#### Notes 8: Model Selection

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#### **Outline of Notes**

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  - Wine Example
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- 2) P-Value Model Selection:
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  - Forward Selection
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- 3) Intelligent Model Selection:
  - Adjusted R<sup>2</sup>
  - Information Criteria
  - Prediction Based

- 4) State Data Example:
  - Data Description
  - P-Value Selection
  - Intelligent Selection

#### The Problem: Which Variables??

The problem of model selection asks the question: which variables should be included in a multiple regression model?

We do not want to include too many predictors.

- Problem of over-fitting data
- Solution may not cross-validate

We do not want to include too few predictors.

- Miss important relationships in data
- Misinterpret relationships in data

#### All Possible Models

We need to consider ALL possible models that could be formed.

If we have p predictors, then (according to binomial theorem) there are

$$\sum_{j=1}^{p} \binom{p}{j} = 2^{p}$$

possible models we could choose.

# Wine Example: Overview

Using Wine Quality data set from UCI Machine Learning: http://archive.ics.uci.edu/ml/datasets/Wine+Quality

#### Predict wine quality from 11 possible physicochemical predictors:

- quality (range 0-10)
- fixed acidity (g/dm<sup>3</sup>)
- volatile acidity (g/dm³)
- citric acid  $(g/dm^3)$
- residual sugar (g/dm³)
- chlorides  $(g/dm^3)$

- free sulfur dioxide (mg/dm<sup>3</sup>)
- total sulfur dioxide (mg/dm<sup>2</sup>)
- density (g/cm<sup>3</sup>)
- pH
- sulphates (g/dm<sup>3</sup>)
- alcohol (% ABV)

# Wine Example: Look at Data

```
> wines=read.table("/Users/Nate/Desktop/winequality-red.csv",
                 sep="; ", header=TRUE)
> wines[1:3,]
 fixed.acidity volatile.acidity citric.acid residual.sugar
                                                 1.9
          7.4
                         0.88
          7.8
                        0.76 0.04
 chlorides free.sulfur.dioxide total.sulfur.dioxide density
                                            54 0.9970
   pH sulphates alcohol quality
1 3.51 0.56 9.4
2 3.20 0.68 9.8
3 3.26 0.65 9.8
```

# Wine Example: Predicting Red Wine Quality

```
> wmod=lm(quality~.,data=wines)
> summary(wmod)
                                   Max
                   Estimate Std. Error t value Pr(>|t|)
volatile.acidity -1.084e+00 1.211e-01 -8.948 < 2e-16 ***
citric.acid -1.826e-01 1.472e-01 -1.240 0.2150
residual.sugar 1.633e-02 1.500e-02 1.089 0.2765
chlorides -1.874e+00 4.193e-01 -4.470 8.37e-06 ***
free.sulfur.dioxide 4.361e-03 2.171e-03 2.009 0.0447 *
               -4.137e-01 1.916e-01 -2.159 0.0310 *
```

# Wine Example: Problems with Model

Model on previous slide is very complicated, so interpretation of the coefficients is problematic.

• Remember conditional interpretation of  $b_i$  parameters

Model on previous slide has included many effects which may not be needed to predict wine quality.

Model is not likely to cross-validate well.

How do we select which of the physicochemical predictors are needed to predict wine quality??

### The Solution: Model Selection Strategies

We can use different statistical model selection strategies to choose which predictors to include.

There are a variety of strategies we can use:

- P-value based methods (NOT good)
- Adjusted R<sup>2</sup> (better)
- Information criteria (best)
- Prediction/cross-validation (best)

#### Overview of P-Value Model Selection

P-value model selection strategies choose which terms to include based on the significance of the terms (i.e., p-values of *F* tests).

There are three popular p-value based selection strategies:

- Backwards elimination
- Forward selection
- Stepwise selection

There is no guarantee that these selection strategies will produce a reasonable (or the same) model!

# **Backwards Elimination Algorithm**

Given a threshold  $\alpha^*$ , backwards elimination algorithm is:

- Begin with all possible predictors in model
- 2 Remove predictor with largest p-value above  $\alpha^*$
- **3** Refit and repeat step 2 until all p-values below  $\alpha^*$

Note that  $\alpha^*$  doesn't have to be the magical 0.05; typically set  $\alpha^*$  larger (e.g., 0.10 or 0.15) if ultimately interested in prediction.

