Ridge, Best Subsets and LASSO

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Outline

High-dimensional data

- In the past 20 years, new technologies have changed the way that data are collected in fields as diverse as finance, marketing, and medicine
- It is now commonplace to collect a large number p of predictors
- While p can be extremely large, the number of observations n is often limited due to cost, sample availability, or other considerations
- Data sets containing more predictors than observations, i.e.

$$p > n$$

  are often referred to as high-dimensional
- Classical approaches such as least squares linear regression are not appropriate in this setting
- The slides about ridge regression are based on *Lecture notes on ridge regression* by van Wieringen (2015)

Linear regression

- $n \geq p$
- Training data: $\underset{n \times 1}{\mathbf{y}}$, $\underset{n \times p}{\mathbf{X}}$
- OLS estimator: $\underset{p \times 1}{\hat{\boldsymbol{\beta}}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$
- Fit on training data: $\underset{n \times 1}{\hat{\mathbf{y}}} = \mathbf{X} \hat{\boldsymbol{\beta}}$
- Test data: $\underset{m \times 1}{\mathbf{y}^*}$, $\underset{m \times p}{\mathbf{X}^*}$
- Prediction on test data: $\underset{m \times 1}{\hat{\mathbf{y}}^*} = \mathbf{X}^* \hat{\boldsymbol{\beta}}$

High-dimensional regression

- **Case** $p < n$

$\mathrm{rank}(\mathbf{X}) = p$: it exists an unique solution $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$

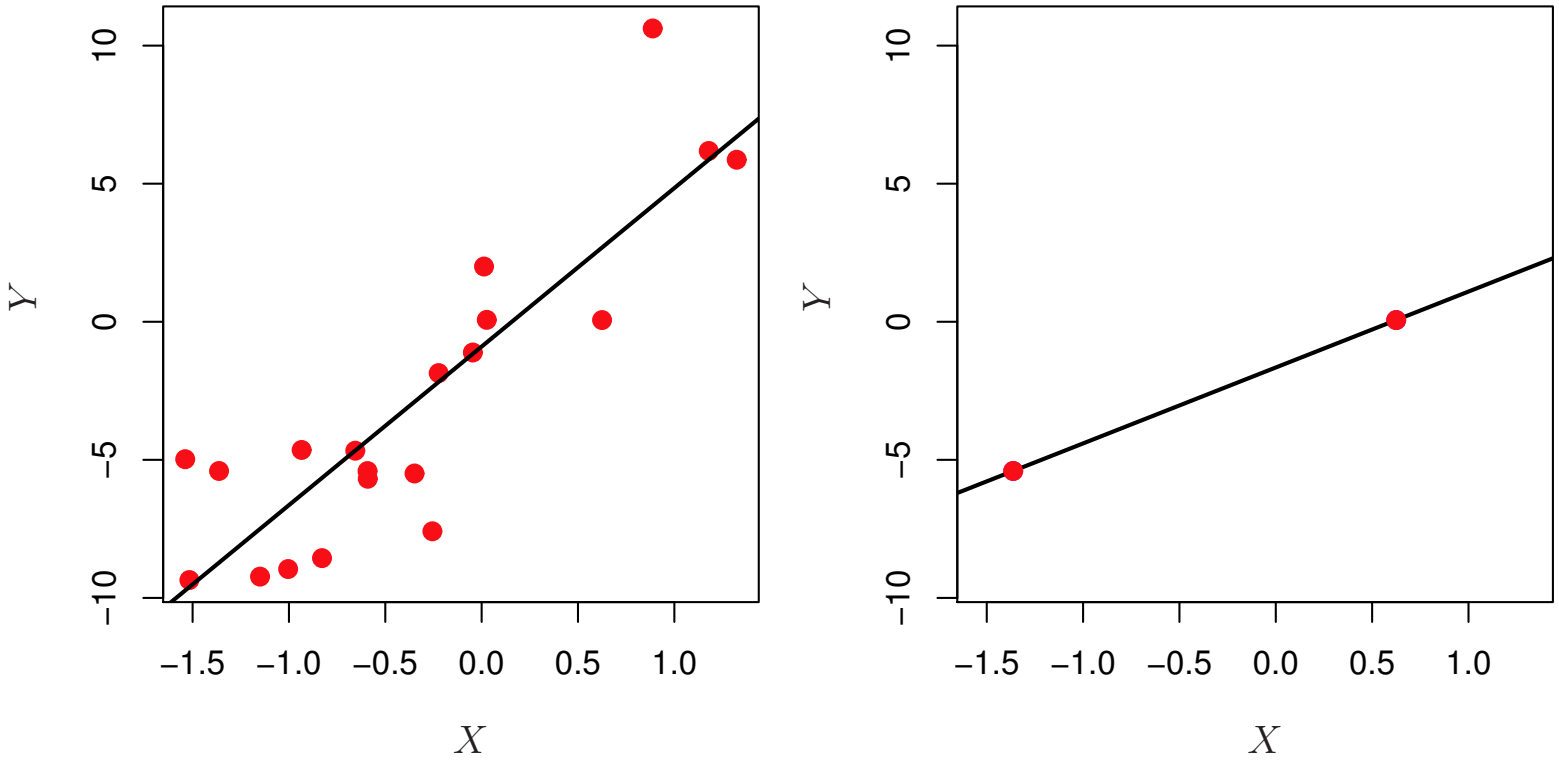
- **Case** $p \to n$

Even if $\mathbf{X}^\top \mathbf{X}$ can be inverted, $\mathbf{X}^\top \mathbf{X}$ approaches singularity and $\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}) = \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}$ increases without bound

- **Case** $p > n$

$\mathrm{rank}(\mathbf{X}) < p$: $\mathbf{X}^\top \mathbf{X}$ is singular and does not have an inverse. $\hat{\boldsymbol{\beta}}$ is not defined since there are infinitely many solutions $\hat{\boldsymbol{\beta}}$

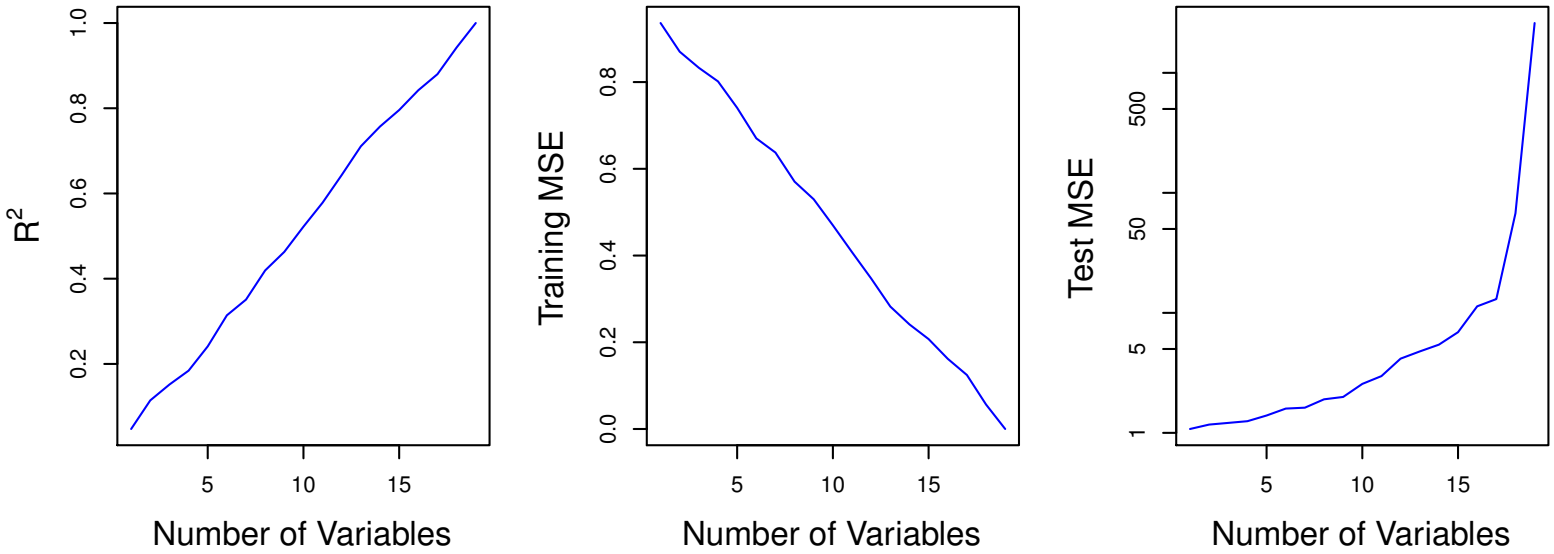
$p = n$



- Left: Least squares regression in the low-dimensional setting
- Right: Least squares regression with $n = 2$ observations and two parameters to be estimated (intercept+slope)

Source: ISL p. 240 Figure 6.22

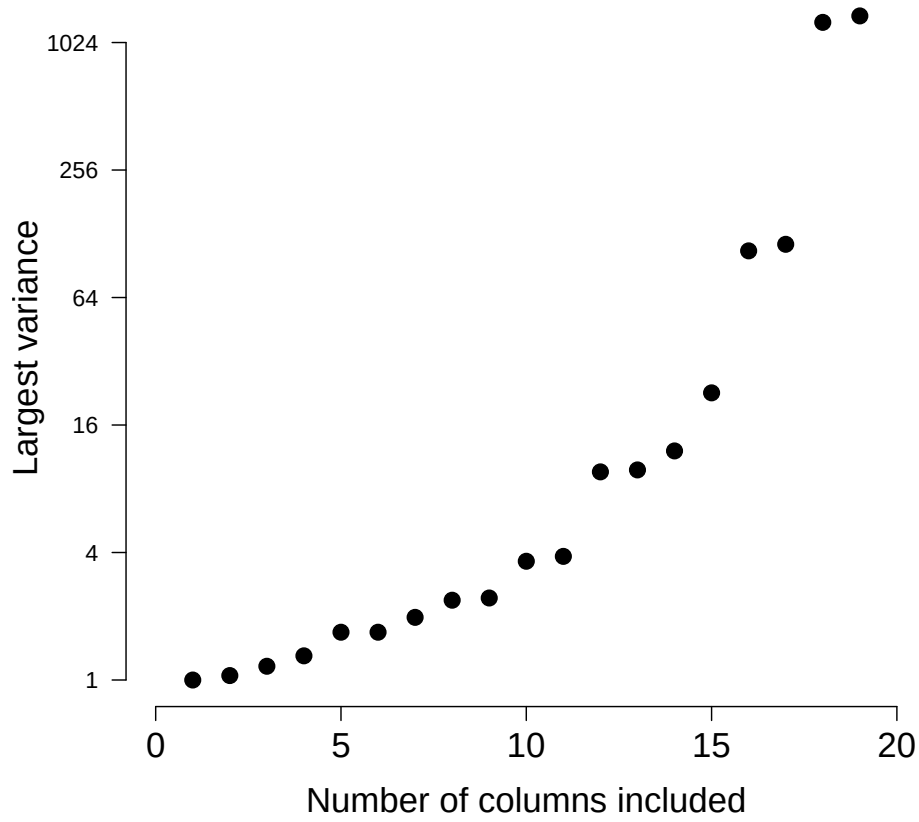
$p \longrightarrow n$



- Simulated example with $n = 20$ and predictors that are completely unrelated to the response are added to the model
- Left: The R^2 increases to 1 as more predictors are included
- Center: $\mathrm{MSE}_{\mathrm{Tr}}$ decreases to 0 as more predictors are included
- Right: $\mathrm{MSE}_{\mathrm{Te}}$ increases as more predictors are included

Source: ISL p. 241 Figure 6.23

Consider $\mathbf{X}$ with $n = 20$ and whose elements consist of independent, normally distributed random numbers; the figure below plots the largest variance of the $\hat{\beta}_j$ estimates as we increase the number of columns in $\mathbf{X}$



Source: P. Breheny

Collinearity

- Collinearity in regression refers to the event of two (or multiple) predictors in $\mathbf{X}$ being highly linearly related
- Then, the subspace spanned by the columns of $\mathbf{X}$ is close to not being of full rank
- When the subspace onto which $\mathbf{y}$ is projected, is close to rank deficient, it is almost impossible to separate the contribution of the individual predictors
- The uncertainty with respect to the predictors responsible for the variation explained in $\mathbf{y}$ is often reflected in the fit of the linear regression model to data by a large error of the estimates of the regression parameters corresponding to the collinear predictors

```
n = 20
set.seed(123)
x1 <- rnorm(n)
x2 <- rnorm(n)
x3 <- rnorm(n,mean=x2,sd=.01)
y <- 1 + 1*x1 + 3*x2 + 3*x3 + rnorm(n)
summary( lm(y ~ x1 + x2 + x3 ) )
```

```
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   0.8949     0.2301   3.889 0.001305 **
x1            1.1254     0.2402   4.685 0.000248 ***
x2           19.3422    24.4470   0.791 0.440405
x3          -13.0406    24.4209  -0.534 0.600686
```

