

3 Model Building

3.1 Introduction

The following sections will discuss various topics regarding constructing a good representative regression model for your data. Three main topics will be considered.

First, multicollinearity deals with the problem of linear relationships between your regressions. We already know that we require the columns of the design matrix to be linearly independent in order to solve for the least squares estimate. However, it is possible to have near dependencies among the columns. This can lead to numerical stability issues and unnecessary redundancy among the regressors.

Second, there are many different variable selection techniques in existence. Given a large number of regressors to can be included in a model, the question is, which should and which should not be included? We will discuss various techniques such as forward and backward selection as well as different tools for comparing models.

Third, penalized regression will be discussed. This section introduces two modern and quite powerful approaches to linear regression: ridge regression from the 1970's and LASSO from the 1990's. Both arise from modifying how we estimate the parameter vector $\hat{\beta}$. Up until now, we have chosen $\hat{\beta}$ to minimize the sum of the squared error. Now, we will add a penalty term to this optimization problem, which will encourage choices of $\hat{\beta}$ with small-in-magnitude or just zero entries.

3.2 Multicollinearity

The concept of multicollinearity is intuitively simple. Say we have a model of the form

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon.$$

This results in a design matrix of the form

$$X = \begin{pmatrix} 1 & x_{1,1} & x_{1,2} \\ \vdots & \vdots & \vdots \\ 1 & x_{n,1} & x_{n,2} \end{pmatrix}$$

Then, we can consider a new model of the form

$$x_2 = \alpha_0 + \alpha_1 x_1 + \varepsilon.$$

If this simple regression has a strong fit—e.g. A significant F-test or R^2 value—then the addition of the regressor x_2 to the original model is unnecessary as almost all of the explanatory information provided by x_2 with regards to predicting y is already provided by x_1 . Hence, the inclusion of x_2 in our model is superfluous.

Taking a more mathematical approach, it can be shown that such near linear dependencies lead to a very high variance for the least squares estimator $\hat{\beta}$. Furthermore, the magnitude of the vector is much larger than it should be.

Assuming that the errors have a covariance matrix $\text{Var}(\varepsilon) = \sigma^2 I_n$, then we have from before that

$$\begin{aligned}\text{Var}(\hat{\beta}) &= \text{Var}((X^T X)^{-1} X^T Y) = \\ &= (X^T X)^{-1} X^T \text{Var}(Y) X (X^T X)^{-1} = \sigma^2 (X^T X)^{-1}.\end{aligned}$$

With some effort, it can be shown that the diagonal entries of the matrix $(X^T X)^{-1}$ are equal to $(1 - R_0^2)^{-1}, \dots, (1 - R_p^2)^{-1}$ where R_j is the coefficient of determination for the model

$$x_j = \alpha_0 + \alpha_1 x_1 + \dots + \alpha_{j-1} x_{j-1} + \alpha_{j+1} x_{j+1} + \dots + \alpha_p x_p + \varepsilon,$$

which is trying to predict the j th regressor by the other $p - 1$ regressors. If the remaining regressors are good predictors for x_j , then the value R_j^2 will be close to 1. Hence,

$$\text{Var}(\hat{\beta}_j) = \frac{\sigma^2}{1 - R_j^2}$$

will be very large.

Furthermore, this implies that the expected Euclidean distance between $\hat{\beta}$ and β will be quite large as well. Indeed, we have

$$\mathbb{E} \left((\hat{\beta} - \beta)^T (\hat{\beta} - \beta) \right) = \sum_{i=0}^p \mathbb{E} \left(\hat{\beta}_i - \beta_i \right)^2 = \sum_{i=0}^p \text{Var}(\hat{\beta}_i) = \sigma^2 \text{tr}((X^T X)^{-1})$$

where $\text{tr}(\cdot)$ denotes the trace of a matrix—i.e. the sum of the diagonal entries. Hence, if at least one of the R_j^2 is close to 1, then the expected distance from our estimator to the true β will be quite large.

The trace of a matrix is also equal to the sum of its eigenvalues. Hence, if we denote the eigenvalues of $X^T X$ by $\lambda_1, \dots, \lambda_{p+1}$, then

$$\text{tr}((X^T X)^{-1}) = \sum_{i=1}^{p+1} \lambda_i^{-1}.$$

Hence, an equivalent condition to check for multicollinearity is the presence of eigenvalues of $X^T X$ very close to zero, which would make the above sum very large.

3.2.1 Identifying Multicollinearity

$$\text{VIF} = 1/(1-R^2)$$

To identify the presence of multicollinearity in our linear regression, there are many measures to consider.

We already established that near linear dependencies will result in large values for the diagonal entries of $(X^T X)^{-1}$. These values are known as the *Variance Inflation Factors* and sometimes written as $VIF_i = (1-R_i^2)^{-1}$.

An interesting interpretation of the VIF is in terms of confidence intervals. Recall that for β_j , we can construct a $1 - \alpha$ confidence interval as

$$-t_{\alpha/2, n-p-1} \sqrt{(X^T X)_{j,j}^{-1} \frac{SS_{\text{res}}}{n-p-1}} \leq \beta_j - \hat{\beta}_j \leq t_{\alpha/2, n-p-1} \sqrt{(X^T X)_{j,j}^{-1} \frac{SS_{\text{res}}}{n-p-1}}.$$

If all $i \neq j$ regressors are orthogonal to the j th regressor, then $R_j^2 = 0$ and the term $(X^T X)_{j,j}^{-1} = 1$. Under

multicollinearity, $(X^T X)_{j,j}^{-1} \gg 1$. Hence, the confidence interval is expanded by a factor of $\sqrt{(X^T X)_{j,j}^{-1}}$ when the regressors are not orthogonal.

We can alternatively examine the eigenvalues of the matrix $X^T X$. Recall that finding the least squares estimator is equivalent to solving a system of linear equations of the form

$$X^T X \hat{\beta} = X^T Y.$$

To measure the stability of a solution to a system of equations to small perturbations, a term referred to as the *condition number* is used. This term arises in more generality in numerical analysis; See [Condition Number](#). It is

$$\kappa = \lambda_{\max} / \lambda_{\min}$$

where λ_{\max} and λ_{\min} are the maximal and minimal eigenvalues, respectively. According to Montgomery, Peck, & Vining, values of κ less than 100 are not significant whereas values greater than 1000 indicate severe multicollinearity.

If the minimal eigenvalue is very small, we can use the corresponding eigenvector to understand the nature of the linear dependency. That is, consider the eigenvector $u = (u_0, u_1, \dots, u_p)$ for the matrix $X^T X$ corresponding to the eigenvalue λ_{\min} . Recall that this implies that

$$(X^T X)u = \lambda_{\min} u \approx 0,$$

which is approximately zero because λ_{\min} is close to zero. Hence, for regressors 1, x_1, \dots, x_p ,

$$u_0 + u_1 x_1 + \dots + u_p x_p \approx 0.$$

Thus, we can use the eigenvectors with small eigenvalues to get a linear relationship between the regressors.

Remark 3.1. If you are familiar with the concept of the [Singular Value Decomposition](#), then you could alternatively consider the ratio between the maximal and minimal singular values of the design matrix X . Furthermore, you can also analyze the singular vectors instead of the eigen vectors.

3.2.2 Correcting Multicollinearity

Ideally, we would design a model such that the columns of the design matrix X are linearly independent. Of course, in practice, this is often not achievable. When confronted with real world data, there are still some options available.

First, the regressors can be *respecified*. That is, if x_1 and x_2 are near linearly related, then instead of including both terms in the model, we can include a single combination term like $x_1 x_2$ or $(x_1 + x_2)/2$. Second, one of the two variables can be dropped from the model, which will be discussed below when we consider variable selection.

More sophisticated solutions to this problem include penalized regression techniques, which we will discuss below. Also, principal components regression—See Montgomery, Peck, Vining Sections 9.5.4 for more on PC regression—and partial least squares are two other methods that can be applied to deal with multicollinear data.

Remark 3.2. A common thread among all of these alternatives is that they result in a biased estimate for β unlike the usual least squares estimator. Often in statistics, we begin with unbiased estimators, but can often

achieve a better estimator by adding a small amount of bias. This is the so-called [bias-variance tradeoff](#).

3.3 Variable Selection

In general, if we have p regressors, we may want to build a model consisting only of the best regressors for modelling the response variable. In some sense, we could compare all possible subset models. However, there are many issues with this, which we will address in the following subsections. First, what are the effects of removing regressors from your model? Second, how do we compare models if they are not nested? Third, there are 2^p possible models to consider. Exhaustively fitting and comparing all of these models may be computational impractical or impossible. Hence, how do we find a good subset of the regressors?

3.3.1 Subset Models

What happens to the model when we remove some regressors? Assume we have a sample of n observations and $p + q$ regressors and want to remove q of them.

The full model would be

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_{p+q} x_{p+q} + \varepsilon.$$

This can be written in terms of the design matrix and partitioned over the two sets of regressors as

$$\begin{aligned} Y &= X\beta + \varepsilon \\ &= X_p \beta_p + X_q \beta_q + \varepsilon \end{aligned}$$

where $X_p \in \mathbb{R}^{n \times p}$, $X_q \in \mathbb{R}^{n \times q}$, $\beta_p \in \mathbb{R}^p$, $\beta_q \in \mathbb{R}^q$, and

$$X = (X_p \quad X_q), \quad \beta = \begin{pmatrix} \beta_p \\ \beta_q \end{pmatrix}$$

We have two models to compare. The first is the full model, $Y = X\beta + \varepsilon$, where we denote the least squares estimator as $\hat{\beta} = (X^T X)^{-1} X^T Y$ as usual with components

$$\hat{\beta} = \begin{pmatrix} \hat{\beta}_p \\ \hat{\beta}_q \end{pmatrix}.$$

The second is the reduced model obtained by deleting q regressors: $Y = X_p \beta_p + \varepsilon$. The least squares estimator for this model will be denoted as $\tilde{\beta}_p = (X_p^T X_p)^{-1} X_p^T Y$

3.3.1.1 Bias may increase

The first concern with the reduced model is that the estimator $\tilde{\beta}_p$ can be biased as

$$\begin{aligned} E\tilde{\beta}_p &= (X_p^T X_p)^{-1} X_p^T EY = (X_p^T X_p)^{-1} X_p^T (X_p \beta_p + X_q \beta_q) = \\ &= \beta_p + (X_p^T X_p)^{-1} X_p^T X_q \beta_q = \beta_p + A\beta_q. \end{aligned}$$

Hence, our reduced estimator is only unbiased in two cases. Case one is when $A = 0$, which occurs if the p regressors and q regressors are orthogonal resulting in $X_p^T X_q = 0$. Case two is when $\beta_q = 0$, which occurs if those regressors have no effect on the given response. If neither of these cases occurs, then $A\beta_q \neq 0$ and represents the bias in our estimator $\tilde{\beta}_p$. Note that the matrix A is referred to as the *alias matrix*.

