Variable selection

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Statistical inference

Types of statistical inference:

- looking at a focal predictor - e.g. is the coefficient of that predictor equal to zero?
- predicting future values of response from predictors
- finding a plausible range of values for a parameter of interest
- finding which predictors are *active* predictors

Variable or model selection is a type of inference

Example: Respiratory muscle strength in cystic fibrosis

Measurements of a number of clinical variables were taken on 25 patients with cystic fibrosis aged from 7 to 23 years. The response variable is maximum expiratory pressure (`pemax`).[1]

- What variables are useful predictors of `pemax`?
- What is a useful prediction model for `pemax`?

Response

- `pemax`: maximum expiratory pressure

(decrease is an index of malnutrition effect on pressures)

[1]: Dalgaard 2008, Introductory Statistics with R, Springer; O'Neill et al. 1983, Am. Rev. Respir. Dis., 128:1051–1054.

Example: Cystic fibrosis

- `age`: age (yr)
- `sex`: coded 0: male, 1:female
- `height`: height (cm)
- `weight`: weight (kg)
- `bmp`: body mass (% of normal)

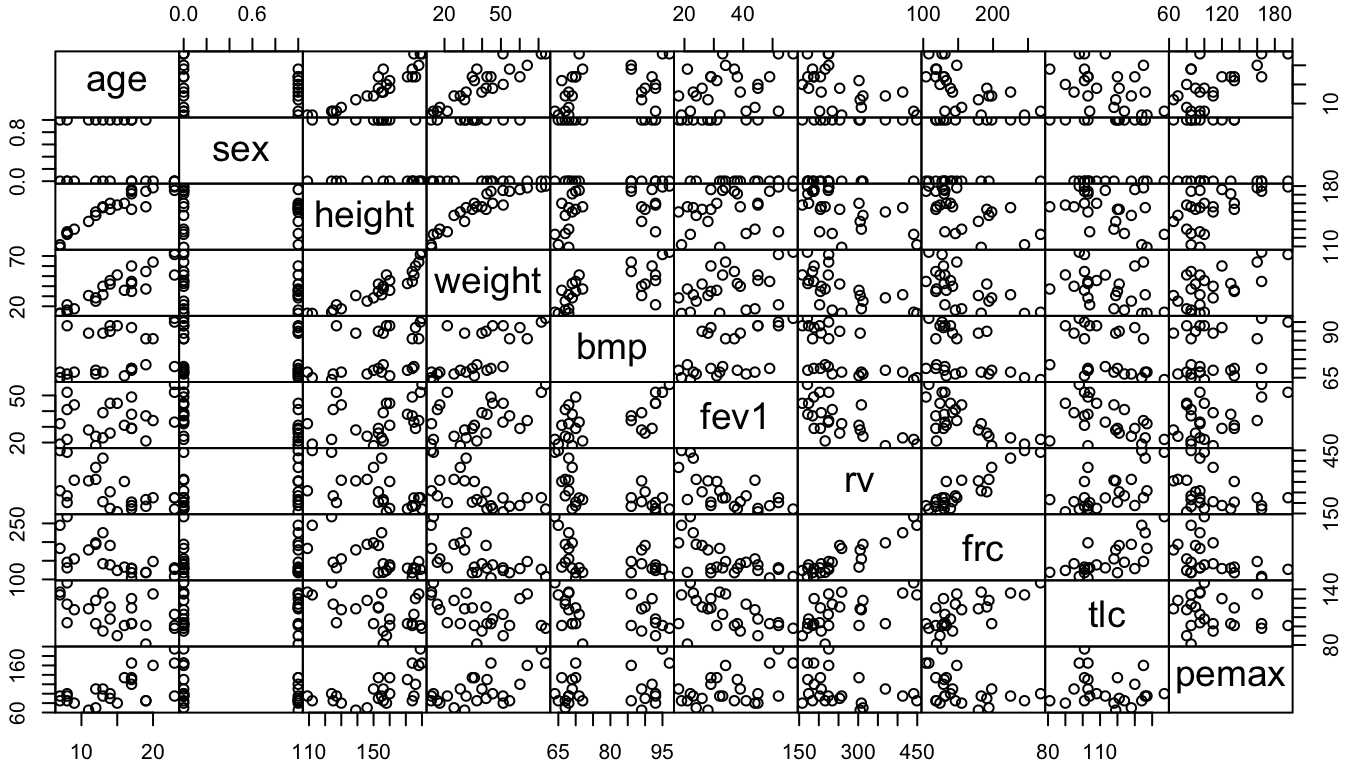
Lung function indicators

- `fev1`: forced expiratory volume
- `rv`: residual volume
- `frc`: functional residual capacity
- `tlc`: total lung capacity

Example: Cystic fibrosis - variables

```
## 'data.frame':    25 obs. of  10 variables:
##  $ age   : int  7 7 8 8 8 9 11 12 12 13 ...
##  $ sex   : int  0 1 0 1 0 0 1 1 0 1 ...
##  $ height: int  109 112 124 125 127 130 139 150 146 155 ...
##  $ weight: num  13.1 12.9 14.1 16.2 21.5 17.5 30.7 28.4 25.1 31.5 ...
##  $ bmp   : int  68 65 64 67 93 68 89 69 67 68 ...
