Linear Modelling: Multiple Regression

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Linear models:

Simple/single regression: $$\boldsymbol{y} = \alpha + \beta \boldsymbol{x} + \boldsymbol{\varepsilon}$$

Multiple regression: $$\boldsymbol{y} = \beta_0 + \beta_1 \boldsymbol{x_1} + \beta_2 \boldsymbol{x_2} + \cdots + \beta_n \boldsymbol{x_n} + \boldsymbol{\varepsilon}$$

$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon}$$

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Parameter estimation:

Minimise sum of squares of residuals:

$$SS_{\mathrm{error}} = \boldsymbol{\varepsilon}^{\mathrm{T}}\boldsymbol{\varepsilon} = (\boldsymbol{y} - \boldsymbol{X\beta})^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{X\beta}) \to \min$$

Solution: $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y}$

Compare with the simple case: $\hat{\beta} = \frac{\sum_i (y_i - \bar{y})(x_i - \bar{x})}{\sum_i (x_i - \bar{x})^2} = \frac{\mathrm{cov}(\boldsymbol{x}, \boldsymbol{y})}{\mathrm{var}(\boldsymbol{x})}$

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$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon}$$

Assumptions:

1. Model is linear in parameters.
2. Gaussian error model. $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$
3. Additive error model.
4. Independence of errors. $\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0$
5. Homoscedasticity. $\mathrm{Var}(\boldsymbol{\varepsilon}|\boldsymbol{x}) = \sigma^2\mathbf{I}$

   and…
6. Lack of multicollinearity in the predictors (highly correlated variables).

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Multiple Regression:

Example: *Predicting timber volume of felled black cherry trees*

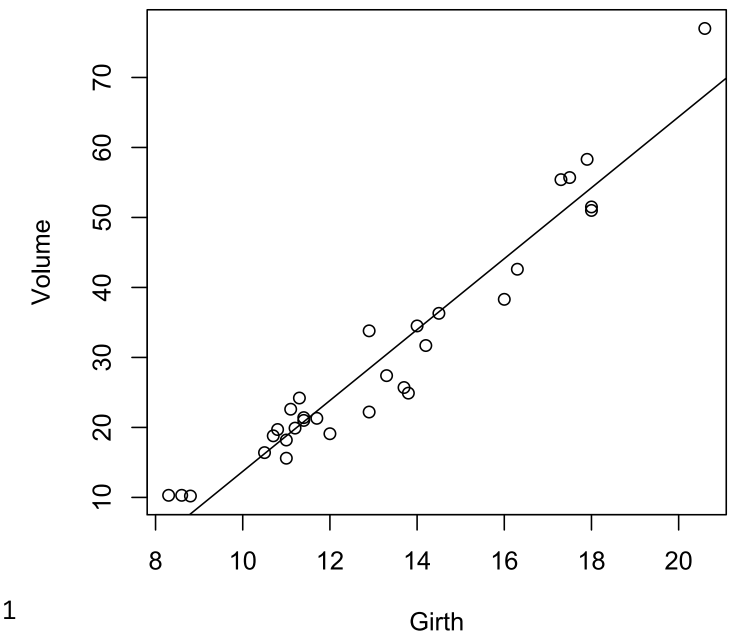
$$y = \alpha + \beta x + \varepsilon$$

```
Call:
lm(formula = Volume ~ Girth, data = trees)

Residuals:
   Min     1Q Median     3Q    Max 
-8.065 -3.107  0.152  3.495  9.587 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) -36.9435     3.3651  -10.98 7.62e-12 ***
Girth         5.0659     0.2474   20.48  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 4.252 on 29 degrees of freedom
Multiple R-squared:  0.9353,	Adjusted R-squared:  0.9331 
F-statistic: 419.4 on 1 and 29 DF,  p-value: < 2.2e-16
```



Response: y = Volume

Predictor: x = Girth

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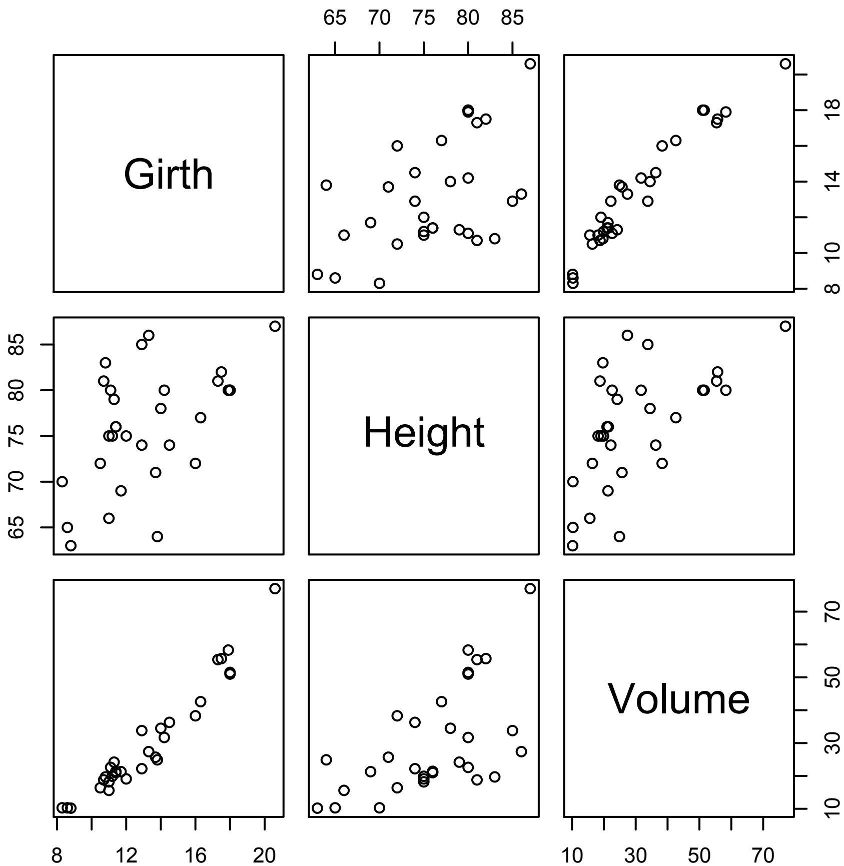
Example: *Predicting timber volume of cherry trees*