Super-collinearity

- The case of two (or multiple) predictors in $\mathbf{X}$ being perfectly linearly dependent is referred as super-collinearity
- An high-dimensional $\mathbf{X}$ suffers from super-collinearity
- If $p > n$, then $\mathrm{rank}(\mathbf{X}) \leq n < p$. This implies that the columns of $\mathbf{X}$ are linearly dependent

$$\exists \mathbf{v} \in \mathbb{R}^p, \mathbf{v} \neq \mathbf{0} : \mathbf{X}\mathbf{v} = \mathbf{0}$$

- If $p > n$, then $\mathrm{rank}(\mathbf{X}) = \mathrm{rank}(\mathbf{X}^\mathsf{T}\mathbf{X}) < p$. This implies that the square matrix $\mathbf{X}^\mathsf{T}\mathbf{X}$ is singular with $\det(\mathbf{X}^\mathsf{T}\mathbf{X}) = 0$ and it does not have an inverse $(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}$

Outline

Ridge regression

- To obtain an estimate of the regression parameter $\boldsymbol{\beta}$ when $\mathbf{X}$ is super-collinear, Hoerl and Kennard (1970) proposed an ad-hoc fix to resolve the singularity of $\mathbf{X}^\top\mathbf{X}$
- Simply replace $\mathbf{X}^\top\mathbf{X}$ by $\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_{p\times p}$ with $\lambda > 0$
- The scalar λ is a tuning parameter, henceforth called the penalty parameter
- The ridge regression estimator is defined as

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

- The set of all ridge regression estimates $\{\hat{\boldsymbol{\beta}}^\lambda : \lambda \in [0, \infty)\}$ is called the solution path of the ridge estimator

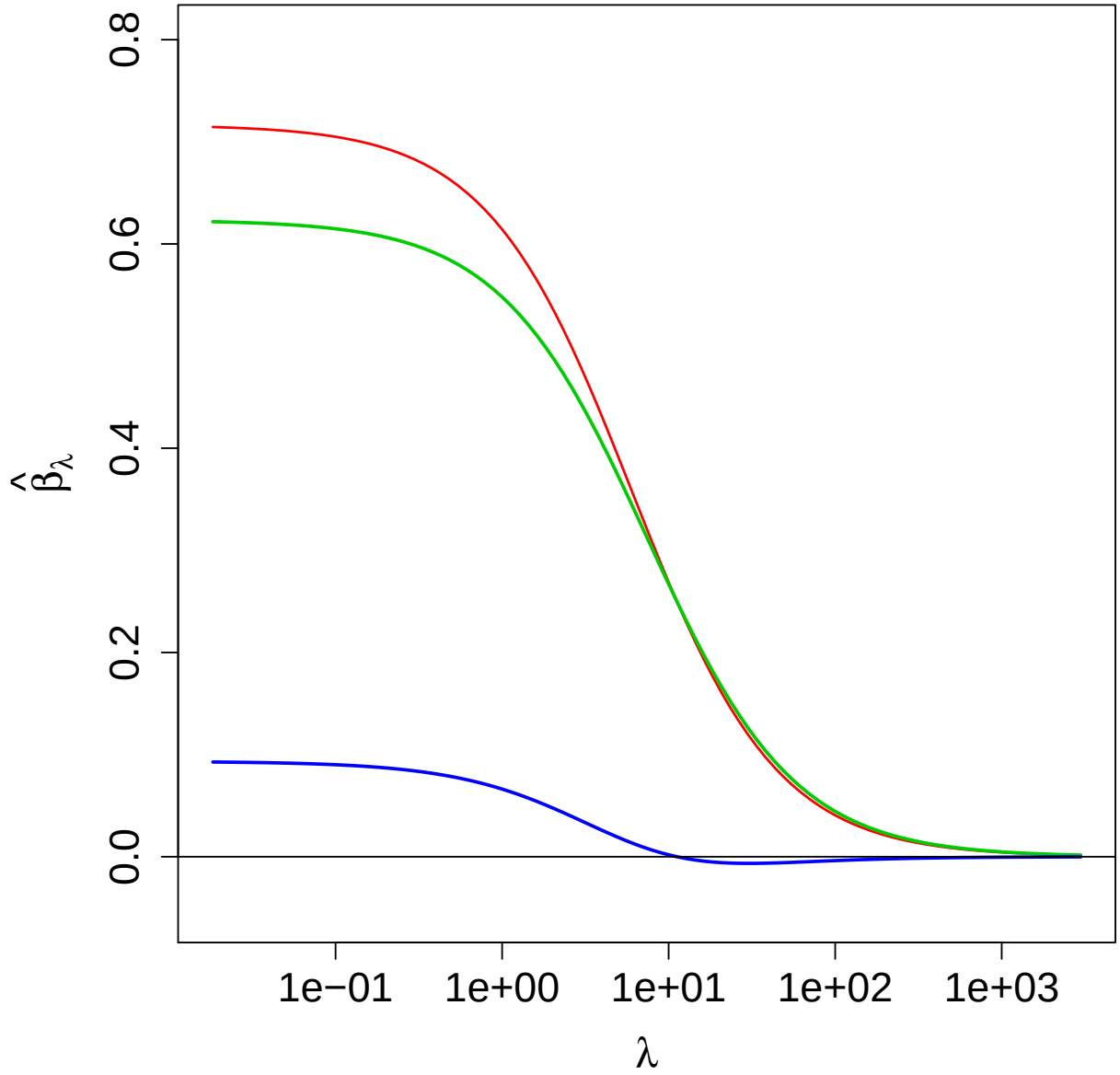
Ridge regression fit

- Ridge regression fit on the training data $\hat{\mathbf{y}}^{\lambda} = \mathbf{H}^{\lambda}\mathbf{y}$ with

$$\mathbf{H}^{\lambda} = \mathbf{X}(\mathbf{X}^{\mathsf{T}}\mathbf{X} + \lambda \mathbf{I}_{p\times p})^{-1}\mathbf{X}^{\mathsf{T}}$$

- If $\mathrm{rank}(\mathbf{X}) = p$ and $\lambda = 0$, the OSL fit $\hat{\mathbf{y}}^{0} = \hat{\mathbf{y}}$ is the projection of $\mathbf{y}$ onto the subspace spanned by the columns of $\mathbf{X}$
- With $\lambda > 0$, the fit $\hat{\mathbf{y}}^{\lambda}$ is not the projection of $\mathbf{y}$ onto the subspace spanned by the columns of $\mathbf{X}$, i.e. $\mathbf{H}^{\lambda}$ is not a projection matrix. Consequently, the ridge residuals $\mathbf{y} - \hat{\mathbf{y}}^{\lambda}$ are not orthogonal to the fit $\hat{\mathbf{y}}^{\lambda}$

Solution path



```
X = matrix(c(1,1,1,1,-1,0,2,1,2,1,-1,0), byrow=F, ncol=3)
p = ncol(X)
qr(X)$rank
y = c(1.3,-.5,2.6,.9)

lambdas = exp(seq(-4,8,length.out = 100))
hatbetas =sapply(lambdas, function(lambda)
solve(t(X)%*%X + lambda*diag(p)) %*% t(X) %*%y
)
plot(lambdas, hatbetas[1,], type="l", log="x")
lines(lambdas, hatbetas[2,])
lines(lambdas, hatbetas[3,])
```

Expectation

- Assume the linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}_n(\mathbf{0}, \sigma^2 \mathbf{I}_{n\times n})$$

- The expectation of the ridge estimator

$$\mathbb{E}(\hat{\boldsymbol{\beta}}^{\lambda}) = \mathbf{X}^{\mathsf{T}}\mathbf{X}(\lambda \mathbf{I}_{p\times p} + \mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\boldsymbol{\beta}$$

- Clearly, $\mathbb{E}(\hat{\boldsymbol{\beta}}^{\lambda}) \neq \boldsymbol{\beta}$ for any $\lambda \neq 0$. Hence the ridge estimator is biased

Shrinkage

- The expectation of the ridge estimator vanishes as λ tends to infinity

$$\lim_{\lambda \to \infty} \mathbb{E}(\hat{\boldsymbol{\beta}}^{\lambda}) = \mathbf{0}$$

- All regression coefficients are shrunken towards zero as the penalty parameter λ increases
- This behaviour is not strictly monotone in λ: $\lambda_a > \lambda_b$ does not necessarily imply $|\hat{\beta}_j^{\lambda_a}| < |\hat{\beta}_j^{\lambda_b}|$
- If $\mathbf{X}$ is an orthonormal matrix, i.e. $\mathbf{X}^{\top}\mathbf{X} = \mathbf{I}_{p \times p} = (\mathbf{X}^{\top}\mathbf{X})^{-1}$, the relation between OLS $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}^0$ and ridge estimator $\hat{\boldsymbol{\beta}}^{\lambda}$ is

$$\hat{\boldsymbol{\beta}}^{\lambda} = \frac{1}{1+\lambda}\hat{\boldsymbol{\beta}}$$

Variance

- The linear operator

$$\mathbf{W}^{\lambda} = [\mathbf{I}_{p\times p} + \lambda(\mathbf{X}^{\top}\mathbf{X})^{-1}]^{-1}$$

  transforms the OLS estimator into the ridge estimator

$$\mathbf{W}^{\lambda}\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}^{\lambda}$$

- The variance of the ridge estimator

$$\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}^{\lambda}) = \mathbf{W}^{\lambda}\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}})(\mathbf{W}^{\lambda})^{\top} = \sigma^2\mathbf{W}^{\lambda}(\mathbf{X}^{\top}\mathbf{X})^{-1}(\mathbf{W}^{\lambda})^{\top}$$

- Like the expectation the variance of the ridge estimator vanishes as λ tends to infinity

$$\lim_{\lambda\to\infty} \mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}^{\lambda}) = \mathbf{0}$$

- If $\mathbf{X}$ is an orthonormal matrix, then $\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}) = \sigma^2\mathbf{I}_{p\times p}$ and

$$\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}^{\lambda}) = \frac{\sigma^2}{(1+\lambda)^2}\mathbf{I}_{p\times p}$$

Variance comparison

- The difference

$$\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}) - \mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}^{\lambda})$$

  is non-negative definite
- In words, the variance of the OLS estimator is larger than of the ridge estimator (in the sense that their difference is not-negative definite)
- The variance inequality

$$\mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}) \succeq \mathbb{V}\mathrm{ar}(\hat{\boldsymbol{\beta}}^{\lambda})$$

  can be interpreted in terms of the uncertainty of the estimate

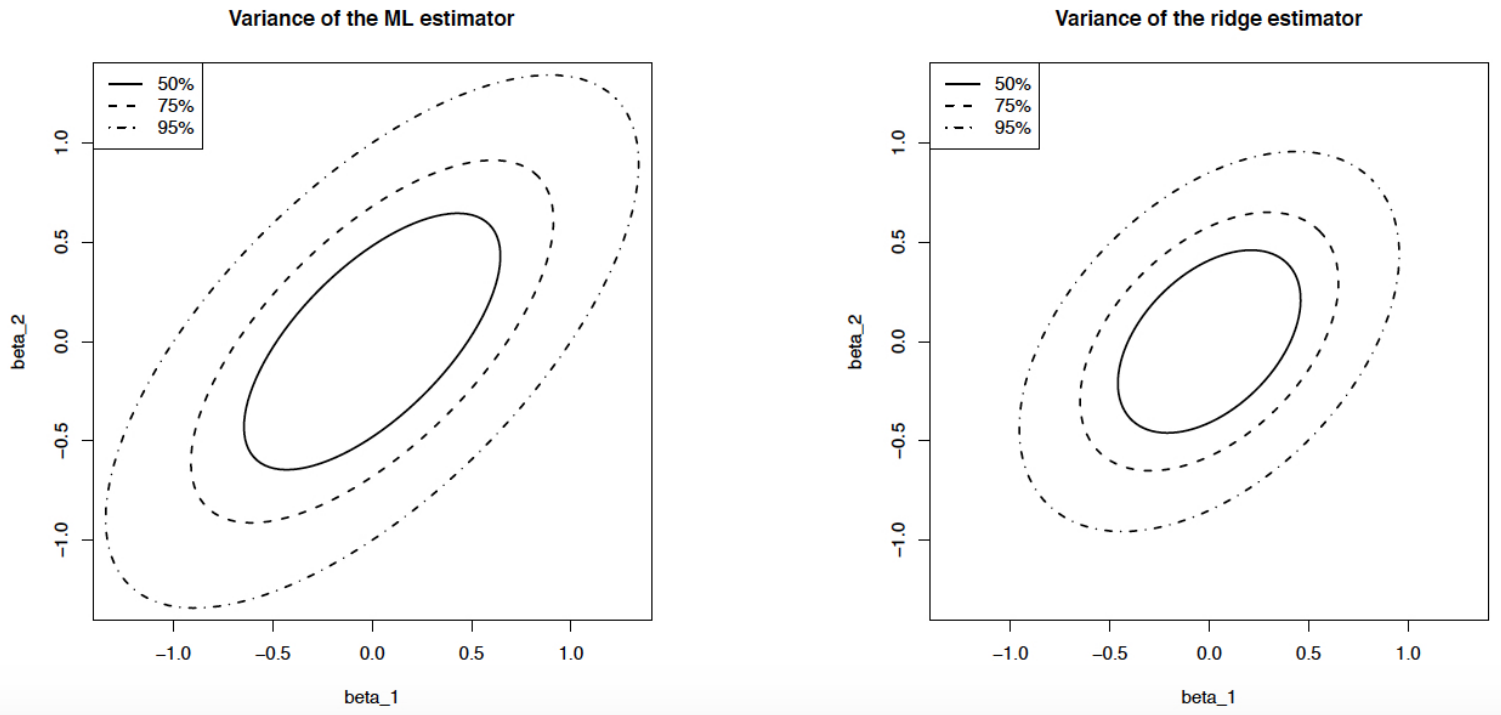
Example 1.5 *Variance comparison*
Consider the design matrix:

$$\mathbf{X} = \begin{pmatrix} -1 & 2 \\ 0 & 1 \\ 2 & -1 \\ 1 & 0 \end{pmatrix}.$$

