Feature Selection and Engineering

Prof Wells

STA 295: Stat Learning

March 7th, 2024

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
- Discuss ways to create and modify predictors

Section 1

Explaratory Data Analysis

Molecular Solubility

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

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solTest <- cbind(solTestX, Solubility = solTestY)
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- We'll ignore these predictors for now.

```
library(dplyr)
solTest <- solTest %>% select(!starts_with("FP"))
solTrain <- solTrain %>% select(!starts_with("FP"))
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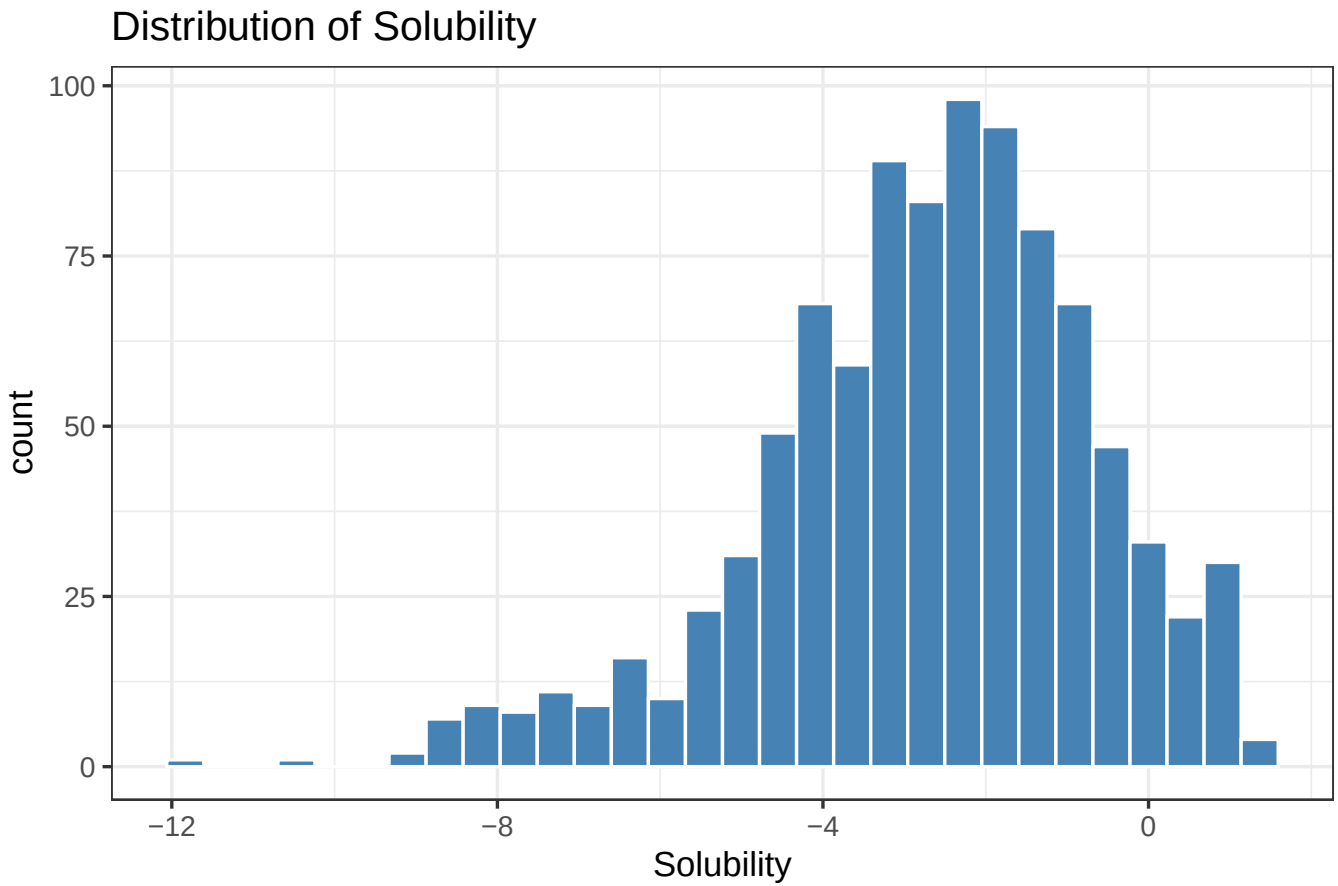
  - But we don't have any categorical variables in this data set
- We should also assess whether we have any missing values

Response Histogram

```
ggplot(solTrain, aes(x = Solubility))+
  geom_histogram(color = "white", fill = "steelblue")
```



Response Summary Statistics

```
solTrain %>% summarize(
  min = min(Solubility),
  Q1 = quantile(Solubility, 0.25),
  median = median(Solubility),
  Q3 = quantile(Solubility, 0.75),
  max = max(Solubility),
  mean = mean(Solubility),
  sd = sd(Solubility))
```