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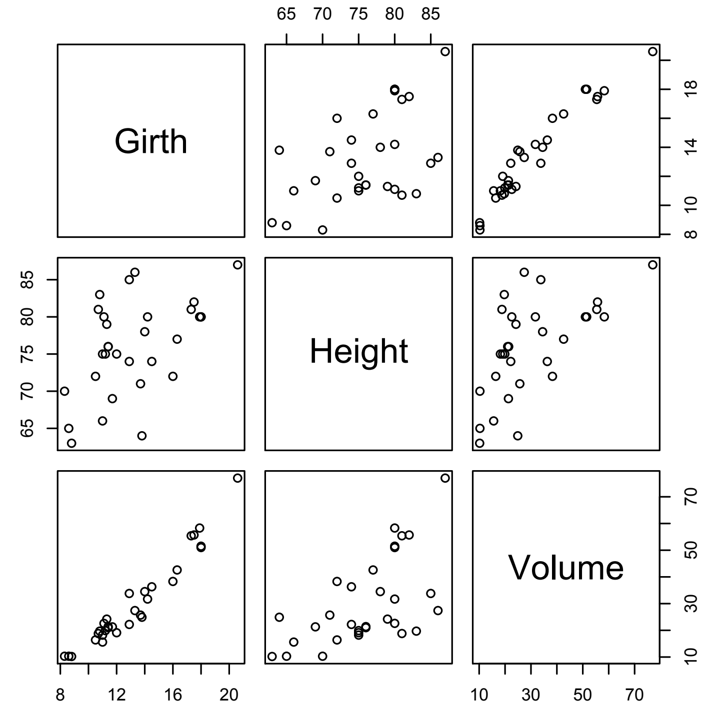

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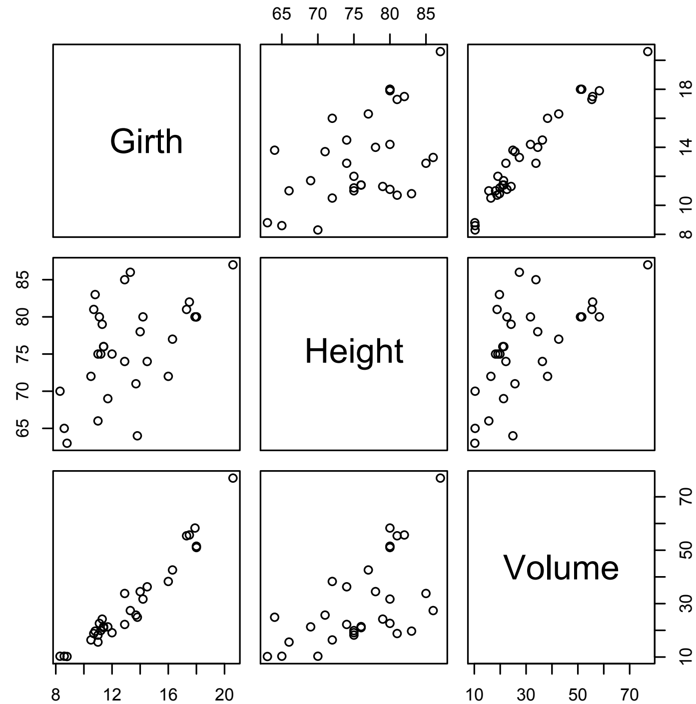

$$y = \alpha + \beta x + \varepsilon$$

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$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