The variances of the ML and ridge (with $\lambda = 1$) estimates of the regression coefficients then are:

$$\text{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2 \begin{pmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{pmatrix} \quad \text{and} \quad \text{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2 \begin{pmatrix} 0.1524 & 0.0698 \\ 0.0698 & 0.1524 \end{pmatrix}.$$

These variance can be used to construct confidence intervals of the estimates. The 50%, 75% and 95% confidence intervals for the ML and ridge estimates are plotted in Figure 1.2. In line with inequality (1.3) the confidence intervals of the ridge estimate are smaller than that of the ML estimate. □



Source: van Wieringen (2015) p. 8 Figure 1.2

Penalized estimation

- The ad-hoc fix of Hoerl and Kennard (1970) to super-collinearity of the design matrix (and, consequently the singularity of $\mathbf{X}^\top\mathbf{X}$) has been motivated post-hoc
- The ridge estimator minimizes the ridge loss function

$$\begin{aligned} & \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2 + \lambda\|\boldsymbol{\beta}\|_{\ell_2}^2 \\ = & \sum_{i=1}^{n}(y_i - x_i\boldsymbol{\beta})^2 + \lambda\sum_{j=1}^{p}\beta_j^2 \end{aligned}$$

  where $\|\underset{p\times 1}{v}\|_{\ell_2} = \sqrt{\sum_{j=1}^{p} v_j^2}$ denotes the ℓ_2 norm
- This loss function is the traditional residual sum-of-squares (RSS) $\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2$ augmented with a penalty $\lambda\sum_{j=1}^{p}\beta_j^2$

Penalized estimation

- The minimum of the RSS is attained at $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}$
- The minimum of the ridge penalty is attained at $\boldsymbol{\beta} = \mathbf{0}$
- The $\boldsymbol{\beta}$ that minimizes the ridge loss function balances the RSS and the penalty:

$$\hat{\boldsymbol{\beta}}^{\lambda} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\arg\min} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2 + \lambda \|\boldsymbol{\beta}\|_{\ell_2}^2$$

- The effect of the penalty in this balancing act is to shrink the regression coefficients towards zero, its minimum

Constrained estimation

- The penalized minimization problem

$$\min_{\boldsymbol{\beta}\in\mathbb{R}^p} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2 + \lambda\|\boldsymbol{\beta}\|_{\ell_2}^2$$

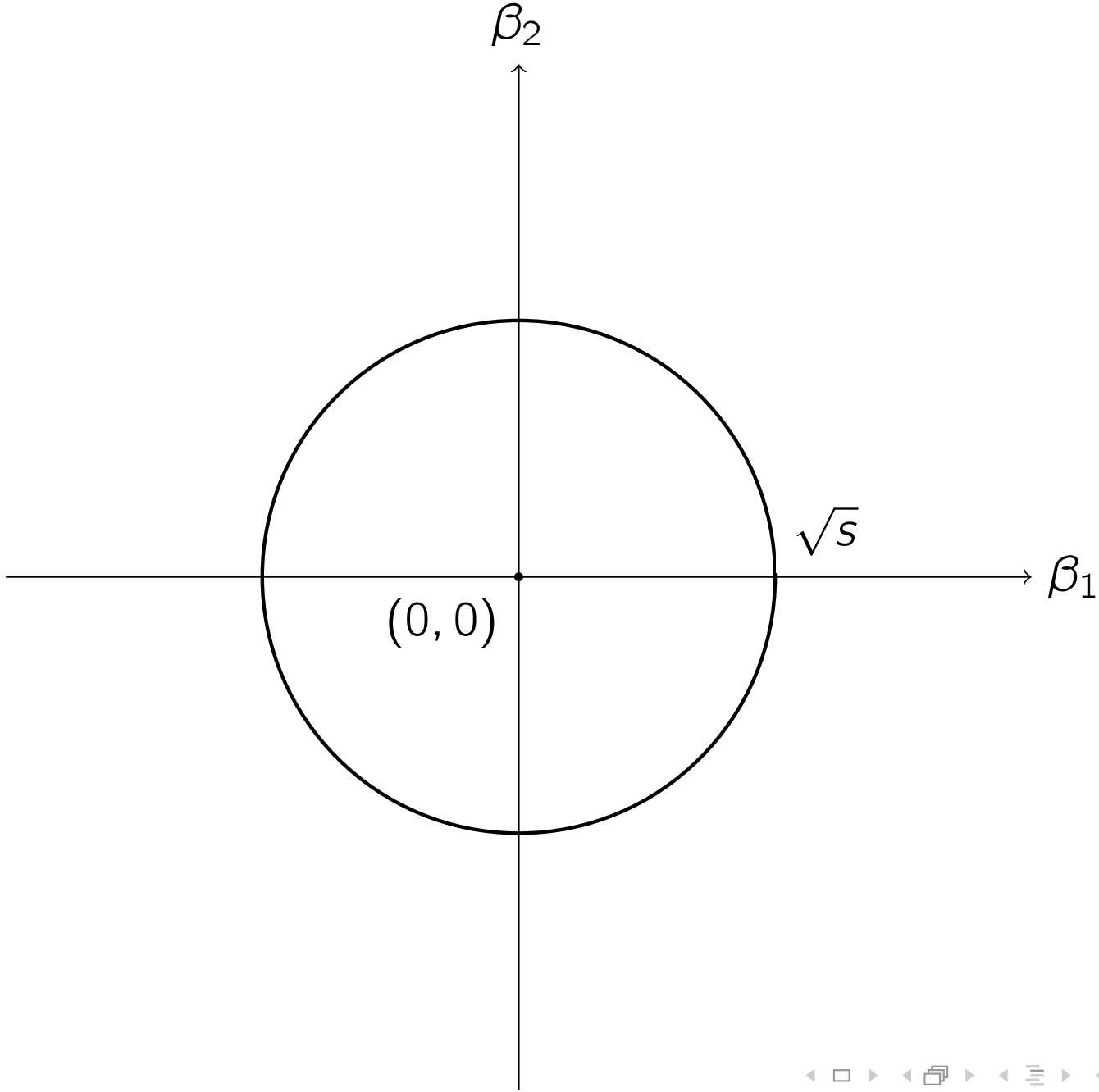
  can be reformulated into the following constrained minimization problem

$$\min_{\boldsymbol{\beta}:\|\boldsymbol{\beta}\|_{\ell_2}^2 \leq s} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2$$

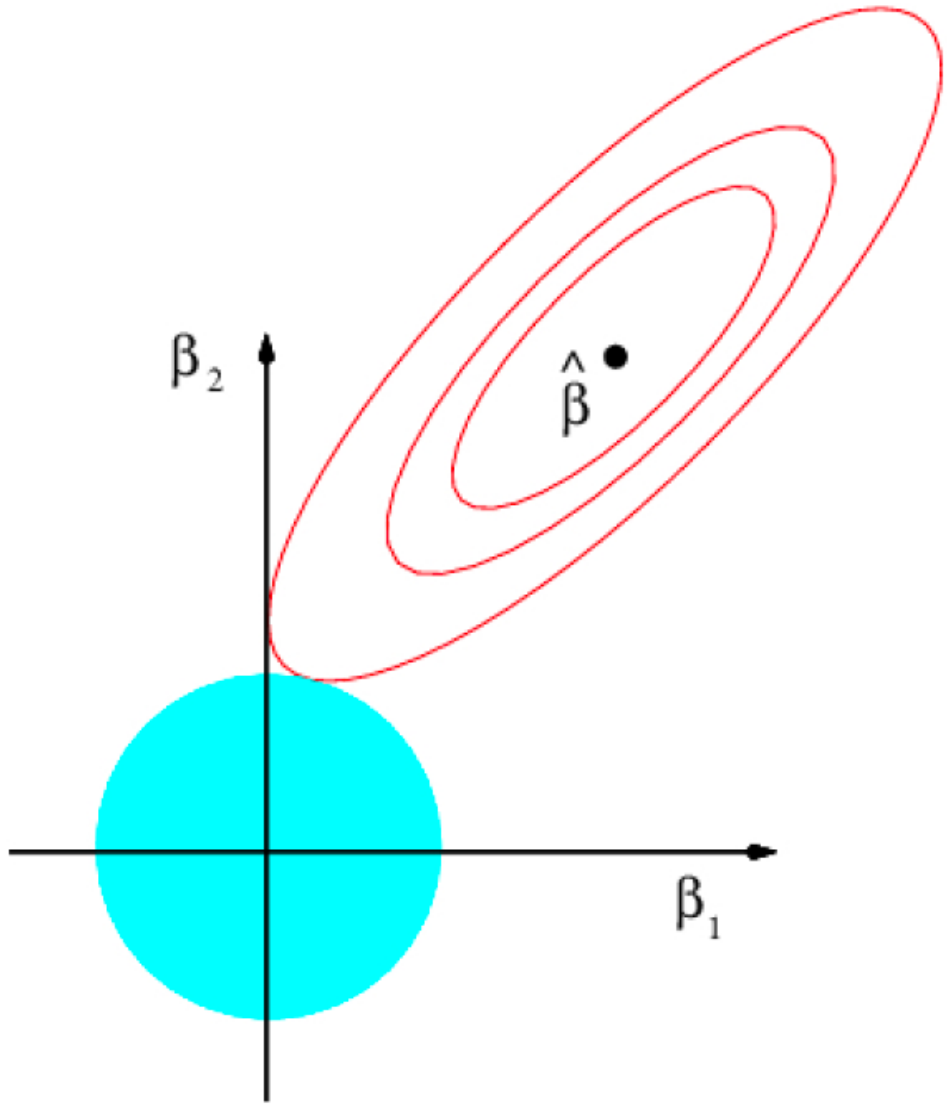
  for some suitable $s > 0$

- The constrained problem can be solved by means of the Karuch-Kuhn-Tucker (KTT) multiplier method, which minimizes a function subject to inequality constraint

Constraint $\beta_1^2 + \beta_2^2 \leq s$



Constrained estimation



Source: Hastie et al. (2009) p. 71

Penalized and constrained problems

- There is a one-to-one correspondence between the penalized problem and the constrained problem
- For each value s, there is a corresponding value λ that yields the same solution
- Conversely, the solution $\hat{\boldsymbol{\beta}}^{\lambda}$ to the penalized problem solves the constrained problem with $s = \|\hat{\boldsymbol{\beta}}^{\lambda}\|_{\ell_2}^2$

Overfitting in high-dimensions

- The relevance of viewing the ridge regression estimator as the solution to a constrained estimation problem becomes obvious when considering a typical threat to high-dimensional data analysis: overfitting
- Overfitting refers to the phenomenon of modelling the noise rather than the signal
- In high-dimensional settings overfitting is a real threat. The number of predictors exceeds the number of observations. It is thus possible to form a linear combination of the predictors that perfectly explains the response, including the noise
- Large estimates of regression coefficients (in absolute value) are often an indication of overfitting
- The estimation procedure with a constraint on the regression coefficients is a simple remedy to large parameter estimates. As a consequence it decreases the probability of overfitting

Example 1.6 *(Overfitting)*
Consider an artificial data set comprising of ten observations on a response Y_i and nine covariates $X_{i,j}$. All covariate data are sampled from the standard normal distribution: $X_{i,j} \sim \mathcal{N}(0,1)$. The response is generated by $Y_i = X_{i,1} + \varepsilon_i$ with $\varepsilon_i \sim \mathcal{N}(0, 1/4)$. Hence, only the first covariate contributes to the response.

