STAT540-Lecture 19: Variables Selection

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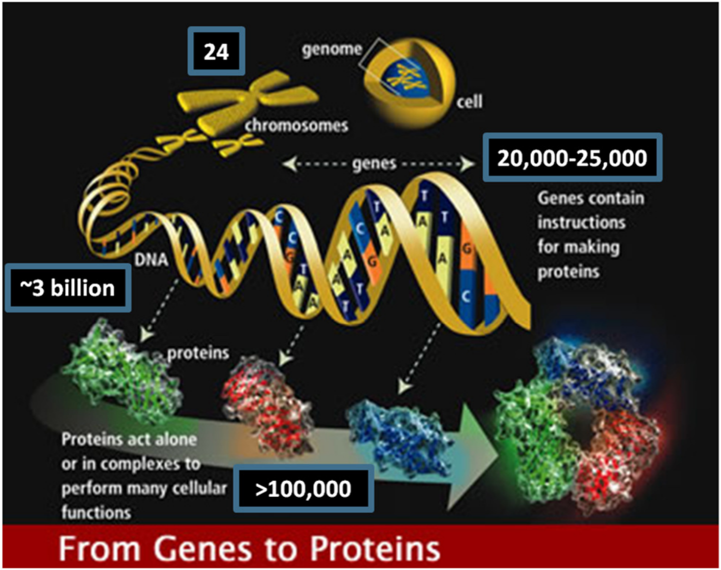
When biology speaks, we listen.

... but it may get too loud, too noisy...



http://www.ornl.gov/sci/techresources/Human_Genome/project/info.shtml

Biomarkers Studies

1. **Identify** molecular biomarkers of a disease
2. Based on the identified markers, **build** a molecular signature of the disease
3. Build a classifier to **predict** the outcome of samples

Are these 3 sequential but unrelated steps?

Notation

Let y be the response (also denoted *target*) we want to predict:

- **Classification**: y takes values from a finite set of labels (e.g., $\{$benign, malignant$\}$)
- **Regression**: y is a real number (e.g., tumor size)

We want to predict y based on the values of p variables called covariates (also known as inputs or predictors, $\boldsymbol{X} \in \mathbb{R}^p$)

This lecture is focused on regression but the same ideas apply for classification.

Goal: prediction!

... based on what information??

- In -omics studies p $>>$ n (i.e., the number of potential covariates is much larger than the number of samples) e.g., $\sim$thousands genes and $\sim$hundreds samples
- Among the p covariates available, many may be highly correlated, e.g., many genes from a common pathway
  - Do we need to listen to the whole rock band? or can we just listen to the singer?

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Which covariates should be included in the model??

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Model Selection

Linear Regression Models

Assume a linear model of the form:

$$\mathbf{y} = \boldsymbol{\beta}^T \mathbf{x} + \varepsilon$$

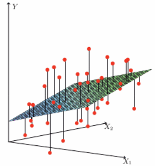

FIGURE 3.1. *Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of X that minimizes the sum of squared residuals from Y.*

Then, the **Least Squares** (LS) estimators of β are those that minimize the residuals sum-of-squares (RSS) [1]:

$$\hat{\boldsymbol{\beta}} = \min_{\boldsymbol{\beta} \in \mathbb{R}^p} \sum_{i=1}^{n} \left(y_i - \mathbf{x}_i^T \boldsymbol{\beta}\right)^2 = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

In matrix notation:

$$\text{RSS} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T \mathbf{X}^T \mathbf{X} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

[1] Note that the intercept can be capture in β adding a column of 1s to $\mathbf{x}$.Image: The Elements of Statistical Learning, Hastie, Tibshirani, Friedman

Pros and Cons of LS

- $\hat{\beta}$ has the smallest variance among all linear unbiased estimates.
- However, if we sacrifice bias, there may be other estimators with lower variance
- Lower variance may result in better prediction accuracy (remember that prediction is our main goal!!)
- The model may be difficult to interpret when there are *many* covariates (e.g., 1000 genes ?!)
- When covariates are highly correlated, the LS estimators can become very unstable

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Model Selection

Model / feature selection - Subset Selection

- **Best subset regression** finds the subset of size k with the smallest RSS. Even using an efficient algorithm, this procedure is unfeasible if more than 40 covariates are available.

- **Forward stepwise selection** (or similarly backward, or both), sequentially adds the best covariate that most improves the fit (or even some measure of prediction). In general it has higher bias than best-subset but with lower variance.