3.3.1.2 Variance may decrease

While deleting regressors can result in the addition of bias to our estimate, it can also result in a reduction in the variance of our estimator. Namely,

$$\text{Var}(\tilde{\beta}_p) = \sigma^2(X_p^T X_p)^{-1}, \text{ while}$$

$$\text{Var}(\hat{\beta}_p) = \sigma^2(X_p^T X_p)^{-1} + \sigma^2 A[X_q^T (I - P_p) X_q]^{-1} A^T,$$

where $P_p = X_p(X_p^T X_p)^{-1} X_p^T$. This expression can be derived via the formula for [inverting a block matrix](#).

The matrix $A[X_q^T (I - P_p) X_q]^{-1} A^T$ is symmetric positive semi-definite, so the variance for $\hat{\beta}_p$ can only be larger than $\tilde{\beta}_p$.

3.3.1.3 MSE may or may not improve

Generally in statistics, when deciding whether or not the increase in the bias is worth the decrease in the variance, we consider the change in the *mean squared error* (MSE) of our estimate.

This is,

$$\begin{aligned} \text{MSE}(\tilde{\beta}_p) &= E\left((\tilde{\beta}_p - \beta_p)(\tilde{\beta}_p - \beta_p)^T\right) \\ &= E\left((\tilde{\beta}_p - E\tilde{\beta}_p + E\tilde{\beta}_p - \beta_p)(\tilde{\beta}_p - E\tilde{\beta}_p + E\tilde{\beta}_p - \beta_p)^T\right) \\ &= \text{var}(\tilde{\beta}_p) + \text{bias}(\tilde{\beta}_p)^2 \\ &= \sigma^2(X_p^T X_p)^{-1} + A\beta_q\beta_q^T A^T. \end{aligned}$$

For the full model,

$$\text{MSE}(\hat{\beta}_p) = \text{var}(\hat{\beta}_p) = \sigma^2(X_p^T X_p)^{-1} + \sigma^2 A[X_q^T (I - P_p) X_q]^{-1} A^T,$$

If $\text{MSE}(\hat{\beta}_p) - \text{MSE}(\tilde{\beta}_p)$ is positive semi-definite, then the mean squared error has decreased upon the removal of the regressors in X_q .

3.3.2 Model Comparison

We have already compared models in Chapter 1 with the partial F-test. However, for that test to make sense, we require the models to be nested—i.e. the larger model must contain all of the parameters of the smaller model. But, given a model

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \varepsilon,$$

we may want to compare two different subset models that are not nested. Hence, we have some different measures to consider.

Note that ideally, we would compare all possible subset models. However, given p regressors, there are 2^p different models to consider, which will often be computationally infeasible. Hence, we will consider two approaches to model selection that avoid this combinatorial problem.

Remark 3.3. To avoid confusion and awkward notation, assume that all subset models will always contain the intercept term β_0

3.3.2.1 Residual Sum of Squares

For two subset models with p_1 and p_2 regressors, respectively, with $p_1 < p$ and $p_2 < p$, we can compare the mean residual sum of squares for each

$$\frac{SS_{\text{res}}(p_1)}{n - p_1 - 1} \quad \text{vs} \quad \frac{SS_{\text{res}}(p_2)}{n - p_2 - 1}$$

and choose the model with the smaller value.

We know from before that the mean of the residual sum of squares for the full model, $SS_{\text{res}}/(n - p - 1)$, is an unbiased estimator for σ^2 . Similar to the calculations in the previous section, we can show that

$$E\left(\frac{SS_{\text{res}}(p_1)}{n - p_1 - 1}\right) \geq \sigma^2 \quad \text{and} \quad E\left(\frac{SS_{\text{res}}(p_2)}{n - p_2 - 1}\right) \geq \sigma^2,$$

which is that these estimators for subset models are upwardly biased.

3.3.2.2 Mallows' C_p

We can also compare different models by computing Mallows' C_p . The goal of this value is to choose the model that minimizes the mean squared prediction error, which is

$$MSPE = \sum_{i=1}^n \frac{E(\tilde{y}_i - E\tilde{y}_i)^2}{\sigma^2}$$

where \tilde{y}_i is the i th fitted value of the submodel and $E\tilde{y}_i$ is the i th fitted value of the true model. Furthermore, let \hat{y}_i be the i th fitted value for the full model. This is the expected squared difference between what the submodel predicts and what the real value is. As usual with mean squared errors in statistics, we rewrite this in terms of the variance plus the squared bias, which is

$$\begin{aligned} MSPE &= \frac{1}{\sigma^2} \sum_{i=1}^n [E(\tilde{y}_i - E\tilde{y}_i + E\tilde{y}_i - E\hat{y}_i)^2] \\ &= \frac{1}{\sigma^2} \sum_{i=1}^n [E(\tilde{y}_i - E\tilde{y}_i)^2 + (E\tilde{y}_i - E\hat{y}_i)^2] \\ &= \frac{1}{\sigma^2} \sum_{i=1}^n [\text{Var}(\tilde{y}_i) + \text{bias}(\tilde{y}_i)^2] \end{aligned}$$

Recall that the variance of the fitted values for the full model is $\text{Var}(\hat{y}) = \sigma^2 P_x$ where $P_x = X(X^T X)^{-1} X^T$. For a submodel with $p_1 < p$ regressors and design matrix X_{p_1} , we get the similar $\text{Var}(\tilde{y}) = \sigma^2 X_{p_1} (X_{p_1}^T X_{p_1})^{-1} X_{p_1}^T$. As $X_{p_1} (X_{p_1}^T X_{p_1})^{-1} X_{p_1}^T$ is a rank $p_1 + 1$ projection matrix, we have that

$$\sum_{i=1}^n \text{Var}(\tilde{y}_i) = \sigma^2 \text{tr}(X_{p_1} (X_{p_1}^T X_{p_1})^{-1} X_{p_1}^T) = \sigma^2(p_1 + 1).$$

For the bias term, consider the expected residual sum of squares for the submodel:

$$\begin{aligned}
 \mathbb{E}(SS_{\text{res}}(p_1)) &= \mathbb{E} \sum_{i=1}^n (y_i - \tilde{y}_i)^2 \\
 &= \mathbb{E} \sum_{i=1}^n (y_i - \mathbb{E}\tilde{y}_i + \mathbb{E}\tilde{y}_i - \mathbb{E}y_i + \mathbb{E}y_i - \tilde{y}_i)^2 \\
 &= \sum_{i=1}^n [\text{Var}(\tilde{r}_i) + (\mathbb{E}\tilde{y}_i - \mathbb{E}y_i)^2] \\
 &= (n - p_1 - 1)\sigma^2 + \sum_{i=1}^n \text{bias}(\tilde{y}_i)^2.
 \end{aligned}$$

Hence, rearranging the terms above gives

$$\sum_{i=1}^n \text{bias}(\tilde{y}_i)^2 = \mathbb{E}(SS_{\text{res}}(p_1)) - (n - p_1 - 1).$$

Combining the bias and the variance terms derived above results in Mallows' C_p statistic for a submodel with $p_1 < p$ regressors: %\begin{multiline}

$$C_{p_1} = \frac{\mathbb{E}(SS_{\text{res}}(p_1))}{\sigma^2} - n + 2p_1 + 2 \approx \frac{SS_{\text{res}}(p_1)}{SS_{\text{res}}/(n - p - 1)} - n + 2p_1 + 2.$$

%\end{multiline} Here, we estimate $\mathbb{E}(SS_{\text{res}}(p_1))$ by $SS_{\text{res}}(p_1)$ and estimate σ^2 by $SS_{\text{res}}/(n - p - 1)$.

Remark 3.4. Note that if we compute Mallows' C_p for the full model, we get

$$C_p = \frac{SS_{\text{res}}}{SS_{\text{res}}/(n - p - 1)} - n + 2p + 2 = p + 1.$$

Hence, Mallows' C_p in this case is just the number of parameters in the model. In general, we want to find submodels with C_p value smaller than $p + 1$.

3.3.2.3 Information Criteria

Information criteria are concerned with quantifying the amount of information in a model. With such a measure, we can choose a model that optimizes this measurement. A main requirement for these methods is that the response y is the same. Hence, we should not use the measures below when comparing transformed models—e.g. different linearized models—without the necessary modifications.

The first such measure is the Akaike Information Criterion or AIC, which is a measure of the entropy of a model. Its general definition is

$$\text{AIC} = -2 \log(\text{Likelihood}) + 2(\# \text{ parameters})$$

where p is the number of parameters in the model. This can be thought of a measurement of how much information is lost when modelling complex data with a p parameter model. Hence, the model with the minimal AIC will be optimal in some sense.

In our least squares regression case with normally distributed errors,

$$\text{AIC} = n \log(SS_{\text{res}}/n) + 2(p + 1)$$

where $p + 1$ is for the p regressors and 1 intercept term. Thus, adding more regressors will decrease SS_{res} but will increase p . The goal is to find a model with the minimal AIC. This can be shown to give the same ordering as Mallows' C_p when the errors are normally distributed.

The second such measure is the closely related Bayesian Information Criterion or BIC, which, in general, is

$$\text{BIC} = -2 \log(\text{Likelihood}) + (\# \text{ parameters}) \log n.$$

In the linear regression setting with normally distributed errors,

$$\text{BIC} = n \log(SS_{\text{res}}/n) + (p + 1) \log n.$$

Remark 3.5. Using AIC versus using BIC for model selection can sometimes result in different final choices. In some cases, one may be preferred, but often both can be tried and discrepancies, if they exist, can be reported.

There are also other information criterion that are not as common in practise such as the Deviation Information Criterion (DIC) and the Focused Information Criterion (FIC).

3.3.3 Forward and Backward Selection

Ideally, we choose a measure for model selection from the previous section and then compare all possible models. However, for p possible regressors, this will result in 2^p models to check, which may be computationally infeasible. Hence, there are iterative approaches that can be effective.

Forward selection is the process of starting with the constant model

$$y = \beta_0 + \varepsilon$$

and choosing the best of the p regressors with respect to the model selection criterion. This gives

$$y = \beta_0 + \beta_1 x_1 + \varepsilon.$$

This process will continue to add terms to the model as long as it results in an improvement in the criterion. For example, computing the AIC at each step.

Backwards selection is the reverse of forward selection. In this case, the algorithm begins with the full model,

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \varepsilon,$$

and iteratively removes the regressor that gives the biggest improvement in the model selection criterion. If the best choice is to remove no regressors, then the process terminates.

A third option is *stepwise selection*, which incorporates both forward and backward steps. In this case, we begin with the constant model as in forward selection. However, at every step, we choose either to add a new regressor to our model or remove one that is already in the model depending on which choice improves the criterion the most.