Do not want to miss important predictors

#### Backwards Elimination: R Function

#### We can write our own R function to perform backwards elimination:

```
bslm<-function(y, X, alpha=0.1, maxstep=NA, printdrop=TRUE, stepc=0L) {
 mymod=lm(y\sim ., data=X)
  if (is.na(maxstep)) {maxstep=length(xnames)+stepc}
  notsig=TRUE; nstep=0L+stepc
  while (notsig && nstep<maxstep) {
   nstep=nstep+1L
   mydrop=drop1 (mymod, test="F")
   pvals=mvdrop[,6]; mxidx=which.max(pvals)
    if (pvals[mxidx]>alpha) {
     dropname=rownames (mydrop) [mxidx]
     myform=as.formula(paste(".~.-", dropname))
     mymod=update(mymod, myform)
     if(printdrop) {print(paste("Step", nstep, ":", "Dropping", dropname))}
    } else{notsig=FALSE}
 mvmod
```

# Backwards Elimination: Wine Example

```
> bswmod=bslm(wines$quality,wines[,-12])
[1] "Step 2 : Dropping fixed.acidity"
[1] "Step 3 : Dropping residual.sugar"
[1] "Step 4 : Dropping citric.acid"
> summary(bswmod)
                    # I deleted some output
                      Estimate Std. Error t value Pr(>|t|)
                    -2.0178138 0.3975417 -5.076 4.31e-07 ***
                    -0.4826614 0.1175581 -4.106 4.23e-05 ***
                               0.1099084 8.031 1.86e-15 ***
Multiple R-squared: 0.3595, Adjusted R-squared: 0.3567
```

#### Note that we dropped

- density
- ② fixed.acidity
- 3 residual.sugar
- 4 citric.acid

# Forward Selection Algorithm

Given a threshold  $\alpha^*$ , forward selection algorithm is:

- Begin with no predictors in model
- 2 Add predictor with smallest p-value below  $\alpha^*$
- **3** Refit and repeat step 2 until no new p-values below  $\alpha^*$

Note that  $\alpha^*$  doesn't have to be the magical 0.05; typically set  $\alpha^*$  larger (e.g., 0.10 or 0.15) if ultimately interested in prediction.

Do not want to miss important predictors

### Forward Selection in R

### We can write our own R function to perform forward selection:

```
fslm<-function(y, X, alpha=0.1, maxstep=NA, printadd=TRUE, stepc=0L, inidx=NULL) {
 X=data.frame(X):
                      xnames=names(X)
 if(is.null(inidx)){
    mymod=lm(y~1); anames=NULL
  } else {
    anames=xnames[inidx]; xnames=xnames[-inidx]
    myform=as.formula(paste("y",paste(anames,collapse="+"),sep="~"))
    mvmod=lm(mvform,data=X)
  if (is.na(maxstep)) {maxstep=length(xnames)+stepc}
 notsig=TRUE: nstep=0L+stepc
 while (notsig && nstep<maxstep) {
    nstep=nstep+1L
    myform=as.formula(paste("~",paste(c(anames,xnames),collapse="+")))
    mvadd=add1 (mvmod, scope=mvform, x=model.matrix (mvform, data=X), test="F")
    pvals=myadd[,6]; mnidx=which.min(pvals)
    if(pvals[mnidx]<alpha){
      anames=c(anames,rownames(mvadd)[mnidx])
      addname=rownames(myadd)[mnidx]
      myform=as.formula(paste(".~.+",addname))
      mvmod=update(mvmod,mvform,data=X)
      if (printadd) {print(paste("Step", nstep, ":", "Adding", addname))}
      xnames=xnames[-(mnidx-1L)]
    } else{notsig=FALSE}
 mymod
```

# Forward Selection: Wine Example

```
> fswmod=fslm(wines$quality, wines[,-12])
[1] "Step 1 : Adding alcohol"
[1] "Step 2 : Adding volatile.acidity"
[1] "Step 3 : Adding sulphates"
[1] "Step 4 : Adding total.sulfur.dioxide"
[1] "Step 5 : Adding chlorides"
[1] "Step 5 : Adding pH"
[1] "Step 7 : Adding free.sulfur.dioxide"
> summary(fswmod) # I deleted some output
```

```
Estimate Std. Error t value Pr(>|t|) (Intercept) 4.4300987 0.4029168 10.995 < 2e-16 *** alcohol 0.2893028 0.0167958 17.225 < 2e-16 *** volatile.acidity -1.0127527 0.1008429 -10.043 < 2e-16 *** sulphates 0.8826651 0.1099084 8.031 1.86e-15 *** total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 *** chlorides -2.0178138 0.3975417 -5.076 4.31e-07 *** pH -0.4826614 0.1175581 -4.106 4.23e-05 *** free.sulfur.dioxide 0.0050774 0.0021255 2.389 0.017 *-- Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1 Residual standard error: 0.6477 on 1591 degrees of freedom Multiple R-squared: 0.3556 Adjusted R-squared: 0.3567
```

#### Note we did NOT add

- fixed.acidity
- citric.acid
- residual.sugar
- density

# Stepwise Selection Algorithm

Given thresholds  $\alpha_F^*$  and  $\alpha_B^*$ , stepwise selection algorithm is:

- Begin with no predictors in model
- 2 Forward step: add predictor with smallest p-value below  $\alpha_F^*$
- Backward step: remove predictor with largest p-value above  $\alpha_B^*$
- Repeat steps 2–3 until convergence (or max steps reached)

Note that  $\alpha_F^*$  and  $\alpha_B^*$  do not have to be the magical 0.05; typically set  $\alpha^*$  larger (e.g., 0.10 or 0.15) if ultimately interested in prediction.