Response: y = Volume
Predictor: x_1 = Girth
Predictor: x_2 = Height

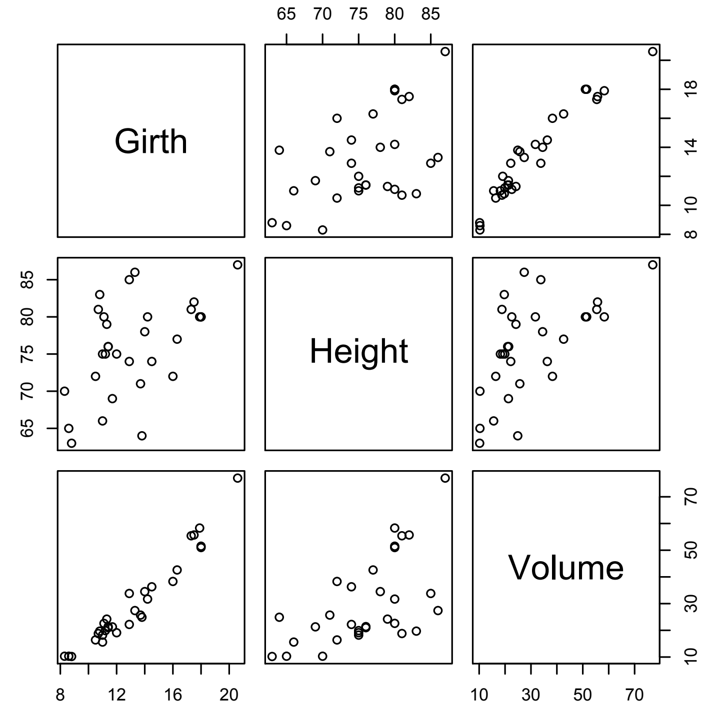
```
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -57.9877     8.6382  -6.713 2.75e-07 ***
Girth         4.7082     0.2643  17.816  < 2e-16 ***
Height        0.3393     0.1302   2.607   0.0145 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 3.882 on 28 degrees of freedom
Multiple R-squared:  0.948,   Adjusted R-squared:  0.9442
F-statistic:   255 on 2 and 28 DF,  p-value: < 2.2e-16
```

Multiple regression model:
R^2 is improved
Height term not significant

Multiple Regression:

Example: *Predicting timber volume of cherry trees*



$$\boldsymbol{y} = \beta_0 + \beta_1 \boldsymbol{x_1} + \beta_2 \boldsymbol{x_2} + \boldsymbol{\varepsilon}$$

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$$\boldsymbol{y} = \beta_0 + \beta_1 \boldsymbol{x_1} + \beta_2 \boldsymbol{x_2} + \beta_3 \boldsymbol{x_1 x_2} + \boldsymbol{\varepsilon}$$

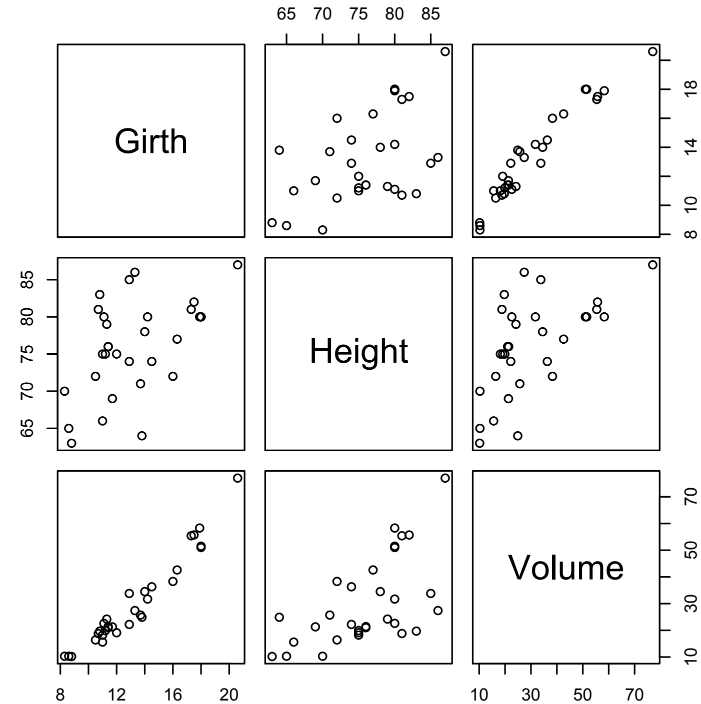
```
             Estimate Std. Error t value Pr(>|t|)    
(Intercept)  69.39632   23.83575   2.911  0.00713 ** 
Girth        -5.85585    1.92134  -3.048  0.00511 ** 
Height       -1.29708    0.30984  -4.186  0.00027 ***
Girth:Height  0.13465    0.02438   5.524 7.48e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.709 on 27 degrees of freedom
Multiple R-squared:  0.9756,  Adjusted R-squared:  0.9728 
F-statistic: 359.3 on 3 and 27 DF,  p-value: < 2.2e-16
```

Include interaction term:
R^2 is improved
Height term is significant (!)
All terms are significant

Multiple Regression:

Example: *Predicting timber volume of cherry trees*



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$$\log(\boldsymbol{y}) = \beta_0 + \beta_1 \log(\boldsymbol{x_1}) + \beta_2 \log(\boldsymbol{x_2}) + \boldsymbol{\varepsilon}$$

```
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) -6.63162    0.79979  -8.292 5.06e-09 ***
log(Girth)   1.98265    0.07501  26.432  < 2e-16 ***
log(Height)  1.11712    0.20444   5.464 7.81e-06 ***
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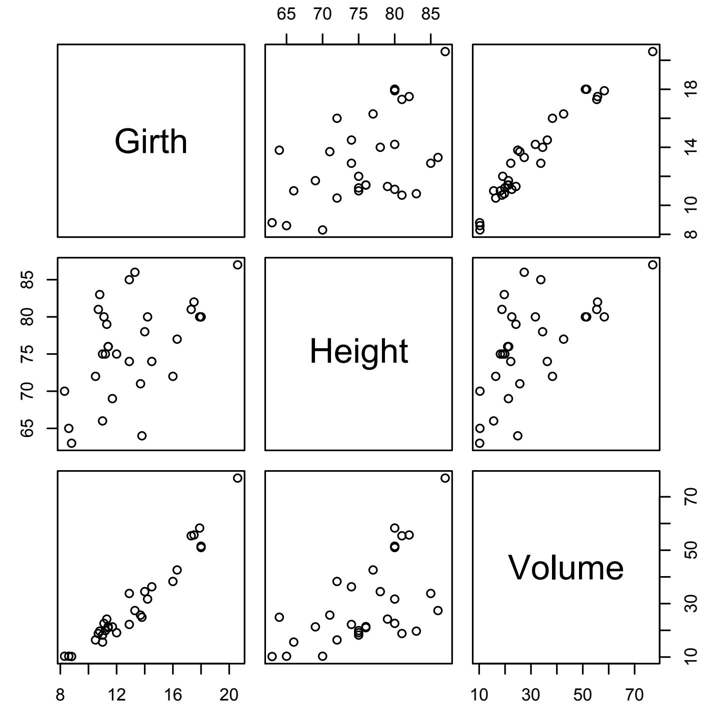
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.08139 on 28 degrees of freedom
Multiple R-squared:  0.9777,  Adjusted R-squared:  0.9761 
F-statistic: 613.2 on 2 and 28 DF,  p-value: < 2.2e-16
```

Log-transform variables:
R^2 is improved
Fewer parameters
All terms are significant
Residual standard error!!!

Multiple Regression:

Example: *Predicting timber volume of cherry trees*



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```
                        Estimate Std. Error t value Pr(>|t|)
(Intercept)             -3.6869     7.6996  -0.479    0.636
log(Girth)               0.7942     3.0910   0.257    0.799
log(Height)              0.4377     1.7788   0.246    0.808
log(Girth):log(Height)   0.2740     0.7124   0.385    0.704