The regression model :

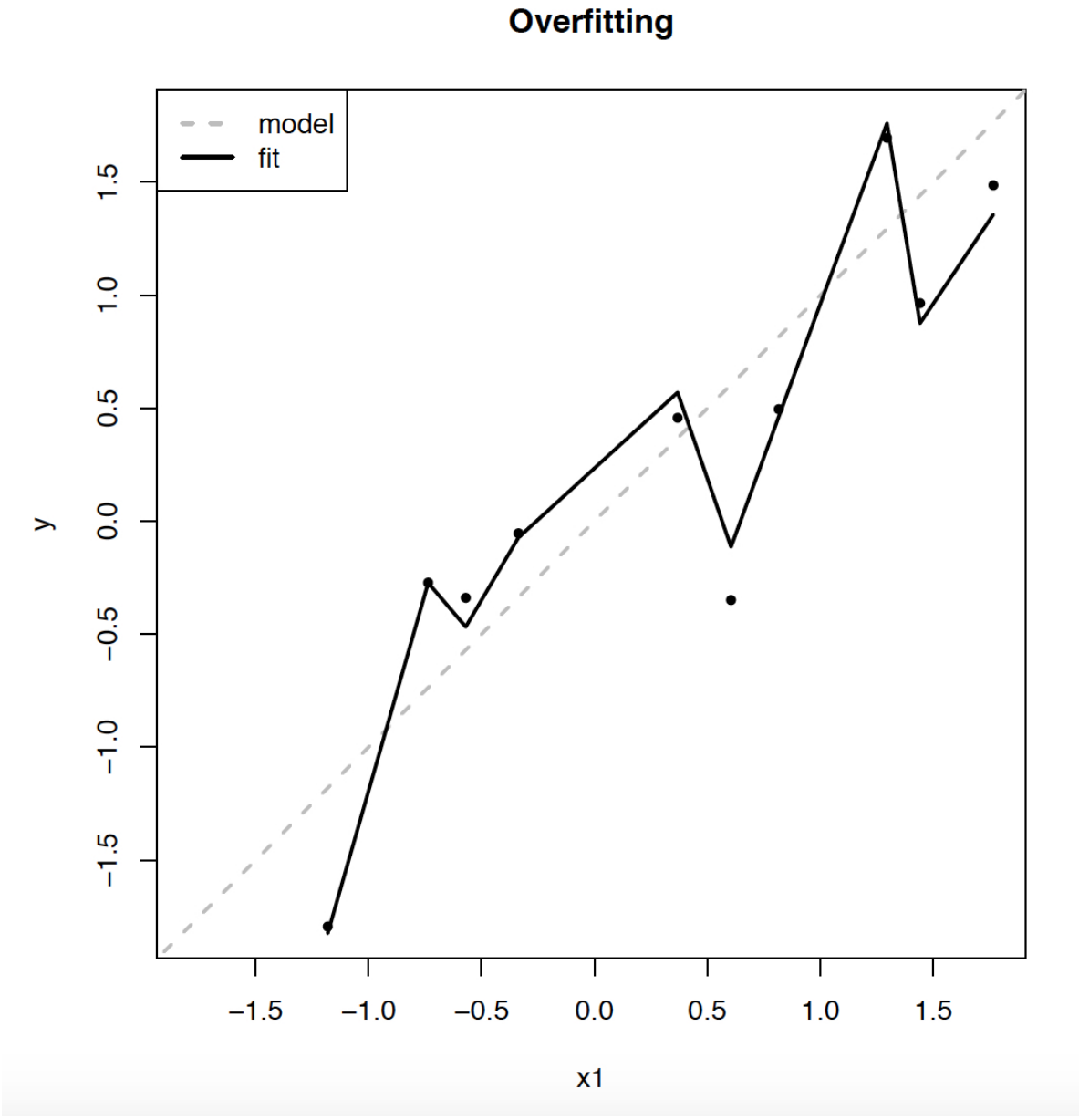
$$Y_i \quad = \quad \sum_{j=1}^{9} X_{i,j}\beta_j + \varepsilon_i$$

is fitted to the artificial data using `R`. This yields the regression parameter estimates:

$$\hat{\boldsymbol{\beta}}^\top \quad = \quad (0.048, -2.386, -5.528, 6.243, -4.819, 0.760, -3.345, -4.748, 2.136).$$

As $\boldsymbol{\beta}^\top = (1, 0, \ldots, 0)$, many regression coefficient are clearly over-estimated.

Source: van Wieringen (2015) p. 11



Source: van Wieringen (2015) p. 10 Figure 1.3

Perfect overfit: $p = n$

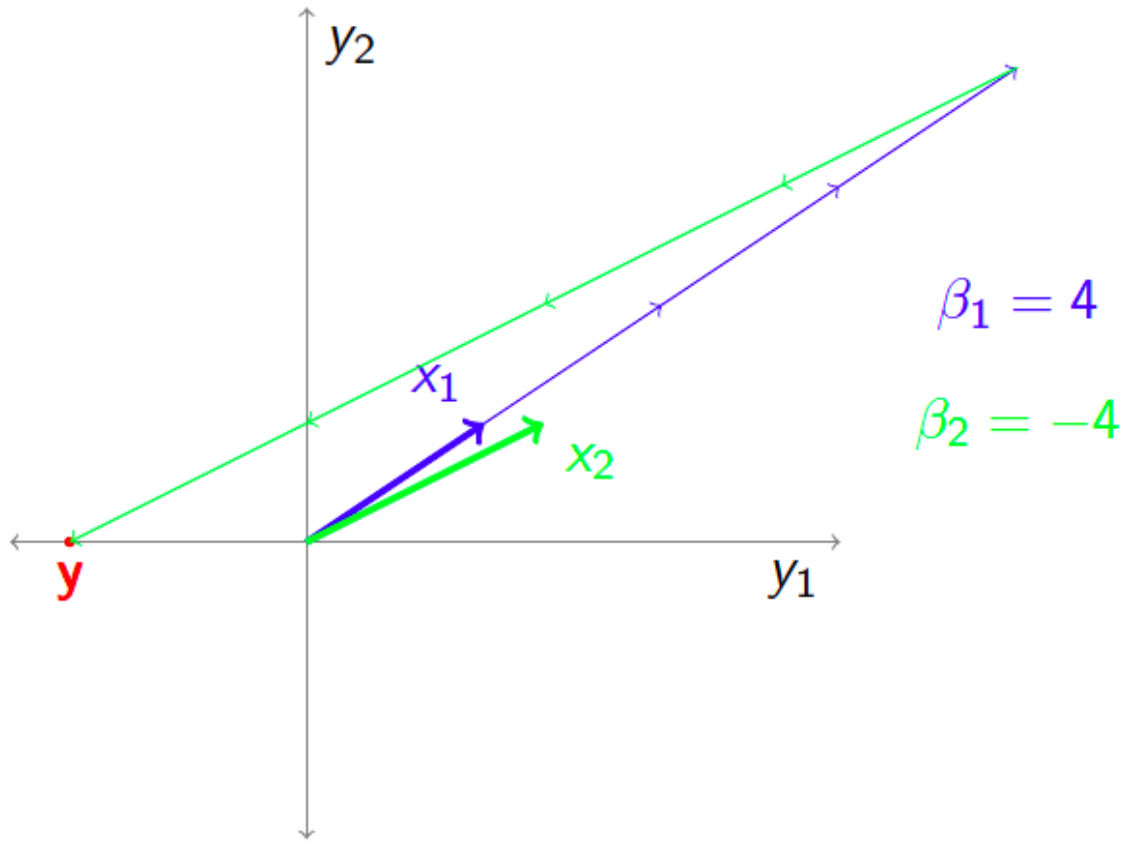
```
y = c(-1,0); x1 = c(.75,.5); x2 = c(1,.5)
summary(lm(y~0+x1+x2))

Residuals:
ALL 2 residuals are 0: no residual degrees of freedom!

Coefficients:
   Estimate Std. Error t value Pr(>|t|)
x1        4         NA      NA       NA
x2       -4         NA      NA       NA

Residual standard error: NaN on 0 degrees of freedom
Multiple R-squared:      1,Adjusted R-squared:    NaN
F-statistic:   NaN on 2 and 0 DF,  p-value: NA
```

Perfect overfit: $p = n$



Source: J. Goeman *Lasso, Ridge and Cross-validation* slides

Shrinkage

Estimates are shrunk towards zero

Consequence

- Introduces bias
- Reduces variance

Predicting a Gaussian random variable

- $Y = \mu + \varepsilon$ with $\varepsilon \sim \mathcal{N}(0, \sigma^2)$
- Training data: $Y_1, \ldots, Y_n$
- Sample mean: $\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i$
- Bias-Variance decomposition

$$\begin{aligned} \mathbb{E}\{[Y - \bar{Y}]^2\} &= \sigma^2 + [\mathbb{B}\mathrm{ias}(\bar{Y})]^2 + \mathbb{V}\mathrm{ar}(\bar{Y}) \\ &= \sigma^2 + 0 + \sigma^2/n \end{aligned}$$

Question

Rao-Blackwell theorem says that $\bar{Y}$ has lower variance than any other unbiased estimator. Is $\bar{Y}$ the optimal prediction for Y ?

Shrunken sample mean

- Shrunken sample mean: $\hat{Y} = \lambda \bar{Y}$ with $\lambda \in [0, 1]$
- Bias-Variance decomposition

$$\begin{aligned}\mathbb{E}\{[Y - \hat{Y}]^2\} &= \sigma^2 + [\mathbb{B}\mathrm{ias}(\hat{Y})]^2 + \mathbb{V}\mathrm{ar}(\hat{Y}) \\ &= \sigma^2 + [\mu - \lambda\mu]^2 + \lambda^2(\sigma^2/n)\end{aligned}$$

- Solving $\frac{\partial}{\partial\lambda}\mathbb{E}\{[Y - \hat{Y}]^2\} = 0$ gives the value

$$\lambda = \frac{\mu^2}{\mu^2 + \sigma^2/n}$$

  that minimizes $\mathbb{E}\{[Y - \hat{Y}]^2\}$
- However, the optimal λ depends on unknown parameters

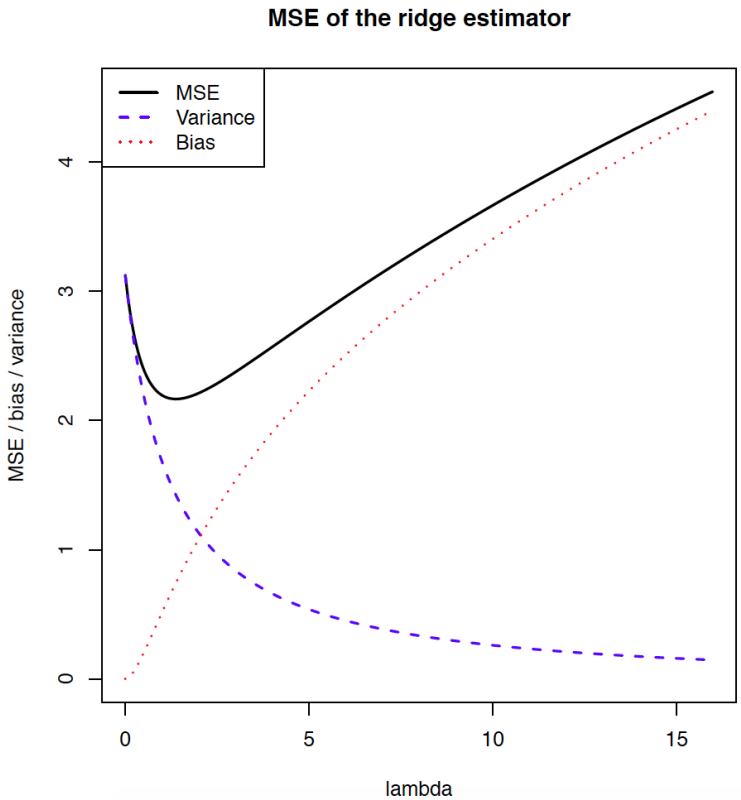
Theorem

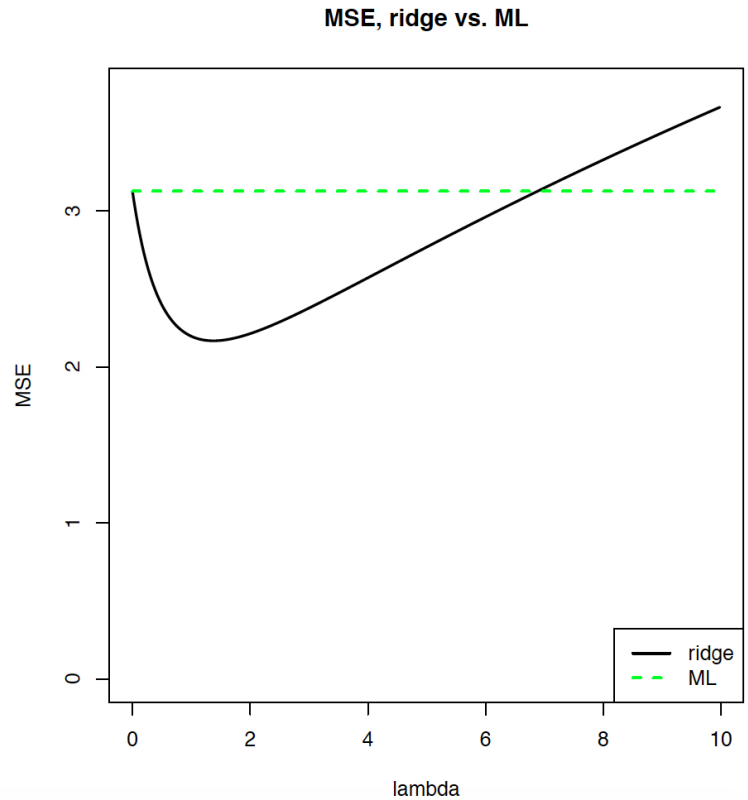
- There exists $\lambda > 0$ such that $(\mathbb{B}\mathrm{ias})^2 + \mathbb{V}\mathrm{ar}$ of the ridge regression estimator is lower than the OLS estimator (Theorem 2 of Theobald, 1974)
- For a certain value of λ, the decrease in variance of the ridge regression estimator exceeds the increase in its bias
- The optimal choice of λ depends on the quantities $\boldsymbol{\beta}$ and σ^2. These are unknown in practice
- If $\mathbf{X}$ is an orthonormal matrix, the bias-variance decomposition is

