Model Selection

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Model selection

- Regression problems often have many predictors
- The number of possible models increase rapidly with number of predictors
- Even if we one of these models is "correct", how do we find it?

Why does it matter?

- One solution could be to use all the predictors
- This is technically a valid model
- Unfortunately this usually leads to unnecessarily high prediction error
- Alternative: find "smallest" model for which F-test comparing to full model is accepted
- This leads to multiple testing, inflated Type I error probability (and no obvious fix)
- Model selection is usually based on some alternative criteria developed specifically for that purpose

Underfitting vs overfitting: the bias-variance trade-off

- The basic problem in model selection is the familiar bias-variance trade-off problem
- Underfitting leads to biased coefficient estimates
- Overfitting leads to coefficient estimates with higher variance
- Formally, suppose we fit the two models

$$\begin{aligned} E(\mathbf{y}) &= \mathbf{X}_1\beta_1 \\ E(\mathbf{y}) &= \mathbf{X}_1\beta_1 + \mathbf{X}_2\beta_2 = \mathbf{X}\beta \end{aligned}$$

- If the second model is correct, then $\hat{\beta}_1^{(1)}$ obtained by fitting the first model will be *biased* for β_1 in general
- If the first model is correct, then $\hat{\beta}_1^{(2)}$ obtained by fitting the second model will be unbiased for β_1
- However, in that case, $\hat{\beta}_1^{(2)}$ will have higher variance than $\hat{\beta}_1^{(1)}$ in general; i.e., for any vector $\mathbf{u}$,

$$V\left(\mathbf{u}^T\hat{\beta}_1^{(2)}\right) \geq V\left(\mathbf{u}^T\hat{\beta}_1^{(1)}\right)$$

- Proof: exercise

Model selection criteria

- Overly simple and overly complex models are both bad
- Best model usually lies somewhere in the middle
- How do we find this ideal model?
- Most common approach: some model-selection criterion measuring overall quality of a model
- To be useful, such a criterion must punish both overly simple and overly complex models
- Once criterion is determined, fit a number of different models and choose the best (details later)
- We will first discuss some possible criteria

Coefficient of determination

- The simplest model quality measure is R^2

$$R^2 = \frac{T^2 - S^2}{T^2} = \frac{\frac{T^2}{n} - \frac{S^2}{n}}{\frac{T^2}{n}}$$

- Always increases when more predictors are added (does not penalize complexity)
- Can compare models of same size, but not generally useful for model selection
- Possible alternative: Adjusted R^2 (substitute unbiased estimators of σ^2)

$$R^2_{adj} = \frac{\frac{T^2}{n-1} - \frac{S^2}{n-p}}{\frac{T^2}{n-1}} = 1 - \frac{n-1}{n-p}(1 - R^2)$$

- Maximizing R^2 equivalent to minimizing SSE (or $\hat{\sigma}^2_{MLE}$)
- Maximizing R^2_{adj} equivalent to minimizing unbiased $\hat{\sigma}^2$
- Other than simplicity of interpretation, no particular justification

Cross-validation SSE

- Use cross-validation to directly assess prediction error
- Define

$$T_p^2 = \sum_{i=1}^{n} \left(y_i - \bar{y}_{(-i)}\right)^2$$

and

$$S_p^2 = \sum_{i=1}^{n} \left(y_i - \hat{y}_{i(-i)}\right)^2 = \sum_{i=1}^{n} \left(\frac{e_i}{1 - h_i}\right)^2$$

- The predictive R^2 is defined as

$$R_p^2 = \frac{T_p^2 - S_p^2}{T_p^2}$$

- Equivalently, minimize predictive sum of squares S_p^2 (often abbreviated as PRESS)

Directly estimating bias and variance

- More sophisticated approaches attempt to directly estimate bias and variance
- Suppose true expected value of y_i is μ_i
- Total mean squared error of a model fit is

$$MSE = E\sum_i(\hat{y}_i - \mu_i)^2 = \sum_i\left[(E\hat{y}_i - \mu_i)^2 + V(\hat{y}_i)\right]$$

- The first term is the "bias sum of squares" BSS (equals zero if no bias)
- The second term simplifies to

$$\sum_i V(\hat{y}_i) = \sigma^2\sum_i \mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i = \sigma^2\sum_i h_i = p\sigma^2$$

- On the other hand

$$E(RSS) = E\sum_i(y_i - \hat{y}_i)^2 = E(\mathbf{y}^T(\mathbf{I} - \mathbf{H})\mathbf{y})$$

- This equals $(n-p)\sigma^2$ when $\hat{y}_i$-s are unbiased
- If $\hat{y}_i$-s are biased, it can be shown that this term equals $BSS + (n-p)\sigma^2$
- This gives the following estimator of MSE (up to unknown σ^2)

$$RSS - (n-p)\sigma^2 + p\sigma^2 = RSS + (2p-n)\sigma^2$$

Mallow's C_p

- Dividing by σ^2 on both sides, this gives Mallow's C_p criterion

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

- This requires an estimate of σ^2
- It is customary to use $\hat{\sigma}^2$ from the largest model
- If model has no bias, then $C_p \approx p$ (exact for largest model by definition)
- An alternative expression for C_p is (exercise)

$$C_p = (p_f - p)(F - 1) + p$$

- where
  - p_f is the number of coefficients in the largest model (used to estimate σ^2)
  - F is the F-statistic comparing the model being evaluated with the largest model
- Again, if the model is "correct", then $F \approx 1$, so $C_p \approx p$

Likelihood based criterion

- A more general approach is to prefer models that improve the expected log-likelihood

$$E \sum_i \log P_{\hat{\theta}}(y_i)$$

- Here the expectation is over two independent sets of the true distribution of $\mathbf{y}$
- One set of $\mathbf{y}$ is used to estimate $\hat{\theta}$
- Akaike showed that

$$-2E \sum_i \log P_{\hat{\theta}}(y_i) \approx -2E(\text{loglik}) + 2p$$

- Here loglik is the maximized log-likelihood for the fitted model

Akaike Information Criterion

- This suggests the Akaike Information Criterion (AIC)

$$\text{AIC} = -2\text{loglik} + 2p$$

- For linear models, this is equivalent to (up to a constant)

$$\text{AIC} = n \log RSS + 2p$$

- An advantage of AIC over C_p is that it does not require an estimate of σ^2
- It is also applicable more generally (e.g., for GLMs)

Bayesian Information Criterion

- A similar criterion is the Bayesian Information Criterion (BIC)

$$\text{BIC} = -2\text{loglik} + p \log n$$

- As suggested by its name, this is derived using a Bayesian approach
- The complexity penalty for BIC is higher (except for small n), so favours simpler models