3.3.3.1 Variable Selection Example

Consider the same example as in the spline section where $x \in [0, 2]$ and

$$y = 2 + 3x - 4x^5 + x^7 + \varepsilon$$

with a sample of $n = 41$ observations. We can fit two regression models, an empty and a saturated model,

respectively,

$$y = \beta_0 + \varepsilon \text{ and } y = \beta_0 + \sum_{i=1}^7 \beta_i x^i + \varepsilon.$$

and use the R function `step()` to choose a best model with respect to AIC.

```
set.seed(256)
# Generate Data from a degree-7 polynomial
xx = seq(0,2,0.05)
len = length(xx)
yy = 2 + 3*xx - 4*xx^5 + xx^7 + rnorm(len,0,4)
# Fit the null and saturated models
# Note: never ever fit a polynomial model
#       like this. We are trying to create
#       a model with high multicollinearity
#       for educational purposes.
md0 = lm(yy~1);
md7 = lm(
  yy~xx+I(xx^2)+I(xx^3)+I(xx^4)+I(xx^5)+I(xx^6)+I(xx^7)
)
summary(md0)
```

Call:

```
lm(formula = yy ~ 1)
```

Residuals:

Min	1Q	Median	3Q	Max
-10.4234	-3.9053	0.8976	4.0282	9.4048

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.6483	0.7630	0.85	0.401

Residual standard error: 4.886 on 40 degrees of freedom

```
summary(md7)
```

Call:

```
lm(formula = yy ~ xx + I(xx^2) + I(xx^3) + I(xx^4) + I(xx^5) +
  I(xx^6) + I(xx^7))
```

Residuals:

Min	1Q	Median	3Q	Max
-7.7630	-2.3611	-0.7164	2.2562	7.3220

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.529	3.554	0.149	0.883
xx	-26.747	70.159	-0.381	0.705
I(xx^2)	271.061	434.342	0.624	0.537

I(xx^3)	-799.042	1158.236	-0.690	0.495
I(xx^4)	1124.811	1557.892	0.722	0.475
I(xx^5)	-824.786	1108.239	-0.744	0.462
I(xx^6)	300.118	397.719	0.755	0.456
I(xx^7)	-42.561	56.669	-0.751	0.458

Residual standard error: 3.982 on 33 degrees of freedom

Multiple R-squared: 0.4518, Adjusted R-squared: 0.3356

F-statistic: 3.886 on 7 and 33 DF, p-value: 0.003437

First, we note that this (non-orthogonal) polynomial model is very poorly specified. That is, the estimated coefficients vary wildly and are effectively trying to counter balance each other. None of our t-statistics are significant meaning that we can remove any of these terms individually without harming the fit of the model. The F-statistic is significant indicating that, globally, this model is significantly reducing the residual sum of squares.

First, we apply backwards variable selection. The result is an AIC that drops from 120.42 to 113.29 and the following fitted model:

$$y = 0.56 + 20.47x^2 - 18.59x^3 + 1.09x^6.$$

In this case, we did not recover the model that was used to generate the data. However, this one still fits the noisy data well.

```
# Perform a backward variable selection
md.bck = step(md7)
```

Start: AIC=120.42

yy ~ xx + I(xx^2) + I(xx^3) + I(xx^4) + I(xx^5) + I(xx^6) + I(xx^7)

	Df	Sum of Sq	RSS	AIC
- xx	1	2.3052	525.69	118.60
- I(xx^2)	1	6.1770	529.56	118.90
- I(xx^3)	1	7.5484	530.93	119.00
- I(xx^4)	1	8.2678	531.65	119.06
- I(xx^5)	1	8.7846	532.17	119.10
- I(xx^7)	1	8.9462	532.33	119.11
- I(xx^6)	1	9.0311	532.42	119.12
<none>		523.39	120.42	

Step: AIC=118.6

yy ~ I(xx^2) + I(xx^3) + I(xx^4) + I(xx^5) + I(xx^6) + I(xx^7)

	Df	Sum of Sq	RSS	AIC
- I(xx^7)	1	7.4088	533.10	117.17
- I(xx^6)	1	7.9536	533.64	117.21
- I(xx^5)	1	8.3113	534.00	117.24
- I(xx^4)	1	8.7075	534.40	117.27
- I(xx^3)	1	9.8197	535.51	117.36
- I(xx^2)	1	13.0549	538.75	117.60
<none>		525.69	118.60	

Step: AIC=117.17

yy ~ I(xx^2) + I(xx^3) + I(xx^4) + I(xx^5) + I(xx^6)

	Df	Sum of Sq	RSS	AIC
- I(xx^5)	1	1.5784	534.68	115.29
- I(xx^4)	1	1.5872	534.69	115.29
- I(xx^6)	1	2.1726	535.27	115.34
- I(xx^3)	1	2.6951	535.79	115.38
- I(xx^2)	1	6.2706	539.37	115.65
<none>			533.10	117.17

Step: AIC=115.29

yy ~ I(xx^2) + I(xx^3) + I(xx^4) + I(xx^6)

	Df	Sum of Sq	RSS	AIC
- I(xx^4)	1	0.0096	534.69	113.29
- I(xx^3)	1	3.4790	538.16	113.56
- I(xx^6)	1	7.0789	541.76	113.83
- I(xx^2)	1	12.5541	547.23	114.24
<none>			534.68	115.29

Step: AIC=113.29

yy ~ I(xx^2) + I(xx^3) + I(xx^6)

	Df	Sum of Sq	RSS	AIC
<none>			534.69	113.29
- I(xx^2)	1	143.39	678.08	121.03
- I(xx^3)	1	197.82	732.50	124.20
- I(xx^6)	1	229.28	763.96	125.92

`summary(md.bck)`

Call:

`lm(formula = yy ~ I(xx^2) + I(xx^3) + I(xx^6))`

Residuals:

Min	1Q	Median	3Q	Max
-8.3054	-2.4655	0.0047	2.3310	6.7750

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)							
(Intercept)	0.5640	1.3500	0.418	0.678528							
I(xx^2)	20.4701	6.4984	3.150	0.003226 **							
I(xx^3)	-18.5896	5.0245	-3.700	0.000698 ***							
I(xx^6)	1.0863	0.2727	3.983	0.000306 ***							

Signif. codes:	0	'***'	0.001	'**'	0.01	'*'	0.05	'.'	0.1	' '	1

Residual standard error: 3.801 on 37 degrees of freedom

Multiple R-squared: 0.44, Adjusted R-squared: 0.3946

F-statistic: 9.691 on 3 and 37 DF, p-value: 7.438e-05

Next, doing forward selection, we drop the AIC from 131.07 to 113.36, which is almost the same ending AIC as in the backwards selection performed above. In this case, the fitted model is

$$y = 0.78 + 17.19x^2 - 14.86x^3 + 0.41x^7.$$

```
# Perform a forward variable selection
md.fwd = step(md0,direction = "forward",scope = list(upper=md7))
```

Start: AIC=131.07

yy ~ 1

	Df	Sum of Sq	RSS	AIC
+ I(xx ²)	1	189.254	765.55	124.01
+ I(xx ³)	1	178.275	776.53	124.59
+ xx	1	151.475	803.33	125.98
+ I(xx ⁴)	1	150.951	803.85	126.01
+ I(xx ⁵)	1	121.568	833.23	127.48
+ I(xx ⁶)	1	95.317	859.48	128.75
+ I(xx ⁷)	1	73.561	881.24	129.78
<none>		954.80	131.06	

Step: AIC=124.01

yy ~ I(xx²)

	Df	Sum of Sq	RSS	AIC
+ I(xx ⁷)	1	44.476	721.07	123.55
<none>		765.55	124.01	
+ I(xx ⁶)	1	33.044	732.50	124.20
+ I(xx ⁵)	1	21.043	744.50	124.86
+ xx	1	15.086	750.46	125.19
+ I(xx ⁴)	1	9.728	755.82	125.48
+ I(xx ³)	1	1.583	763.96	125.92

Step: AIC=123.55

yy ~ I(xx²) + I(xx⁷)

	Df	Sum of Sq	RSS	AIC
+ I(xx ³)	1	185.46	535.61	113.36
+ I(xx ⁴)	1	178.81	542.26	113.87
+ xx	1	170.88	550.19	114.46
+ I(xx ⁵)	1	170.31	550.76	114.51
+ I(xx ⁶)	1	161.22	559.85	115.18
<none>		721.07	123.55	

Step: AIC=113.36

yy ~ I(xx²) + I(xx⁷) + I(xx³)

	Df	Sum of Sq	RSS	AIC
<none>		535.61	113.36	
+ xx	1	2.72717	532.89	115.15
+ I(xx ⁴)	1	1.21296	534.40	115.27
+ I(xx ⁵)	1	1.01714	534.60	115.28
+ I(xx ⁶)	1	0.93707	534.68	115.29

```
summary(md.fwd)
```

Call:
`lm(formula = yy ~ I(xx^2) + I(xx^7) + I(xx^3))`

Residuals:

Min	1Q	Median	3Q	Max
-8.0984	-2.3891	0.0842	2.4374	6.7973

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)							
(Intercept)	0.7795	1.3253	0.588	0.560027							
I(xx^2)	17.1905	5.7868	2.971	0.005195 **							
I(xx^7)	0.4142	0.1043	3.972	0.000317 ***							
I(xx^3)	-14.8630	4.1525	-3.579	0.000984 ***							

Signif. codes:	0	'***'	0.001	'**'	0.01	'*'	0.05	'.'	0.1	' '	1

Residual standard error: 3.805 on 37 degrees of freedom

Multiple R-squared: 0.439, Adjusted R-squared: 0.3935

F-statistic: 9.652 on 3 and 37 DF, p-value: 7.672e-05

3.3.4 Hypothermic Half Marathon Data, Revisited

In this section, we will revisit the hypothermic half marathon data from the previous chapter. This time, we will consider the predictors age, sex, and date as three categorical variables. There are 6 levels for age, 2 for sex, and 2 for race date.

```

hypoDat = read.csv("data/hypoHalf.csv",) [, -1]
hypoDat$DIV  <- as.factor(hypoDat$DIV)
hypoDat$date <- as.factor(hypoDat$date)
hypoDat$sex   <- as.factor(hypoDat$sex)
hypoDat$ageGroup <- as.factor(hypoDat$ageGroup)

levels( hypoDat$ageGroup )

```

```
[1] "0119" "2029" "3039" "4049" "5059" "60+"
```

```
levels( hypoDat$sex )
```

```
[1] "female" "male"
```

```
levels( hypoDat$date )
```

```
[1] "1" "2"
```

When we fit a model taking into account age, sex, and date, we can also consider interaction terms like $age \times sex$, which could be significant, for example, if age affects male and female runners differently with respect to their finishing time. The model that contains all pairwise interactions is fit below using the notation `(ageGroup + sex + date)^2`, which does *not* fit a quadratic polynomial model, but instead fits a model with the three main inputs and the $\binom{3}{2} = 3$ pairwise interactions.

```
summary(
  lm( time~(ageGroup + sex + date)^2, data=hypoDat )
)
```

Call:

```
lm(formula = time ~ (ageGroup + sex + date)^2, data = hypoDat)
```

Residuals:

Min	1Q	Median	3Q	Max
-51.172	-13.483	-0.944	11.212	76.509

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	137.0333	21.3140	6.429	5.7e-10 ***
ageGroup2029	-0.3606	21.8178	-0.017	0.987
ageGroup3039	5.1578	21.6055	0.239	0.811
ageGroup4049	7.9163	21.9381	0.361	0.718
ageGroup5059	4.9225	23.6578	0.208	0.835
ageGroup60+	29.6652	23.9378	1.239	0.216
sexmale	2.4778	24.6113	0.101	0.920
date2	-12.7856	25.2010	-0.507	0.612
ageGroup2029:sexmale	-11.1589	25.2088	-0.443	0.658
ageGroup3039:sexmale	-20.7837	25.0266	-0.830	0.407
ageGroup4049:sexmale	-14.5883	25.3120	-0.576	0.565
ageGroup5059:sexmale	0.2885	26.9407	0.011	0.991
ageGroup60+:sexmale	-18.2491	27.9274	-0.653	0.514
ageGroup2029:date2	4.2395	25.4660	0.166	0.868
ageGroup3039:date2	5.4182	25.0613	0.216	0.829
ageGroup4049:date2	2.2504	25.2425	0.089	0.929
ageGroup5059:date2	28.8170	26.9407	1.070	0.286
ageGroup60+:date2	-7.9524	27.8594	-0.285	0.776
sexmale:date2	3.7244	5.4197	0.687	0.493

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1				

Residual standard error: 21.31 on 273 degrees of freedom

Multiple R-squared: 0.1759, Adjusted R-squared: 0.1216

F-statistic: 3.238 on 18 and 273 DF, p-value: 1.627e-05

What we see in the summary of this regression model is that none of the t-tests for individual inputs is significant in this model except for the intercept term.