•  $\alpha_F^*$  and  $\alpha_B^*$  do not have to be equal

# Stepwise Selection in R

#### We can write our own R function to perform stepwise selection:

```
swlm<-function(y, X, alpha=c(0.1, 0.1), maxstep=20, printad=TRUE) {
 X=data.frame(X);
                      xnames=names(X)
 notsig=TRUE; nstep=0L; inidx=oldidx=NULL
 while (notsig && nstep<maxstep) {
   nstep=nstep+1L
    # forward step
   mymod=fslm(y, X, alpha[1], nstep, printad, (nstep-1L), inidx)
    innames=attr(mymod$terms,"term.labels")
    inidx=match(innames,xnames)
    # backwards step
   if (nstep>1L) {
     Xin=data.frame(X[,inidx]); names(Xin)=innames
     mymod=bslm(y, Xin, alpha[2], nstep, printad, (nstep-1L))
      innames=attr(mymod$terms, "term.labels")
      inidx=match(innames, xnames)
    # check convergence
    if(length(inidx) == length(oldidx) && any(inidx! = oldidx) == FALSE) {notsig=FALSE}
    oldidx=inidx
 mymod
```

# Stepwise Selection: Wine Example

```
> stmmod=swlm(wines$quality, wines[,-12])
[1] "Step 1 : Adding alcohol"
[1] "Step 2 : Adding volatile.acidity"
[1] "Step 3 : Adding sulphates"
[1] "Step 4 : Adding total.sulfur.dioxide"
[1] "Step 5 : Adding chlorides"
[1] "Step 5 : Adding pH"
[1] "Step 7 : Adding free.sulfur.dioxide"
> summary(stwmod) # I deleted some output
```

#### Note we did not include

- fixed.acidity
- citric.acid
- residual.sugar
- density

```
Estimate Std. Error t value Pr(>|t|) (Intercept) 4.4300987 0.4029168 10.995 < 2e-16 *** alcohol 0.2893028 0.0167958 17.225 < 2e-16 *** volatile.acidity -1.0127527 0.1008429 -10.043 < 2e-16 *** sulphates 0.8826651 0.1099084 8.031 1.86e-15 *** total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 *** chlorides -2.0178138 0.3975417 -5.076 4.31e-07 *** pH -0.4826614 0.1175581 -4.106 4.23e-05 *** free.sulfur.dioxide 0.0050774 0.0021255 2.389 0.017 * --- Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 `' 1 Residual standard error: 0.6477 on 1591 degrees of freedom Multiple R-squared: 0.3595, Adjusted R-squared: 0.3567
```

# Selection Summary: Wine Example

Bad example where all three methods choose same model.

- Note that selected model is NOT easily interpretable
- Note that selected model is NOT theoretically motivated

Although we have "systematically selected" this model, there is no guarantee that this is a good (i.e., valid and useful) model.

It would be best to use some theory to guide model building.

# Selection Summary: Toy Example

```
> set.seed(1120)
> x1=rnorm(100)
> x2 = rnorm(100)
> x3 = (x1+x2)/2 + rnorm(100, sd=.1)
> X=as.data.frame(cbind(x1,x2,x3))
> y=x1+x2+rnorm(100)
> bstest=bslm(y,X) # picks correct model
[1] "Step 1 : Dropping x3"
> fstest=fslm(y,X)
                  # picks wrong model
[1] "Step 1 : Adding x3"
> swtest=swlm(y,X) # picks wrong model
[1] "Step 1 : Adding x3"
```

### Coefficient of Multiple Determination (revisited)

Consider the MLR model  $y_i = b_0 + \sum_{j=1}^p b_j x_{ij} + e_i$  with  $e_i \stackrel{\text{iid}}{\sim} N(0, \sigma^2)$ .

Remember: the coefficient of multiple determination is defined as

$$R^{2} = \frac{SSR}{SST}$$
$$= 1 - \frac{SSE}{SST}$$

and gives the amount of variation in  $y_i$  that is explained by the linear relationships with  $x_{i1}, \ldots, x_{ip}$ .

# Adjusted $R^2$ (revisited)

Including more predictors in a MLR model can artificially inflate  $R^2$ :

- Capitalizing on spurious effects present in noisy data
- Phenomenon of over-fitting the data

The adjusted  $R^2$  is a relative measure of fit:

$$\begin{aligned} R_{\rm a}^2 &= 1 - \frac{SSE/df_E}{SST/df_T} \\ &= 1 - \frac{\hat{\sigma}^2}{s_V^2} \end{aligned}$$

where  $s_Y^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1}$  is the sample estimate of the variance of Y.

# Adjusted R<sup>2</sup> for Model Selection

If p is not too large, could calculate  $R_a^2$  for all  $2^p$  possible models.

• Pick model with largest  $R_a^2$ .

Implemented in leaps function (leaps package).

