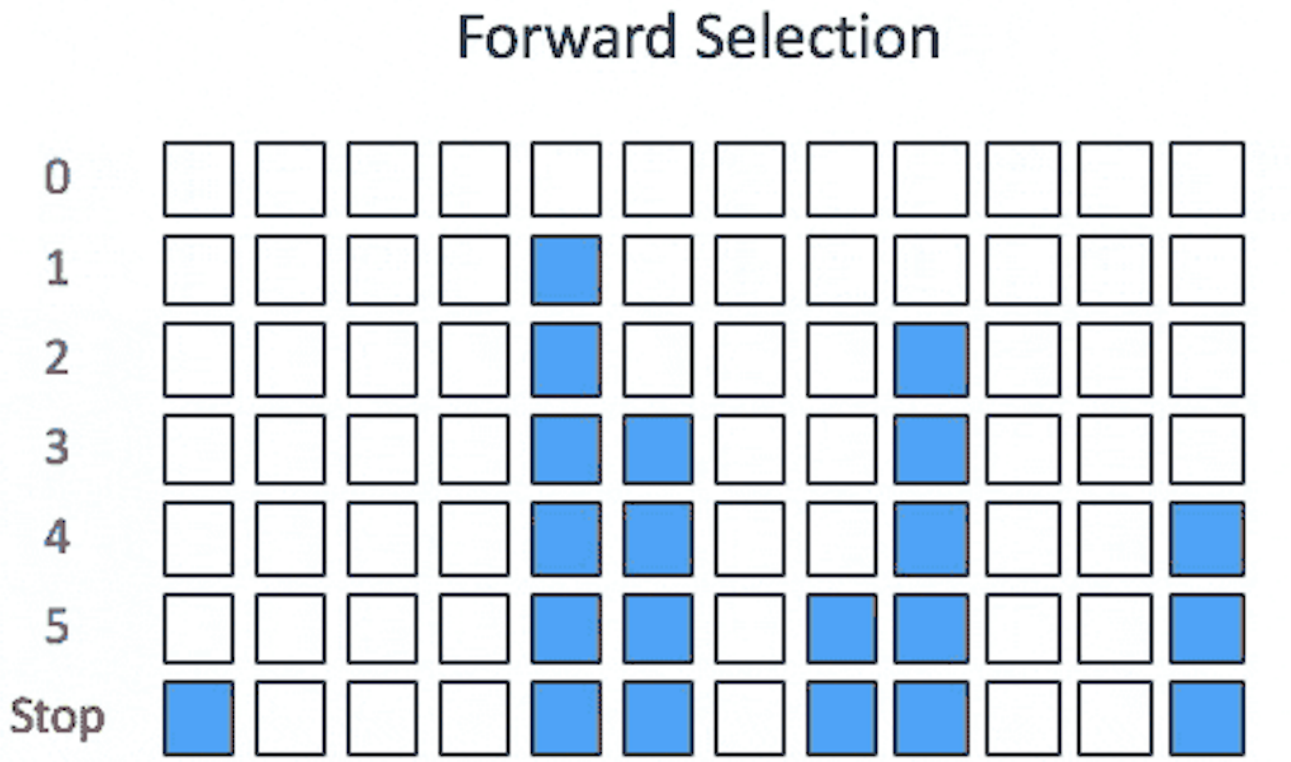
STAT 380:
Variable Selection, Ridge, and Lasso Regression

An Example using .... Data

United Arab Emirates University

Variable Selection in Regression

Forward variable selection



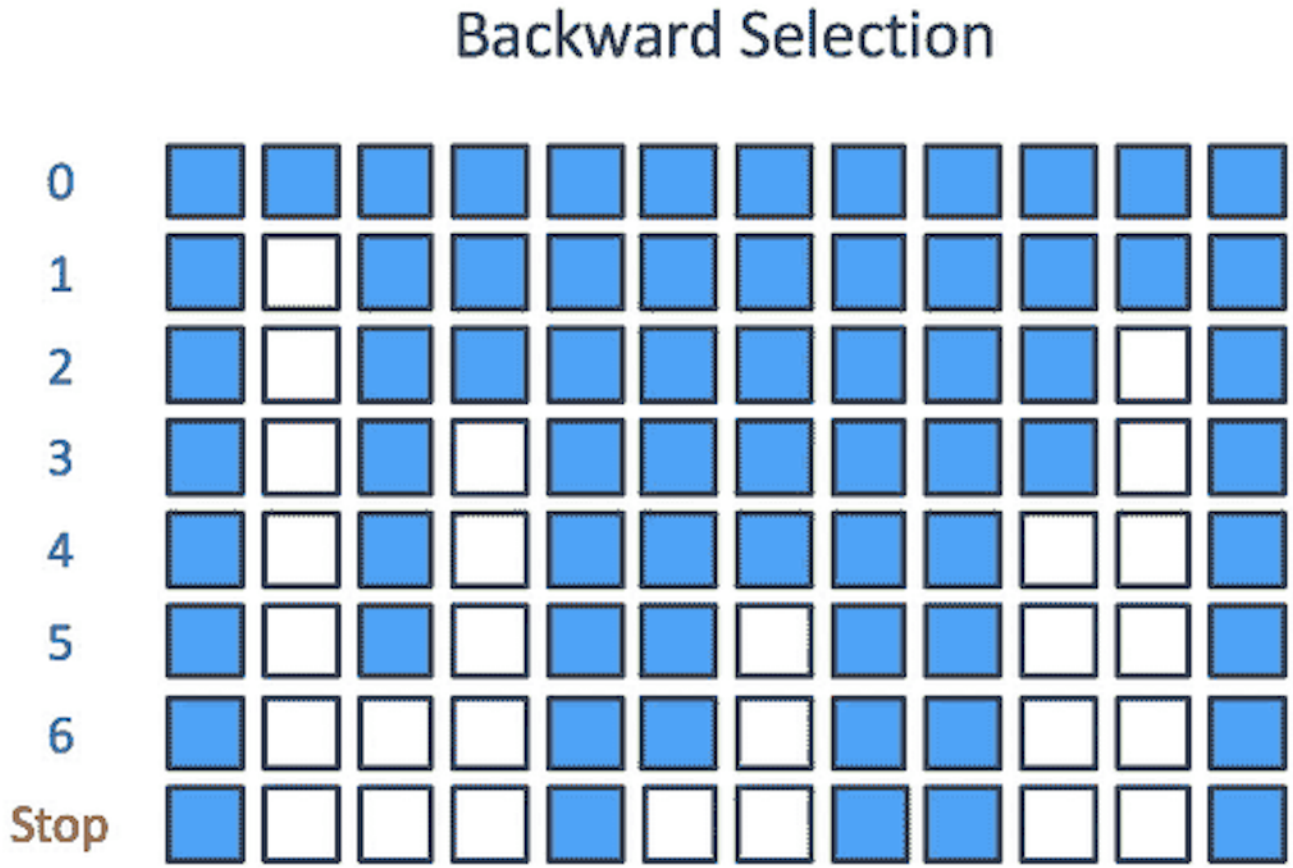
- The first blue point is the variable with the lowest p-value.

