STAT406- Methods of Statistical Learning Lecture 4

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Proper use of CV

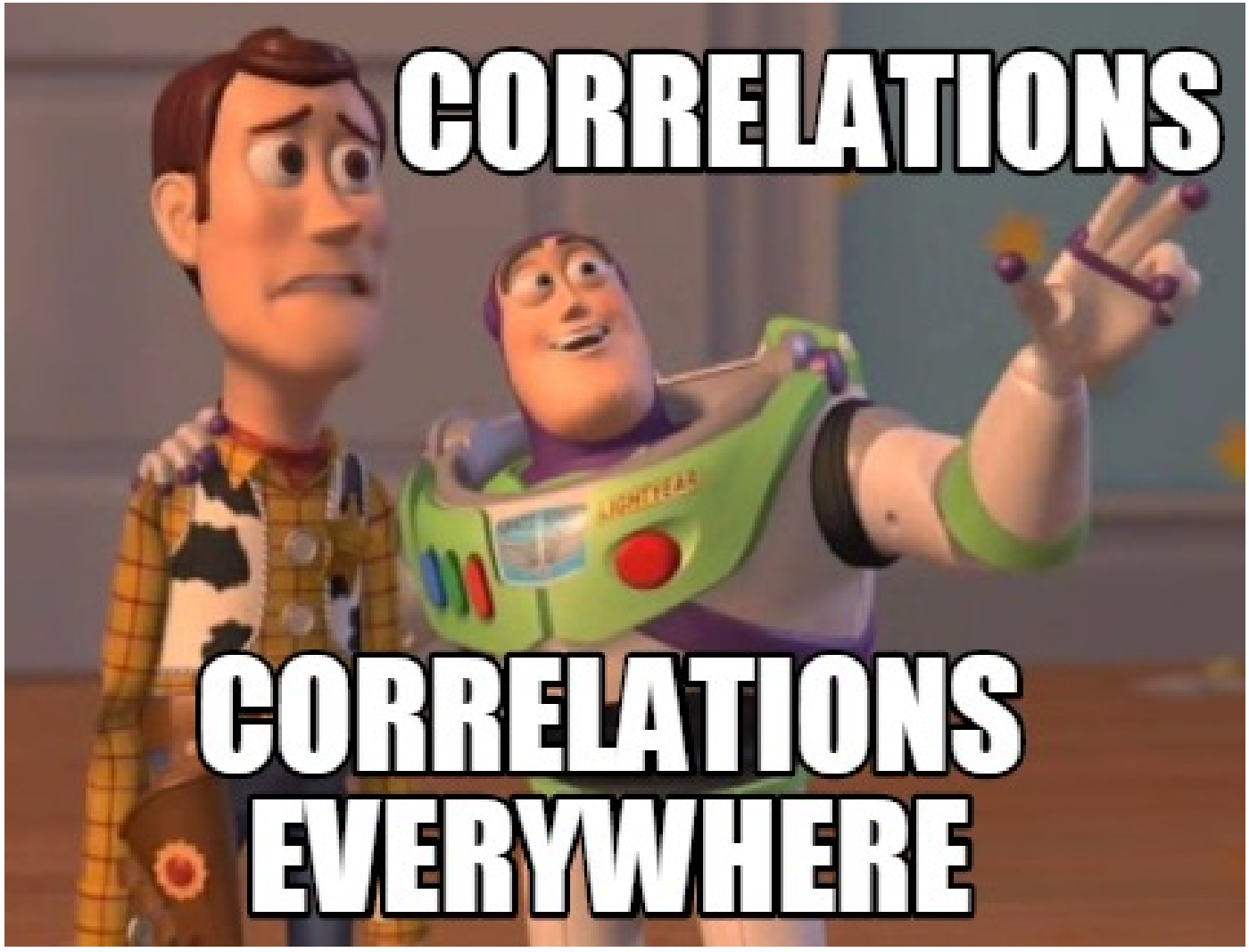
- An example of the importance and relevance of what we discussed in our last class:

  Ambroise, C. and McLachlan, G.J. Selection bias in gene extraction on the basis of microarray gene-expression data, PNAS, 2002, 99 (10), 6562-6566.

  https://doi.org/10.1073/pnas.102102699

Discussion points

- Why? Why would anybody want to **not** use all available features?
- “Somewhat obvious”: model parsimony, identify features that are relevant for the process under study.
- “Not so obvious?”: does prediction suffer if we use fewer variables? how much variability is induced by the feature selection step?


