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Laboratory of
Molecular Biology

Linear Modelling: Multiple Regression

10th of May 2018

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Linear models:

Simple/single regression:

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

Multiple regression:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \varepsilon$$

$$y = X\beta + \varepsilon$$

Linear models:

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

Multiple regression: $\mathbf{y} = \beta_0 + \beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 + \cdots + \beta_n \mathbf{x}_n + \boldsymbol{\varepsilon}$

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

Parameter estimation:

Minimise sum of squares of residuals: $\sum_i \varepsilon_i^2 \rightarrow \min$

$$SS_{\text{error}} = \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \rightarrow \min$$

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

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

Linear models:

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

Multiple regression: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n + \varepsilon$

$$y = X\beta + \varepsilon$$

Assumptions:

1. Model is linear in parameters.

2. Gaussian error model.

$$\varepsilon \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$$

3. Additive error model.

4. Independence of errors.

$$\text{Cov}(\varepsilon_i, \varepsilon_j) = 0$$

5. Homoscedasticity.

$$\text{Var}(\varepsilon|\mathbf{x}) = \sigma^2 \mathbf{I}$$

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:

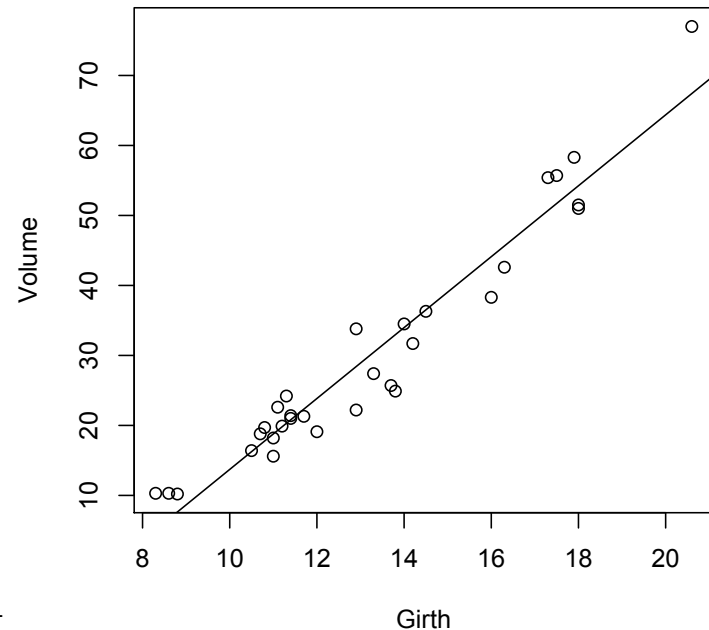
Min	1Q	Median	3Q	Max
-8.065	-3.107	0.152	3.495	9.587

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

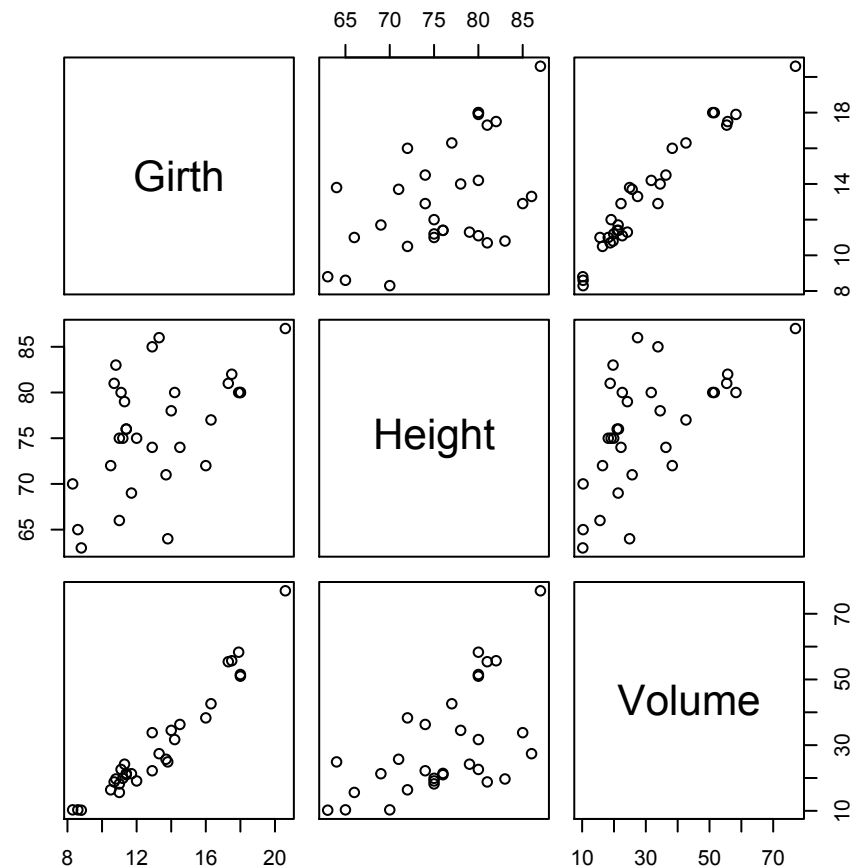
Residual standard error: 4.252 on 29 degrees of freedom
Multiple R-squared: 0.9353, Adjusted R-squared: 0.9331
F-statistic: 419.4 on 1 and 29 DF, p-value: < 2.2e-16



