Model selection

Overview

Quick review of multicollinearity and polynomial regression

Model selection

- Overfitting
- Statistics and methods useful for model selection

Review: polynomial regression

Polynomial regression extends linear regression to non-linear relationships by including nonlinear transformations of predictors

$$\text{salary} = \beta_0 + \beta_1 \cdot \text{endowment} + \beta_2 \cdot (\text{endowment})^2 + \beta_3 \cdot (\text{endowment})^3 + \varepsilon$$

Still a linear equation but non-linear in original predictors

Polynomial regression

Polynomial regression extends linear regression to non-linear relationships by including nonlinear transformations of covariates

We can compare model fits by:

- Assessing if higher order terms are statistically significant
- Looking at the r^2 values
- Running hypothesis tests comparing nested models
- Any many more methods…

Let’s explore this a little more in R…

Model selection

Model selection

Model selection is the process of selecting a statistical model from a set of candidate models

- E.g., which explanatory variables, interaction terms, transformations of variables, etc. to include in a final model

Model selection is a bit of an art

- "All models are wrong but some are useful"
  - But there is definitely some bad art out there

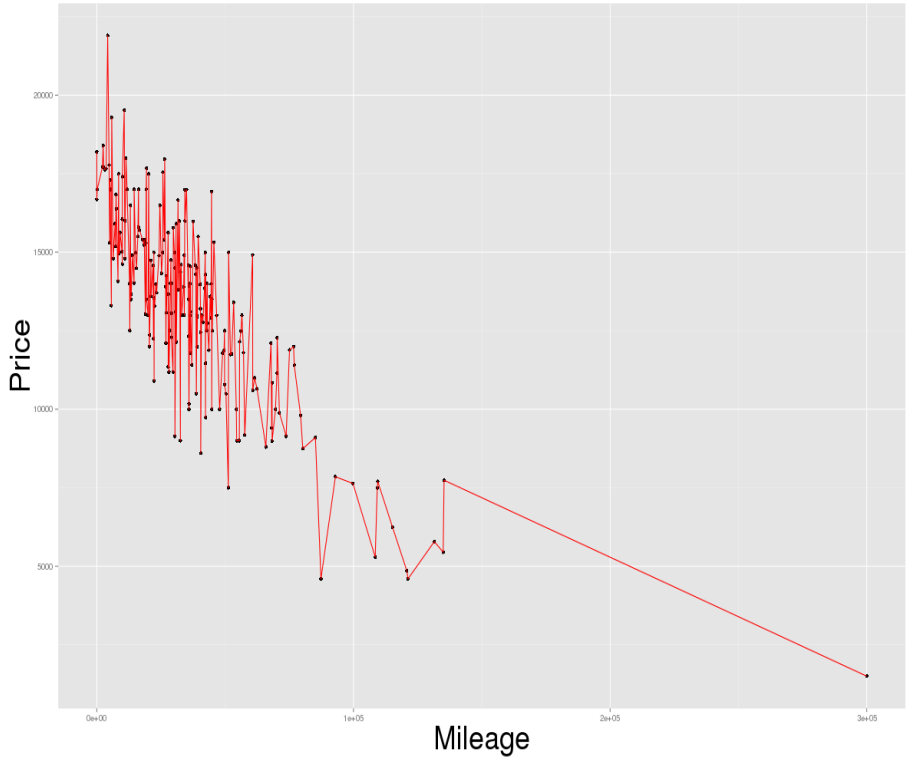
Model selection

Model selection depends on our goal, which usually is either:

