STAT 380: Variable Selection, Ridge, and Lasso Regression

An Example using .... Data

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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.

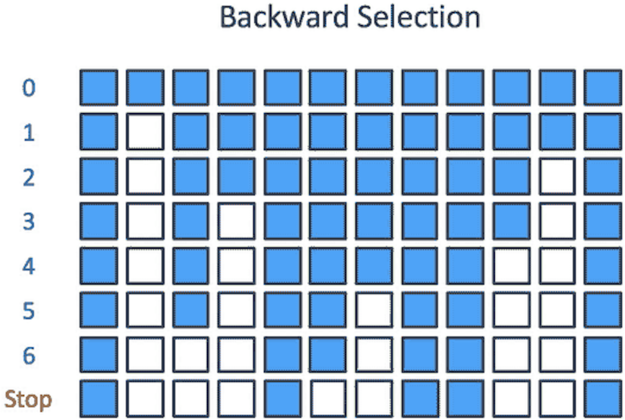
  Minimum AIC: Comparing all the models adding one more variable

  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

```r
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:

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

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.

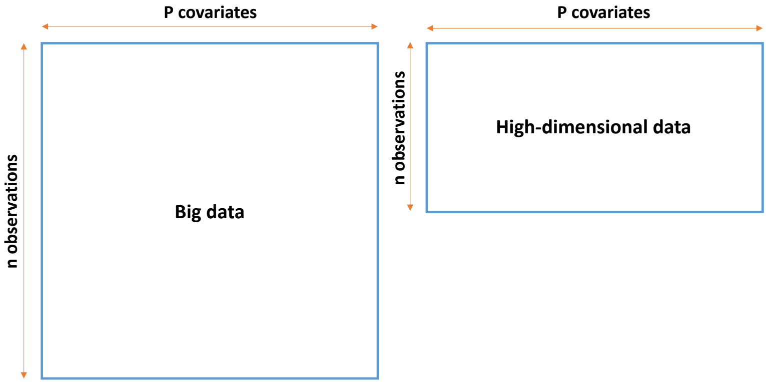
Penalized regression: when?

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)

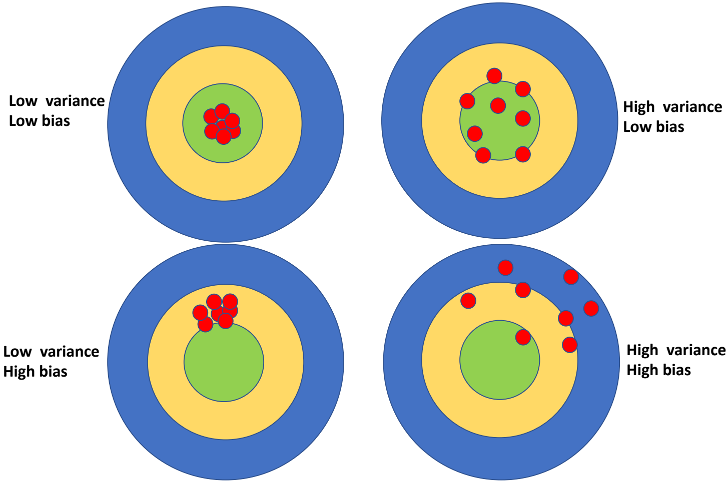
MSE of a predictor: remeber

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:

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

, $\lambda > 0$.

