Model Selection

Chapter 2 of LMWR2, Chapter 2 and 3 of ALR4

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Overview

Why Model Selection?

Variable selection is intended to (objectively) find the “best” subset of predictors.

Reasons for this include:

- We want the simplest model that adequately explains the data.
- Unnecessary regressors will add noise to all model estimates.
- Degrees of freedom are wasted.
- A smaller model might achieve more precise estimates and predictions.
- Removing excess regressors aids in interpretation and helps to prevent problems with linearly dependent regressors.
- If the model is to be used for prediction, we can save time and/or money by not having to measure extra predictors (and improve our prediction!).

Caution

Variable selection is affected by: • Outliers/influential observations. • Transformation of variables.

Iteration and experimentation are essential to finding better models, BUT be very careful not to overtrain your model to the sample data!

Two aspects

There are two aspects to variable selection:

- The criterion used to compare models.
- The strategy used to search for the “optimal” model.

Selection Criteria

p-values

P-values are a common criterion for selecting regressors to keep in our regression model.

This criterion keeps the regressors with the smallest p-values in the model, specifically the regressors with p-values less than some threshold, α_{crit}.

Information Criteria

Akaike's Information Criterion (AIC) and the **Bayesian Information Criterion (BIC)** are two information-based criteria for variable selection.

- $AIC(\mathcal{M}) = -2L(\mathcal{M}) + 2p_{\mathcal{M}}$, where $\mathcal{M}$ is the model, $L(\mathcal{M})$ is the log likelihood of the model using the MLE estimates of the parameters, and $p_{\mathcal{M}}$ is the number of regression coefficients in model $\mathcal{M}$.

- $BIC(\mathcal{M}) = -2L(\mathcal{M}) + \log(n)p_{\mathcal{M}}$.

For linear regression models, $-2L(\mathcal{M}) = n\log(RSS_{\mathcal{M}}/n) + c$, where c is a constant that depends only on the observed data and not on the model, and $RSS_{\mathcal{M}}$ is the RSS of model $\mathcal{M}$.

- c can be ignored when comparing between models.

Smaller the better

The information criteria capture two aspects of model fit:

- The $-2L(\mathcal{M})$ measures how well the fitted model matches the observed data.
- The second component penalizes the model according to the number of parameters it includes (its complexity).
- The more parameters, the larger the penalty.
- Models with more parameters will fit better (reducing the RSS), but will be penalized more for having additional parameters.
- AIC and BIC provide criteria for balancing model fit with model complexity.

AIC vs BIC

BIC tends to penalize complex models more heavily than AIC (anytime $\log(n) > 2$, i.e., $n \geq 8$), so it tends to suggest simpler models than the AIC criterion.

AIC and BIC are used as selection criteria for many types of models, not just linear regression models.

Predictive Value

R^2 never decreases as new regressors are added to the model.

- It is useless for comparing models with different numbers of regressors.

Adjusted R^2, R_a^2, is a better criterion for assessing model fit.

- The adjusted R^2 criterion penalizes for the number of parameters in the model.

For model $\mathcal{M}$ with $p_{\mathcal{M}}$ regression coefficients,

$$R_a^2 = 1 - \frac{\frac{RSS_{\mathcal{M}}}{n-p_{\mathcal{M}}}}{\frac{TSS}{n-1}} = 1 - \left(\frac{n-1}{n-p_{\mathcal{M}}}\right)(1-R^2) = 1 - \frac{\hat{\sigma}_{\mathcal{M}}^2}{\hat{\sigma}_{null}^2}$$

Why R_a^2

Adding a regressor to a model only increases R_a^2 if the regressor has some predictive value.

- This is because minimizing the variance of the prediction error amounts to minimizing $\hat{\sigma}^2_{\mathcal{M}}$, which in turn maximizes R_a^2.

We favor models that produce larger R_a^2.

Mallow’s C_p Statistic

Mallow’s C_p statistic is a criterion designed to quantify the predictive usefulness of a model.