- Making accurate predictions
- Understanding relationships in our data

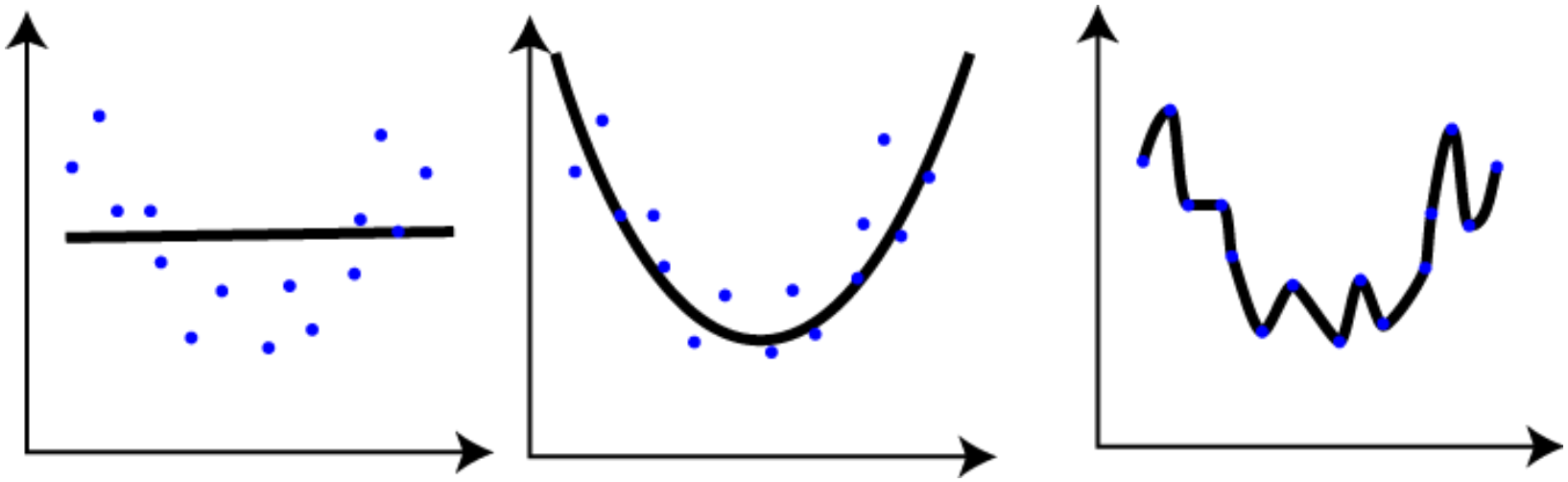
If we fit our model too closely to the data sample we have, we are likely to fail in both of these goals

- i.e., it will be hard to understand relationships between explanatory and response variables
- and model will not make good predictions on new data



Overfitting

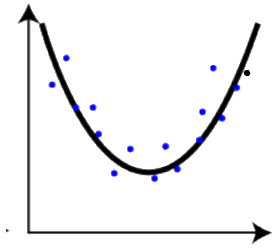
Overfitting occurs when we generate a function that too closely matches random sample we have, but does not generalize to the full probability distribution

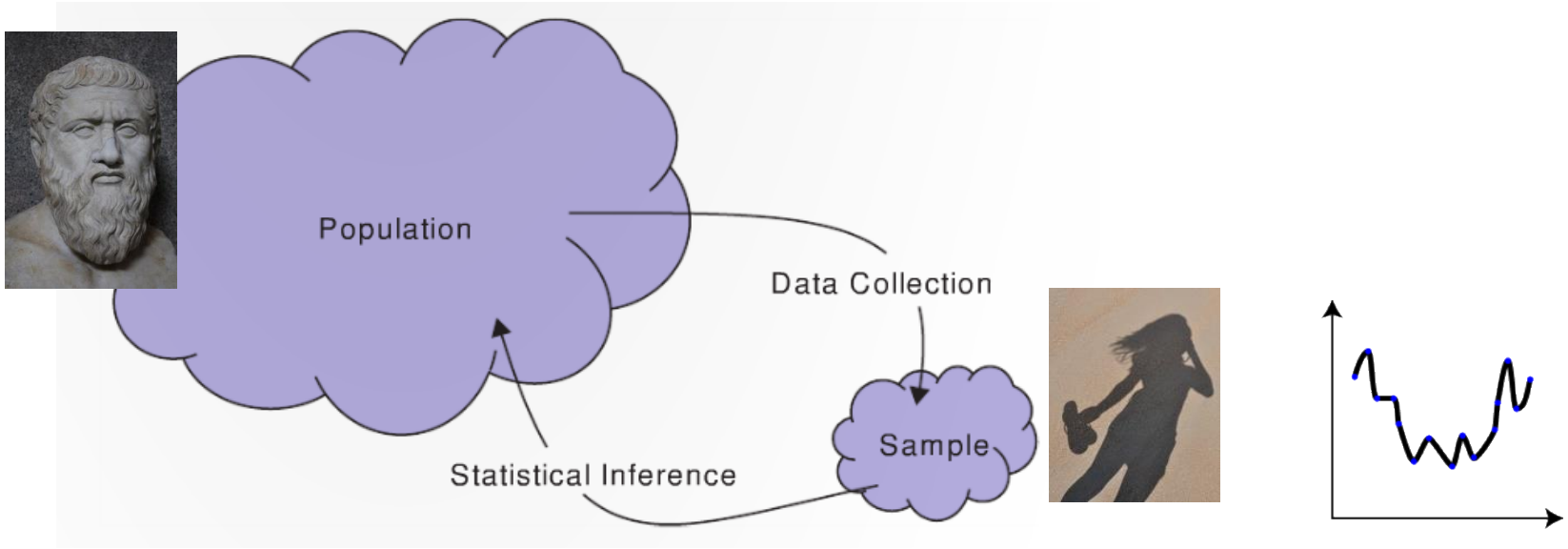


Overfitting

Overfitting occurs when we generate a function that too closely matches random sample we have, but does not generalize to the full probability distribution