Example: SLID data — comparing pre-determined set of models

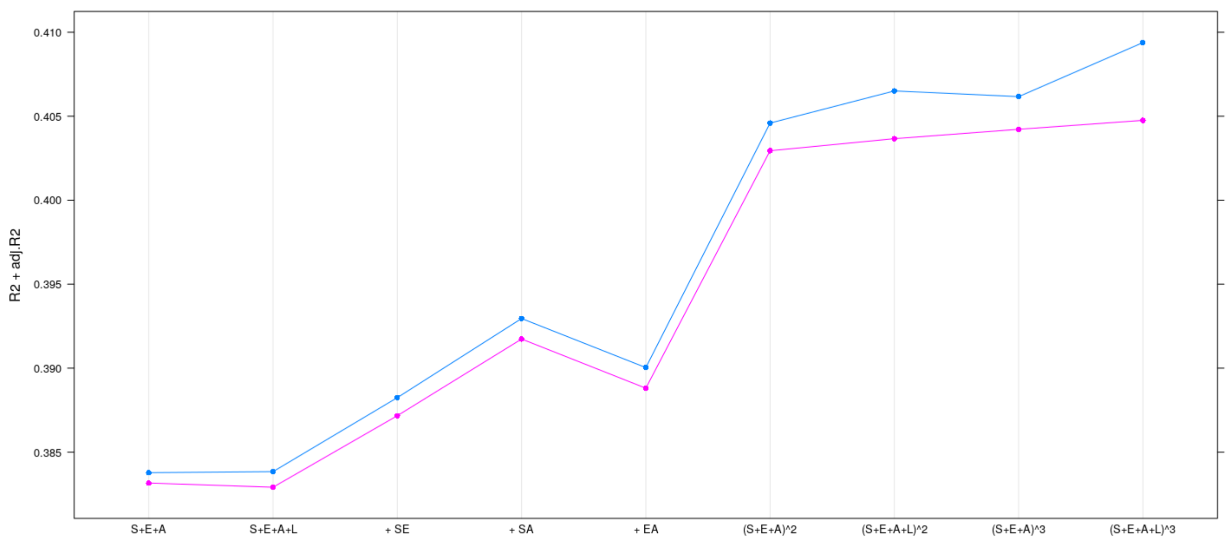
```
SLID2 <- transform(na.omit(SLID), log.wages = log(wages), edu.sq = education^2)
SLID2 <- SLID2[c("log.wages", "sex", "edu.sq", "age", "language")]
str(SLID2)
```

```
'data.frame':   3987 obs. of  5 variables:
 $ log.wages: num  2.36 2.4 2.88 2.64 2.1 ...
 $ sex      : Factor w/ 2 levels "Female","Male": 2 2 2 1 2 1 1 1 2 2 ...
 $ edu.sq   : num  225 174 196 256 225 ...
 $ age      : int  40 19 46 50 31 30 61 46 43 17 ...
 $ language : Factor w/ 3 levels "English","French",..: 1 1 3 1 1 1 1 3 1 1 ...
```

```r
fm <- list()
fm[["S+E+A"]] <- lm(log.wages ~ sex + edu.sq + poly(age, 2), data = SLID2)
fm[["S+E+A+L"]] <- lm(log.wages ~ sex + edu.sq + poly(age, 2) + language, data = SLID2)
fm[["+ SE"]] <- update(fm[[2]], . ~ . + sex:edu.sq)
fm[["+ SA"]] <- update(fm[[2]], . ~ . + sex:poly(age, 2))
fm[["+ EA"]] <- update(fm[[2]], . ~ . + edu.sq:poly(age, 2))
fm[["(S+E+A)^2"]] <- update(fm[[2]], . ~ . + (sex + edu.sq + poly(age, 2))^2)
fm[["(S+E+A+L)^2"]] <- update(fm[[2]], . ~ . + (sex + edu.sq + poly(age, 2) + language)^2)
fm[["(S+E+A)^3"]] <- update(fm[[2]], . ~ . + (sex + edu.sq + poly(age, 2))^3)
fm[["(S+E+A+L)^3"]] <- update(fm[[2]], . ~ . + (sex + edu.sq + poly(age, 2) + language)^3)
models <- factor(names(fm), levels = names(fm))
```

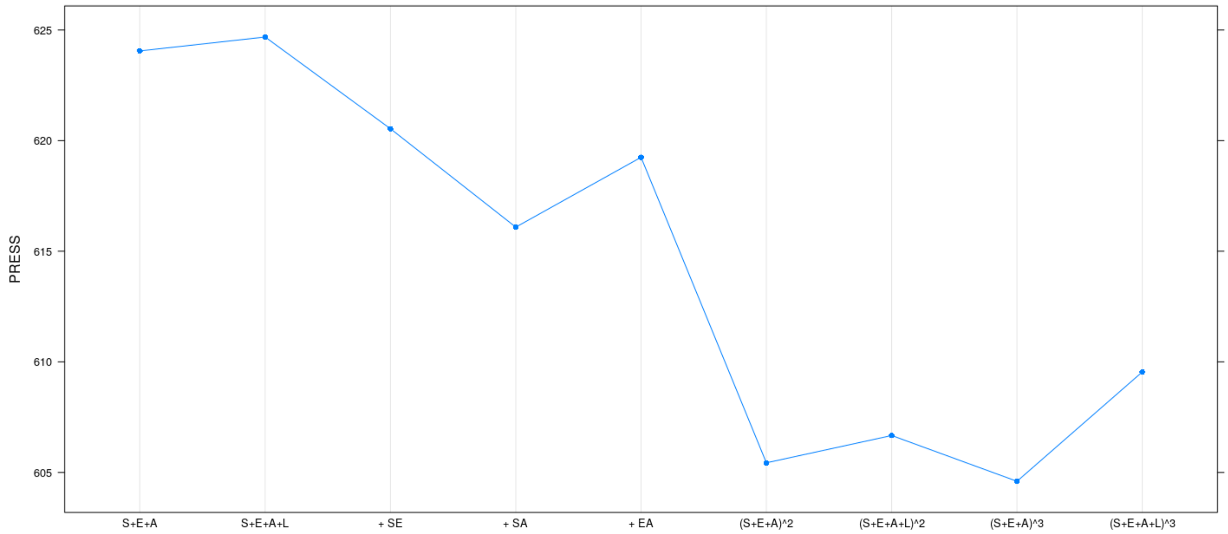
Example: SLID data — R^2 and adjusted R^2

```r
R2 <- sapply(fm, function(fit) summary(fit)$r.squared)
adj.R2 <- sapply(fm, function(fit) summary(fit)$adj.r.squared)
dotplot(R2 + adj.R2 ~ models, type = "o", pch = 16)
```



