02_Regularized_Regression

June 25, 2019

Day 2: Regularized Regression

```
In [1]: # Package "glmnet" contains the LASSO function
        # install.packages( 'glmnet' )
        library( glmnet )

        # Package "glmnetUtils" allows the use of R formulas for
        # specifying glmnet models (as opposed to converting to matrices)
        #library(devtools)
        #install_github("hong-revo/glmnetUtils")
        library(glmnetUtils)

        # Metapackage "tidyverse" imports libraries
        # for data manipulation (dplyr) and plotting (ggplot2)
        library( tidyverse )

        # Package "skimr" has excellent descriptive statistics
        # function skim_to_wide()
        library( skimr )

        # Package "GGally" has ggplot2-style scatterplot matrices
        library( GGally )

        # Package tictoc has functions to time function calls
        library( tictoc )

        # Library car has variance inflation factor function (vif())
        library( car )
```

```
Loading required package: Matrix
Loading required package: foreach
Loaded glmnet 2.0-18


Attaching package: glmnetUtils

The following objects are masked from package:glmnet:
```

```
    cv.glmnet, glmnet

Registered S3 methods overwritten by 'ggplot2':
  method         from
  [.quosures     rlang
  c.quosures     rlang
  print.quosures rlang
Registered S3 method overwritten by 'rvest':
  method            from
  read_xml.response xml2
 Attaching packages  tidyverse 1.2.1
 ggplot2 3.1.1      purrr   0.3.2
 tibble  2.1.1      dplyr   0.8.1
 tidyr   0.8.3      stringr 1.4.0
 readr   1.3.1      forcats 0.4.0
 Conflicts  tidyverse_conflicts()
 purrr::accumulate() masks foreach::accumulate()
 tidyr::expand()     masks Matrix::expand()
 dplyr::filter()     masks stats::filter()
 dplyr::lag()        masks stats::lag()
 purrr::when()       masks foreach::when()

Attaching package: skimr

The following object is masked from package:stats:

    filter

Registered S3 method overwritten by 'GGally':
  method from
  +.gg   ggplot2

Attaching package: GGally

The following object is masked from package:dplyr:

    nasa

Loading required package: carData

Attaching package: car

The following object is masked from package:dplyr:

    recode

The following object is masked from package:purrr:
```

```
some
```

```
In [2]: library( broom )
```

```
In [3]: options(repr.plot.width=4, repr.plot.height=3)
```

```
In [4]: uniform_noise <- function( min, max ) {
            runif( n=200, min, max )
        }
```

```
In [5]: gaussian_noise <- function( c=1 ) {
            rnorm( n=200 ) * c
        }
```

1 Generate fake data

```
In [6]: set.seed( 42 )
```

```
In [7]: GenerateFake <- function (){
            Y <- uniform_noise( -10, 10 ) + 7
            X1 <- Y + gaussian_noise(1)
            X2 <- Y + gaussian_noise(2)
            X3 <- Y + gaussian_noise(4)
            trash1 <- gaussian_noise(10)
            trash2 <- gaussian_noise(10)
            trash3 <- gaussian_noise(10)
            fake_data <- data.frame( Y, X1, X2, X3, trash1, trash2, trash3 )
            return( fake_data )
        }
```

```
In [8]: fake_data <- GenerateFake()
```

```
In [9]: library( rsample )
```

```
In [10]: dim( fake_data )
```