Residual standard error: 0.08265 on 27 degrees of freedom
Multiple R-squared:  0.9778,  Adjusted R-squared:  0.9753
F-statistic: 396.4 on 3 and 27 DF,  p-value: < 2.2e-16
```

Include interaction term:
R^2 marginally improved
No terms are significant!!!

Multiple Regression:

Example: *Predicting timber volume of cherry trees*

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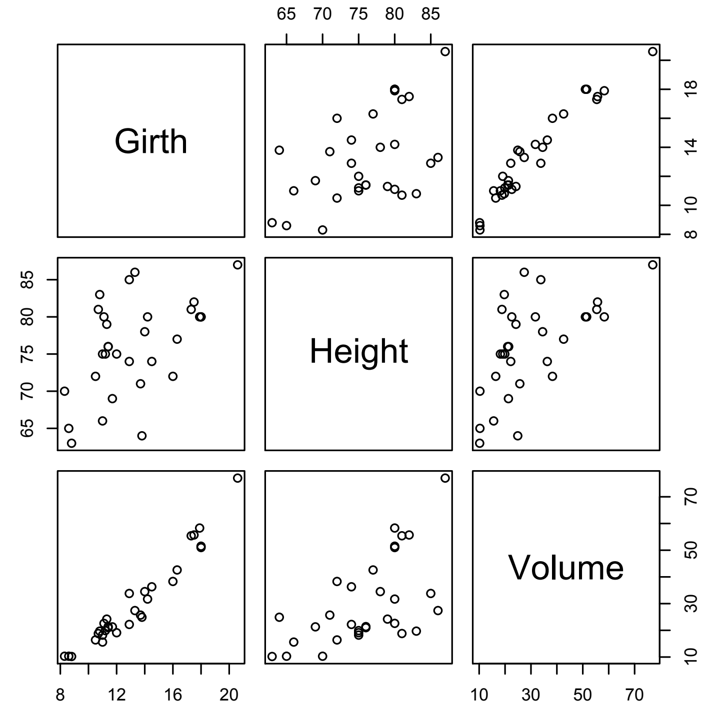

Response: y = Volume
Predictor: x_1 = Girth
Predictor: x_2 = Height

$$\boldsymbol{y} = e^{\beta_0} \boldsymbol{x_1}^{\beta_1} \boldsymbol{x_2}^{\beta_2} e^{\boldsymbol{\varepsilon}}$$

Volume ∝ Girth^2 x Height

Confidence Intervals:

	2.5 %	97.5 %
(Intercept)	-8.269912	-4.993322
log(Girth)	1.828998	2.136302
log(Height)	0.698353	1.535894

$$\hat{\beta}_1 \approx 2$$
$$\hat{\beta}_2 \approx 1$$

Multiple Regression:

Example: *Predicting timber volume of cherry trees*

$$\log(\boldsymbol{y}) = \beta_0 + \beta_1 \log(\boldsymbol{x_1}) + \beta_2 \log(\boldsymbol{x_2}) + \boldsymbol{\varepsilon}$$

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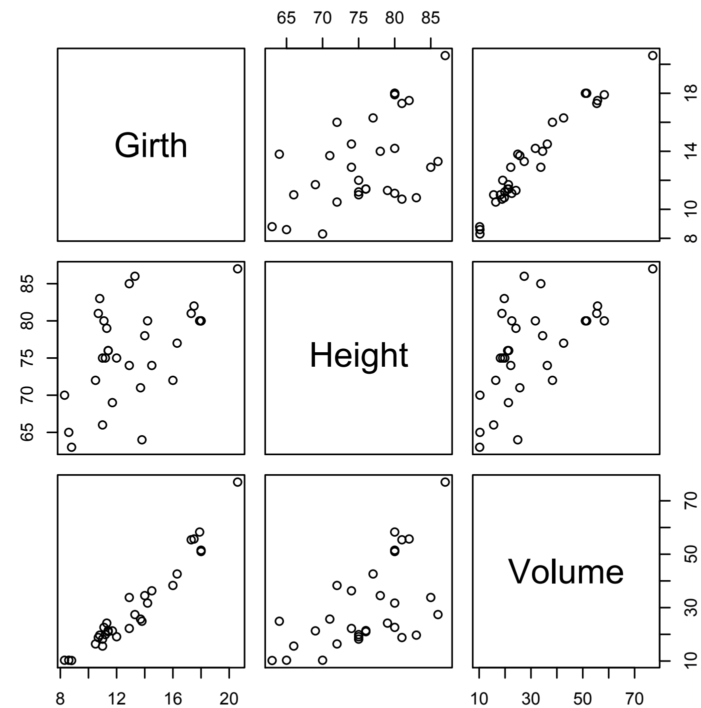

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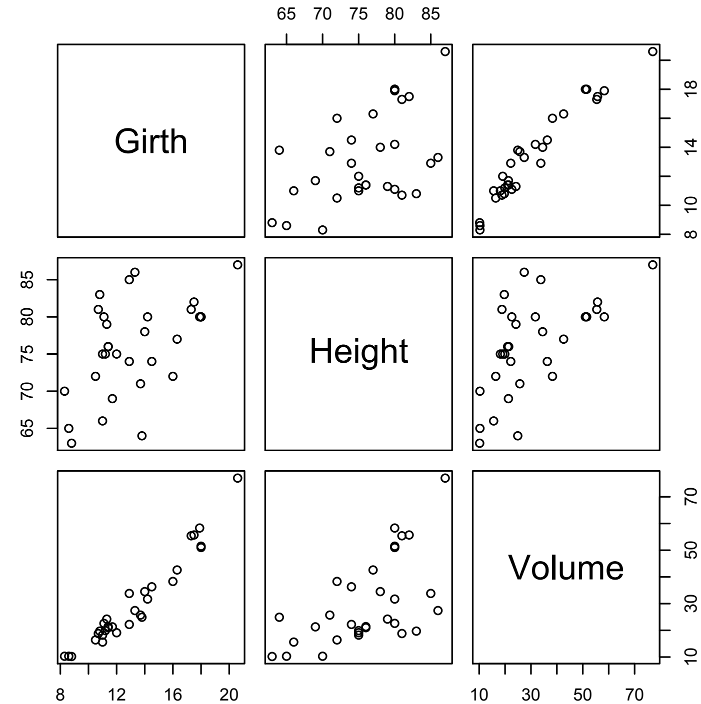


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$$\log(\boldsymbol{y}) = \beta_0 + 2\log(\boldsymbol{x_1}) + \log(\boldsymbol{x_2}) + \boldsymbol{\varepsilon}$$

$$\log\left(\frac{\boldsymbol{y}}{\boldsymbol{x_1}^2 \boldsymbol{x_2}}\right) = \beta_0 + \boldsymbol{\varepsilon}$$

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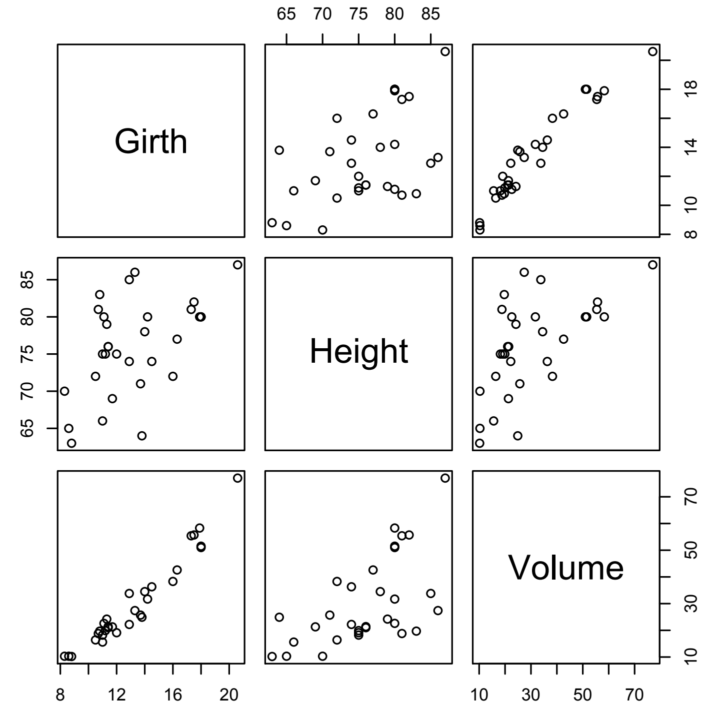

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$$\log\left(\frac{\boldsymbol{y}}{\boldsymbol{x_1^2 x_2}}\right) = \beta_0 + \boldsymbol{\varepsilon}$$