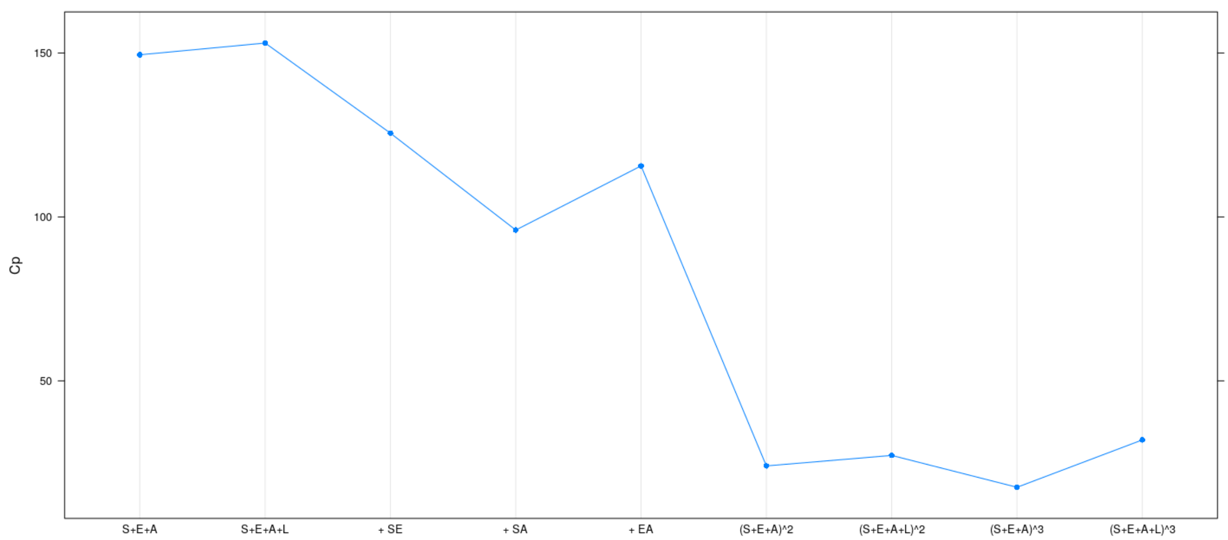
Example: SLID data — prediction SS

```r
PRESS <- sapply(fm, function(fit) sum((residuals(fit) / (1-hatvalues(fit)))^2))
dotplot(PRESS ~ models, type = "o", pch = 16)
```



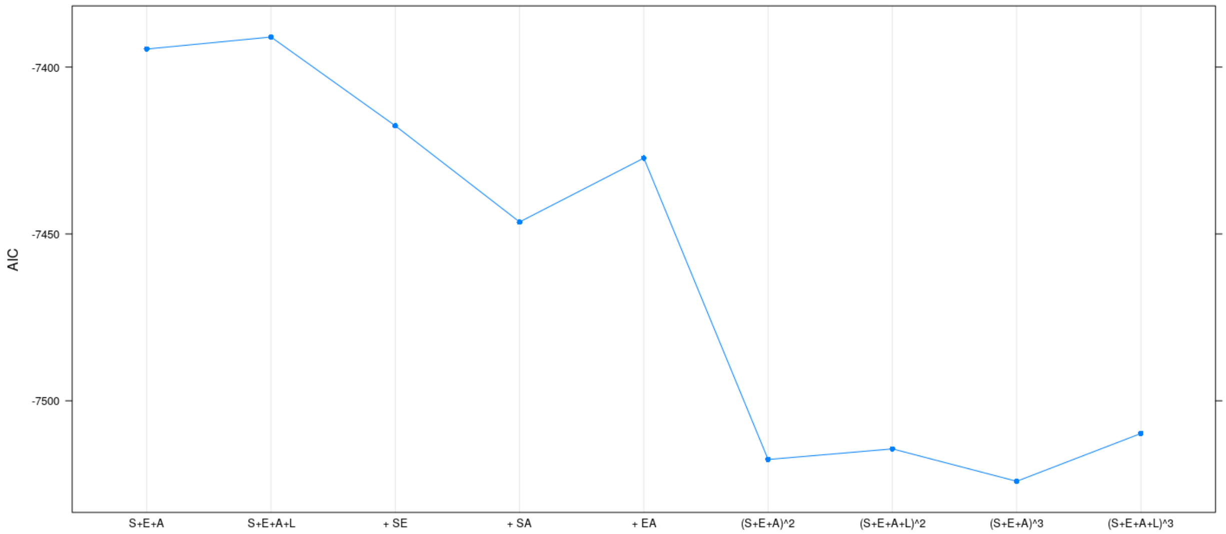
Example: SLID data — Mallow's C_p

```
sigma.sq <- summary(fm[[9]])$sigma^2 # common 'scale' for all fits
Cp <- sapply(fm, function(fit) extractAIC(fit, scale = sigma.sq)[2])
dotplot(Cp ~ models, type = "o", pch = 16)
```



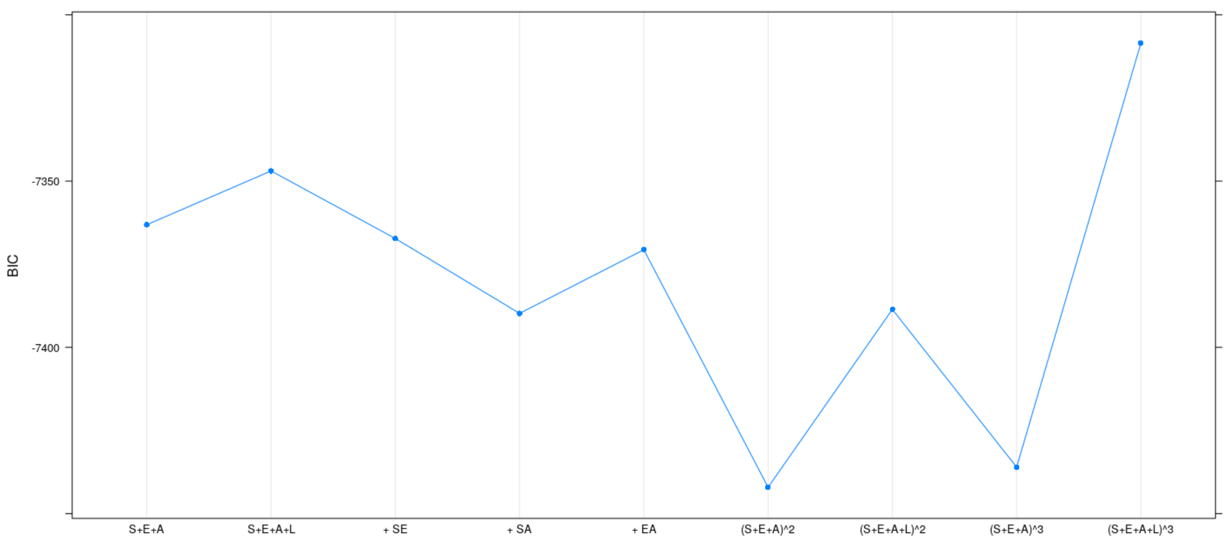
Example: SLID data — AIC

```
AIC <- sapply(fm, function(fit) extractAIC(fit)[2])
dotplot(AIC ~ models, type = "o", pch = 16)
```



Example: SLID data — BIC

```
n <- nrow(SLID2)
BIC <- sapply(fm, function(fit) extractAIC(fit, k = log(n))[2])
dotplot(BIC ~ models, type = "o", pch = 16)
```