However, the F-statistic returns a very significant p-value. This indicates that we likely have too many inputs in our regression model. Performing backwards variable selection with respect to AIC results in the removal of all of the pairwise interaction terms leaving only the three main inputs as predictors for this model.

```
md.step = step(
  lm( time~(ageGroup + sex + date)^2, data=hypoDat )
)
```

Start: AIC=1805.02

time ~ (ageGroup + sex + date)^2

```

          Df Sum of Sq    RSS    AIC
- ageGroup:sex  5  2287.93 126308 1800.4
- ageGroup:date 5  2866.26 126886 1801.7
- sex:date      1   214.54 124235 1803.5
<none>                      124020 1805.0

```

Step: AIC=1800.36

```
time ~ ageGroup + sex + date + ageGroup:date + sex:date
```

```

          Df Sum of Sq    RSS    AIC
- ageGroup:date 5  2315.9 128624 1795.7
- sex:date      1   146.6 126455 1798.7
<none>                      126308 1800.4

```

Step: AIC=1795.67

```
time ~ ageGroup + sex + date + sex:date
```

```

          Df Sum of Sq    RSS    AIC
- sex:date      1   116 128740 1793.9
<none>                      128624 1795.7
- ageGroup      5   11262 139886 1810.2

```

Step: AIC=1793.93

```
time ~ ageGroup + sex + date
```

```

          Df Sum of Sq    RSS    AIC
<none>                      128740 1793.9
- date          1   2398.4 131138 1797.3
- ageGroup      5   11266.3 140006 1808.4
- sex           1   10116.2 138856 1814.0

```

```
summary(md.step)
```

Call:

```
lm(formula = time ~ ageGroup + sex + date, data = hypoDat)
```

Residuals:

Min	1Q	Median	3Q	Max
-69.267	-14.331	-1.126	12.157	79.624

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	148.070	9.757	15.176	< 2e-16 ***
ageGroup2029	-9.454	9.857	-0.959	0.3383
ageGroup3039	-8.994	9.761	-0.921	0.3576
ageGroup4049	-4.202	9.898	-0.425	0.6715
ageGroup5059	11.981	10.719	1.118	0.2646
ageGroup60+	8.672	11.159	0.777	0.4377
sexmale	-12.069	2.555	-4.724	3.64e-06 ***
date2	-6.055	2.632	-2.300	0.0222 *

```
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 21.29 on 284 degrees of freedom

Multiple R-squared: 0.1446, Adjusted R-squared: 0.1235

F-statistic: 6.856 on 7 and 284 DF, p-value: 1.545e-07

In the final model, none of the t-tests for `ageGroup` levels are significant. These t-tests are testing the hypotheses, *is the average finishing time of this age group different from the 0119 category* after already taking the variables `sex` and `date` into account. Note that while none of the t-tests are significant, the `ageGroup` variable is still included in the regression model even after variable selection.

Since `ageGroup` is an ordered categorical variable, we can also re-encode it as a polynomial to identify that there is a significant linear increase in the finishing times across the age groups as well as some significance in the quadratic term. This coincides with what was seen in the previous chapter.

```
hypoDat$ageGroup <- as.ordered(hypoDat$ageGroup)
contrasts( hypoDat$ageGroup, how.many=2 ) <- contr.poly
summary(
  lm( time~ageGroup + sex + date, data=hypoDat )
)
```

Call:

```
lm(formula = time ~ ageGroup + sex + date, data = hypoDat)
```

Residuals:

Min	1Q	Median	3Q	Max
-61.057	-14.637	-1.708	11.890	78.831

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	146.443	2.645	55.360	< 2e-16 ***
ageGroup.L	18.125	4.910	3.692	0.000267 ***
ageGroup.Q	10.101	4.813	2.099	0.036727 *
sexmale	-11.921	2.557	-4.662	4.81e-06 ***
date2	-6.502	2.627	-2.475	0.013889 *

```
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 21.35 on 287 degrees of freedom

Multiple R-squared: 0.1306, Adjusted R-squared: 0.1185

F-statistic: 10.78 on 4 and 287 DF, p-value: 3.739e-08

3.4 Penalized Regressions

No matter how we design our model, thus far we have always computed the least squares estimator, $\hat{\beta}$, by minimizing the sum of squared errors

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^{p+1}} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 \right\}.$$

This is an unbiased estimator for β . However, as we have seen previously, the variance of this estimator can be

quite large. Hence, we *shrink* the estimator towards zero adding bias but decreasing the variance. General idea of shrinkage is attributed to Stein (1956) and the so-called [Stein Estimator](#). In the context of regression, we add a penalty term to the above minimization to get a new estimator

$$\hat{\beta}^{\text{pen}} = \arg \min_{\beta \in \mathbb{R}^{p+1}} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 + \text{penalty}(\beta) \right\},$$

which increases as β increases thus attempting to enforce smaller choices for the estimated parameters. We will consider some different types of penalized regression. In [R](#), the [glmnet](#) package has a lot of functionality to fit different types of penalized general linear models ::: {#rem-penalIntercept} We generally do not want to penalize the intercept term β_0 . Often to account for this, the regressors and response are centred—i.e. Y is replaced with $Y - \bar{Y}$ and each X_j is replaced with $X_j - \bar{X}_j$ for $j = 1, \dots, p$ —in order to set the intercept term to zero. :::

3.4.1 Ridge Regression

The first method we consider is ridge regression, which arose in statistics in the 1970's—see Hoerl, A.E.; R.W. Kennard (1970)—but similar techniques arise in other areas of computational mathematics. In short, a quadratic penalty is applied to the least squares estimator resulting in

$$\hat{\beta}_\lambda^R = \arg \min_{\beta \in \mathbb{R}^p} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$

for any $\lambda \geq 0$. When $\lambda = 0$, we have the usual least squares estimator. As λ grows, the β 's are more strongly penalized.

To solve for $\hat{\beta}_\lambda^R$, we proceed as before with the least squares estimator $\hat{\beta}$ by setting the partial derivatives equal to zero

$$0 = \frac{\partial}{\partial \beta_k} \left\{ \sum_{i=1}^n (y_i - \beta_1 x_{i,1} - \dots - \beta_p x_{i,p})^2 + \lambda \sum_{j=1}^p \beta_j^2 \right\}.$$

This results in the system of equations

$$X^T Y - (X^T X) \hat{\beta}_\lambda^R - \lambda \hat{\beta}_\lambda^R = 0$$

with the ridge estimator being $\hat{\beta}_\lambda^R = (X^T X + \lambda I_n)^{-1} X^T Y$

The matrix $X^T X$ is positive semi-definite even when $p > n$ —i.e. the number of parameters exceeds the sample size. Hence, any positive value λ will make $X^T X + \lambda I_n$ invertible as it adds the positive constant λ to all of the eigenvalues. Increasing the value of λ will increase the numerical stability of the estimator—i.e. decrease the condition number of the matrix. Furthermore, it will decrease the variance of the estimator while increasing the bias. It can also be shown that the bias of $\hat{\beta}_\lambda^R$ is

$\lambda \uparrow, v \downarrow, B \uparrow$

$$E \hat{\beta}_\lambda^R - \beta = -\lambda (X^T X + \lambda I_n)^{-1} \beta,$$

which implies that the estimator does, in fact, shrink towards zero as λ increases.

3.4.2 Best Subset Regression

Another type of penalty related to the variable selection techniques from the previous section is the Best Subset Regression approach, which counts the number of non-zero β 's and adds a larger penalty as more terms are included in the model. The optimization looks like

$$\hat{\beta}_\lambda^B = \arg \min_{\beta \in \mathbb{R}^p} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 + \lambda \sum_{j=1}^p \mathbf{1}[\beta_j \neq 0] \right\}.$$

The main problem with this method is that the optimization is non-convex and becomes severely difficult to compute in practice. This is why the forwards and backwards selection methods are used for variable selection.

3.4.3 LASSO

The last method we consider is the Least Absolute Shrinkage and Selection Operator, which is commonly referred to as just LASSO. This was introduced by Tibshirani (1996) and has since been applied to countless areas of statistics. The form is quite similar to ridge regression with one small but profound modification,

$$\hat{\beta}_\lambda^L = \arg \min_{\beta \in \mathbb{R}^p} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 + \lambda \sum_{j=1}^p |\beta_j| \right\},$$

which is that the penalty term is now the sum of the absolute values instead of a sum of squares.

The main reason for why this technique is popular is that it combines shrinkage methods like ridge regression with variable selection and still results in a convex optimization problem. Delving into the properties of this estimator requires convex analysis and will be left for future investigations.

3.4.4 Elastic Net

The [elastic net regularization](#) method combines both ridge and lasso regression into one methodology. Here, we include a penalty term for each of the two methods:

$$\hat{\beta}_\lambda^{EN} = \arg \min_{\beta \in \mathbb{R}^p} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 + \lambda_1 \sum_{j=1}^p |\beta_j| + \lambda_2 \sum_{j=1}^p \beta_j^2 \right\}.$$

This method has two tuning parameters $\lambda_1 \geq 0$ and $\lambda_2 \geq 0$. In the `R` library `glmnet`, a *mixing* parameter α and a *scale* parameter λ is specified to get

$$\hat{\beta}_\lambda^{EN} = \arg \min_{\beta \in \mathbb{R}^p} \left\{ \sum_{i=1}^n (y_i - X_i^T \beta)^2 + \lambda \sum_{j=1}^p \left[\alpha |\beta_j| + \frac{1-\alpha}{2} \beta_j^2 \right] \right\}.$$

The intuition behind this approach is to combine the strengths of both ridge and lasso regression. Namely, ridge regression shrinks the coefficients towards zero reducing the variance while lasso selects a subset of the parameters to remain in the model.