$$(\mathbb{B}\mathrm{ias})^2 + \mathbb{V}\mathrm{ar} = \frac{\lambda^2}{(1+\lambda)^2}\boldsymbol{\beta}^\mathsf{T}\boldsymbol{\beta} + \frac{p\sigma^2}{1+\lambda}$$

and the optimal choice is $\lambda = p\sigma^2/\boldsymbol{\beta}^\mathsf{T}\boldsymbol{\beta}$

Bias-variance trade-off





Source: van Wieringen (2015) p. 14 Figure 1.4

Degrees of freedom

- In in ordinary regression, model complexity can be measured by the degrees of freedom consumed by the model
- In ordinary regression, the degrees of freedom consumed by the model is $\mathrm{trace}(\mathbf{H}) = p$, the trace of the projection matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}$
- By analogy, the ridge version of $\mathbf{H}$ (which is not a projection matrix) is

$$\mathbf{H}^\lambda = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X} + \lambda\mathbf{I}_{p\times p})^{-1}\mathbf{X}^\mathsf{T}$$

- The degrees of freedom consumed by ridge regression (effective degrees of freedom) is

$$\mathrm{trace}(\mathbf{H}^\lambda) = q$$

- The degrees of freedom consumed by ridge regression is monotone in λ. In particular

$$\lim_{\lambda\to\infty} \mathrm{trace}(\mathbf{H}^\lambda) = 0$$

Choice of the penalty parameter

- Throughout the introduction of ridge regression and the subsequent discussion of its properties the penalty parameter λ is considered known or 'given'
- In practice, it is unknown and the user needs to make an informed decision on its value
- Information criteria measure the balance between model fit and model complexity (degrees of freedom):
  $\text{AIC} = n \log(\text{MSE}_{\text{Tr}}) + 2q$, $\text{BIC} = n \log(\text{MSE}_{\text{Tr}}) + q \log(n)$
- Generalized cross-validation $= \text{MSE}_{\text{Tr}} / (1 - q/n)^2$
- Cross-validation
- Cross-validated log-likelihood (R package `penalized`)

Prostate cancer data

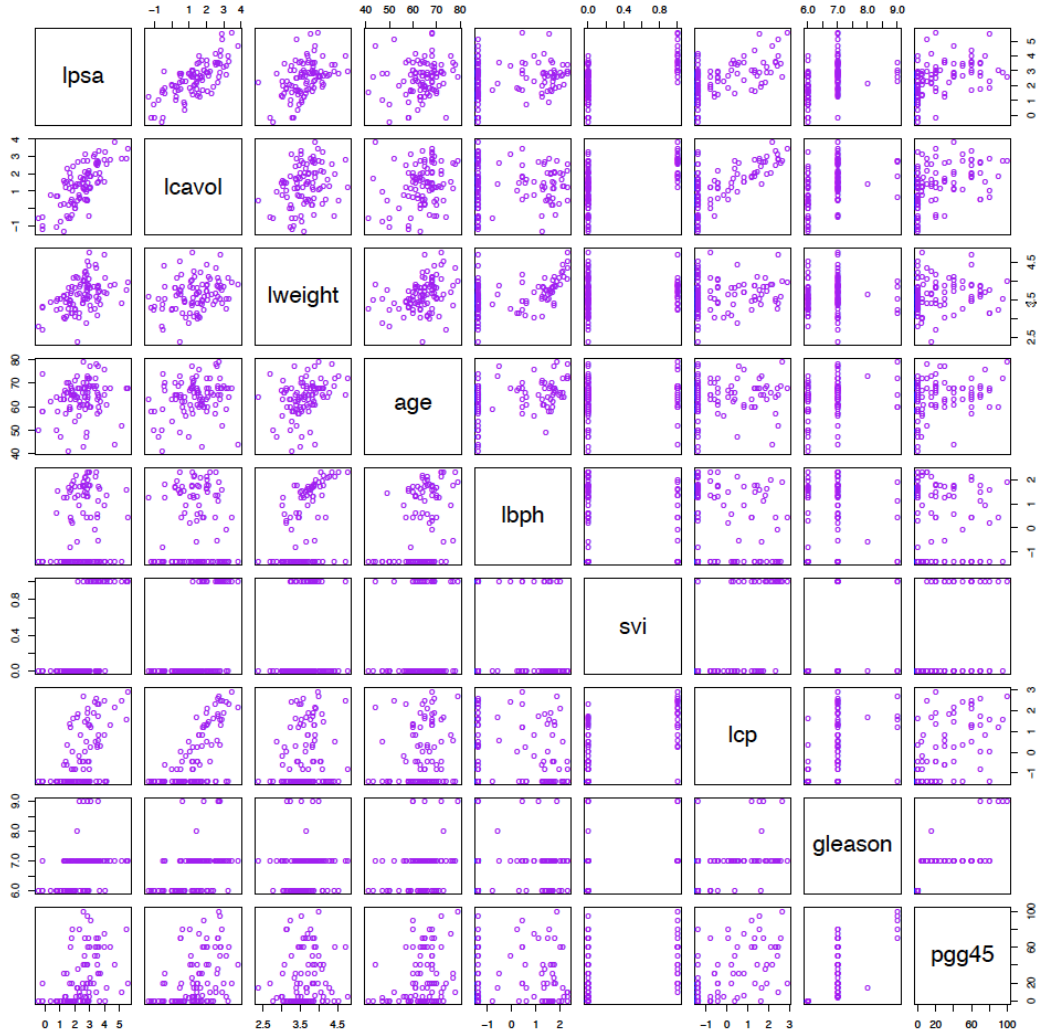


FIGURE 1.1. *Scatterplot matrix of the prostate cancer data. The first row shows the response against each of the predictors in turn. Two of the predictors,* `svi` *and* `gleason`*, are categorical.*