Automatic model selection

- This process still requires us to construct a list of models to consider
- In general, the number of possible models can be large
- With k predictors, there are 2^k additive models, many more with interactions

- How do we select the “best” out of all possible models?
- Two common strategies
  - Best subset selection: exhaustive search of all possible models
  - Stepwise selection: add or drop one term at a time (only benefit: needs less time)

Best subset selection: exhaustive search

```
library(leaps)
reg.sub <- regsubsets(log.wages ~ (sex + edu.sq + poly(age, 2) + language)^3,
                      data = SLID2, nbest = 2, nvmax = 100)
t(summary(reg.sub)$outmat)
```

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edu.sq                               "*"       "*"       "*"       "*"       "*"       "*"       "*"
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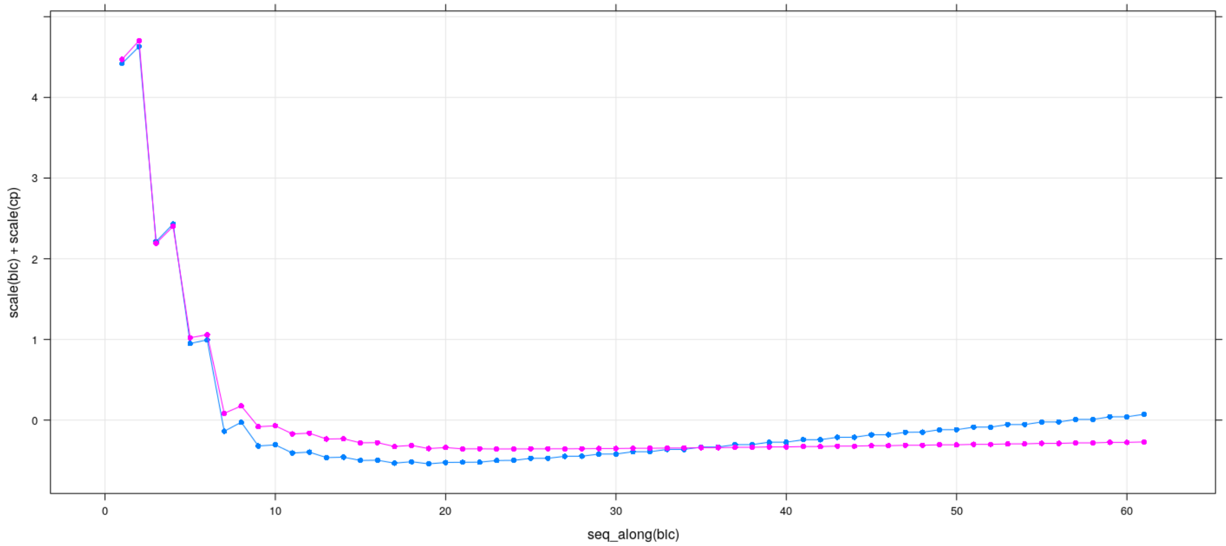
poly(age, 2)2                        "*"       "*"       "*"       "*"       "*"       "*"       "*"
languageFrench                       " "       "*"       " "       " "       " "       "*"       " "
languageOther                        " "       " "       " "       " "       " "       " "       " "
sexMale:edu.sq                       "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)1                "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2                "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:languageFrench               "*"       " "       "*"       "*"       "*"       " "       "*"
sexMale:languageOther                "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)1                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:languageFrench                " "       " "       " "       "*"       " "       " "       " "
edu.sq:languageOther                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)1:languageFrench         " "       " "       " "       " "       " "       " "       " "
poly(age, 2)2:languageFrench         " "       " "       " "       " "       " "       " "       " "
poly(age, 2)1:languageOther          " "       " "       " "       " "       " "       " "       "*"
poly(age, 2)2:languageOther          " "       " "       " "       " "       " "       " "       " "
sexMale:edu.sq:poly(age, 2)1         "*"       "*"       "*"       "*"       "*"       "*"       "*"
```

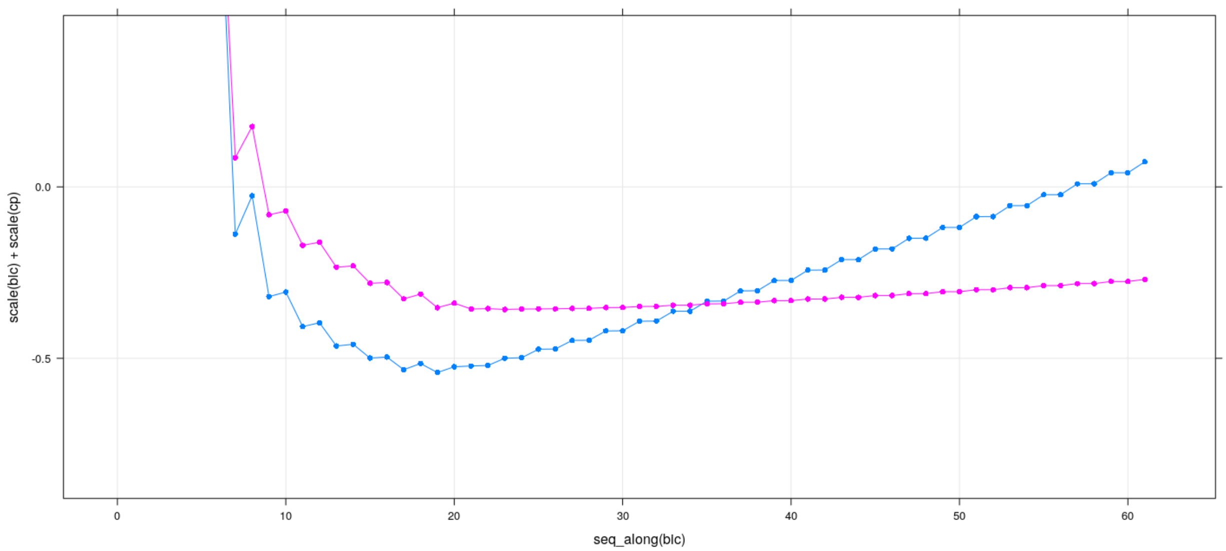
```
sexMale:edu.sq:poly(age, 2)2         "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:languageFrench        "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:languageOther         " "       " "       " "       " "       " "       " "       " "
sexMale:poly(age, 2)1:languageFrench "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2:languageFrench " "       " "       " "       " "       " "       " "       " "
sexMale:poly(age, 2)1:languageOther  "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2:languageOther  "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)1:languageFrench  " "       " "       " "       " "       "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageFrench  " "       " "       " "       " "       " "       " "       " "
edu.sq:poly(age, 2)1:languageOther   " "       " "       "*"       " "       "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageOther   " "       " "       " "       " "       " "       " "       " "
                                     22  ( 1 ) 22  ( 2 ) 23  ( 1 ) 23  ( 2 ) 24  ( 1 ) 24  ( 2 ) 25  (
sexMale                              "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq                               "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)1                        "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)2                        "*"       "*"       "*"       "*"       "*"       "*"       "*"
languageFrench                       "*"       " "       "*"       " "       " "       "*"       " "
languageOther                        " "       " "       " "       " "       " "       " "       " "
sexMale:edu.sq                       "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)1                "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2                "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:languageFrench               " "       "*"       " "       "*"       "*"       "*"       "*"
sexMale:languageOther                "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)1                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:languageFrench                " "       " "       " "       "*"       "*"       " "       "*"
edu.sq:languageOther                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)1:languageFrench         "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)2:languageFrench         " "       " "       " "       " "       " "       " "       "*"
poly(age, 2)1:languageOther          "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)2:languageOther          " "       " "       " "       " "       " "       " "       " "
sexMale:edu.sq:poly(age, 2)1         "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:poly(age, 2)2         "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:languageFrench        "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:languageOther         " "       " "       "*"       " "       "*"       "*"       "*"
sexMale:poly(age, 2)1:languageFrench "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2:languageFrench " "       " "       " "       " "       " "       " "       " "
sexMale:poly(age, 2)1:languageOther  "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2:languageOther  "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)1:languageFrench  "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageFrench  " "       " "       " "       " "       " "       " "       " "
edu.sq:poly(age, 2)1:languageOther   "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageOther   " "       " "       " "       " "       " "       " "       " "
                                     26  ( 1 ) 26  ( 2 ) 27  ( 1 ) 27  ( 2 ) 28  ( 1 ) 28  ( 2 ) 29  (
sexMale                              "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq                               "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)1                        "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)2                        "*"       "*"       "*"       "*"       "*"       "*"       "*"
languageFrench                       " "       " "       " "       " "       " "       "*"       "*"
languageOther                        " "       " "       " "       " "       " "       " "       " "
sexMale:edu.sq                       "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)1                "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2                "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:languageFrench               "*"       "*"       "*"       "*"       "*"       "*"       "*"
```