3.4.5 Penalized Regression: An Example

Consider a sample of size $n = 100$ generated by the model

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_{50} x_{50} + \varepsilon$$

where $\beta_{27} = 2$, $\beta_{34} = -2$, all other $\beta_i = 0$, and $\varepsilon \sim \mathcal{N}(0, 16)$. Even though only two of the regressors have

any effect on the response y , feeding all 50 regressors into R's `lm()` function can result in many false positives as in the code below. In this example, we have three terms in the model that have weakly small p-values around 6% - 7%, two false positive p-values significant at the 5% level, and the two true positive results—entries 27 and 34—which both have very significant p-values.

```
set.seed(256)
# simulate some data
xx = matrix(
  rnorm(100*50,0,1), 100, 50
)
yy = 2*xx[,27] - 2*xx[,34] + rnorm(100,0,4)
dat.sim = data.frame( yy,xx )
# fit a least squares model with all 50 inputs
md.lm = lm( yy ~ ., data=dat.sim )
summary(md.lm)
```

Call:

```
lm(formula = yy ~ ., data = dat.sim)
```

Residuals:

Min	1Q	Median	3Q	Max
-8.4593	-1.7764	0.0529	1.3162	8.6453

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-0.114956	0.604874	-0.190	0.85006
X1	-0.186314	0.501304	-0.372	0.71175
X2	0.293722	0.698205	0.421	0.67583
X3	0.846036	0.635611	1.331	0.18933
X4	-0.617202	0.719074	-0.858	0.39489
X5	0.947231	0.573410	1.652	0.10494
X6	1.226520	0.530814	2.311	0.02510 *
X7	-0.316981	0.585094	-0.542	0.59044
X8	0.133680	0.563881	0.237	0.81359
X9	0.583568	0.515985	1.131	0.26357
X10	0.130990	0.472349	0.277	0.78270
X11	-0.017902	0.469984	-0.038	0.96977
X12	-1.269013	0.668925	-1.897	0.06372 .
X13	0.427024	0.564001	0.757	0.45260
X14	0.295055	0.679860	0.434	0.66620
X15	-0.008477	0.565341	-0.015	0.98810
X16	0.684455	0.507938	1.348	0.18401
X17	-0.852380	0.655739	-1.300	0.19973
X18	-1.482044	0.788183	-1.880	0.06601 .
X19	-0.582075	0.567622	-1.025	0.31018
X20	1.184024	0.720145	1.644	0.10655
X21	-0.825218	0.549479	-1.502	0.13956
X22	0.368528	0.600818	0.613	0.54246
X23	-0.846930	0.623998	-1.357	0.18092
X24	-0.066278	0.526772	-0.126	0.90039
X25	0.982897	0.644828	1.524	0.13387
X26	0.444571	0.513192	0.866	0.39056

X27	1.733198	0.552519	3.137	0.00289	**
X28	-0.263400	0.510541	-0.516	0.60823	
X29	0.287366	0.623317	0.461	0.64682	
X30	-0.460872	0.505887	-0.911	0.36675	
X31	-0.057786	0.493507	-0.117	0.90727	
X32	0.522936	0.503179	1.039	0.30378	
X33	0.338087	0.581553	0.581	0.56367	
X34	-3.384722	0.537832	-6.293	8.25e-08	***
X35	0.635258	0.530874	1.197	0.23721	
X36	0.942947	0.500341	1.885	0.06542	.
X37	0.385363	0.565600	0.681	0.49887	
X38	0.517330	0.628746	0.823	0.41461	
X39	-0.305261	0.535436	-0.570	0.57120	
X40	-0.539736	0.532697	-1.013	0.31594	
X41	-1.357445	0.608486	-2.231	0.03030	*
X42	-0.102478	0.657813	-0.156	0.87684	
X43	0.573256	0.681116	0.842	0.40408	
X44	-0.291538	0.591831	-0.493	0.62449	
X45	0.512879	0.571004	0.898	0.37347	
X46	0.235569	0.561770	0.419	0.67681	
X47	0.475641	0.565423	0.841	0.40432	
X48	0.308767	0.596236	0.518	0.60689	
X49	0.196569	0.535140	0.367	0.71496	
X50	-0.878138	0.578599	-1.518	0.13552	

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4 on 49 degrees of freedom

Multiple R-squared: 0.7283, Adjusted R-squared: 0.4511

F-statistic: 2.627 on 50 and 49 DF, p-value: 0.0004624

We could attempt one of the stepwise variable selection procedures from the previous section. Running backwards and forwards selection results in the many terms being retained in the model, which furthermore are deemed to be statistically significant from the t-test.

In particular, backwards selection results in 18 of 50 terms kept in the model with 10 significant at the 5% level. Meanwhile, forward selection results in 17 of 50 terms kept in the model with 4 significant at the 5% level and another 7 terms just above the classic 5% threshold.

```
md0 = lm(yy~1,data=dat.sim)
md.bck = step(
  md.lm, direction = "backward", trace=0
)
summary(md.bck)
```

Call:

```
lm(formula = yy ~ X5 + X6 + X9 + X12 + X14 + X17 + X20 + X21 +
  X23 + X25 + X27 + X34 + X35 + X36 + X38 + X41 + X45 + X50,
  data = dat.sim)
```

Residuals:

Min	1Q	Median	3Q	Max
-7.1215	-1.9121	-0.0406	1.7660	10.7895

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)							
(Intercept)	0.02405	0.40411	0.060	0.9527							
X5	0.55510	0.36882	1.505	0.1362							
X6	0.83115	0.38887	2.137	0.0356 *							
X9	0.54329	0.35032	1.551	0.1248							
X12	-0.93968	0.45563	-2.062	0.0424 *							
X14	0.86042	0.42725	2.014	0.0473 *							
X17	-0.84374	0.39494	-2.136	0.0357 *							
X20	0.67458	0.44559	1.514	0.1339							
X21	-0.99140	0.41366	-2.397	0.0188 *							
X23	-0.81608	0.36562	-2.232	0.0284 *							
X25	0.64772	0.44846	1.444	0.1525							
X27	1.85091	0.37052	4.996	3.32e-06 ***							
X34	-3.16199	0.38734	-8.163	3.58e-12 ***							
X35	0.50745	0.38561	1.316	0.1919							
X36	0.91381	0.34915	2.617	0.0106 *							
X38	0.82018	0.42639	1.924	0.0579 .							
X41	-0.99945	0.41261	-2.422	0.0177 *							
X45	0.66715	0.38839	1.718	0.0897 .							
X50	-0.52955	0.39024	-1.357	0.1786							

Signif. codes:	0	'***'	0.001	'**'	0.01	'*'	0.05	'.'	0.1	' '	1

Residual standard error: 3.49 on 81 degrees of freedom

Multiple R-squared: 0.658, Adjusted R-squared: 0.582

F-statistic: 8.659 on 18 and 81 DF, p-value: 2.152e-12

```
md.fwd = step(
  md0, direction = "forward", trace=0, scope = list(upper=md.lm)
)
summary(md.fwd)
```

Call:

```
lm(formula = yy ~ X34 + X27 + X29 + X50 + X23 + X41 + X25 + X36 +
  X45 + X21 + X5 + X17 + X12 + X6 + X48 + X8 + X9, data = dat.sim)
```

Residuals:

Min	1Q	Median	3Q	Max
-7.818	-2.077	0.162	1.371	10.639

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.1072	0.3931	0.273	0.78584
X34	-3.1401	0.3868	-8.117	4.10e-12 ***
X27	1.9382	0.3809	5.088	2.26e-06 ***
X29	0.5857	0.4051	1.446	0.15198
X50	-0.6915	0.3859	-1.792	0.07679 .
X23	-0.5109	0.3562	-1.434	0.15537
X41	-1.1933	0.4098	-2.912	0.00463 **
X25	0.7984	0.4472	1.785	0.07790 .

```

X36      0.6600  0.3486  1.893  0.06186 .
X45      0.7560  0.3979  1.900  0.06091 .
X21     -1.0932  0.4203 -2.601  0.01102 *
X5       0.6229  0.3679  1.693  0.09425 .
X17     -0.7021  0.4025 -1.744  0.08484 .
X12     -0.8150  0.4439 -1.836  0.06997 .
X6       0.5831  0.3835  1.521  0.13217
X48      0.6162  0.3868  1.593  0.11503
X8      -0.5647  0.3906 -1.446  0.15208
X9       0.4483  0.3461  1.295  0.19888
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

Residual standard error: 3.516 on 82 degrees of freedom
 Multiple R-squared: 0.6487, Adjusted R-squared: 0.5759
 F-statistic: 8.909 on 17 and 82 DF, p-value: 1.866e-12

Hence, both of these procedures retain too many regressors in the final model. The stepwise selection method was also run, but returned results equivalent to forward selection.

Applying ridge regression to this dataset will result in all 50 of the estimated parameters being shrunk towards zero. The code and plot below demonstrate this behaviour. The vertical axis corresponds to the values of $\beta_1, \dots, \beta_{50}$. The horizontal axis corresponds to increasing values of the penalization parameter λ . As λ increases, the estimates for the β 's tend towards zero. Hence we see all 50 of the curves bending towards the zero.

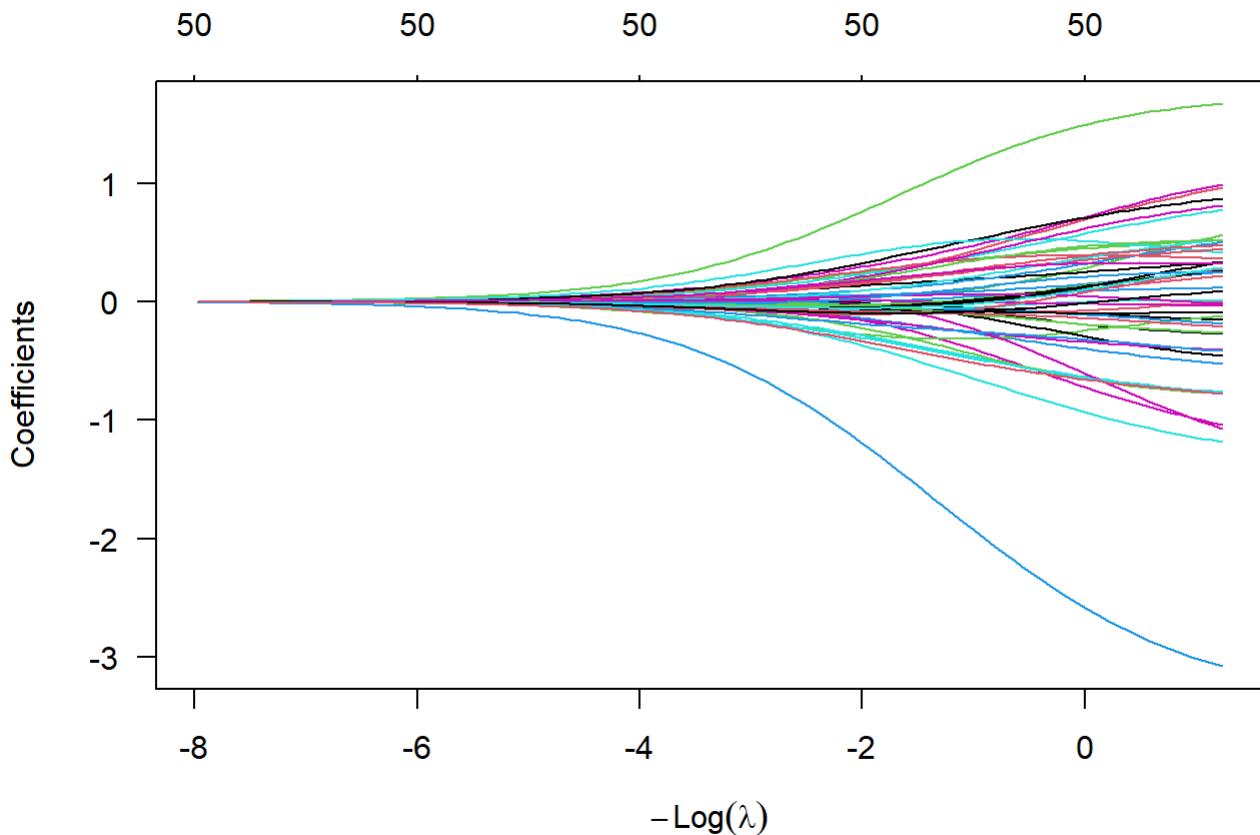
```
# Load in the glmnet package
library(glmnet)
```

Warning: package 'glmnet' was built under R version 4.5.2

Loading required package: Matrix

Loaded glmnet 4.1-10

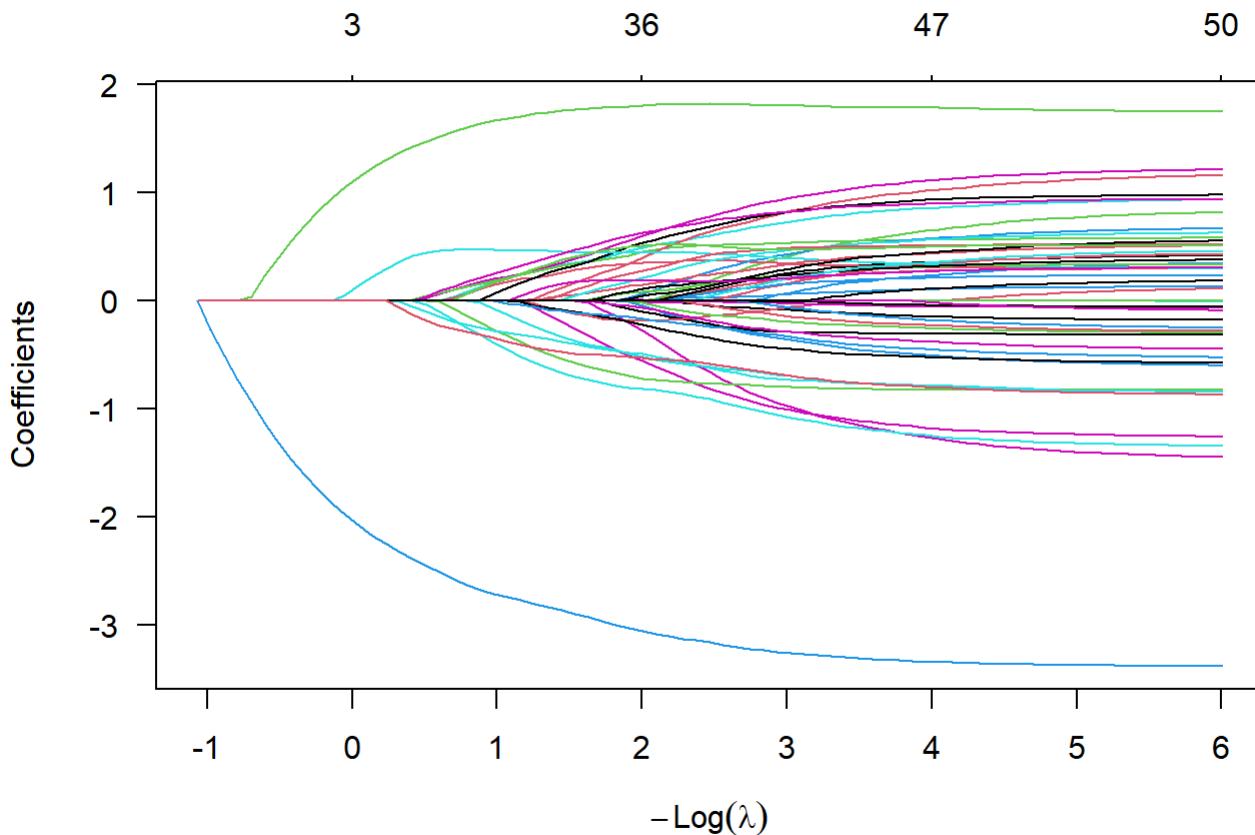
```
# Run a ridge regression
md.ridge = glmnet( xx,yy,alpha=0 )
plot( md.ridge,las=1 )
```



Applying LASSO to the dataset results in a different set of paths from the ridge regression. The plot below displays the LASSO paths. In this case, the horizontal axis corresponds to some K such that $\|\hat{\beta}_\lambda^L\|_1 < K$, which is equivalent to adding the penalty term $\lambda \sum_{j=1}^p |\beta_j|$. As this bound K grows, more variables will enter the model. The blue and green lines represent the regressors x_{34} and x_{27} , which are the first two terms to enter the model.

Eventually, as the penalty is relaxed, many more terms begin to enter the model. Hence, choosing a suitable K , or equivalently λ , is a critical problem for this method.

```
# Run a lasso regression
md.lasso = glmnet( xx,yy,alpha=1 )
plot( md.lasso,las=1 )
```



3.5 US Communities and Crime Dataset

This section considers a dataset entitled “Communities and Crime”, which was downloaded from the UCI Machine Learning Repository.¹ From the short description on the UCI website, *the data combines socio-economic data from the 1990 US Census, law enforcement data from the 1990 US LEMAS survey, and crime data from the 1995 FBI UCR*. For our purposes, the dataset has 128 columns, but after removing those with missing values and some categorical variables, we have a dataset with $p = 99$ predictors and a sample of $n = 1994$ communities. The goal of the following regression models is to predict `ViolentCrimesPerPop`, which is the total number of violent crimes per 100,000 people.

If we fit a standard linear regression model, we see many significant predictor variables, but also have a large problem with multicollinearity as can be seen by computing the VIF values for each input to the model. We see some inputs with very low vif values and others with very high vif values. The three highest and lowest are summarized in the following table.

Variable	VIF	Description
indianPerCap	1.17	per capita income for native americans
AsianPerCap	1.56	per capita income for people with asian heritage
LemasPctOfficDrugUn	1.58	percent of officers assigned to drug units
...

Variable	VIF	Description
PctPersOwnOccup	568.98	percent of people in owner occupied households
OwnOccMedVal	577.52	owner occupied housing - median value
TotalPctDiv	1037.33	percentage of population who are divorced

```
# load car package for vif()
library(car)
```

Warning: package 'car' was built under R version 4.5.2

Loading required package: carData

Warning: package 'carData' was built under R version 4.5.2

```
# read in data
dat.cc <- read.csv("data/crimeDat.csv") [,-1]
# fit OLS model
md.ols <- lm( ViolentCrimesPerPop~, data=dat.cc )
# compute vif values
sort(vif(md.ols))
```

indianPerCap	AsianPerCap	LemasPctOfficDrugUn
1.170277	1.561501	1.578085
pctWFarmSelf	PctW0FullPlumb	HispPerCap
1.931995	1.994314	2.162989
blackPerCap	PctVacantBoarded	MedOwnCostPctIncNoMtg
2.175619	2.485693	2.542223
NumStreet	PctVacMore6Mos	MedNumBR
2.559441	2.573746	2.812721
PctUsePubTrans	LandArea	MedRentPctHousInc
3.204282	3.300431	3.478678
PctHous0occup	PopDens	pctWRetire
4.126627	4.348160	4.354717
MedOwnCostPctInc	PctEmplManu	NumInShelters
4.757836	4.816572	4.966596
MedYrHousBuilt	NumImmig	pctUrban
5.180590	5.284101	5.529765
PctEmplProfServ	racePctAsian	PctSameCity85
5.877700	5.886797	6.667340
PctWorkMomYoungKids	PctTeen2Par	PctUnemployed
7.177116	7.629905	7.768671
PctSameState85	PctBornSameState	PctHousNoPhone
8.194955	8.262952	8.332114
PctImmigRecent	PctWorkMom	PctHousLess3BR
9.238551	10.180738	11.702095
pctWPubAsst	PctSameHouse85	PctYoungKids2Par
11.964125	12.469516	12.727784
Pct0occupManu	PctIlleg	HousVacant
13.635199	13.658336	13.797805

PctImmigRec10	15.470409	NumIlleg	MalePctNevMarr
pctWInvInc	16.550890	racePctHisp	racepctblack
PctEmploy	21.581210	PctImmigRec5	householdszie
PctPopUnderPov	23.469586	racePctWhite	PctLess9thGrade
RentLowQ	24.716495	PctNotSpeakEnglWell	PersPerRentOccHous
PctImmigRec8	27.654191	PctPersDenseHous	PctSpeakEnglOnly
PctOccupMgmtProf	29.586770	PctBSorMore	pctWWage
agePct12t21	30.826378	NumUnderPov	30.517782
pctWSocSec	39.545215	PctNotHSGrad	agePct65up
RentHighQ	52.265807	agePct12t29	PctForeignBorn
PersPerOwnOccHous	80.189980	agePct16t24	MedRent
whitePerCap	92.712971	85.484471	87.214942
PctKids2Par	117.310433	PctRecentImmig	medFamInc
perCapInc	148.700025	94.964943	115.656168
PersPerOccupHous	205.076410	PctFam2Par	RentMedian
MalePctDivorce	233.733489	medIncome	OwnOccHiQuart
population	290.456635	149.478200	171.793014
FemalePctDiv	336.318105	PctLargHouseFam	PctLargHouseOccup
PctPersOwnOccup	569.984167	225.969285	233.094839
		OwnOccLowQuart	numbUrban
		237.789803	281.558920
		PctRecImmig10	PctRecImmig5
		301.610537	312.448675
		PctRecImmig8	PctHousOwnOcc
		478.170602	550.685258
		OwnOccMedVal	TotalPctDiv
		577.523898	1037.327141

3.5.1 Variable Selection

We can try to fix this problem of multicollinearity by using forwards or backwards variable selection, which will remove terms from our model if removing those terms improves the AIC. Note that with $p = 99$, there are $2^{99} \approx 6.3 \times 10^{29}$ possible regression models to consider, which is much too many to exhaustively search through.

Backwards variable selection finished with $p = 53$ inputs remaining in the model with the largest VIF now at 202.03. Forwards variable selection finished with $p = 37$ inputs in the model with the largest VIF only at 88.14.

