Chapter 6: Linear Model Selection & Regularization

In the regression setting, the standard linear model is commonly used to describe the relationship between a response Y and a set of variables $X_1, \ldots, X_p$.

$$Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \varepsilon.$$

typically fit w/ least squares.

Upcoming: more general models (non-linear).

The linear model has distinct advantages in terms of inference and is often surprisingly competitive for prediction. How can it be improved?

replace least squares with alternative fitting procedures.

We can yield both better *prediction accuracy* and *model interpretability*:

prediction accuracy: If the true relationship is ≈ linear, least squares will have low bias

If $n >> p$ => also have low variance => perform well on test data.

But if n is not much larger than p => high variability => poor performance.

If $p > n$: no longer a unique solution => variance = ∞ => cannot be used at all!

goal: reduce variance without adding too much bias.

model interpretability: often many variables used in a regression are not in fact associated with the response.

By removing them (setting $\hat{\beta}_i = 0$) we could obtain a more easily interpretable model.

Note: least squares will hardly ever result in $\hat{\beta}_i = 0$.

=> need variable selection.

Same ideas apply to logistic regression.

1 Subset Selection

We consider methods for selecting subsets of predictors.

1.1 Best Subset Selection.

To perform *best subset selection*, we fit a separate least squares regression for each possible combination of the p predictors. ← $\binom{p}{2} = \frac{p(p-1)}{2}$ models w/ exactly 2 predictors, etc.

Algorithm:

1. Let $\mathcal{M}_0$ denote null model - no predictors.
2. For $k = 1, \ldots, p$
   (a) Fit all $\binom{p}{k}$ models that contain k predictors.
   (b) Pick the best of those ($\mathcal{M}_k$). Best is defined by ↓RSS (↑R^2).
3. Select a single best model from $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using CV error, C_p, AIC/BIC, or adjusted R^2 more later.

Why can't we use R^2 for step 3? as p↑, R^2↑ always. Why might we not want to do this? Fitting 2^p models! $p = 10 \Rightarrow$ 1000 models!

We can perform something similar with logistic regression.

1.2 Stepwise Selection

For computational reasons, best subset selection cannot be performed for very large p. → impossible with $p \geq 40$.

Best subset may also suffer when p large because w/ a large search space we can find spurious good models that work on training data but perform poorly w/ test data.

Stepwise selection is a computationally efficient procedure that considers a much smaller subset of models.

Forward Stepwise Selection:

Start w/ no predictors and add predictors one at a time until all predictors are in the model. Choose the "best" from these.

1. Let $\mathcal{M}_0$ denote the null model - no predictors.
2. For $k = 0, \ldots, p-1$
   (a) Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$ with 1 additional predictor.
   (b) Choose the best among those $p-k$ and call it $\mathcal{M}_{k+1}$ (↑R^2, ↓RSS).
3. Select a single best model from $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using CV error, C_p, AIC/BIC, adj R^2.

- Now we fit $1 + \sum_{k=0}^{p-1}(p-k) = 1 + \frac{p(p+1)}{2}$ models.

Backward Stepwise Selection: Begin w/ full model and take predictors away one at a time until we get to null model.

1. Let M_p denote the full model — contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:
   (a) consider all k models that contain all predictors except one of predictors in M_k ($k-1$ predictors).
   (b) choose best among these and call it M_{k-1} (↑ R^2, ↓ RSS).
3. Select the single best model from $M_0, \ldots, M_p$ using CV error, C_p, AIC/BIC, adj R^2.

* Neither forward nor backwards stepwise selection are guaranteed to find the best model containing a subset of the p predictors.

forward selection can be used when $p > n$ (but only up to $n-1$ predictors, not p!).

1.3 Choosing the Optimal Model

Need a way to pick "best" model that depends on test error (training error not a good estimate of this)
↳ either estimate this directly or adjust training errors for model size.

$C_p = \frac{1}{n}(RSS + 2d\hat{\sigma}^2)$ ← estimate of variance for full model.
↑ # of predictors in subset model

add penalty to training error (RSS) to adjust for underestimate of test error.

as d↑, C_p↑ (choose model w/ lowest value).

(gives us proportional some answer)

AIC & BIC can use for maximum likelihood fits

$AIC = \frac{1}{n\hat{\sigma}^2}(RSS + 2d\hat{\sigma}^2)$

$BIC = \frac{1}{n\hat{\sigma}^2}(RSS + \log(n)d\hat{\sigma}^2)$

choose model w/ low value, since $\log(n) > 2$ for $n \geq 7$ => heavier penalty on models w/ many variables
=> results in smaller models.

