REGULARIZATION METHODS

Jan-Philipp Kolb

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REGULARIZATION

ELITEDATASCIENCE.COM DEFINITION

Regularization is a technique used to prevent overfitting by artificially penalizing model coefficients.

- It can discourage large coefficients (by dampening them).
- ▶ It can also remove features entirely (by setting their coefficients to 0).
- ▶ The "strength" of the penalty is tunable.

WIKIPEDIA DEFINITION OF REGULARIZATION

Regularization is the process of adding information in order to solve an ill-posed problem or to prevent overfitting.

STRENGHTS AND WEAKNESSES OF REGULARIZATION

STRENGTHS:

Linear regression is straightforward to understand and explain, and can be regularized to avoid overfitting. In addition, linear models can be updated easily with new data

WEAKNESSES:

Linear regression in general performs poorly when there are non-linear relationships. They are not naturally flexible enough to capture more complex patterns, and adding the right interaction terms or polynomials can be tricky and time-consuming.

Three regularized regression algorithms







Lasso Regression

Ridge Regression

Elastic-Net

LASSO REGRESSION

- Absolute size of coefficients is penalized.
- ► Coefficients can be exactly 0.

RIDGE REGRESSION

- Squared size of coefficients is penalized.
- ▶ Smaller coefficients, but it doesn't force them to 0.

ELASTIC-NET

A mix of both absolute and squared size is penalzied.

PREPARATIONS

Most of the following slides are based on the UC Business
 Analytics R Programming Guide

NECESSARY PACKAGES

```
library(rsample) # data splitting
library(glmnet) # implementing regularized regression approach
library(dplyr) # basic data manipulation procedures
library(ggplot2) # plotting
library(knitr) # for tables
```

THE EXAMPLE DATASET

library(AmesHousing)

ames_data <- AmesHousing::make_ames()</pre>

	MS_SubClass	MS_Zoning \$	Lot_Frontage	Lot_Area	Street	Alley \$	Lot_Shape
1	One_Story_1946_and_Newer_All_Styles	Residential_Low_Density	141	31770	Pave	No_Alley_Access	Slightly_Irregular
2	$One_Story_1946_and_Newer_All_Styles$	Residential_High_Density	80	11622	Pave	No_Alley_Access	Regular
3	$One_Story_1946_and_Newer_All_Styles$	Residential_Low_Density	81	14267	Pave	No_Alley_Access	Slightly_Irregular
4	One_Story_1946_and_Newer_All_Styles	Residential_Low_Density	93	11160	Pave	No_Alley_Access	Regular
5	Two_Story_1946_and_Newer	Residential_Low_Density	74	13830	Pave	No_Alley_Access	Slightly_Irregular
6	Two_Story_1946_and_Newer	Residential_Low_Density	78	9978	Pave	No_Alley_Access	Slightly_Irregular
7	One_Story_PUD_1946_and_Newer	Residential_Low_Density	41	4920	Pave	No_Alley_Access	Regular
8	One_Story_PUD_1946_and_Newer	Residential_Low_Density	43	5005	Pave	No_Alley_Access	Slightly_Irregular
9	One_Story_PUD_1946_and_Newer	Residential_Low_Density	39	5389	Pave	No_Alley_Access	Slightly_Irregular
10	Two_Story_1946_and_Newer	Residential_Low_Density	60	7500	Pave	No_Alley_Access	Regular

Create training (70%) and test (30%) sets

- set.seed is used for reproducibility
- initial_split is used to split data in training and test data

Insufficient Solution

- ▶ When the number of features exceed the number of observations (p > n), the OLS solution matrix is not invertible.
- ▶ This causes significant issues because it means:
- 1. The least-squares estimates are not unique. There are an infinite set of solutions available and most of these solutions overfit the data.
- 2. In many instances the result will be computationally infeasible.
- ► To resolve this issue we can remove variables until p < n and then fit an OLS regression model.
- ▶ Although we can use pre-processing tools to apply this manual approach (**Kuhn and Johnson**, 2013, pp. 43-47), it can be cumbersome and prone to errors.