- The model is fit to closely to the shadows and not getting at the Truth





Overfitting song

https://www.youtube.com/watch?v=DQWI1kvmwRg

Selecting models methods

There are a number of different methods for selecting models. Four we will briefly discuss are:

1. Creating measures of fit (statistics) that penalize models with more predictors

2. Creating simpler models by removing predictors

3. Evaluating models using cross-validation

4. If there is time: methods that shrink regression coefficients

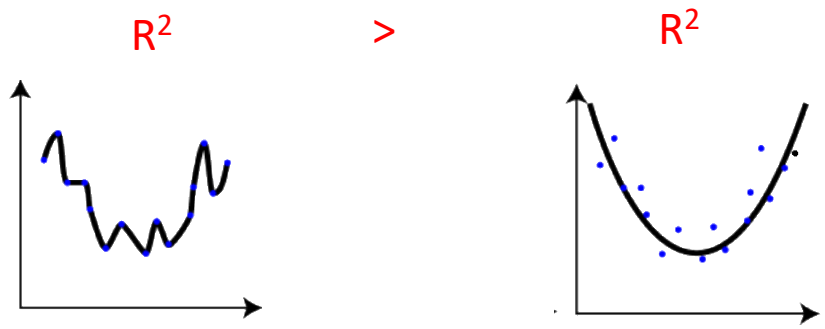
Model method selection 1: Selected models using statistics that penalize larger models

R^2 as a measure of model fit

We have used the coefficient of multiple determination (R^2) to determine how well our model is fitting the data:

$$R^2 = \frac{SSModel}{SSTotal} = 1 - \frac{SSResidual}{SSTotal} = 1 - \frac{\Sigma_{i=1}^{n}(y_i - \hat{y})^2}{\Sigma_{i=1}^{n}(y_i - \bar{y})^2}$$

R^2 always increases with more predictors x_i because the response variable y can always fit more closely with more predictors



Recall: the standard deviation of the errors: σ_ε

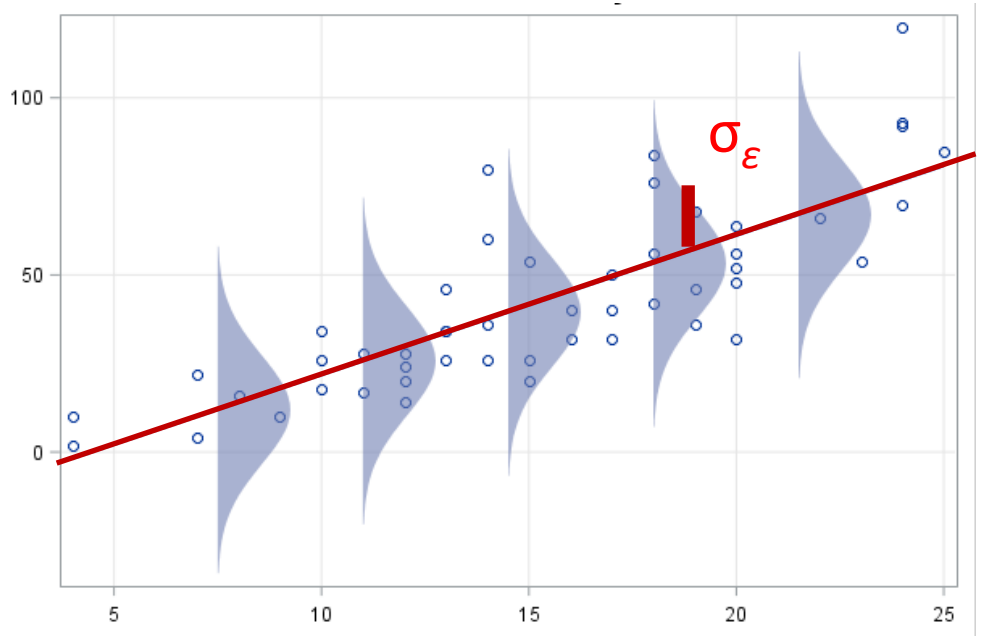
Recall for simple linear regression, the standard deviation of error is denoted $\boldsymbol{\sigma_\varepsilon}$ and shows how far the points fall off the true regression line.