##  $ fev1  : int  32 19 22 41 52 44 28 18 24 23 ...
##  $ rv    : int  258 449 441 234 202 308 305 369 312 413 ...
##  $ frc   : int  183 245 268 146 131 155 179 198 194 225 ...
##  $ tlc   : int  137 134 147 124 104 118 119 103 128 136 ...
##  $ pemax : int  95 85 100 85 95 80 65 110 70 95 ...
```

Example: Cystic fibrosis - all pairs plot



Example: Cystic fibrosis - summary statistics

```
##            mean          sd IQR   50%  n
## age      14.480   5.0589854   6  14.0 25
## sex       0.440   0.5066228   1   0.0 25
## height  152.800  21.5000000  35 156.0 25
## weight   38.404  17.8981256  26  37.2 25
## bmp      78.280  12.0052766  22  71.0 25
## fev1     34.720  11.1971723  18  33.0 25
## rv      255.200  86.0169557 117 225.0 25
## frc     155.400  43.7187984  56 139.0 25
## tlc     114.000  16.9681073  27 113.0 25
## pemax   109.120  33.4369058  45  95.0 25
```

Example: Cystic fibrosis - correlations

```
##            age    sex height weight    bmp   fev1     rv    frc    tlc pemax
## age       1.00 -0.17   0.93   0.91   0.38   0.29 -0.55 -0.64 -0.47  0.61
## sex      -0.17  1.00  -0.17  -0.19  -0.14  -0.53  0.27  0.18  0.02 -0.29
## height    0.93 -0.17   1.00   0.92   0.44   0.32 -0.57 -0.62 -0.46  0.60
## weight    0.91 -0.19   0.92   1.00   0.67   0.45 -0.62 -0.62 -0.42  0.64
## bmp       0.38 -0.14   0.44   0.67   1.00   0.55 -0.58 -0.43 -0.36  0.23
## fev1      0.29 -0.53   0.32   0.45   0.55   1.00 -0.67 -0.67 -0.44  0.45
## rv       -0.55  0.27  -0.57  -0.62  -0.58  -0.67  1.00  0.91  0.59 -0.32
## frc      -0.64  0.18  -0.62  -0.62  -0.43  -0.67  0.91  1.00  0.70 -0.42
## tlc      -0.47  0.02  -0.46  -0.42  -0.36  -0.44  0.59  0.70  1.00 -0.18
## pemax     0.61 -0.29   0.60   0.64   0.23   0.45 -0.32 -0.42 -0.18  1.00
```