REGULARIZED REGRESSION

- When we experience these concerns, one alternative to OLS regression is to use regularized regression (also commonly referred to as penalized models or shrinkage methods) to control the parameter estimates.
- Regularized regression puts contraints on the magnitude of the coefficients and will progressively shrink them towards zero. This constraint helps to reduce the magnitude and fluctuations of the coefficients and will reduce the variance of our model.

THE OBJECTIVE FUNCTION OF REGULARIZED REGRESSION METHODS...

- ▶ is very similar to OLS regression;
- ► And a penalty parameter (P) is added.

$$minimize{SSE + P}$$

- ▶ There are two main penalty parameters, which have a similar effect.
- ▶ They constrain the size of the coefficients such that the only way the coefficients can increase is if we experience a comparable decrease in the sum of squared errors (SSE).

RIDGE REGRESSION

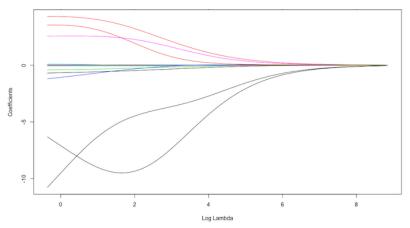
- ▶ Ridge regression (Hoerl, 1970) controls the coefficients by adding $\lambda \sum_{j=1}^{p} \beta_{j}^{2}$ to the objective function.
- ► This penalty parameter is referred to as "L2" as it signifies a second-order penalty being used on the coefficients.

$$\mathsf{minimize}\{\mathsf{SSE} + \lambda \sum_{j=1}^p \beta_j^2\}$$

- ▶ This penalty parameter can take on a wide range of values, which is controlled by the tuning parameter λ .
- ▶ When $\lambda = 0$, there is no effect and our objective function equals the normal OLS regression objective function of simply minimizing SSE.
- \blacktriangleright As $\lambda\to\infty,$ the penalty becomes large and forces our coefficients to zero.

EXEMPLAR COEFFICIENTS

Exemplar coefficients have been regularized with λ ranging from 0 to over 8,000 (log(8103)=9).



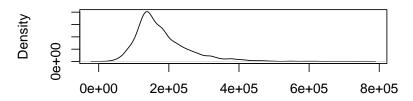
How to choose the right λ

- ▶ Although these coefficients were scaled and centered prior to the analysis, you will notice that some are extremely large when $\lambda \to 0$.
- ▶ We have a large negative parameter that fluctuates until $log(\lambda) \approx 2$ where it then continuously shrinks to zero.
- ▶ This is indicitive of multicollinearity and likely illustrates that constraining our coefficients with $log(\lambda) > 2$ may reduce the variance, and therefore the error, in our model.
- ▶ But how do we find the amount of shrinkage (or λ) that minimizes our error?

IMPLEMENTATION IN GLMNET

- ▶ glmnet does not use the formula method $(y \sim x)$ so prior to modeling we need to create our feature and target set.
- ► The model.matrix function is used on our feature set, which will automatically dummy encode qualitative variables
- ▶ We also log transform our response variable due to its skeweness.

plot(density(ames_data\$Sale_Price),main="")



TRAINING AND TESTING FEATURE MODEL MATRICES AND RESPONSE VECTORS.

▶ We use model.matrix(...)[, -1] to discard the intercept

```
ames_train_x <- model.matrix(Sale_Price ~ ., ames_train)[, -1]
ames_train_y <- log(ames_train$Sale_Price)

ames_test_x <- model.matrix(Sale_Price ~ ., ames_test)[, -1]
ames_test_y <- log(ames_test$Sale_Price)

# What is the dimension of of your feature matrix?
dim(ames_train_x)

## [1] 2054 307</pre>
```

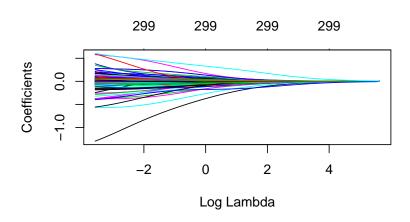
BEHIND THE SCENES

- ▶ The alpha parameter tells glmnet to perform a Ridge ($\alpha = 0$), Lasso ($\alpha = 1$), or Elastic Net ($0 \le \alpha \le 1$) model.
- Behind the scenes, glmnet is doing two things that you should be aware of:
- (1.) It is essential that predictor variables are standardized when performing regularized regression. glmnet performs this for you. If you standardize your predictors prior to glmnet you can turn this argument off with standardize=FALSE.
- (2.) glmnet will perform Ridge models across a wide range of λ parameters, which are illustrated in the figure on the next slide.

```
ames_ridge <- glmnet(x = ames_train_x,y = ames_train_y,
    alpha = 0)</pre>
```