Adjusted R^2 (least squares models)

$R^2 = 1 - \frac{RSS}{TSS}$ always ↑ as d↑

$Adj\ R^2 = 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)}$

choose model w/ highest adj R^2.

Validation and Cross-Validation

- Directly estimate test error w/ validation or CV and choose model w/ lowest est. error.
- Very general, can be used w/ any model, even when it's not clear how many "predictors" we have.

Now have fast computers => these are preferred.

2 Shrinkage Methods

The subset selection methods involve using least squares to fit a linear model that contains a subset of the predictors. As an alternative, we can fit a model with all p predictors using a technique that constrains (*regularizes*) the estimates.

↳ shrink estimates towards zero.

Shrinking the coefficient estimates can significantly reduce their variance!

Help us to avoid overfitting!

2.1 Ridge Regression

Recall that the least squares fitting procedure estimates $\beta_1, \ldots, \beta_p$ using values that minimize

$$RSS = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij}\right)^2$$

residual sum of squares.

Ridge Regression is similar to least squares, except that the coefficients are estimated by minimizing

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij}\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

note we are not penalizing β_0

we want to penalize the relationships not the intercept (mean value of response when $x_{i1} = \ldots = x_{ip} = 0$)

$\lambda \geq 0$ tuning parameter (determined separately of the fitting procedure).

trades off 2 criteria: minimize RSS to fit data well

$\lambda \sum_{j=1}^{p} \beta_j^2$ shrinkage penalty small when β_j's close to zero $\Rightarrow$ shrinks estimates towards zero.

The tuning parameter λ serves to control the impact on the regression parameters.

When $\lambda = 0$ penalty has no effect and ridge regression = least squares.

As $\lambda \to \infty$, impact of the penalty grows and $\hat{\beta}^R \to 0$.

Ridge regression will produce a different set of coefficients for each penalty ($\hat{\beta}_\lambda^R$).

Selecting a good λ is critical! How to choose? Cross validation!

The standard least squares coefficient estimates are scale invariant.

Multiplying X_j by a constant c leads to a scaling of least squares estimates by a factor of $\frac{1}{c}$.

$\Rightarrow$ regardless of how j^{th} predictor is scaled, $X_j\hat{\beta}_j$ will remain the same.

In contrast, the ridge regression coefficients $\hat{\beta}^R_\lambda$ can change substantially when multiplying a given predictor by a constant.

e.g. say we have an income variable in ① dollars vs. ② thousands of dollars.

① = 1000 × ②

due to the sum of squared coef. terms this change will not simply result in the coefficient estimate to change by a factor of 1000.

$\Rightarrow X_j \hat{\beta}^R_{j,\lambda}$ depends not only on λ, but also on the scaling of X_j

(may even depend on the scaling of other predictors!)

Therefore, it is best to apply ridge regression *after standardizing the predictors* so that they are on the same scale:

i.e. standard deviation of one.

$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}}$$

s.t. dev. of j^{th} predictor.

nice in workflow, recipe

① standardize data

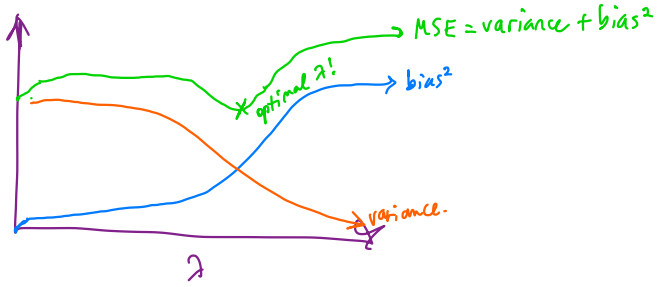
1.5 tune model to choose λ (using CV)

② fit ridge regression on training data using chosen λ.

Why does ridge regression work?

Because of the bias-variance trade-off!

As $\lambda \uparrow$, flexibility of the ridge regression fit $\downarrow$
$\downarrow$ variability and $\uparrow$ bias



In situations where relationship between response and predictors $\approx$ linear least squares estimate will have low bias.

When p is almost as large as n $\Rightarrow$ least squares has high variability!
If $p > n$ least squares doesn't even have a unique solution!

ridge regression can still perform well in these scenarios by trading off a small amount of bias for decrease in variance.

