Model Selection

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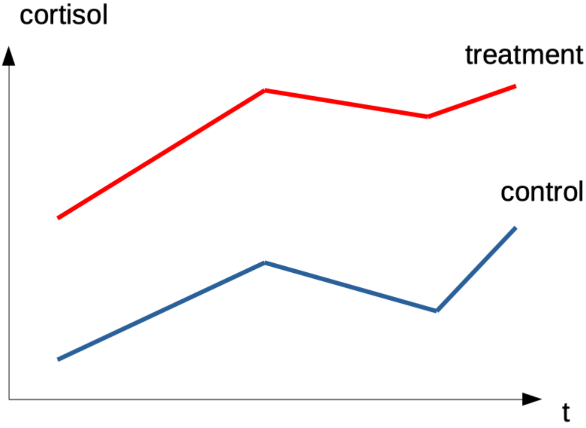
Why Statistical Modelling?

Some people believe, they do not need statistics. For them it is enough to look at a diagram

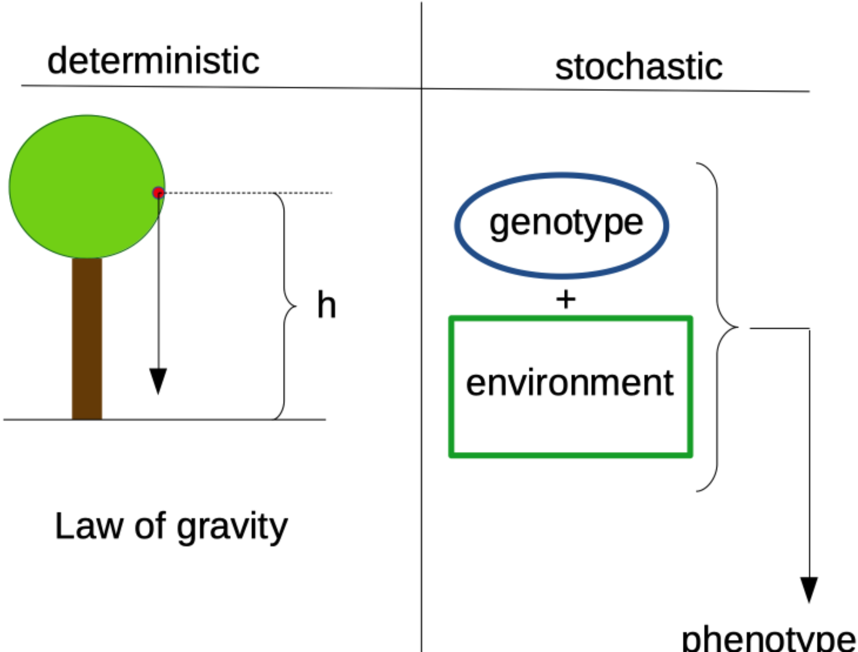


Statistical Modelling Because ...

Two types of dependencies between physical quantities

1. deterministic
2. stochastic

Deterministic Versus Stochastic



Statistical Model

- stochastic systems contains many sources of uncertainty
- statistical models can handle uncertainty
- components of a statistical model
  - response variable y
  - predictor variables $x_1, x_2, \ldots, x_k$
  - error term e
  - function $m(x)$

How Does A Statistical Model Work?

- predictor variables $x_1, x_2, \ldots, x_k$ are transformed by function $m(x)$ to explain the response variable y
- uncertainty is captured by error term.
- as a formula, for observation i

$$y_i = m(x_i) + e_i$$

Which function $m(x)$?

- class of functions that can be used as $m(x)$ is infinitely large
- restrict to linear functions of predictor variables

Which predictor variables?

