NYC DATA SCIENCE ACADEMY

Regularization and Cross Validation

Data Science Bootcamp

Outline

- Part 1: Ridge & Lasso Regression
- Part 2: Cross-Validation
- Part 3: Review

PART 1

Ridge & Lasso Regression

Subset Selection

- In subset selection, we identify a subset of p predictors that we believe are related to the response. We then fit a model using least squares regression on the reduced set of variables.

- Subset selection can be performed in a myriad of ways:
  - Best subset selection
  - Forward stepwise regression
  - Backward stepwise regression
  - Both stepwise regression

- Select a model based on selected criteria:
  - AIC
  - BIC
  - $R^2_{Adj.}$

Shrinkage/Regularization

- In shrinkage/regularization, we fit a model involving all predictors; however, the estimated coefficients are shrunken towards 0 relative to the least squares estimates. As a result:
  - Estimate variance is reduced.
  - Variable selection can be performed.

- In order to regularize the coefficient estimates, we must further constrain the original least squares minimization problem. How do we do this?
  - Ridge regression
  - Lasso regression

Multiple Linear Regression: Mathematically

- Recall that in multiple linear regression we wish to quantify the relationship between X and Y as follows:

$$Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p$$

- Our original task was to find the estimates of $\beta_0, \beta_1, \beta_2, \ldots, \beta_p$ that reduce the sum of the squared vertical distances from the observations to the regression surface (i.e., the RSS) as much as possible.
  - Solved the minimization problem using basic calculus and linear algebra.

$$RSS = \sum_{i=1}^{n} e_i^2$$

Ridge Regression: Mathematically

- Ridge regression is an extension of the minimization problem posed by multiple linear regression; rather than attempting to simply reduce the RSS, ridge regression attempts to minimize the following:

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

- **NB:** Here, λ is a tuning parameter that essentially determines how the ridge regression will operate.

Ridge Regression: Mathematically

- As in the multiple linear regression setting, ridge regression attempts to find coefficient estimates that render the RSS as small as possible, thus fitting the data well.

- Additionally, there is an added shrinkage penalty (the extra term containing the tuning parameter λ).
  - Notice, the shrinkage penalty is simply the sum of the squared coefficient estimates. This penalty will be small when the estimates are close to 0. Therefore, it has the effect of shrinking the coefficient estimates as a group!

- The value of λ determines the relative impact of the RSS and shrinkage penalty terms on the resulting coefficient estimates.
  - A small λ penalizes the RSS more than the shrinkage penalty.
  - A large λ penalizes the shrinkage penalty more than the RSS.

Ridge Regression: Mathematically

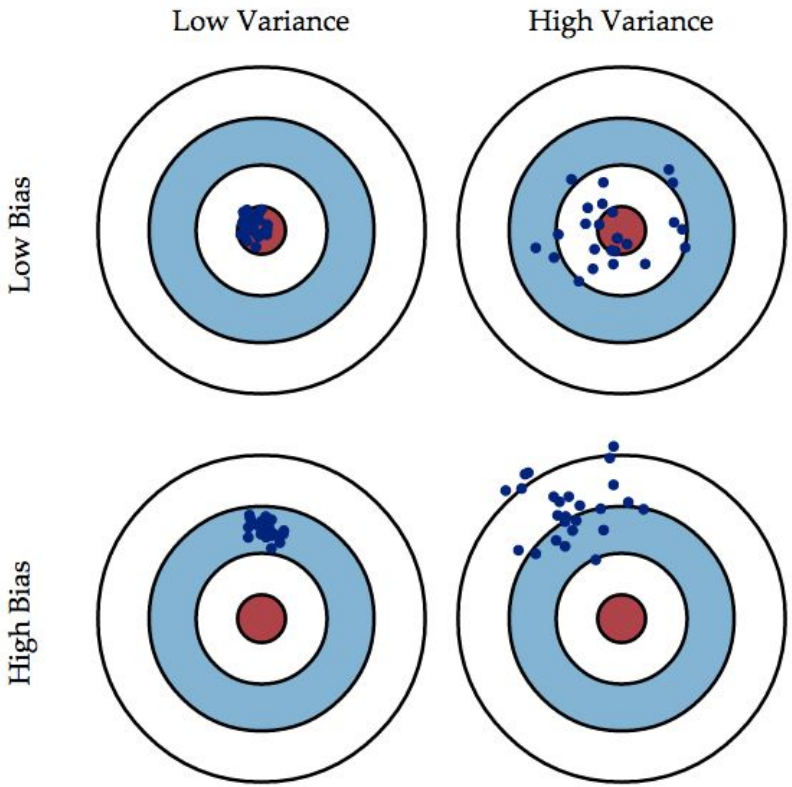
- Recall that the standard least squares coefficient estimates are scale equivariant: if we multiply a predictor variable by a constant, the corresponding least squares coefficient estimate will be scaled down by the same constant.
  - Regardless of how a predictor variable is scaled, the resulting product with the corresponding estimated coefficient will remain the same.

