Feature Selection

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Math 243: Stat Learning

October 4th, 2021

Outline

In today's class, we will...

- Perform some exploratory data analysis on a new data set
- Investigate algorithms for selecting good subsets of predictors

Section 1

Explaratory Data Analysis

Molecular Solubility

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- Finally, the data contains 4 continuous descriptors, such as "molecular weight" or "surface area"

We are interested in determining solubility based on these 20 chemical descriptors.

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- It will be easier to have predictors and response in the same set, so we'll bind columns together:

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solTest <- data.frame(solTestX, Solubility = solTestY)
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- The data also contains 218 binary "fingerprints" for each compound indicating presence of particular chemical substructure, each beginning with "FP"
- We'll ignore these predictors.

```
solTest <- solTest %>% select(!starts_with("FP"))
solTrain <- solTrain %>% select(!starts_with("FP"))
```

Distribution of Response

We'll take a look just at the training data for now. (Why?)

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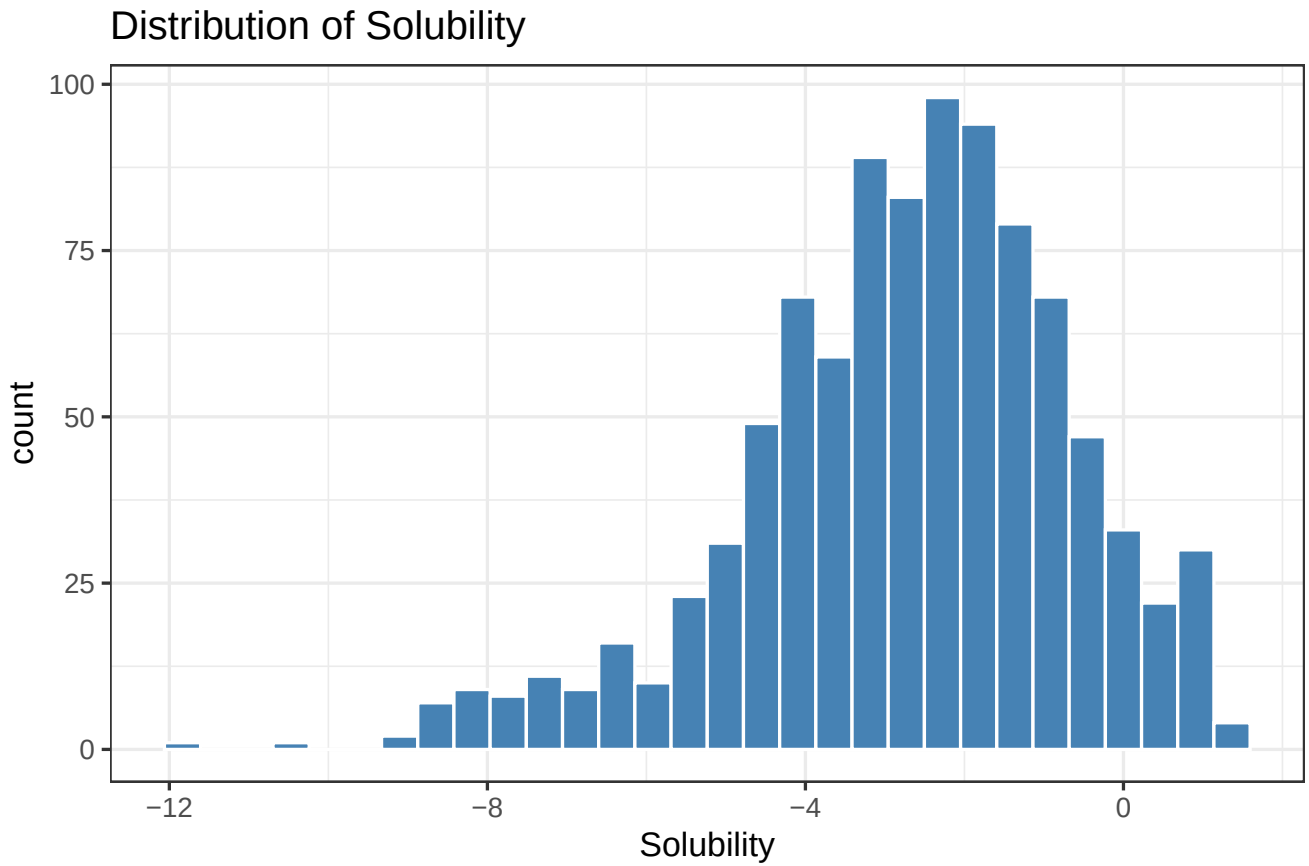
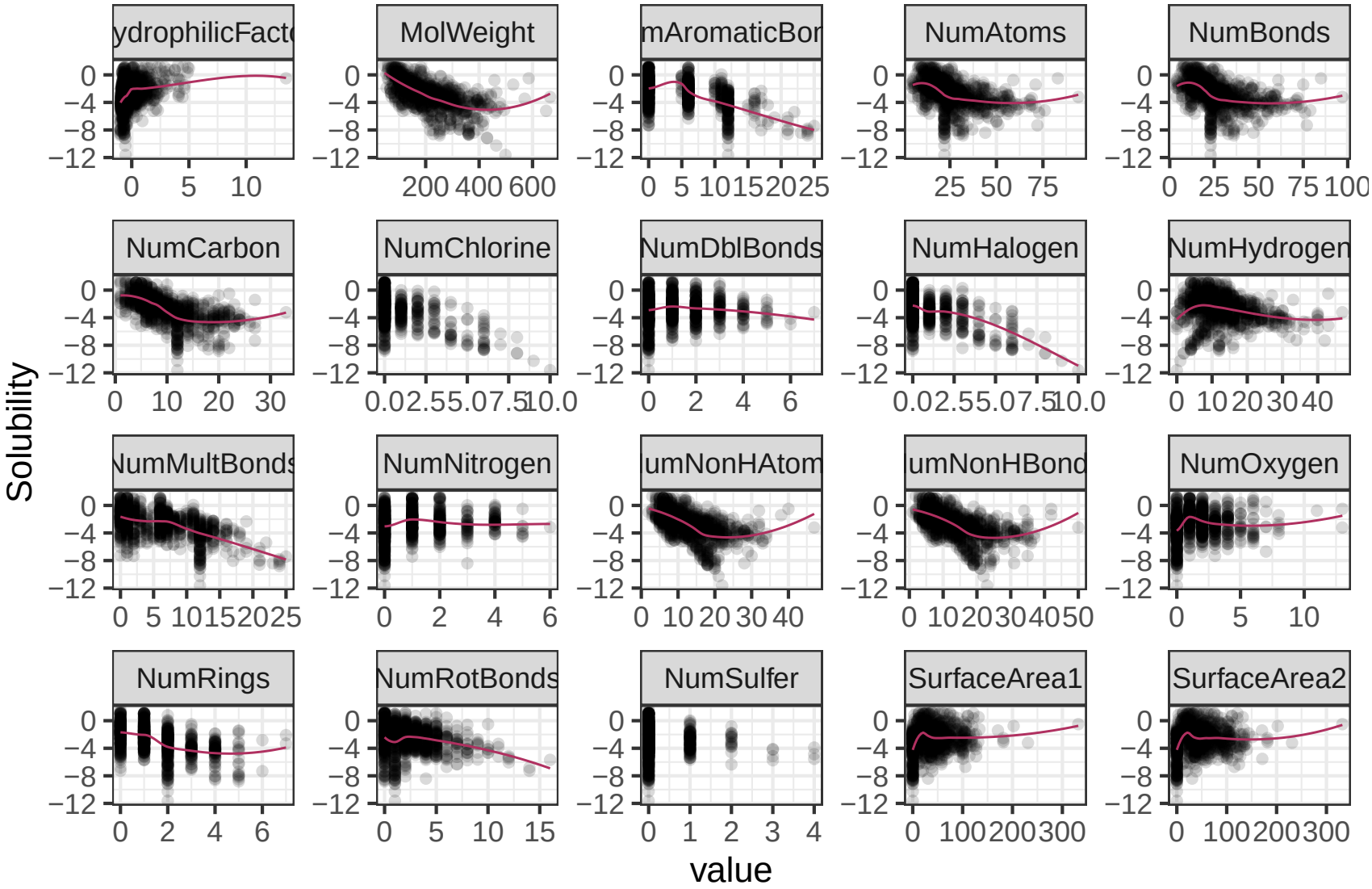


Pairwise Scatterplots



Correlation Matrix

```
library(GGally)
ggcorr(solTrain, hjust = 1, size = 2, layout.exp = 5)
```

Collinearity

- What are downsides of fitting the full model?

Collinearity

- What are downsides of fitting the full model?
- Let's do it anyway!