Prostate cancer data

Response

`lpsa` for $n = 67$ subjects

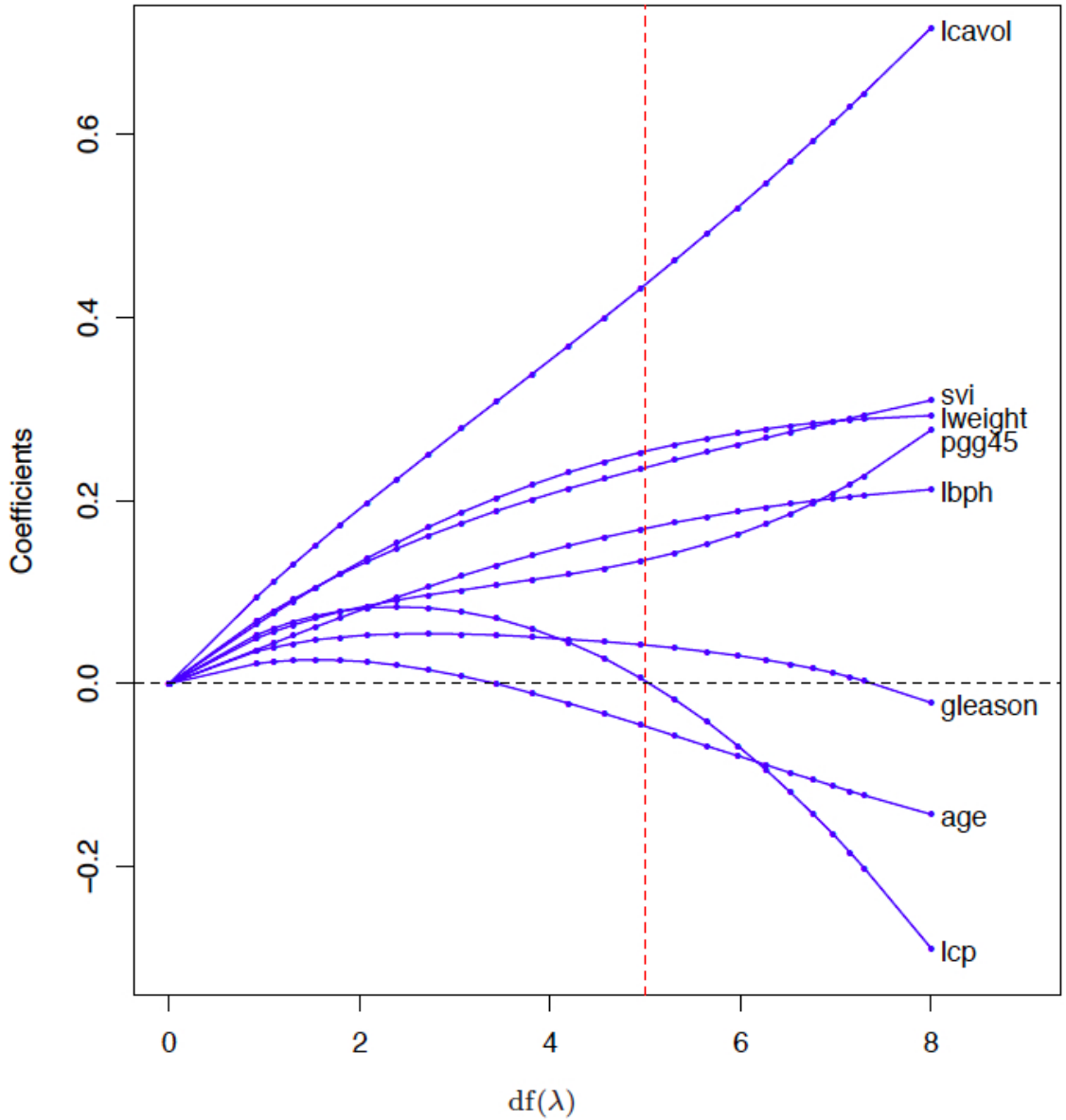
Predictors

`1`, `lcavol`, `lweight`, `age`, `lbph`, `svi`, `lcp`, `gleason`, `pgg45`

Test set

$m = 30$ subjects

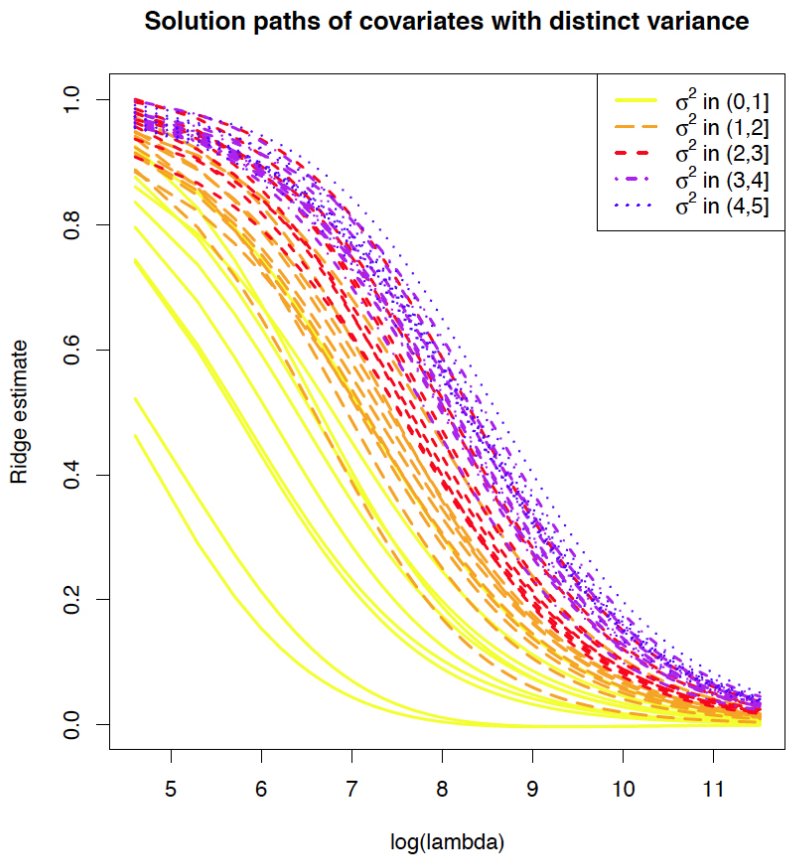
Prostate Cancer Data

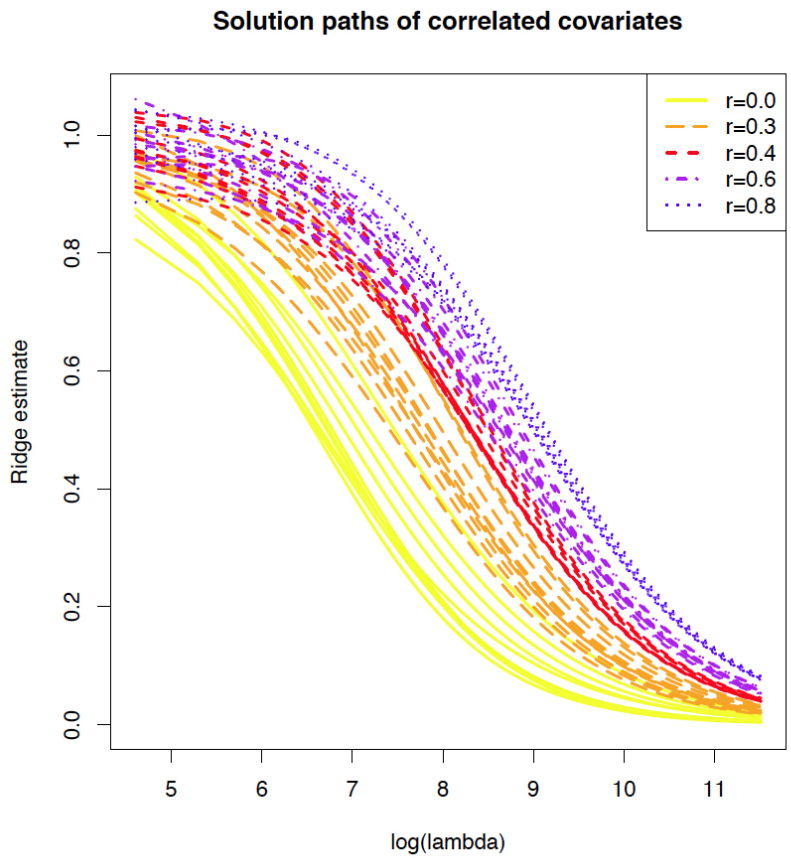


Source: Hastie et al (2009) p. 65

Standardization

- Usually the intercept is not included in the penalty, unless you have some reason to think that the mean of the response should be 0
- Usually both the response and the predictors are standardized to have mean 0 and standard deviation 1 prior to the execution of the ridge regression
- This is because ridge regularization path of coefficients corresponding to predictors with a large variance dominate those with low variances
- Ridge regression is not invariant to scaling: ridge estimates prior or posterior to scaling of predictors do not simply differer by a factor





Source: van Wieringen (2015) p. 19 Figure 1.6

Ridge regression and collinearity

- Suppose that X_1 and X_2 are strongly positively correlated
- We can write the linear model as

$$\mathbb{E}(Y|X_1, X_2) = \beta_1 X_1 + \beta_2 X_2$$
$$\mathbb{E}(Y|X_1, X_2) + \gamma(X_1 - X_2) = (\beta_1 + \gamma)X_1 + (\beta_2 - \gamma)X_2$$

  where $X_1 - X_2 \approx 0$ because $X_1 \approx X_2$
- Then $3X_1 + 3X_2$, $4X_1 + 2X_2$, $5X_1 + X_2$ etc. all have very similar fit, and least squares estimation can't easily distinguish them

Ridge regression and collinearity

- For large enough λ, ridge regression favors the fits that minimize
$$(\beta_1 + \gamma)^2 + (\beta_2 - \gamma)^2$$
- This expression is minimized at $\gamma = (\beta_2 - \beta_1)/2$, giving
$$\frac{(\beta_1 + \beta_2)}{2} X_1 + \frac{(\beta_1 + \beta_2)}{2} X_2$$
- Ridge regression favors coefficient estimates for which strongly correlated predictors have similar effect sizes

Ridge regression and collinearity

```
n = 20
set.seed(123)
x1 <- rnorm(n)
x2 <- rnorm(n,mean=x1,sd=.01)
y <-  10 + 3*x1 + 3*x2 + rnorm(n)

lm(y~x1+x2)$coef
(Intercept)          x1          x2
  10.127965   -7.155559   13.040228

require(MASS)
lm.ridge(y~x1+x2, lambda=1)
                   x1         x2
10.144123  2.858528  2.875259
```

Source: P. Breheny

glmnet

Read *Glmnet Vignette* by Hastie and Qian
https://web.stanford.edu/~hastie/glmnet/glmnet_alpha.html

```
glmnet(X, y,
family="gaussian",
alpha = 0, # default = 1 (LASSO)
nlambda = 100,
standardize = TRUE, # both response and predictors
intercept=TRUE
)
```

Outline

Sp rsi y

- Bet on sparsity principle: in high dimensions, it is wise to proceed under the assumption that only a small number of predictors have an effect, i.e. have $\beta_j \neq 0$
- We would like our estimator $\hat{\boldsymbol{\beta}}$ to be sparse, meaning that most $\hat{\beta}_j$'s are zero
- Ridge regression estimator $\hat{\boldsymbol{\beta}}^{\lambda}$ is not sparse
- Variable selection methods use the data in order decide which predictors have $\beta_j \neq 0$

Source: Steven L. Scott (for the title)

The variable selection problem

Select the "optimal" subset of predictors among $X_1, \ldots, X_p$

Bias-variance trade-off

- Including many predictors leads to low bias and high variance
- Including few predictors leads to high bias and low variance

Number of possible subsets

With p predictors, there are 2^p possible subsets

Best subsets selection

Solve the constrained minimization problem

$$\min_{\boldsymbol{\beta}:\|\boldsymbol{\beta}\|_{\ell_0}\leq s} \|\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2$$

where $\|\boldsymbol{\beta}\|_{\ell_0} = \sum_{j=1}^{p} I\{\beta_j \neq 0\}$ is the ℓ_0 norm

The solution is known as best subsets selection

However, the above problem is nonconvex (NP-hard): it requires searching through all 2^p subsets

Best subsets selection algorithm

Set B_0 as the null model (only intercept)

For $k = 1, \ldots, p$:

1. Fit all $\binom{p}{k}$ models that contain exactly k predictors
2. Pick the *best* among these $\binom{p}{k}$ models, and call it B_k, where *best* is defined having the smallest residual sum of squares $\text{RSS} = n\text{MSE}_{\text{Tr}}$

Select a single best model from among $B_0, B_1, \ldots, B_p$ using AIC, BIC, cross-validation, etc.