At its core, Mallow’s C_p statistic is trying to estimate the standardized total mean square prediction error, given by

$$\frac{1}{\sigma^2}\sum_i E\big(\hat{y}_i - E(y_i)\big)^2 = \frac{1}{\sigma^2}\sum_i MSE(\hat{y}_i),$$

where $MSE(\hat{y}_i) = var(\hat{y}_i) + Bias(\hat{y}_i)^2$

For model

For model $\mathcal{M}$ with $p_{\mathcal{M}}$ regression coefficients, this quantity is estimated by

$$C_{p_{\mathcal{M}}} = RSS_{\mathcal{M}}/\hat{\sigma}^2_{\Omega} + 2p_{\mathcal{M}} - n$$

where $\hat{\sigma}^2_{\Omega}$ is the estimated error variance for the model with all regressors and $RSS_{\mathcal{M}}$ is the residual sum of squares for model $\mathcal{M}$.

Notes on Mellow's C_p

- For the model with all regressors (model Ω with p_Ω regression coefficients), $C_{p_\Omega} = p_\Omega$.

- If a model with $p_\mathcal{M}$ regression coefficients fits the data well and has little or no bias, then $E(C_{p_\mathcal{M}}) \approx p_\mathcal{M}$.

- A model with a biased fit will have $C_{p_\mathcal{M}}$ much larger than $p_\mathcal{M}$. (Models with $C_{p_\mathcal{M}}$ less than $p_\mathcal{M}$ do not show evidence of bias).

- It is common to plot $C_{p_\mathcal{M}}$ versus $p_\mathcal{M}$ and compare this to 45^o line $(C_{p_\mathcal{M}} = p_\mathcal{M})$.

We favor models with small $p_\mathcal{M}$ and $C_{p_\mathcal{M}}$ close to $p_\mathcal{M}$.

MSE

The **mean squared error (MSE)** for prediction is simply the average of the squared deviations between the fitted values and the observed data, i.e., $\frac{1}{n}\sum(y_i - \hat{y}_i)^2$

- We favor models with smaller mean squared error, but the search algorithm is very important, otherwise you just use the model with the most regressors.

- The RMSE (root mean squared error) is simply the square root of the MSE, and is sometimes used in place of the MSE.

- The RMSE or MSE will produce identical variable selection results since they are 1-1 transformations of each other.

Cross-Validation

Cross-validation breaks the data into a **training** dataset and a **test** dataset to get a more accurate assessment of the predictive accuracy of a model.

- A model is fit to the training dataset and then the fitted model is used to predict the responses of the test dataset, from which an error criterion (e.g, the MSE) is calculated for the test dataset.
- We favor the model the minimizes the MSE (or optimizes some other measure of prediction accuracy).

Variations of CV

There are many variations of how to choose the training and testing datasets for crossvalidation.

- Leave-one-out crossvalidation uses each observation (individually) as a test data set, using the other n-1 observations as the training data.
- In principle, we must fit n models to find the mean squared error, though this can be done using only a single model if you scale things correctly..
- k-fold crossvalidation breaks the data into k unique sets.
- For each set, the other $k-1$ sets are used as training data, and then the fitted model is used to predict the responses for the kth testing set.
- We must fit k models to determine the mean squared error.
- There are other mechanisms for choosing the training and test datasets, but these are the most common.

Selection Criterion for CV

When using cross-validation as your selection criterion, we prefer the model that produces the lowest MSE or RMSE.

- You typically don’t do an exhaustive search or stepwise selection search.
- You often use one of the other selection criteria/search strategies to narrow down the possible models to a few final candidate models and then use cross-validation to make a final decision.

Search Strategies

Exhaustive Search

An **exhaustive search** looks at all possible models using all available regressors.

- This is not feasible unless the number of regressors is relatively small.
- If the number of regressors (including the intercept) is p_{Ω}, there are $2^{p_{\Omega}}$ possible models.

Because of our error criteria, our search often simplifies to finding the model that minimizes $RSS_{\mathcal{M}}$ for each value of $p_{\mathcal{M}}$.

- This is the best subset searching strategy.
- It’s really just a smart way to do an exhaustive search.

Stepwise Selection

When the previous strategies may take too long, **stepwise selection** can be used to iteratively build models, choosing the next model as the one that maximizes or minimizes the criterion of interest.

- Backwards selection starts with the model having all regressors, then prunes the regressors one at a time until we can no longer improve the error criterion by removing a single regressor.
- Forward selection starts with the null model (only an intercept), and adds regressors one at a time until we can no longer improve the error criterion by adding a single regressor.
- “Both” (or commonly, stepwise selection) is similar to backward selection, except that we can add a regressor back into the model if it improves the error criterion.

Additional Notes

- Stepwise selection can miss the optimal model because we do not consider all possible models due to the one-at-a-time nature of adding/removing regressors.