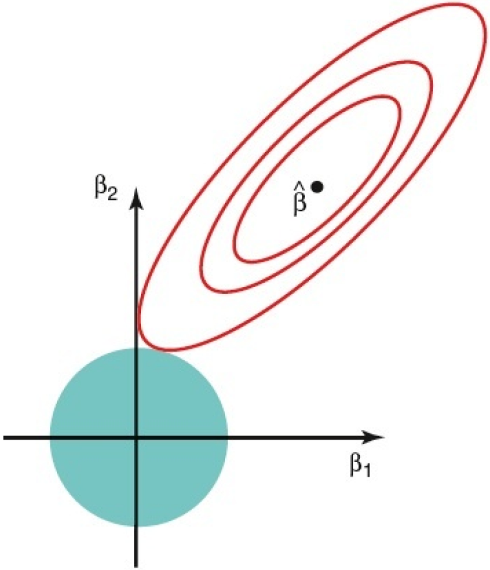
$$\boxed{\hat{\beta}_{\text{ridge},\lambda} = (\boldsymbol{X}^T\boldsymbol{X} + \lambda I_p)^{-1}\boldsymbol{X}^T\mathbf{y},}$$

The role of λ

Ridge Regression: The objective function

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

$\lambda > 0$.

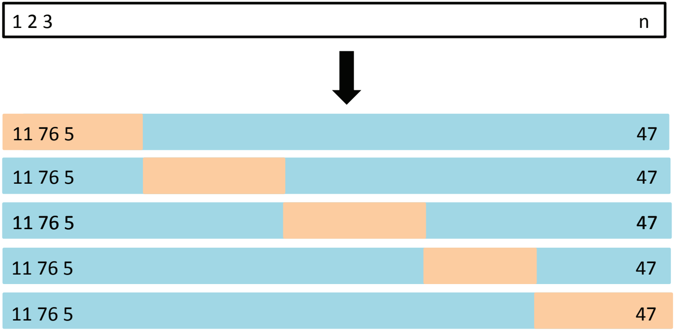


β_2
$\hat{\beta}$
β_1

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



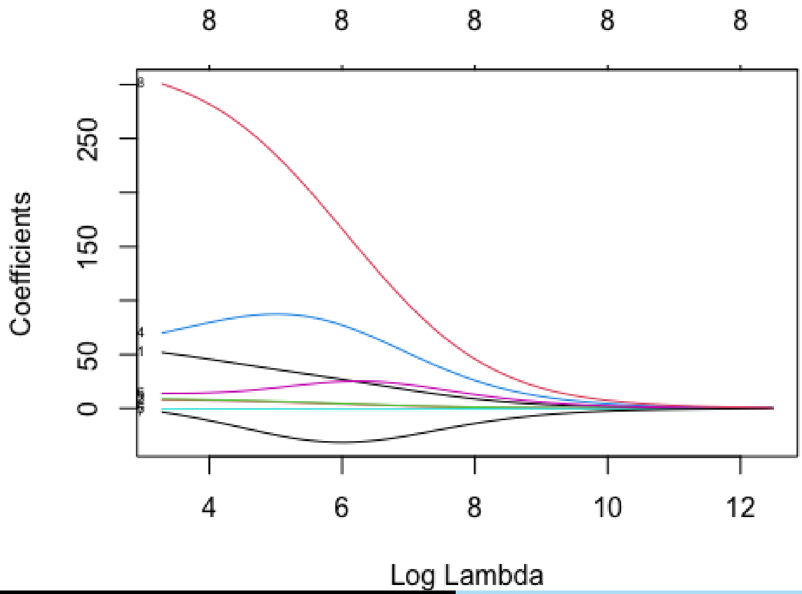
A set of n observations is randomly split into 5 non-overlapping groups. Each of these fifths acts as a validation set, and the remainder as a training set. The test error is estimated by averaging the 5 resulting MSE estimates.

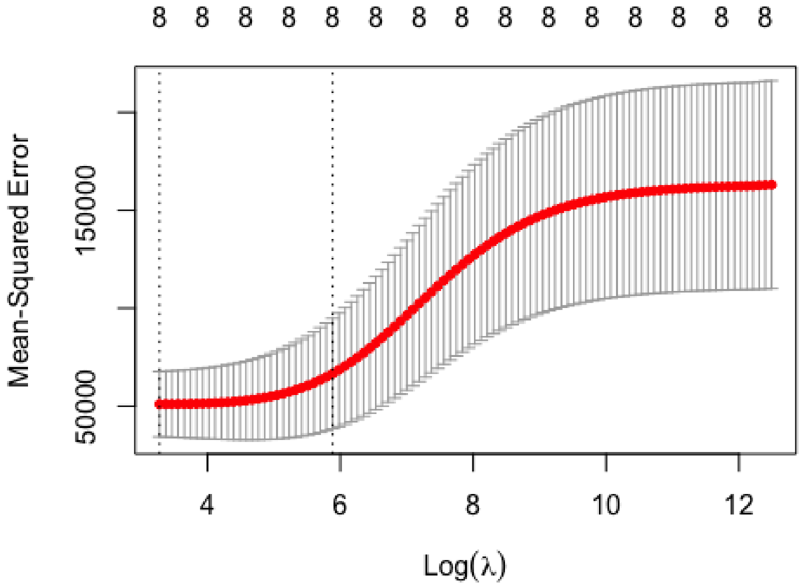
Selection of λ

```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
50000
150000
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

