Model Selection

We created 100 explanatory variables and a response variable where the true model is linear in the first 5 of these variables.

The sample size is 500.

We fit a bunch of models to the data.

```
mod0 = lm(y~X[,1])
mod1 = lm(y~X[,1:3])
mod1.4 = lm(y~X[,1:5])
mod1.5 = lm(y~X[,1:5])
mod1.6 = lm(y~X[,1:6])
mod1.7 = lm(y~X[,1:7])
mod1.8 = lm(y~X[,1:8])
mod1.9 = lm(y~X[,1:9])
mod2 = lm(y~X[,1:10])
mod2.5 = lm(y~X[,1:20])
mod3 = lm(y~X[,1:30])
mod4 = lm(y~X[,1:50])
mod5 = lm(y~X[,1:50])
mod5 = lm(y~X[,1:50])
mod1.8", "mod1.9", "mod2.5", "mod3", "mod4", "mod5")
```

Here is a function that we can use to plot the model selection criteria against the model size.

Now we examine the various model selection criteria, including Mallow's Cp, AIC, BIC, and leave-one-out cross validation.

Mallow's C_n

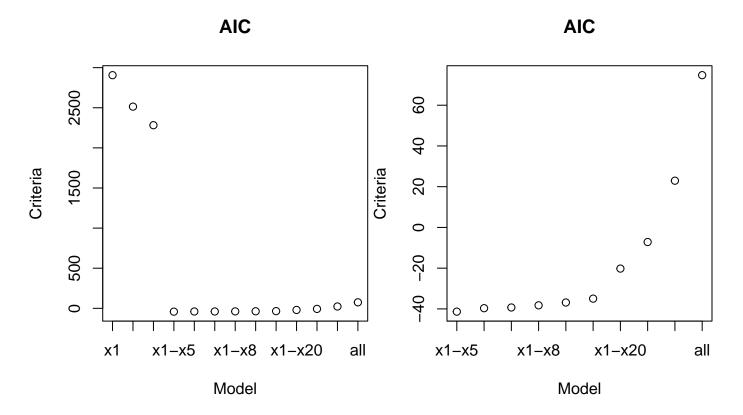
We calculate Mallow's Cp for each of the models that we fit. Recall the alternative representation of Mallow's Cp as

$$2(p(m)+1)-n+ErrSS(m)/s_e^2$$

Mallow's Cp Mallow's Cp 0 0 -350-300 0 -400 0 0 -400 0 0 -450 0 0 0 0 0 0 0 x1-x5 х1 x1-x8 x1-x20 all x1-x5 x1-x8 x1-x20 all Model Model

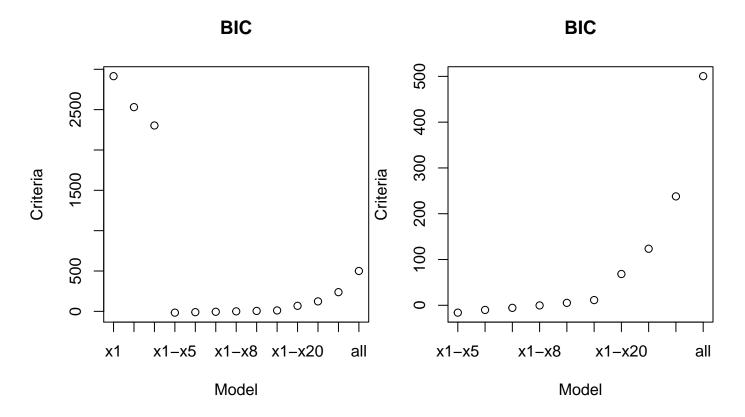
AIC

Find AIC for these various models.



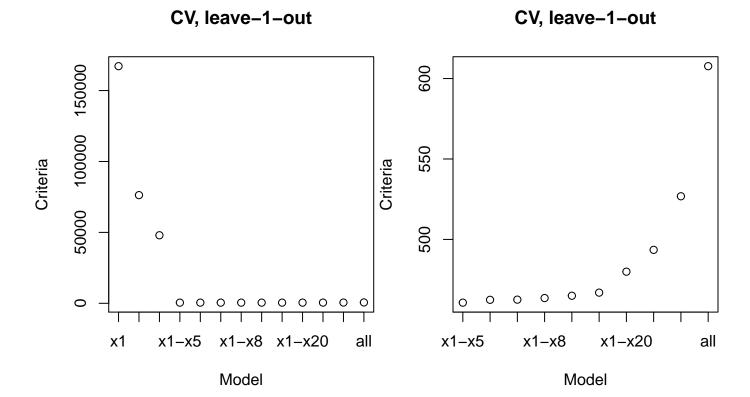
BIC

Find BIC for various models.