Forward Selection

- Only intercept is considered in the very first model. Thereafter, one variable is **added** to the model at a time. Based on the slected model selection criteria.
  - Minimum AIC: Comparing all the models adding one more variable
  - Minimum BIC: Comparing all the models adding one more variable
  - Include the variable in the model taht has Minimum p- value of the corresponding regression coefficient when adding it the existing model..

- The inclusion of the variables are stopped when a pre determined p-value/AIC/BIC is achieved.

Backward variable selection



- The first white point is the variable with the highest p-value.

Backward Selection

All the variables are considered in the very first model. Thereafter, one variable is removed from the model at a time. Based on the slected model selection criteria.

- Minimum AIC: Comparing all the models removing one more variable
- Minimum BIC: Comparing all the models removing one more variable
- Each Step remove the variable that has Maximum p- value of the corresponding coefficient.

The Elimination of the variables are stopped when a pre determined p-value/AIC/BIC is achieved.

the data set named ‘surgical’

Available in the R - package

library(olsrr)

A dataset containing data about survival of patients undergoing liver operation. *Kutner, MH, Nachtscheim CJ, Neter J and Li W., 2004

It is a R data-frame with 54 rows and 8 covariates and response is the 'Survival time'

bcs : blood clotting score

enzyme_test : enzyme function test score

pindex : prognostic index

liver_test : liver function test score

age : In years

Gender : Iindicator variable for gender (0 = male, 1 = female)

alc_mod : indicator variable for history of alcohol use (0 = None, 1 = Moderate)

alc_heavy : indicator variable for history of alcohol use (0 = None, 1 = Heavy)

Forward Selection: R code

```
library(olsrr)
data(surgical)
model <- lm(y ~ ., data = surgical)
step_forward<-ols_step_forward_p(model, details = TRUE)
step_forward
plot(step_forward)
```

Elimination Summary

Step	Variable Removed	R-Square	Adj. R-Square	C(p)	AIC	RMSE
1	alc_mod	0.7818	0.7486	7.0141	734.4068	199.2637
2	gender	0.7814	0.7535	5.0870	732.4942	197.2921
3	age	0.7809	0.7581	3.1925	730.6204	195.4544

Backward Selection: R code

```
model <- lm(y ~ ., data = surgical)
step_backward<-ols_step_backward_p(model, details = TRUE)
step_backward
plot(step_backward)
```

Selection Summary

Step	Variable Entered	R-Square	Adj. R-Square	C(p)	AIC	RMSE
1	liver_test	0.4545	0.4440	62.5119	771.8753	296.2992
2	alc_heavy	0.5667	0.5498	41.3681	761.4394	266.6484
3	enzyme_test	0.6590	0.6385	24.3379	750.5089	238.9145
4	pindex	0.7501	0.7297	7.5373	735.7146	206.5835
5	bcs	0.7809	0.7581	3.1925	730.6204	195.4544

Selection the best combination comparing all the sebsets

- All the 2^p models are fitted if there are p variables in total.

Minimum AIC: Comparing all the models best model is chosen based on the AIC/BIC/RMSE/R^2 criterion.

```r
# stepwise aic regression
model <- lm(y ~ ., data = surgical)
ols_step_both_aic(model, details = TRUE)
```

```r
model <- lm(y ~., data = surgical)
allPossible <- ols_step_all_possible(model)
allPossible
plot(allPossible)
```

Penalized Regression

Penalized Regression: Matrix Notation

Let $(y_i, \underset{\sim}{\mathbf{x}}_i) \in \mathbb{R} \times \mathbb{R}^p$ for $i = 1, \ldots n$ are observed data. A Penalized Regression estimator is via following minimization (with respect to $\underset{\sim}{\beta}$) problem:

$$\|\mathbf{y} - \boldsymbol{X}\underset{\sim}{\beta}\|^2 + \lambda \text{ Penalty Function}.$$

Penalized Regression: idea behind

- They are also known as shrinkage methods or regularization models.
- We would like to continue using linear regression models, but we need to **adjust** them to be usable with big or high-dimensional datasets.
- We introduce a **penalty** for too many or too large coefficients.
- We can fit a model containing all p predictors using a technique that **constrains** or **regularizes** the coefficient estimates, or equivalently, that **shrinks** the coefficient estimates towards zero.

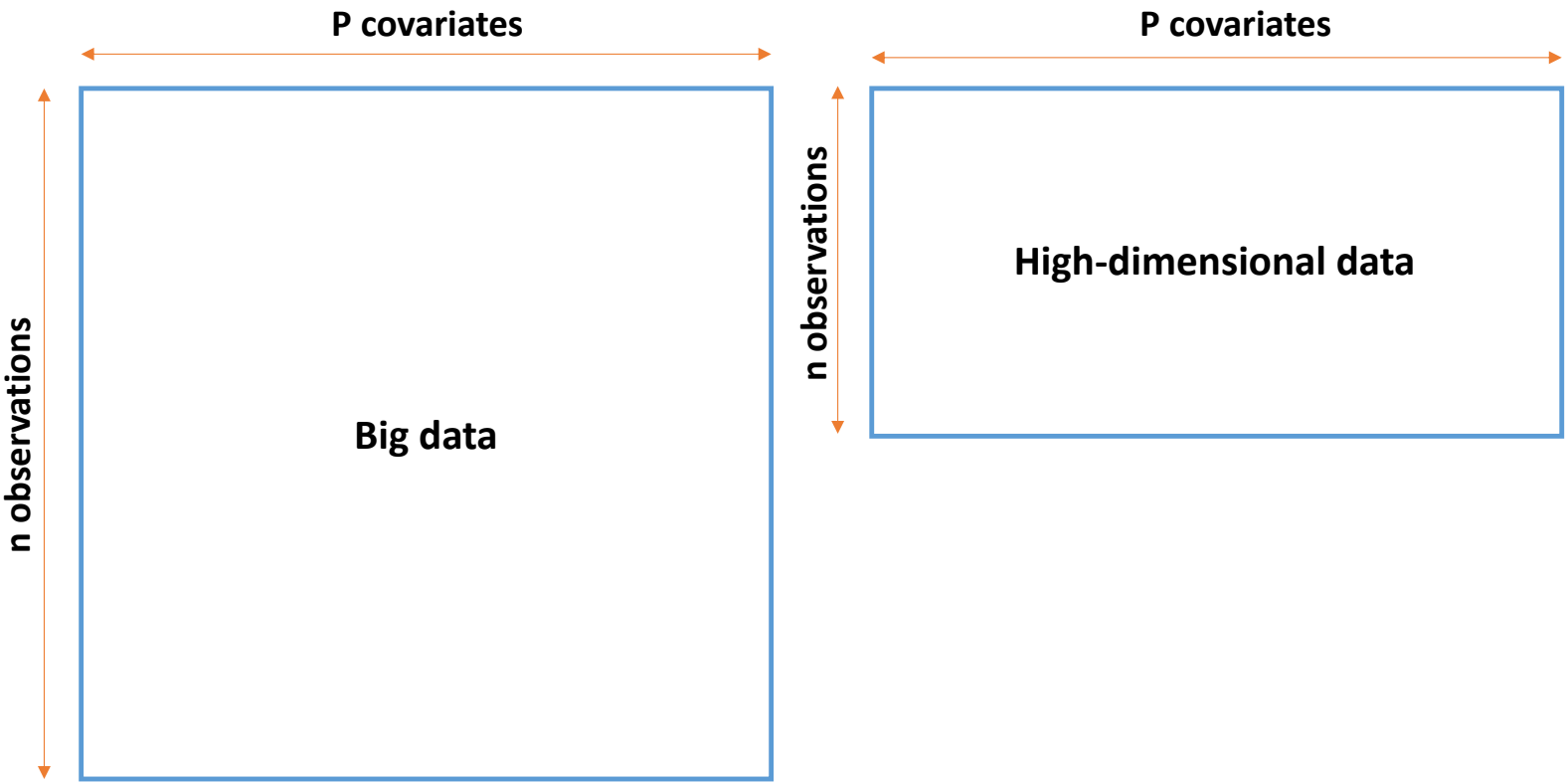
Penalized regression: when?