```
sexMale:languageOther                "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)1                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:languageFrench                "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:languageOther                 "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)1:languageFrench         "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)2:languageFrench         "*"       " "       "*"       "*"       "*"       "*"       "*"
poly(age, 2)1:languageOther          "*"       "*"       "*"       "*"       "*"       "*"       "*"
poly(age, 2)2:languageOther          " "       " "       "*"       " "       "*"       "*"       "*"
sexMale:edu.sq:poly(age, 2)1         "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:poly(age, 2)2         "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:languageFrench        "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:edu.sq:languageOther         "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)1:languageFrench "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2:languageFrench " "       " "       " "       " "       " "       " "       " "
sexMale:poly(age, 2)1:languageOther  "*"       "*"       "*"       "*"       "*"       "*"       "*"
sexMale:poly(age, 2)2:languageOther  "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)1:languageFrench  "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageFrench  " "       "*"       " "       "*"       "*"       " "       "*"
edu.sq:poly(age, 2)1:languageOther   "*"       "*"       "*"       "*"       "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageOther   "*"       "*"       "*"       "*"       "*"       "*"       "*"
                                     30  ( 1 ) 30  ( 2 ) 31  ( 1 )
sexMale                              "*"       "*"       "*"
edu.sq                               "*"       "*"       "*"
poly(age, 2)1                        "*"       "*"       "*"
poly(age, 2)2                        "*"       "*"       "*"
languageFrench                       "*"       "*"       "*"
languageOther                        " "       "*"       "*"
sexMale:edu.sq                       "*"       "*"       "*"
sexMale:poly(age, 2)1                "*"       "*"       "*"
sexMale:poly(age, 2)2                "*"       "*"       "*"
sexMale:languageFrench               "*"       "*"       "*"
sexMale:languageOther                "*"       "*"       "*"
edu.sq:poly(age, 2)1                 "*"       "*"       "*"
edu.sq:poly(age, 2)2                 "*"       "*"       "*"
edu.sq:languageFrench                "*"       "*"       "*"
edu.sq:languageOther                 "*"       "*"       "*"
poly(age, 2)1:languageFrench         "*"       "*"       "*"
poly(age, 2)2:languageFrench         "*"       "*"       "*"
poly(age, 2)1:languageOther          "*"       "*"       "*"
poly(age, 2)2:languageOther          "*"       "*"       "*"
sexMale:edu.sq:poly(age, 2)1         "*"       "*"       "*"
sexMale:edu.sq:poly(age, 2)2         "*"       "*"       "*"
sexMale:edu.sq:languageFrench        "*"       "*"       "*"
sexMale:edu.sq:languageOther         "*"       "*"       "*"
sexMale:poly(age, 2)1:languageFrench "*"       "*"       "*"
sexMale:poly(age, 2)2:languageFrench "*"       " "       "*"
sexMale:poly(age, 2)1:languageOther  "*"       "*"       "*"
sexMale:poly(age, 2)2:languageOther  "*"       "*"       "*"
edu.sq:poly(age, 2)1:languageFrench  "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageFrench  "*"       "*"       "*"
edu.sq:poly(age, 2)1:languageOther   "*"       "*"       "*"
edu.sq:poly(age, 2)2:languageOther   "*"       "*"       "*"
```

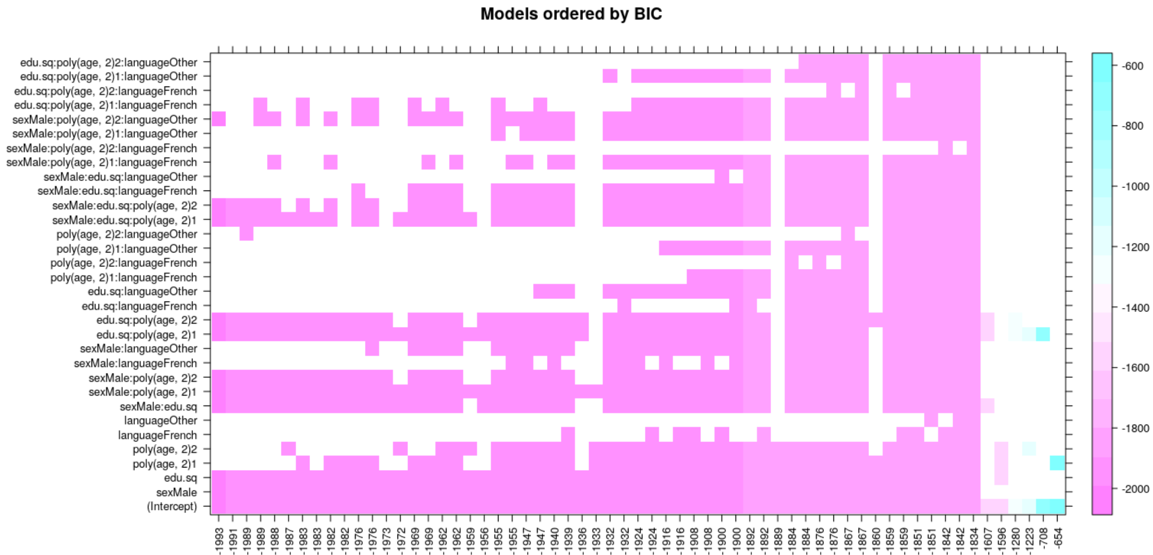
```r
xyplot(scale(bic) + scale(cp) ~ seq_along(bic), data = summary(reg.sub), grid = TRUE,
       type = "o", pch = 16)
```



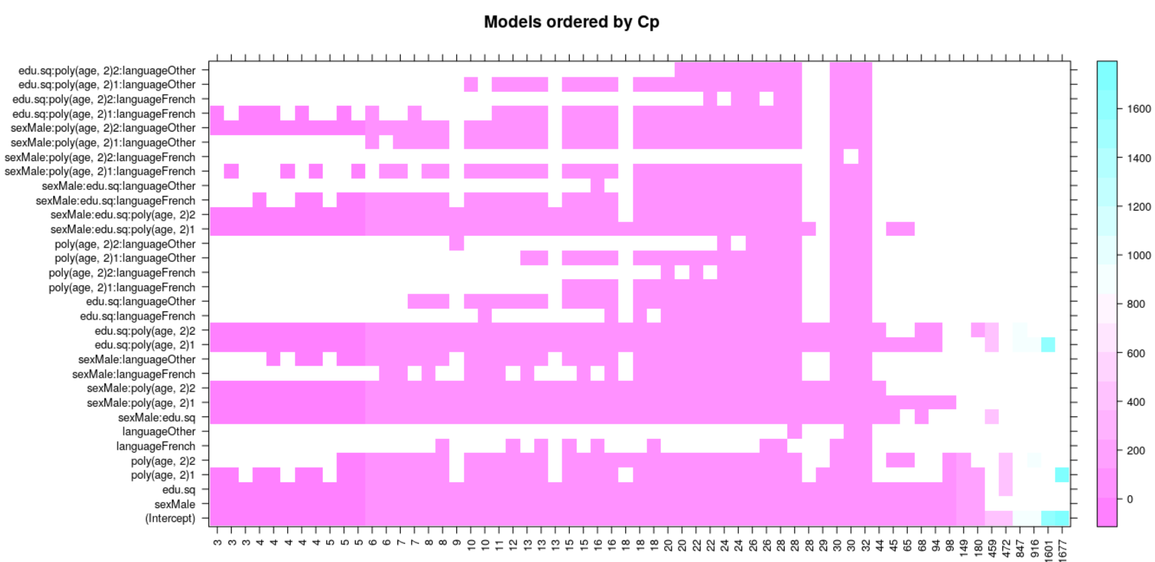