- **Forward stagewise regression** sequentially adds covariates to the model but at each steps the algorithm identifies the variable most correlated with the current residual.

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- **Forward stagewise regression** sequentially adds covariates to the model but at each steps the algorithm identifies the variable most correlated with the current residual.

These models discretely selects covariates (*in* or *out*)

Thus, often exhibit high variance

Select coefficients in a more continuous way by adding a bound to their size

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For example,

LASSO: least absolute shrinkage and selection operator (Tibshirani, *JRSS*, 1996)

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) = \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta}\right)^2$$

subject to

$$\sum_{j=1}^{p} |\boldsymbol{\beta}_j| \leq C \text{ for some } C > 0$$

Model / feature selection - Penalized methods

Equivalently, LASSO minimizes a *penalized* RSS:

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) = \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta} \right)^2 + \lambda \sum_{j=1}^{p} |\boldsymbol{\beta}_j| \right\}$$

for some $\lambda > 0$.

Penalized Estimators

More general, one can define

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) \; = \; \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \; \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta} \right)^2 \; + \; \lambda P(\boldsymbol{\beta}) \right\}$$

where P is a penalty function and λ controls the amount of penalization. **Examples:**

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Ridge regression

The ridge coefficients minimize the RSS,

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}})_R \;=\; \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \; \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta}\right)^2$$

subject to

$$\sum_{j=1}^{p} \boldsymbol{\beta}_j^2 \;\leq\; C \;\; \text{for some } C > 0.$$

or equivalently, the penalized RSS:

$$\text{RSS}(\lambda) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) + \lambda \boldsymbol{\beta}^T \boldsymbol{\beta}$$

Given this constrain on the slopes, the estimated coefficient will not adjust to different scales in the covariates.

- Thus, we need to standardize the covariates before using regularized methods.
- It can be shown that if we center the predictors, then $\hat{\alpha}_R = \bar{y}$, and $\hat{\boldsymbol{\beta}}_R$ can be estimated separately.

Ridge regression (cont.)

If the covariates are centered

$$\hat{\boldsymbol{\beta}}_R = \left(\mathbf{X}^T\mathbf{X} + \lambda\,\mathbf{I}\right)^{-1} \mathbf{X}^T\mathbf{y}$$

- There is a solution for each λ (path of solutions).
- λ controls the size of the coefficients (i.e., amount of regularization). If $\lambda = 0$, $\hat{\boldsymbol{\beta}}_R = \hat{\boldsymbol{\beta}}_{LS}$. The $\hat{\boldsymbol{\beta}}_R$ shrink as λ increases and tend to 0 as λ goes to infinity.
- If the explanatory variables are highly correlated, $\mathbf{X}^T\mathbf{X}$ is close to being singular (i.e., LS are very unstable). This problem is solved by ridge regression. In fact, this was its original motivation.
- It can also be thought as a way of reducing the variance of $\hat{\boldsymbol{\beta}}_R$

Toy example

```r
library(MASS)

set.seed(123)
x1 <- rnorm(506)
x2 <- rnorm(506, mean = 2, sd = 1)


x3 <- rexp(506, rate = 1)
x4 <- x2 + rnorm(506, sd = 0.1)
x5 <- x1 + rnorm(506, sd = 0.1)
x6 <- x1 - x2 + rnorm(506, sd = 0.1)
x7 <- x1 + x3 + rnorm(506, sd = 0.1)

# Let's make x1 and x2 important covariates

y <- x1 * 3 + x2/3 + rnorm(506, sd = 2.2)

x <- data.frame(y = y, x1 = x1, x2 = x2, x3 = x3, x4 = x4, x5 = x5, x6 = x6,
    x7 = x7)

summary(lm(y ~ ., data = x))
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   0.0346     0.2302    0.15    0.881
x1            3.2261     1.6809    1.92    0.056 .
x2            0.2387     1.3936    0.17    0.864
x3           -0.3593     0.9868   -0.36    0.716
x4           -0.6936     0.9902   -0.70    0.484
x5            0.0927     0.9116    0.10    0.919
x6           -0.7389     1.0111   -0.73    0.465
x7            0.3165     0.9861    0.32    0.748
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.15 on 498 degrees of freedom
Multiple R-squared: 0.635,    Adjusted R-squared: 0.63
F-statistic:  124 on 7 and 498 DF,  p-value: <2e-16
```

Nothing is significant!