- In ridge regression, this is not the case. Coefficient estimates can change dramatically when multiplying a given predictor by a constant due to the shrinkage penalty; it depends on the sum of the squared coefficients!

- To avoid the issue of overvaluing or undervaluing certain predictor variables simply based on their magnitudes, we must standardize the variables prior to performing ridge regression.

Ridge Regression: Mathematically

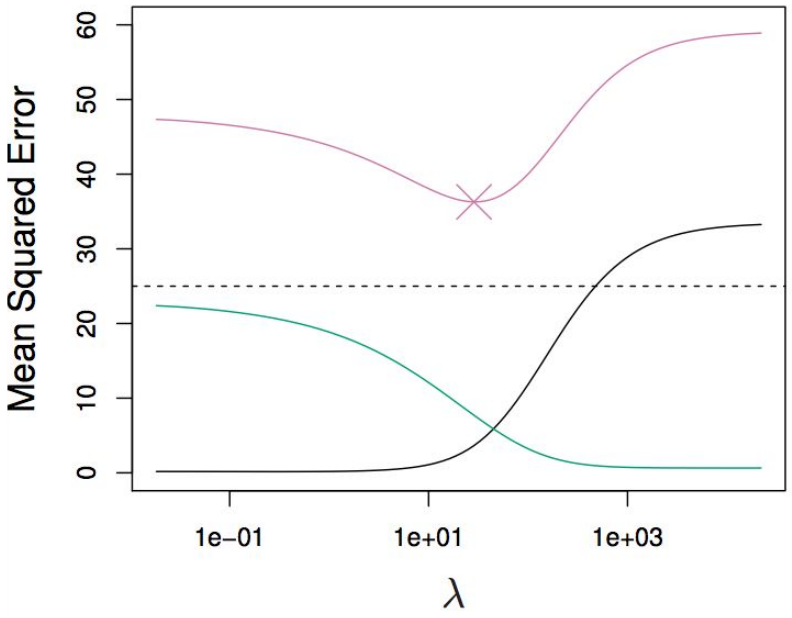
- Ideally, in any scenario, we hope to uncover a model that has:
  - Low bias (i.e., high accuracy)
  - Low variance (i.e., high precision)