- Branch-and-bound search through all possible subsets
- Use method="adjr2" option to select via adjusted R2

# Adjusted R<sup>2</sup> Selection: Wine Example

```
> X=wines[,-12]
> arsqmod=leaps(x=X,y=wines$quality,method="adjr2")
> widx=which.max(arsqmod$adjr2)
  xidx=(1:ncol(X))[arsqmod$which[widx,]]
> Xin=data.frame(X[,xidx])
 arsqmod=lm(wines$quality~.,data=Xin)
```

# Adjusted R<sup>2</sup> Selection: Wine Example (continued)

```
> summarv(arsqmod)  # I deleted some output
                     Estimate Std. Error t value Pr(>|t|)
                   4.6680876 0.4608410 10.129 < 2e-16 ***
volatile.acidity -1.0736123 0.1159362 -9.260 < 2e-16 ***
citric.acid -0.1295444 0.1217717 -1.064 0.2876
                -1.9494185 0.4026906 -4.841 1.42e-06 ***
free.sulfur.dioxide 0.0047601 0.0021463 2.218 0.0267 *
total.sulfur.dioxide -0.0033658 0.0006954 -4.840 1.42e-06 ***
                   -0.5491501 0.1331350 -4.125 3.90e-05 ***
                  0.8914283 0.1102122 8.088 1.19e-15 ***
alcohol
                    0.2928780 0.0171280 17.099 < 2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 0.6477 on 1590 degrees of freedom
Multiple R-squared: 0.3599, Adjusted R-squared: 0.3567
F-statistic: 111.8 on 8 and 1590 DF, p-value: < 2.2e-16
> summary(stwmod)$adi
> summary(arsqmod)$adj
```

# Likelihood Function (revisited)

Remember that  $(\mathbf{y}|\mathbf{X}) \sim N(\mathbf{Xb}, \sigma^2 \mathbf{I}_n)$ , which implies that  $\mathbf{y}$  has pdf

$$f(\mathbf{y}|\mathbf{X}, \mathbf{b}, \sigma^2) = (2\pi)^{-n/2} (\sigma^2)^{-n/2} e^{-\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\mathbf{b})'(\mathbf{y} - \mathbf{X}\mathbf{b})}$$

As a result, the log-likelihood of  $(\mathbf{b}, \sigma^2)$  given  $(\mathbf{y}, \mathbf{X})$  is

$$\ln\{L(\mathbf{b},\sigma^2|\mathbf{y},\mathbf{X})\} = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln(\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\mathbf{b})'(\mathbf{y}-\mathbf{X}\mathbf{b})$$

#### Maximized Likelihood Functions

Remember that the MLEs of **b** and  $\sigma^2$  are

$$\hat{\mathbf{b}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$
 $\tilde{\sigma}^2 = SSE/n$ 

where  $SSE = (\mathbf{y} - \mathbf{X}\hat{\mathbf{b}})'(\mathbf{y} - \mathbf{X}\hat{\mathbf{b}})$  is the sum-of-squared errors.

As a result, the *maximized* log-likelihood of  $(\mathbf{b}, \sigma^2)$  given  $(\mathbf{y}, \mathbf{X})$  is

$$\begin{split} \ln\{L(\hat{\mathbf{b}}, \tilde{\sigma}^2|\mathbf{y}, \mathbf{X})\} &= -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln(\tilde{\sigma}^2) - \frac{1}{2\tilde{\sigma}^2}(\mathbf{y} - \mathbf{X}\hat{\mathbf{b}})'(\mathbf{y} - \mathbf{X}\hat{\mathbf{b}}) \\ &= -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln(\tilde{\sigma}^2) - \frac{n}{2} \end{split}$$

#### Likelihoods and Information Criteria

Information criteria define model fit using maximized likelihoods that are penalized according to model complexity.

Defining  $\hat{\mathcal{L}} = \ln\{L(\hat{\mathbf{b}}, \tilde{\sigma}^2 | \mathbf{y}, \mathbf{X})\}$ , Akaike's (1974) AIC is defined as

$$AIC = -2\hat{\mathcal{L}} + 2q$$

where q is number of parameters; note that AIC stands for an information criterion, but people typically refer to it as Akaike's.

The Bayesian Information Criterion (BIC; Schwarz, 1978) is

$$BIC = -2\hat{\mathcal{L}} + \ln(n)q$$

# Information Criteria in Regression

Using the definition  $\hat{\mathcal{L}} = -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\tilde{\sigma}^2) - \frac{n}{2}$ , we have that

$$AIC = n + n\ln(2\pi) + n\ln(\tilde{\sigma}^2) + 2c$$

$$BIC = n + n \ln(2\pi) + n \ln(\tilde{\sigma}^2) + \ln(n)c$$

where c = p + 1 is the number of columns of the model design matrix.

In some cases the constant  $n + n \ln(2\pi)$  is dropped, such as

$$AIC = n\ln(\tilde{\sigma}^2) + 2c$$

$$BIC = n\ln(\tilde{\sigma}^2) + \ln(n)c$$

#### Information Criteria and Model Selection

AIC and BIC are theoretical optimal criteria for model selection.