Example: Cystic fibrosis - regression model

Model: multivariable linear regression

```
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 176.0582   225.8912  0.7794   0.4479
## age          -2.5420     4.8017 -0.5294   0.6043
## sex          -3.7368    15.4598 -0.2417   0.8123
## height       -0.4463     0.9034 -0.4940   0.6285
## weight        2.9928     2.0080  1.4905   0.1568
## bmp          -1.7449     1.1552 -1.5105   0.1517
## fev1          1.0807     1.0809  0.9998   0.3333
## rv            0.1970     0.1962  1.0039   0.3314
## frc          -0.3084     0.4924 -0.6264   0.5405
## tlc           0.1886     0.4997  0.3774   0.7112

## [1] Adjusted R-sq = 0.4197       p value = 0.032
```

Example: Cystic fibrosis - collinearity

Global P value small, no P values for model coefficients small?

Correlations among variables are interfering with estimated standard errors - *collinearity*

Check via *variance inflation factor*

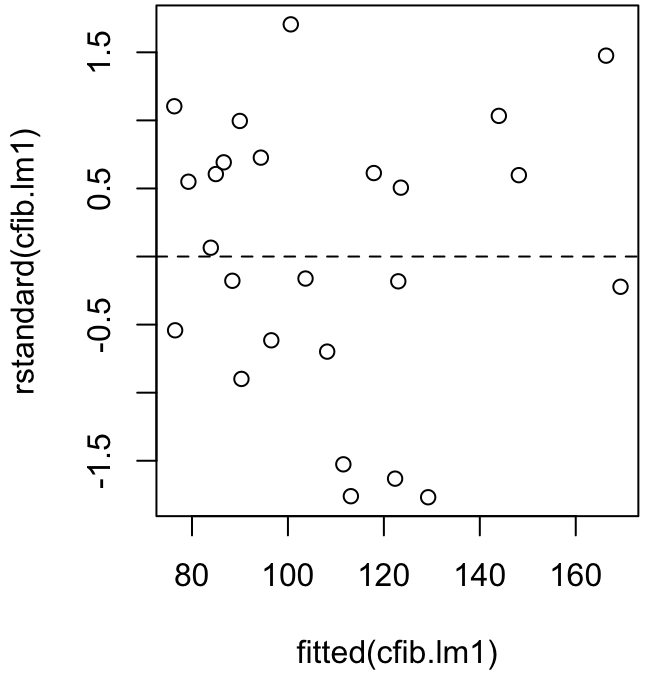
```
##    age    sex height weight    bmp   fev1     rv    frc    tlc
## 21.830  2.269 13.955 47.781  7.116  5.420 10.538 17.143  2.660
```

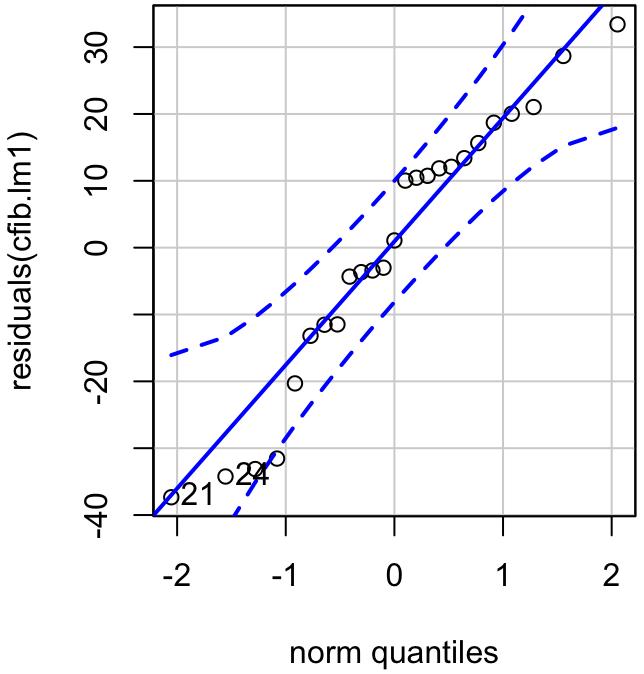
Values of VIF > 10 show concerning collinearity