Response: $y = \text{Volume}$
Predictor: $x = \text{Girth}$

Multiple Regression:

Example: *Predicting timber volume of cherry trees*



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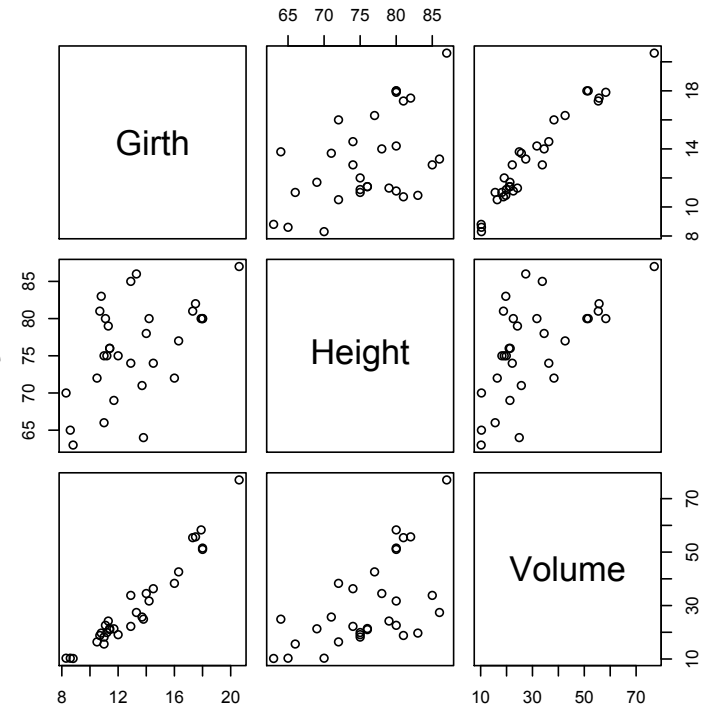
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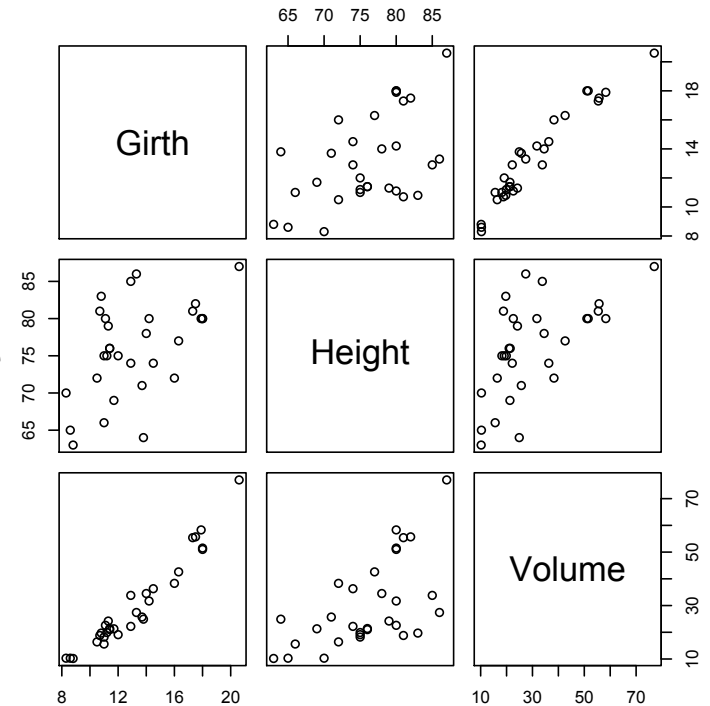
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