```
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -6.16917    0.01421  -434.3   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.0791 on 30 degrees of freedom
```

Constrain parameters:

No R^2

Intercept is significant

Again, can’t compare RSE…

Multiple Regression:

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$$\log\left(\frac{y}{x_1^2 x_2}\right) = \beta_0 + \varepsilon$$

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Residual standard error: 0.0791 on 30 degrees of freedom
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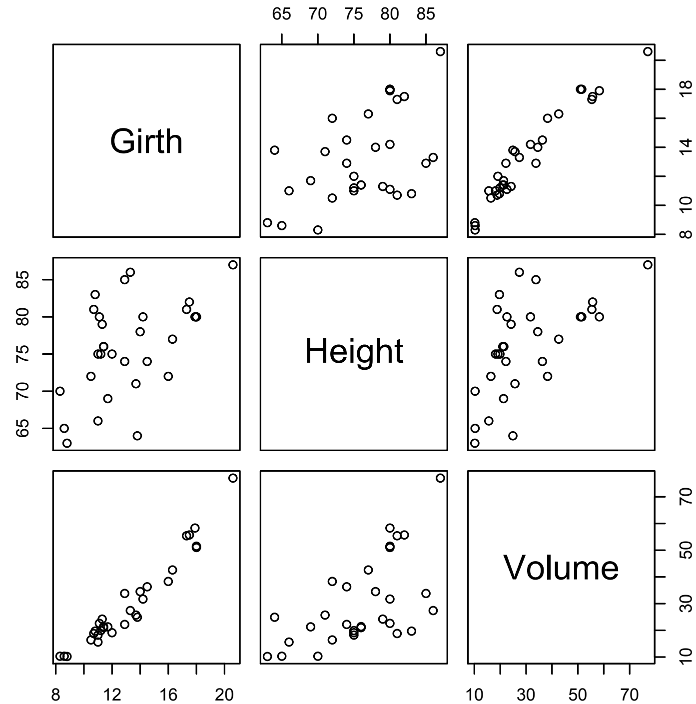

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Predictor: x_2 = Height

$$y = \beta_1 x_1^2 x_2 + \varepsilon$$

```
                  Estimate Std. Error t value Pr(>|t|)
I(Girth^2):Height 2.108e-03  2.722e-05   77.44   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.455 on 30 degrees of freedom
Multiple R-squared:  0.995,   Adjusted R-squared:  0.9949
F-statistic:  5996 on 1 and 30 DF,  p-value: < 2.2e-16
```

Simple regression, no intercept:
R^2 incomparable
Again, can’t compare RSE…

exp(-6.16917) = 2.092e-03 …?!

Multiple Regression:

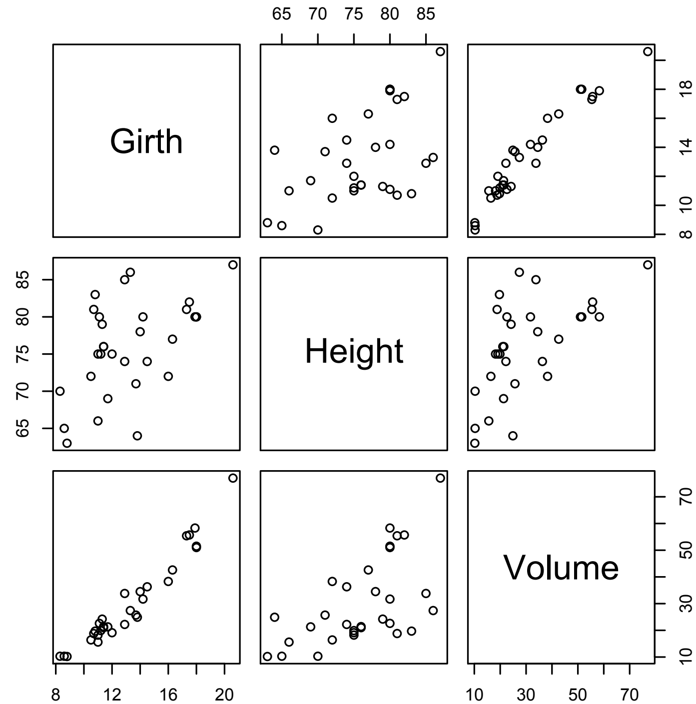
Example: *Predicting timber volume of cherry trees*

$$\log\left(\frac{\boldsymbol{y}}{\boldsymbol{x}_1^2\boldsymbol{x}_2}\right) = \beta_0 + \boldsymbol{\varepsilon}$$

$$\boldsymbol{y} = \beta_1 \boldsymbol{x}_1^2 \boldsymbol{x}_2 e^{\boldsymbol{\varepsilon}}$$

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -6.16917    0.01421  -434.3   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.0791 on 30 degrees of freedom
```