Model Summary

```
##
## Call:
## lm(formula = Solubility ~ ., data = solTrain)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.8499 -0.5963  0.0232  0.5842  2.7848
##
## Coefficients: (3 not defined because of singularities)
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)        0.344876   0.149393   2.309 0.021189 *
## MolWeight         -0.008074   0.001325  -6.093 1.61e-09 ***
## NumAtoms           0.275577   0.086182   3.198 0.001432 **
## NumNonHAtoms       1.536062   0.450948   3.406 0.000687 ***
## NumBonds          -0.612747   0.127856  -4.792 1.92e-06 ***
## NumNonHBonds             NA         NA      NA       NA
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## NumOxygen         -0.300338   0.424632  -0.707 0.479563
## NumSulfer          0.621244   0.298101   2.084 0.037432 *
## NumChlorine       -0.374042   0.061636  -6.069 1.87e-09 ***
## NumHalogen        -1.579937   0.459350  -3.440 0.000609 ***
## NumRings                 NA         NA      NA       NA
## HydrophilicFactor  0.162663   0.073229   2.221 0.026570 *
## SurfaceArea1       0.047692   0.013827   3.449 0.000587 ***
## SurfaceArea2      -0.070007   0.013245  -5.285 1.56e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9044 on 933 degrees of freedom
## Multiple R-squared:  0.8082,  Adjusted R-squared:  0.8047
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## Multiple R-squared:  0.8082, Adjusted R-squared:  0.8047
## F-statistic: 231.3 on 17 and 933 DF,  p-value: < 2.2e-16
```
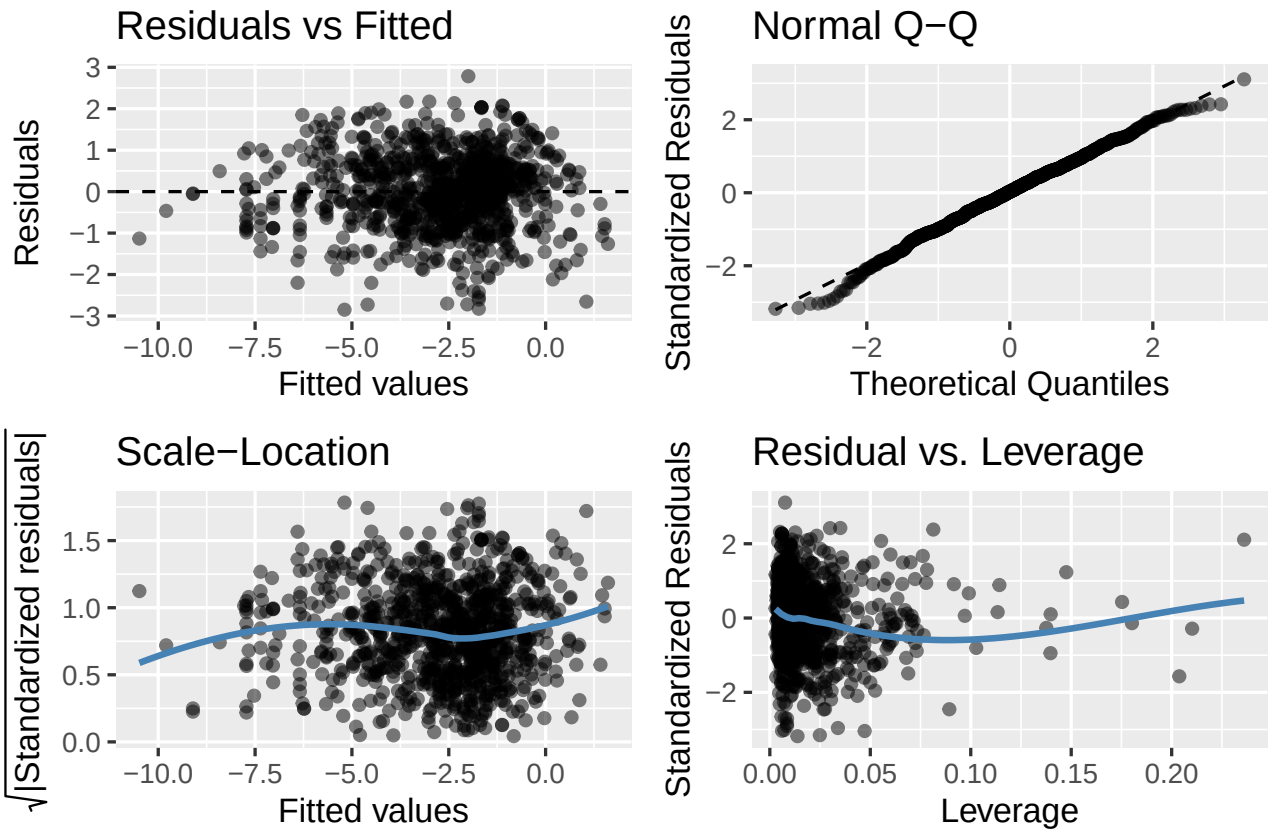

Model Diagnostics

```
library(gglm)
gglm(sol_mod)
```



Section 2

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  - Bayesian information criterion (BIC): uses method of maximum likelihood and Bayes' Rule

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

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- We are performing a large number of *tests*, which corresponds to a relatively flexible model. Likely to overfit.