Response: $y = \text{Volume}$
 Predictor: $x_1 = \text{Girth}$
 Predictor: $x_2 = \text{Height}$

	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:

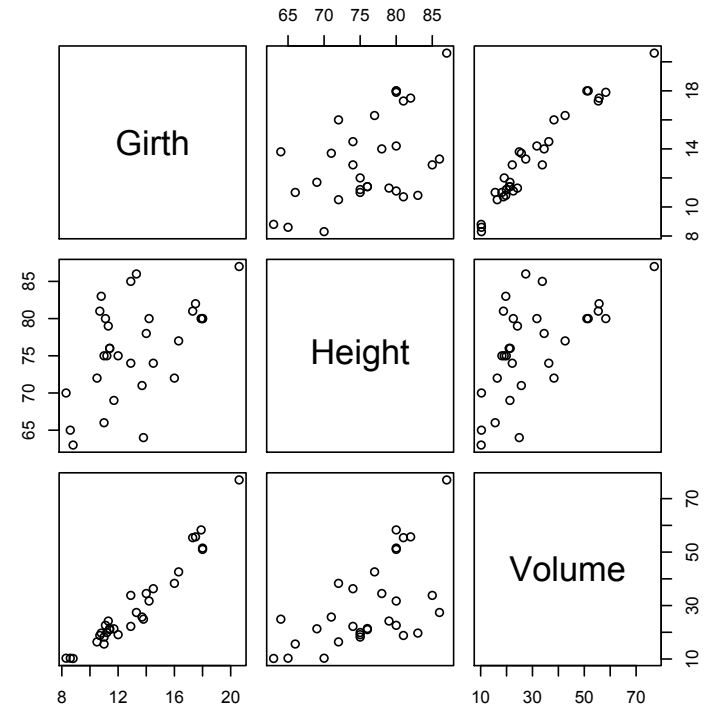
Example: *Predicting timber volume of cherry trees*

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

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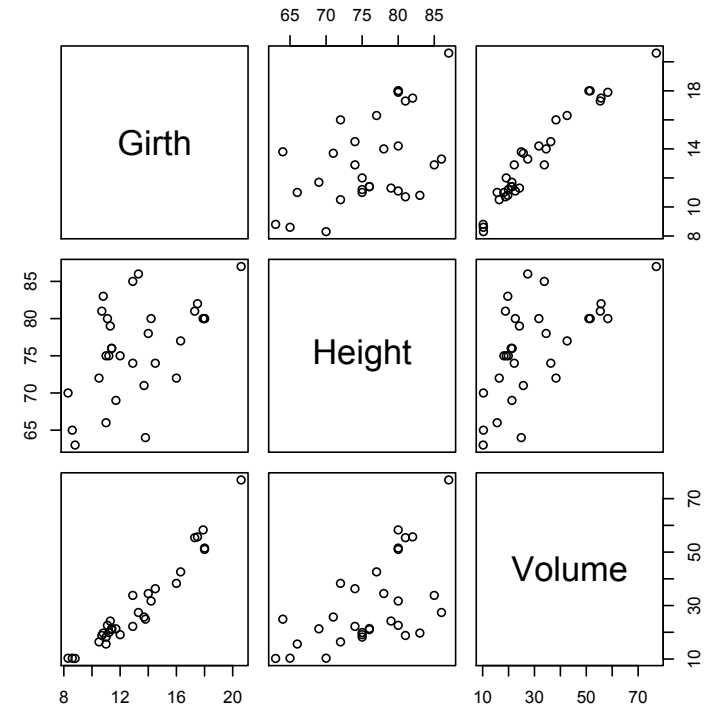
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$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \varepsilon$$

	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



Response: $y = \text{Volume}$
 Predictor: $x_1 = \text{Girth}$
 Predictor: $x_2 = \text{Height}$

Include interaction term:

R^2 is improved

Height term is significant (!)