VIF values show why individual P values are not smaller

Example: Cystic fibrosis - model assumptions

Check model assumptions






```
## [1] 21 24
```

Model or variable selection - criteria and methods

Criteria used (well or not!) for deciding the fate of a variable:

- P value derived from some statistic (t, F, χ^2)
- measure of model fit - mean squared error (residual mean square), adjusted R^2
- information criterion - AIC, BIC (combination of measure of model fit and penalty for larger model)

For all of these, smaller is better

Model or variable selection - criteria and methods

Methods

- stepwise methods - forwards, backwards, both (1960)
  - one variable added or removed at each step
- validation methods
  - measure how well models predict using new data (1990s)
  - randomly split data set into training and test sets
  - all subsets combined with k-fold cross-validation
- penalised estimation methods - model coefficient estimates forced towards zero
  - penalty term is based on magnitude of model coefficients
  - LASSO (1996)

Model or variable selection - criteria and methods

Use expert knowledge first to *simplify* your model

- eliminate unnecessary predictors

Stepwise methods

- no statistical justification but if you must …
- do not use P values for decisions
  - hypothesis testing not appropriate for model selection as no a priori hypothesis is tested
  - multiple testing problems
- use information criterion (AIC, BIC)

Model or variable selection - criteria and methods

Validation methods

- common criterion is mean squared error
- good for comparing predictive capability of models and so model selection
- choose appropriate “k” for k-fold cross-validation - one recommendation:
  - leave-one-out (i.e. N-fold c.v.) if n < 20
  - 10-fold c.v. for 20<n<100
  - 5-fold c.v. for n>100

Penalised estimation methods

- main goal is predictive capability of model
- good when many parameters or small sample

Model or variable selection - criteria and methods

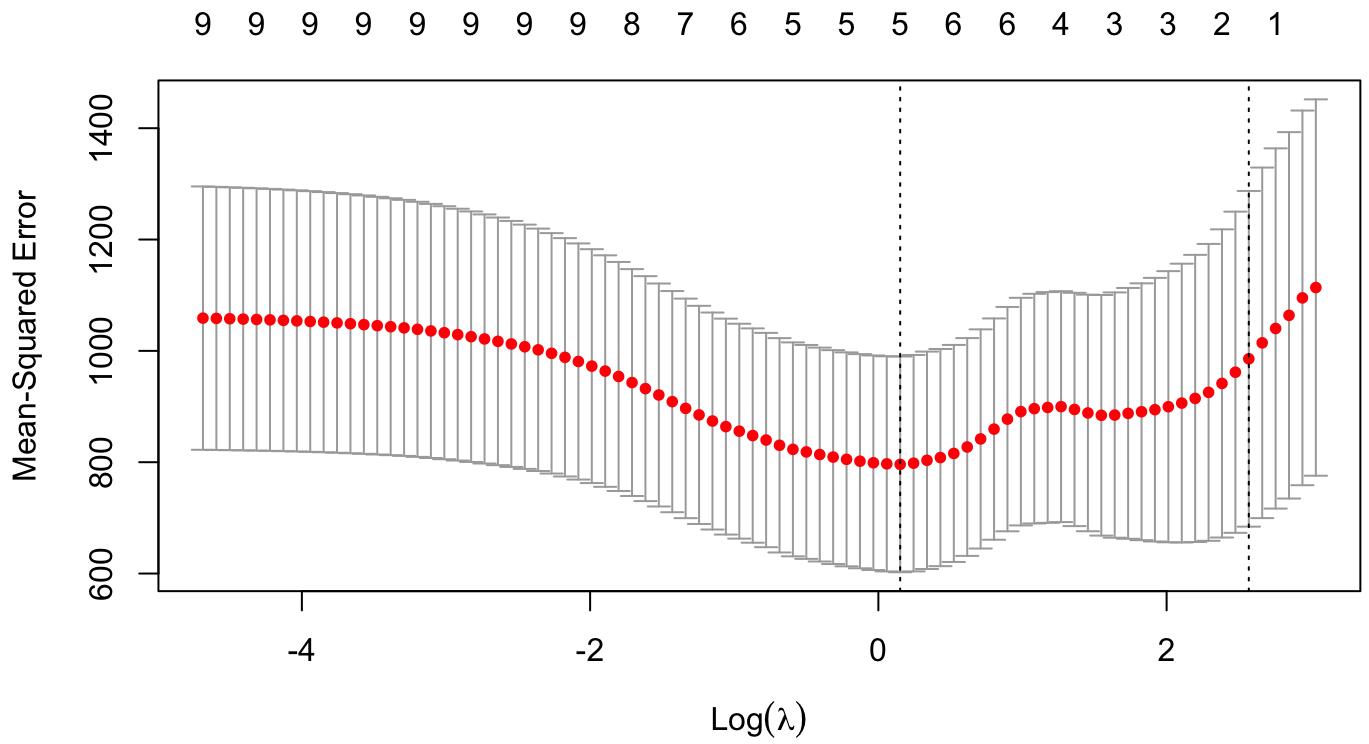
Each method also has its *limitations* and *disadvantages*

