3.1 Best Subset Selection

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2. For $k = 1, 2, \ldots, p$:
   (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.
   (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Here best is defined as having the smallest RSS = SSE, or equivalently largest R^2.
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3.2 Stepwise Selection: Forward

1. Let $\mathcal{M}_0$ denote the null model, which contains no predictors. This model simply predicts the sample mean for each observation.
2. For $k = 0, 1, \ldots, p - 1$:
   (a) Consider all $p - k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor.
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1. Let $\mathcal{M}_p$ denote the full model, which contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:
   (a) Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
   (b) Choose the best among these k models, and call it $\mathcal{M}_{k-1}$. Here best is defined as having smallest RSS or highest R^2.
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Data example

- 50 states data collected by U.S. Bureau of the Census
- Response: life expectancy

```r
#read data and load package
library(faraway)
data(state)
statedata <- data.frame(state.x77,row.names=state.abb)
head(statedata)
```

```
##    Population Income Illiteracy Life.Exp Murder HS.Grad Frost   Area
## AL       3615   3624        2.1    69.05   15.1    41.3    20  50708
## AK        365   6315        1.5    69.31   11.3    66.7   152 566432
## AZ       2212   4530        1.8    70.55    7.8    58.1    15 113417
## AR       2110   3378        1.9    70.66   10.1    39.9    65  51945
## CA      21198   5114        1.1    71.71   10.3    62.6    20 156361
## CO       2541   4884        0.7    72.06    6.8    63.9   166 103766
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R package: leaps

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library(leaps)
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regsubsets: R function for model selection

- method: exhaustive search, forward or backward stepwise

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b <- regsubsets(Life.Exp~.,data=statedata, method="exhaustive")
rs <- summary(b)
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- for each size of model p, it finds the variables that produce the minumum RSS .

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rs$which
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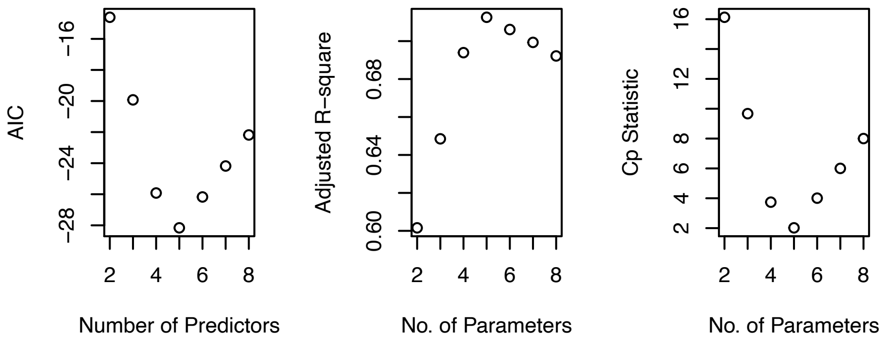
```r
AIC <- 50*log(rs$rss/50) + (2:8)*2
par(mfrow=c(1,3))
plot(AIC ~ c(2:8), ylab="AIC", xlab="Number of Predictors")
plot(2:8, rs$adjr2, xlab="No. of Parameters", ylab="Adjusted R-square")
plot(2:8,rs$cp,xlab="No. of Parameters",ylab="Cp Statistic")
```



[MS 4] Validation and Cross-Validation

Prediction Error

- Arguably, the goal of a regression analysis is to "build" a model that predicts well.
- One way to measure this is in the expected prediction error of the model.
  - Estimate model parameters $\hat{\beta}$ from training data.
  - Consider future data $(X_{\text{new}}, Y_{\text{new}})$
  - Given X_{new}. Predict Y_{new} by $\hat{Y}_{\text{new}} = X_{\text{new}}\hat{\beta}$.
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Model Validation

Model validation refers to checking a selected model against independent data.

1. Collect new data as validation data set.
2. Split data into training and validation set.

- Estimate model by a training set.
- Evaluate Mean Squared Prediction Error by

$$\text{MSPE} = \frac{\sum_{i \in \mathcal{V}} (Y_i - \hat{Y}_i)^2}{|\mathcal{V}|}$$

  - $|\mathcal{V}|$ is the sample size of the validation data set.
  - Y_i is the i th observed response in the validation data set.
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Leave-One-Out Cross-Validation

- Suppose we have n observations $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$.
- For $i = 1, \ldots, n$
  - Fit a model with observations exclusing i-th observation.
  - Make a prediciton $\hat{y}_i$ using the fitted model.
  - Define $\mathrm{MSE}_i = (y_i - \hat{y}_i)^2$ (prediction error).
- Define LOOCV estimate

$$\mathrm{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \mathrm{MSE}_i$$

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k-Fold Cross-Validation

- Split data randomly into K roughly equal parts.
- For $k = 1, \ldots, K$, fit the model using all but the k th part of the data and obtain predicted values $\hat{Y}_{ki}$
- Compute the prediction error mean sum of squares

$$\mathrm{CV}_k = \frac{1}{n_k} \sum_{i=1}^{n_k} \left(Y_{ki} - \hat{Y}_{ki} \right)^2$$

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Example on LOOCV

```r
library(ISLR)
library(boot)
```

- Auto Data: Including MPG, horsepower, and other information for 392 vehicles.
- LOOCV: done by `cv.glm` in the package `boot`.

```r
glm.fit = glm(mpg ~ horsepower, data =Auto)
```

- glm gives the same fit as lm but can be input for cv.glm

```r
cv.err = cv.glm( Auto, glm.fit)
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```r
cv.err$delta[1] #LOOCV estimate
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## [1] 24.23151
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Example on K-fold CV

- Set K option in cv.glm

```
cv.glm( Auto, glm.fit, K=10)$delta[1]

## [1] 24.14184
```

- Similar value to LOOCV.
- K-fold CV can be less computationally demanding compared to LOOCV under general models.

Example on K-fold CV

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cv.glm( Auto, glm.fit, K=10)$delta[1]
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[MS 5] Bias-Variance Tradeoff

Decomposing PE

- Expected prediction error/ Mean squared error

$$\mathrm{MSE} = \mathrm{E}(\mathrm{PE}) = \mathrm{E}\,\|Y_{\mathrm{new}} - \hat{Y}_{\mathrm{new}}\|^2$$

- We have

$$\begin{aligned}\mathrm{MSE} &= \|\,\mathrm{E}(Y_{\mathrm{new}}) - \mathrm{E}(\hat{Y}_{\mathrm{new}})\|^2 + \mathrm{tr}\{\mathrm{var}(Y_{\mathrm{new}} - \hat{Y}_{\mathrm{new}})\} \\ &= \mathrm{bias}^2 + \mathrm{variance}\end{aligned}$$

  - $\hat{Y}_{\mathrm{new}}$ is from old (training) data.
  - Y_{new} is from new data.
    - When independent, variance $= \mathrm{tr}\{\mathrm{var}(\epsilon_{\mathrm{new}}) + \mathrm{var}(\hat{Y}_{\mathrm{new}})\}$
    - $\mathrm{tr}\{\mathrm{var}(\epsilon_{\mathrm{new}})\}$ is the irreducible variane while $\mathrm{tr}\{\mathrm{var}(\hat{Y}_{\mathrm{new}})\}$ depends on model.

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