A WIDE RANGE OF λ PARAMETERS

plot(ames_ridge, xvar = "lambda")



λ VALUES IN GLMNET

- ▶ We can see the exact λ values applied with ames_ridge\$lambda.
- You can specify your own λ values,
- ▶ By default glmnet applies 100 λ values that are data derived.
- lacktriangle Normally you will have little need to adjust the default λ values.

head(ames_ridge\$lambda)

[1] 279.1035 254.3087 231.7166 211.1316 192.3752 175.2851

ACCESS THE COEFFICIENTS WITH COEF.

- The coefficients are stored for each model in order of largest to smallest λ.
- ▶ The coefficients for the Gr_Liv_Area and TotRms_AbvGrd features for the largest λ (279.1035) and smallest λ (0.02791035) are visible.
- ▶ The largest λ value has pushed these coefficients to nearly 0.

```
coef(ames_ridge)[c("Gr_Liv_Area", "TotRms_AbvGrd"),100]
## Gr_Liv_Area TotRms_AbvGrd
## 0.0001004011 0.0096383231
coef(ames_ridge)[c("Gr_Liv_Area", "TotRms_AbvGrd"), 1]
## Gr_Liv_Area TotRms_AbvGrd
## 5.551202e-40 1.236184e-37
```

▶ But how much improvement we are experiencing in our model.

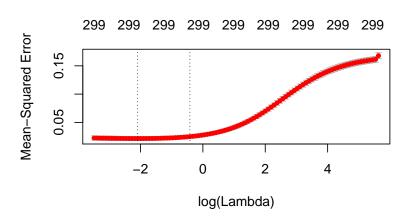
TUNING

- Recall that λ is a tuning parameter that helps to control our model from over-fitting to the training data.
- ▶ To identify the optimal λ value we need to perform cross-validation (CV).
- cv.glmnet provides a built-in option to perform k-fold CV, and by default, performs 10-fold CV.

```
ames_ridge <- cv.glmnet(x = ames_train_x,y = ames_train_y,
    alpha = 0)</pre>
```

RESULTS OF CV RIDGE REGRESSION

plot(ames_ridge)



The plot explained (I)

- As we constrain our coefficients with $log(\lambda) \le 0$ penalty, the MSE rises considerably.
- ▶ The numbers at the top of the plot (301) just refer to the number of variables in the model.
- Ridge regression does not force any variables to exactly zero so all features will remain in the model.

THE PLOT EXPLAINED (II)

```
min(ames ridge$cvm) # minimum MSE
## [1] 0.02147691
ames ridge$lambda.min  # lambda for this min MSE
## [1] 0.1236602
# 1 st.error of min MSE
ames_ridge$cvm[ames_ridge$lambda == ames_ridge$lambda.1se]
## [1] 0.02488411
ames_ridge$lambda.1se # lambda for this MSE
## [1] 0.6599372
```

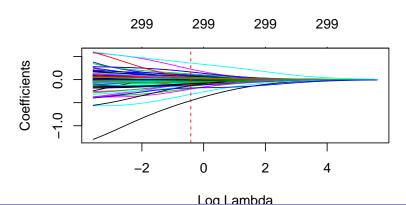
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THE PLOT EXPLAINED (III)

- ▶ The advantage of identifying the λ with an MSE within one standard error becomes more obvious with the Lasso and Elastic Net models.
- ▶ For now we can assess this visually.
- ▶ We plot the coefficients across the λ values and the dashed red line represents the largest λ that falls within one standard error of the minimum MSE.
- ► This shows you how much we can constrain the coefficients while still maximizing predictive accuracy.

```
ames_ridge_min <- glmnet(x = ames_train_x,y = ames_train_y,
    alpha = 0)</pre>
```