- P-values should not be taken as very accurate in stepwise or best subset searches because we are bound to see small p-values due to chance alone.

- Stepwise selection tends to produce simpler models that are not necessarily the best for prediction.

Model Hierarchy

We must respect hierarchy in models when it is naturally present.

- In polynomial models, x^2 is a higher order term than x.
- A lower order term should be retained if a higher order term is retained to increase the flexibility.
    - E.g., for the model $y = \beta_0 + \beta_2 x^2 + \epsilon$, the maximum/minimum value MUST occur at $x = 0$.
    - For the model $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$, the maximum/minimum value can occur anywhere along the real line (depending on what the data suggest).

Example: If we fit the model $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$ and β_1 is not significant, it would NOT make sense to remove x from the model but still keep x^2.

Example

The U.S. Bureau of the Census collected data from the 50 states in the 1970s. Measured variables include:

- `Population`: population estimate as of July 1, 1975
- `Income`: per capita income (1974)
- `Illiteracy`: illiteracy (1970, percent of population)
- `Life.Exp`: life expectancy in years (1969–71)
- `Murder`: murder and non-negligent manslaughter rate per 100,000 population (1976)
- `HS Grad`: percent high-school graduates (1970)
- `Frost`: mean number of days with minimum temperature below freezing (1931–1960) in capital or large city
- `Area`: land area in square miles

Backward selection using p-values and α_{crit}.

```r
statedata = data.frame(state.x77)
lmod_full <- lm(Life.Exp ~ ., data = statedata)
knitr::kable(summary(lmod_full)$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	70.9432241	1.7479754	40.5859402	0.0000000
Population	0.0000518	0.0000292	1.7747731	0.0831835
Income	-0.0000218	0.0002444	-0.0892060	0.9293422
Illiteracy	0.0338203	0.3662799	0.0923346	0.9268712
Murder	-0.3011232	0.0466207	-6.4589973	0.0000001
HS.Grad	0.0489295	0.0233233	2.0978818	0.0419718
Frost	-0.0057350	0.0031432	-1.8245568	0.0751868
Area	-0.0000001	0.0000017	-0.0442593	0.9649075

Remove Least Significant Predictor

```
lmod <- lm(Life.Exp ~ .-Area, data = statedata)
knitr::kable(summary(lmod)$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	70.9893185	1.3874544	51.1651541	0.0000000
Population	0.0000519	0.0000288	1.8022535	0.0785181
Income	-0.0000244	0.0002343	-0.1043161	0.9174036
Illiteracy	0.0284588	0.3416329	0.0833023	0.9339978
Murder	-0.3018231	0.0433443	-6.9633836	0.0000000
HS.Grad	0.0484723	0.0206673	2.3453662	0.0236917
Frost	-0.0057758	0.0029702	-1.9445503	0.0583888

Remove Least Significant Predictor (Illiteracy)

```
lmod <- update(lmod,. ~ . - Illiteracy)
knitr::kable(summary(lmod)$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	71.0657509	1.0289415	69.0668559	0.0000000
Population	0.0000511	0.0000271	1.8877836	0.0656610
Income	-0.0000248	0.0002316	-0.1069555	0.9153104
Murder	-0.3000077	0.0370418	-8.0991613	0.0000000
HS.Grad	0.0477580	0.0185908	2.5689048	0.0136703
Frost	-0.0059099	0.0024678	-2.3948100	0.0209534

Remove Least Significant Predictor (Income)

```
lmod <- update(lmod,. ~ . - Income)
knitr::kable(summary(lmod)$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	71.0271285	0.9528530	74.541541	0.0000000
Population	0.0000501	0.0000251	1.996017	0.0520051
Murder	-0.3001488	0.0366095	-8.198669	0.0000000
HS.Grad	0.0465822	0.0148271	3.141704	0.0029681
Frost	-0.0059433	0.0024209	-2.455017	0.0180178

Remove **`Population`**?

Whether we should remove Population is a close call. We should probably keep it if it makes the model more interpretable.

```
lmod <- update(lmod,. ~ . - Population)
knitr::kable(summary(lmod)$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	71.0363788	0.9832622	72.245614	0.0000000
Murder	-0.2830652	0.0367313	-7.706370	0.0000000
HS.Grad	0.0499487	0.0152011	3.285856	0.0019504
Frost	-0.0069117	0.0024475	-2.824025	0.0069877

All variables are now significant at $\alpha_{\text{crit}} = 0.05$.

How did we do?