All terms are significant

Multiple Regression:

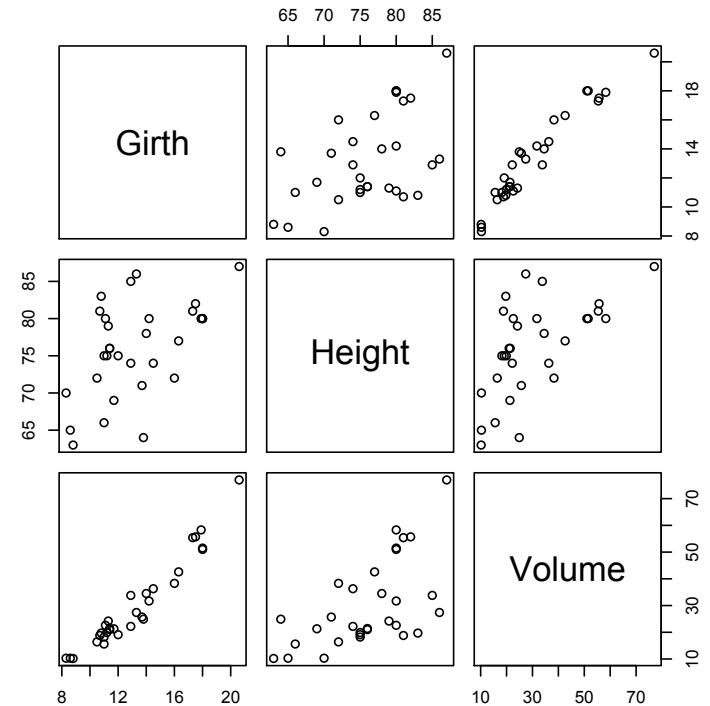
Example: *Predicting timber volume of cherry trees*

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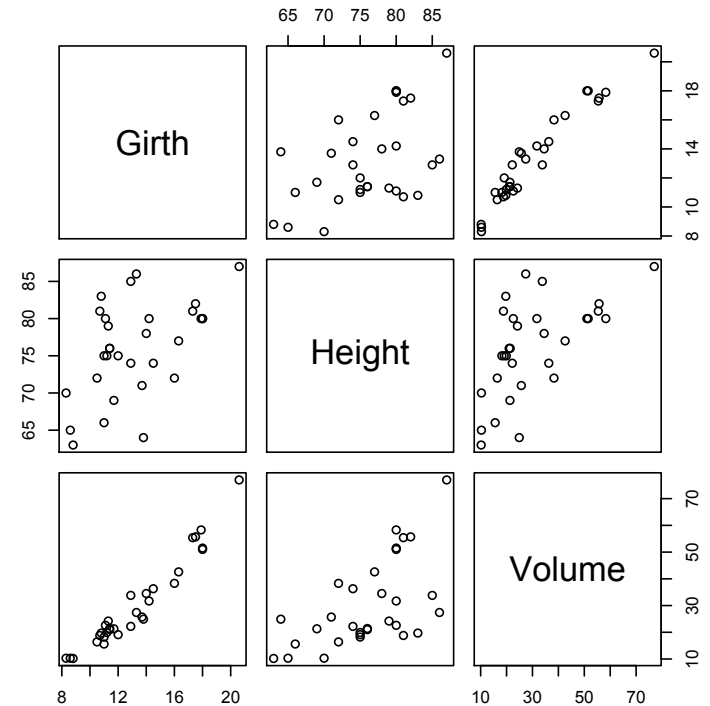
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$$\log(y) = \beta_0 + \beta_1 \log(x_1) + \beta_2 \log(x_2) + \varepsilon$$

	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	***

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



Response: $y = \text{Volume}$
Predictor: $x_1 = \text{Girth}$
Predictor: $x_2 = \text{Height}$

Log-transform variables:

R^2 is improved

Fewer parameters

All terms are significant

Residual standard error!!!

