\lambda)\} = \lambda \boldsymbol{s}_j, \qquad j \in \mathcal{A},$$

  where $s_j \in \{-1, 1\}$ indicates the **sign of the covariance**.

- On the other hand, let $\mathcal{A}_{\text{lasso}}$ be the active set of the lasso. For these variables, the penalized lasso loss is differentiable, obtaining:

$$\text{cov}(\tilde{\boldsymbol{x}}_j, \boldsymbol{r}(\lambda)) = \frac{1}{n}\sum_{i=1}^{n} x_{ij}\{y_i - \boldsymbol{x}_i^T\beta(\lambda)\} = \lambda \text{sign}(\beta_j), \qquad j \in \mathcal{A}_{\text{lasso}},$$

  which **coincide** with the LAR solution if $s_j = \text{sign}(\beta_j)$, which is **almost always the case**.

Uniqueness of the lasso solution

- The lasso can be computed even when $p > n$. In these cases, will it be **unique**?

Three uniqueness results (Tibshirani, 2013)

- If $\boldsymbol{X}$ has **full rank** $\mathrm{rk}(\boldsymbol{X}) = p$, which implies $p \leq n$, then $\hat{\beta}_{\text{lasso}}$ is uniquely determined.
- If **all** the values of $\boldsymbol{X}$ are **different**, then $\hat{\beta}_{\text{lasso}}$ is uniquely determined, even when $p > n$.
- The **predictions** $\boldsymbol{X}\hat{\beta}_{\text{lasso}}$ are always uniquely determined.

- Non-uniqueness may occur in the presence of **discrete-valued** data. It is of practical concern only whenever $p > n$ and if we are interested in interpreting the coefficients.
- Much more **general** sufficient conditions for the uniqueness of $\hat{\beta}_{\text{lasso}}$ are known, but they are quite technical and complex to check in practice.

The degrees of freedom of the lasso

- In ridge regression, the **effective degrees of freedom** have a simple formula.
- **Miraculously**, for the lasso with a fixed penalty parameter λ, the number of nonzero coefficients $|\mathcal{A}_{\text{lasso}}(\lambda)|$ is an **unbiased estimate** of the degrees of freedom.

Degrees of freedom (Zhou, Hastie, and Tibshirani, 2007, Tibshirani and Taylor, 2012)