```
##      min     Q1 median    Q3  max     mean       sd
## 1 -11.62 -3.955  -2.51 -1.36 1.58 -2.71857 2.046641
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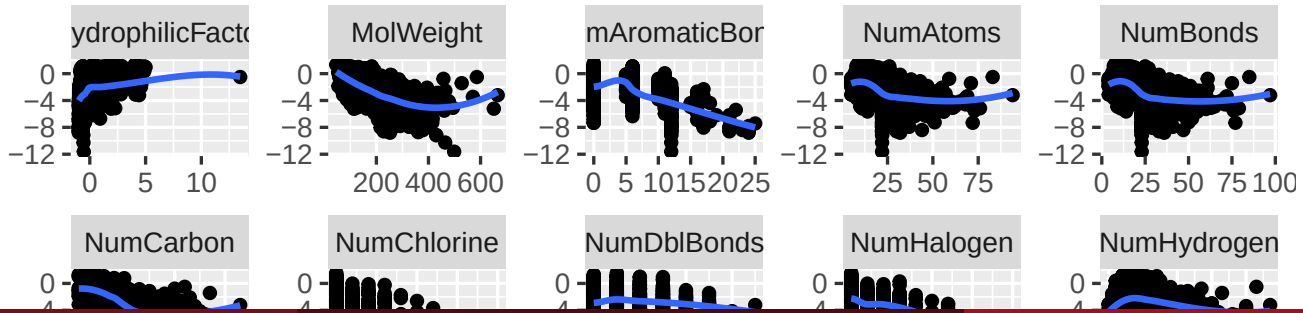
- But with many predictors, that's lots of redundant coding.
  - Instead, we can make use of the `pivot_longer` function from `tidyr`:

```
solTrain %>% pivot_longer(-Solubility, names_to = "variables",
                          values_to = "value") %>%
  ggplot(aes(x = value, y = Solubility ))+
    geom_point()+
  geom_smooth(se = F)+
  facet_wrap(~variables, scales = "free")
```



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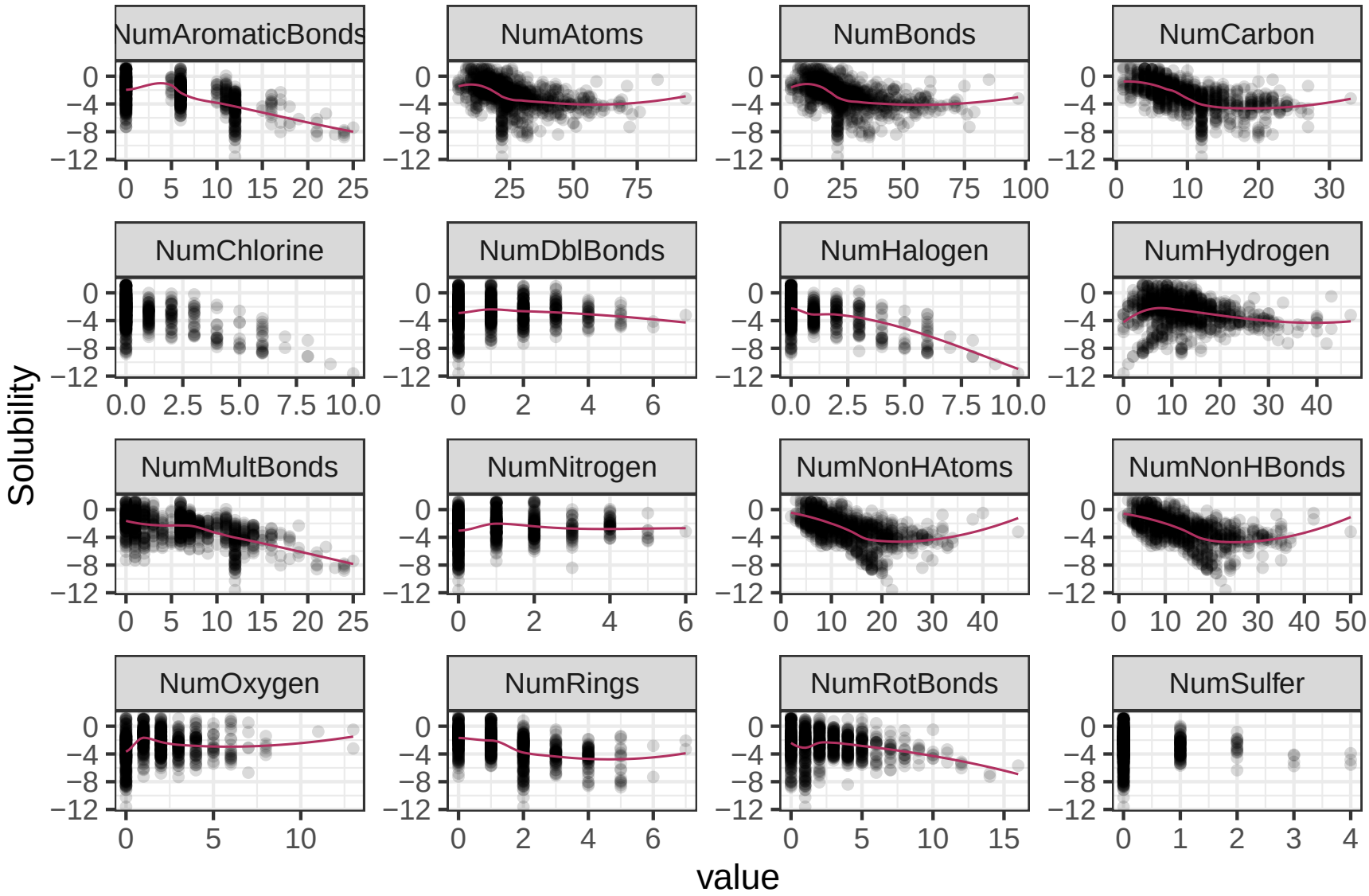