CORRELATIONS
CORRELATIONS
EVERYWHERE

Model / feature selection

- Simple example:

```
set.seed(123)
x1 <- rnorm(506)
x2 <- rnorm(506, mean=2, sd=1)
x3 <- rexp(506, rate=1)
x4 <- x2 + rnorm(506, sd=.1)
x5 <- x1 + rnorm(506, sd=.1)
x6 <- x1 - x2 + rnorm(506, sd=.1)
x7 <- x1 + x3 + rnorm(506, sd=.1)
y <- x1*3 + x2/3 + rnorm(506, sd=2.2)
```

- Variables X_1 and X_2 are clearly important. But they are also highly correlated to X_4, X_5, X_6 and X_7.

Model / feature selection

- However, nothing is significant?

```
> summary(lm(y~., data=x))

Call:
lm(formula = y ~ ., data = x)
Residuals:
   Min     1Q Median     3Q    Max
-6.882 -1.474 -0.033  1.415  5.823

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.03457    0.23018   0.150   0.8807
x1           3.22612    1.68088   1.919   0.0555 .
x2           0.23867    1.39355   0.171   0.8641
x3          -0.35926    0.98680  -0.364   0.7160
x4          -0.69359    0.99025  -0.700   0.4840
x5           0.09271    0.91162   0.102   0.9190
x6          -0.73887    1.01114  -0.731   0.4653
x7           0.31651    0.98610   0.321   0.7484
---
Signif. codes:  0 ’***’ 0.001 ’**’ 0.01 ’*’ 0.05 ’.’ 0.1 ’ ’ 1

Residual standard error: 2.148 on 498 degrees of freedom
Multiple R-squared: 0.6353,Adjusted R-squared: 0.6302
F-statistic: 123.9 on 7 and 498 DF,  p-value: < 2.2e-16
```

Model / feature selection

- But...

```
> summary(lm(y~x1+x2, data=x))

Call:
lm(formula = y ~ x1 + x2, data = x)

Residuals:
    Min      1Q  Median      3Q     Max
-6.9303 -1.5736 -0.0068  1.3840  5.9567

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.00733    0.20900   0.035  0.97204
x1           2.89168    0.09806  29.490  < 2e-16 ***
x2           0.27903    0.09249   3.017  0.00268 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.141 on 503 degrees of freedom
Multiple R-squared: 0.6343,Adjusted R-squared: 0.6328
F-statistic: 436.2 on 2 and 503 DF,  p-value: < 2.2e-16
```

Model / feature selection

- Even worse...

```
> summary(lm(y~x1+x2+x4, data=x))

Call:
lm(formula = y ~ x1 + x2 + x4, data = x)

Residuals:
    Min      1Q  Median      3Q     Max
-6.8064 -1.5229 -0.0308  1.4226  5.8861

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.0001127  0.2093588   0.001    1.000
x1           2.8964461  0.0983390  29.454   <2e-16 ***
x2           0.9740807  0.9917783   0.982    0.326
x4          -0.6934442  0.9851714  -0.704    0.482
---
Signif. codes:  0 ’***’ 0.001 ’**’ 0.01 ’*’ 0.05 ’.’ 0.1 ’ ’ 1

Residual standard error: 2.142 on 502 degrees of freedom
Multiple R-squared: 0.6347,Adjusted R-squared: 0.6325
F-statistic: 290.7 on 3 and 502 DF,  p-value: < 2.2e-16
```