Response: y = Volume
Predictor: x_1 = Girth
Predictor: x_2 = Height

$$\boldsymbol{y} = \beta_1 \boldsymbol{x}_1^2 \boldsymbol{x}_2 + \boldsymbol{\varepsilon}$$

```
                 Estimate Std. Error t value Pr(>|t|)
I(Girth^2):Height 2.108e-03  2.722e-05   77.44   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.455 on 30 degrees of freedom
Multiple R-squared:  0.995,   Adjusted R-squared:  0.9949
F-statistic:  5996 on 1 and 30 DF,  p-value: < 2.2e-16
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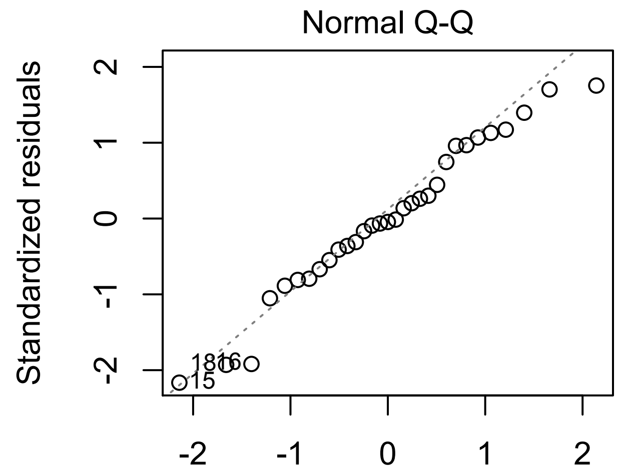

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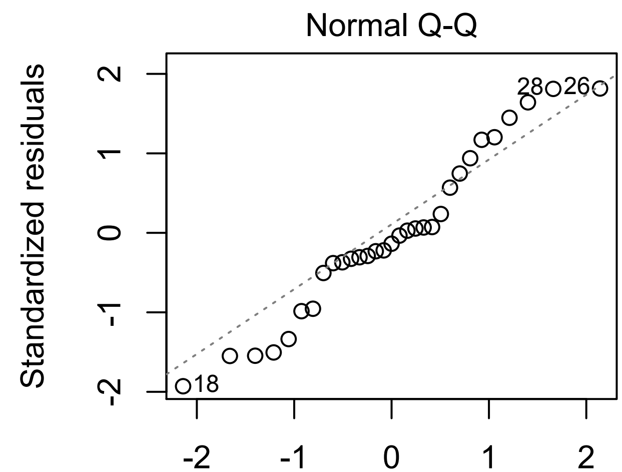

Multiple Regression:

Shapiro-Wilk test p-value: 0.5225

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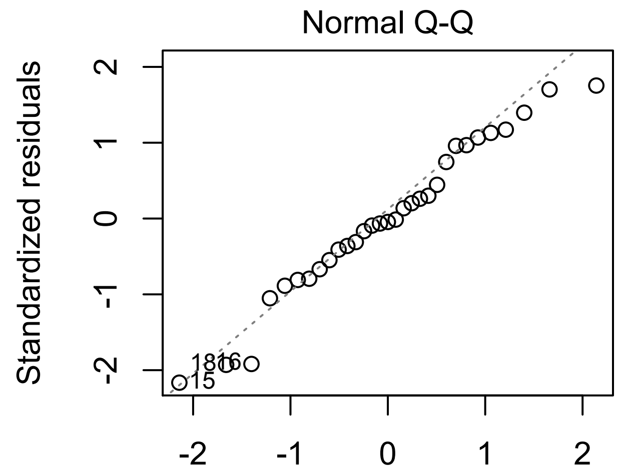

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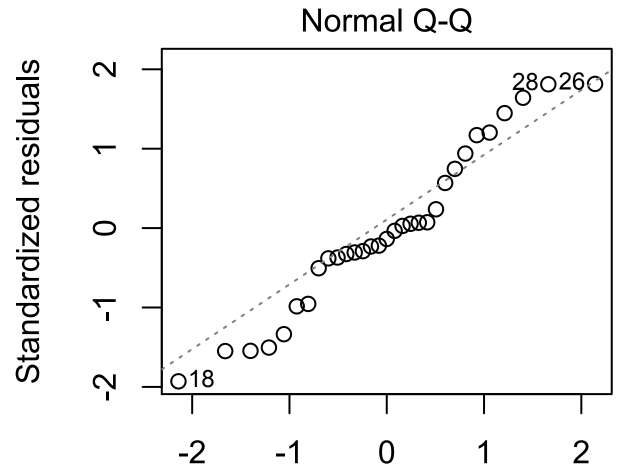

Shapiro-Wilk test p-value: 0.2655

Model Selection: Choosing the best model

Occam's Razor:
Among competing hypotheses, the one with the fewest assumptions should be selected

Parsimonious modelling:
Only choose a more complex model if the benefits are sufficiently substantial.

We want:
1. The model that fits the data the best
2. Not to suffer from excessive overfitting

Objective solution: use information criteria.

Model Selection: Choosing the best model

Akaike's Information Criterion:

$$\mathrm{AIC} = 2k - 2\log(\hat{L})$$

k : number of parameters
$\hat{L}$: maximum of the likelihood function.

The model with the smallest AIC is deemed the best.

Other information criteria exist.
Notably Bayesian Information Criterion (BIC), which more heavily penalises parameters.
Careful with small sample sizes… corrections exist.

Model Selection: Choosing the best model

Model	R^2	AIC
$\boldsymbol{y} = \alpha + \beta\boldsymbol{x} + \boldsymbol{\varepsilon}$	0.9353	181.6
$\boldsymbol{y} = \beta_0 + \beta_1\boldsymbol{x_1} + \beta_2\boldsymbol{x_2} + \boldsymbol{\varepsilon}$	0.9480	176.9
$\boldsymbol{y} = \beta_0 + \beta_1\boldsymbol{x_1} + \beta_2\boldsymbol{x_2} + \beta_3\boldsymbol{x_1}\boldsymbol{x_2} + \boldsymbol{\varepsilon}$	0.9756	155.5
$\log(\boldsymbol{y}) = \beta_0 + \beta_1\log(\boldsymbol{x_1}) + \beta_2\log(\boldsymbol{x_2}) + \boldsymbol{\varepsilon}$	0.9777	-62.71
$\log(\boldsymbol{y}) = \beta_0 + \beta_1\log(\boldsymbol{x_1}) + \beta_2\log(\boldsymbol{x_2}) + \beta_3\log(\boldsymbol{x_1})\log(\boldsymbol{x_2}) + \boldsymbol{\varepsilon}$	0.9778	-60.88
$\log\left(\frac{\boldsymbol{y}}{\boldsymbol{x_1}^2\boldsymbol{x_2}}\right) = \beta_0 + \boldsymbol{\varepsilon}$	NA	-66.34
$\boldsymbol{y} = \beta_1\boldsymbol{x_1}^2\boldsymbol{x_2} + \boldsymbol{\varepsilon}$	0.9950	146.6

Response: y = Volume
Predictor: x_1 = Girth
Predictor: x_2 = Height

Model Selection: Choosing the best model

Sometimes selecting the best model can be difficult (time consuming & subjective)

Especially when there are a huge number of independent variables

Stepwise Regression – automatically selects "the best" model:

- Start from a given model
- Add or remove terms one at a time
- Score model (AIC)
- Repeat until optimal solution is found

Two options:

- Forward selection – start from simple model and add terms one at a time
- Backward elimination – start from a complex model and remove terms one at a time

Warning:
These strategies can lead to different models being selected
Neither strategy guarantees the optimal solution, but they are quick

Stepwise Regression:

Example: *Swiss fertility and socioeconomic indicators*

Regress Fertility against all available indicators:

```
                 Estimate Std. Error t value Pr(>|t|)    
(Intercept)      66.91518   10.70604   6.250 1.91e-07 ***
Agriculture      -0.17211    0.07030  -2.448  0.01873 *  
Examination      -0.25801    0.25388  -1.016  0.31546    
Education        -0.87094    0.18303  -4.758 2.43e-05 ***
Catholic          0.10412    0.03526   2.953  0.00519 ** 
Infant.Mortality  1.07705    0.38172   2.822  0.00734 ** 
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 7.165 on 41 degrees of freedom
Multiple R-squared:  0.7067,  Adjusted R-squared:  0.671 
F-statistic: 19.76 on 5 and 41 DF,  p-value: 5.594e-10
```

Stepwise Regression:

Example: *Swiss fertility and socioeconomic indicators*

Regress Fertility against all available indicators:

```
Start:  AIC=190.69
Fertility ~ Agriculture + Examination +
Education + Catholic + Infant.Mortality

                   Df Sum of Sq    RSS    AIC
- Examination       1     53.03 2158.1 189.86
<none>                          2105.0 190.69
- Agriculture       1    307.72 2412.8 195.10
- Infant.Mortality  1    408.75 2513.8 197.03
- Catholic          1    447.71 2552.8 197.75
-  Education        1   1162.56 3267.6 209.36
```

```
Step:  AIC=189.86
Fertility ~ Agriculture + Education + Catholic
+ Infant.Mortality

                   Df Sum of Sq    RSS    AIC
<none>                          2158.1 189.86
- Agriculture       1    264.18 2422.2 193.29
- Infant.Mortality  1    409.81 2567.9 196.03
- Catholic          1    956.57 3114.6 205.10
- Education         1   2249.97 4408.0 221.43
```

Stepwise Regression:

Example: *Swiss fertility and socioeconomic indicators*

Regress Fertility against all available indicators:

```
                 Estimate Std. Error t value Pr(>|t|)    
(Intercept)      62.10131    9.60489   6.466 8.49e-08 ***
Agriculture      -0.15462    0.06819  -2.267  0.02857 *  
Education        -0.98026    0.14814  -6.617 5.14e-08 ***
Catholic          0.12467    0.02889   4.315 9.50e-05 ***
Infant.Mortality  1.07844    0.38187   2.824  0.00722 ** 
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.168 on 42 degrees of freedom
Multiple R-squared:  0.6993,  Adjusted R-squared:  0.6707 
F-statistic: 24.42 on 4 and 42 DF,  p-value: 1.717e-10
```

- Compared to before stepwise regression, R^2 is lower, and RSE is higher
- AIC favoured the model with fewer parameters.
- Not all terms have significant utility, but the model is worse without them

Final Message:

Linear regression is well-suited to dealing with continuous data…

However it is also suited to:

- Discrete data (e.g. Poisson, Binomial)
- Categorical data (indicator variables, factors)
- Binary data (e.g. Bernoulli)

We have already seen a linear model be used to estimate the mean…

Consider similarities to other techniques:

One-sample Student's t-test: $$Y_i = \mu + \varepsilon_i$$

Two independent sample t-test:
One-way ANOVA: $$Y_{i(g)} = \mu + \delta_g + \varepsilon_{i(g)}$$

Two-way ANOVA: $$Y_{i(gk)} = \mu + \delta_g + \delta_k + \delta_{gk} + \varepsilon_{i(gk)}$$

These are all linear models! The only difference is in the questions we ask…
Linear modelling is extremely flexible.