Coefficients across the λ values

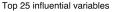


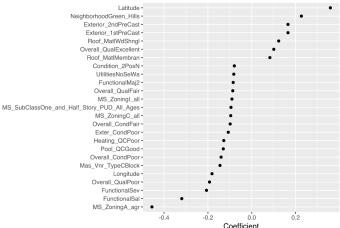
Advantages and Disadvantages

- ► The Ridge regression model has pushed many of the correlated features towards each other rather than allowing for one to be wildly positive and the other wildly negative.
- ▶ Many of the non-important features have been pushed closer to zero.
- We have reduced the noise in our data ⇒ more clarity in identifying the true signals.

```
coef(ames_ridge, s = "lambda.1se") %>%
  filter(row != "(Intercept)") %>%
  top_n(25, wt = abs(value)) %>%
  ggplot(aes(value, reorder(row, value))) +
  geom_point() +
  ggtitle("Top 25 influential variables") +
  xlab("Coefficient") +
  ylab(NULL)
```

Top 25 influential variables





RIDGE AND LASSO

A Ridge Model...

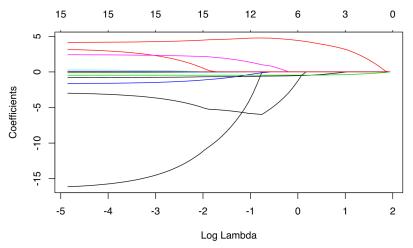
- ▶ ... is good if we need to retain all features, yet reduce the noise that less influential variables may create and minimize multicollinearity.
- ... does not perform feature selection. If greater interpretation is necessary where you need to reduce the signal in your data to a smaller subset then a Lasso model may be preferable.
- We could remove less important variables.
- We can do that manually by examining p-values of coefficients and discarding those variables whose coefficients are not significant.
- But this can become tedious for classification problems with many independent variables

LASSO REGRESSION

- Originally introduced in geophysics literature in 1986
- ► The least absolute shrinkage and selection operator (Lasso) model was rediscovered and popularized in 1996 by Robert Tibshirani
- It is an alternative to Ridge regression that has a small modification to the penalty in the objective function.
- ▶ Rather than the L_2 penalty we use the following L_1 penalty $\lambda \sum_{i=1}^{p} |\beta_i|$ in the objective function.

$$\mathsf{minimize}\{\mathsf{SSE} + \lambda \sum_{j=1}^{p} |\beta_j|\}$$

LASSO PENALTY PUSHES COEFFICIENTS TO ZERO



Lasso improves the model with regularization and conducts automated feature selection.

THE REDUCTION OF COEFFICIENTS

- ▶ 15 variables for $\log(\lambda) = -5$
- ▶ 12 variables for $\log(\lambda) = -1$
- ▶ 3 variables for $log(\lambda) = 1$

When a data set has many features, Lasso can be used to identify and extract those features with the largest (and most consistent) signal.

IMPLEMENTATION LASSO REGRESSION TO AMES DATA

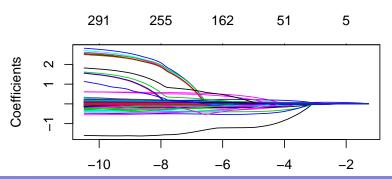
▶ Implementing Lasso follows the same logic as implementing the Ridge model, we just need to switch $\alpha = 1$ within glmnet.

```
ames_lasso<-glmnet(x=ames_train_x,y=ames_train_y,alpha=1)</pre>
```

A QUICK DROP IN NUMBER OF FEATURES

- Very large coefficients for ols (highly correlated)
- ▶ As model is constrained these noisy features are pushed to 0.
- ightharpoonup CV is necessary to determine right value for λ

```
plot(ames_lasso, xvar = "lambda")
```



TUNING WITH CV.GLMNET

cv.glmnet with alpha=1 is used to perform cv.