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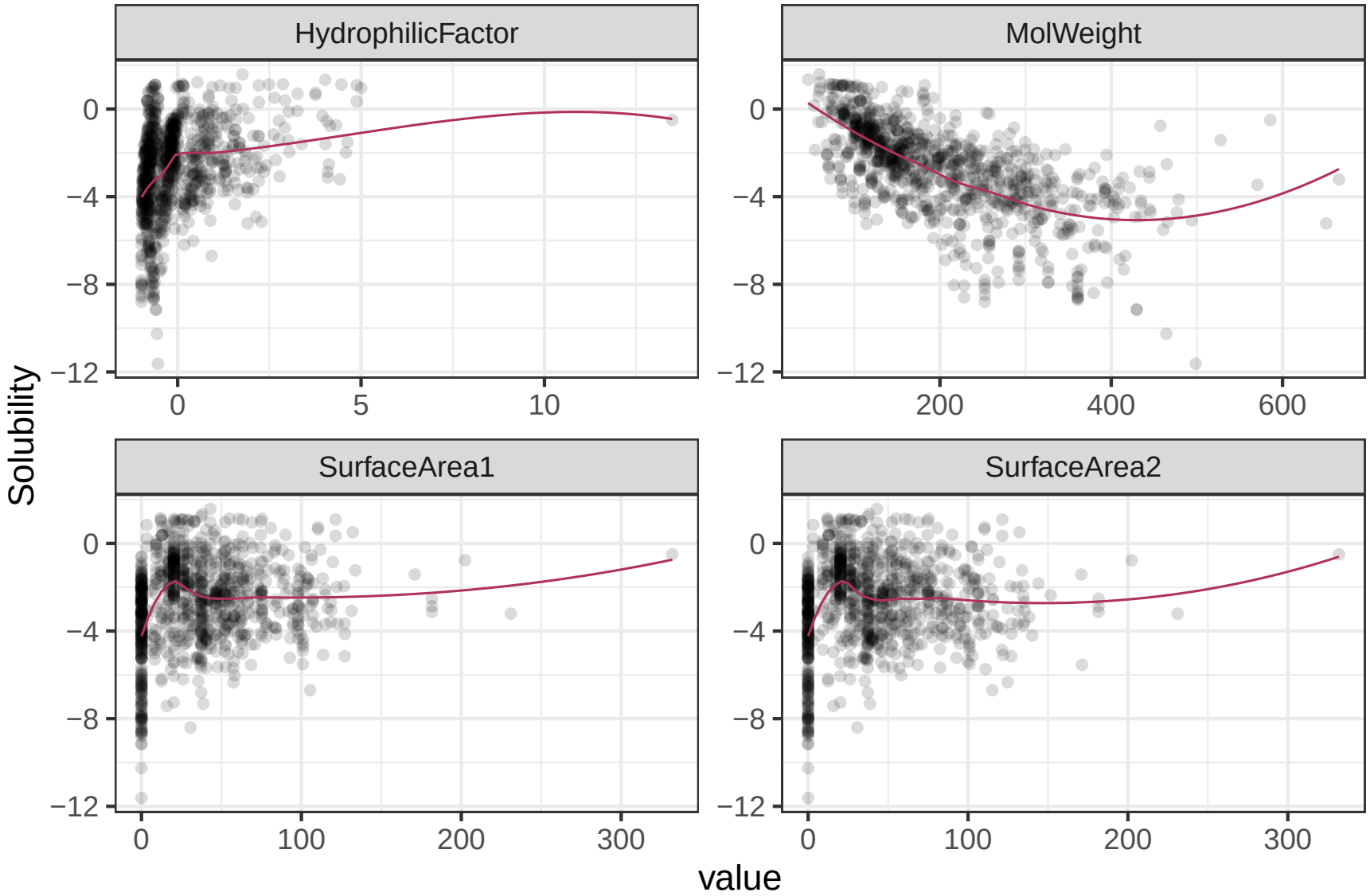

Correlation with Response

```
cor_values <- cor(solTrain[,-21], solTrain$Solubility)
# obtains correlations between each variable and the response
# stores results as a 1 x 20 matrix

cor_names <- rownames(cor_values)
# extracts names for each variable

cor_df <- data.frame(correlation = as.numeric(cor_values), variable =  cor_names)
# creates data frame with correlations and variable names
# as.numeric coerces the cor_values matrix into a vector
```

Correlation with Response

```
cor_df
```

```
##     correlation          variable
## 1  -0.629163885         MolWeight
## 2  -0.398943188          NumAtoms
## 3  -0.544646707      NumNonHAtoms
## 4  -0.420459121          NumBonds
## 5  -0.551457131      NumNonHBonds
## 6  -0.525248387      NumMultBonds
## 7  -0.149343282       NumRotBonds
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## 14 -0.091418407         NumSulfer
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cor_df %>% arrange(desc(abs(correlation)))
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- We can use the ggcorr function from the GGally package to quickly create a visual correlation matrix:

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

# hjust changes the position of the names
# size changes the size of names
# layout.exp expands the horizontal axis to prevent text clipping
# other options are possible (use ?ggcorr)
```

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full_mod <- lm(Solubility ~ ., data = solTrain)
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Model Summary

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## Call:
## lm(formula = Solubility ~ ., data = solTrain)
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## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.8499 -0.5963  0.0232  0.5842  2.7848
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## Coefficients: (3 not defined because of singularities)
##                   Estimate Std. Error t value Pr(>|t|)
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## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9044 on 933 degrees of freedom
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## F-statistic: 231.3 on 17 and 933 DF,  p-value: < 2.2e-16
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- As a result, R dropped the linearly related variables.