- Question, about which predictor variables to use is answered by model selection

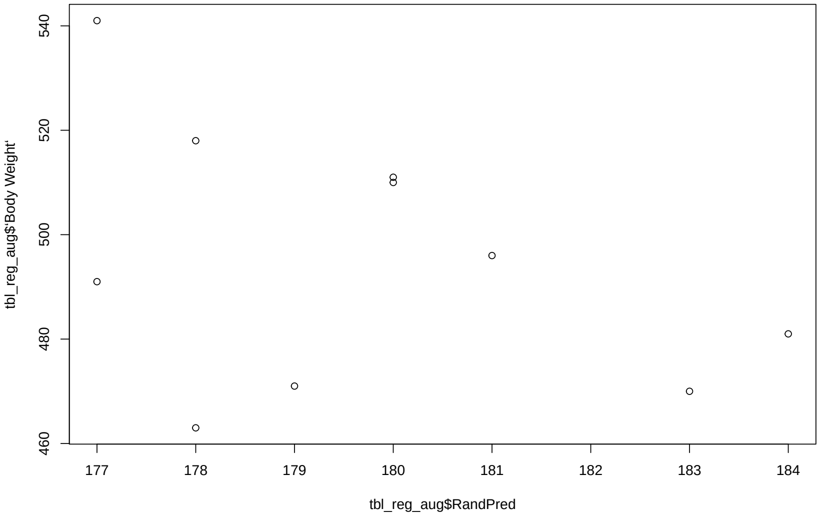
Why Model Selection

- Many predictor variables are available
- Are all of them `relevant`?
- What is the meaning of `relevant` in this context?

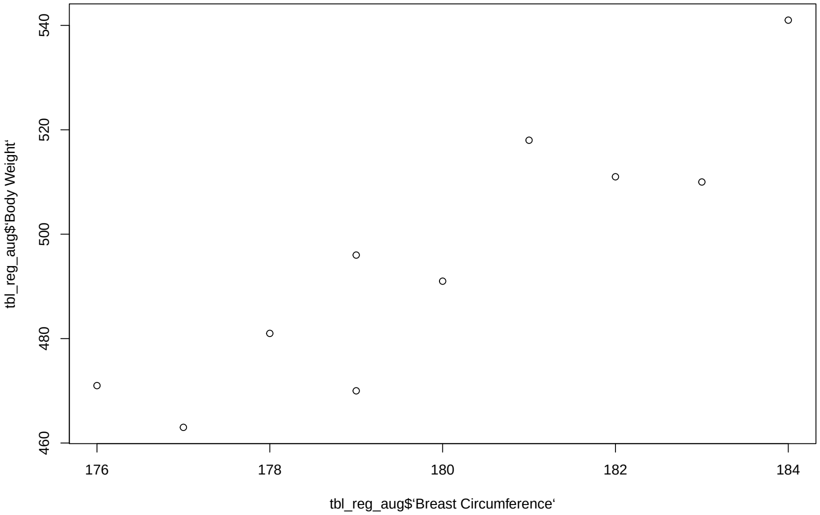
Example Dataset

Animal	Breast Circumference	Body Weight	RandPred
1	176	471	179
2	177	463	178
3	178	481	184
4	179	470	183
5	179	496	181
6	180	491	177
7	181	518	178
8	182	511	180
9	183	510	180
10	184	541	177

No Relevance of Predictors



Relevance of Predictors



Fitting a Regression Model

```
##
## Call:
## lm(formula = `Body Weight` ~ RandPred, data = tbl_reg_aug)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -39.163 -14.365   4.769  15.981  34.741
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 1231.246    602.814   2.042   0.0754 .
## RandPred      -4.096      3.354  -1.221   0.2568
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 24.21 on 8 degrees of freedom
## Multiple R-squared:  0.1571, Adjusted R-squared:  0.05175
## F-statistic: 1.491 on 1 and 8 DF,  p-value: 0.2568
```

Fitting a Regression Model II

```
##
## Call:
## lm(formula = `Body Weight` ~ `Breast Circumference`, data = tbl_reg_aug)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -17.3941  -6.5525  -0.0673   9.3707  13.2594
##
## Coefficients:
##                         Estimate Std. Error t value Pr(>|t|)
## (Intercept)            -1065.115    255.483  -4.169 0.003126 **
## `Breast Circumference`     8.673      1.420   6.108 0.000287 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 11.08 on 8 degrees of freedom
## Multiple R-squared:  0.8234, Adjusted R-squared:  0.8014
## F-statistic: 37.31 on 1 and 8 DF,  p-value: 0.000287
```

Multiple Regression

```
##
## Call:
## lm(formula = `Body Weight` ~ `Breast Circumference` + RandPred,
##     data = tbl_reg_aug)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -12.778 -10.062   2.941   7.955  11.139
##
## Coefficients:
##                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)            -721.333    449.542  -1.605 0.152618
## `Breast Circumference`    8.269      1.496   5.529 0.000879 ***
## RandPred                 -1.509      1.617  -0.933 0.381831
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 11.17 on 7 degrees of freedom
## Multiple R-squared:  0.843,  Adjusted R-squared:  0.7981
## F-statistic: 18.79 on 2 and 7 DF,  p-value: 0.001535
```

Which model is better?