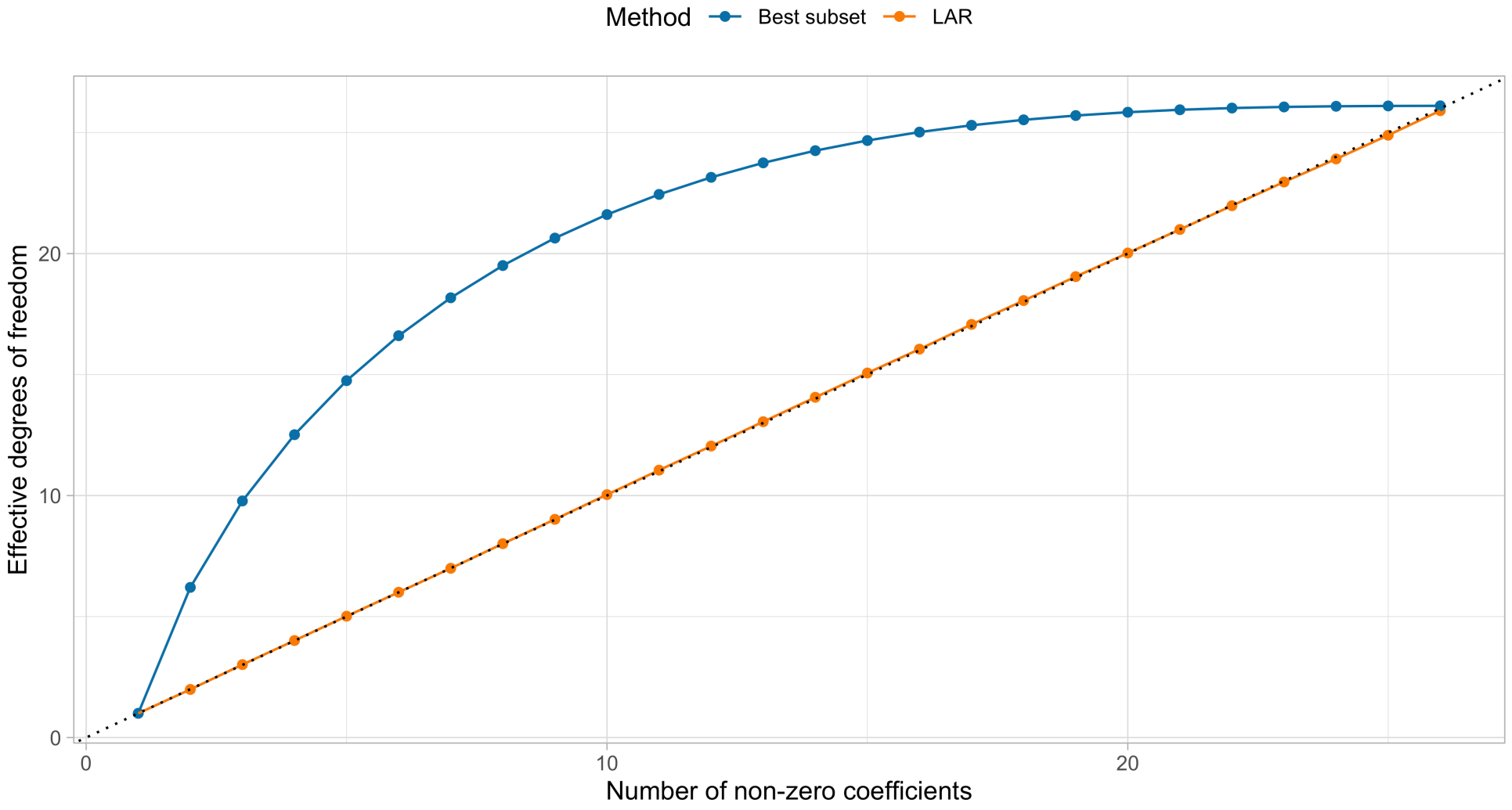
- Suppose $\boldsymbol{X}$ has **full rank** $\text{rk}(\boldsymbol{X}) = p$ and $\boldsymbol{y}$ follows a Gaussian law. Then:

$$\text{df}_{\text{lasso}} = 1 + \mathbb{E}|\mathcal{A}_{\text{lasso}}(\lambda)|.$$

- Under further regularity conditions, the above relationship is **exact** if we consider the **LAR active set**, therefore implicitly using a different set of λ values for any fit:

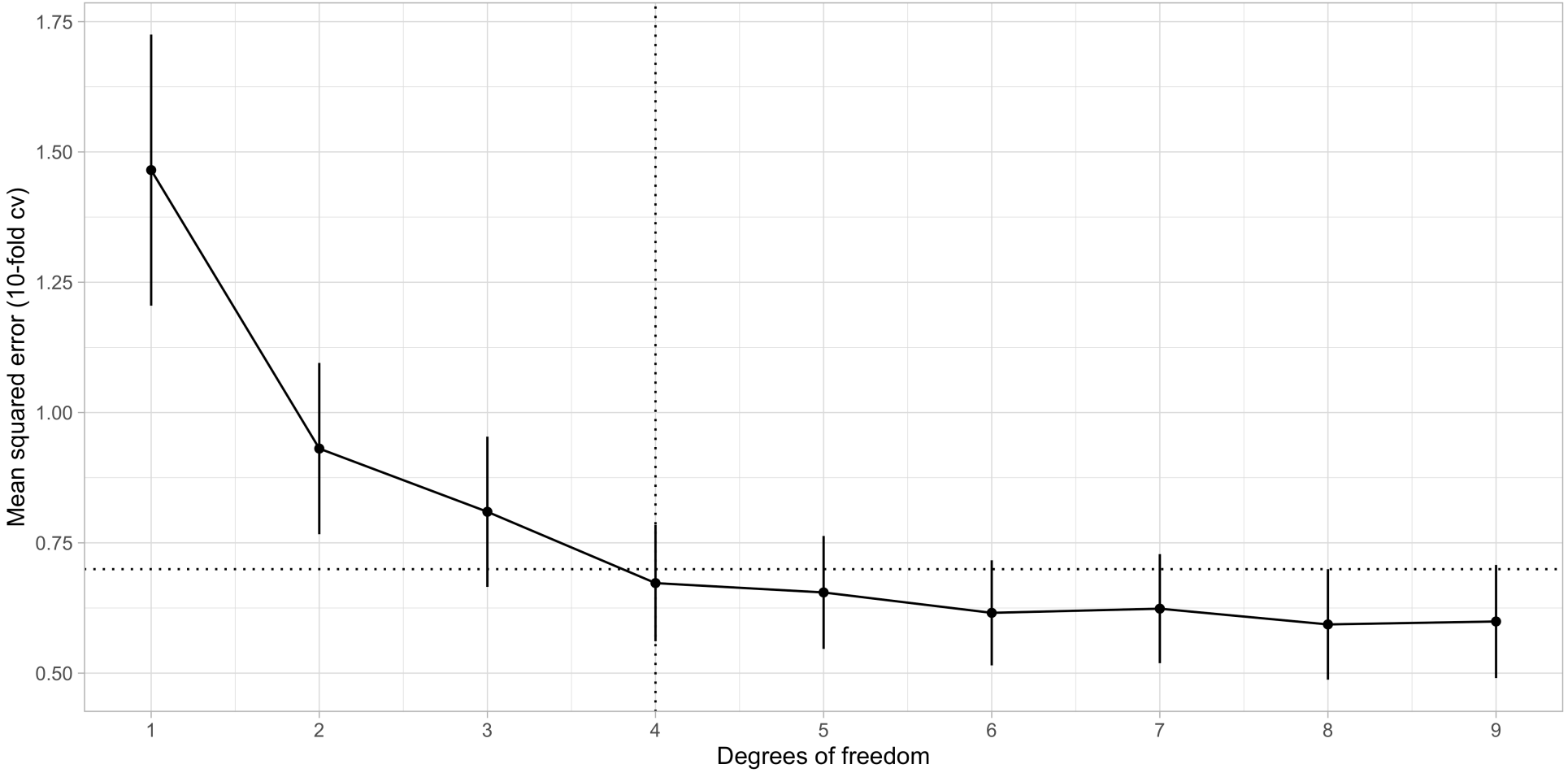
$$\text{df}_{\text{lar}} = 1 + |\mathcal{A}|.$$