Multiple Regression:

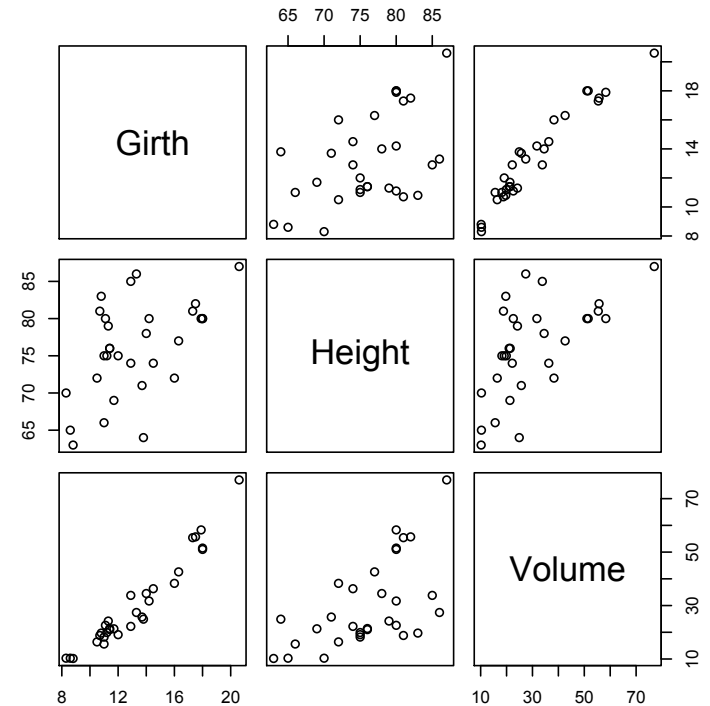
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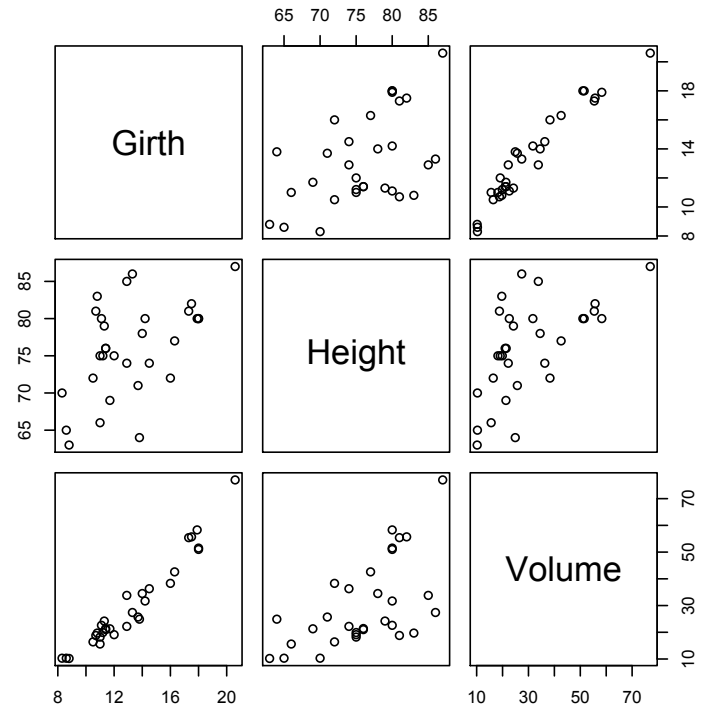
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	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-3.6869	7.6996	-0.479	0.636
log(Girth)	0.7942	3.0910	0.257	0.799
log(Height)	0.4377	1.7788	0.246	0.808
log(Girth):log(Height)	0.2740	0.7124	0.385	0.704

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:
R² marginally improved
No terms are significant!!!

Multiple Regression:

Example: *Predicting timber volume of cherry trees*

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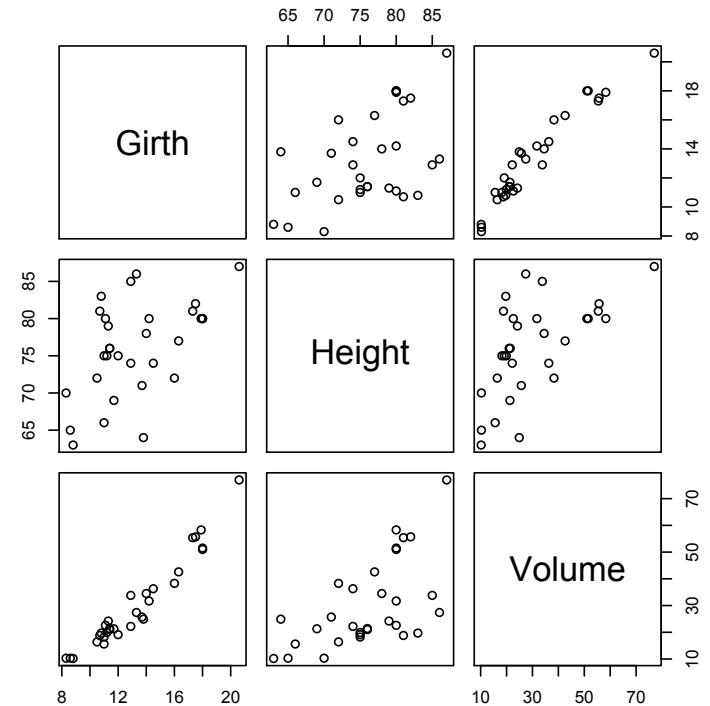
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$$y = e^{\beta_0} x_1^{\beta_1} x_2^{\beta_2} e^{\varepsilon}$$

Confidence Intervals:

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



Response: $y = \text{Volume}$
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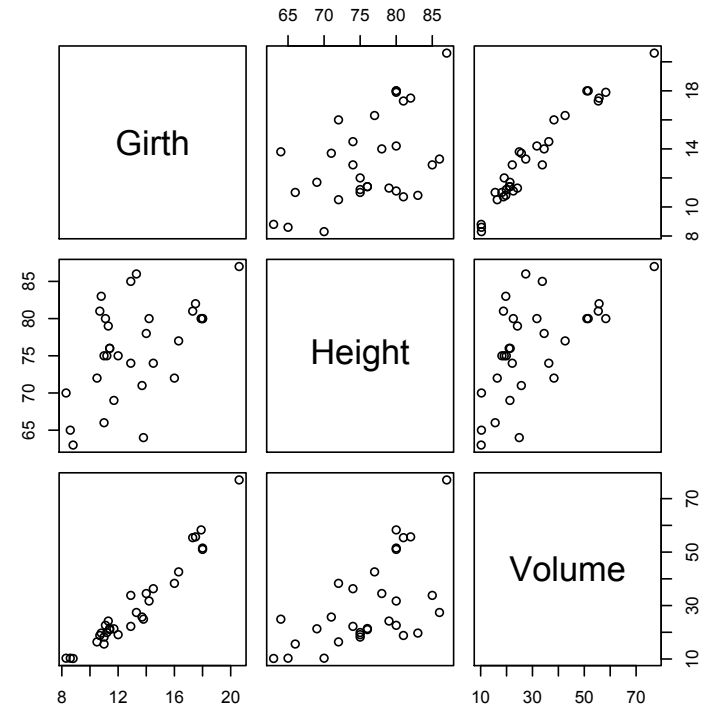
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$\hat{\beta}_1 \approx 2$
 $\hat{\beta}_2 \approx 1$



Response: $y = \text{Volume}$
Predictor: $x_1 = \text{Girth}$
Predictor: $x_2 = \text{Height}$

$$\text{Volume} \propto \text{Girth}^2 \times \text{Height}$$

Multiple Regression:

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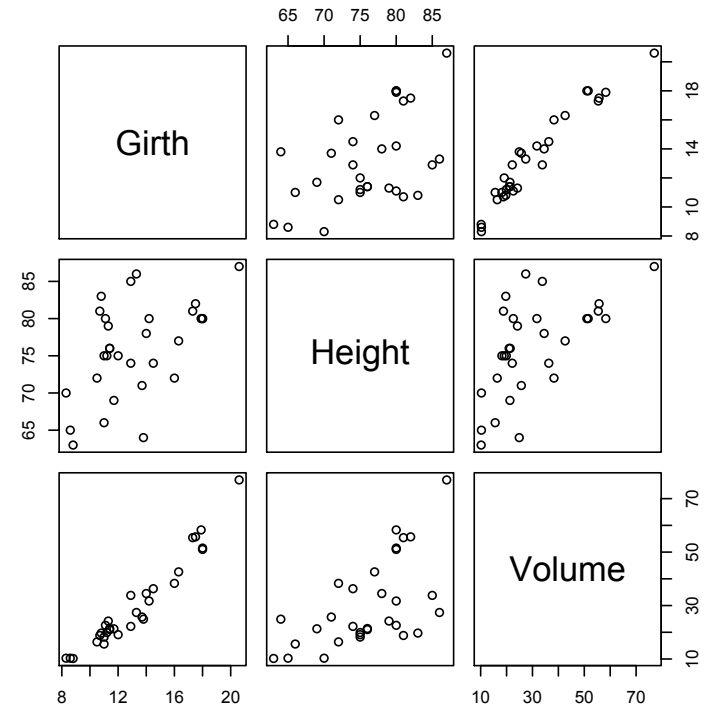
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Response: $y = \text{Volume}$
Predictor: $x_1 = \text{Girth}$
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$$\text{Volume} \propto \text{Girth}^2 \times \text{Height}$$