- Stepwise methods can be undermined by collinearity
- AIC and BIC rely on model being close to correct
- Cross-validation requires only independent splits for training and test data but different results for different “k”
- LASSO estimates are biased and no standard errors are available

Example: Cystic fibrosis - active predictors

- What variables are useful predictors of `pemax`?

LASSO



Example: Cystic fibrosis - active predictors

```
## 9 x 1 sparse Matrix of class "dgCMatrix"
##                 s0
## age      .
## sex      .
## height   .
## weight   1.48240558
## bmp     -1.03833881
## fev1     1.17164094
## rv       0.05732589
## frc      .
## tlc      0.12969407
```

Available output:

- active predictors and model coefficients
- no P values
- no standard errors

Example: Cystic fibrosis - prediction model

- What is a useful prediction model for `pemax`?

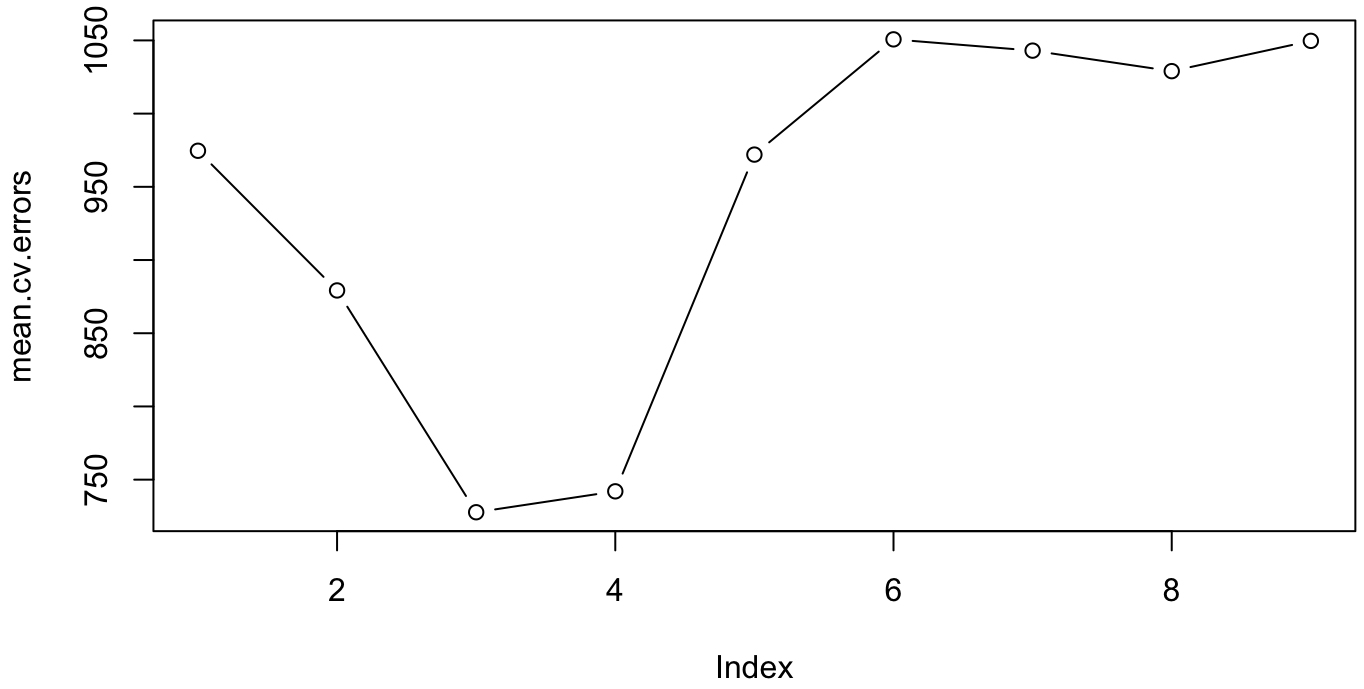
k-fold cross validation (k = 1, leave-one-out) with all subsets in each fold

```
## folds
##  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
##  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
## 24 25
##  1  1
```

```
##         1         2         3         4         5         6         7
##  974.6263  879.2297  727.7373  742.0240  972.0102 1050.7182 1043.0226
##         8         9
## 1029.0064 1049.6921
```

```
## [1] "No. of predictors in final model = 3"
```

Example: Cystic fibrosis - prediction model



Example: Cystic fibrosis - prediction model

```
## (Intercept)      weight         bmp        fev1
##  126.333557    1.536475   -1.465406    1.108629
```