Model / feature selection

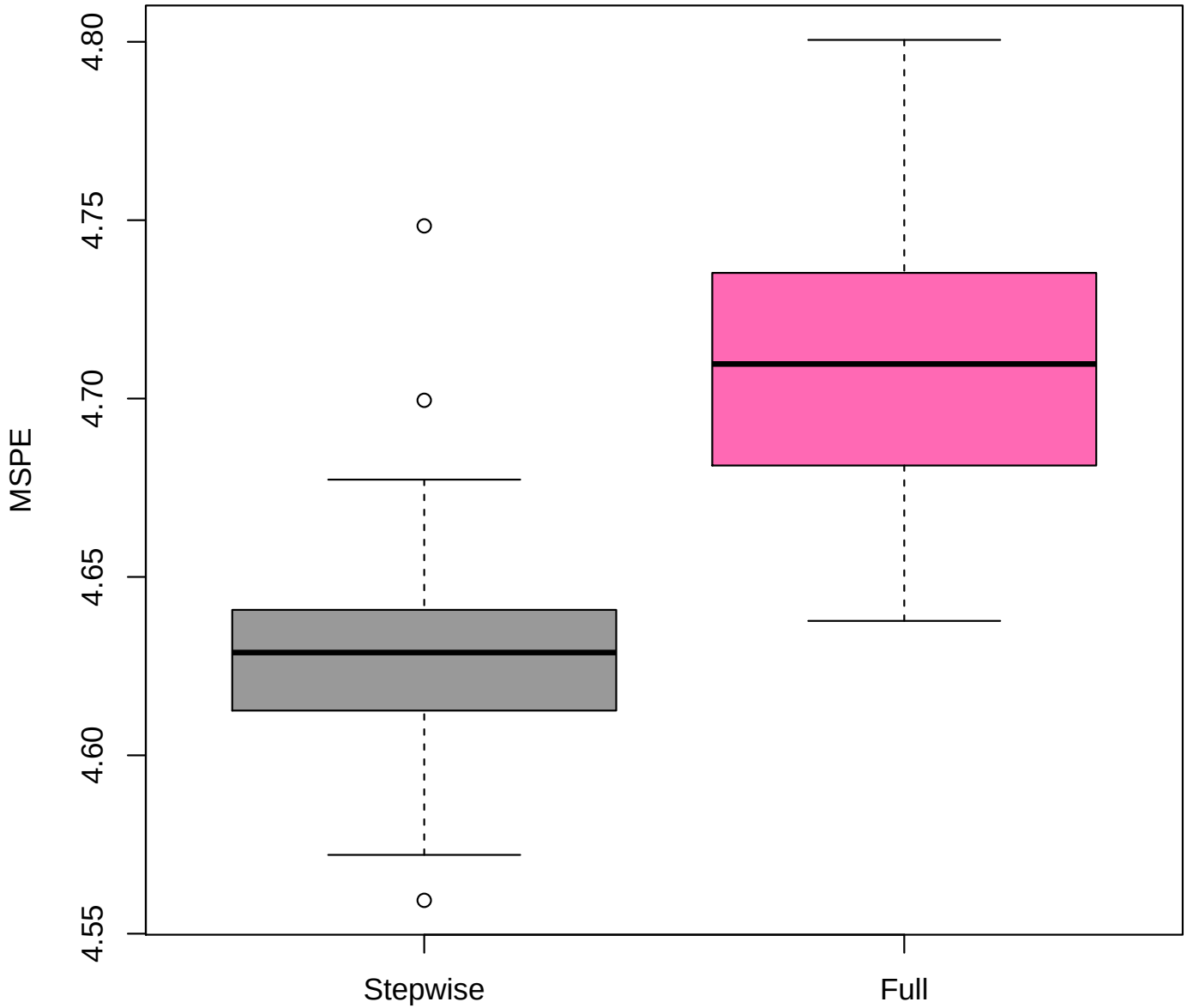
- If we use AIC

```
> st <- stepAIC(null,
      scope=list(lower=null, upper=full))
> st

Call:
lm(formula = y ~ x1 + x6, data = x)

Coefficients:
(Intercept)           x1           x6
  -0.000706     3.175239    -0.282906
```