$\Rightarrow$ ridge regression works very well in high variance scenarios.

Also
Cost advantage over subset selection
b/c for fixed λ, only fit one model! (very fast model to fit).

Ridge regression improves predictive performance.

Does it also help us w/ interpretation? No

2.2 The Lasso

Ridge regression does have one obvious disadvantage.

Unlike best subset, forward/backward selection (generally select model w/ a subset of variables) ridge regression will include all p variables in the final model.

penalty $\lambda \sum_{j=1}^{p} \beta_j^2$ will shrink $\beta_j \to 0$, but $\beta_j \neq 0$ (unless $\lambda = \infty$)!

This may not be a problem for prediction accuracy, but it could be a challenge for model interpretation when p is very large.

We will always have all variables in the model, whether there is a relationship or not.

Least absolute shrinkage and selection operator.

The *lasso* is an alternative that overcomes this disadvantage. The lasso coefficients $\hat{\beta}_\lambda^L$ minimize

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij}\right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| = \text{RSS} + \lambda \boxed{\sum_{j=1}^{p} |\beta_j|}$$

$\|\beta\|_1$ ℓ_1 norm.

ℓ_1 penalty

vs.

$\left(\sum_{j=1}^{p} \beta_j^2 = \text{"}\ell_2 \text{ penalty"}\right)$.

As with ridge regression, the lasso shrinks the coefficient estimates towards zero.

ℓ_1 penalty also has the effect of forcing some coefficients to be exactly zero when λ sufficiently large!

$\Rightarrow$ much like best subset selection lasso perform variable selection!

As a result, lasso models are generally easier to interpret.

Why does the lasso result in estimates that are exactly equal to zero but ridge regression does not? One can show that the lasso and ridge regression coefficient estimates solve the following problems

In other words, when we perform the lasso we are trying to find the set of coefficient estimates that lead to the smalled RSS, subject to the contraint that there is a budget s for how large $\sum_{j=1}^{p} |\beta_j|$ can be.

2.3 Tuning

We still need a mechanism by which we can determine which of the models under consideration is “best”.

For both the lasso and ridge regression, we need to select λ (or the budget s).

How?

3 Dimension Reduction Methods

So far we have controlled variance in two ways:

We now explore a class of approaches that

We refer to these techniques as *dimension reduction* methods.

The term *dimension reduction* comes from the fact that this approach reduces the problem of estimating $p + 1$ coefficients to the problem of estimating $M + 1$ coefficients where $M < p$.

Dimension reduction serves to constrain β_j, since now they must take a particular form.

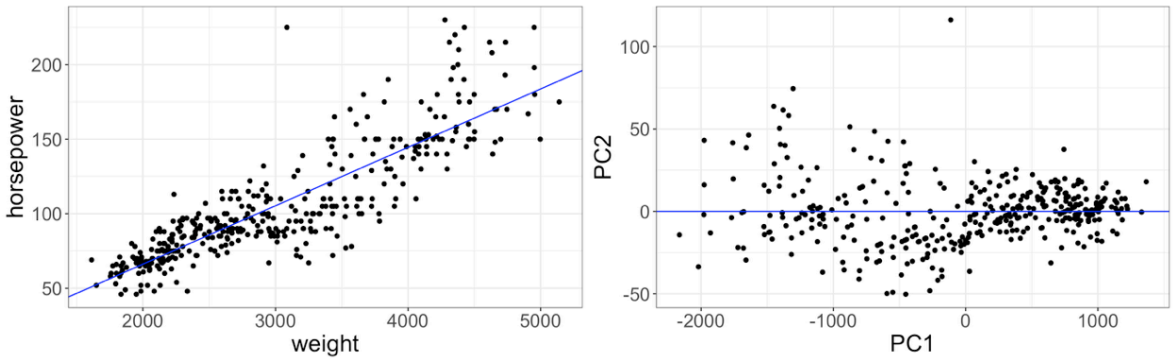
All dimension reduction methods work in two steps.

3.1 Principle Component Regression

Principal Components Analysis (PCA) is a popular approach for deriving a low-dimensional set of features from a large set of variables.

The *first principal component* directions of the data is that along which the obervations vary the most.

We can construct up to p principal components, where the 2nd principal component is a linear combination of the variables that are uncorrelated to the first principal component and has the largest variance subject to this constraint.



The Principal Components Regression approach (PCR) involves

1.

2.