Leave one out CV

For each model, we fit the model with least squares, we find the residual sum of squares for the model, and we find the hat values for each observations. These give us the leave-one-out cross-validated residual sum of squares.



Best subset regression

Rather than compare the 13 models that we constructed earlier, we can examine all possible models based on all possible subsets of variables. (Note this is problematic for categorical explanatory variables). We start with the Cp for all subsets of the full model. The leaps() function reports Mallow's Cp for the 10 best models for each model size. Included in the return value are the variables that belong to the 10 best models.

Here are the top 10 one-variable models and the top ten two-variable models. The TRUE and FALSE indicate which variables belong in the model. Note that we show only the first 12 of the 30 variables here.

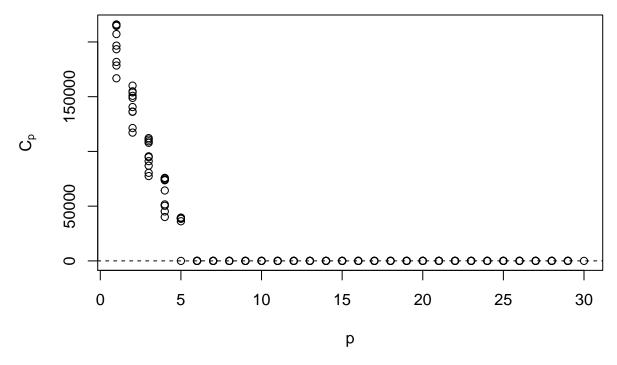
```
outs$which[1:20, 1:12]
```

```
Х7
##
                          X1
                                              Х2
                                                                  ХЗ
                                                                                      Х4
                                                                                                          X5
                                                                                                                             Х6
                                                                                                                                                                     Х8
                                                                                                                                                                                         Х9
                                                                                                                                                                                                          X10
                                                                                                                                                                                                                              X11
                                                                                                                                                                                                                                                 X12
         1 FALSE FALSE FALSE
                                                                                                  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
                   TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
                                       TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 1 FALSE
                                                          TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
        1 FALSE FALSE
        1 FALSE FALSE FALSE
                                                                              TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
         1 FALSE FALSE FALSE FALSE FALSE
                                                                                                                                       TRUE FALSE FALSE FALSE FALSE
         1 FALSE FALSE
         1 FALSE FALSE
         1 FALSE FALS
        1 FALSE FALSE
                   TRUE TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
```

```
## 2 FALSE FALSE TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 FALSE FALSE FALSE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 TRUE FALSE TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## 2 FALSE TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## 3 FALSE TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## 4 PALSE TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## 5 FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## 5 FALSE FA
```

Plot the Cp for the best 10 models for each model size.

```
plot(outs$size, outs$Cp, xlab = "p", ylab = expression(C[p]))
abline(a = 0, b = 1, lty = 2, untf = TRUE)
```



```
plot(outs$size, outs$Cp, xlab = "p",
    ylab = expression(C[p]),ylim=c(min(outs$Cp),median(outs$Cp)))
abline(a = 0, b = 1, lty = 2, untf=TRUE)
```

```
10
                                   0
                                  0
    2
တ္
    0
             5
      0
              5
                     10
                            15
                                   20
                                          25
                                                 30
                             p
```