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NAs in the table mean we have a perfect linear relationship among some of the predictors

- As a result, R dropped the linearly related variables.
- For better clarity, we should refit the model without them

Model Summary

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## Call:
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## Residuals:
##     Min      1Q  Median      3Q     Max
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- None of the estimates or p-values changed after refitting the model

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- None of the estimates or p-values changed after refitting the model
- However, extraneous rows were removed (and the table now fits on the slide. Yay!)

Model Diagnostics

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library(gglm)
gglm(full_mod)
```

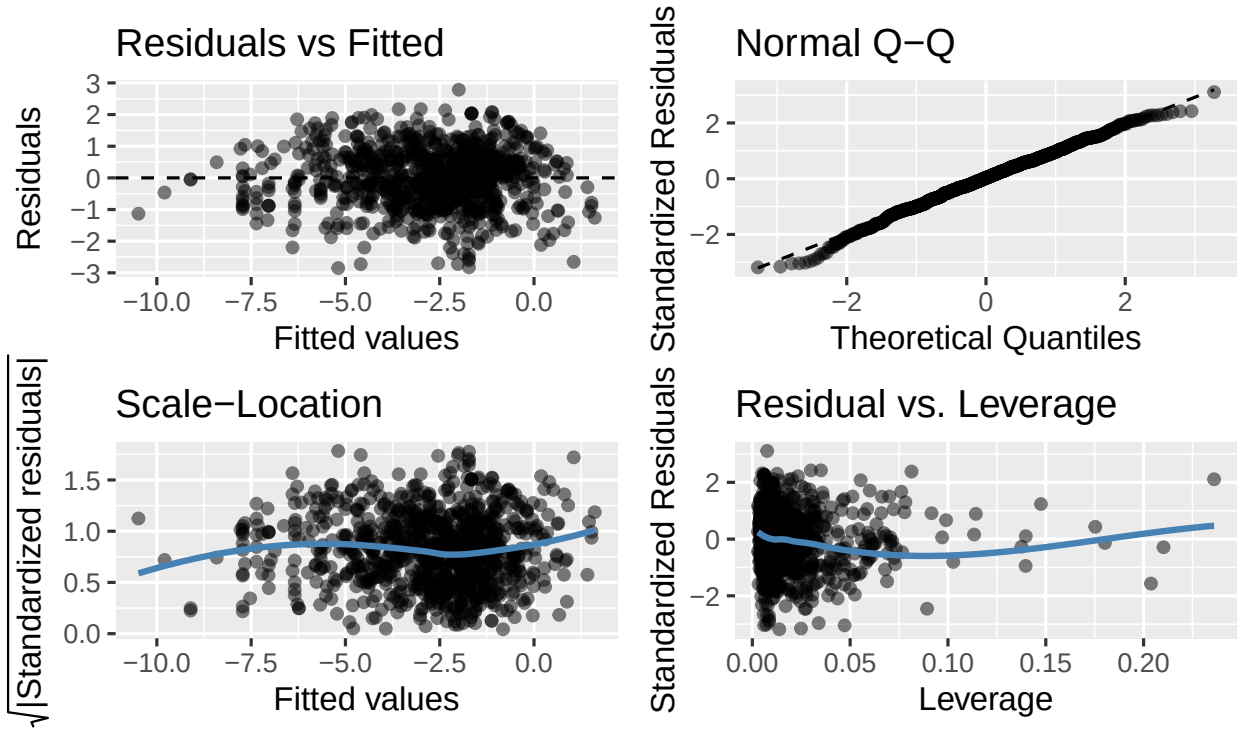

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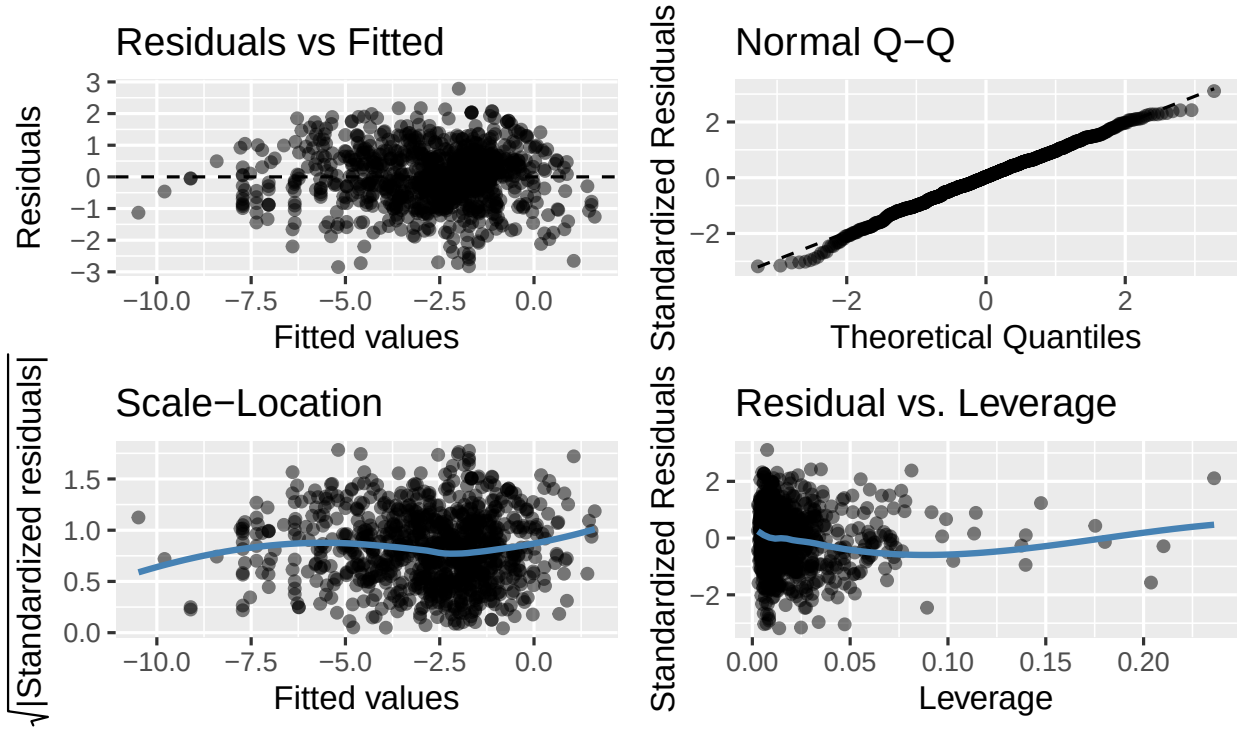

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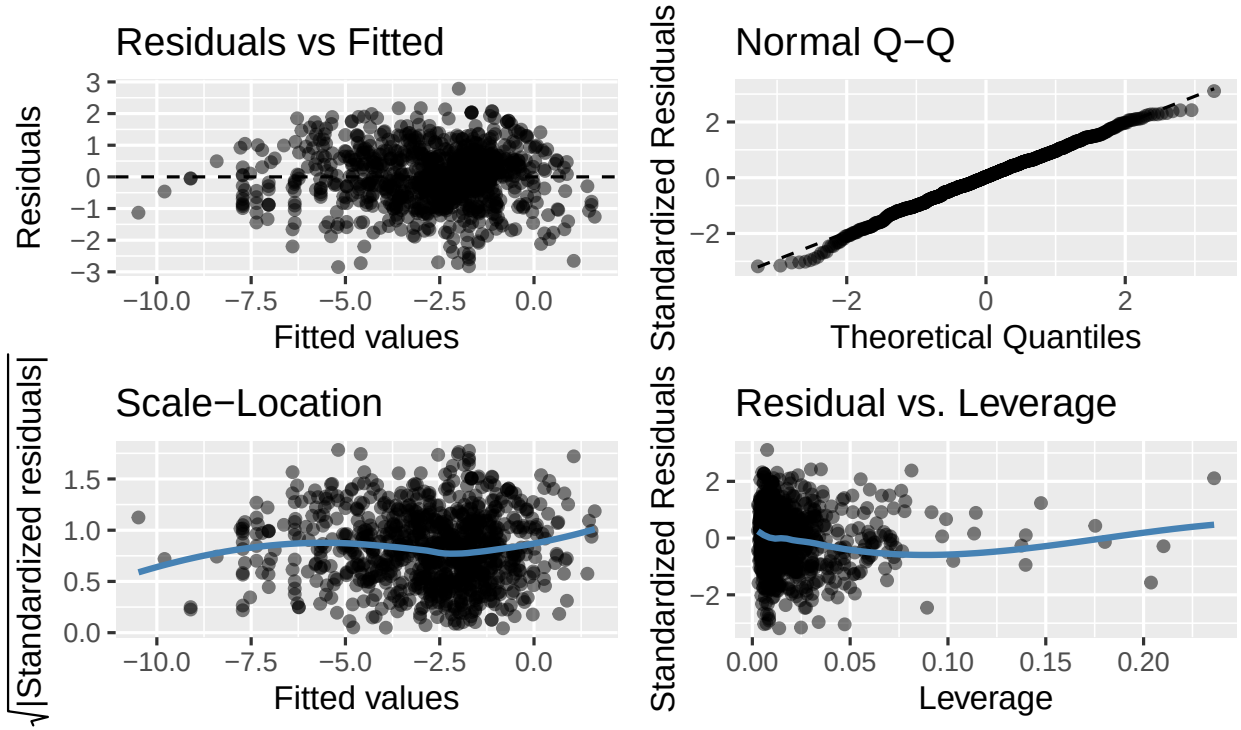

- Diagnostic plots reveal no concerns about model assumptions.
- But we likely still have multicollinearity, and some variables might not be that helpful

Section 2

Subset Selection

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- **Validation set**: Subject to variability in test/training split; but can be alright for large data sets, or initial exploration