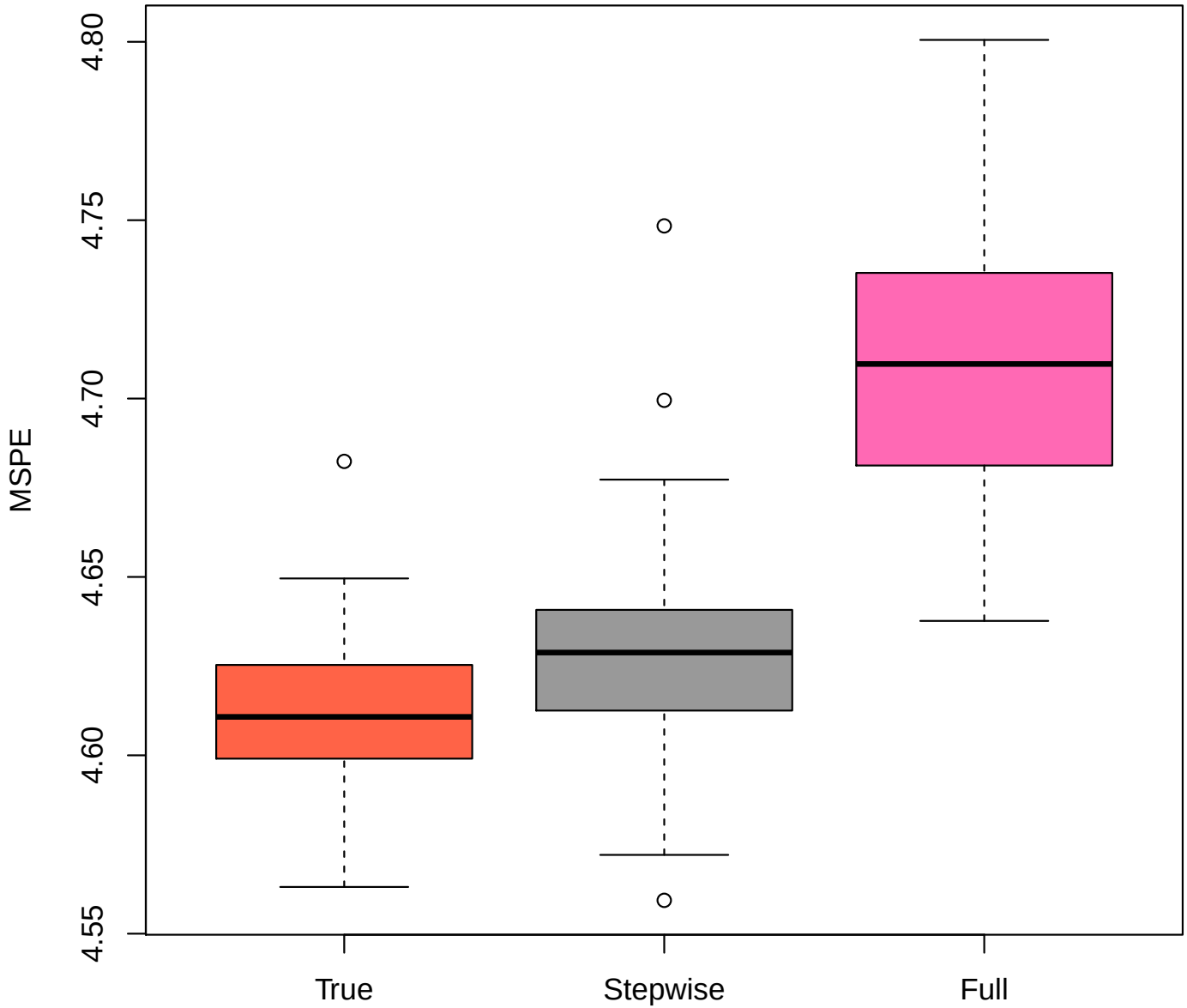
Discussion points

- Modeling problem (important variables may be missed)
- Prediction? Does stepwise give “the best” predicting model?