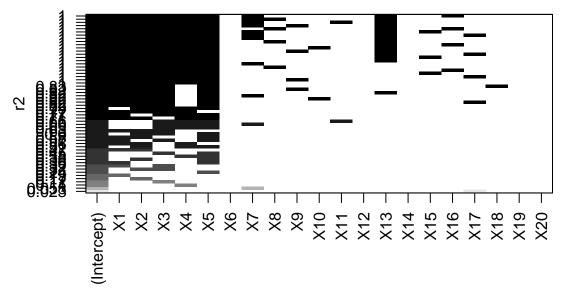
```
mydata = data.frame(y, X[ , 1:20])
leaps = regsubsets(y ~ ., data = mydata, nbest = 7)
summary(leaps)
```

```
## Subset selection object
## Call: regsubsets.formula(y ~ ., data = mydata, nbest = 7)
  20 Variables (and intercept)
##
       Forced in Forced out
## X1
           FALSE
                      FALSE
## X2
                      FALSE
           FALSE
## X3
           FALSE
                      FALSE
## X4
           FALSE
                      FALSE
## X5
           FALSE
                      FALSE
## X6
                      FALSE
           FALSE
## X7
           FALSE
                      FALSE
## X8
           FALSE
                      FALSE
## X9
           FALSE
                      FALSE
## X10
           FALSE
                      FALSE
## X11
           FALSE
                      FALSE
## X12
           FALSE
                      FALSE
## X13
           FALSE
                      FALSE
## X14
           FALSE
                      FALSE
## X15
           FALSE
                      FALSE
## X16
           FALSE
                      FALSE
## X17
           FALSE
                      FALSE
## X18
           FALSE
                      FALSE
## X19
           FALSE
                      FALSE
## X20
           FALSE
                      FALSE
## 7 subsets of each size up to 8
## Selection Algorithm: exhaustive
            X1 X2 X3 X4 X5 X6 X7 X8 X9 X10 X11 X12 X13 X14 X15 X16
##
```

```
## 4
```

```
X17 X18 X19 X20
## 1 (1)"""""""
## 1 (2) " " " " " " "
## 1 (3)"""""""
## 1 (4) " " " " " " "
## 1 (5)"""""""
## 1 (6) " " " " " " "
## 1 (7) "*" " " " " "
## 2 (1) " " " " " " "
## 2 (2) " " " " " " "
## 2 (3) " " " " " " "
## 2 (4) " " " " " " "
## 2 (5)"""""""
   (6)"""""""
## 2
## 2 (7) " " " " " " "
## 3 (1) " " " " " " "
## 3 (2) " " " " " " "
## 3 (3)"""""""
## 3 (4)"""""""
## 3 (5)"""""""
## 3 (6) " " " " " " "
   (7)"""""""
## 3
## 4 (1)"""""""
## 4 (2) " " " " " " "
## 4 (3)"""""""
## 4 (4) " " " " " " "
## 4 (5)"""""""
## 4 (6) " " " " " " "
   (7)"""""""
## 4
## 5 (1) " " " " " " "
## 5 (2) " " * " " " "
## 5 (3)"""""""
   (4)"""""""
## 5
## 5 (5) " " " " " " "
## 5 (6) " " " " " " "
## 5 (7) "*" " " " " "
   (1)"""""""
## 6
## 6 (2) " " " " " " "
## 6 (3) " " " " " " "
## 6 (4) " " " " " " "
## 6 (5) " " " " " " "
## 6 ( 6 ) "*" " " " " "
## 6 (7) " " " " " " "
##7 (1)"""""""
   (2)"""""""
## 7
##7 (3)"""""""
## 7 (4) " " " " " " "
   (5)"""""""
## 7
## 7 (6) "*" " " " " "
##7 (7) " " " " " " "
## 8 (1) " " " " " " "
## 8 (2) " " " " " " "
```

```
plot(leaps, scale="r2")
```



We can also distinguish the Cp for the variaous models with the Cpplot function.

```
#show all models
library(faraway)
Cpplot(outs)
```

Forward and Backward selection of variables

Forward selection of variables

We fit the starting model, i.e., the minimum model

```
min.model = lm(y ~ 1, data = mydata)
```

Then we specify the largest model with

```
biggest = formula(lm(y ~ ., mydata))
biggest
```

```
## y ~ X1 + X2 + X3 + X4 + X5 + X6 + X7 + X8 + X9 + X10 + X11 + 
## X12 + X13 + X14 + X15 + X16 + X17 + X18 + X19 + X20
```