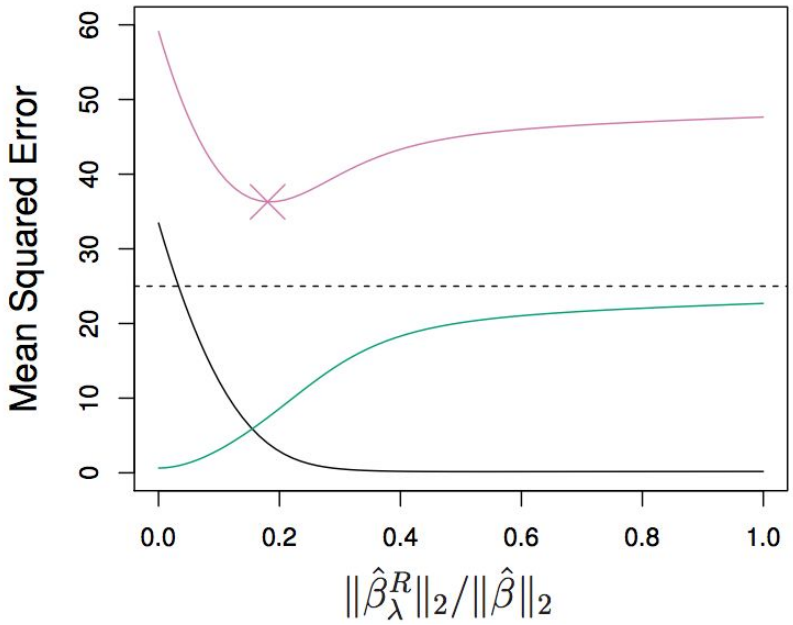


Image

Ridge Regression: Mathematically

- By shrinking the coefficient estimates towards 0 by increasing λ, we see that:
  - The bias (black) increases slightly but remains relatively small.
  - The variance (green) reduces substantially.
  - The mean squared error (red) of the predictions drops.





Lasso Regression: Mathematically

- The main disadvantage of ridge regression is that, while parameter estimates are shrunken, they only asymptotically approach 0 as we increase the value of λ.
  - Thus, the resulting model still includes estimates for all parameters.

- Lasso regression is another extension of the minimization problem posed by multiple linear regression; rather than attempting to simply reduce the RSS, lasso regression attempts to minimize the following:

$$RSS + \lambda \sum_{j=1}^{p} |\beta_j|$$

- **NB:** The only difference between the lasso and ridge regressions is that lasso implements the l_1 penalty (norm) rather than the l_2 penalty.

Lasso Regression: Mathematically

- While both ridge and lasso regression have the effect of shrinking coefficient estimates towards 0, the lasso necessarily forces some coefficient estimates to be exactly 0 (when λ is sufficiently large).

- Lasso regression has the added advantage of essentially performing variable selection, yielding models that are both accurate and parsimonious.

- Once again, the value of λ determines the relative impact of the RSS and shrinkage penalty terms on the resulting coefficient estimates.
  - In both ridge and lasso regression, it is important to select an appropriate value of λ by means of cross-validation.

Lasso VS Ridge

- Why is it the case that lasso regression results in coefficient estimates that are exactly 0? Why does ridge regression only end up shrinking the coefficients?

- We can restate the optimization problems of lasso and ridge regression, respectively, as the following Lagrangian multiplier scenarios:

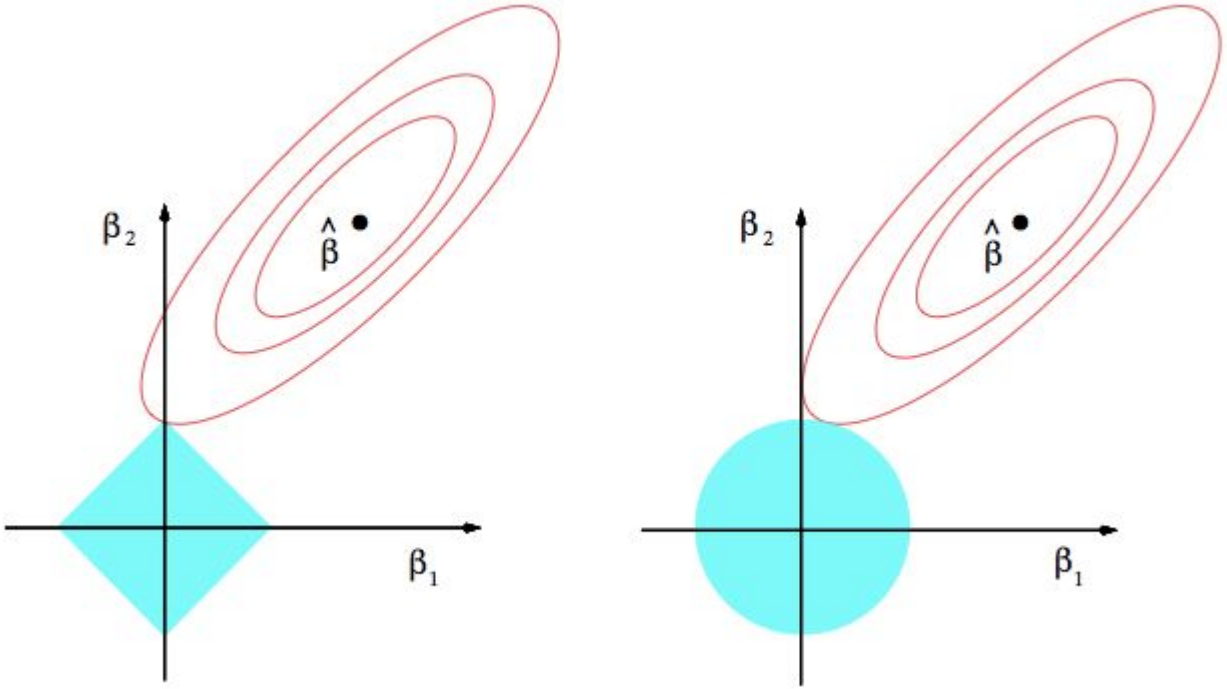
$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s$$