- **Training set assessment**: using RSS alone on training will lead to overfitting and biased estimate of test MSE;
  - Instead, can apply penalty to RSS based on number of predictors in the model, in order to better estimate test MSE
  - However, can use if validation set is not available, or if large number of models need to be considered.

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Criteria Formulas:

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  - Hence, for *fixed* number of variables, we can choose the model that has the **smallest** RSS.

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- The best model for each fixed number of predictors is determined by *RSS*
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Best Subset in R

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

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- The `regsubsets` function returns *RSS*, $\text{adj}R^2$, C_p, *BIC* for the best model of each number of predicts.
- The **overall** best model can be selected using any of these criteria.

Using regsubsets

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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.

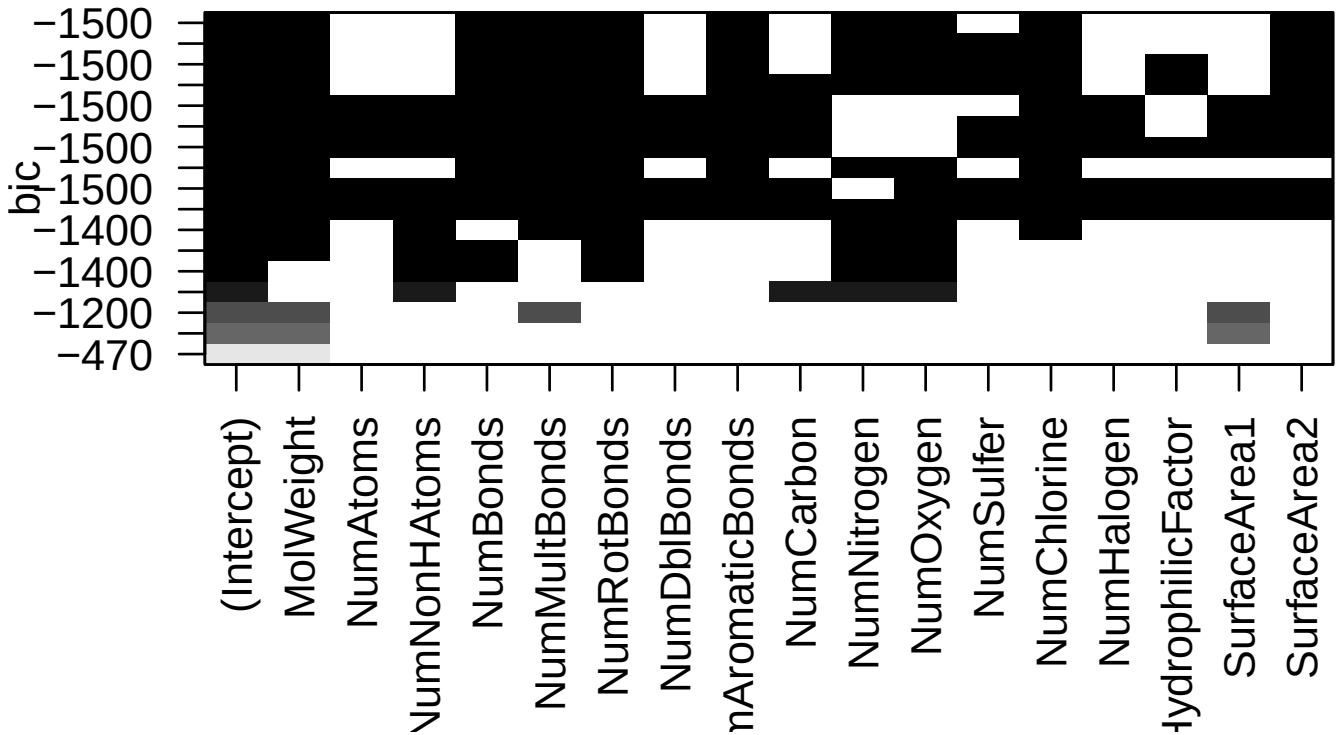
```
d <- data.frame(model = 1:17,
  adjr2 = summary(best_subset)$adjr2,
  rss = summary(best_subset)$rss,
  cp = summary(best_subset)$cp,
  bic = summary(best_subset)$bic)
d %>% head()
```