- Smaller AIC (or BIC) means better model.
- AIC < BIC whenever  $n \ge 8 \Longrightarrow AIC$  tends to pick larger models

AIC is optimal model selection criterion if trying to find model that best describes data among possible candidate models

True model is unknown and not one of candidate models

BIC is optimal model selection criterion if trying to find true model among possible candidate models

True model is one of candidate models

#### AIC and BIC Model Selection in R

You can perform AIC and BIC model selection using step function.

- Default use performs stepwise AIC selection (direction="both" and k=2)
- Use direction="backward" or direction="forward" to change selection algorithm
- Set k=log(n) to perform BIC selection

# Wine Example: Backward AIC Selection

```
> wmod=lm(quality~.,data=wines)
> bwine=step(wmod,direction="backward",trace=0)
> summary(bwine)
   total.sulfur.dioxide + pH + sulphates + alcohol, data = wines)
                                       Max
             -2.0178138 0.3975417 -5.076 4.31e-07 ***
total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 ***
                    -0.4826614 0.1175581 -4.106 4.23e-05 ***
```

# Wine Example: Forward AIC Selection

```
> wnames=names(wines)[-12]
> wmod=lm(qualitv~1,data=wines)
> wform=as.formula(paste("quality~",paste(wnames,collapse="+")))
> fwine=step(wmod,scope=wform,direction="forward",trace=0)
> summary(fwine)
   total.sulfur.dioxide + chlorides + pH + free.sulfur.dioxide,
   data = wines)
total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 ***
                   -2.0178138 0.3975417 -5.076 4.31e-07 ***
                   -0.4826614 0.1175581 -4.106 4.23e-05 ***
free.sulfur.dioxide 0.0050774 0.0021255 2.389 0.017 *
```

# Wine Example: Stepwise AIC Selection

```
> wnames=names(wines)[-12]
> wmod=lm(qualitv~1,data=wines)
> wform=as.formula(paste("quality~",paste(wnames,collapse="+")))
> swine=step(wmod,scope=wform,trace=0)
> summary(swine)
   total.sulfur.dioxide + chlorides + pH + free.sulfur.dioxide,
   data = wines)
total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 ***
                   -2.0178138 0.3975417 -5.076 4.31e-07 ***
                   -0.4826614 0.1175581 -4.106 4.23e-05 ***
free.sulfur.dioxide 0.0050774 0.0021255 2.389 0.017 *
```

# Wine Example: Backward BIC Selection

```
> wmod=lm(quality~.,data=wines)
> bwine=step(wmod, direction="backward", k=log(1599), trace=0)
> summary(bwine)
    pH + sulphates + alcohol, data = wines)
    Min
                                         Max
                      Estimate Std. Error t value Pr(>|t|)
F-statistic: 147.4 on 6 and 1592 DF, p-value: < 2.2e-16
```

#### Wine Example: Forward BIC Selection

```
> wnames=names(wines)[-12]
> wmod=lm(quality~1,data=wines)
> wform=as.formula(paste("quality~", paste(wnames, collapse="+")))
> fwine=step(wmod,scope=wform,direction="forward",k=log(1599),trace=0)
> summary(fwine)
                    4.2957316 0.3995603 10.751 < 2e-16 ***
total.sulfur.dioxide -0.0023721 0.0005064 -4.684 3.05e-06 ***
F-statistic: 147.4 on 6 and 1592 DF, p-value: < 2.2e-16
```

#### Wine Example: Stepwise BIC Selection

```
> wnames=names(wines)[-12]
> wmod=lm(quality~1,data=wines)
> wform=as.formula(paste("quality~", paste(wnames, collapse="+")))
> swine=step(wmod,scope=wform,k=log(1599),trace=0)
> summary(swine)
                    4.2957316 0.3995603 10.751 < 2e-16 ***
total.sulfur.dioxide -0.0023721 0.0005064 -4.684 3.05e-06 ***
F-statistic: 147.4 on 6 and 1592 DF, p-value: < 2.2e-16
```

#### Toy Example: AIC Selection

```
> set.seed(1120)
> x1=rnorm(100)
> x2=rnorm(100)
> x3=(x1+x2)/2+rnorm(100.sd=.1)
> X=as.data.frame(cbind(x1,x2,x3))
> v=x1+x2+rnorm(100)
> mymod=lm(v~.,data=X)
> amod=step(mymod,trace=0)
> amodScoef
(Intercept) x1
> mymod=lm(y~.,data=X)
> bmod=step(mymod,direction="backward",trace=0)
> bmodscoef
(Intercept) x1
> mymod=lm(y~1,data=X)
> fmod=step(mymod, y~x1+x2+x3, direction="forward", trace=0)
> fmod$coef
> mvmod=lm(v~1,data=X)
> smod=step(mymod,y~x1+x2+x3,trace=0)
> smod$coef
```