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

Multiple Regression:

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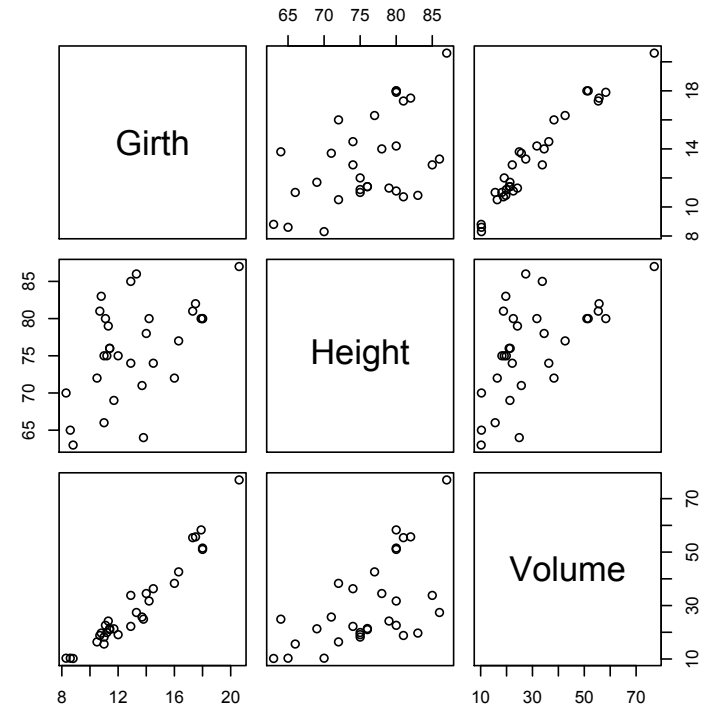
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Volume \propto Girth² x Height

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

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



Response: $y = \text{Volume}$
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```

              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 ***
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```