```
##   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 = "bic")
```



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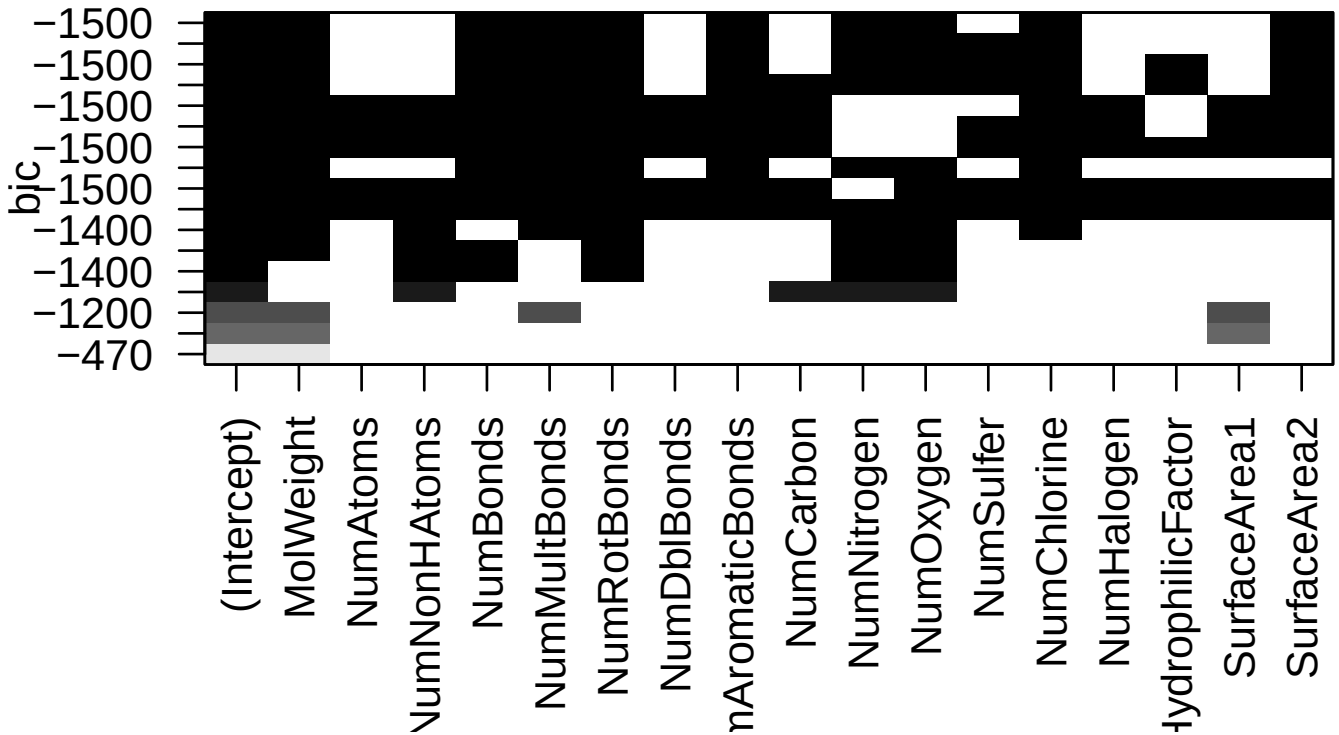
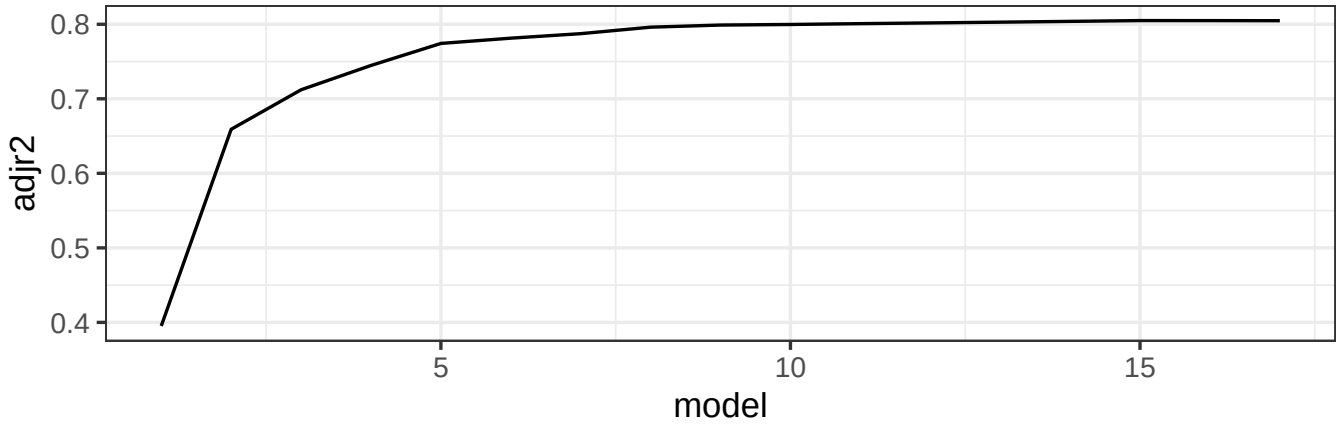


- Models are ordered by values of BIC criteria. Dark rectangles indicate variable is present in the best model for that criteria's value.

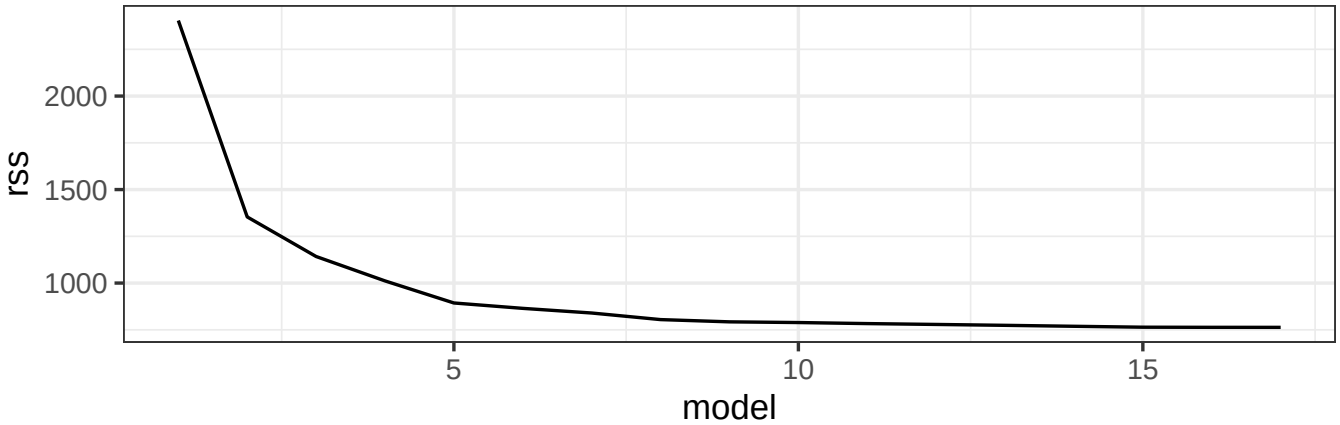
Plotting

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()
```