```r
xyplot(scale(bic) + scale(cp) ~ seq_along(bic), data = summary(reg.sub), grid = TRUE,
       type = "o", pch = 16, ylim = c(NA, 0.5))
```




```r
with(summary(reg.sub), {
        o <- order(bic); w <- which; is.na(w) <- w == FALSE
        wbic <- w * bic
        levelplot(wbic[o, ], xlim = as.character(round(bic))[o], xlab = NULL, ylab = NULL,
                  scales = list(x = list(rot = 90)), main = "Models ordered by BIC")
    })
```




```r
with(summary(reg.sub), {
        o <- order(cp); w <- which; is.na(w) <- w == FALSE
        wcp <- w * cp
        levelplot(wcp[o, ], xlim = as.character(round(cp))[o], xlab = NULL, ylab = NULL,
                  scales = list(x = list(rot = 90)), main = "Models ordered by Cp")
    })
```



Handling dummy variables, interactions, etc.

- One problem with this approach: considers each column of $\mathbf{X}$ separately
- Usually we would keep or drop all columns for a term (factor, polynomial) together
- Similarly, an interaction term usually not meaningful without main effects and lower order interactions

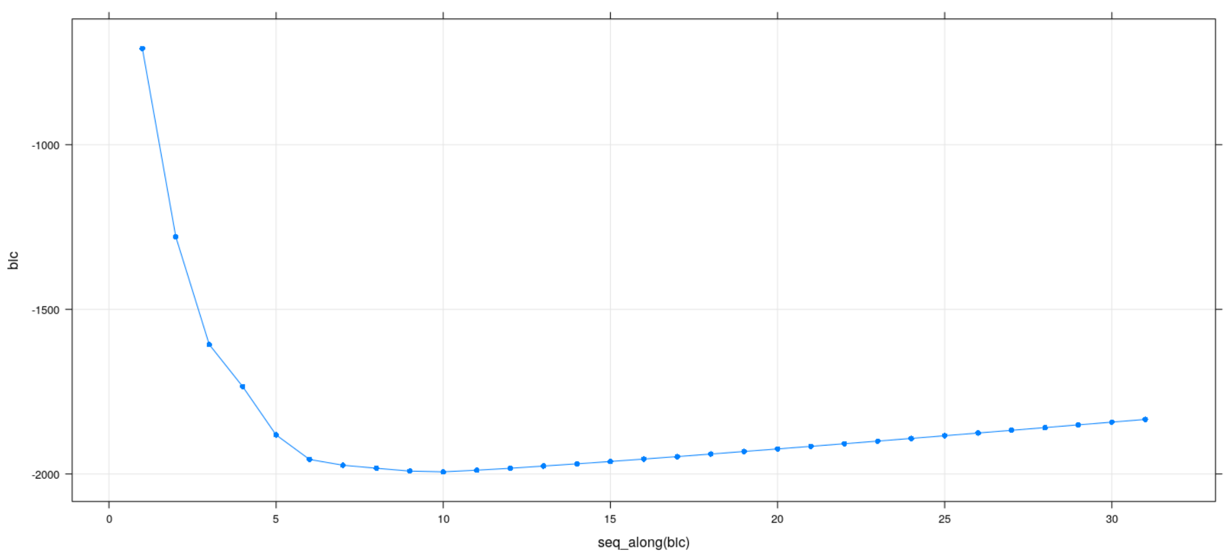
- Such considerations are not automated by `regsubsets()` and have to be handled manually

Best subset selection: stepwise search

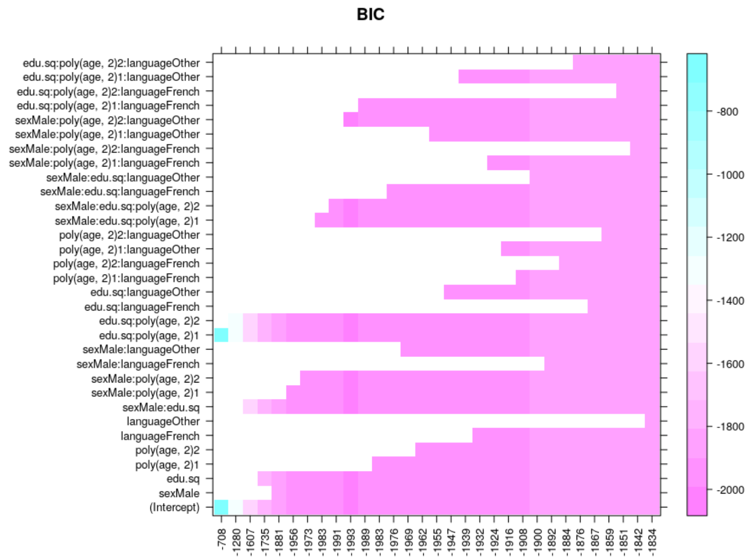
- Stepwise selection methods are *greedy algorithms* that add or drop one predtctor at a time
- This greatly limits the number of subsets evaluated
- Makes the problem tractable if number of predictors is large
- On the other hand, stepwise methods explore only a fraction of possible subsets
- For many predictors, rarely finds the optimal model
- Forward selection
  - Find best one-variable model
  - Find best two-variable model by adding another variable
  - and so on
- That is, do not look at all two-variable models; only ones that contain the best one-variable model
- Backward selection: start with full model and eliminate variables successively
- Sequential replacement: consider both adding and dropping in each step
- Stepwise selection is supported by `regsubsets()`
- Also implemented in `MASS::stepAIC()` and `stats::step()`

Best subset selection: forward selection