Prostate cancer data

Response

`lpsa` for $n = 67$ subjects

Predictors

`1`, `lcavol`, `lweight`, `age`, `lbph`, `svi`, `lcp`, `gleason`, `pgg45`

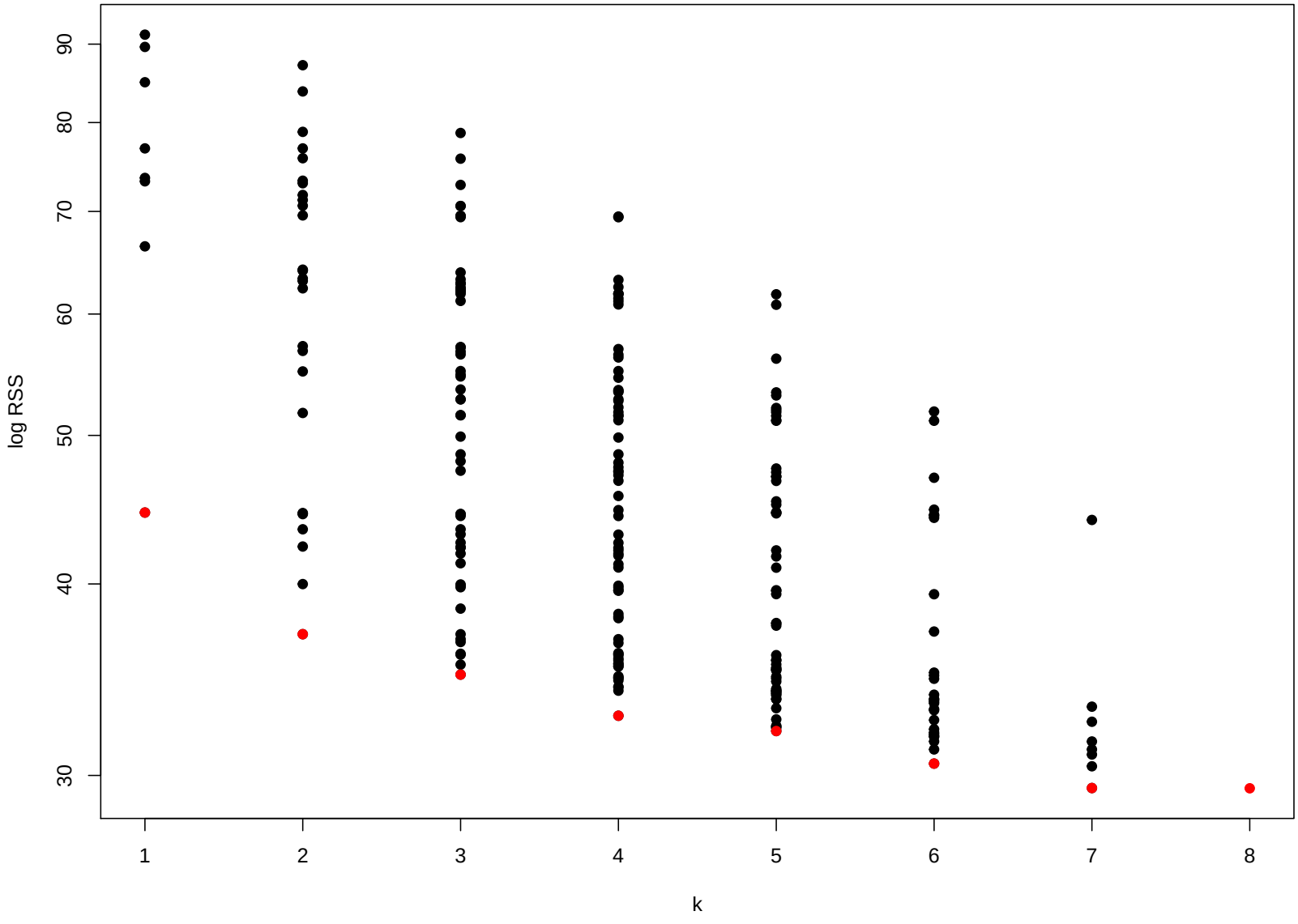
Variable selection problem

Select the "optimal" subset of predictors

Number of possible subsets

$2^p = 256$

Residual sum of squares

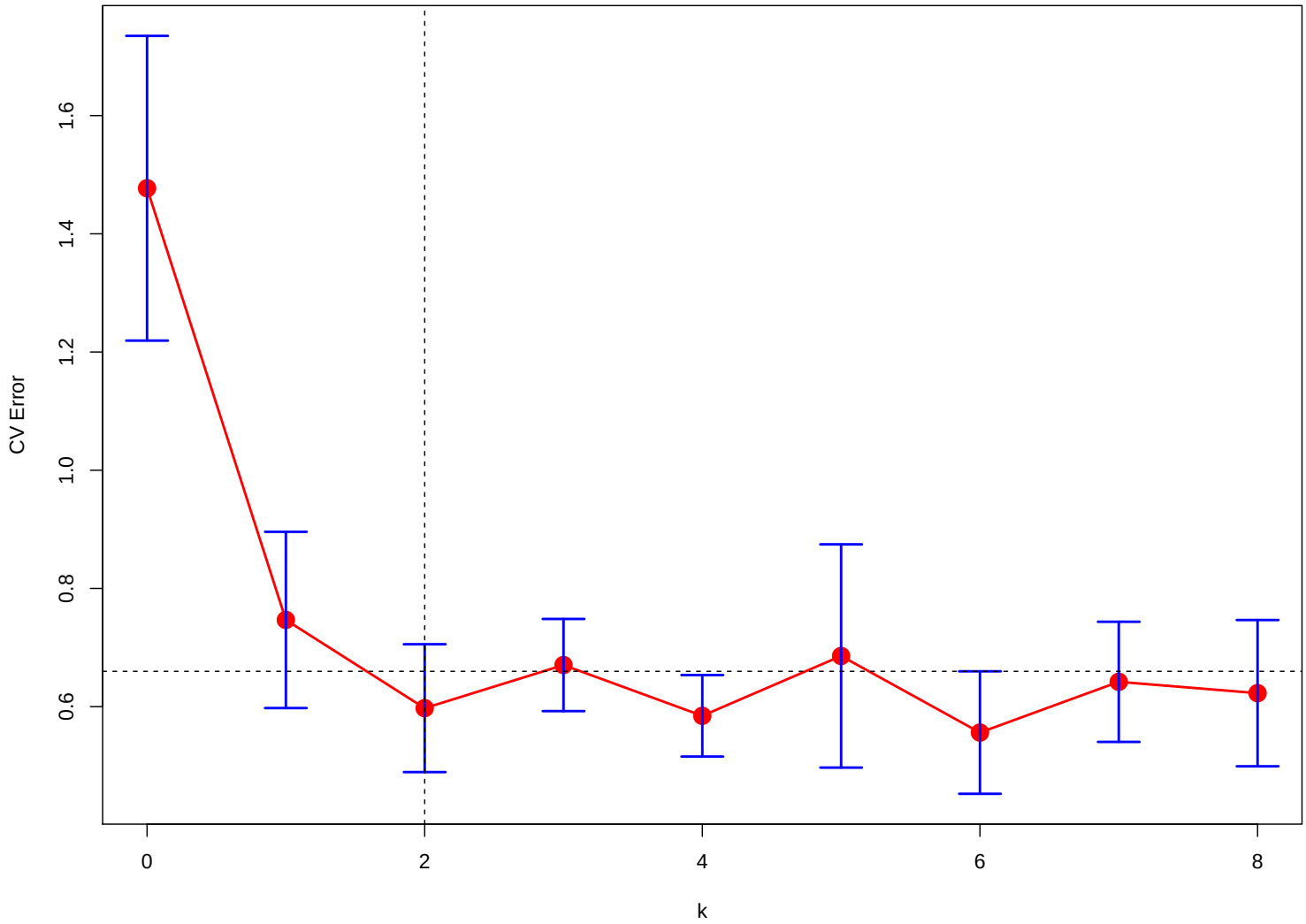


Best subsets

k	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	RSS	Cp	BIC
1	•								44.53	24.77	-43.26
2	•	•							37.09	12.11	-51.30
3	•	•			•				34.91	9.80	-51.16
4	•	•		•	•				32.81	7.68	-51.09
5	•	•		•	•			•	32.07	8.21	-48.43
6	•	•		•	•	•		•	30.54	7.19	-47.50
7	•	•	•	•	•	•		•	29.44	7.02	-45.76
8	•	•	•	•	•	•	•	•	29.43	9.00	-41.58

Best k?

5-fold CV with 1-sd rule



Backward Stepwise Selection

Set S_p as the full model (all p predictors)
For $k = p, p-1, \ldots, 1$:

1. Consider all k models that contain all but one of the predictors in S_k, for a total of $k-1$ predictors
2. Choose the *best* among these k models and call it S_{k-1}, where *best* is defined having the smallest RSS

Select a single best model from among $S_0, S_1, \ldots, S_p$ using AIC, BIC, cross-validation, etc.

- *greedy algorithm* sub-optimal to Best Subsets Selection but computationally efficient
- applicable only when $n > p$

Forward stepwise selection

Set S_0 as the null model (only intercept)
For $k = 0, \ldots, \min(n-1, p-1)$:

1. Consider all $p - k$ models that augment the predictors in S_k with one additional predictor
2. Choose the *best* among these $p - k$ models and call it S_{k+1}, where *best* is defined having the smallest RSS

Select a single best model from among $S_0, S_1, S_2, \ldots$ using AIC, BIC, cross-validation, etc.

- *greedy algorithm* sub-optimal to Best Subsets Selection but computationally efficient
- applicable also when $p > n$ to construct the sequence $S_0, S_1, \ldots, S_{n-1}$

Forward with AIC-based stopping rule

Set S_0 as the null model and $k = 0$

1. Consider all $p - k$ models that augment the predictors in S_k with one additional predictor
2. Choose the *best* among these $p - k$ models and call it S_{k+1}, where *best* is defined having the smallest AIC
3. If $\text{AIC}(S_{k+1}) < \text{AIC}(S_k)$, set $k = k + 1$ and go to ① , otherwise STOP

Forward with AIC-based stopping rule

k	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	AIC
1	•								-23.37
2	•	•							-33.62
3	•	•			•				-35.68
4	•	•		•	•				-37.83
5	•	•		•	•			•	-37.36

Outline

ℓ_q norm

$$\|\boldsymbol{\beta}\|_{\ell_q} = (|\beta_1|^q + \ldots + |\beta_p|^q)^{1/q} = (\sum_{j=1}^{p} |\beta_j|^q)^{1/q}$$

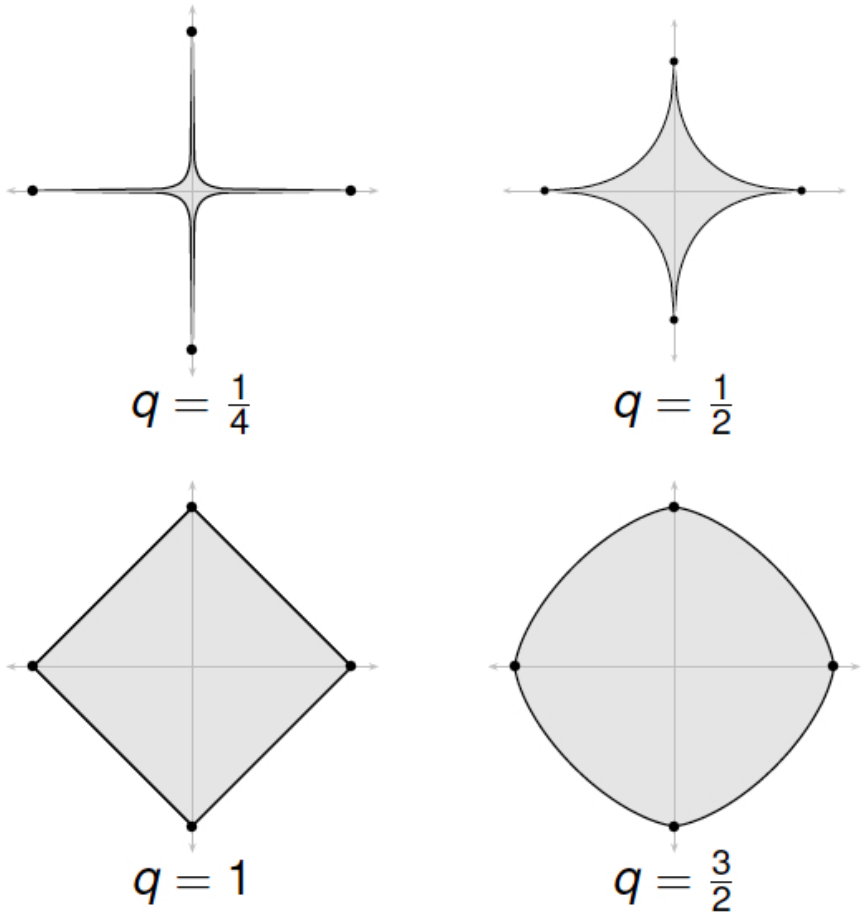
Which values of q are sensitive to sparsity?

$$\begin{array}{rrcccccc} \text{sparse:} & \boldsymbol{\alpha} & = (& 1 & , & 0 & , \ldots , & 0 &) \\ \text{not sparse:} & \boldsymbol{\beta} & = (& 1/\sqrt{p} & , & 1/\sqrt{p} & , \ldots , & 1/\sqrt{p} &) \end{array}$$

	BS $q = 0$	? $q = 1$	Ridge $q = 2$
$\|\boldsymbol{\alpha}\|_{\ell_q}$	1	1	1
$\|\boldsymbol{\beta}\|_{\ell_q}$	p	$\sqrt{p}$	1
sensitive?	yes	yes	no

Source: L. Wasserman

ℓ_q norm

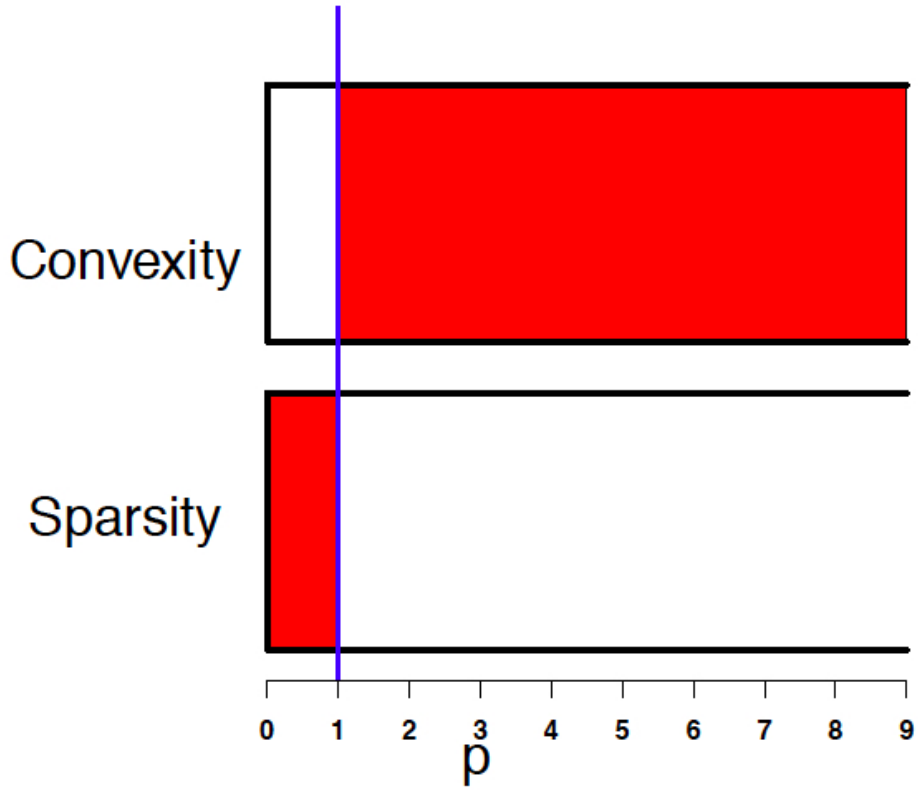


Source: L. Wasserman

Where Sparsity and Convexity Meet

Sensitivity to sparsity: $q \leq 1$

Convexity: $q \geq 1$



Source: L. Wasserman

Lasso

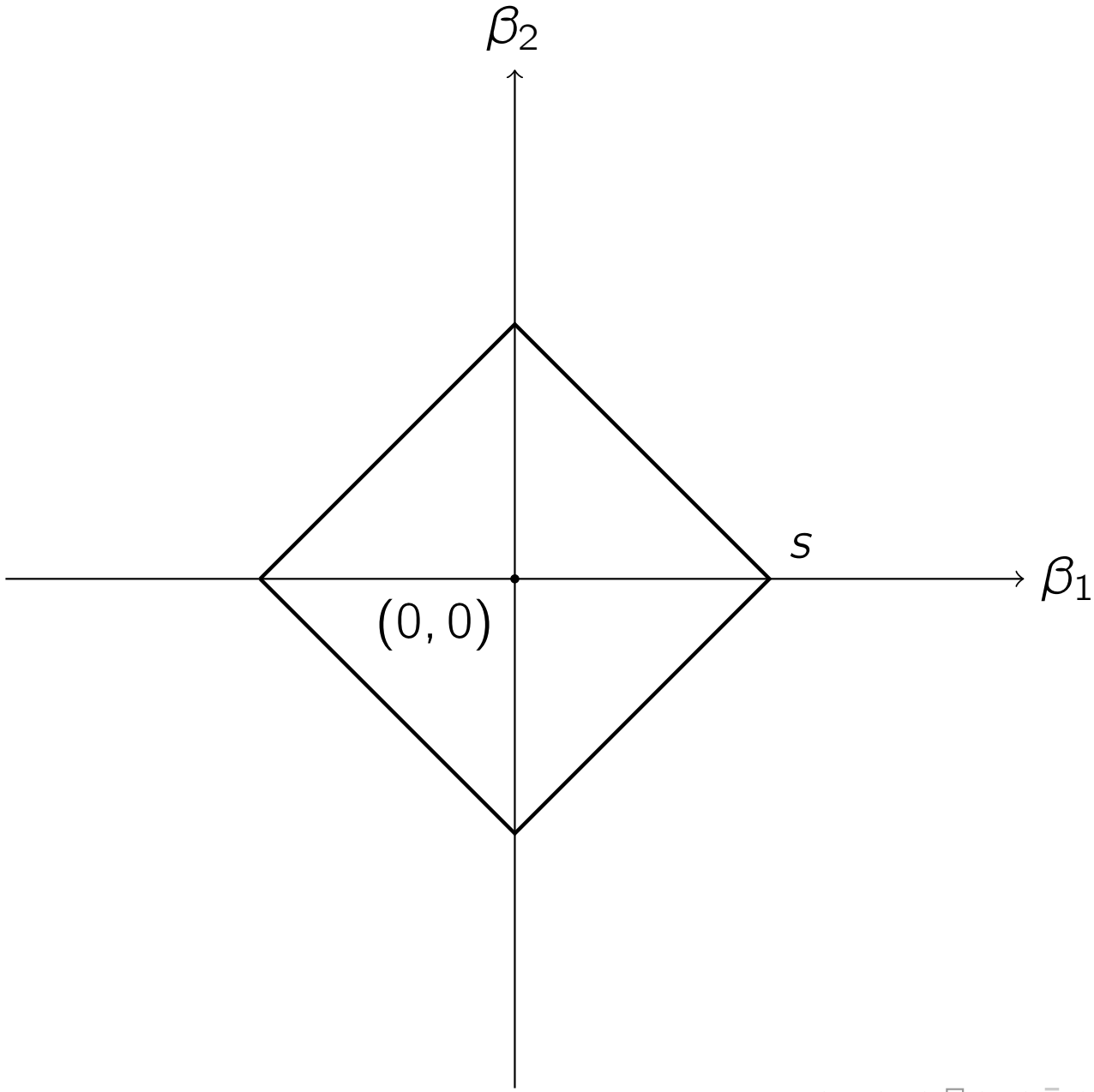
Solve the constrained minimization problem