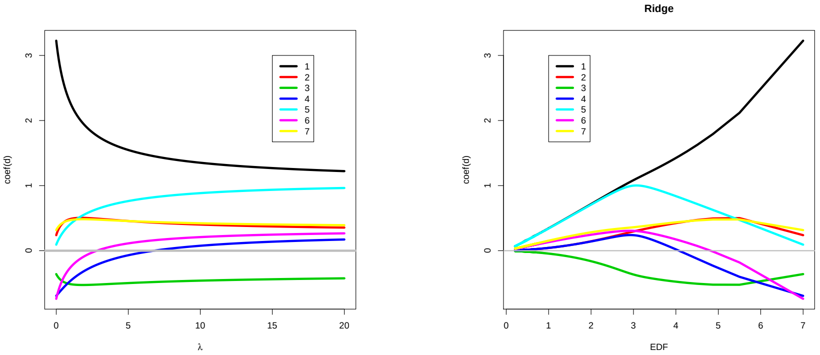
```
summary(lm(y ~ x1 + x2, data = x))
```

```
##
## Call:
## lm(formula = y ~ x1 + x2, data = x)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -6.930 -1.574 -0.007  1.384  5.957
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.00733    0.20900    0.04   0.9720
## x1           2.89168    0.09806   29.49   <2e-16 ***
## x2           0.27903    0.09249    3.02   0.0027 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.14 on 503 degrees of freedom
## Multiple R-squared: 0.634,	Adjusted R-squared: 0.633
## F-statistic:  436 on 2 and 503 DF,  p-value: <2e-16
```

```
summary(lm(y ~ x1 + x2 + x4, data = x))
```

```
##
## Call:
## lm(formula = y ~ x1 + x2 + x4, data = x)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -6.806 -1.523 -0.031  1.423  5.886
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.000113   0.209359    0.00     1.00
## x1           2.896446   0.098339   29.45   <2e-16 ***
## x2           0.974081   0.991778    0.98     0.33
## x4          -0.693444   0.985171   -0.70     0.48
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.14 on 502 degrees of freedom
## Multiple R-squared: 0.635,	Adjusted R-squared: 0.632
## F-statistic:  291 on 3 and 502 DF,  p-value: <2e-16
```

Ridge Coefficients

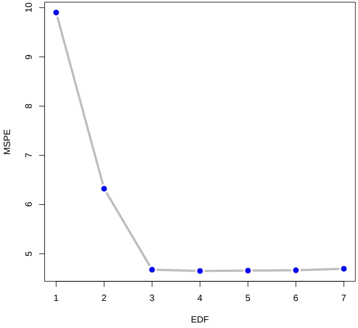


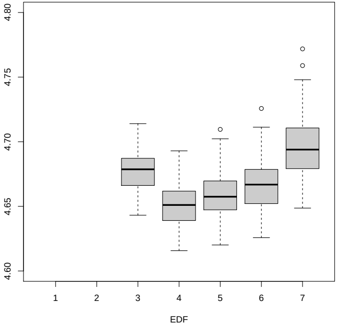
- The effective degrees of freedom $\text{EDF}(\lambda) = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2+\lambda}$, where d_j are the single values of $\mathbf{X}$.
- What is a good amount of shrinkage? (i.e., choosing λ)
- We might want to look at their predictive power!

Choosing λ

A standard practice is to use cross-validation to select a good λ.

I've used 100 10-fold CV estimates of the mean squared prediction error (MSPE).





Choosing λ (cont.)

		lambda	x1	x2	x3	x4	x5	x6	x7
	1	2809.521	0.344	0.043	-0.045	0.043	0.342	0.132	0.154
	2	662.711	0.716	0.145	-0.161	0.142	0.707	0.245	0.283
	3	66.671	1.084	0.296	-0.366	0.239	1.000	0.305	0.360
->	4	8.001	1.406	0.419	-0.472	0.034	0.850	0.183	0.432
	5	2.667	1.792	0.495	-0.522	-0.230	0.627	-0.012	0.479
	6	1.333	2.118	0.501	-0.523	-0.401	0.472	-0.180	0.480
	7	0.000	3.226	0.239	-0.359	-0.694	0.093	-0.739	0.317

LASSO: least absolute shrinkage and selection operator

The lasso coefficients minimize the RSS

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}})_L \;=\; \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta}\right)^2$$

subject to a different constrain on the coefficients, i.e.,

$$\sum_{j=1}^{p} |\boldsymbol{\beta}_j| \;\leq\; C \;\text{ for some } C > 0.$$

or equivalently, a penalized RSS:

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}})_L \;=\; \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta}\right)^2 \;+\; \lambda \sum_{j=1}^{p} |\boldsymbol{\beta}_j| \right\}$$

- Again, we have a tuning parameter λ that controls the amount of regularization.