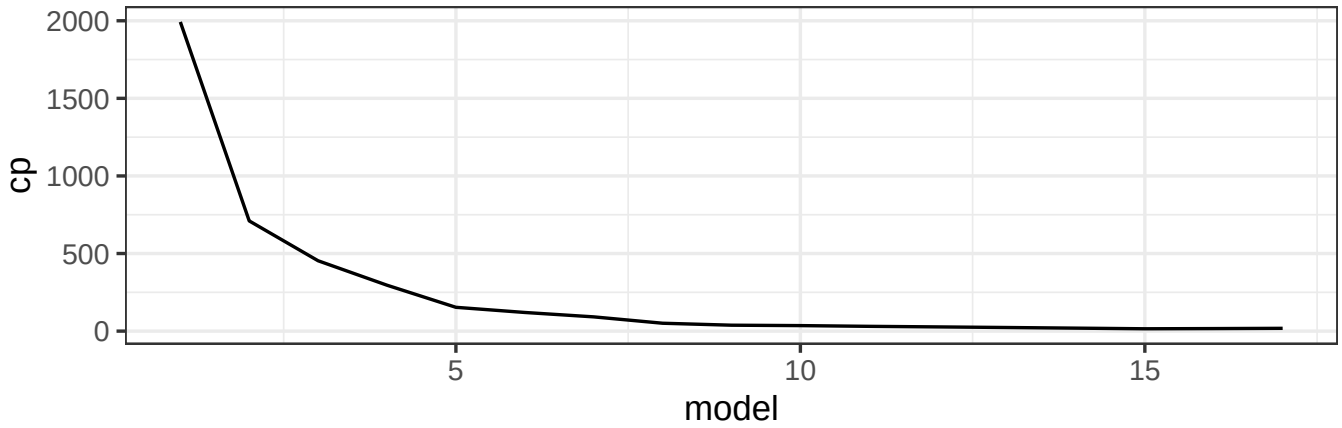



```
ggplot(d, aes(x = model, y = rss))+geom_line()+theme_bw()
```