```
summary(lmod_full)$r.squared
```

```
## [1] 0.7361563
```

```
summary(lmod)$r.squared
```

```
## [1] 0.7126624
```

```
summary(lmod_full)$adj.r.squared
```

```
## [1] 0.6921823
```

```
summary(lmod)$adj.r.squared
```

```
## [1] 0.693923
```

The R^2 for the full model is 0.736. Our final model has an R^2 of 0.713, which is only slightly lower.

- Removal of four predictors causes only a minor reduction in fit. This is NOT surprising.
- A better question might be: what would the effect of removing these variables be on a new independent sample?

Replace `HS.Grad` with `Illiteracy`

```
knitr::kable(summary(lm(Life.Exp ~ Illiteracy + Murder + Frost, statedata))$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	74.5567171	0.5842507	127.610835	0.0000000
Illiteracy	-0.6017607	0.2989270	-2.013069	0.0499811
Murder	-0.2800474	0.0433940	-6.453594	0.0000001
Frost	-0.0086910	0.0029595	-2.936708	0.0051663

Replace `HS.Grad` with `Illiteracy`

```
knitr::kable(summary(lm(Life.Exp ~ Illiteracy + Murder + Frost, statedata))$coefficients)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	74.5567171	0.5842507	127.610835	0.0000000
Illiteracy	-0.6017607	0.2989270	-2.013069	0.0499811
Murder	-0.2800474	0.0433940	-6.453594	0.0000001
Frost	-0.0086910	0.0029595	-2.936708	0.0051663

- Illiteracy does have some association with life expectancy
- High school graduation rate and illiteracy are likely correlated
- Impossible to know which is the important/causal variable
- Both could be important or both could be proxies for a third variable.

Example 2

Use best subset selection to minimize the AIC criterion.

- The regsubsets function in the leaps package can be used to do this.
- For each number of regression coefficients p, it finds the model that minimizes the RSS.
- For each value of p, the model that minimizes the RSS will have the smallest AIC, BIC, R_a^2, and Mallow's C_p.
- NOTE: By default, regsubsets only goes up to p=9. You have to set nvmax = j, where j is the number of regressors you want to consider.

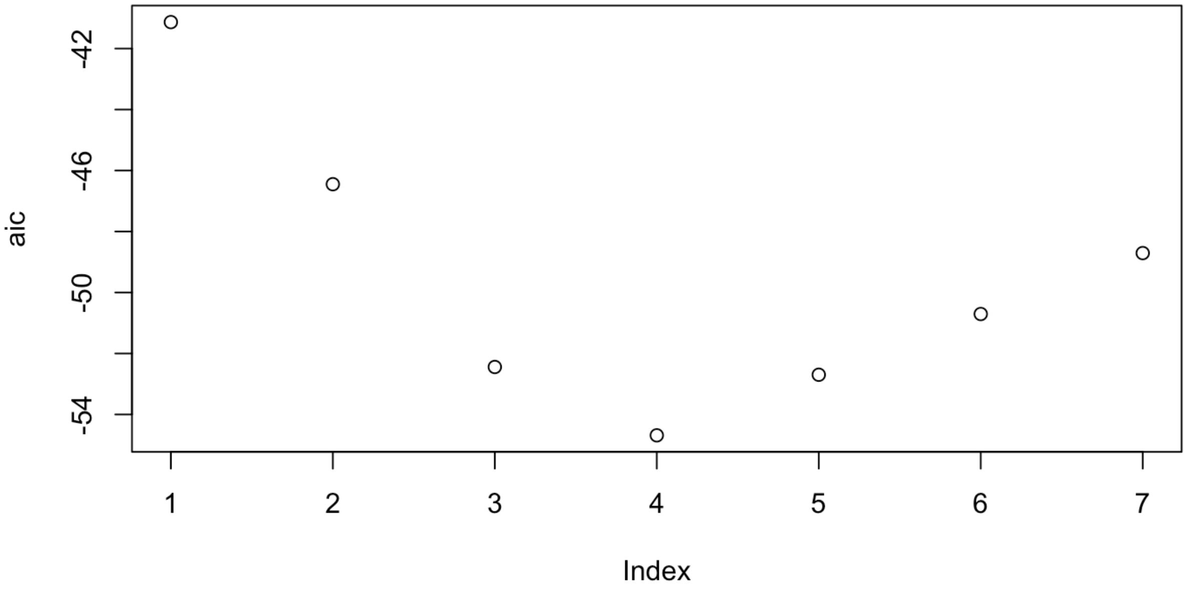
Example 2