Regularization methods can be used when at least one of the following conditions is met

- large number of variables
- more variables than observations $n \ll p$
- strong multicollinearity
- a sparse solution is wanted/needed (feature selection)
- "The word 'high-dimensional' refers to a situation where the number of unknown parameters which are to be estimated is one or several orders of magnitude larger than the number of samples in the data."[2]

[2] Peter Bühlmann, Sara van de Geer - Statistics for High-Dimensional Data, Springer 2011

Big data vs. high-dimensional data



Examples of high-dimensional data

Typically, high-dimensional data arise in a number of settings:

- genomics (microarrays, proteomics)
- signal processing
- image analysis
- market basket data and portfolio allocation
- industry (3d-printing)

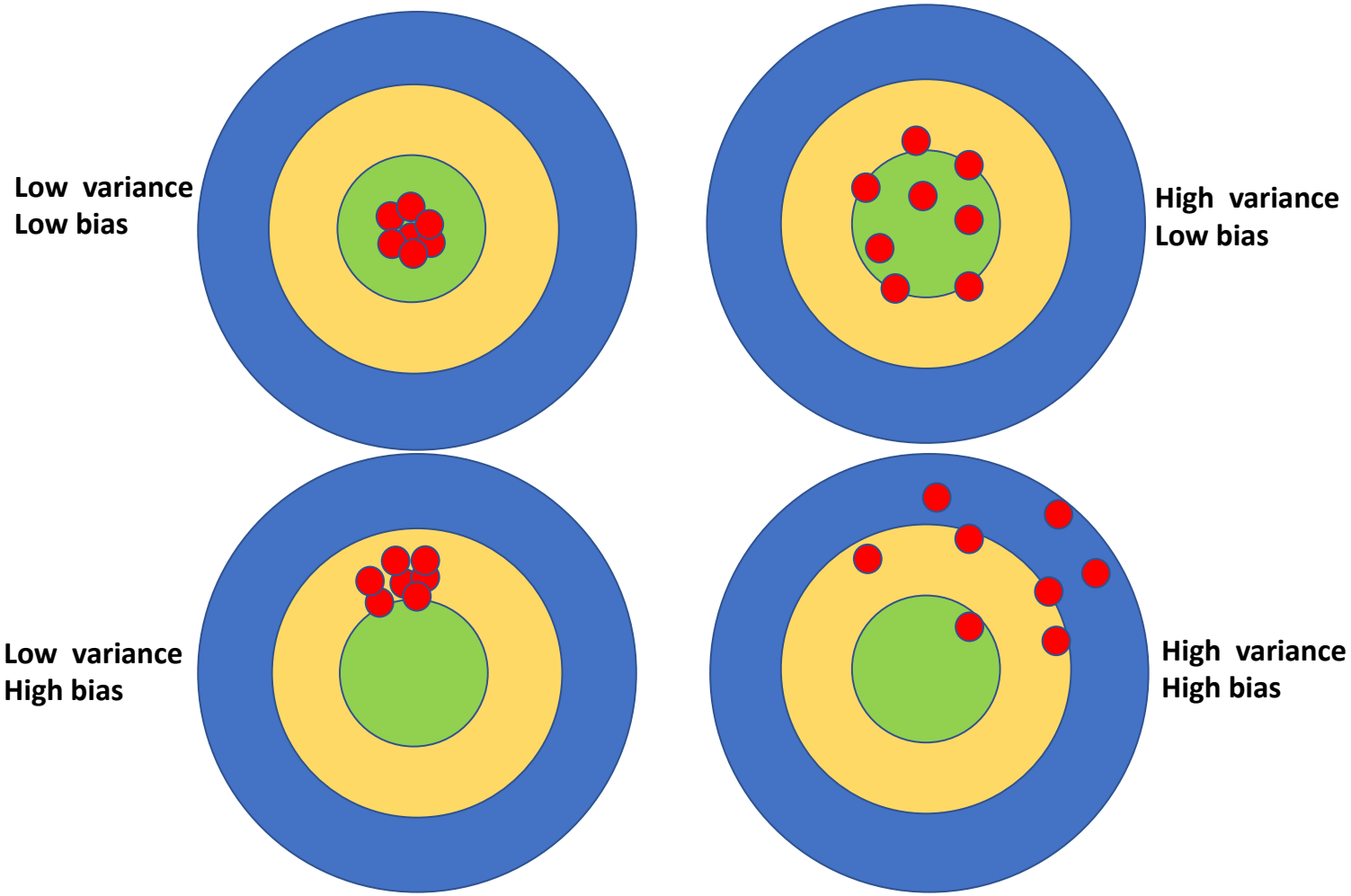
MSE of a predictor: remeber

We use the MSE together with cross validation to assess our model fit.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(\hat{Y}_i - Y_i\right)^2$$

Or more exactly, the mean squared prediction error.

Bias-variance trade-off



Ridge Regression

Definition of ridge regression

- The ridge estimate is defined by

$$\hat{\beta}^{ridge} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{p} \beta_j^2 \leq t.$$

- Or equivalently in *Lagrangian form*

$$\hat{\beta}^{ridge} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\},$$

with $\lambda \geq 0$.

Ridge Regression: Matrix Notation

Let $(y_i, \underset{\sim}{\mathbf{x}}_i) \in \mathbb{R} \times \mathbb{R}^p$ for $i = 1, \ldots n$ are observed data. A Ridge Regression estimator $\hat{\beta}_{\text{ridge},\lambda}$ is via following minimization problem:

$$\hat{\beta}_{\text{ridge},\lambda} = \text{Argmin}_{\beta} \boxed{\|\mathbf{y} - \boldsymbol{X}\underset{\sim}{\beta}\|^2 + \lambda\|\beta\|^2}.$$

, $\lambda > 0$.