and

$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s,$$

Lasso VS Ridge: Visually

- The red ellipses represent the contours of the least squares error function.
- The blue regions represent the constrained regions for lasso and ridge, respectively.



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Selecting the Tuning Parameter: λ

- How do we choose the best value of λ?
- Let's take a look at the method of cross-validation.

PART 2

Cross-Validation

The Training & Test Sets

- When conducting cross-validation, we generally split the observations in our data into different (non-overlapping) sections:
  - The training set
  - The test set

- We use the observations in the training set to fit an initial model, but then can calculate the error in different ways:
  - The training error is calculated by applying the fitted model to the observations used to create the initial model (the training set).
  - The test error is calculated by applying the fitted model to the observations not used to create the initial model (the test set); this is like assessing the predictions of new observations.

- Why does the training error underestimate the test error?

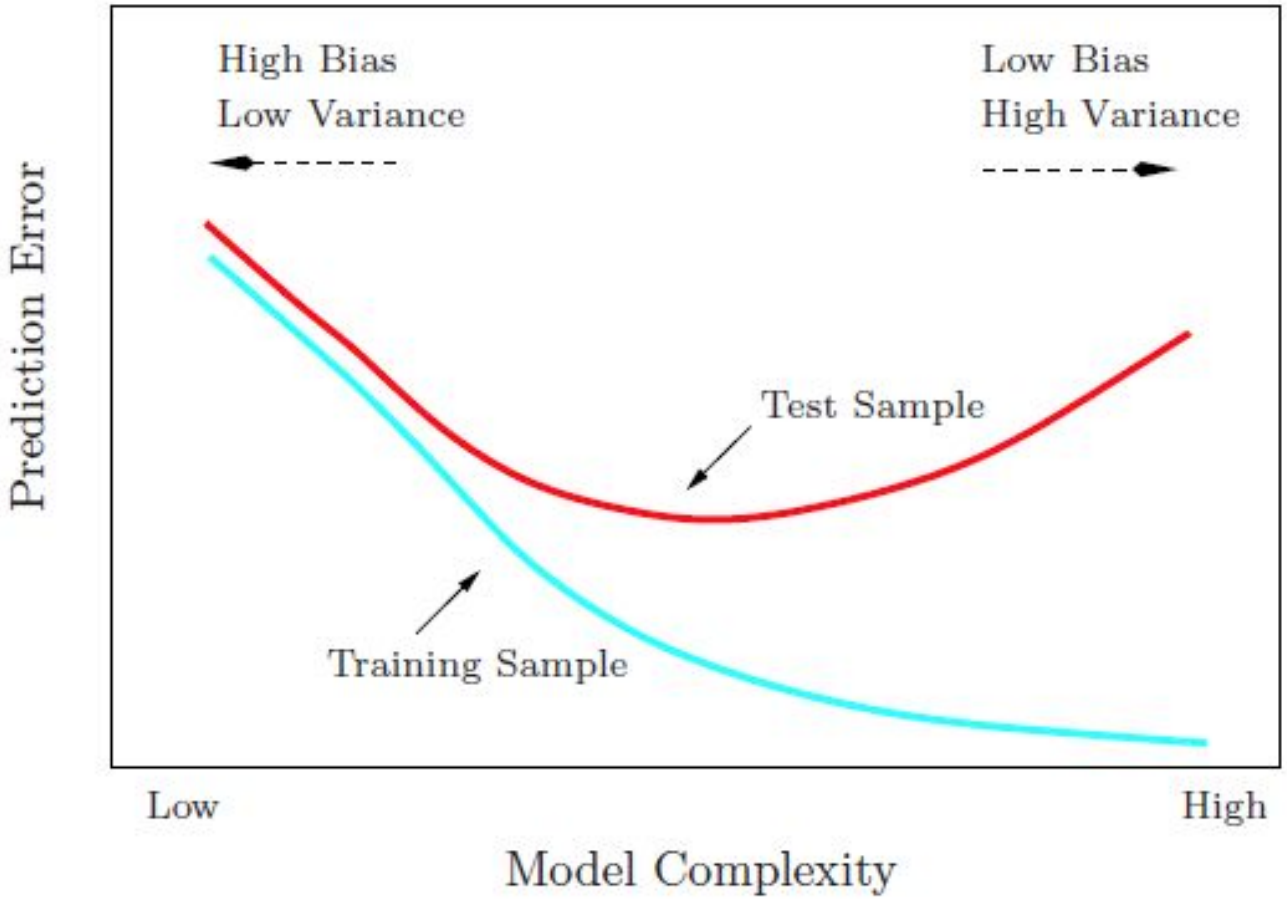
The Bias-Variance Tradeoff

- Recall that:
  - Bias is how far off on the average the model is from the truth.
  - Variance is how much the estimate varies about its average.

- With low model complexity:
  - Bias is high because predictions are more likely to stray from the truth with an inflexible model.
  - Variance is low because there are only few parameters being fit.

- With high model complexity:
  - Bias is low because the model can adapt to more subtleties in the data.
  - Variance is high because we have more parameters to estimate from the same amount of data.

The Bias-Variance Tradeoff



K-Fold Cross-Validation

- The results of K-fold cross-validation can help determine the best model at hand by estimating the test error among ultimate models.

- The process boils down to the following steps:
  - Divide your data into K (relatively) equal parts.
  - Leave out one of the K parts (call it part k), and put it to the side.