Look at terms in 4-predictor model from c.v. runs

```
## (Intercept)      weight         bmp        fev1          rv
##  63.9466933   1.7489143  -1.3772433   1.5476984   0.1257152
```

Strange:

- both weight and bmp are in model when cor(weight, bmp) = 0.67
- coef of bmp is negative when cor(pemax, bmp) = 0.23

Possible overfitting?

Example: Cystic fibrosis - prediction model

Optimal model from cross-validation with all subsets fitted on full data set

```
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 126.3336    34.7199  3.6387   0.0015
## weight        1.5365     0.3644  4.2162   0.0004
## bmp          -1.4654     0.5793 -2.5297   0.0195
## fev1          1.1086     0.5144  2.1553   0.0429

## [1] Adjusted R-sq = 0.5086       p value = 4e-04
```

Example: Cystic fibrosis - prediction model

For prediction models:

- some overfitting is not a problem
- some collinearity is not a problem

Example: Cystic fibrosis - active predictors

Simplify the model

- use logic from expert knowledge - consider groups of predictors

Lung function: `fev1`, `rv`, `frc`, `tlc`

Remove these other lung function indicators as a group

Model comparison criteria:

- AIC - overfits, better for prediction model
- BIC - penalises larger models harder, good for active predictors
- As models are *nested*, can use an F test

Example: Cystic fibrosis - active predictors

Simplify the model contd

```
## [1] AIC full model: 242.05
```

```
## [1] AIC reduced model: 239.56
```

```
## [1] AIC_full - AIC_red = 2.49
```

```
## [1] BIC full model: 255.46
```

```
## [1] BIC reduced model: 248.09
```

```
## [1] BIC_full - BIC_red = 7.37
```