LASSO: Example

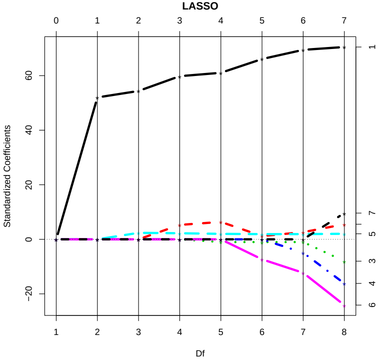
```
# using LASSO
b <- lars(x = as.matrix(x)[, -1], y = y, type = "lasso")
b
```

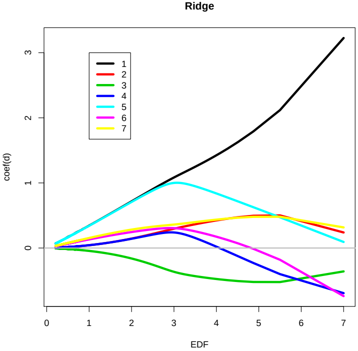
```
##
## Call:
## lars(x = as.matrix(x)[, -1], y = y, type = "lasso")
## R-squared: 0.635
## Sequence of LASSO moves:
##      x1 x5 x2 x3 x6 x4 x7
## Var   1  5  2  3  6  4  7
## Step  1  2  3  4  5  6  7
```

```
round(coef(b), 3)
```

```
##         x1    x2     x3     x4    x5     x6    x7
## [1,] 0.000 0.000  0.000  0.000 0.000  0.000 0.000
## [2,] 2.380 0.000  0.000  0.000 0.000  0.000 0.000
## [3,] 2.489 0.000  0.000  0.000 0.108  0.000 0.000
## [4,] 2.737 0.228  0.000  0.000 0.102  0.000 0.000
## [5,] 2.794 0.275 -0.045  0.000 0.091  0.000 0.000
## [6,] 3.025 0.052 -0.046  0.000 0.087 -0.225 0.000
## [7,] 3.179 0.113 -0.045 -0.211 0.087 -0.376 0.000
## [8,] 3.226 0.239 -0.359 -0.694 0.093 -0.739 0.317
```

LASSO: Example





- The y-axis of the LASSO plot shows each coefficient scaled by the size of the corresponding covariate ("Standardized Coefficients").
- Large enough λ (or small enough C) will set some of the LASSO coefficients exactly equal to 0. (i.e., model selection)!

Ridge *vs.* LASSO

Elements of Statistical Learning (2nd Ed.) ©Hastie, Tibshirani & Friedman 2009 Chap 3

$$\text{RSS} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T\mathbf{X}^T\mathbf{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

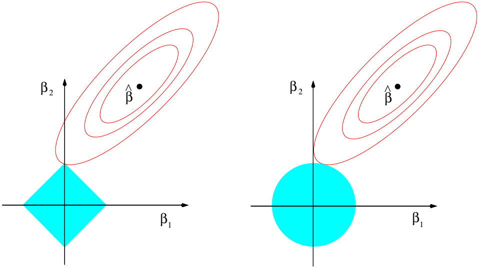


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \le t$ *and* $\beta_1^2 + \beta_2^2 \le t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

Limitations of Ridge and LASSO

- In general, Ridge (and Bridge) does not give sparse solutions (i.e., it is not a variable selection method).
- If $p > n$, LASSO can select at most n variables out of p candidates (Efron et al., 2004)
- If there is a group of highly correlated variables, LASSO tends to select only one covariate from the group, and in general its prediction performance is dominated by ridge regression.
- As these situations are common in -omics studies, LASSO does not seem to be the most convenient method.

Elastic Net

The Elastic Net coefficients minimize the RSS:

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}})_{EN} = \min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta}\right)^2$$

subject to

$$\sum_{j=1}^{p} (1-\alpha)|\boldsymbol{\beta}_j| + \alpha(\boldsymbol{\beta}_j)^2 \leq C \text{ for some } C > 0.$$

or equivalently a penalized RSS:

$$\min_{\beta_0, \boldsymbol{\beta} \in \mathbb{R}^p} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \boldsymbol{\beta}^T \mathbf{x}_i\right)^2 + \lambda \left((1-\alpha) \sum_{j=1}^{p} |\boldsymbol{\beta}_j| + \alpha \sum_{j=1}^{p} (\boldsymbol{\beta}_j)^2 \right) \right\}$$

A convex combination of the lasso and ridge penalties!