The step() function does the stepwise fitting for us. We provide the starting model, the direction (forward, backward, or both), and the largest model to consider

```
## Start: AIC=3009
## y \sim 1
##
##
          Df Sum of Sq
                        RSS AIC
## + X5
                 49523 155065 2872
           1
## + X1
           1
                 38700 165887 2906
## + X2
                 35553 169034 2916
           1
## + X3
                 24586 180001 2947
           1
## + X4
                 21529 183059 2955
           1
## + X7
               11784 192803 2981
           1
## + X17
           1
                 4778 199810 2999
## + X14
                 4514 200074 3000
           1
## + X20
                  3093 201495 3003
           1
## + X13
                  2976 201611 3004
           1
## + X11
                  1507 203081 3007
           1
## + X9
           1
                  1151 203437 3008
## + X10
           1
                  1056 203532 3008
## + X16
                  918 203669 3009
## <none>
                       204588 3009
                  700 203887 3009
## + X8
           1
## + X19
                   574 204014 3010
           1
## + X12
           1
                   547 204041 3010
## + X15
                   180 204408 3011
           1
## + X18
                   131 204456 3011
          1
## + X6
           1
                   25 204563 3011
##
## Step: AIC=2872
## y ~ X5
##
          Df Sum of Sq
                        RSS AIC
              42065 113000 2716
## + X3
           1
## + X4
           1
                 28164 126901 2774
## + X2
          1
                 28145 126920 2774
## + X1
           1
                 24784 130281 2787
## + X7
           1
                 11735 143330 2835
## + X16
                 5276 149789 2857
           1
## + X20
           1
                 3741 151324 2862
## + X17
                  2668 152397 2866
           1
## + X11
           1
                  2262 152803 2867
## + X9
                  1722 153343 2869
           1
## + X19
                  1565 153500 2869
           1
## + X10
                  1524 153541 2870
           1
## + X8
           1
                  1154 153911 2871
## + X18
           1
                  719 154346 2872
                       155065 2872
## <none>
## + X13
                  549 154516 2873
           1
## + X12
           1
                   309 154756 2873
## + X14
           1
                  102 154963 2874
## + X6
                    9 155056 2874
           1
## + X15
                     8 155057 2874
           1
##
```

```
## Step: AIC=2716
## y \sim X5 + X3
##
          Df Sum of Sq
                        RSS AIC
##
                 40694 72306 2495
## + X4
           1
## + X2
                 31815 81185 2553
           1
## + X1
                 25084 87916 2593
           1
## + X7
                  8405 104595 2680
           1
## + X11
           1
                  5273 107727 2694
## + X9
                  3290 109710 2703
           1
## + X18
           1
                  3224 109776 2704
## + X20
                  2570 110430 2707
           1
## + X16
                  2298 110702 2708
           1
## + X12
                  1076 111924 2713
           1
## + X8
                  883 112117 2714
           1
## + X10
           1
                   485 112515 2716
## <none>
                       113000 2716
## + X13
           1
                   301 112699 2717
## + X19
                   214 112786 2717
           1
## + X14
                   190 112810 2717
           1
## + X6
           1
                   89 112911 2718
## + X15
                   71 112929 2718
           1
## + X17
                   33 112967 2718
           1
##
## Step: AIC=2495
## y \sim X5 + X3 + X4
##
##
          Df Sum of Sq RSS AIC
## + X2
                 29922 42384 2230
          1
## + X1
                 24316 47990 2292
           1
## + X11
           1
                  3581 68725 2472
## + X7
           1
                  3207 69099 2474
## + X13
                  2705 69602 2478
           1
## + X12
                  1831 70475 2484
           1
## + X16
           1
                  1193 71113 2489
## + X8
           1
                  1174 71132 2489
## + X20
                  768 71538 2492
## + X17
           1
                  414 71892 2494
## + X14
           1
                   368 71938 2494
## + X9
                   310 71996 2495
           1
## <none>
                      72306 2495
                   129 72177 2496
## + X15
           1
## + X10
                   64 72242 2497
           1
## + X19
                    58 72248 2497
           1
## + X18
                    35 72271 2497
           1
## + X6
                    27 72279 2497
           1
##
## Step: AIC=2230
## y \sim X5 + X3 + X4 + X2
##
##
          Df Sum of Sq
                       RSS AIC
## + X1
          1 41934
                         449 -41
## + X12
           1
                 1820 40564 2210
## + X11
                 1778 40606 2211
           1
```

```
## + X8
           1
                  1691 40693 2212
## + X7
                  1618 40766 2212
           1
## + X20
                  1520 40864 2214
## + X16
                   626 41758 2225
           1
## + X10
           1
                   358 42026 2228
## + X19
                   339 42045 2228
           1
## + X13
                   333 42051 2228
           1
## + X9
                   319 42064 2228
           1
## + X14
           1
                   188 42196 2230
## <none>
                       42384 2230
## + X15
           1
                   23 42361 2232
## + X18
                    20 42363 2232
           1
## + X17
           1
                    15 42369 2232
## + X6
                    11 42373 2232
           1
##
## Step: AIC=-41.34
## y \sim X5 + X3 + X4 + X2 + X1
##
##
         Df Sum of Sq RSS AIC
## + X13
             2.037 447 -41.6
## <none>
                       449 -41.3
## + X7
                1.619 448 -41.1
## + X8
                1.231 448 -40.7
           1
## + X16
           1
                0.964 448 -40.4
## + X15
                0.750 449 -40.2
           1
## + X17
           1
                0.680 449 -40.1
## + X9
                0.458 449 -39.9
           1
## + X14
                0.423 449 -39.8
           1
## + X10
                0.379 449 -39.8
           1
## + X6
                0.275 449 -39.7
           1
## + X20
           1
                0.275 449 -39.7
## + X19
           1
                0.264 449 -39.6
## + X18
           1
                 0.248 449 -39.6
## + X11
                 0.223 449 -39.6
           1
## + X12
           1
                 0.104 449 -39.5
##
## Step: AIC=-41.62
## y \sim X5 + X3 + X4 + X2 + X1 + X13
##
##
          Df Sum of Sq RSS AIC
## <none>
              447 -41.6
## + X7
                1.465 446 -41.3
           1
## + X8
                0.983 446 -40.7
           1
## + X16
                0.859 447 -40.6
           1
## + X10
                 0.769 447 -40.5
           1
## + X9
                0.516 447 -40.2
           1
## + X17
           1
                 0.506 447 -40.2
## + X15
                 0.469 447 -40.1
           1
## + X6
           1
                 0.433 447 -40.1
## + X11
           1
                 0.419 447 -40.1
## + X14
                 0.319 447 -40.0
           1
## + X20
                0.206 447 -39.8
           1
## + X19
           1
                0.197 447 -39.8
## + X12
                0.092 447 -39.7
           1
```

```
## + X18 1 0.067 447 -39.7
```