#### Toy Example: BIC Selection

```
> set.seed(1120)
> x1 = rnorm(100)
> x2=rnorm(100)
> x3=(x1+x2)/2+rnorm(100.sd=.1)
> X=as.data.frame(cbind(x1,x2,x3))
> v=x1+x2+rnorm(100)
> mymod=lm(v~.,data=X)
> amod=step(mymod,k=log(100),trace=0)
> amodScoef
(Intercept) x1
> mymod=lm(y~.,data=X)
> bmod=step(mymod,direction="backward",k=log(100),trace=0)
> bmodscoef
(Intercept) x1
> mymod=lm(y~1,data=X)
> fmod=step(mymod,y~x1+x2+x3,direction="forward",k=log(100),trace=0)
> fmod$coef
> mvmod=lm(v~1,data=X)
> smod=step(mymod, y~x1+x2+x3, k=log(100), trace=0)
> smod$coef
```

#### Prediction and Model Selection

If we are ultimately interested in prediction, we can use predictionbased criteria to select our model.

Idea: minimize prediction SSE (instead of SSE for given data).

Most implementations do exhaustive (or branch-and-bound) searches, but you could use these criterion in a stepwise fashion too.

#### Mallow's $C_p$

Consider the model  $\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{e}$  where  $\mathbf{X}$  is  $n \times m$  and  $\mathbf{e} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$ .

If we want to estimate the mean-squared prediction error (MSPE)

$$\frac{1}{\sigma^2} \sum_{i=1}^n E\left\{ \left[ \hat{y}_i - E(y_i | \mathbf{x}_i) \right]^2 \right\}$$

we can use Mallow's (1973)  $C_p$ 

$$C_p = \frac{SSE_p}{\hat{\sigma}^2} - n + 2p$$

where

- $SSE_p$  is the SSE with p < m columns of **X** used in fit
- $\hat{\sigma}^2 = SSE/(n-m)$  is the MSE of full model

## Mallow's $C_p$ in R

Implemented in leaps function (leaps package).

- Branch-and-bound search through all possible subsets
- ullet Use default method="Cp" option to select via Mallow's  $C_p$

We could also use the drop1 and add1 functions

- These were called within bslm, fslm, swlm, and step
- Use scale= input to get Mallow's  $C_p$

# Mallow's $C_p$ : Wine Example

```
> X=wines[,-12]
> cpmod=leaps(x=X,v=wines$quality,method="Cp")
> widx=which.min(cpmod$Cp)
> xidx=(1:ncol(X))[cpmod$which[widx,]]
> Xin=data.frame(X[,xidx])
> cpmod=lm(wines$quality~.,data=Xin)
> summary(cpmod)
lm(formula = wines$quality ~ ., data = Xin)
total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 ***
                    -0.4826614 0.1175581 -4.106 4.23e-05 ***
F-statistic: 127.6 on 7 and 1591 DF, p-value: < 2.2e-16a
```

## Mallow's $C_p$ : Wine Example (continued)

```
> wmod=lm(quality~.,data=wines)
> sigmasg=summary(wmod)$sigma^2
> drop1 (wmod, scale=sigmasg)
     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
volatile.acidity 1 33.620 700.03 90.063
citric.acid 1 0.646 667.06 11.539 residual.sugar 1 0.498 666.91 11.185 chlorides 1 8.391 674.80 29.982 free.sulfur.dioxide 1 1.694 668.10 14.035
total.sulfur.dioxide 1 8.427 674.84 30.069
density 1 0.287 666.70 10.683 pH 1 1 057 600 pp 1 1 1
```

Drop density because it has the smallest  $C_p$  score below  $p_0 = 12$ .

#### Predicted Residual Sum-of-Squares (PRESS)

The Predicted Residual Sum-of-Squares (PRESS) statistic is

PRESS = 
$$\sum_{i=1}^{n} (y_i - \hat{y}_{[-i]})^2 = \sum_{i=1}^{n} (\frac{\hat{e}_i}{1 - h_{ii}})^2$$

#### where

- $\hat{y}_{[-i]} = \mathbf{x}_i \hat{\mathbf{b}}_{[-i]}$  and  $\hat{\mathbf{b}}_{[-i]}$  is estimate of **b** without *i*-th observation
- $\hat{e}_i$  is *i*-th estimated residual from full model
- $h_{ii}$  is i-th leverage score from full model

#### PRESS Statistic in R

```
getpress<-function(indx, y, Xmat) {</pre>
  ivec=(1:ncol(X))[indx]
  mymod=lm(y~.,data=data.frame(Xmat[,ivec]))
  sum((mymod$residuals/(1-hatvalues(mymod)))^2)
presslm<-function(y, X) {</pre>
  X=data.frame(X); np=ncol(X)
  xlist=vector("list", np)
  for(j in 1:np) {xlist[[j]]=c(TRUE, FALSE)}
  xall=expand.grid(xlist); nxall=nrow(xall)
  xall=as.matrix(xall[1:(nxall-1),])
  allpress=apply(xall, 1, getpress, y=y, Xmat=X)
  list (which=xall, press=allpress)
```