We can use the **standard deviation of residuals ($\hat{\sigma}_\varepsilon$)** as an estimate for σ_ε

For simple linear regression we had:

$$\hat{\sigma}_\epsilon = \sqrt{\frac{1}{n-2} SSRes}$$

$$= \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$

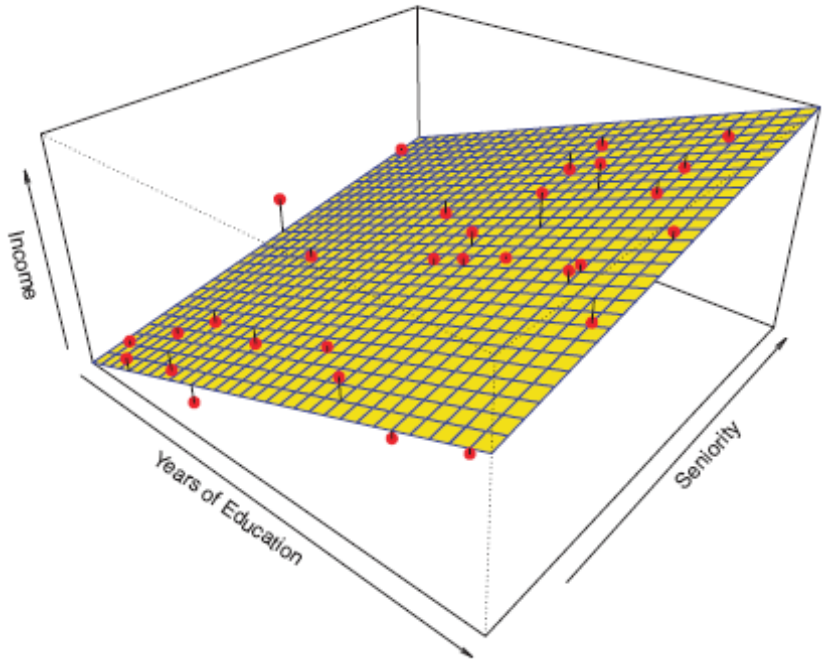


Recall: the standard deviation of the errors: σ_ε

For multiple regression, we with k parameters (i.e., k - 1 predictors) an (almost) unbiased estimate of $\hat{\sigma}_\varepsilon$ is:

$$\hat{\sigma}_\epsilon = \sqrt{\frac{1}{n-k} SSRes}$$

$$= \sqrt{\frac{1}{n-k} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$



The residual standard error $\hat{\sigma}_\varepsilon$ corrects for bias by dividing the SSResidual by 1/(n - k)

This estimate does not always decrease with more predictors x

Adjusted R^2

The **adjusted R^2** helps account for the number of predictors in the model by using $\hat{\sigma}_\varepsilon^2$

$$R^2_{adj} = 1 - \frac{SSRes/(n-k)}{SSTotal/n-1} = 1 - \frac{\hat{\sigma}^2_\epsilon}{s^2_y}$$

The adjusted R^2 does not always give a higher values to the model with the more predictors

- i.e., using this statistic, we will not always say that a model with the most predictors is a “better” fit to the data

Other statistics that penalize larger models

There are several other statistics that also ***penalize models that have more predictors***

- These statistics are only meaningful for within data set comparisons

Akaike information criterion: $AIC = 2 \cdot k + n \cdot ln(SSRes)$ R: AIC(lm_fit)

Bayesian information criterion: $BIC = k \cdot ln(n) + n \cdot ln(SSRes/n)$ R: BIC(lm_fit)

One should select the model with the lowest value on these statistics

Let’s try it in R…

Model method selection 2: Using algorithms to select a subset of variables

Brief mention: Variable selection

Variable selection refers to finding models that rely on a small subset of predictors

- This can help make the regression model more interpretable as well

We could use individual feature p-values to determine which predictors to use, however…

- Some of these will be spuriously significant
  - i.e., if H_0 is true for all predictors, ~5 will be significant at $\alpha = .05$ level
- The p-values change as predictors are added and removed
  - Due to multicollinearity

```
lm_fit_mult <-
    lm(log(endowment)  ~
     salary_tot,
     salary_men,
     salary_women
    )
```