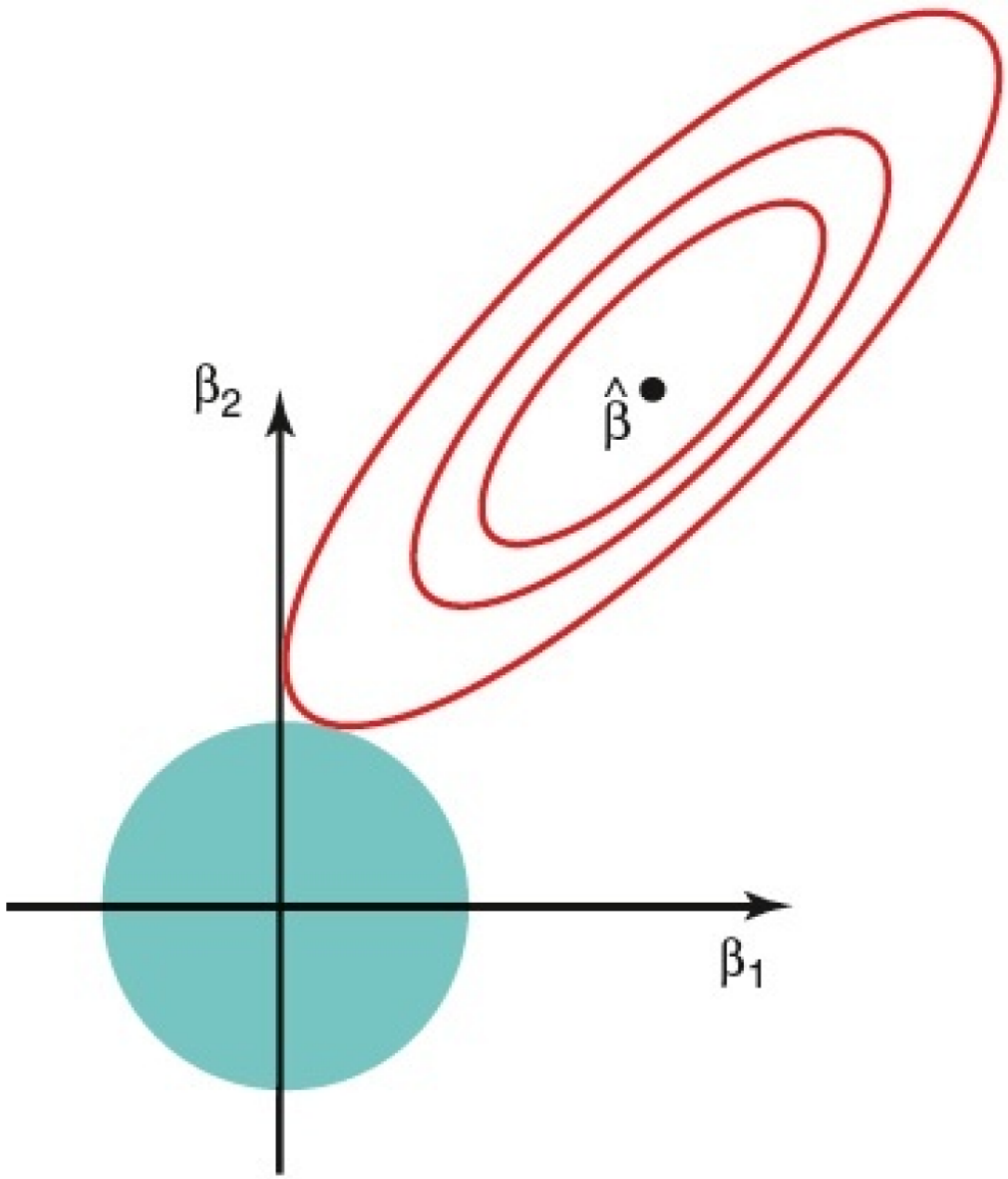
$$\hat{\beta}_{\text{ridge},\lambda} = (\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)^{-1}\boldsymbol{X}^T\mathbf{y},$$

The role of λ

Ridge Regression: The objective function

$$\|\mathbf{y} - \boldsymbol{X}\underset{\sim}{\boldsymbol{\beta}}\|^2 + \lambda\|\beta\|^2.$$

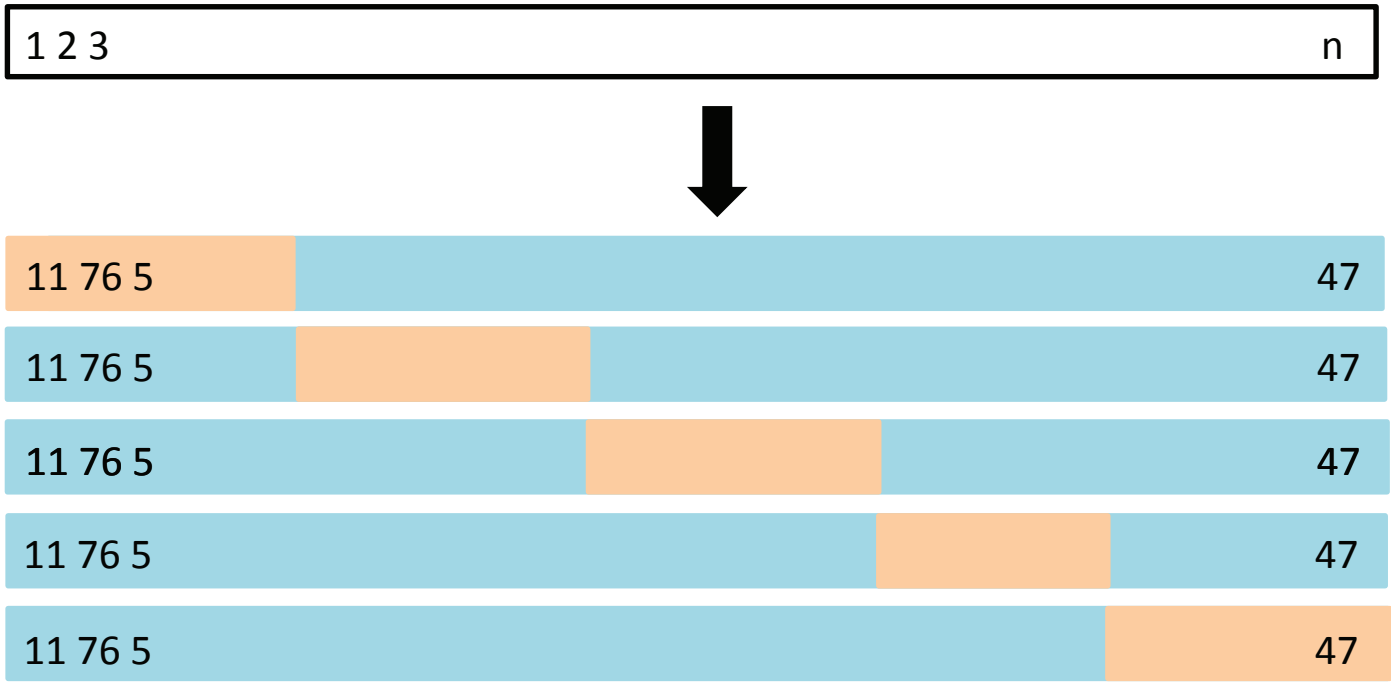
$\lambda > 0$.