Effective degrees of freedom of LAR and best subset



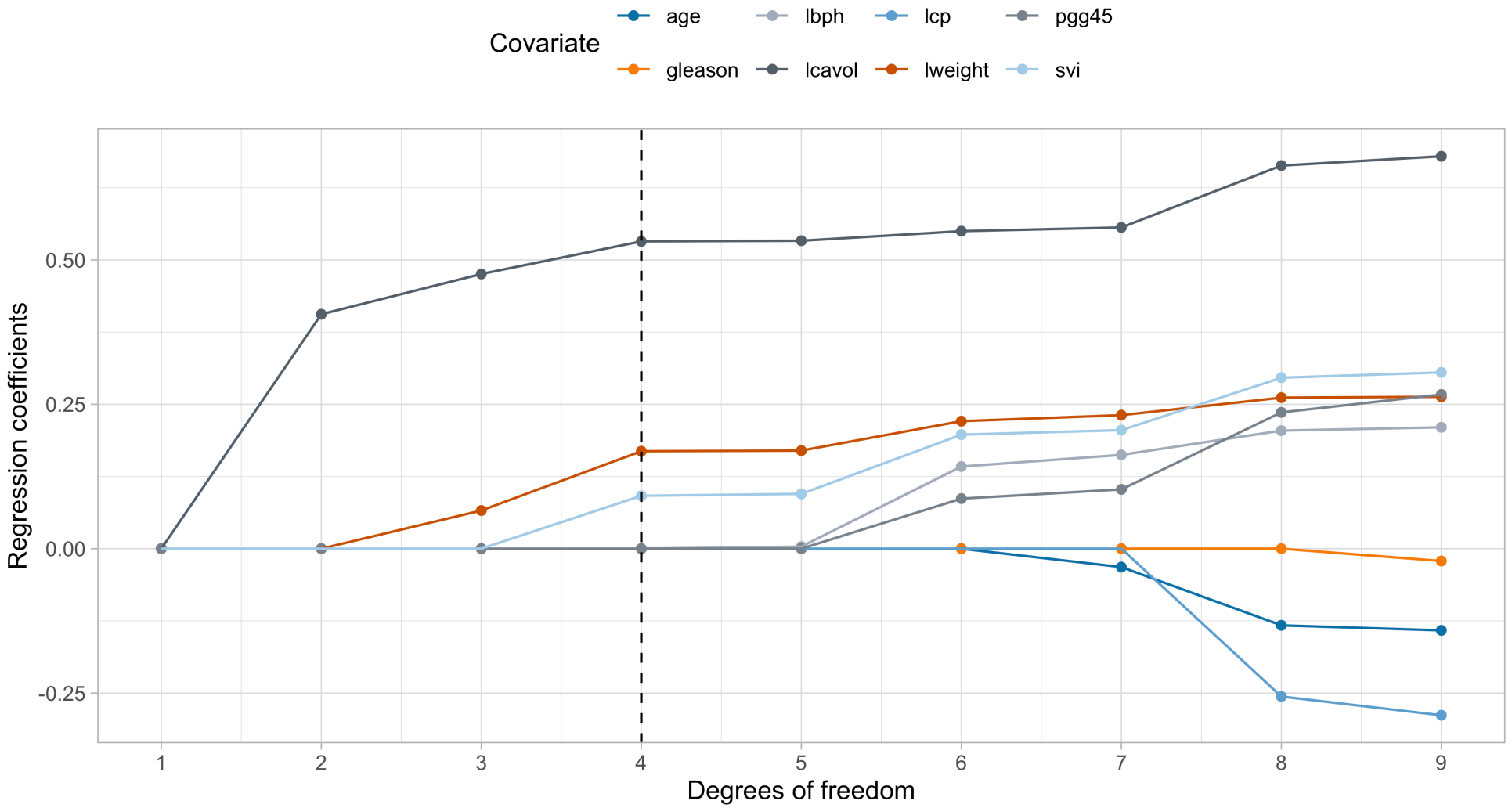
Home page

Cross-validation for lasso



Home page

The LAR (lasso) estimate



Home page

Other properties of LAR and lasso

- **Bayesian interpretation**: the penalty can be interpreted as a Laplace prior on β.
- As mentioned, under certain conditions the LAR algorithm can be seen as the limiting case of a **boosting procedure**, in which small corrections to predictions are iteratively performed.
- The **nonnegative garrote** (Breiman, 1995) is a two-stage procedure with a close relationship to the lasso. Breiman's paper was the inspiration for Tibshirani (1996).
- There is a large body of theoretical work on the behavior of the lasso, focused on:
  - the mean-squared-error consistency of the lasso;
  - the recovery of the nonzero support set of the true regression parameters, sometimes called **sparsistency**.
- The interested reader work may have a look at the (very technical) Chapter 11 of Hastie, Tibshirani and Wainwright (2015)

Summary of LARS and lasso

Pros

- LAR and Lasso are extremely efficient approaches that perform both **variable selection** and **shrinkage** at the same time.
- Lasso produces a **parsimonious** model.