## PRESS Statistic: Wine Example

```
> X=wines[,-12]
> pressmod=presslm(wines$quality,X)
> widx=which.min(pressmod$press)
> xidx=(1:ncol(X))[pressmod$which[widx,]]
> Xin=data.frame(X[,xidx])
> pressmod=lm(wines$quality~.,data=Xin)
> summary (pressmod)
lm(formula = wines$quality ~ ., data = Xin)
total.sulfur.dioxide -0.0034822 0.0006868 -5.070 4.43e-07 ***
                    -0.4826614 0.1175581 -4.106 4.23e-05 ***
```

#### R State Facts Data

The state.x77 matrix contains 8 variables (columns) collected from the 50 states (rows) during the early 1970s

- Population: estimate of state population (1975)
- Income: per capita income (1974)
- Illiteracy: percent illiterate (1970)
- Life Exp: life expectancy (1969–1971)
- Murder: murder rate per 100,000 people (1976)
- HS Grad: percent high-school graduates (1970)
- Frost: mean number of days with minimum temperature below freezing (1931–1960)
- Area: land area in square miles

#### Look at State Facts Data

- > states=data.frame(state.x77,row.names=state.abb)
- > states[1:15,]

	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
ΑZ	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
CT	3100	5348	1.1	72.48	3.1	56.0	139	4862
DE	579	4809	0.9	70.06	6.2	54.6	103	1982
FL	8277	4815	1.3	70.66	10.7	52.6	11	54090
GA	4931	4091	2.0	68.54	13.9	40.6	60	58073
ΗI	868	4963	1.9	73.60	6.2	61.9	0	6425
ID	813	4119	0.6	71.87	5.3	59.5	126	82677
IL	11197	5107	0.9	70.14	10.3	52.6	127	55748
IN	5313	4458	0.7	70.88	7.1	52.9	122	36097
IA	2861	4628	0.5	72.56	2.3	59.0	140	55941

#### State Data: Backward Elimination

```
> bsmod=bslm(states$Murder, states[,-5])
[1] "Step 1 : Dropping Income"
[1] "Step 2 : Dropping HS.Grad"
> summary(bsmod) # I deleted some output
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.202e+02 1.718e+01 6.994 1.17e-08 ***
Population 1.780e-04 5.930e-05 3.001 0.00442 **
Illiteracy 1.173e+00 6.801e-01 1.725 0.09161.
Life.Exp -1.608e+00 2.324e-01 -6.919 1.50e-08 ***
Frost -1.373e-02 7.080e-03 -1.939 0.05888.
Area 6.804e-06 2.919e-06 2.331 0.02439 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.712 on 44 degrees of freedom
Multiple R-squared: 0.8068, Adjusted R-squared: 0.7848
F-statistic: 36.74 on 5 and 44 DF, p-value: 1.221e-14
```

#### State Data: Forward Selection

```
> fsmod=fslm(states$Murder, states[,-5])
[1] "Step 1 : Adding Life.Exp"
[1] "Step 2 : Adding Frost"
[1] "Step 3: Adding Population"
[1] "Step 4 : Adding Area"
[1] "Step 5 : Adding Illiteracy"
> summary(fsmod) # I deleted some output
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.202e+02 1.718e+01 6.994 1.17e-08 ***
Life.Exp -1.608e+00 2.324e-01 -6.919 1.50e-08 ***
Frost -1.373e-02 7.080e-03 -1.939 0.05888.
Population 1.780e-04 5.930e-05 3.001 0.00442 **
Area 6.804e-06 2.919e-06 2.331 0.02439 *
Illiteracy 1.173e+00 6.801e-01 1.725 0.09161.
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.712 on 44 degrees of freedom
Multiple R-squared: 0.8068, Adjusted R-squared: 0.7848
F-statistic: 36.74 on 5 and 44 DF, p-value: 1.221e-14
```

# State Data: Stepwise Selection

```
> swmod=swlm(states$Murder, states[,-5])
[1] "Step 1 : Adding Life.Exp"
[1] "Step 2 : Adding Frost"
[1] "Step 3: Adding Population"
[1] "Step 4 : Adding Area"
[1] "Step 5 : Adding Illiteracy"
> summary(swmod)  # I deleted some output
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.202e+02 1.718e+01 6.994 1.17e-08 ***
Life.Exp -1.608e+00 2.324e-01 -6.919 1.50e-08 ***
Frost -1.373e-02 7.080e-03 -1.939 0.05888.
Population 1.780e-04 5.930e-05 3.001 0.00442 **
Area 6.804e-06 2.919e-06 2.331 0.02439 *
Illiteracy 1.173e+00 6.801e-01 1.725 0.09161.
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.712 on 44 degrees of freedom
Multiple R-squared: 0.8068, Adjusted R-squared: 0.7848
F-statistic: 36.74 on 5 and 44 DF, p-value: 1.221e-14
```