β_2
$\hat{\beta}$
β_1

Ridge regression does not exclude variables, but reduces effect estimates to near zero. It is therefore not suited for finding parsimonious models.

W use the `glmnet` r package to fit it.

5-fold cross-validation: A schematic display



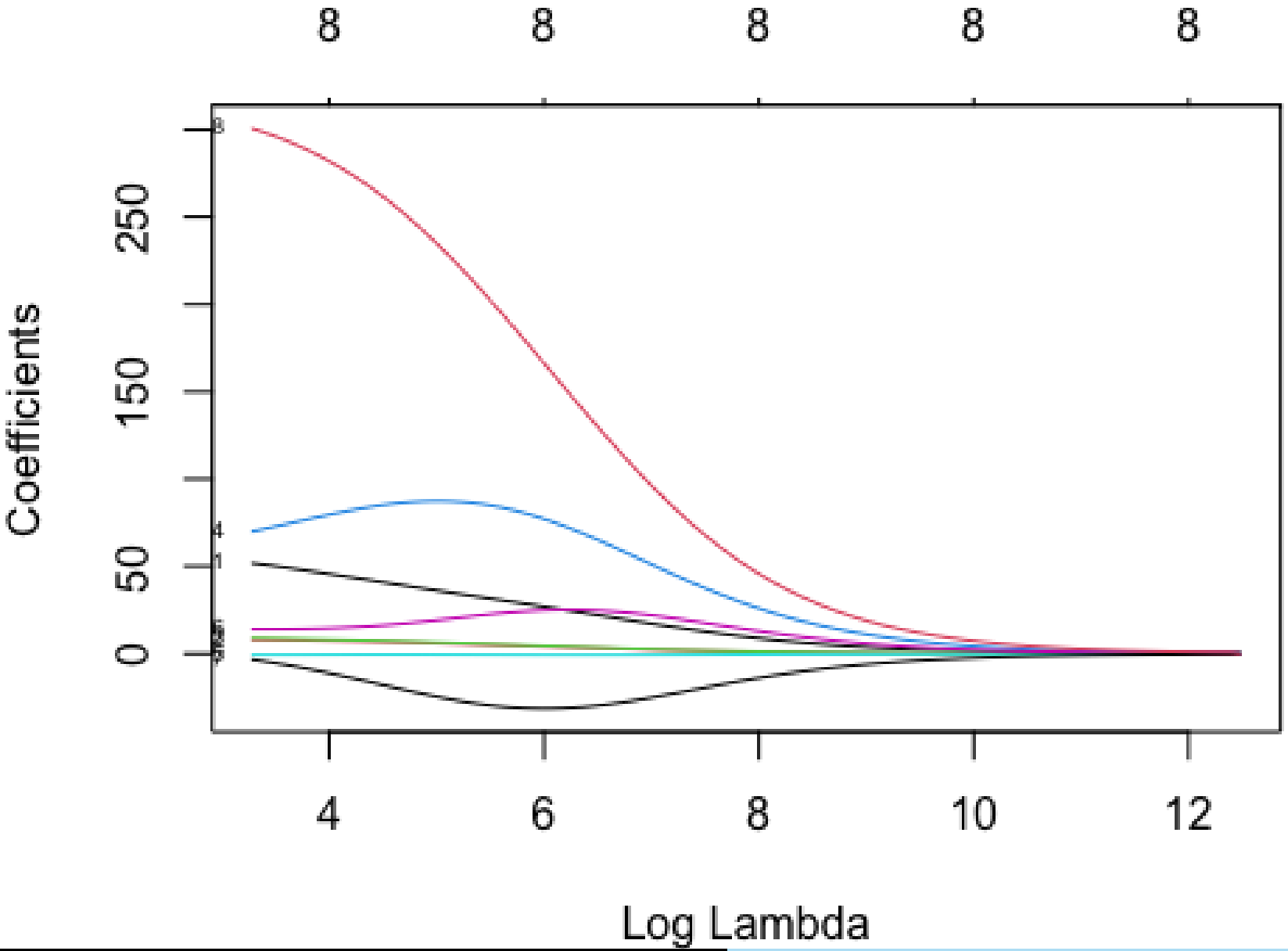
A set of n observations is randomly split into 5 non-overlapping groups. Each of these fifths acts as a validation set, and the remainder as a training set. The test error is estimated by averaging the 5 resulting MSE estimates.

