## Set S04 - Model comparison

STAT 401 (Engineering) - Iowa State University

April 24, 2017

## Comparing nested models

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How do we compare non-nested models?

## $R^2$ always increases as explanatory variables are added

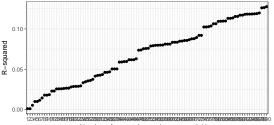
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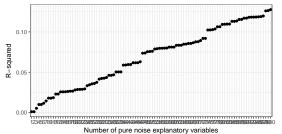
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Number of pure noise explanatory variables

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For this reason, sometimes  $R^2$  is reported with a subscript that indicates the number of  $\beta$ s in the model.

## Adjusted R-squared

One way to remedy this is to use "adjusted  ${\cal R}^2$ " which can be calculated using the formula

$$\overline{R}^2 = 1 - \frac{(1 - R^2)(n - 1)}{n - p - 1}$$

#### where

- ullet  $R^2$  is the unadjusted  $R^2$
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The idea with adjusted  $R^2$  is that it only increases if the inclusion of a new explanatory variable is more than one would expect to see by chance.

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- AIC:  $-2 \log L(\hat{\theta}_{MLE}) + 2p$
- BIC:  $-2 \log L(\hat{\theta}_{MLE}) + p \log(n)$
- AICc:  $-2 \log L(\hat{\theta}_{MLE}) + 2p(p+1)/(n-p-1)$

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There are a number of alternatives that also modify the "fit" component:

- DIC:  $-2 \log L(E[\theta|y]) + 2p_D$  (effective number of parameters)
- BPIC:  $-2 \log p(\tilde{y}|E[\theta|y]) + 2p_D$
- •

# Obtaining AIC/BIC in R

```
lm1 <- lm(Fertility ~ . , data = swiss)</pre>
AIC(lm1)
[1] 326.0716
BIC(lm1)
Γ17 339.0226
lm2 <- update(lm1, . ~ . -Examination)</pre>
AIC(lm1, lm2)
    df ATC
lm1 7 326.0716
lm2 6 325.2408
BIC(lm1, lm2)
    df
       BIC
lm1 7 339.0226
lm2 6 336.3417
```

## Obtaining AICc in R

```
AICcmodavg::AICc(lm1)
Γ17 328.9434
AICcmodavg::AICc(1m2)
[1] 327.3408
sme::AICc(lm1)
Γ17 328.9434
sme::AICc(lm2)
[1] 327.3408
```

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$$p(M_j|y) = \frac{p(y|M_j)p(M_j)}{\sum_i p(y|M_i)p(M_i)} = \frac{1}{1 + \sum_{i \neq j} \frac{p(y|M_i)}{p(y|M_j)} \frac{p(M_i)}{p(M_j)}}$$

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This integral provides a natural penalty for increased number of parameters. BIC is an asymptotic approximation to  $p(y|M_j)$ .

## Bayes Factors in R

```
library("bayess")
m <- BayesReg(swiss$Fertility, swiss[,-1])
         PostMean PostStError Log10bf EvidAgaH0
Intercept 70.1426
                     1.0339
         -3.7865 1.5463 0.4357
                                         (*)
x1
         -1.9939 1.9614 -0.6087
x2
         -8.1123 1.7043 3.3083
                                     (****)
x3
x4
         4.2062 1.4240 0.9664
                                        (**)
x5
          3.0389
                     1.0767 0.8215
                                       (**)
Posterior Mean of Sigma2: 50.2438
Posterior StError of Sigma2: 71.877
```

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## Bayesian model averaging

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$$p(\mu|y) = \sum_{j=1}^{J} p(\mu|M_j, y) p(M_j|y)$$

and model averaging for an unknown predictive value  $\tilde{y}$  is

$$p(\tilde{y}|y) = \sum_{j=1}^{J} p(\tilde{y}|M_j, y) p(M_j|y).$$

## AIC model averaging

You can also perform AIC model averaging using Akaike weights:

$$w_j = \frac{e^{-\Delta_j}/2}{\sum_{i=1}^{J} e^{-\Delta_i}/2}$$

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Since there is no notion of a posterior distribution, we calculate an estimate and standard error of quantities of interest. For example, a model averaged mean estimate is

$$\hat{\mu} = \sum_{j=1}^{J} \hat{\mu}_j w_j.$$

### Step-wise model selection

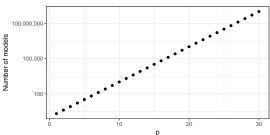
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### Step-wise model selection

Once you have chosen a criteria, a common approach is to choose the model that optimizes that criteria. But in regression problems there are  $2^p$  models to consider which is often too many to enumerate. An alternative is to use a stepwise selection procedure that compares all neighboring models.