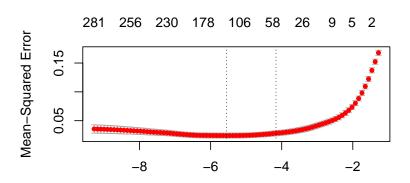
```
ames_lasso<-cv.glmnet(x=ames_train_x,y=ames_train_y,alpha=1)
names(ames_lasso)</pre>
```

```
## [1] "lambda" "cvm" "cvsd" "cvup" "cvl
## [6] "nzero" "name" "glmnet.fit" "lambda.min" "lam
```

MSE FOR CROSS VALIDATION

- ▶ MSE can be minimized with $-6 \le log(\lambda) \le -4$
- ▶ Also the number of features can be reduced (156 $\leq p \leq$ 58)

plot(ames_lasso)



MINIMUM AND ONE STANDARD ERROR MSE AND λ VALUES.

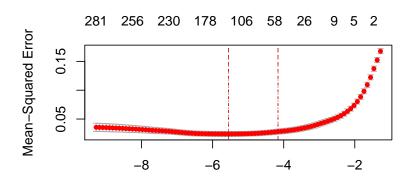
```
min(ames lasso$cvm) # minimum MSE
## [1] 0.02411134
ames lasso$lambda.min # lambda for this min MSE
## [1] 0.003865266
# 1 st.error of min MSE
ames lasso$cvm[ames lasso$lambda == ames lasso$lambda.1se]
## [1] 0.02819356
ames lasso$lambda.1se # lambda for this MSE
## [1] 0.01560415
```

MSE WITHIN ONE STANDARD ERROR

- The advantage of identifying the λ with an MSE within one standard error becomes more obvious.
- If we use the λ that drives the minimum MSE we can reduce our feature set from 307 down to less than 160.
- There is some variability with this MSE and we can assume that we can achieve a similar MSE with a slightly more constrained model (only 63 features).
- If describing and interpreting the predictors is an important outcome of your analysis, this will help.

Model with minimum MSE

```
plot(ames_lasso, xvar = "lambda")
abline(v=log(ames_lasso$lambda.min),col="red",lty="dashed")
abline(v=log(ames_lasso$lambda.1se),col="red",lty="dashed")
```



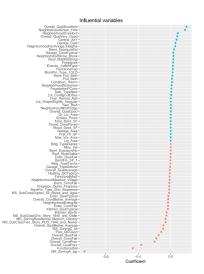
Advantages and Disadvantages

- Similar to Ridge, the Lasso pushes many of the collinear features towards each other rather than allowing for one to be wildly positive and the other wildly negative.
- Unlike Ridge, the Lasso will actually push coefficients to zero and perform feature selection.
- This simplifies and automates the process of identifying those feature most influential to predictive accuracy.

RCODE FOR PLOTTING INFLUENTIAL VARIABLES

```
coef(ames_lasso, s = "lambda.1se") %>%
  tidy() %>%
  filter(row != "(Intercept)") %>%
  ggplot(aes(value, reorder(row, value), color = value > 0)) +
  geom_point(show.legend = FALSE) +
  ggtitle("Influential variables") +
  xlab("Coefficient") +
  ylab(NULL)
```

PLOT INFLUENTIAL VARIABLES



MSE FOR RIDGE AND LASSO

```
# minimum Ridge MSE
min(ames_ridge$cvm)
## [1] 0.02147691
# minimum Lasso MSE
min(ames_lasso$cvm)
## [1] 0.02411134
```

ELASTIC NET

- Elastic-Net is a compromise between Lasso and Ridge.
- ▶ Elastic-Net penalizes a mix of both absolute and squared size.
- ▶ The ratio of the two penalty types should be tuned.
- ► The overall strength should also be tuned.

ELASTIC NETS

A generalization of the Ridge and Lasso models is the Elastic Net (Zou and Hastie, 2005), which combines the two penalties.

$$\textit{minimize} \{\textit{SSE} + \lambda \sum_{j=1}^p \beta_j^2 + \lambda_2 \sum_{j=1}^p |\beta_j| \}$$

SUMMARY OVERVIEW

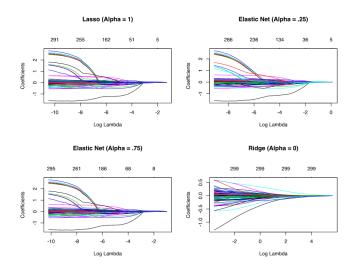
- ▶ A result of Lasso is that typically when two strongly correlated features are pushed towards zero, one may be pushed fully to zero while the other remains in the model.
- ▶ The process of one being in and one being out is not very systematic.
- ▶ In contrast, the Ridge regression penalty is a little more effective in systematically reducing correlated features together.
- ▶ The advantage of the Elastic Net model is that it enables effective regularization via the Ridge penalty with the feature selection characteristics of the Lasso penalty.