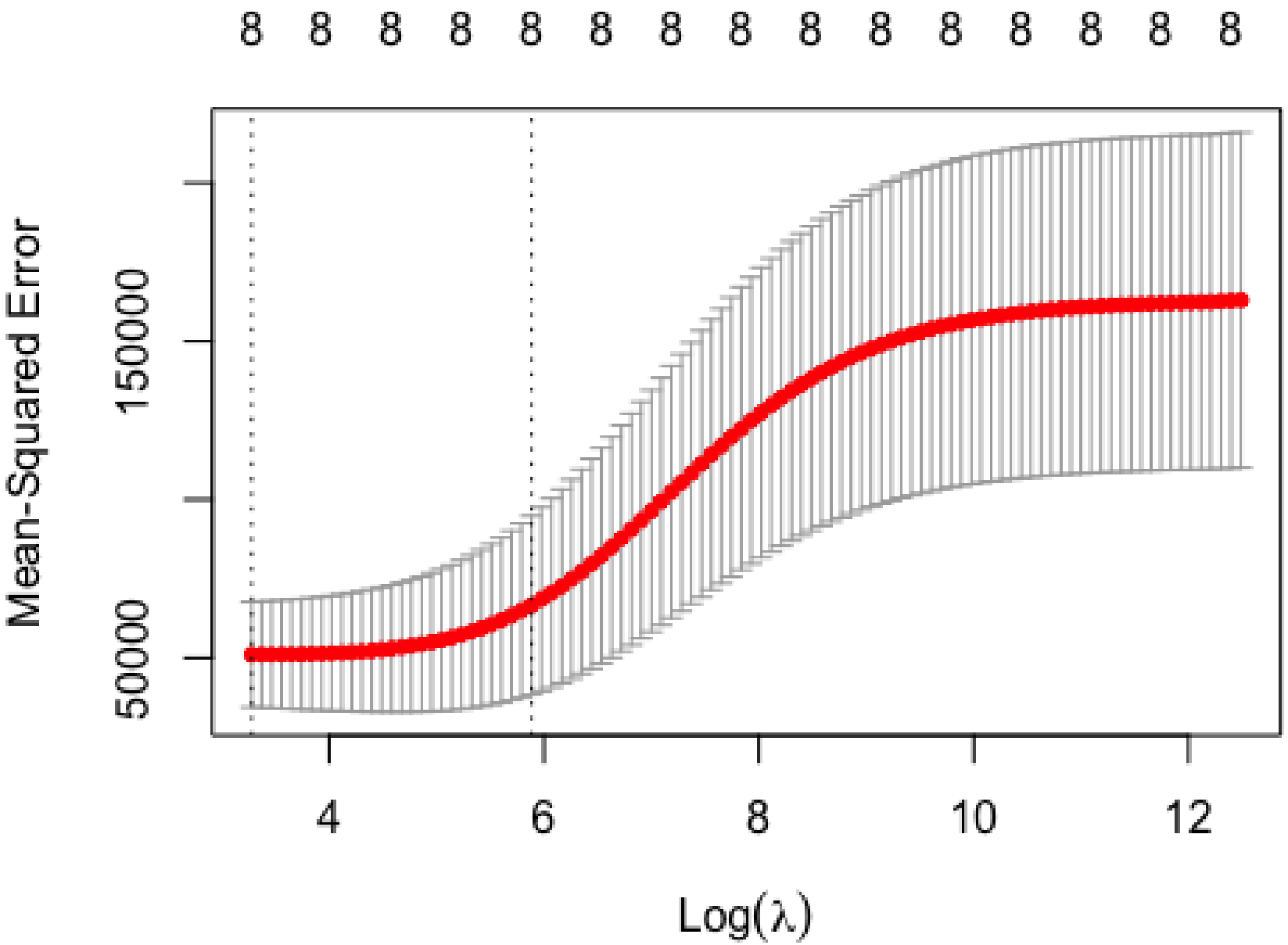
Selection of λ

```r
library(glmnet)
data("surgical") # from the package library(olsrr)
names(surgical[,1:8])
# alpha=0 for fitting a Ridge Regression model
fit_ridge<-glmnet(x =as.matrix(surgical[,1:8]) , y =surgical$y, alpha = 0 )
fit_ridge

plot(fit_ridge, xvar = "lambda", label = TRUE)

# Cross validation to Choose the optimal \Lambda Parameter
cvfit <- cv.glmnet(x =as.matrix(surgical[,1:8]) , y =surgical$y, alpha=0, nfolds = 10)
plot(cvfit)
Ridge_opt_Lambda.model <- glmnet(x=as.matrix(surgical[,1:8]), y=surgical$y,
                      alpha  = 0,
                      lambda = cvfit$lambda.min)
Ridge_opt_Lambda.model


#Alternatively
coef(cvfit, s = "lambda.min")
```

Shrinkage Effect

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


8
8
8
8
8
Coefficients
0
50
150
250
4
6
8
10
12
Log Lambda


8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
Mean-Squared Error
150000
50000
4
6
8
10
12
Log(λ)

```
Call:  glmnet(x = as.matrix(surgical[, 1:8]), y = surgical$y, alpha = 0,      lambda
= cvfit$lambda.min)

  Df  %Dev Lambda
1  8 77.87  26.54
9 x 1 sparse Matrix of class "dgCMatrix"
                          1
(Intercept) -1002.4910407
bcs            51.8370557
pindex          8.0497572
enzyme_test     8.7789615
liver_test     69.9033668
age            -0.6486542
gender         13.9924291
alc_mod        -3.2776238
alc_heavy     300.7347029
```

LASSO Regression

Lasso regression

Least **A**bsolute **S**hrinkage and **S**election **O**perator introduced by Tibshirani in 1996.

Advantages:

- statistical accuracy in prediction
- variable selection
- computational feasibility

Does not perform well, when groups with high collinearity are present.

Definition of lasso regression

The lasso estimate is defined by

$$\hat{\beta}^{lasso} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{p} |\beta_j| \leq t.$$

Or equivalently in *Lagrangian form*

$$\hat{\beta}^{lasso} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\},$$

with $\lambda \geq 0$.

LASSO Regression: Matrix Notation

Let $(y_i, \underset{\sim}{\mathbf{x}}_i) \in \mathbb{R} \times \mathbb{R}^p$ for $i = 1, \ldots n$ are observed data. A LASSO Regression estimator $\hat{\beta}_{\text{lasso},\lambda}$ is via following minimization problem:

$$\hat{\beta}_{\text{lasso},\lambda} = \text{Argmin}_{\underset{\sim}{\beta}} \mathbf{y} - \boldsymbol{X}\underset{\sim}{\beta}\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

, Or

$$\hat{\beta}_{\text{lasso},\lambda} = \text{Argmin}_{\underset{\sim}{\beta}} \|\mathbf{y} - \boldsymbol{X}\underset{\sim}{\beta}\|^2 + \lambda \|\underset{\sim}{\beta}\|_{L_1}.$$