Model without lung function variables appears better

Example: Cystic fibrosis - active predictors

Simplify the model contd

F test for nested models

```
## Analysis of Variance Table
##
## Model 1: pemax ~ age + sex + height + weight + bmp + fev1 + rv + frc +
##     tlc
## Model 2: pemax ~ age + sex + height + weight + bmp
##   Res.Df     RSS Df Sum of Sq      F Pr(>F)
## 1     15  9731.2
## 2     19 12129.2 -4     -2398 0.9241 0.4758
```

Smaller model is no worse than larger model

Example: Cystic fibrosis - active predictors

```
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 280.4482   124.9556  2.2444   0.0369
## age          -3.0750     3.6352 -0.8459   0.4081
## sex         -11.5281    10.3720 -1.1115   0.2802
## height       -0.6853     0.7962 -0.8607   0.4001
## weight        3.5546     1.5281  2.3261   0.0312
## bmp          -1.9613     0.9263 -2.1174   0.0476
```

```
## [1] Adjusted R-sq = 0.429       p value = 0.0064
```

Collinearity still present - possibly obscuring relationships

```
##       age       sex    height    weight       bmp
## 12.715251  1.038066 11.015970 28.123150  4.648941
```

Example: Cystic fibrosis - active predictors

Simplify the model contd

Remove `age`

```
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 251.3973   119.2859  2.1075   0.0479
## sex         -11.5458    10.2979 -1.1212   0.2755
## height       -0.8128     0.7762 -1.0472   0.3075
## weight        2.6947     1.1329  2.3787   0.0275
## bmp          -1.4881     0.7330 -2.0302   0.0558
```

```
## [1] Adjusted R-sq = 0.4371       p value = 0.0033
```

Collinearity still present

```
##       sex    height    weight       bmp
##  1.038062 10.620847 15.678850  2.953131
```

Example: Cystic fibrosis - active predictors

Perhaps no neat ending here in specifying active predictors

cor(height, weight) = 0.92 so possibly one should have been removed at the start

Different methods may lead to different results

Variable selection - Recommendations

- In study design, use expert knowledge to list candidate predictors (do not use the data later to "help" you!) and plan to collect adequate data
- Avoid including too many predictors for your sample size
- Ask yourself whether variable selection is *necessary*; if so
  - do it in a limited, structured way (e.g. consider groups of predictor variables)
  - use *minimal* backwards elimination steps if you want parsimony (active predictors) rather than accuracy (good predictions) and use model validation techniques[2]

[2]: Harrell 2015, Regression Modeling Strategies, Springer, 2nd ed., s. 4.12

Variable selection - Recommendations

- What is the role of modelling in your field?
  - systems biology - complex problems addressed by computational modelling and simulation[3]
  - business - big data - Netflix Prize (100 million records)[4]
  - clinical science and health - diagnostic and prognostic inferences … for care decisions … policy[5]
  - more generally - how statistical modelling decisions connect with answering scientific questions[6]

[3]: Macleod 2018 https://doi.org/10.1007/s40656-017-0183-9
[4]: Hastie 2015 Statistical learning with big data https://web.stanford.edu/~hastie/TALKS/SLBD_new.pdf
[5]: Henley 2020 https://doi.org/10.1080/24709360.2019.1618653
[6]: Navarro 2019 https://doi.org/10.1007/s42113-018-0019-z

Variable selection - future seminar topics?

Many issues not raised:

- how many variables is it feasible to start with in a model?
- after you've done model selection, how much can you trust P values for model parameter estimates?
- what methods can be used for models with multiple categorical predictor variables?
- what about mixed models with fixed and random effects - i.e. where the data records are not independent, such as observations made on subjects in different groups?
- what methods can be used with other types of model - e.g. non-linear models or where response variable is binary, small count, categorical, …?