Elastic Net Penalty

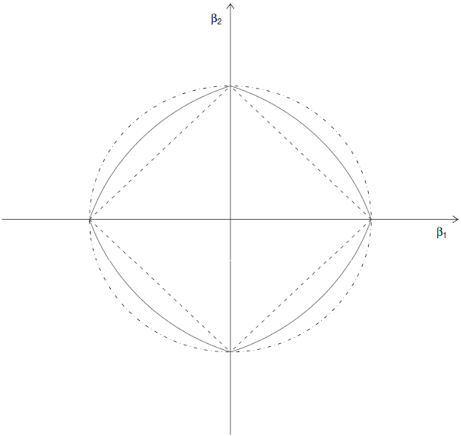


Fig. 1. Two-dimensional contour plots (level 1) (· - · - · -, shape of the ridge penalty; - - - - - - -, contour of the lasso penalty; ———, contour of the elastic net penalty with $\alpha = 0.5$): we see that singularities at the vertices and the edges are strictly convex; the strength of convexity varies with α

Elastic Net Algorithms

- Two famous algorithms can be used to compute EN coefficient with respective packages in R:
  - lars-en proposed in Zou and Hastie (2005)
  - glmnet in Friedman et al., (2010)
- In general, the latter is computationally more efficient and demonstrated better prediction performance (Friedman et al., 2010).
- glmnet can also be used to obtain LASSO estimates, and for classification (family=”binomial”)!.

Elastic Net: Example

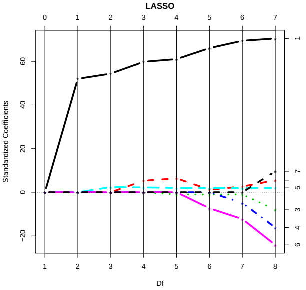
```
en <- glmnet(x = as.matrix(x)[, -1], y = y, family = "gaussian", nlambda = 10,
    standardize = TRUE)
print(en)
```

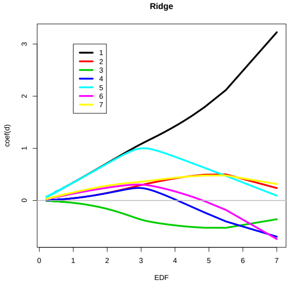
```
##
## Call:  glmnet(x = as.matrix(x)[, -1], y = y, family = "gaussian", nlambda = 10,      standardize = TRUE)
##
##       Df  %Dev   Lambda
##  [1,]  0 0.000 2.800000
##  [2,]  1 0.547 1.000000
##  [3,]  2 0.617 0.361000
##  [4,]  3 0.631 0.130000
##  [5,]  4 0.634 0.046600
##  [6,]  4 0.634 0.016800
##  [7,]  4 0.634 0.006020
##  [8,]  7 0.635 0.002160
##  [9,]  7 0.635 0.000778
## [10,]  7 0.635 0.000280
```

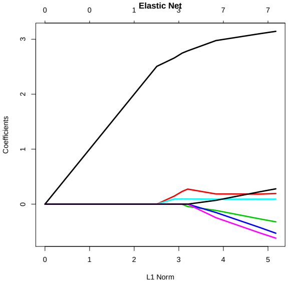
```
t(round(coef(en)[-1, ], 3))
```

```
## 10 x 7 sparse Matrix of class "dgCMatrix"
##       x1    x2     x3     x4    x5     x6    x7
## s0 .     .      .      .      .     .      .
## s1 1.844 .      .      .      .     .      .
## s2 2.506 .      .      .      0.001 .      .
## s3 2.659 0.146  .      .      0.093 .      .
## s4 2.747 0.231 -0.003  .      0.094 .      .
## s5 2.778 0.262 -0.033  .      0.095 .      .
## s6 2.789 0.274 -0.043  .      0.095 .      .
## s7 2.975 0.185 -0.114 -0.152 0.090 -0.246 0.069
## s8 3.101 0.183 -0.269 -0.426 0.091 -0.524 0.225
## s9 3.143 0.193 -0.322 -0.529 0.091 -0.619 0.279
```

Elastic Net: Example (cont.)