Feature selection: deciding which variables to use

Ideally we would like to try all combinations of predictors, however, if there are k features, there are 2^k possible models which can be intractable

A few heuristic methods exist for selecting smaller models

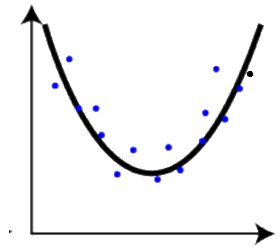
- Forward selection: start with a model with no predictors and add predictors (until you have enough)
- Backward selection: Start with the full model and delete predictors
- Mixed selection: Use a combination of forward and backward selection

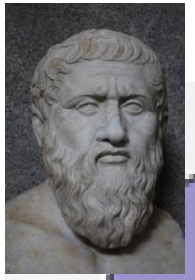
```
Coefficients:
                Estimate  Std. Error t value             Pr(>|t|)
(Intercept)  12.85948900  0.17913330  71.787 < 0.0000000000000002 ***
salary_tot    0.00013686  0.00003950   3.465             0.000551 ***
salary_men   -0.00001569  0.00002019  -0.777             0.437160
salary_women -0.00004304  0.00002156  -1.997             0.046099 *
```

In R: leaps::regsubsets()

Model method selection 3: Choosing a model through cross-validation

Cross-validation

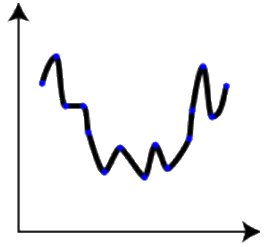




Population

Training set

Sample



Test set

Sample

Good predictions on the test set give an estimate of how accurate the model will be on new data from the population

Cross-validation

We run cross-validation by splitting data into two sets:

A training set in which the parameters of a regression model are fit

A test set in which the prediction accuracy of our model is assessed

Mean squared prediction error

To evaluate how effective a model is, we can use the mean squared prediction error (MSPE) using the following steps:

1. Fit a model using the training data
2. Make predictions on the test data
3. We can use the MSPE to assess how accurate the predictions are:

$$MSPE = \frac{1}{n_t}\sum_{i=1}^{n_t}(y_i - \hat{y}_i)^2 = \frac{1}{n_t}\sum_{i=1}^{n_t}(y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_1 + \ldots + \hat{\beta}_k x_k))^2$$

Actual y values in the test set

Predicted y values on the test set

Parameters estimated on the training set

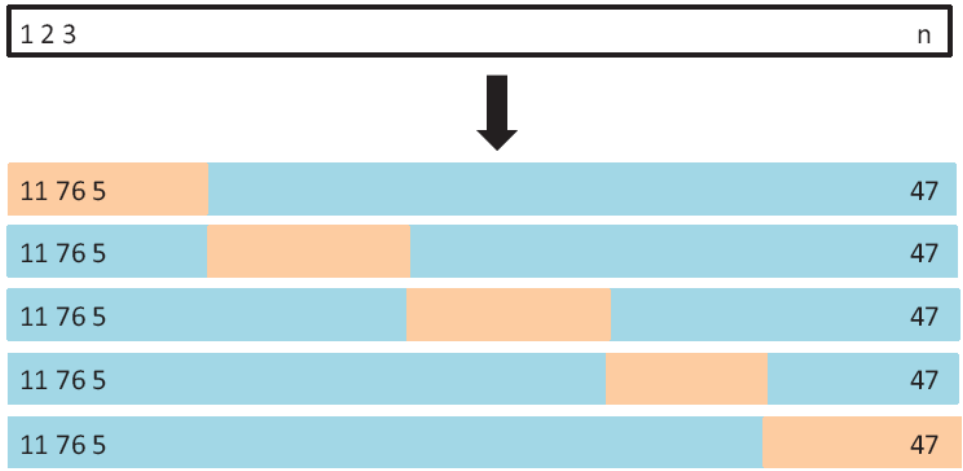
Predictions assessed on the test set

n_t is the number of points in the test set

K-fold cross-validation

K-fold cross-validation

- Split the data into k parts
- Train on k-1 of these parts and test on the left out part
- Repeat this process for all k parts
- Average the prediction accuracies to get a final estimate of the generalization error