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- The `regsubsets` function returns *RSS*, R^2, C_p, *AIC*, *BIC* for the best model of each number of predicts.
- The **overall** best model can be selected using any of these criteria.
- Why does `regsubsets` only use *RSS* to determine best model for each number predictors?

Using regsubsets

```
library(leaps)
best_subset<-regsubsets(Solubility~.-NumNonHBonds -NumHydrogen -NumRings,
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- The `regsubsets` function itself outputs a special `regsubsets` object, which contains data but is not user-accessible.
- We'll use the `summary` function, which provides the following elements:
  - `which`: a list of which predictors are in each model
  - `outmat`: a version of `which` for printing
  - Several metrics: `rsq`, `rss`, `adjr2`, `cp`, `bic`

Summary of regsubsets

- Stars indicate variable is included in model.
- For readability, I've only shown models with 5 or fewer variables

```
summary(best_subset)$outmat
```

```
##          MolWeight NumAtoms NumNonHAtoms NumBonds NumMultBonds NumRotBonds
## 1  ( 1 ) "*"       " "      " "          " "      " "          " "
## 2  ( 1 ) "*"       " "      " "          " "      " "          " "
## 3  ( 1 ) "*"       " "      " "          " "      "*"          " "
## 4  ( 1 ) " "       " "      "*"          " "      " "          " "
## 5  ( 1 ) " "       " "      "*"          "*"      " "          "*"
##          NumDblBonds NumAromaticBonds NumCarbon NumNitrogen NumOxygen NumSulfer
## 1  ( 1 ) " "         " "              " "       " "         " "       " "
## 2  ( 1 ) " "         " "              " "       " "         " "       " "
## 3  ( 1 ) " "         " "              " "       " "         " "       " "
## 4  ( 1 ) " "         " "              "*"       "*"         "*"       " "
## 5  ( 1 ) " "         " "              " "       "*"         "*"       " "
##          NumChlorine NumHalogen HydrophilicFactor SurfaceArea1 SurfaceArea2
## 1  ( 1 ) " "         " "         " "               " "          " "
## 2  ( 1 ) " "         " "         " "               "*"          " "
## 3  ( 1 ) " "         " "         " "               "*"          " "
## 4  ( 1 ) " "         " "         " "               " "          " "
## 5  ( 1 ) " "         " "         " "               " "          " "
```

Other Selection Metrics

The summary function can return selection metrics for each model.

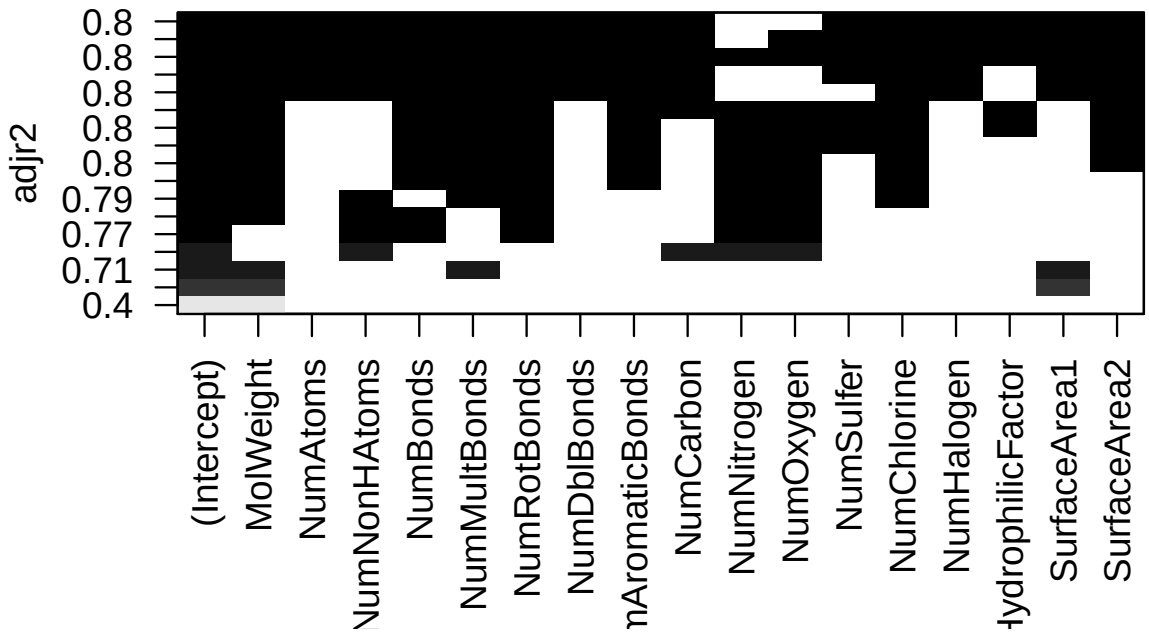
```
d <- data.frame(model = 1:17,
  adjr2 = summary(best_subset)$adjr2,
  rss = summary(best_subset)$rss,
  cp = summary(best_subset)$cp,
  bic = summary(best_subset)$bic)
d %>% head()
```