```r
library(leaps)
b <- regsubsets(Life.Exp ~ ., data = statedata)
rs <- summary(b) # summarize model that minimizes RSS for each p
knitr::kable(rs$which) # best subset models (in terms of RSS)
```

(Intercept)	Population	Income	Illiteracy	Murder	HS.Grad	Frost	Area
TRUE	FALSE	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE
TRUE	FALSE	FALSE	FALSE	TRUE	TRUE	FALSE	FALSE
TRUE	FALSE	FALSE	FALSE	TRUE	TRUE	TRUE	FALSE
TRUE	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE	FALSE
TRUE	TRUE	TRUE	FALSE	TRUE	TRUE	TRUE	FALSE
TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE
TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE

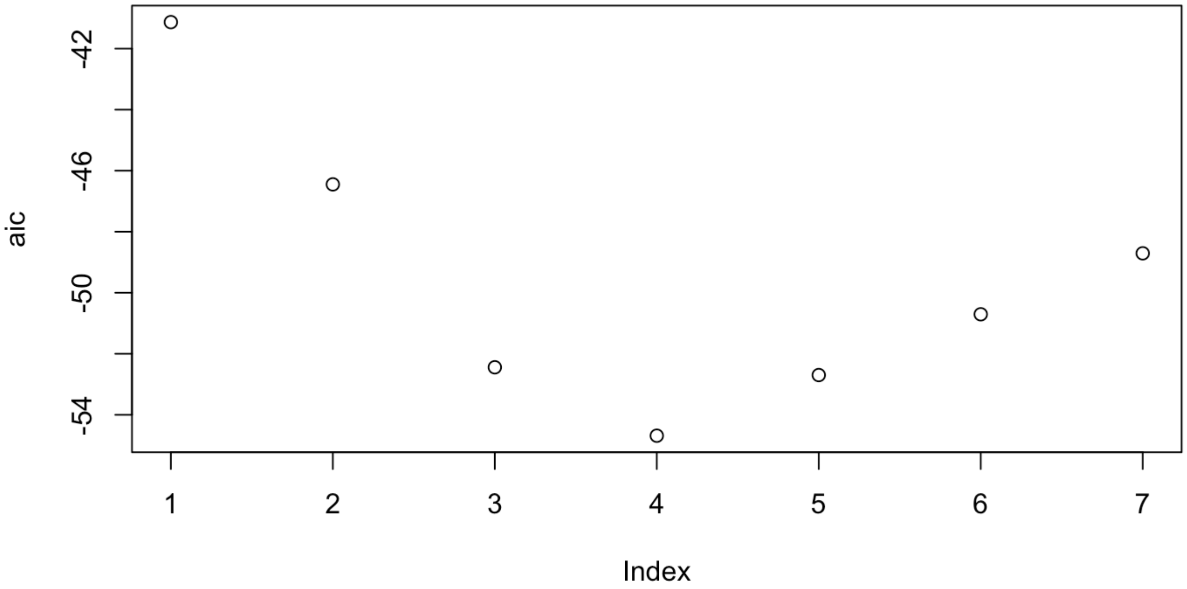
Use AIC