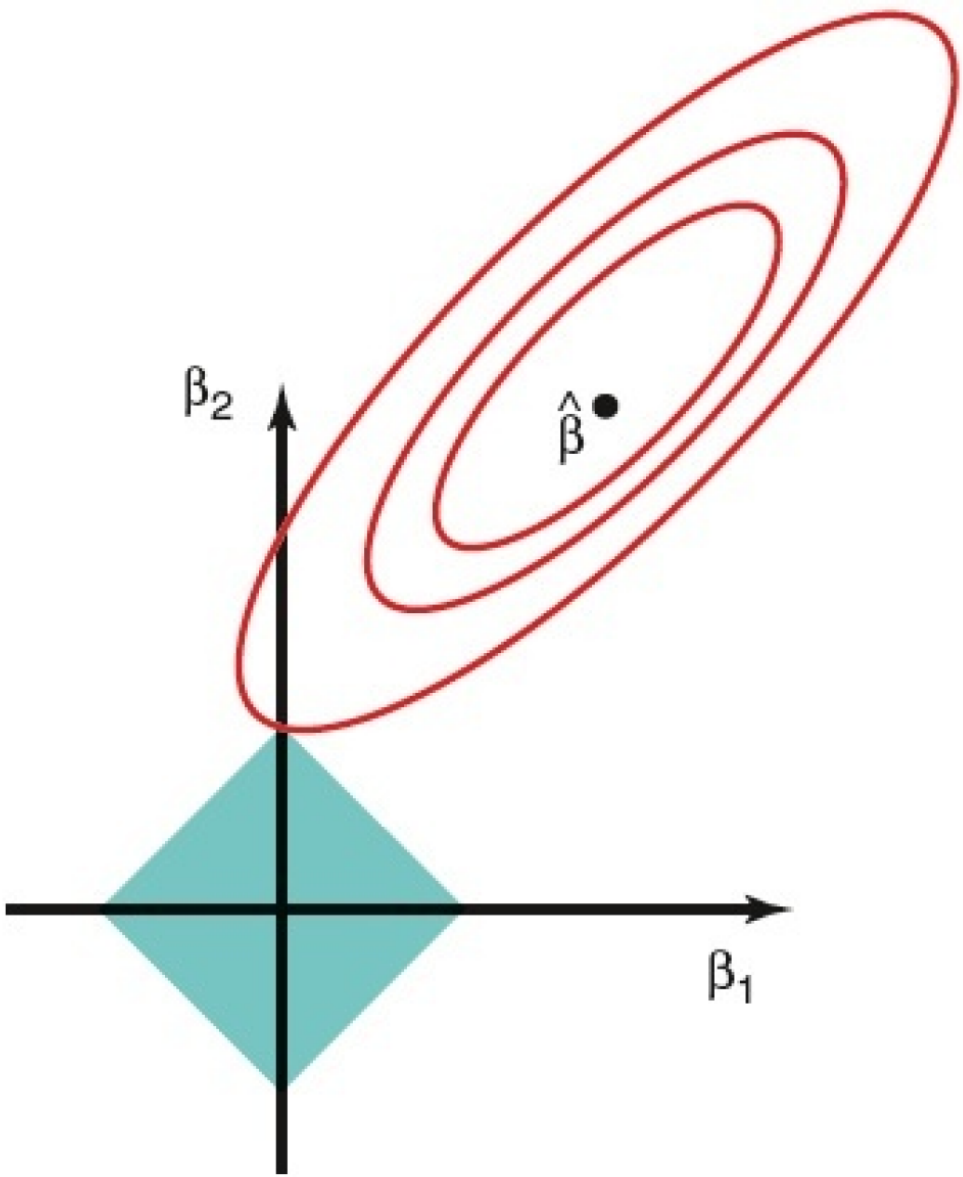
$\lambda > 0$

The role of λ

Ridge Regression: The objective function

$$\|\mathbf{y} - \boldsymbol{X}\underset{\sim}{\beta}\|^2 + \lambda \|\underset{\sim}{\beta}\|_{L_1}.$$

$\lambda > 0$

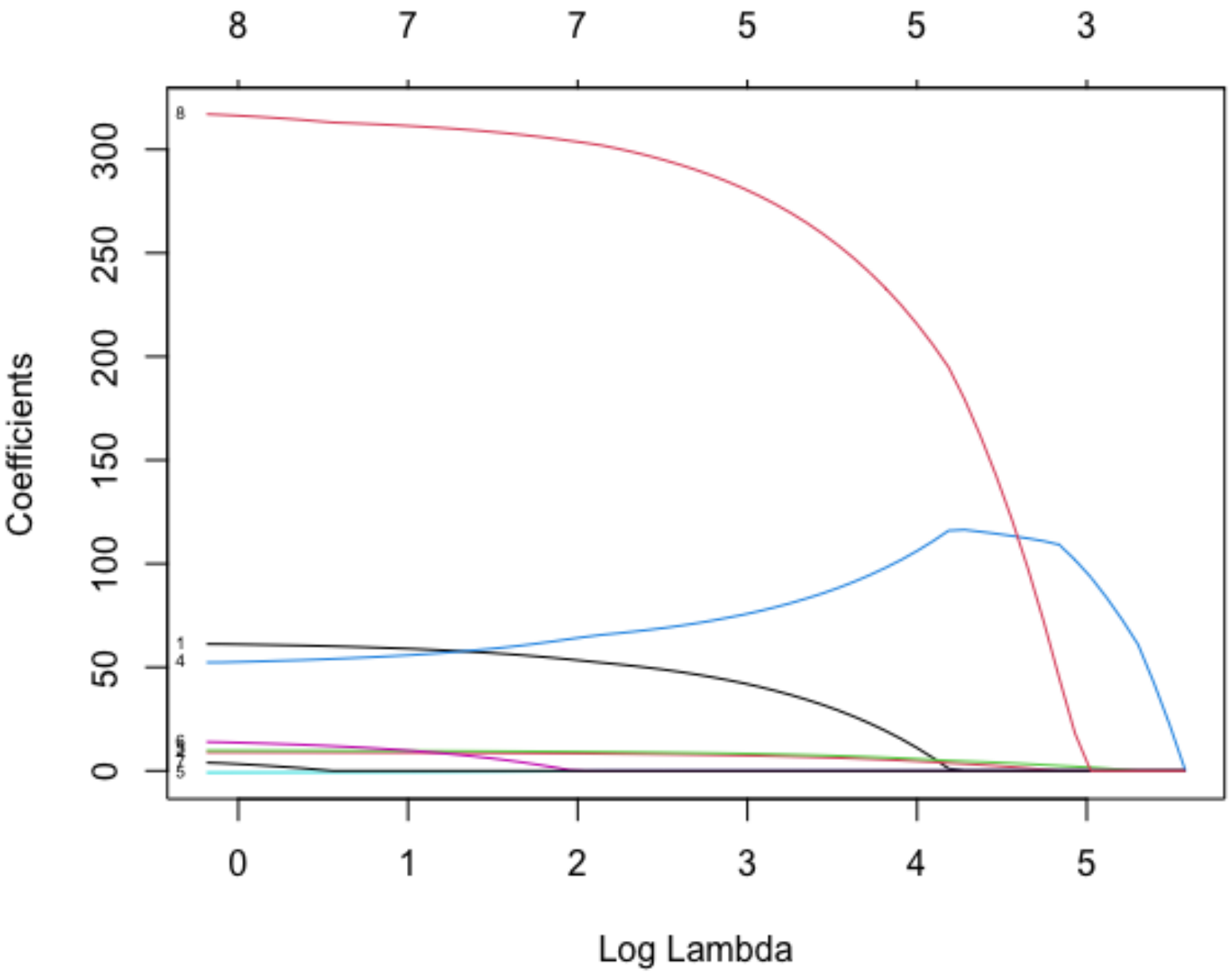

β_2
$\hat{\beta}$
β_1

Lasso regression can estimate a regression coefficient to be Exactly zero,. Therefore it has the ability to perform variable selection. It is often used to find parsimonious models.

W use the `glmnet` r package to fit it.