Cons

- Lasso can be applied when $p > n$, but there might be **uniqueness** issues. Moreover, the lasso selects at most n variables.
- If there is a group of variables with high pairwise correlations, the lasso tends to "randomly" select only one variable from the group.
- When $p < n$, if there are **high correlations** between predictors, it has been empirically observed that the prediction performance of the lasso is dominated by ridge regression.

The prostate dataset. A summary of the estimates

	Least squares	Best subset	PCR	Ridge	Lasso
(Intercept)	2.465	2.477	2.455	2.467	2.468
lcavol	0.680	0.740	0.287	0.588	0.532
lweight	0.263	0.316	0.339	0.258	0.169
age	-0.141	.	0.056	-0.113	.
lbph	0.210	.	0.102	0.201	.
svi	0.305	.	0.261	0.283	0.092
lcp	-0.288	.	0.219	-0.172	.
gleason	-0.021	.	-0.016	0.010	.
pgg45	0.267	.	0.062	0.204	.

The results on the test set

- At the beginning of this unit, we split the data into **training** set and **test** set. Using the training, we selected λ via cross-validation or the C_p index.
- Using the final test set with 30 observations, we will assess which model is **preferable**.

	OLS	**Best subset**	**PCR**	**Ridge**	**Lasso**
Test error (MSE)	0.521	0.492	0.496	0.496	0.48

- All the approaches presented in this unit perform better than ordinary least squares.
- The **lasso** is the approach with **lowest mean squared error**. At the same time, it is also a **parsimonious** choice.
- Best subset is the second best, doing a good job in this example... but here $p = 8$, so there were no computational difficulties!

Elastic-net and pathwise algorithms

Elastic-net

- The **elastic-net** is a compromise between ridge and lasso. It selects variables like the lasso and shrinks together the coefficients of correlated predictors like ridge.
- Having removed the intercept, the elastic-net estimator $\hat{\beta}_{\text{en}}$ is the **minimizer** of:

$$\frac{1}{2n}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^T\beta)^2 + \lambda\sum_{j=1}^{p}\left(\alpha|\beta_j| + \frac{(1-\alpha)}{2}\beta_j^2\right),$$

  where $0 < \alpha < 1$ and the **complexity parameter** $\lambda > 0$.

- **Ridge regression** is a special case, when $\alpha = 0$. **Lasso** is also a special case, when $\alpha = 1$.
- It is often **not worthwhile** to estimate α using cross-validation. A typical choice is $\alpha = 0.5$.
- An advantage of the elastic-net is that it has a **unique solution**, even when $p > n$.
- Another nice property, shared by ridge, is that whenever $\tilde{\boldsymbol{x}}_j = \tilde{\boldsymbol{x}}_\ell$, then $\hat{\beta}_{j,\text{en}} = \hat{\beta}_{\ell,\text{en}}$. On the other hand, the **lasso** estimator would be **undefined**.

Convex optimization

- The estimators OLS, ridge, lasso, and elastic-net have a huge **computational advantage** compared, e.g., to best subset: they are all **convex optimization problems**.
- A function $f : \mathbb{R}^p \to \mathbb{R}$ is **convex** if for any values $\boldsymbol{b}_1, \boldsymbol{b}_2 \in \mathbb{R}^p$ and $t \in [0, 1]$ it holds that

$$f(t\boldsymbol{b}_1 + (1-t)\boldsymbol{b}_2) \leq tf(\boldsymbol{b}_1) + (1-t)f(\boldsymbol{b}_2).$$

  Replacing $\leq$ with $<$ for $t \in (0, 1)$ gives the definition of **strict convexity**.
- **OLS** and the **lasso** are, for a general design matrix $\boldsymbol{X}$, convex problems. On the other hand, **ridge** and **elastic net** are strictly convex, as well as OLS and lasso when $\mathrm{rk}(\boldsymbol{X}) = p$.

Properties of convex optimization

- In a **convex** optimization problem, every local minimum is a **global minimum**;
- In a **strictly convex** optimization problem, there exists a **unique** global minimum.