```
# Backwards Variable Selection
md.back <- step(md.ols, trace=0)
sort(vif(md.back))
```

indianPerCap	LemasPctOfficDrugUn	pctWFarmSelf
1.141616	1.496937	1.769121
pctUrban	HispPerCap	PctVacMore6Mos
1.893758	2.025846	2.198193
MedOwnCostPctIncNoMtg	PctVacantBoarded	NumStreet
2.212207	2.296319	2.445900
PctUsePubTrans	MedNumBR	PctWorkMom
2.613058	2.685736	2.767703
MedRentPctHousInc	PctHous0ccup	pctWRetire
2.960188	3.032502	3.534648
NumImmig	MedOwnCostPctInc	PctEmplManu
3.607630	3.787314	4.110466
NumInShelters	HousVacant	PctLess9thGrade
4.679666	5.940583	7.018809
racepctblack	NumIlleg	racePctHisp
7.165975	7.234419	8.506237
PctHousLess3BR	MalePctNevMarr	PctIlleg
10.236929	11.029312	11.405678
agePct12t29	PctOccupManu	PctForeignBorn
11.603578	11.846101	11.995279
PctOccupMgmtProf	PctEmploy	pctWInvInc
12.075506	12.579787	13.266811
PctPopUnderPov	PctLargHouse0ccup	RentLowQ
15.050398	16.063152	16.758133
pctWSocSec	PctNotSpeakEnglWell	PersPerRent0ccHous
19.202997	19.642101	21.943281
whitePerCap	PctPersDenseHous	pctWWage
22.255426	22.628408	22.755048
PctKids2Par	MalePctDivorce	PersPerOccupHous
27.162936	32.780138	33.099839
medFamInc	TotalPctDiv	RentHighQ
39.285294	40.667122	43.859596
MedRent	OwnOccLowQuart	OwnOccMedVal
48.267116	154.292084	156.122860
PctHous0wn0cc	PctPersOwn0ccup	
173.515817	202.028631	

```
# Forwards Variable Selection
md.0 <- lm( ViolentCrimesPerPop~1, data=dat.cc )
md.forw <- step(
  md.0, trace=0, direction="forward",
  scope = list(lower=md.0, upper=md.ols)
)
sort(vif(md.forw))
```

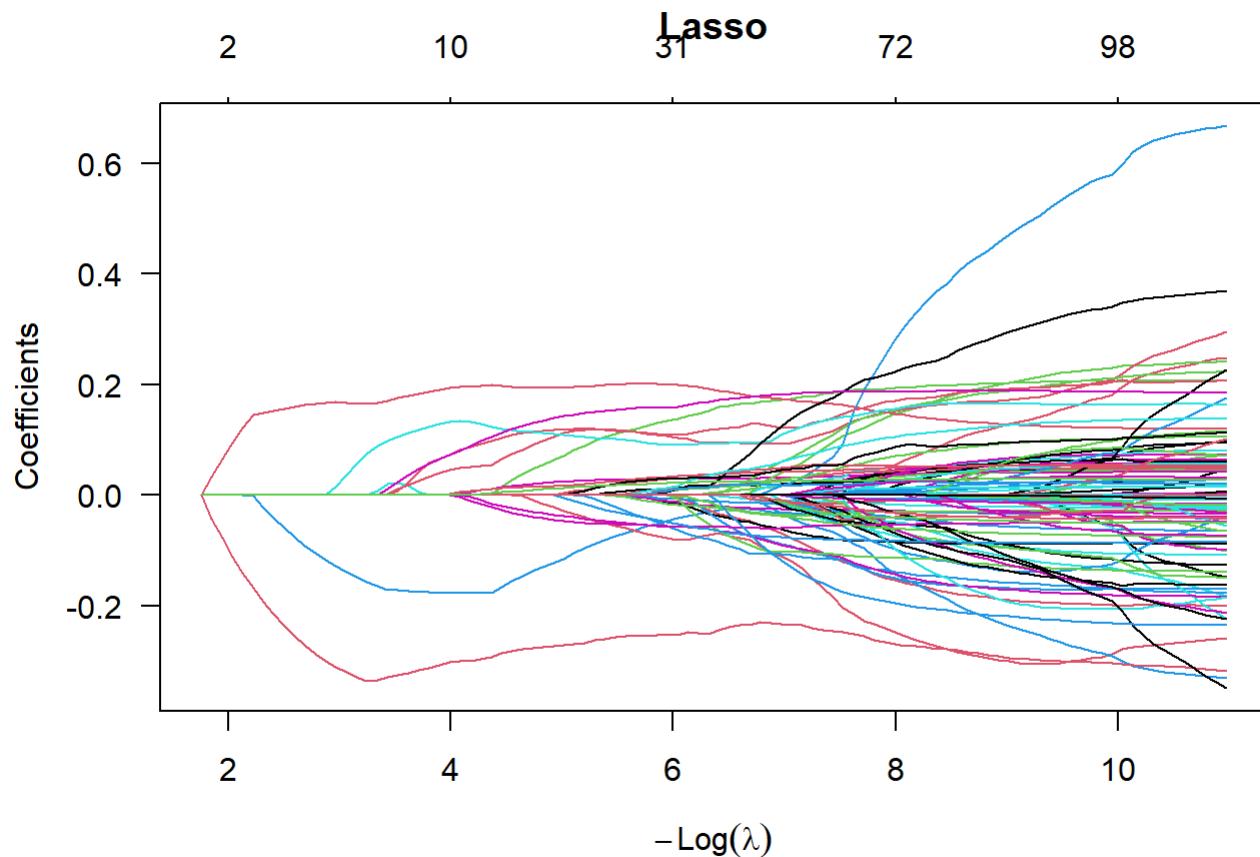
indianPerCap	LemasPctOfficDrugUn	AsianPerCap
1.124833	1.457492	1.470653
PctEmplManu	pctWFarmSelf	MedOwnCostPctIncNoMtg
1.642768	1.699459	1.817426
NumStreet	pctUrban	HispPerCap
1.853679	1.890667	1.991065
PctVacMore6Mos	PctVacantBoarded	PctWorkMom
2.014917	2.147307	2.361651

MedRentPctHousInc	MedOwnCostPctInc	pctWRetire
2.697115	2.986114	3.097814
PctLess9thGrade	HousVacant	PctLargHouseFam
4.955276	6.893231	6.942874
agePct12t21	MalePctNevMarr	numbUrban
6.954019	7.616776	7.719742
pctWWage	PctIlleg	pctWInvInc
9.862223	9.937225	10.821914
PctEmploy	racepctblack	PctPopUnderPov
11.118442	11.519250	11.860735
PctPersDenseHous	racePctWhite	agePct12t29
12.485013	13.838907	14.560154
RentLowQ	MedRent	PctKids2Par
15.681439	17.993276	24.552975
MalePctDivorce	TotalPctDiv	whitePerCap
28.494673	36.357173	68.199024
perCapInc		
88.142344		

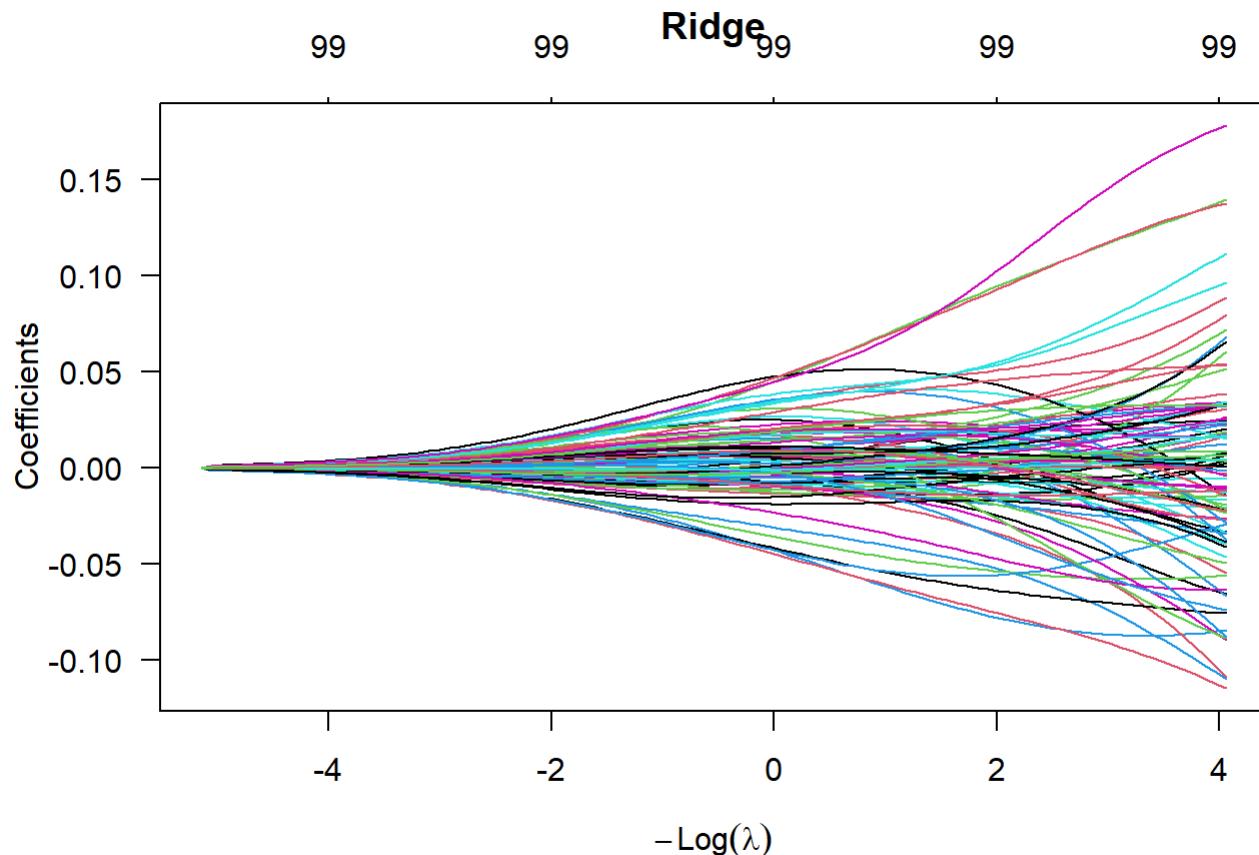
3.5.2 Penalized Regression

Another approach to this data is to use penalized regression methods discussed about like LASSO and Ridge Regression. In the plots below, from left to right, we see λ going to zero or $-\log \lambda$ increasing. As this happens, more input variables enter the regression model and the value of these coefficients change.

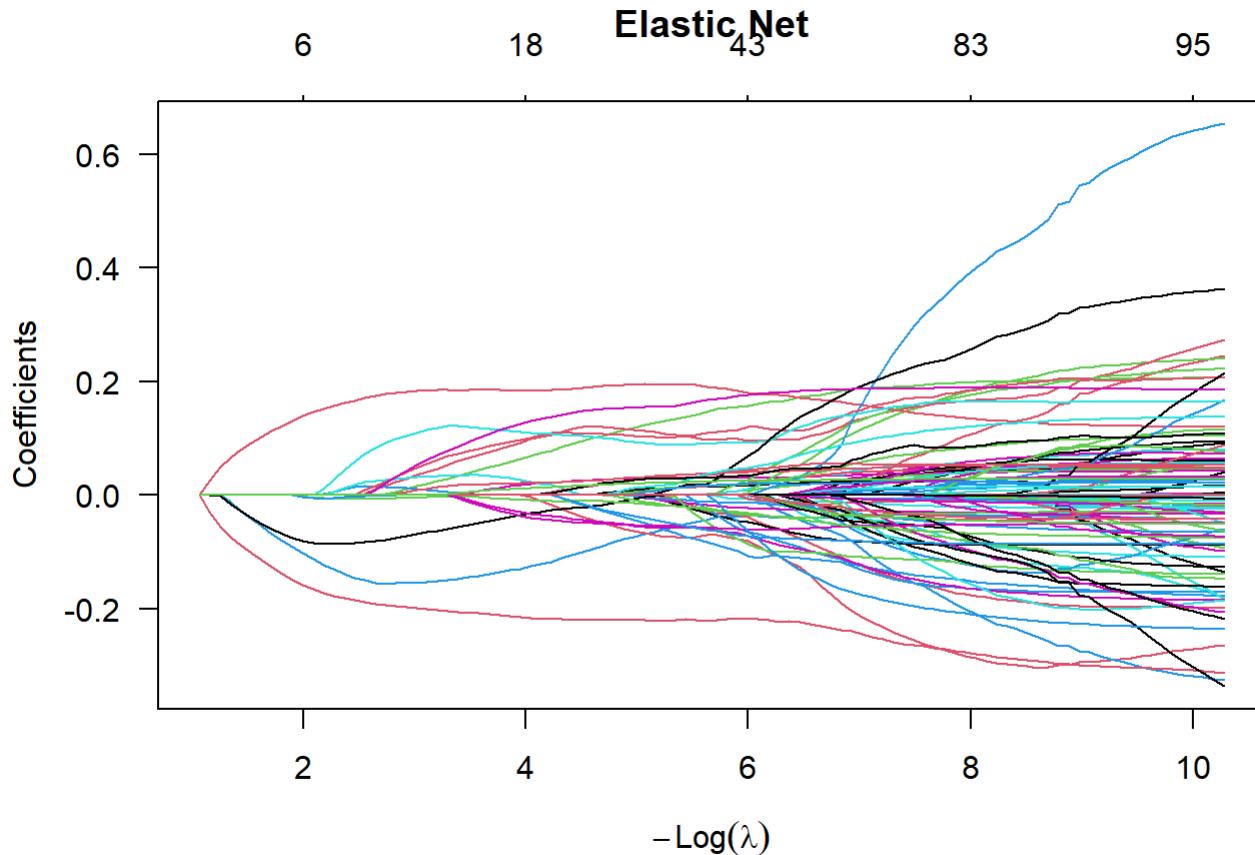
```
# load in the glmnet package
library(glmnet)
# fit a lasso model
md.la <- glmnet(
  x=dat.cc[,-100], y=dat.cc[,100], alpha=1
)
# fit a ridge model
md.rd <- glmnet(
  x=dat.cc[,-100], y=dat.cc[,100], alpha=0
)
# fit an elastic net model
md.en <- glmnet(
  x=dat.cc[,-100], y=dat.cc[,100], alpha=0.5
)
# plot the variable paths
plot(md.la, las=1, main="Lasso")
```