# Stepwise selection in R

```
d \leftarrow data.frame(X = X) \% \% mutate(Y = 10 * X.1 + 10 * X.2 + 10 * X.3 
                                                                                                                           X.4 + X.5 + X.6 +
                                                                                                              .1 * X.7 + .1 * X.8 + .1 * X.9 +
                                                                                                       rnorm(n()))
m \leftarrow step(lm(y \sim ., data = d), k = 2, trace=FALSE) # AIC
summary(m)
Call:
lm(formula = y ~ X.1 + X.2 + X.3 + X.4 + X.5 + X.6 + X.7 + X.8 +
           X.9 + X.12 + X.13 + X.17 + X.21 + X.27 + X.28 + X.30 + X.31 +
           X.34 + X.48 + X.49 + X.61 + X.62 + X.67 + X.71 + X.82 + X.83 +
           X.93, data = d)
 Residuals:
              Min
                                           10 Median
                                                                                              30
                                                                                                                     Max
-2.68780 -0.67529 -0.02836 0.63979 2.73789
Coefficients:
                                   Estimate Std. Error t value Pr(>|t|)
X.1
                                  X.2
                                                                   0.02999 334.288 < 2e-16 ***
                                 10.02637
Х.3
                                 9.96052
                                                                   0.03106 320.687 < 2e-16 ***
X.4
                                   0.97607
                                                                    0.03151 30.973 < 2e-16 ***
X.5
                                                                    0.03187 33.030 < 2e-16 ***
                                   1.05271
X.6
                                                                    0.02914 33.522 < 2e-16 ***
                                    0.97690
X.7
                                    0.09115
                                                                     0.03149 2.895 0.003881 **
X.8
                                  0.11682
                                                                     0.02966
                                                                                             3.938 8.79e-05 ***
X.9
                                 0.11488
                                                                     0.03156
                                                                                              3.640 0.000287 ***
X.12
                                   -0.06478
                                                                     0.03002 -2.158 0.031194 *
```

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## Assessing predictive performance

Sometimes, we are just interested in developing a model with a good predictive performance.

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- training data set
- testing data set

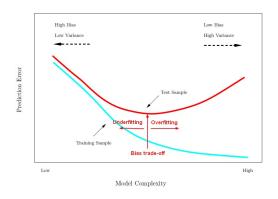
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- training data set
- testing data set

Use the training data set to build your model and then use your testing data set to evaluate the fit.

## Overfitting



https://gerardnico.com/wiki/data\_mining/overfitting

# Example splitting in R

```
d \leftarrow data.frame(X = X) \%\% mutate(y = 10 * X.1 + 10 * X.2 + 10 * X.3 + 10 * X
                                                                                                                                                            X.4 + X.5 + X.6 +
                                                                                                                                            .1 * X.7 + .1 * X.8 + .1 * X.9 +
                                                                                                                                   rnorm(n()),
                                                                                                                            train = rbinom(n(), 1, 0.5))
train <- d %>% filter(train == 1) %>% dplyr::select(-train)
test <- d %>% filter(train == 0) %>% dplyr::select(-train)
m <- step(lm(y ~ ., data = train), k = log(nrow(train)), trace=FALSE)
m
Call:
lm(formula = v ~ X.1 + X.2 + X.3 + X.4 + X.5 + X.6 + X.8 + X.9 +
              X.42, data = train)
 Coefficients:
 (Intercept)
                                                                                                                           X.2
                                                                                                                                                                                                                          X.4
                                                                                                                                                                                                                                                                                                                         X.6
                                                                                                                                                                                                                                                                                                                                                                         X.8
                                                                           X.1
                                                                                                                                                                          X.3
                                                                                                                                                                                                                                                                          X.5
                                                      10.02275 10.09242
                                                                                                                                                             9.93224
                                                                                                                                                                                                             1.02931
                                                                                                                                                                                                                                                            0.96461
                                                                                                                                                                                                                                                                                                           1.02814
                                                                                                                                                                                                                                                                                                                                                           0.10513
              0.02409
                                                                                                                                                                                                                                                                                                                                                                                                          0.1
                         X 42
            -0.13081
test <- test %>% bind_cols(data.frame(prediction = predict(m, newdata = test)))
# Calculate mean sum of squared errors
with(test, mean((y-prediction)^2))
```

[1] 1.14051

The model chosen by the test-training split will be sensitive to the test data set chosen.

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#### Two special cases:

- Leave-one-out cross-validation (LOO-CV)
- k-fold cross validation

### Cross-validation in R

```
library(DAAG)
m <- lm(y~., data = d %>% dplyr::select(-train))
cv <- cv.lm(data = d, form.lm = m, m=nrow(d)/5, plotit=FALSE)
Analysis of Variance Table
Response: y
           Df Sum Sg Mean Sg F value Pr(>F)
            1 104960 104960 1.04e+05 < 2e-16 ***
X.1
X.2
            1 114848 114848 1.14e+05 < 2e-16 ***
X.3
            1 97843
                      97843 9.73e+04 < 2e-16 ***
X.4
               1064 1.06e+03 < 2e-16 ***
X.5
               992
                       992 9.87e+02 < 2e-16 ***
X.6
               1110
                        1110 1.10e+03 < 2e-16 ***
X.7
                  11
                          11 1.09e+01 0.00097 ***
X.8
                           2 1.51e+00 0.21926
X.9
                           7 7.38e+00 0.00673 **
X.10
                   0
                           0 2.70e-01 0.60023
X.11
                   0
                           0 4.00e-02 0.84768
X.12
                   0
                           0 4.00e-01 0.52756
X.13
                   0
                           0 2.50e-01 0.61982
X.14
                   0
                           0 1.40e-01 0.71302
X.15
                           1 5.20e-01 0.47089
X.16
                   0
                           0 4.10e-01 0.51996
X.17
                   0
                           0 1.20e-01 0.72433
X.18
                           4 3.97e+00 0.04656 *
X.19
                           1 1.14e+00 0.28620
X.20
                           1 1.00e+00 0.31700
X.21
                   0
                           0 1.60e-01 0.69183
X.22
                           0 1.50e-01 0.69504
```