Elastic-net with a single predictor

- The elastic-net estimate $\hat{\beta}_{\text{en}}$ is typically obtained through the **coordinate descent** algorithm, which works well here due **convexity** and the following **property**.
- In the **single-predictor** scenario the elastic-net minimization problem simplifies to

$$\hat{\beta}_{\text{en}} = \arg\min_{\beta} \frac{1}{2n} \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda \left(\alpha|\beta| + \frac{(1-\alpha)}{2}\beta^2 \right).$$

- It can be shown that an **explicit expression** for $\hat{\beta}_{\text{en}}$ is available, which is

$$\hat{\beta}_{\text{en}} = \frac{1}{1 + (1-\alpha)\lambda} \mathcal{S}_{\alpha\lambda}(\hat{\beta}_{\text{ols}}),$$

where $\mathcal{S}_\lambda(x) = \text{sign}(x)(|x| - \lambda)_+$ is the **soft-thresholding** operator and the **least square estimate** is $\hat{\beta}_{\text{ols}} = n^{-1} \sum_{i=1}^{n} x_i y_i$.

Coordinate descent

- The **coordinate descent** algorithm is based on a simple principle: optimize one coefficient (coordinate) at a time, keeping the others fixed.
- We can **re-write** the objective function of the elastic-net in a more convenient form:

$$\frac{1}{2n}\sum_{i=1}^{n}\left(y_i - \sum_{k\neq j} x_{ik}\beta_k - x_{ij}\beta_j\right)^2 + \lambda\left(\alpha|\beta_j| + \frac{(1-\alpha)}{2}\beta_j^2\right) + \underbrace{\lambda\sum_{k\neq j}^{p}\{\alpha|\beta_k| + \frac{(1-\alpha)}{2}\beta_k^2\}}_{\text{does not depend on } \beta_j},$$

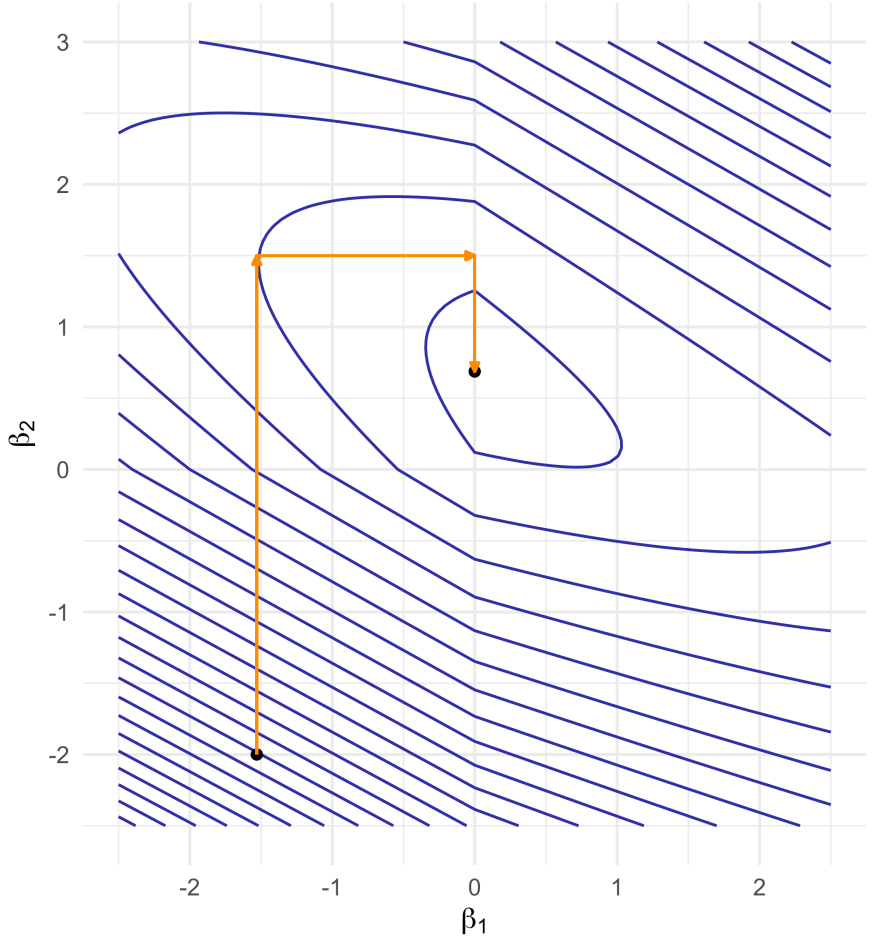
- Let us define the **partial residuals** $r_i^{(j)} = y_i - \sum_{k\neq j} x_{ik}\beta_k$. Then the updated β_j is