Why not taking all predictors?

- Additional parameters must be estimated from data
- Predictive power decreased with too many predictors (cannot be shown for this data set, because too few data points)
- Bias-variance trade-off

Bias-variance trade-off

- Assume, we are looking for optimum prediction

$$s_i = \sum_{r=1}^{q} \hat{\beta}_{j_r} x_{ij_r}$$

with q relevant predictor variables

- Average mean squared error of prediction s_i

$$MSE = n^{-1} \sum_{i=1}^{n} E\left[(m(x_i) - s_i)^2\right]$$

where $m(.)$ denotes the linear function of the unknown true model.

Bias-variance trade-off II

- MSE can be split into two parts

$$MSE = n^{-1}\sum_{i=1}^{n}\left(E\left[s_i\right] - m(x_i)\right)^2 + n^{-1}\sum_{i=1}^{n} var(s_i)$$

where $n^{-1}\sum_{i=1}^{n}\left(E\left[s_i\right] - m(x_i)\right)^2$ is called the squared **bias**

- Increasing q leads to reduced bias but increased variance ($var(s_i)$)
- Hence, find s_i such that MSE is minimal
- Problem: cannot compute MSE because $m(.)$ is not known

$\rightarrow$ estimate MSE

Mallows C_p statistic

- For a given model $\mathcal{M}$, $SSE(\mathcal{M})$ stands for the residual sum of squares.
- MSE can be estimated as

$$\widehat{MSE} = n^{-1}SSE(\mathcal{M}) - \hat{\sigma}^2 + 2\hat{\sigma}^2|\mathcal{M}|/n$$

where $\hat{\sigma}^2$ is the estimate of the error variance of the full model, $SSE(\mathcal{M})$ is the residual sum of squares of the model $\mathcal{M}$, n is the number of observations and $|\mathcal{M}|$ stands for the number of predictors in $\mathcal{M}$

$$C_p(\mathcal{M}) = \frac{SSE(\mathcal{M})}{\hat{\sigma}^2} - n + 2|\mathcal{M}|$$

Searching The Best Model

- Exhaustive search over all sub-models might be too expensive
- For p predictors there are $2^p - 1$ sub-models
- With $p = 16$, we get 6.5535×10^4 sub-models

$\rightarrow$ step-wise approaches

Forward Selection

1. Start with smallest sub-model $\mathcal{M}_0$ as current model
2. Include predictor that reduces SSE the most to current model
3. Repeat step 2 until all predictors are chosen

$\rightarrow$ results in sequence $\mathcal{M}_0 \subseteq \mathcal{M}_1 \subseteq \mathcal{M}_2 \subseteq \ldots$ of sub-models

4. Out of sequence of sub-models choose the one with minimal C_p

Backward Selection

1. Start with full model $\mathcal{M}_0$ as the current model
2. Exclude predictor variable that increases SSE the least from current model
3. Repeat step 2 until all predictors are excluded (except for intercept)

$\rightarrow$ results in sequence $\mathcal{M}_0 \supseteq \mathcal{M}_1 \supseteq \mathcal{M}_2 \supseteq \ldots$ of sub-models

4. Out of sequence choose the one with minimal C_p

Considerations

- Whenever possible, choose **backward** selection, because it leads to better results
- If $p \geq n$, only forward is possible, but then consider LASSO

Alternative Selection Criteria

- AIC or BIC, requires distributional assumptions.
- AIC is implemented in `MASS::stepAIC()`
- Adjusted R^2 is a measure of goodness of fit, but sometimes is not conclusive when comparing two models
- Try in exercise