IMPLEMENTATION

alpha=.5 performs an equal combination of penalties

```
lasso <- glmnet(ames_train_x, ames_train_y, alpha = 1.0)
elastic1 <- glmnet(ames_train_x, ames_train_y, alpha = 0.25)
elastic2 <- glmnet(ames_train_x, ames_train_y, alpha = 0.75)
ridge <- glmnet(ames_train_x, ames_train_y, alpha = 0.0)</pre>
```

THE FOUR MODEL RESULTS PLOTTET



TUNING THE ELASTIC NET MODEL

- \triangleright λ is the primary tuning parameter in Ridge and Lasso models.
- ▶ With Elastic Nets, we want to tune the λ and the alpha parameters.
- ➤ To set up our tuning, we create a common fold_id, which just allows us to apply the same CV folds to each model.

CREATION OF A TUNING GRID

▶ We then create a tuning grid that searches across a range of alphas from 0-1, and empty columns where we'll dump our model results into.

Iteration over α values - Elastic Net

Now we can iterate over each α value, apply a CV Elastic Net, and extract the minimum and one standard error MSE values and their respective λ values.

The resulting tuning grid

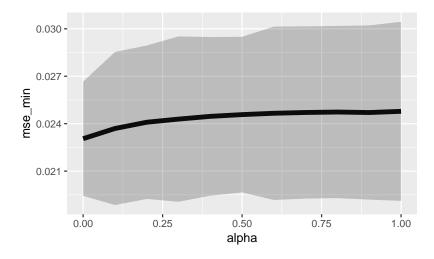
tuning_grid

```
## # A tibble: 11 x 5
##
     alpha mse min mse 1se lambda min lambda 1se
##
     <dbl>
             <dbl>
                    <dbl>
                               <dbl>
                                          <dbl>
##
   1
       0
            0.0230 0.0267
                             0.179
                                        0.795
##
   2
       0.1
            0.0237
                   0.0285
                             0.0387
                                        0.156
##
   3
       0.2
            0.0241
                   0.0289
                             0.0193
                                        0.0856
##
   4
       0.3
            0.0243
                   0.0295
                             0.0129
                                        0.0627
##
       0.4
            0.0245
                   0.0295
                             0.00966
                                        0.0470
##
       0.5
            0.0246
                   0.0295
                             0.00773
                                        0.0376
##
   7
       0.6
            0.0247
                   0.0301
                             0.00644
                                        0.0344
   8
       0.7
            0.0247
                   0.0302
##
                             0.00552
                                        0.0295
       0.8
                   0.0302
##
            0.0247
                             0.00483
                                        0.0258
##
   10
       0.9
            0.0247
                   0.0302
                             0.00429
                                        0.0229
            0.0248
                   0.0304
                             0.00387
##
  11
                                        0.0206
```

PLOT THE MSE

- ▶ If we plot the MSE \pm one standard error for the optimal λ value for each alpha setting, we see that they all fall within the same level of accuracy.
- ▶ We could select a full Lasso model with $\lambda = 0.02062776$, gain the benefits of its feature selection capability and reasonably assume no loss in accuracy.