1. 200 2. 7

```
In [11]: skim_to_wide( fake_data )
```

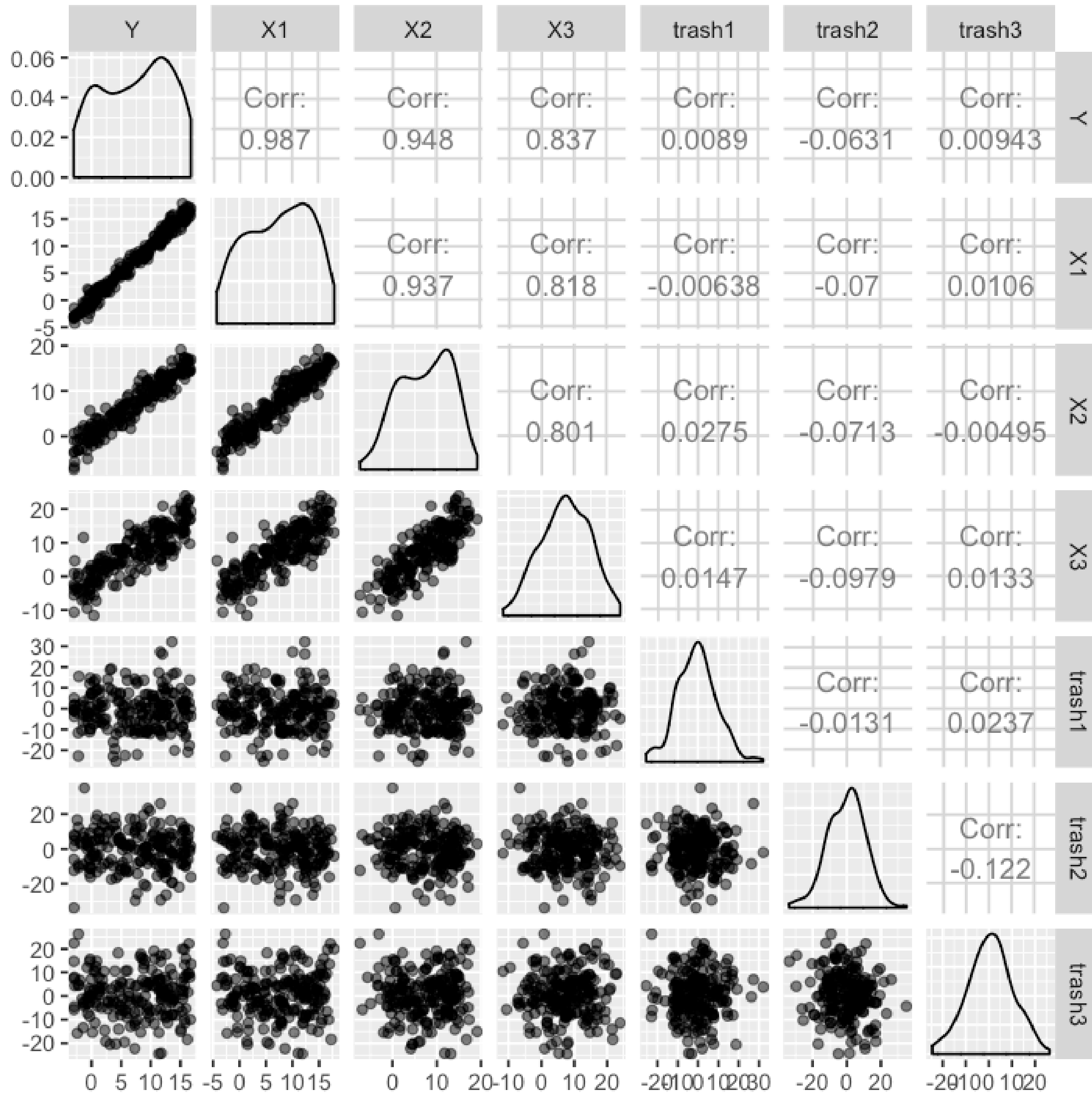
A tibble: 7 Œ 13

type <chr>	variable <chr>	missing <chr>	complete <chr>	n <chr>	mean <chr>	sd <chr>	p0 <chr>	p25 <chr>	p50 <chr>
numeric	trash1	0	200	200	-0.54	9.68	-25.54	-6.76	-0.59
numeric	trash2	0	200	200	-0.22	11	-33.72	-8.45	0.83
numeric	trash3	0	200	200	0.59	9.74	-24.54	-5.7	0.39
numeric	X1	0	200	200	7.4	5.92	-4.29	2.32	7.92
numeric	X2	0	200	200	7.36	5.92	-7.35	2.3	7.81
numeric	X3	0	200	200	7.28	7.42	-11.67	1.9	7.7
numeric	Y	0	200	200	7.44	5.84	-3	2.17	8.11

```
In [12]: library( GGally )
```

```
In [13]: options(repr.plot.width=6, repr.plot.height=6)
```

```
In [14]: ggpairs( fake_data, aes( alpha=0.1) )
```