$$\beta_j \leftarrow \frac{1}{1+(1-\alpha)\lambda}\mathcal{S}_{\alpha\lambda}\left(\frac{1}{n}\sum_{i=1}^{n} x_{ij}r_i^{(j)}\right).$$

We **cycle** this update for $j = 1, \ldots, p$, over and over until convergence.

Coordinate descent - Example

Objective function: $(1-\beta_1-2\beta_2)^2+(3-\beta_1-2\beta_2)^2+5(|\beta_1|+|\beta_2|)$.



Home page

Pathwise coordinate optimization

In a regression model with an elastic-net penalty, the coordinate descent is **theoretically guaranteed** to reach the global minimum.

- The coordinate descent algorithm is implemented in the `glmnet` package. It is, de facto, the default algorithm for penalized generalized linear models.
- The `glmnet` implementation is very efficient due to several additional tricks:
  - The **warm start**. The algorithm for λ_k is initialized at the previous solution using λ_{k-1}.
  - Partial residuals can be efficiently obtained **without re-computing** the whole linear predictor.
  - The code is written in **C++** from version 4.1-3, it used to be written in **Fortran**.
  - Many other tricks are employed: active set convergence, tools for sparse $\boldsymbol{X}$ matrices, etc.
- The same algorithm can also be used to fit ridge regression and lasso, which is often convenient even though alternatives would be available.

Generalized linear models

Generalized linear models

- Almost everything we discussed in this unit for **regression** problems can be **extended to GLMs** and, in particular, to classification problems.

Best subset selection for GLMs

- Best subset selection and its forward and backward greedy approximations are conceptually straightforward to extend to GLMs (using log-likelihood and ML).
- However, computations are much harder: leaps-and-bound approaches can not be applied.

Principal components for GLMs

- Principal components can be straightforwardly applied to GLMs.
- The shrinkage effect and their ability to control the variance remain unaltered, but the theory (e.g., variance of the estimator) holds only in an approximate sense.

Shrinkage methods for GLMs

- Shrinkage methods such as ridge and lasso can also be generalized to GLMs.
- The elastic-net approach for **logistic regression**, which covers ridge and lasso as special cases, becomes:

$$\min_{(\beta_0,\beta)} \left\{ -\frac{1}{n}\sum_{i=1}^{n} y_i(\beta_0 + \boldsymbol{x}_i^T\beta) - \log\{1+\exp(\beta_0+\boldsymbol{x}_i^T\beta)\} + \lambda\sum_{j=1}^{p}\left(\alpha|\beta_j| + \frac{(1-\alpha)}{2}\beta_j^2\right)\right\},$$

  which is an instance of **penalized log-likelihood**.
- **Most of the properties** (e.g. ridge = variance reduction and shrinkage, lasso = variable selection) and other high-level considerations we made so far are **still valid**.
- Computations are somewhat more cumbersome. The `glmnet` package provides the numerical routines for fitting this model, using variants of **coordinate descent**.
- The core idea is to obtain a **quadratic approximation** of the log-likelihood, as for IWLS. Then, the approximated loss becomes a (**weighted**) penalized regression problem.

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