  - Fit the model to the remaining (K - 1) parts all together as your training set.
  - Use part k as your test set to estimate the prediction error.
  - Repeat this process K times, once each for the different splits of your data.

K-Fold Cross-Validation

- The test error can be estimated from the results of this process by essentially computing a weighted average of the K folds as follows:

$$CV_K = \sum_{k=1}^{K} \frac{n_k}{N} MSE_k$$

- Here:
  - K is the number of groups (folds).
  - n_k is the number of observations in fold k out of the total N observations.
  - MSE_k is the mean squared error obtained by using fold k as the test set, and the remaining data as the training set.

- **NB:** For classification problems, the MSE is simply replaced by the error rate.

Yet Again, How do we Choose K?

- 5- or 10-fold cross-validation is typically used because these values have been empirically shown to yield estimates of the test error rate that tend to neither suffer from extreme bias nor high variance.

Selecting the Tuning Parameter: λ

- In order to best implement the ridge and lasso regression methods, we need to have a way of determining the best value of λ (or, equivalently, the constraint s in the Lagrange multiplier formulation of the problem).

- As mentioned earlier, cross-validation helps us check by iterating across a slew of λ values and computing the cross-validation error rate for each.
  - Split the data into training and test sets (10-fold CV).
  - Select the λ for which the cross-validation error is the smallest.

- Lastly, refit the model using all available observations, this time with the best selected value of the tuning parameter.

PART 3

Review

Review

- Part 1: Alternatives to PCA: Ridge & Lasso Regression
  - Alternatives to PCA
  - Subset Selection
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    - Ridge Regression
    - Lasso Regression
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- Part 2: Cross-Validation
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  - Yet Again, How do we Choose K?
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