2 Linear models

2.1 Null model

```
In [15]: model0 <- lm( Y ~ 1, fake_data )
```

```
In [16]: summary( model0 )
```

```
Call:
lm(formula = Y ~ 1, data = fake_data)

Residuals:
     Min       1Q   Median       3Q      Max
-10.4395  -5.2783   0.6639   4.7714   9.3335

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)    7.444      0.413   18.03   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 5.84 on 199 degrees of freedom
```

2.2 With one informative predictor

```
In [17]: model1 <- lm( Y ~ X1, fake_data )
```

```
In [18]: summary( model1 )
```

```
Call:
lm(formula = Y ~ X1, data = fake_data)

Residuals:
     Min       1Q   Median       3Q      Max
-2.89533 -0.52208 -0.03308  0.59546  2.35970

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.24892    0.10757   2.314   0.0217 *
X1           0.97296    0.01136  85.619   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.9495 on 198 degrees of freedom
Multiple R-squared:  0.9737,Adjusted R-squared:  0.9736
F-statistic:  7331 on 1 and 198 DF,  p-value: < 2.2e-16
```

2.3 With additional redundant informative predictor

```
In [19]: model1 <- lm( Y ~ ., fake_data )
```

```
In [20]: summary( model1 )
```

```
Call:
lm(formula = Y ~ ., data = fake_data)

Residuals:
    Min      1Q  Median      3Q     Max 
-2.2072 -0.4907  0.0534  0.4554  2.9097 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 0.192795   0.096240   2.003   0.0465 *  
X1          0.759026   0.030510  24.878  < 2e-16 ***
X2          0.164875   0.029318   5.624 6.49e-08 ***
X3          0.058825   0.014160   4.154 4.90e-05 ***
trash1      0.004954   0.006172   0.803   0.4231    
trash2      0.005524   0.005470   1.010   0.3138    
trash3      0.001290   0.006154   0.210   0.8341    
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.8384 on 193 degrees of freedom
Multiple R-squared:   0.98,Adjusted R-squared:  0.9794 
F-statistic:  1577 on 6 and 193 DF,  p-value: < 2.2e-16
```

2.4 Check variance inflation factor

- High VIF means independent variables have high pairwise correlations (splom or corr)
- VIF 5-10: is danger zone
- VIF > 10: assume bad regression coefficients

```
In [21]: vif( model1 )
```

X1 9.24612568429893 **X2** 8.5305237536944 **X3** 3.12499813445157 **trash1** 1.01049364659881 **trash2** 1.02517312360102 **trash3** 1.01790664676466

3 Multicolinearity discussion

- Want variables of interest to be reasonably independent.
- Multicolinearity increases the variance of the coefficients.
- Famous symptom of multicollinearity is having the wrong sign on the coefficients
- Another symptom: when you add or delete a factor from your model, the regression coefficients change dramatically
- Lose the explanitory part of the model.
- Ask yourself: do I care?

- If predictive model, then no.
- If inference estimating coefficients, then yes.

- Reduce variance of regression coefficients by adding bias.
- Regularization: penalize large coefficients betas. Pushes them to be smaller, is closer to zero.

4 Regularized Regression

- Use case: wide data
- Two objectives: fit the data, AND try to drive the coefficients to zero as much as possible.
- Overfitting: the model will want to fit the noise, which results in a nonzero regression coefficient beta when there should be none.
- Three types of regularized regression: LASSO, Ridge Regression, and ElasticNet
  - In LASSO variables can have regression coefficients that become exactly zero, i.e., drop cleanly out of the analysis. Makes your model more parsimonious, interpretable.
    * Minimize $\frac{1}{N}\sum_{i=1}^{N}(y_i - \beta_0 - x_i^T\beta)^2$ while constraining $\sum_{j=1}^{p}|\beta_j| \leq \lambda$
  - In Ridge Regression, variables don't drop cleanly, but fit metrics (R^2) are generally better.
    * Minimize $\frac{1}{N}\sum_{i=1}^{N}(y_i - \beta_0 - x_i^T\beta)^2$ while constraining $\sum_{j=1}^{p}(\beta_j)^2 \leq \lambda$
  - ElasticNet is a mixture of LASSO and Ridge:
    * Minimize $\hat{\beta} \equiv \underset{\beta}{\operatorname{argmin}}(\|y - X\beta\|^2 + \lambda_2\|\beta\|^2 + \lambda_1\|\beta\|_1)$