```
##   model     adjr2       rss        cp        bic
## 1     1 0.3952106 2404.1073 1992.4929  -465.5206
## 2     2 0.6590876 1353.7381  710.2104 -1004.8309
## 3     3 0.7120856 1142.0806  453.4176 -1159.6606
## 4     4 0.7447217 1011.5526  295.8216 -1268.2214
## 5     5 0.7742668  893.5334  153.5199 -1379.3431
## 6     6 0.7813296  864.6602  120.2167 -1403.7232
```

Vizualizing Variables

The variables present can also be plotted directly using `plot`:

```
plot(best_subset, scale = "adjr2")
```



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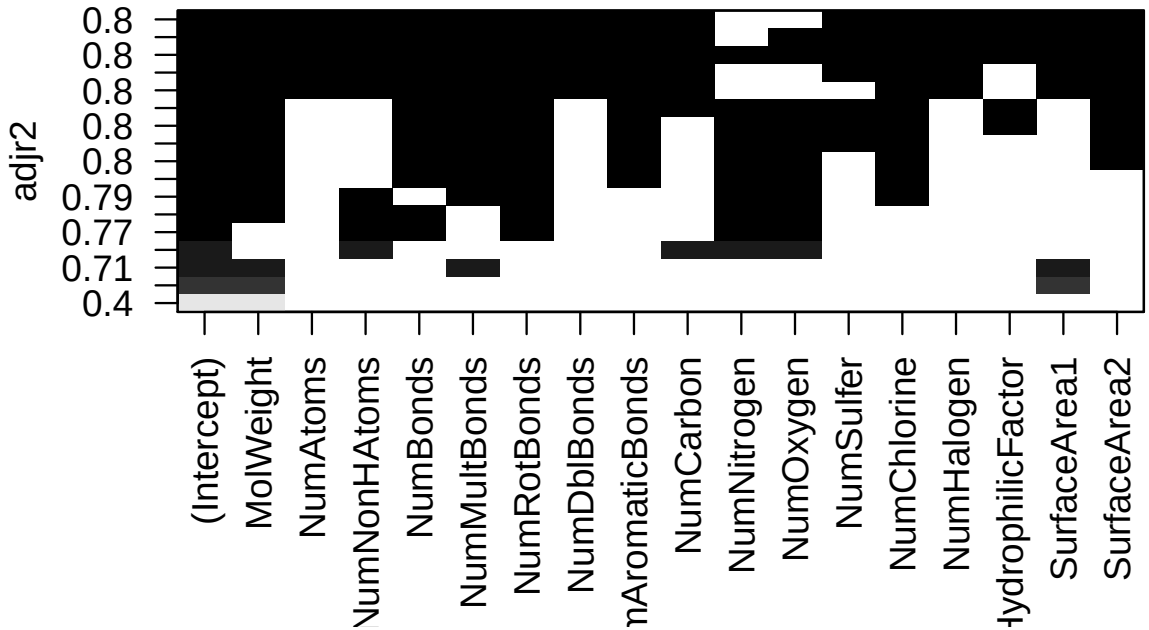
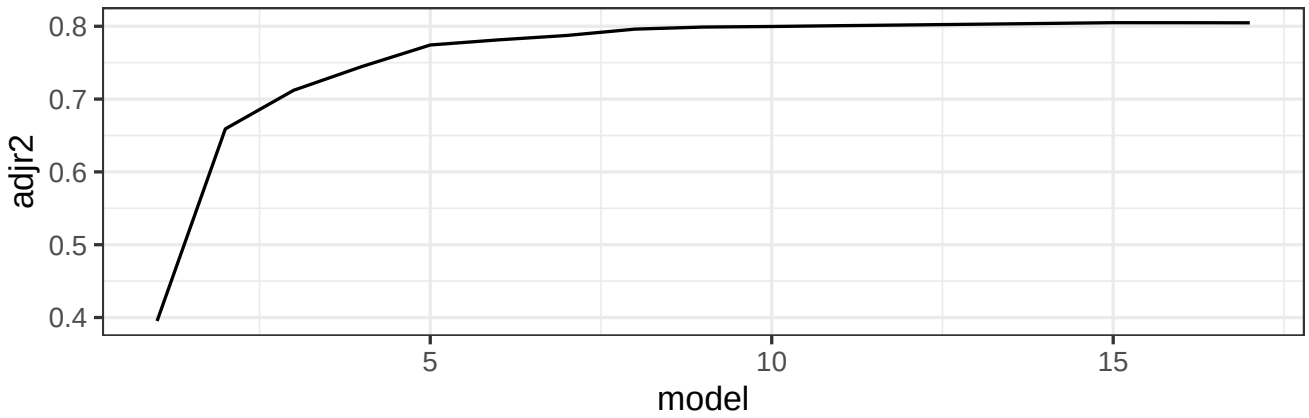


- Models are ordered by by selection statistic. Dark rectangles indicate variable presence

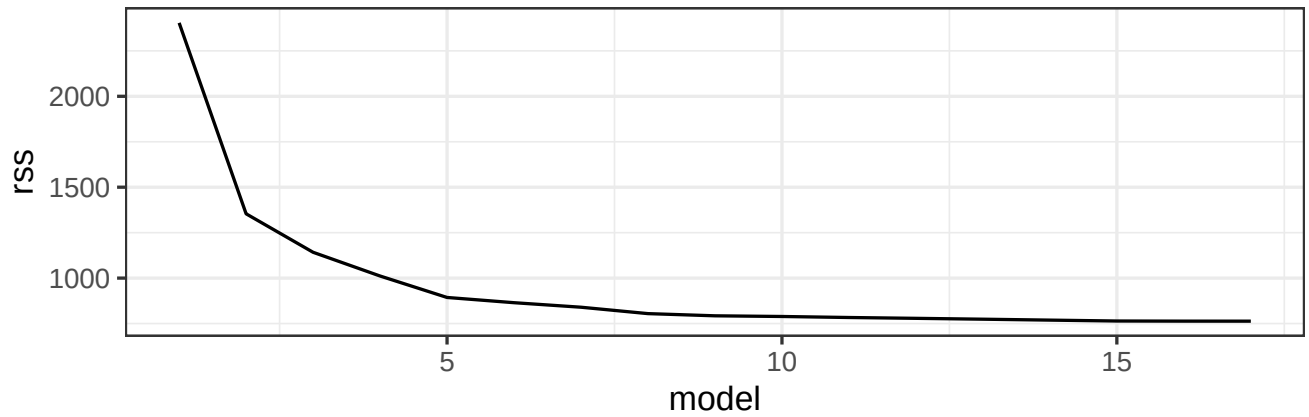
Plotting

We can use ggplot2 to visualize selection metric as a function of variable number

```
ggplot(d, aes(x = model, y = adjr2))+geom_line()+theme_bw()
```

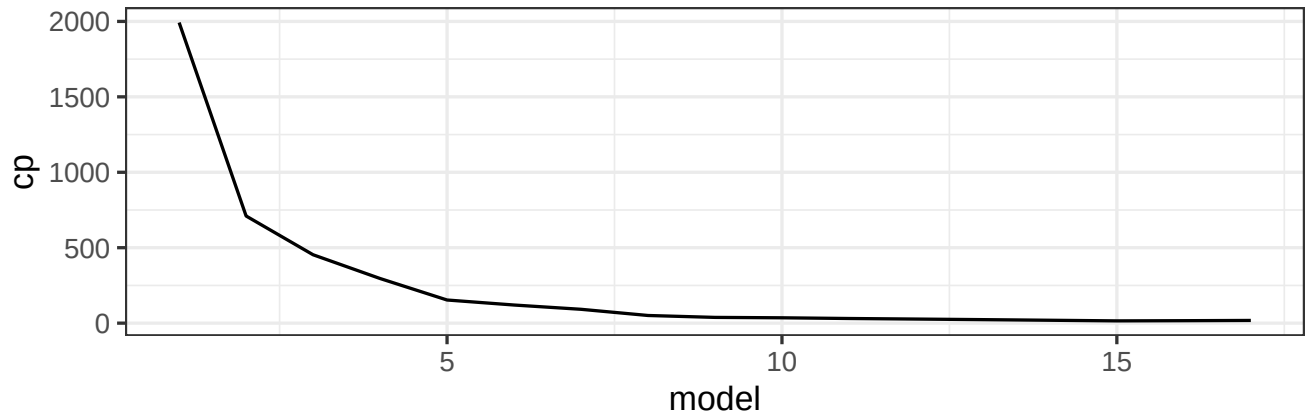