```
p = 1:7
aic <- rs$bic + p*(2-log(50))
plot(aic)
```



Use AIC

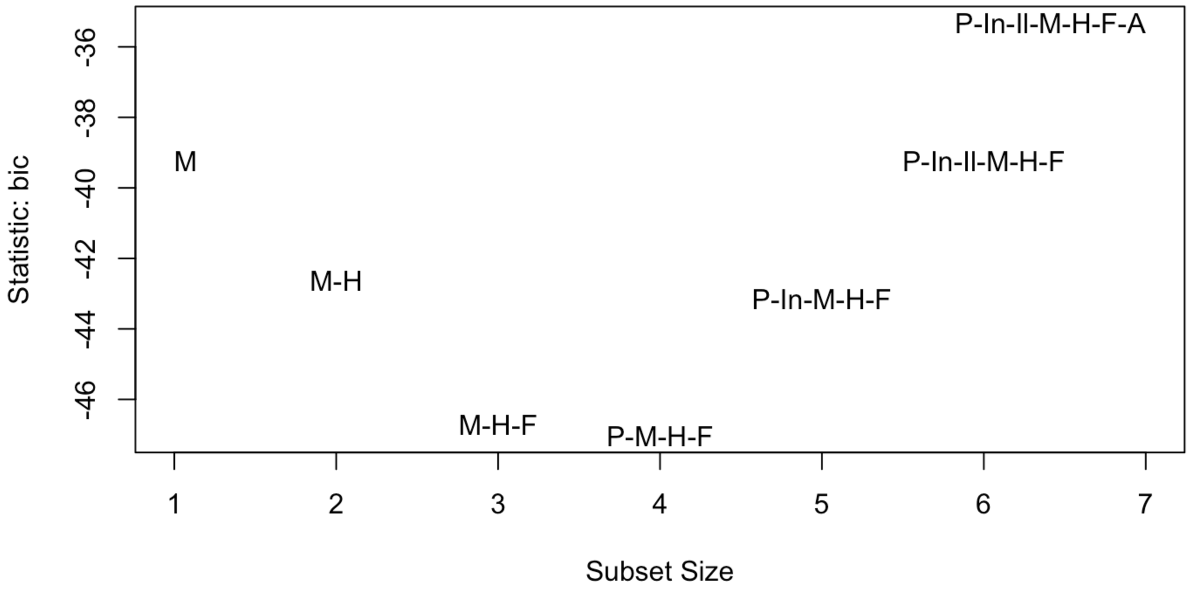
```r
p = 1:7
aic <- rs$bic + p*(2-log(50))
plot(aic)
```



Model $p = 5$: Predictors - 'Population', 'Murder', 'HS.Grad', 'Frost'.

Use BIC

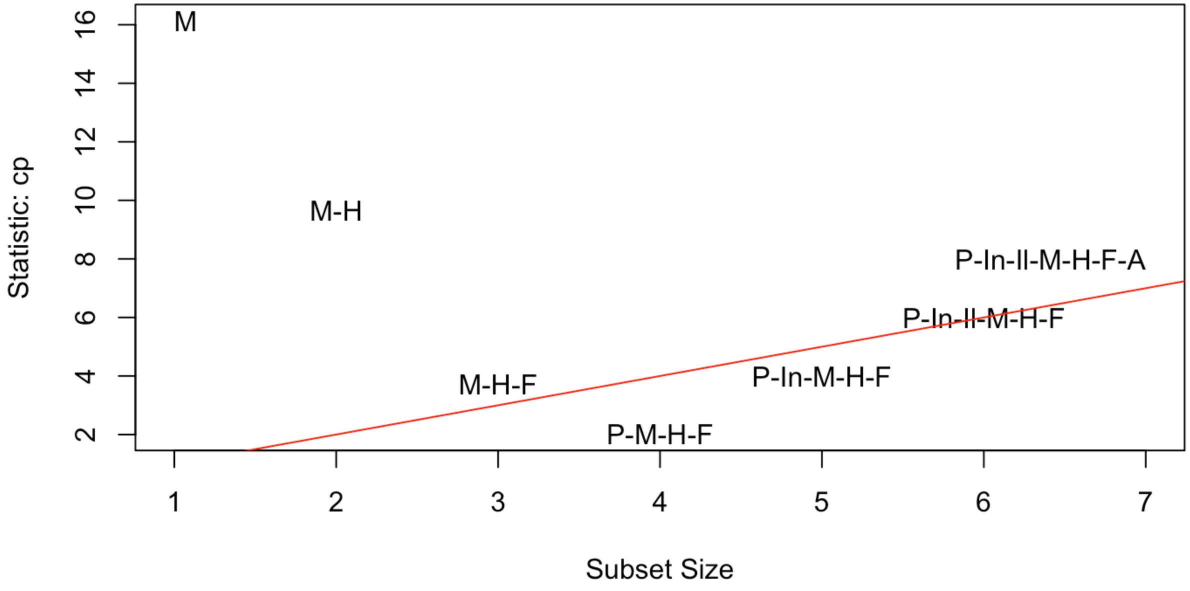
```
car::subsets(b, abbrev = 1, legend = F)
```



We reach a similar conclusion using the BIC criterion.

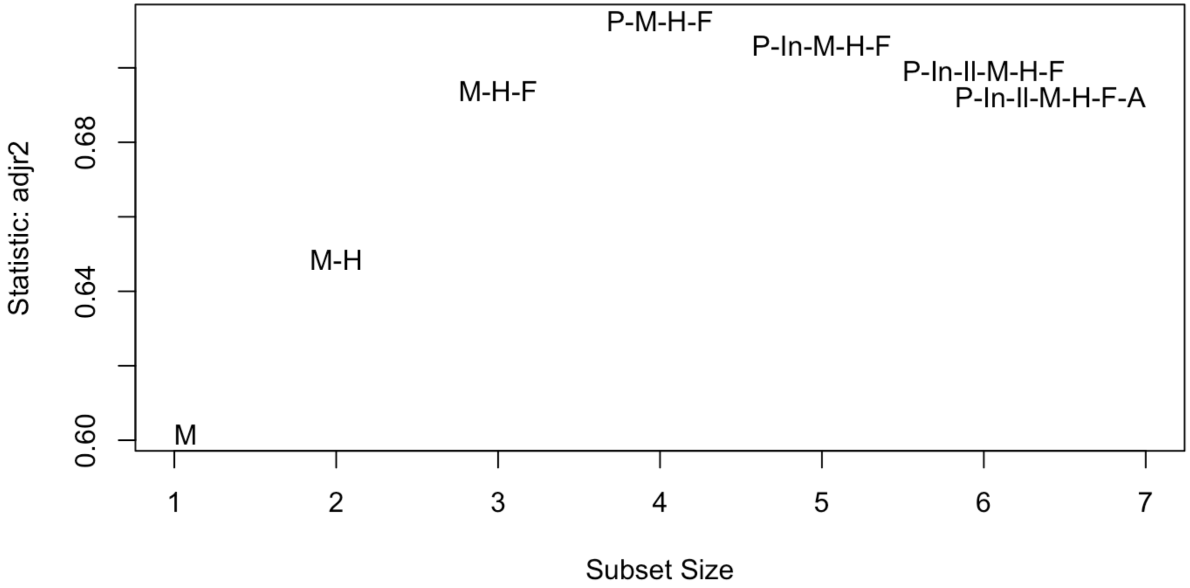
Use C_p