Key idea:

In other words, we assume that the directions in which $X_1, \ldots, X_p$ show the most variation are the directions that are associated with Y.

How to choose M, the number of components?

Note: PCR is not feature selection!

3.2 Partial Least Squares

The PCR approach involved identifying linear combinations that best represent the predictors $X_1, \ldots, X_p$.

Consequently, PCR suffers from a drawback

Alternatively, *partial least squares (PLS)* is a supervised version.

Roughly speaking, the PLS approach attempts to find directions that help explain both the reponse and the predictors.

The first PLS direction is computed,

To identify the second PLS direction,

As with PCR, the number of partial least squares directions is chosen as a tuning parameter.

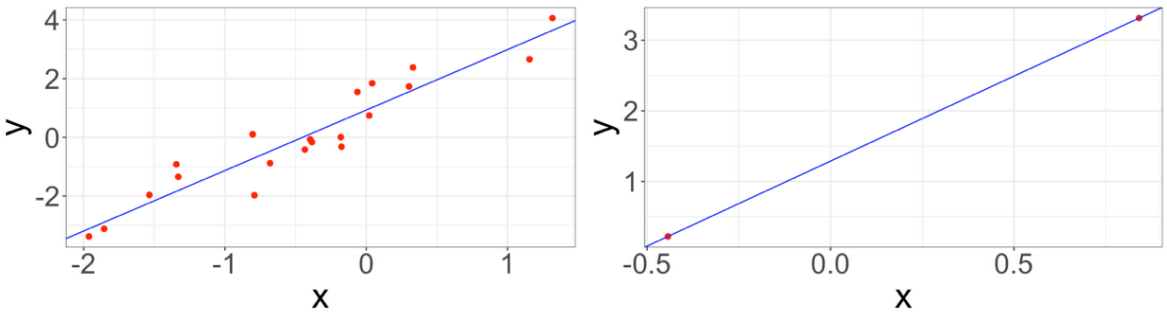
4 Considerations in High Dimensions

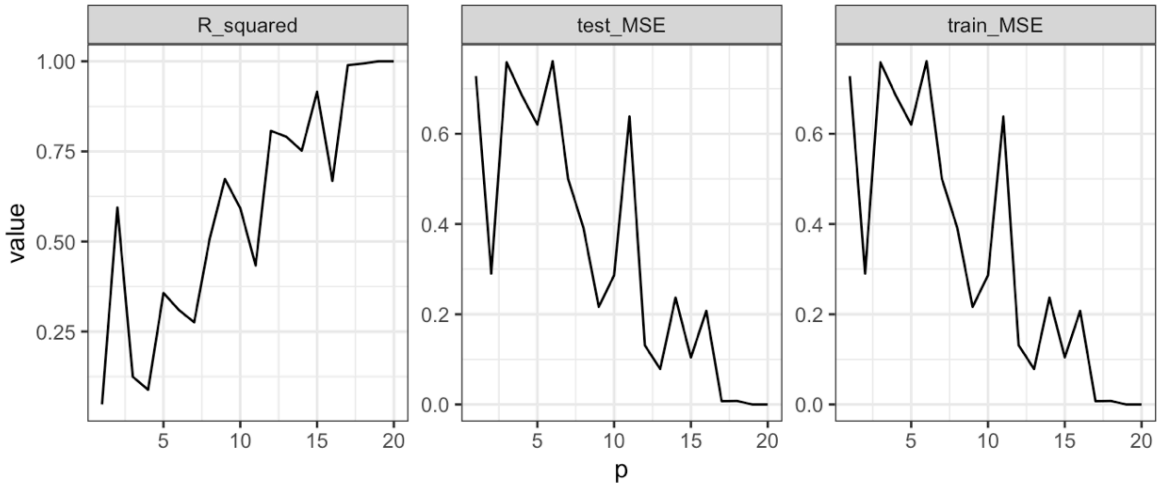
Most traditional statistical techniques for regression and classification are intendend for the low-dimensional setting.

In the past 25 years, new technologies have changed the way that data are collected in many fields. It is not commonplace to collect an almost unlimited number of feature measurements.

Data sets containing more features than observations are often referred to as *high-dimensional*.

What can go wrong in high dimensions?





Many of the methods that we've seen for fitting *less flexible* models work well in the high-dimension setting.

1.

2.

3.

When we perform the lasso, ridge regression, or other regression procedures in the high-dimensional setting, we must be careful how we report our results.