- Different units of different predictor variables you can get different magnitudes of the fitted coefficients.
- glmnet regularization involves standardizing the variables, which also has the effect of eliminating the intercept.
- Use validation set or cross validation to find the optimal λ for LASSO or Ridge Regression.

4.1 Perform LASSO using glmnet package

- glmnet will generate n different models (100 by default) with n different values of the regularization parameter (λ)
- Observe "coefficient paths": the vales of β_i as parameter λ varies
- A reasonable range of lambda vales are selected for you by default
  - Also you can specify your own (or a range of lambdas)

- LASSO corresponds with glmnet with argument $\alpha = 1$ which is default
- glmnet standardized variables by default, so regression coefficients β_i is interpretable as relative importances
- Use `dfmax` argument to limit number of variables included in the model

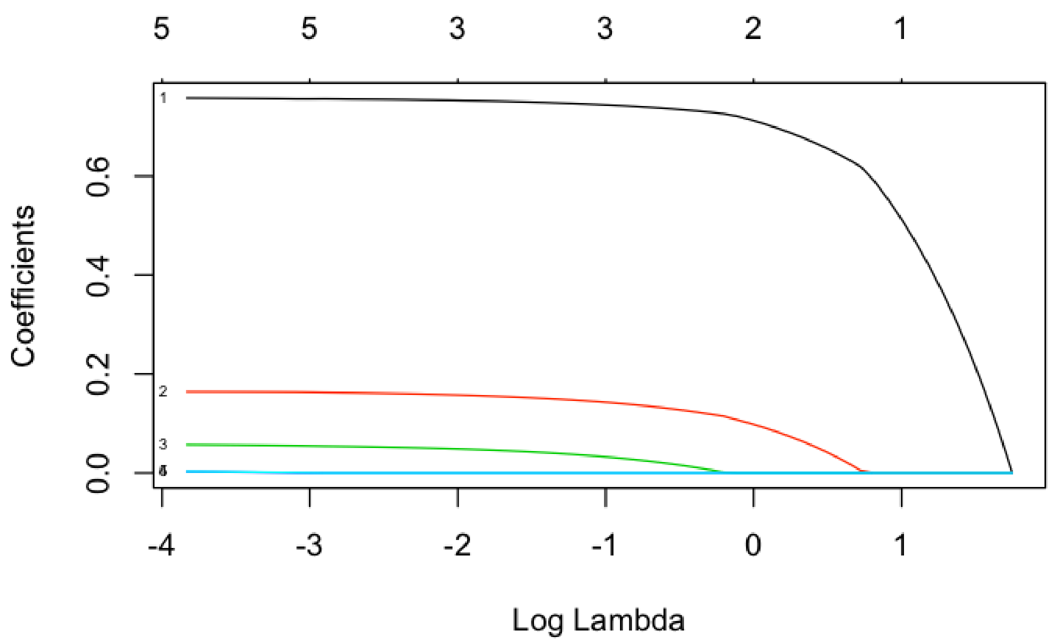
```
In [22]: glmnet_lm_result <- glmnet( Y ~ ., data=fake_data )
```

```
In [23]: print( glmnet_lm_result )
```

```
Call:
glmnet.formula(formula = Y ~ ., data = fake_data)

Model fitting options:
    Sparse model matrix: FALSE
    Use model.frame: FALSE
    Alpha: 1
    Lambda summary:
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
0.02164 0.08738 0.35274 1.05720 1.42401 5.74874
```

```
In [24]: options(repr.plot.width=6, repr.plot.height=4)
         plot( glmnet_lm_result, xvar='lambda', label=TRUE )
```