```
reg.forward <-
    regsubsets(log.wages ~ (sex + edu.sq + poly(age, 2) + language)^3,
               data = SLID2, nvmax = 100, method = "forward")
xyplot(bic ~ seq_along(bic), data = summary(reg.forward), grid = TRUE, type = "o", pch = 16)
```

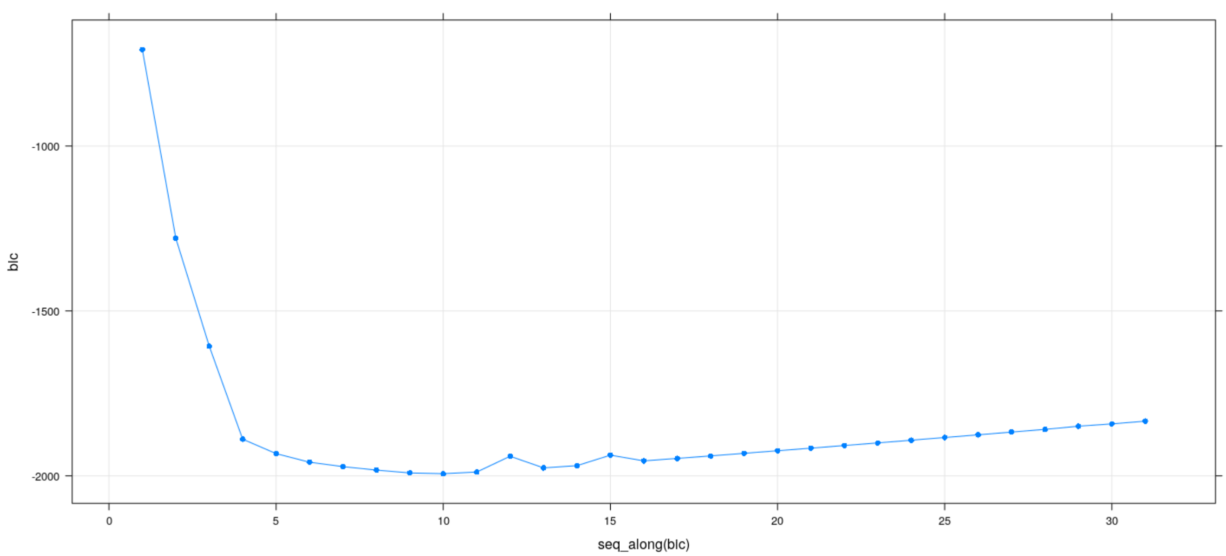


```
with(summary(reg.forward), {
         w <- which; is.na(w) <- w == FALSE
         wbic <- w * bic
         levelplot(wbic, xlim = as.character(round(bic)), xlab = NULL, ylab = NULL,
                   scales = list(x = list(rot = 90)), main = "BIC")
    })
```

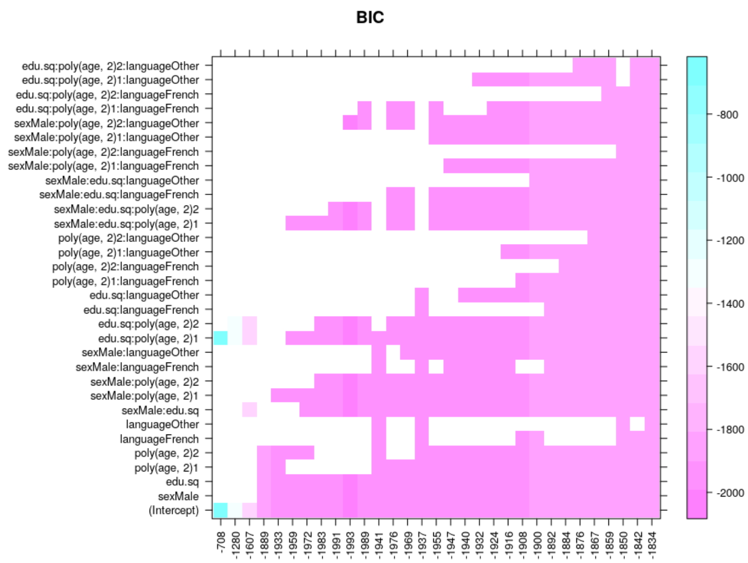


Best subset selection: sequential replacement

```
reg.seqrep <-
    regsubsets(log.wages ~ (sex + edu.sq + poly(age, 2) + language)^3,
               data = SLID2, nvmax = 100, method = "seqrep")
xyplot(bic ~ seq_along(bic), data = summary(reg.seqrep), grid = TRUE, type = "o", pch = 16)
```



```r
with(summary(reg.seqrep), {
         w <- which; is.na(w) <- w == FALSE
         wbic <- w * bic
         levelplot(wbic, xlim = as.character(round(bic)), xlab = NULL, ylab = NULL,
                   scales = list(x = list(rot = 90)), main = "BIC")
    })
```



Benefits and drawbacks of automated model selection

- Can quickly survey a large number of potential models
- However, there are many drawbacks to this approach
- In fact, automated model selection basically invalidates inference
- This is because all derivations assume that model and hypotheses are prespecified
- As a result, for the model chosen by automated selection
  - Test statistics no longer follow t / F distributions
  - Standard errors have negative bias, and confidence intervals are falsely narrow
  - p-values are falsely small
  - Regression coefficients are biased away from 0

Simulation example: no predictive relationship

- Simulate $V_2, \ldots, V_{21} \sim$ i.i.d. $N(0, 1)$
- Simulate independent $V_1 \sim N(0, 1)$
- Regress V_1 on $V_2, \ldots, V_{21}$
- Select model using `stepAIC()`

```r
library(MASS)
d <- as.data.frame(matrix(rnorm(100 * 21), 100, 21))
fm.step <- stepAIC(lm(V1 ~ ., data = d), direction = "both", trace = 0)
```