Choosing λ

- The function `cv.glmnet` runs glmnet to get the λ values for which an additional coefficient is added to the model.
- Given this sequence, cv.glmnet does an n-fold cross-validation (default n = 10) and estimates the prediction error.
- The average error and standard deviation over the folds can be plotted to choose the optimal λ. Note that cv.glmnet does NOT search for values for alpha.
- lambda.min gives the λ that minimizes the error. lambda.1se is the largest value of lambda with an error within 1 standard error from the minimum (i.e., a less complex model at a low cost).

The grouping effect

EN has the ”grouping effect” property (i.e., absolute values of coefficients of highly correlated variables tend to be equal).

Let $Z_1 \sim \mathcal{U}(0, 20)$ and $Z_2 \sim \mathcal{U}(0, 20)$ be latent variables, such that:

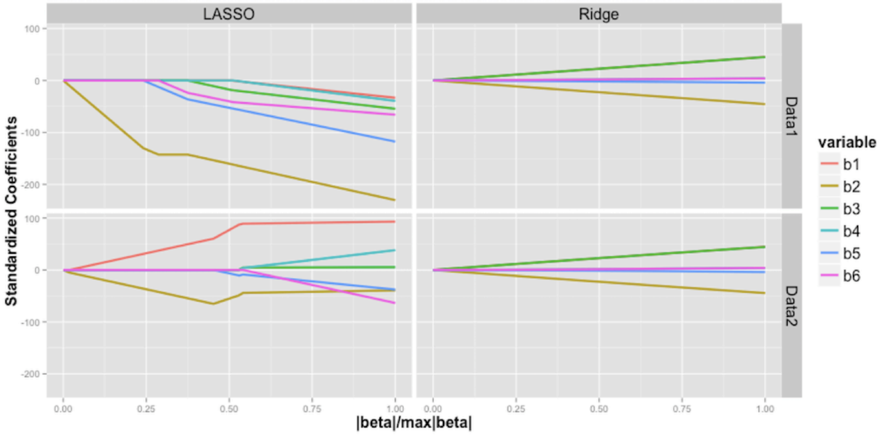
$$y = Z_1 + 0.1Z_2 + \varepsilon, \text{ with } \varepsilon \sim \mathcal{N}(0, 1)$$

Suppose that we observe:

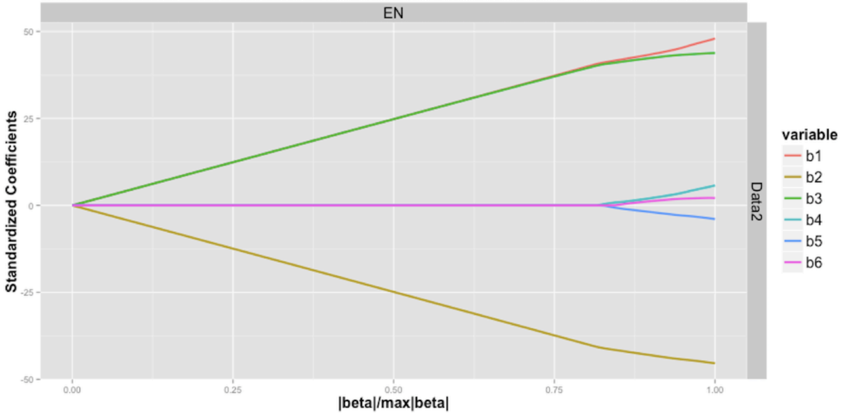
$$x_1 = Z_1 + \varepsilon_1, \; x_2 = -Z_1 + \varepsilon_2, \; x_3 = Z_1 + \varepsilon_3,$$

$$x_4 = Z_2 + \varepsilon_4, \; x_5 = -Z_2 + \varepsilon_5, \; x_6 = Z_2 + \varepsilon_6,$$

with $\varepsilon_i \sim \mathcal{N}(0, 1/16)$


LASSO
Ridge
Data1
Data2
Standardized Coefficients
|beta|/max|beta|
100
0
-100
-200
0.00
0.25
0.50
0.75
1.00
variable
b1
b2
b3
b4
b5
b6

EN penalty with $\alpha = 0.5$



Conclusions

- There are many methods and algorithms to perform classification and regression (more than those covered here).
- There are many variable selection methods (more than those covered here).
- Which one is better? We can evaluate different options using cross-validation.
- There is a trade-off between bias and variance when we fit more complex models.
- Even good CV performance does not mean that you will get good performance in the test set.
- LASSO and Ridge are particular cases of EN. The latter may perform better if covariates are highly correlated (group effect).
- Other extensions of LASSO to solve the grouping problem have been proposed.

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