5 Which lambda gives the best model?

- BEST lambda is given by "lambda.min": the at which the minimal MSE is achieved
- Use `cv.glmnet()` - Perform CROSS-VALIDATION LASSO
- 10-fold cross validation to find optimal lambda parameter

```
In [25]: tic()
         glmnet_cv_result <- cv.glmnet( Y ~ ., data=fake_data )
         toc()
```

```
0.088 sec elapsed
```

```
In [26]: print( glmnet_cv_result )
```

```
Call:
cv.glmnet.formula(formula = Y ~ ., data = fake_data)

Model fitting options:
    Sparse model matrix: FALSE
    Use model.frame: FALSE
    Number of crossvalidation folds: 10
    Alpha: 1
    Deviance-minimizing lambda: 0.06609653  (+1 SE): 0.2668328
```

```
In [27]: glmnet_cv_result$lambda.min
```

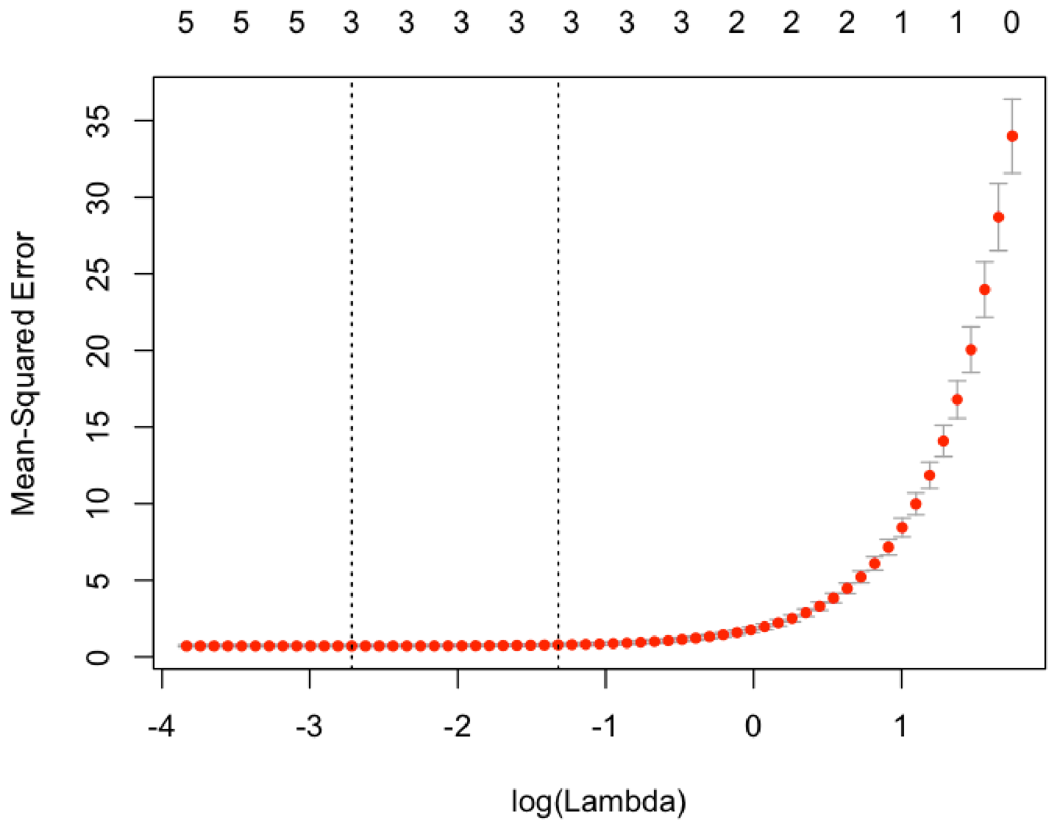
0.0660965280121163

```
In [28]: options(repr.plot.width=6, repr.plot.height=5)
```

```
In [29]: log( glmnet_cv_result$lambda.min )
```

-2.71663905979579

```
In [30]: plot( glmnet_cv_result )
```


5 5 5 3 3 3 3 3 3 3 2 2 2 1 1 0
Mean-Squared Error
0
5
10
15
20
25
30
35
-4
-3
-2
-1
0
1
log(Lambda)