```
car::subsets(b, abbrev = 1, legend = F, statistic = 'cp')
abline(0,1,col='red')
```



Use R_a^2

```
car::subsets(b, abbrev = 1, legend = F, statistic = 'adjr2')
abline(0,1,col='red')
```



Stepwise selection with AIC

```
step_model = step(lmod_full, direction = 'both')
```

```
## Start:  AIC=-22.18
## Life.Exp ~ Population + Income + Illiteracy + Murder + HS.Grad +
##     Frost + Area
##
##              Df Sum of Sq    RSS     AIC
## - Area        1    0.0011 23.298 -24.182
## - Income      1    0.0044 23.302 -24.175
## - Illiteracy  1    0.0047 23.302 -24.174
## <none>                    23.297 -22.185
## - Population  1    1.7472 25.044 -20.569
## - Frost       1    1.8466 25.144 -20.371
## - HS.Grad     1    2.4413 25.738 -19.202
## - Murder      1   23.1411 46.438  10.305
##
## Step:  AIC=-24.18
## Life.Exp ~ Population + Income + Illiteracy + Murder + HS.Grad +
##     Frost
##
##              Df Sum of Sq    RSS     AIC
## - Illiteracy  1    0.0038 23.302 -26.174
```

Final Model using Stepwise AIC

```r
anova(step_model)
```

```
## Analysis of Variance Table
##
## Response: Life.Exp
##            Df Sum Sq Mean Sq  F value    Pr(>F)    
## Population  1  0.409   0.409   0.7895  0.378981    
## Murder      1 57.445  57.445 110.9068 1.002e-13 ***
## HS.Grad     1  4.015   4.015   7.7523  0.007818 ** 
## Frost       1  3.122   3.122   6.0271  0.018018 *  
## Residuals  45 23.308   0.518                       
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Compare full and final model using 10-fold CV

```
library(caret)
# define training/test (control) data
cv_10fold <- trainControl(method="cv", number = 10) # 10-fold crossvalidation train/test data
cv_loo <- trainControl(method="LOOCV") # leave-one-out crossvalidation train/test data
f1 = Life.Exp ~ . # formula for full model
f2 = Life.Exp~Population + Murder + HS.Grad + Frost
modela <- train(f1, data = statedata, trControl=cv_10fold, method = "lm")
modelb <- train(f2, data = statedata, trControl=cv_10fold, method = "lm")
```