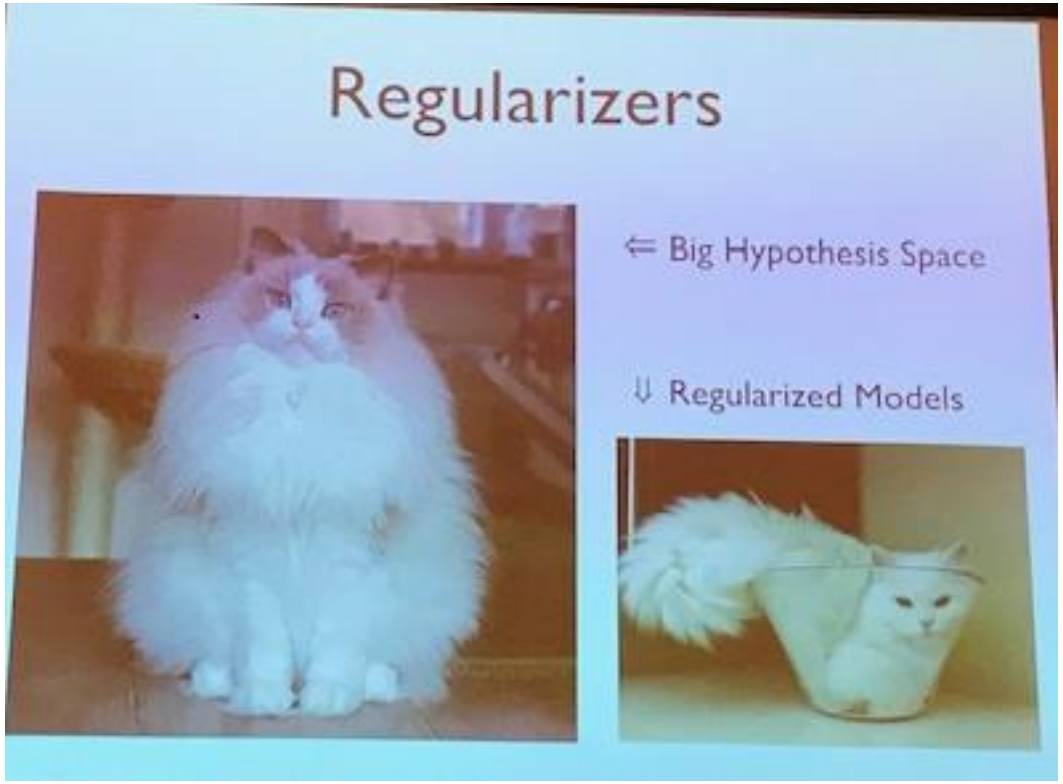
Leave-one-out (LOO) cross-validation: k = n

Let’s try it in R…

Side note: controlling model complexity with regularization

Brief mention: shrinkage methods

Rather than finding the coefficients $\hat{\beta}_i$ by just minimizing the SSRes, one can also add penalties in the fitting procedure to find simpler models



We will very briefly discuss two techniques:

- Ridge regression (l_2 norm penalty)
- The lasso (l_1 norm penalty)

Brief mention: Ridge regression

Ridge regression finds the coefficients $\hat{\beta}_i$ that minimize:

$$\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \sum_{j=1}^{k-1}\hat{\beta}_j x_{ij})^2 + \lambda \sum_{j=1}^{k-1}\hat{\beta}_j^2$$

SSRes

shrinkage penalty

Tuning parameter

What happens if:

- λ = 0
- λ → infinity
- (the coefficients depend on the tuning parameter value)

see the glmnet package

Brief mention: The Lasso

The Lasso finds the coefficients $\hat{\beta}_i$ that minimize:

$$\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \sum_{j=1}^{k-1}\hat{\beta}_j x_{ij})^2 + \lambda \sum_{j=1}^{k-1}|\hat{\beta}_j|$$

SSRes

shrinkage penalty

Tuning parameter

Similar to ridge regression but penalizes $|\hat{\beta}_i|$ instead of $\hat{\beta}_i^2$

- i.e., uses the L_1 penalty instead of the L_2 penalty

<u>Advantages</u>

- Final model will often have many set $\hat{\beta}_i$ to 0
- i.e., does variable selection and creates a 'sparse' model

see the glmnet package

Shrinkage/regularization methods

Regularization methods often work very well when we care about making accurate predictions on new data

Theory suggests that these methods work by minimizing the MSPE through a bias-variance tradeoff

- Average MSPE = bias^2 + variance
- We use a biased method (via regularization) to get models that vary less from one random data set to the next, reducing the average MSPE

To learn more about regularization methods, take a class on Machine Learning!