Selection of λ

```r
library(glmnet)
data("surgical") # from the package library(olsrr)
names(surgical[,1:8])
# alpha=0 for fitting a Ridge Regression model
fit_lasso<-glmnet(x =as.matrix(surgical[,1:8]) , y =surgical$y, alpha = 1 )
fit_lasso

plot(fit_lasso, xvar = "lambda", label = TRUE)

# Cross validation to Choose the optimal \Lambda Parameter
cvfit <- cv.glmnet(x =as.matrix(surgical[,1:8]) , y =surgical$y,alpha=1, nfolds = 10)
plot(cvfit)
Lasso_opt_Lambda.model <- glmnet(x=as.matrix(surgical[,1:8]), y=surgical$y,
                      alpha  = 1,
                      lambda = cvfit$lambda.min)
Lasso_opt_Lambda.model


#Alternatively
coef(cvfit, s = "lambda.min")
```


8
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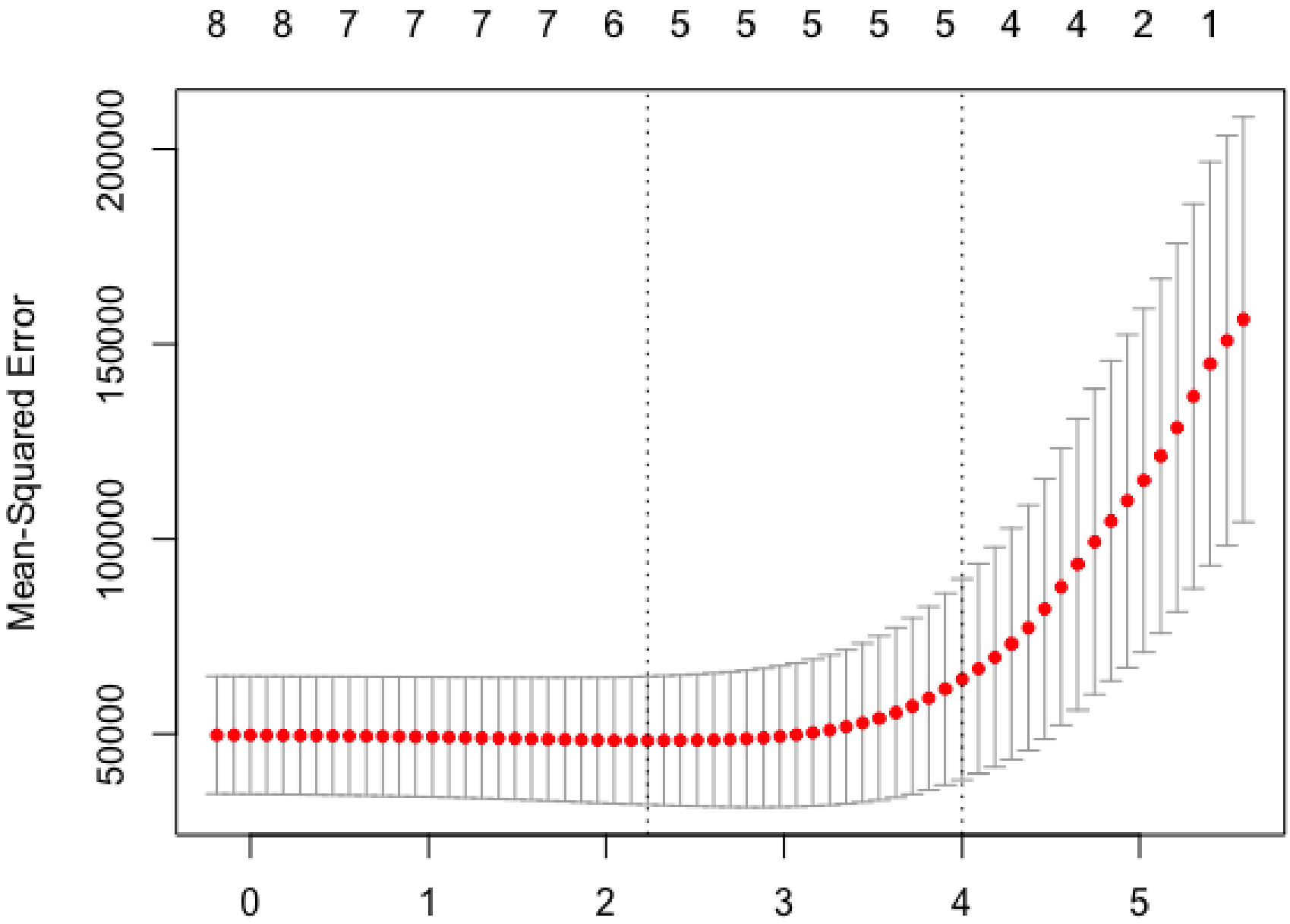
Log Lambda


8 8 7 7 7 7 6 5 5 5 5 5 4 4 2 1
Mean-Squared Error
50000
100000
150000
200000
0
1
2
3
4
5

```
Call:  glmnet(x = as.matrix(surgical[, 1:8]), y = surgical$y, alpha = 1,      lambda
= cvfit$lambda.min)

  Df  %Dev Lambda
1  5 77.86   9.32
9 x 1 sparse Matrix of class "dgCMatrix"
                      1
(Intercept) -1049.793801
bcs            51.473401
pindex          8.189280
enzyme_test     9.058995
liver_test     66.362568
age             .
gender          .
alc_mod         .
alc_heavy     300.440816
```

Regression with Elastic Net Penalty

Elastic net: Ideas behind

- To address the problems of lasso and ridge, the elastic net was created. It generalizes both and combines the l_1 and l_2 penalties.
- The elastic net **combines** the benefits of both lasso and ridge Regression.
  - It will shrink coefficients for groups of highly correlated variables like Ridge
  - It will set variables to zero like Lasso
  - It can give more than n non-zero coefficients in the $n < p$ case

Elastic net definition

The Elastic Net estimate is given by

$$\hat{\beta}^{elnet} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{p} \left(\alpha|\beta_j| + (1-\alpha)\,\beta_j^2 \right) \leq t.$$

Or equivalently in *Lagrangian form*

$$\hat{\beta}^{elnet} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} \left(\alpha|\beta_j| + (1-\alpha)\,\beta_j^2 \right) \right\}$$

with $\lambda \geq 0$ and $\alpha \in [0, 1]$.

Regression with Elsatic Net Penalty: Matrix Notation

Let $(y_i, \underset{\sim}{\mathbf{x}}_i) \in \mathbb{R} \times \mathbb{R}^p$ for $i = 1, \ldots n$ are observed data. A Elsatic Net Regression estimator $\hat{\beta}_{\text{EN},\lambda}$ is via following minimization problem:

$$\hat{\beta}_{\text{EN},\lambda} = \text{Argmin}_{\underset{\sim}{\beta}} \left\| \mathbf{y} - \boldsymbol{X}\underset{\sim}{\beta} \right\|^2 + \lambda \left[(\alpha) \left\| \underset{\sim}{\beta} \right\|_{L_1} + (1-\alpha) \left\| \underset{\sim}{\beta} \right\|^2 \right].$$

$\lambda > 0$, and $0 \leq \alpha \leq 1$.

Try: `https://glmnet.stanford.edu/articles/glmnet.html`

Geneset MicroArray Data

- The covariates are the allele frequencies of 200 Gene sets for 120 subjects. (Scheetz et al., (2006)

  It represents the data of 120 rats with 200 gene probes.

  Response a 120-dimensional vector of, which represents the expression level of 'TRIM32' gene.

  We want to idensity which of the other genes are significantly responsible for the gene counts of the 'TRIM32'.

- Therefore, In terms of the regression terminology: $n = 120$ and $p = 200$.

Thank You