```
ggplot(d, aes(x = model, y = rss))+geom_line()+theme_bw()
```

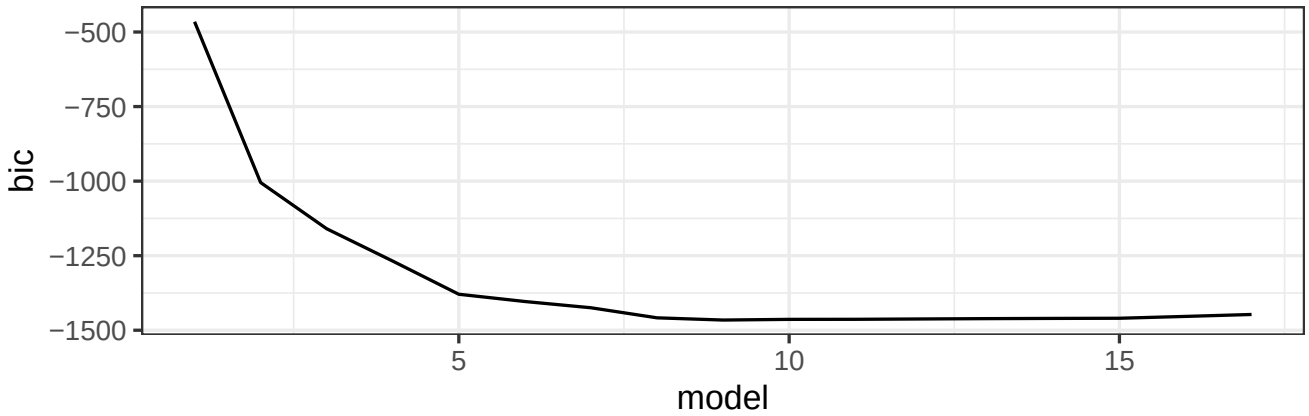


Plotting

```
ggplot(d, aes(x = model, y = cp))+geom_line()+theme_bw()
```




```
ggplot(d, aes(x = model, y = bic))+geom_line()+theme_bw()
```



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adjr2.max <- which.max(summary(best_subset)$adjr2)
rss.min <- which.min(summary(best_subset)$rss)
cp.min <- which.min(summary(best_subset)$cp)
bic.min <- which.min(summary(best_subset)$bic)
data.frame(adjr2.max, rss.min, cp.min, bic.min)
```

```
##   adjr2.max rss.min cp.min bic.min
## 1        15      17     15       9
```

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```

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- So what model is best?
  - Usually the simplest model.

Model Coefficients

- To show coefficients associated with the model with lowest `bic`, use `coef`:

```
coef(best_subset, bic.min)
```

```
##      (Intercept)        MolWeight         NumBonds     NumMultBonds
##      0.179049978     -0.007776351     -0.042507435     -0.368292209
##      NumRotBonds NumAromaticBonds      NumNitrogen        NumOxygen
##     -0.138979290      0.225474767      0.628386933      0.782490751
##      NumChlorine     SurfaceArea2
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- And to get a vector of variable names, use `names`:

```
names(coef(best_subset, bic.min))
```

```
##  [1] "(Intercept)"      "MolWeight"        "NumBonds"         "NumMultBonds"
##  [5] "NumRotBonds"      "NumAromaticBonds" "NumNitrogen"      "NumOxygen"
##  [9] "NumChlorine"      "SurfaceArea2"
```

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Forward/Backward Selection in R

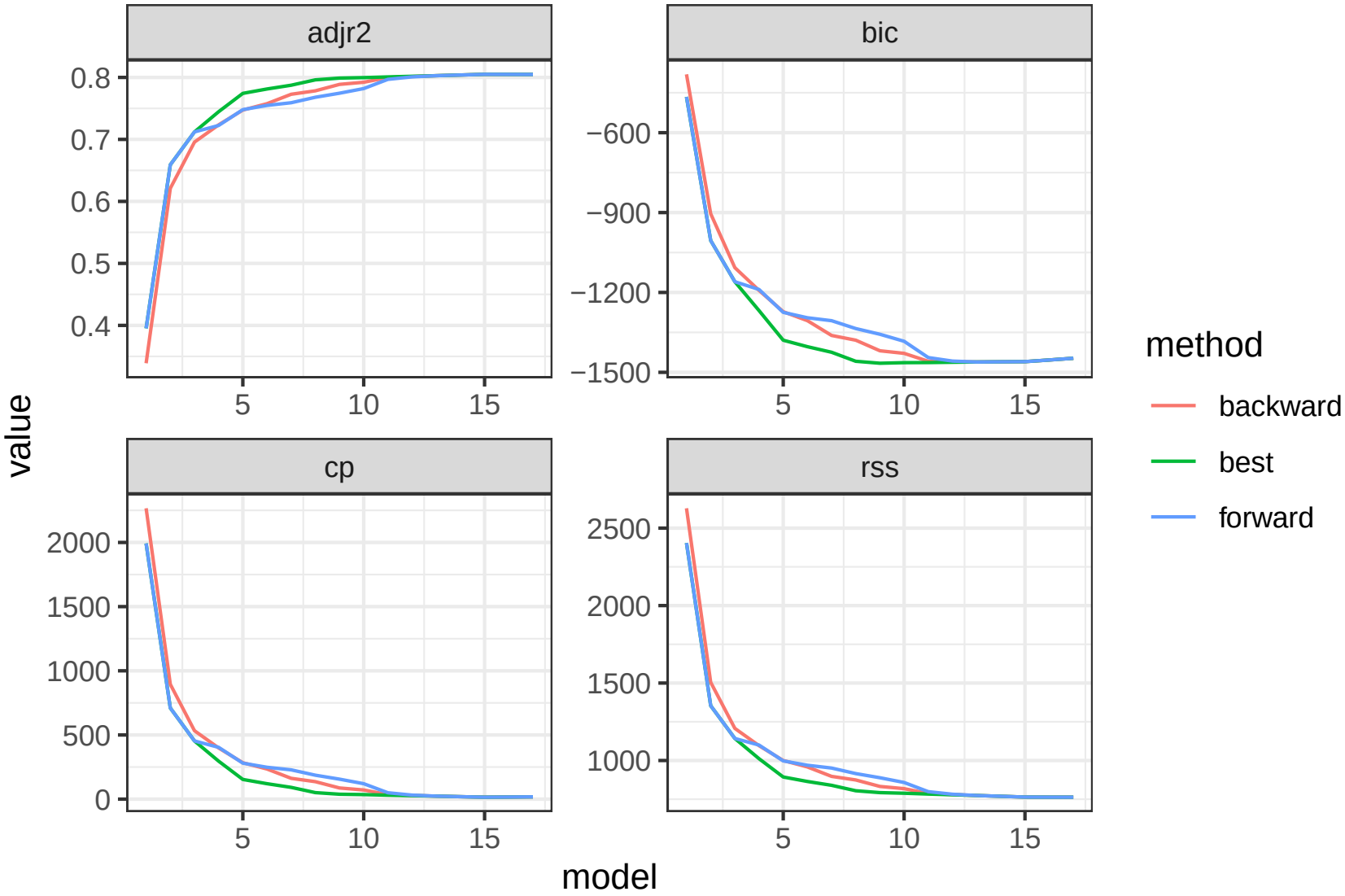
We again use the `regsubsets` function in the `leaps` library.

```
forward_select<-regsubsets(Solubility~.-NumNonHBonds -NumHydrogen -NumRings,
                           data = solTrain, nvmax = 17, method = "forward")

backward_elim<-regsubsets(Solubility~.-NumNonHBonds -NumHydrogen -NumRings,
                           data = solTrain, nvmax = 17, method = "backward")
```

- All of the same tools used for best subsets are available for forward and backward selection

Comparison of Models



Model Testing

- Let's go with 4 models, based on best subset (since we have it)
  - 5 variables (elbow of metric plots)
  - 9 variables (best bic)
  - 15 variables (best adjusted R^2)
  - 17 variables (the full model)
- We'll build each model on the training data, and then compute MSE on the test data.

```
## # A tibble: 4 x 2
##   model      mse
##   <chr>    <dbl>
## 1 model_15 0.928
## 2 model_9  0.966
## 3 model_5  1.13
## 4 model_17 4.31
```