```
plot(md.rd, las=1, main="Ridge")
```



```
plot(md.en, las=1, main="Elastic Net")
```



As an example, when $-\log \lambda = 2$, the lasso model retains $p = 2$ parameters whereas the elastic net model retains $p = 6$ parameters. When $-\log \lambda = 4$, the lasso model retains $p = 10$ parameters whereas the elastic net model retains $p = 18$ parameters. In ridge regression, all variables are included in the model, but the coefficient values are shrunk towards zero.

Lasso selects the two variables `PctIlleg` (percentage of kids born to never married) and `PctKids2Par` (percentage of kids in family housing with two parents) as the most important predictors when highly penalizing the model. When relaxing the penalization a bit, we get the following additional variables:

- `racePctWhite`, percentage of population that is caucasian
- `pctUrban`, percentage of people living in areas classified as urban
- `MalePctDivorce`, percentage of males who are divorced
- `PctWorkMom`, percentage of moms of kids under 18 in labor force
- `PctPersDenseHous`, percent of persons in dense housing
- `HousVacant`, number of vacant households
- `PctVacantBoarded`, percent of vacant housing that is boarded up
- `NumStreet`, number of homeless people counted in the street

Remark 3.6. With this (and really any) dataset, it is worth emphasizing that correlation does not imply causation. If some of these inputs have strong predictive power on the output (total number of violent crimes per 100K population), it only implies that these variables are correlated and not that there is a direct causal link between the inputs and outputs.

```
# Look at the parameters when -log(Lambda) is approx 2 and 4
md.la$lambda[c(4,26)]
```

```
[1] 0.13011052 0.01680442
```

```
md.la$beta[,c(4,26)]
```

```
99 x 2 sparse Matrix of class "dgCMatrix"
           s3      s25
population   .
householdsiz .
racepctblack .
racePctWhite  -0.177643427
racePctAsian  .
racePctHisp   .
agePct12t21   .
agePct12t29   .
agePct16t24   .
agePct65up    .
numbUrban     .
pctUrban      0.002480816
medIncome     .
pctWWage      .
pctWFarmSelf  .
pctWInvInc   .
pctWSocSec   .
pctWPubAsst  .
pctWRetire    .
medFamInc    .
perCapInc    .
whitePerCap  .
blackPerCap  .
indianPerCap .
AsianPerCap   .
HispPerCap   .
NumUnderPov  .
PctPopUnderPov .
PctLess9thGrade .
PctNotHSGrad  .
PctBSorMore   .
PctUnemployed .
PctEmploy     .
PctEmplManu  .
PctEmplProfServ .
PctOccupManu  .
PctOccupMgmtProf .
MalePctDivorce 0.081181639
MalePctNevMarr .
FemalePctDiv   .
TotalPctDiv   .
PersPerFam    .
PctFam2Par    .
PctKids2Par   -0.11118010 -0.300107242
PctYoungKids2Par .
PctTeen2Par   .
PctWorkMomYoungKids .
```

PctWorkMom	.	-0.003477488
NumIlleg	.	.
PctIlleg	0.09491414	0.195131076
NumImmig	.	.
PctImmigRecent	.	.
PctImmigRec5	.	.
PctImmigRec8	.	.
PctImmigRec10	.	.
PctRecentImmig	.	.
PctRecImmig5	.	.
PctRecImmig8	.	.
PctRecImmig10	.	.
PctSpeakEnglOnly	.	.
PctNotSpeakEnglWell	.	.
PctLargHouseFam	.	.
PctLargHouseOccup	.	.
PersPerOccupHous	.	.
PersPerOwnOccHous	.	.
PersPerRentOccHous	.	.
PctPersOwnOccup	.	.
PctPersDenseHous	.	0.048592093
PctHousLess3BR	.	.
MedNumBR	.	.
HousVacant	.	0.133518706
PctHousOccup	.	.
PctHousOwnOcc	.	.
PctVacantBoarded	.	0.005459467
PctVacMore6Mos	.	.
MedYrHousBuilt	.	.
PctHousNoPhone	.	.
PctW0FullPlumb	.	.
OwnOccLowQuart	.	.
OwnOccMedVal	.	.
OwnOccHiQuart	.	.
RentLowQ	.	.
RentMedian	.	.
RentHighQ	.	.
MedRent	.	.
MedRentPctHousInc	.	.
MedOwnCostPctInc	.	.
MedOwnCostPctIncNoMtg	.	.
NumInShelters	.	.
NumStreet	.	0.080640084
PctForeignBorn	.	.
PctBornSameState	.	.
PctSameHouse85	.	.
PctSameCity85	.	.
PctSameState85	.	.
LandArea	.	.
PopDens	.	.
PctUsePubTrans	.	.
LemasPctOfficDrugUn	.	.

```
# Look at the parameters when -log(Lambda) is approx 2 and 4
md.en$lambda[c(12,33)]
```

```
[1] 0.12362608 0.01752368
```

```
md.en$beta[,c(12,33)]
```

```
99 x 2 sparse Matrix of class "dgCMatrix"
           s11        s32
population   .
householdsiz .
racepctblack .
racePctWhite -0.112296761 -0.1252486854
racePctAsian .
racePctHisp  .
agePct12t21  .
agePct12t29  .
agePct16t24  .
agePct65up   .
numbUrban    .
pctUrban     0.0194212436
medIncome    .
pctWWage    .
pctWFarmSelf .
pctWInvInc  .
pctWSocSec   .
pctWPubAsst  .
pctWRetire   .
medFamInc   .
perCapInc   .
whitePerCap  .
blackPerCap  .
indianPerCap .
AsianPerCap  .
HispPerCap  .
NumUnderPov  .
PctPopUnderPov .
PctLess9thGrade .
PctNotHSGrad  .
PctBSorMore   .
PctUnemployed .
PctEmploy    .
PctEmplManu  .
PctEmplProfServ .
PctOccupManu  .
PctOccupMgmtProf .
MalePctDivorce 0.0982854492
MalePctNevMarr  .
FemalePctDiv  .
TotalPctDiv   0.0240915372
PersPerFam   .
PctFam2Par   -0.084158719 -0.0306809156
PctKids2Par  -0.165607053 -0.2154189468
```

PctYoungKids2Par	-0.004186120	-0.0091135229
PctTeen2Par	-0.005214765	.
PctWorkMomYoungKids	.	.
PctWorkMom	.	-0.0396100426
NumIlleg	.	.
PctIlleg	0.145972531	0.1837625182
NumImmig	.	.
PctImmigRecent	.	.
PctImmigRec5	.	.
PctImmigRec8	.	.
PctImmigRec10	.	.
PctRecentImmig	.	.
PctRecImmig5	.	.
PctRecImmig8	.	.
PctRecImmig10	.	.
PctSpeakEnglOnly	.	.
PctNotSpeakEnglWell	.	.
PctLargHouseFam	.	.
PctLargHouseOccup	.	.
PersPerOccupHous	.	.
PersPerOwnOccHous	.	.
PersPerRentOccHous	.	.
PctPersOwnOccup	.	.
PctPersDenseHous	.	0.1017035006
PctHousLess3BR	.	.
MedNumBR	.	.
HousVacant	.	0.1093486938
PctHousOccup	.	-0.0328292382
PctHousOwnOcc	.	.
PctVacantBoarded	.	0.0211353681
PctVacMore6Mos	.	.
MedYrHousBuilt	.	.
PctHousNoPhone	.	.
PctW0FullPlumb	.	.
OwnOccLowQuart	.	.
OwnOccMedVal	.	.
OwnOccHiQuart	.	.
RentLowQ	.	.
RentMedian	.	.
RentHighQ	.	.
MedRent	.	.
MedRentPctHousInc	.	.
MedOwnCostPctInc	.	.
MedOwnCostPctIncNoMtg	.	.
NumInShelters	.	.
NumStreet	.	0.1308971121
PctForeignBorn	.	0.0009972388
PctBornSameState	.	.
PctSameHouse85	.	.
PctSameCity85	.	.
PctSameState85	.	.
LandArea	.	.
PopDens	.	.

PctUsePubTrans	.	.
LemasPctOfficDrugUn	.	0.0125378275

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