$$\min_{\boldsymbol{\beta}:\|\boldsymbol{\beta}\|_{\ell_1}\leq s} \|\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2$$

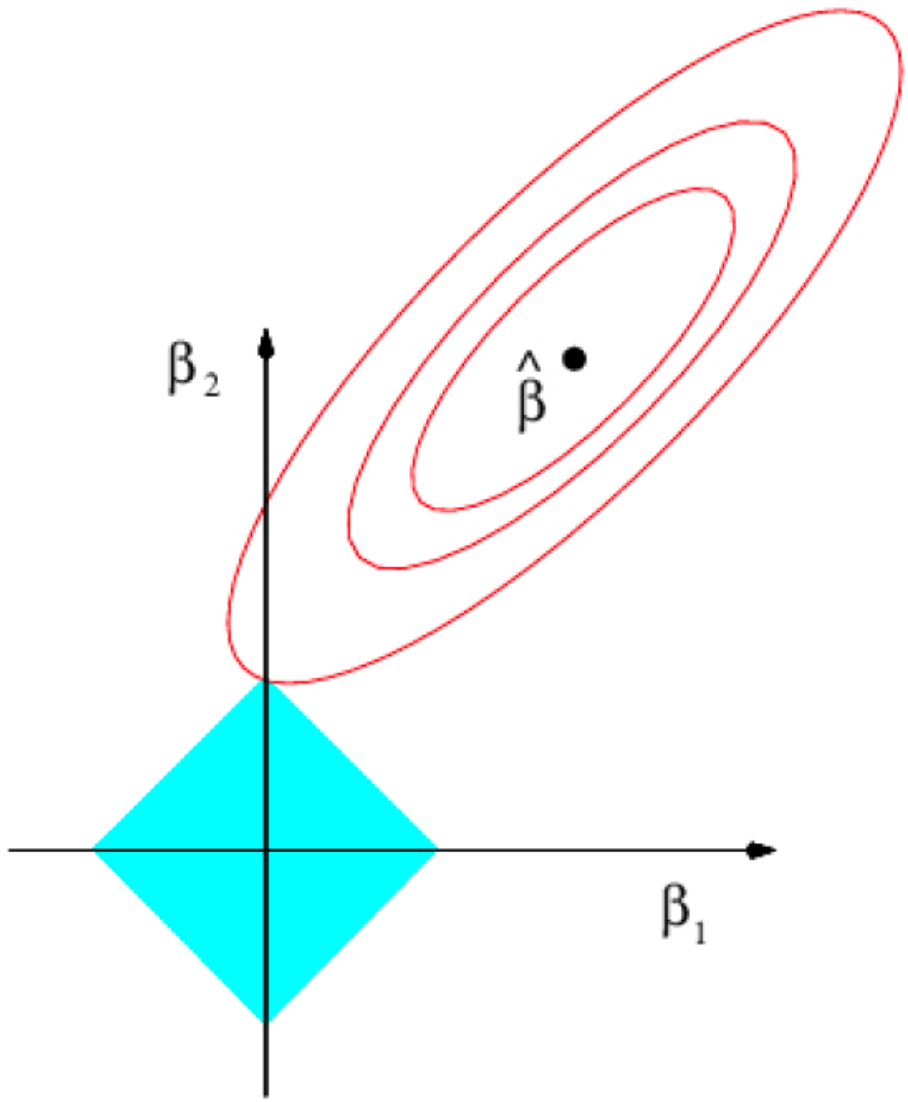
where $\|\boldsymbol{\beta}\|_{\ell_1} = \sum_{j=1}^{p} |\beta_j|$ is the ℓ_1 norm and $s \geq 0$

The solution is known as LASSO: Least Absolute Shrinkage and Selection Operator (Tibshirani, 1996)

Lasso constraint: $|\beta_1| + |\beta_2| \leq s$



Lasso: constrained estimation



Source: Hastie et al. (2009) p. 71

Shrinkage and Selection

Solve the penalized minimization problem

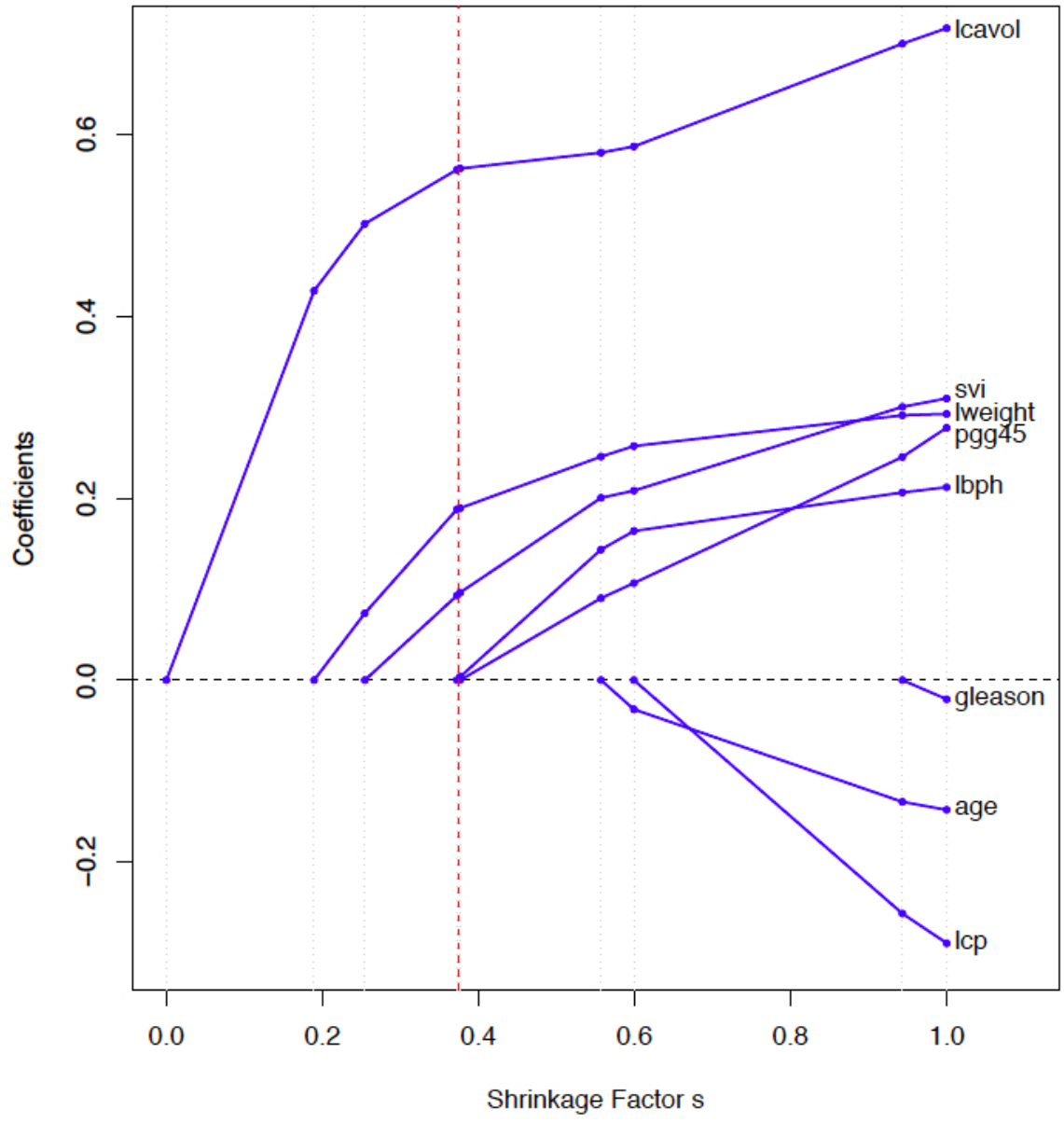
$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2 + \lambda \|\boldsymbol{\beta}\|_{\ell_1}$$

where $\lambda \geq 0$

Shrinkage
$\hat{\boldsymbol{\beta}}^{\lambda}$ is the lasso shrunken estimate

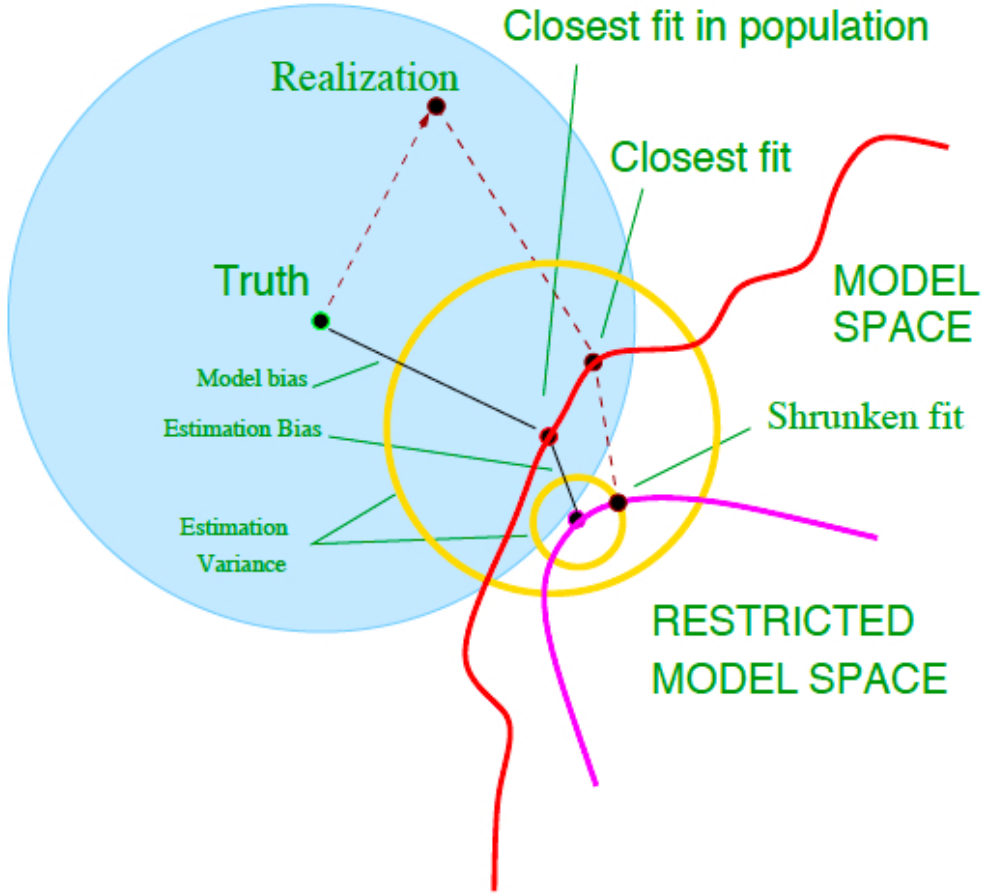
Selection
$\hat{S}^{\lambda} = \{X_j : \hat{\beta}_j^{\lambda} \neq 0\}$ is the set of selected predictors

Prostate Cancer Data



Source: Hastie et al (2009) p. 70

The bias-variance trade-off



Source: Hastie et al. (2009) p. 225