MSE +/- ONE STANDARD ERROR



PREDICTING

- With the preferred model, you can predict the same model on a new data set.
- ▶ The only caveat is you need to supply predict an s parameter with the preferred models λ value.
- ▶ E.g., here we create a Lasso model, with a minimum MSE of 0.022.

```
# some best model
cv_lasso <- cv.glmnet(ames_train_x, ames_train_y, alpha = 1.0)
min(cv_lasso$cvm)
## [1] 0.02276229</pre>
```

▶ I use the minimum λ value to predict on the unseen test set and obtain a slightly lower MSE of 0.015.

```
# predict
pred <- predict(cv_lasso, s = cv_lasso$lambda.min, ames_test_x)
mean((ames_test_y - pred)^2)</pre>
```

THE PACKAGE CARET - CLASSIFICATION AND REGRESSION TRAINING

Vignette for the caret package

OUTPUT FOR CARET MODEL

```
caret mod
## glmnet
##
  2054 samples
##
   307 predictor
##
  Pre-processing: centered (116), scaled (116), remove (191)
  Resampling: Cross-Validated (10 fold)
  Summary of sample sizes: 1848, 1849, 1849, 1848, 1850, 1849,
  Resampling results across tuning parameters:
##
           lambda
                                               MAF.
##
    alpha
                         RMSF.
                                    Rsquared
##
    0 1
           0.0001289530
                         0.1664866
                                    0.8400298
                                               0.1063403
## 0.1 0.0002978982
                         0.1664766
                                    0.8400476
                                               0.1063330
##
    0.1 0.0006881835
                         0.1662662
                                    0.8403949
                                               0.1061256
##
    0.1
           0.0015897932
                         0.1659395
                                    0.8408804
                                               0.1058245
##
    0 1
           0.0036726286 0.1654464 0.8415077 0.1053447
```

REGULARIZATION METHODS

WHICH REGULARIZATION METHOD SHOULD WE CHOOSE?

- ► There's no "best" type of penalty. It depends on the dataset and the problem.
- ► We recommend trying different algorithms that use a range of penalty strengths as part of the tuning process

Advantages and Disadvantages

- ▶ The advantage of the Elastic Net model is that it enables effective regularization via the Ridge penalty with the feature selection characteristics of the Lasso penalty.
- ▶ Elastic Nets allow us to control multicollinearity concerns, perform regression when p > n, and reduce excessive noise in our data so that we can isolate the most influential variables while balancing prediction accuracy.
- ▶ Elastic Nets, and regularization models in general, still assume linear relationships between the features and the target variable.
- ▶ We can incorporate non-additive models with interactions, but it is tedious and difficult for a large number of features.
- When non-linear relationships exist, its beneficial to start exploring non-linear regression approaches.

FURTHER PACKAGES

https://cran.rstudio.com/web/packages/biglasso/biglasso.pdf
install.packages("biglasso")

biglasso: Extending Lasso Model Fitting to Big Data

Extend lasso and elastic-net model fitting for ultrahigh-dimensional, multi-gigabyte data sets that cannot be loaded into memory. It's much more memory- and computation-efficient as compared to existing lasso-fitting packages like 'glmnet' and 'nevreg', thus allowing for very powerful big data analysis even with an ordinary laptop.

Version: 1.3-6

Depends: R (≥ 3.2.0), bigmemory (≥ 4.5.0), Matrix, nevreg

Imports: Rcpp (> 0.12.1), methods

LinkingTo: Rcpp, RcppArmadillo, bigmemory, BH

Suggests: parallel, testthat, R.rsp

Published: 2017-05-04

Author: Yaohui Zeng [aut,cre], Patrick Breheny [ctb]

Lasso for other models than least squares

- Though originally defined for least squares, Lasso regularization is easily extended to a wide variety of statistical models including generalized linear models, generalized estimating equations, proportional hazards models, and M-estimators, in a straightforward fashion.
- Lasso's ability to perform subset selection relies on the form of the constraint and has a variety of interpretations including in terms of geometry, Bayesian statistics, and convex analysis.
- The Lasso is closely related to basis pursuit denoising.

RESOURCES AND LINKS

► Myers (1994) Classical and Modern Regression with Applications

LINKS

A comprehensive beginners guide for Linear, Ridge and Lasso Regression

- Course for statistical learning Youtube Videos
- pcLasso: a new method for sparse regression
- Youtube Lasso regression clearly explained
- glmnet Vignette
- Regularization Methods in R
- A gentle introduction to logistic regression and Lasso regularisation using R
- Penalized Regression in R
- Penalized Logistic Regression Essentials in R
- ▶ All you need to know about Regularization