MSPEs



MSPEs



Discussion points

- Correlated covariates have become prevalent
- Researchers can (and do) collect data “blindly”
- Data are collected without a specific question in mind

Discussion points

- Correlated covariates:
- Mask each other when included simultaneously in a model

- May reduce prediction accuracy

Model / feature selection

One strategy:

- (1): Select models to be considered
- (2): Select a quantitative criterion to compare them (e.g. AIC, C_p, CV-based $\widehat{\text{MSPE}}$)
- (3): Choose a strategy to explore the models under consideration

Model / feature selection

For example:

- (1): Consider all possible models
- (2): Use AIC to compare them
- (3): Best subset search (2^p fits!)
- (3'): Stepwise search

- Is this strategy prediction-based?

AIC?

Why not compare models using residual sum of squares, or R^2?

LS vs MLE

Note that, if we assume that the error distribution is Gaussian, then a least squares fit for a linear regression model is the same as the MLE fit

... or is it?

Comparing models

- Comparing likelihoods / residuals isn’t very useful
- More complex models have higher likelihoods (smaller residuals)
- The Akaike Information Criterion provides a way to compare models with different number of parameters
- There are many different ways to motivate it

Comparing models

- We can measure the “distance” between the true distribution of the data ($f_0(y)$) and our model $f(y, \theta)$

$$d(\theta, f_0) = E_0[-2\,\ell(y, \theta)] =$$

$$\int -2\,\ell(y, \theta)\; f_0(y)\, dy =$$

$$2\left[\mathcal{K}(\theta, f_0) - \int \log(f_0(y))\, f_0(y)\, dy\right]$$

Comparing models

- Given our estimator $\hat{\theta}_n$ we could use

$$d(\hat{\theta}_n, f_0) = E_0 \left[-2 \, \ell(y, \theta) \right]_{\theta = \hat{\theta}_n}$$

  to see "how far" our model-based estimator is from the true distribution
- However, we can't compute $d(\hat{\theta}_n, f_0)$
- Can we use $-2 \, \ell(y, \hat{\theta}_n)$ to estimate $d(\hat{\theta}_n, f_0)$?

Comparing models

- Yes, but this estimator is biased

$$E_0\left[-2\,\ell(y,\hat{\theta}_n)\right] =$$
$$E_0\left\{E_0\left[-2\,\ell(y,\theta)\right]_{\theta=\hat{\theta}_n}\right\} - 2\,p + o(1)$$

Comparing models

- In other words

$$E_0\left[\text{AIC}\right] \approx E_0\left[d(\hat{\theta}_n, f_0)\right]$$

where

$$\text{AIC} = -2\ell(y, \hat{\theta}_n) + 2p$$

Comparing models

- For Gaussian errors we have

$$\text{AIC} = n \log\left(\frac{\text{RSS}}{n}\right) + 2p + \text{constant}$$

where

$$\text{RSS} = \sum_{i=1}^{n} r_i^2 ,$$

the **constant** depends on n, not on p

Comparing models

- However, many times we find

$$\text{AIC} = \frac{1}{n}\frac{1}{\hat{\sigma}^2}\left(\text{RSS} + 2\,p\,\hat{\sigma}^2\right) + \text{constant}$$

(e.g. [JWHT13])

Where does this expression come from?

Comparing models

- Regularity assumptions are needed
  - This is an asymptotic approximation, n should be large
  - One of the models should include truth
  - $\theta_1 \neq \theta_2 \ \Rightarrow f(y, \theta_1) \neq f(y, \theta_2)$
  - Standard large-sample MLE assumptions to obtain asymptotic normality