Compare full and final model using 10-fold CV

```
print(modela)
```

```
## Linear Regression
##
## 50 samples
##  7 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 46, 46, 44, 45, 44, 44, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.8864039  0.6017725  0.7364396
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Compare full and final model using 10-fold CV

```
print(modelb)
```

```
## Linear Regression
##
## 50 samples
##  4 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 46, 45, 46, 45, 45, 44, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.7266738  0.7140054  0.636507
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

The smaller model is preferred (since it has smaller RMSE) using 10-fold crossvalidation

Compare full and final model using LOO CV

```
modelc <- train(f1, data = statedata, trControl=cv_loo, method = "lm")
print(modelc) # full, loo
```

```
## Linear Regression
##
## 50 samples
##  7 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 49, 49, 49, 49, 49, 49, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.9090885  0.5469535  0.7196334
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Compare full and final model using LOO CV

```
modeld <- train(f2, data = statedata, trControl=cv_loo, method = "lm")
print(modeld) # reduced, loo
```

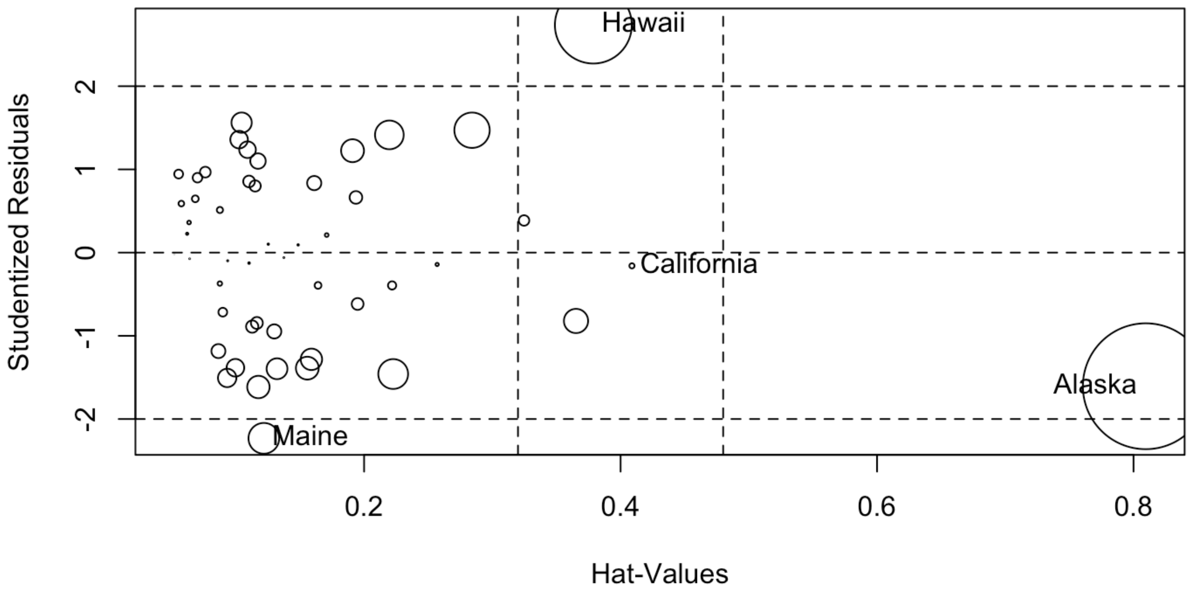
```
## Linear Regression
##
## 50 samples
##  4 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 49, 49, 49, 49, 49, 49, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   0.770042  0.6657615  0.6377097
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

The smaller model is preferred (since it has smaller RMSE) using leave-one-out crossvalidation

Effect of outliers

Alaska is a high leverage point. What’s the effect if we remove it?

```
lmod = lm(Life.Exp ~.,data = statedata)
car::influencePlot(lmod)
```



```
##                StudRes        Hat       CookD
```

Remove Alaska

```r
b <- regsubsets(Life.Exp ~., data = statedata, subset = (state.abb!="AK"))
rs <- summary(b)
rs$which[which.max(rs$adjr), ]
```

```
## (Intercept)  Population      Income  Illiteracy      Murder     HS.Grad
##        TRUE        TRUE       FALSE       FALSE        TRUE        TRUE
##       Frost        Area
##        TRUE        TRUE
```

We now choose a 5 regressor model using R_a^2, whereas we chose 4 before.

Exercise

For the teengamb data in the faraway package, use the methods learned in this chapter to identify the “best” models.