# State Data: Adjusted R<sup>2</sup> Selection

```
> X=states[.-5]
> arsqmod=leaps(x=X, v=states$Murder, method="adjr2")
> widx=which.max(arsqmod$adjr2)
> xidx=(1:ncol(X))[arsqmod$which[widx,]]
> Xin=data.frame(X[,xidx])
> arsqmod=lm(states$Murder~.,data=Xin)
> summary(arsqmod) # I deleted some output
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.202e+02 1.718e+01 6.994 1.17e-08 ***
Population 1.780e-04 5.930e-05 3.001 0.00442 **
Illiteracy 1.173e+00 6.801e-01 1.725 0.09161.
Life.Exp -1.608e+00 2.324e-01 -6.919 1.50e-08 ***
Frost -1.373e-02 7.080e-03 -1.939 0.05888.
Area 6.804e-06 2.919e-06 2.331 0.02439 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.712 on 44 degrees of freedom
Multiple R-squared: 0.8068, Adjusted R-squared: 0.7848
F-statistic: 36.74 on 5 and 44 DF, p-value: 1.221e-14
```

## State Data: Stepwise AIC Selection

```
> smod=lm(states$Murder~.,data=states)
> aicmod=step(smod,trace=0)
> summary(aicmod)  # I deleted some output
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.202e+02 1.718e+01 6.994 1.17e-08 ***
Population 1.780e-04 5.930e-05 3.001 0.00442 **
Illiteracy 1.173e+00 6.801e-01 1.725 0.09161.
Life.Exp -1.608e+00 2.324e-01 -6.919 1.50e-08 ***
Frost -1.373e-02 7.080e-03 -1.939 0.05888.
Area 6.804e-06 2.919e-06 2.331 0.02439 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.712 on 44 degrees of freedom
Multiple R-squared: 0.8068, Adjusted R-squared: 0.7848
F-statistic: 36.74 on 5 and 44 DF, p-value: 1.221e-14
```

#### State Data: Stepwise BIC Selection

```
> smod=lm(states$Murder~.,data=states)
> bicmod=step(smod,k=log(50),trace=0)
> summarv(bicmod) # I deleted some output
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.387e+02 1.369e+01 10.136 3.40e-13 ***
Population 1.581e-04 5.944e-05 2.660 0.010778 *
Life.Exp -1.837e+00 1.946e-01 -9.442 3.04e-12 ***
Frost -2.204e-02 5.299e-03 -4.160 0.000141 ***
Area 7.387e-06 2.962e-06 2.494 0.016374 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.75 on 45 degrees of freedom
Multiple R-squared: 0.7937, Adjusted R-squared: 0.7754
F-statistic: 43.28 on 4 and 45 DF, p-value: 7.106e-15
```

# State Data: Mallow's $C_p$ Selection

```
> X=states[,-5]
> cpmod=leaps(x=X,y=states$Murder,method="Cp")
> widx=which.min(cpmod$Cp)
> xidx=(1:ncol(X))[cpmod$which[widx,]]
> Xin=data.frame(X[,xidx])
> cpmod=lm(states$Murder~.,data=Xin)
> summary(cpmod) # I deleted some output
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.202e+02 1.718e+01 6.994 1.17e-08 ***
Population 1.780e-04 5.930e-05 3.001 0.00442 **
Illiteracy 1.173e+00 6.801e-01 1.725 0.09161.
Life.Exp -1.608e+00 2.324e-01 -6.919 1.50e-08 ***
Frost -1.373e-02 7.080e-03 -1.939 0.05888.
Area 6.804e-06 2.919e-06 2.331 0.02439 *
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 '' 1
Residual standard error: 1.712 on 44 degrees of freedom
Multiple R-squared: 0.8068, Adjusted R-squared: 0.7848
F-statistic: 36.74 on 5 and 44 DF, p-value: 1.221e-14
```

#### State Data: PRESS Selection

```
> X=states[,-5]
> pressmod=presslm(states$Murder, X)
> widx=which.min(pressmod$press)
> xidx=(1:ncol(X))[pressmod$which[widx,]]
> Xin=data.frame(X[,xidx])
> pressmod=lm(states$Murder~.,data=Xin)
> summary(pressmod)  # I deleted some output
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.259e+02 1.777e+01 7.083 8.64e-09 ***
Population 1.946e-04 6.078e-05 3.202 0.00254 **
Illiteracy 1.912e+00 7.620e-01 2.509 0.01587 *
Life.Exp -1.757e+00 2.491e-01 -7.053 9.57e-09 ***
HS.Grad 7.626e-02 4.369e-02 1.746 0.08786.
Frost -1.011e-02 7.199e-03 -1.404 0.16719
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 1.755 on 44 degrees of freedom
Multiple R-squared: 0.797, Adjusted R-squared: 0.7739
F-statistic: 34.54 on 5 and 44 DF, p-value: 3.565e-14
```