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

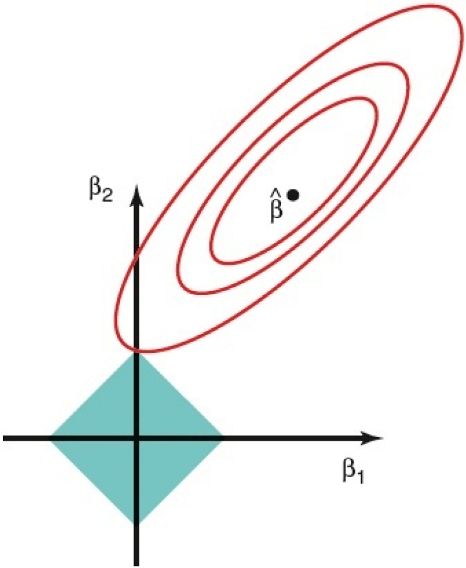
$\lambda > 0$

The role of λ

Ridge Regression: The objective function

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

$\lambda > 0$

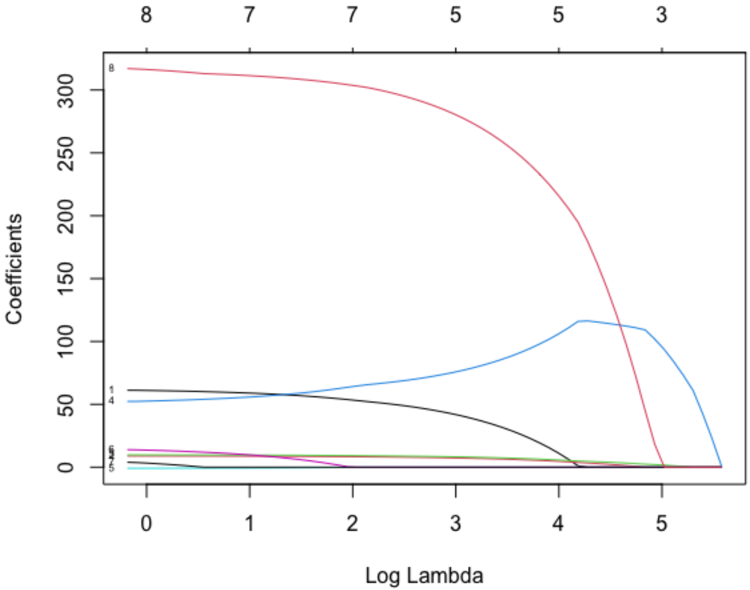

β₂
β̂
β₁

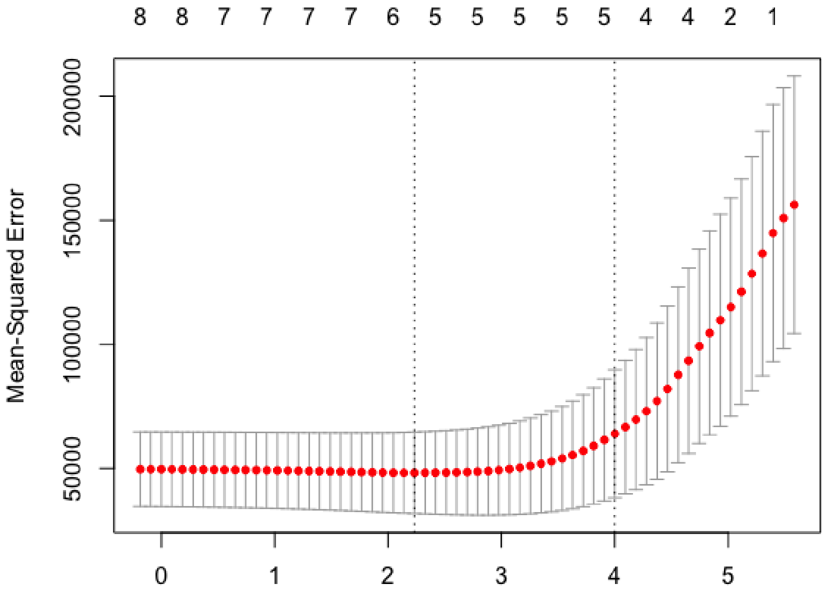
Lasso regression can estimate a regression coefficient to be Exactly zero,. Therefore it has the ability to perform variable selection. It is often used to find parsimonious models.

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

Selection of λ

```
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 7 7 5 5 3
Coefficients
0 50 100 150 200 250 300
0 1 2 3 4 5
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 $\hat{\beta}_{\mathrm{EN},\lambda}$ is via following minimization problem:

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

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

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