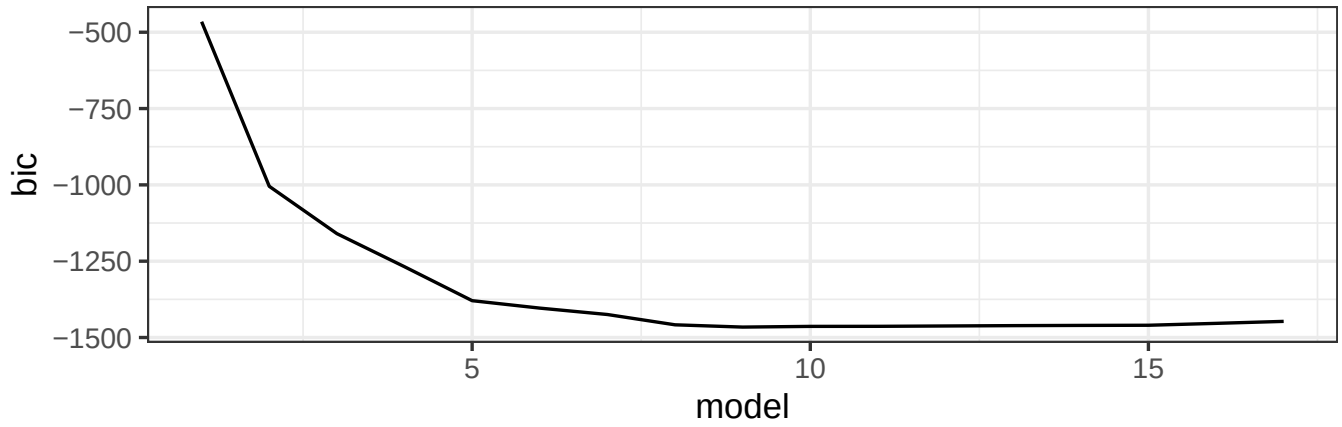


Plotting

```
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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- So what model is best?

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```

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

- 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
##     -0.386474357     -0.008279467
```

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##      NumChlorine     SurfaceArea2
##     -0.386474357     -0.008279467
```

- 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"
```

Model Testing

- Let's go with 4 models, based on best subset (since we have it)
  - 5 variables (elbow of bic plot)
  - 9 variables (best bic)
  - 15 variables (best adjusted R^2 and C_p)
  - 17 variables (the full model)
- We'll use 10-fold cross-validation to compare:

```
##      mod5      mod9     mod15     mod17
## 0.9685227 0.9121188 0.8955325 0.8950262
```

- It appears the full-model performed best!

Code for Cross-Validation (Reference)

```
mod5 <-lm(Solubility ~ NumNonHAtoms + NumBonds + NumRotBonds+
            NumNitrogen + NumOxygen,
          data = solTrain)

mod9 <-lm(Solubility ~ MolWeight + NumBonds + NumMultBonds+
            NumRotBonds + NumAromaticBonds + NumNitrogen +
            NumOxygen + NumChlorine + SurfaceArea2,
          data = solTrain)

mod15 <-lm(Solubility ~.
           -NumNonHBonds -NumHydrogen -NumRings - NumNitrogen - NumOxygen,
           data = solTrain)

mod17 <-lm(Solubility~.
           -NumNonHBonds -NumHydrogen -NumRings  ,
           data = solTrain)
```

Code for Cross-Validation (Reference)

```
set.seed(100)
library(rsample)

my_cv <- vfold_cv(solTrain, v = 5, repeats = 10)

get_rmse <- function(split, model){
  train <- analysis(split)
  test <- assessment(split)
  preds <- predict(model, newdata = test)
  obs <- test$Solubility
  rmse <- sqrt(mean((obs-preds)^2))
  rmse
}
```

Code for Cross-Validation (Reference)

```
library(purrr)
my_rmse_df <- data.frame(
  mod5 = map_dbl(my_cv$splits, get_rmse, model = mod5),
  mod9 = map_dbl(my_cv$splits, get_rmse, model = mod9),
  mod15 = map_dbl(my_cv$splits, get_rmse, model = mod15),
  mod17 = map_dbl(my_cv$splits, get_rmse, model = mod17)
)

map_dbl(my_rmse_df, mean)
```

Section 3

Other Selection Algorithms

Forward Selection

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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