Notice that information about each step is provided. If we do not want to see this, we set trace to 0.

The object contains the final model as well as the actions taken, which we access via the object's anova element.

fwd.model\$anova

```
Deviance Resid. Df Resid. Dev
                                                   AIC
##
      Step Df
## 1
           NA
                     NA
                               499
                                     204587.9 3009.07
## 2
      + X5 -1 49522.717
                               498
                                     155065.2 2872.50
      + X3 -1 42065.391
                                     112999.8 2716.27
                               497
     + X4 -1 40693.600
                                      72306.2 2495.03
                               496
     + X2 -1 29922.342
                               495
                                      42383.8 2229.96
     + X1 -1 41934.425
                               494
                                        449.4
                                               -41.34
## 7 + X13 -1
                  2.037
                               493
                                        447.4 -41.62
```

Backward selection of variables

Backwad regression is similarly carried out. This time we fit the largest model as a starting point and so we need not supply the scope. Although we could supply scope as the smallest model to consider.

```
biggest.model = lm(y ~ ., data = mydata)
bwd.model = step(biggest.model, direction="backward", trace = 0)
```

bwd.model\$anova

```
##
       Step Df Deviance Resid. Df Resid. Dev
                                                  AIC
## 1
            NA
                      NA
                               479
                                         441.5 -20.20
## 2
      - X14
                0.02449
                               480
                                         441.5 -22.18
             1
## 3
      - X19
             1
                0.04119
                               481
                                         441.6 -24.13
## 4
       - X9
             1
                0.06595
                               482
                                         441.6 -26.06
     - X18
             1
                0.09596
                               483
                                         441.7 -27.95
     - X17
                0.09974
## 6
                                         441.8 -29.83
             1
                               484
## 7
      - X20
                0.15596
                                         442.0 -31.66
             1
                               485
## 8
       - X6
             1
                0.34112
                               486
                                         442.3 -33.27
## 9 - X12
             1
                0.31836
                               487
                                         442.7 -34.91
## 10 - X15
             1
                0.31620
                               488
                                         443.0 -36.55
## 11 - X10
             1
                0.78663
                               489
                                         443.8 -37.67
## 12 - X11
                0.55187
                                         444.3 -39.05
             1
                               490
## 13 - X8
             1
                0.82722
                               491
                                         445.1 -40.12
## 14 - X16
             1
                0.76663
                               492
                                         445.9 -41.26
## 15 - X7 1 1.46524
                               493
                                         447.4 -41.62
```

Both directions

When we go in both directions (adding and dropping variables one at a time) we can begin with a viable model and then provide the upper and lower limits of the model via the scope argument. Here we provide only one model to scope so it is taken as the upper limit.

We start with an arbitrary model.

both.model\$anova

```
## Stepwise Model Path
## Analysis of Deviance Table
##
## Initial Model:
## y ~ X1 + X5 + X12 + X20
##
## Final Model:
## y \sim X1 + X5 + X2 + X3 + X4 + X13
##
##
##
      Step Df Deviance Resid. Df Resid. Dev
                                                 AIC
## 1
                              495
                                   129275.0 2787.54
## 2 + X2 1 4.582e+04
                             494
                                    83456.4 2570.74
## 3 + X3 1 4.632e+04
                                    37136.6 2167.87
                             493
## 4 + X4 1 3.669e+04
                                      448.9 -37.86
                              492
## 5 - X12 1 1.895e-01
                              493
                                      449.1 -39.65
## 6 - X20 1 2.749e-01
                              494
                                      449.4 -41.34
## 7 + X13 1 2.037e+00
                              493
                                      447.4 -41.62
```

Note that in this case the final model is the same in all three approaches. That need not be the case generally.