```r
summary(fm.step)
```

```

Call:
lm(formula = V1 ~ V2 + V3 + V6 + V9 + V13, data = d)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.20598 -0.59320 -0.05848  0.56056  2.34801 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)   
(Intercept) -0.03006    0.08906  -0.338  0.73645   
V2           0.13104    0.09139   1.434  0.15493   
V3          -0.16376    0.08943  -1.831  0.07026 . 
V6          -0.29802    0.10074  -2.958  0.00391 **
V9           0.15936    0.08864   1.798  0.07542 . 
V13          0.17006    0.08214   2.070  0.04116 * 
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.8665 on 94 degrees of freedom
Multiple R-squared:  0.1932,	Adjusted R-squared:  0.1503 
F-statistic: 4.501 on 5 and 94 DF,  p-value: 0.001011
```

```r
with(summary(fm.step), pf(fstatistic[1], fstatistic[2], fstatistic[3], lower.tail = FALSE))
```

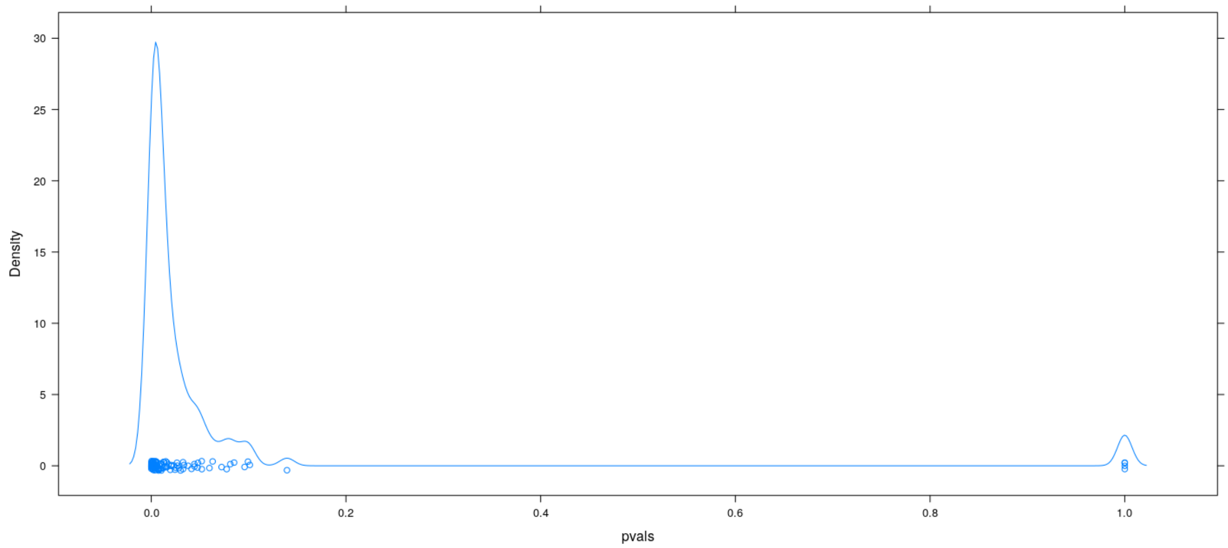
```
     value 
0.00101054 
```

```r
## Replicate this experiment
pvals <-
    replicate(100,
    {
        d <- as.data.frame(matrix(rnorm(100 * 21), 100, 21))
        fm.step <- stepAIC(lm(V1 ~ ., data = d), direction = "both", trace = 0)
        if (length(coef(fm.step)) > 1)
            with(summary(fm.step), pf(fstatistic[1], fstatistic[2], fstatistic[3], lower.tail = FALSE))
        else 1
    })
sum(pvals < 0.05)
```

```
[1] 84
```

Simulation example: no predictive relationship

```r
densityplot(~ pvals)
```

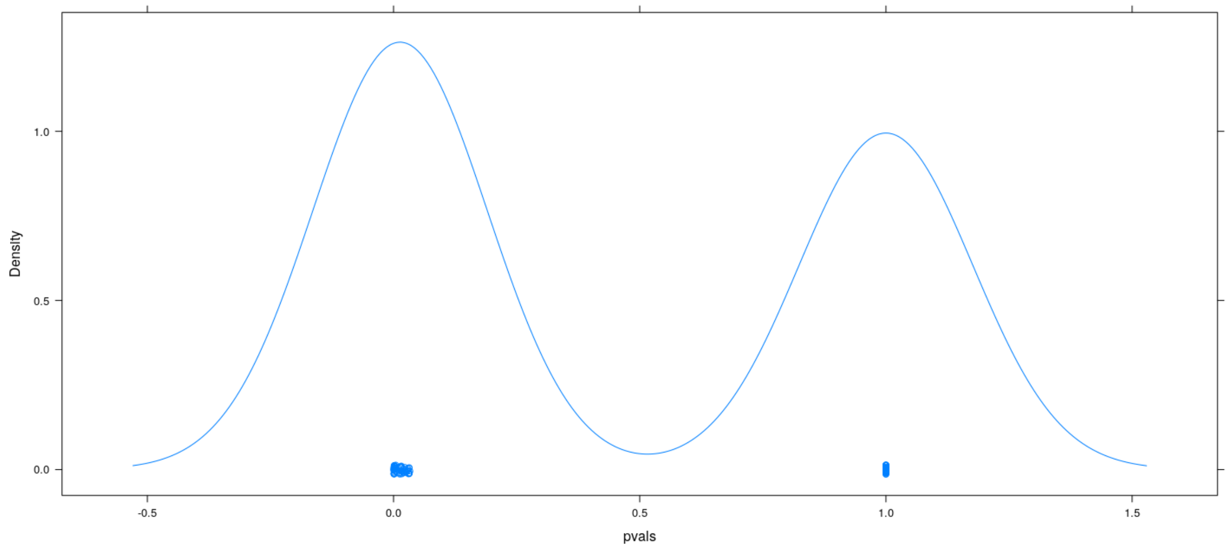


- Results are slightly better when using BIC rather than AIC, but still bad
- Select model using `stepAIC(..., k = log(n))`

```
pvals <-
    replicate(100,
    {
        d <- as.data.frame(matrix(rnorm(100 * 21), 100, 21))
        fm.step <- stepAIC(lm(V1 ~ ., data = d), direction = "both", trace = 0, k = log(100))
        if (length(coef(fm.step)) > 1)
            with(summary(fm.step), pf(fstatistic[1], fstatistic[2], fstatistic[3], lower.tail = FALSE))
        else 1
    })
sum(pvals < 0.05)
```

```
[1] 56
```

```
densityplot(~ pvals)
```



Summary

- Automated model selection has its uses
- However, blindly applying it without thinking about the problem is dangerous
- Many applied studies have no prespecified hypothesis
- Especially in observational studies (e.g., public health and social sciences)
- Model is often chosen by automated selection, but interpreted as if prespecified
- Result: much more than 5% of “significant” results are probably false