Residual standard error: 0.08139 on 28 degrees of freedom
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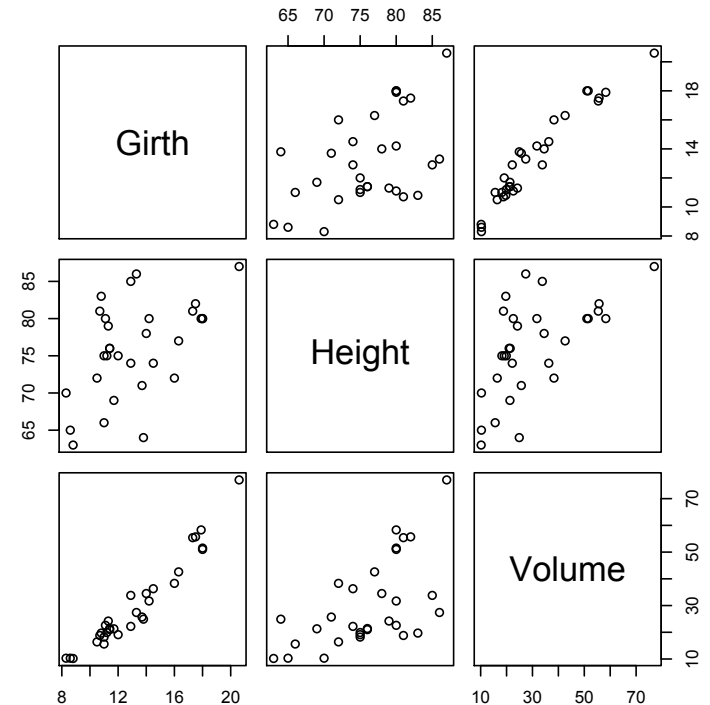
$$\log\left(\frac{y}{x_1^2 x_2}\right) = \beta_0 + \varepsilon$$

```

              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: $y = \text{Volume}$
 Predictor: $x_1 = \text{Girth}$
 Predictor: $x_2 = \text{Height}$

Constrain parameters:

No R^2

Intercept is significant

Again, can't compare RSE...

Multiple Regression:

Example: *Predicting timber volume of cherry trees*

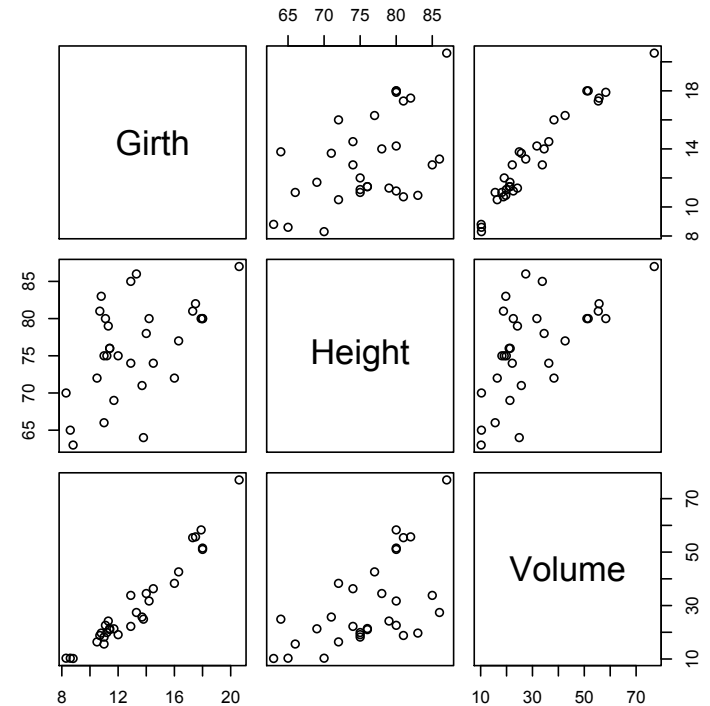
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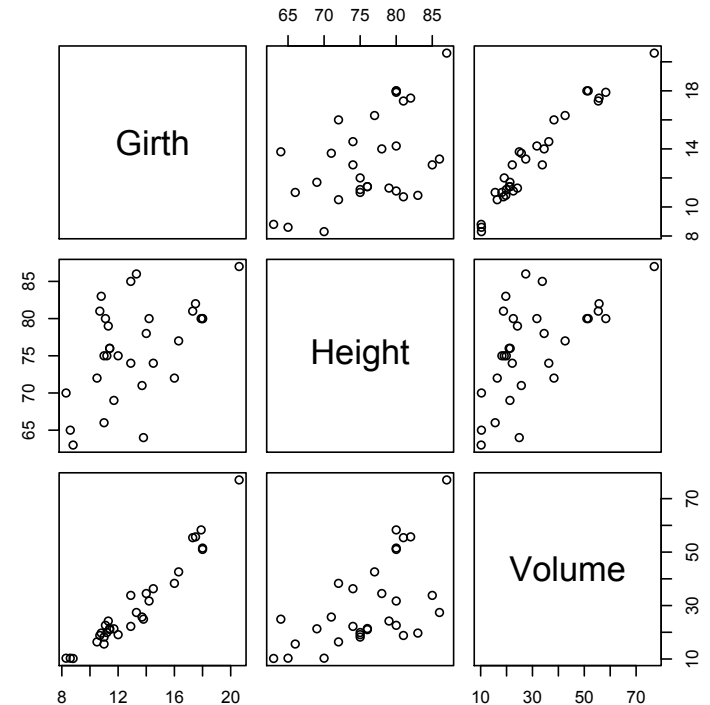
$$y = \beta_1 x_1^2 x_2 + \varepsilon$$

```

              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

```



Response: $y = \text{Volume}$
 Predictor: $x_1 = \text{Girth}$
 Predictor: $x_2 = \text{Height}$

Simple regression, no intercept:
 R^2 incomparable
 Again, can't compare RSE...

$\exp(-6.16917) = 2.092e-03 \dots?!$

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Example: *Predicting timber volume of cherry trees*

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

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

```

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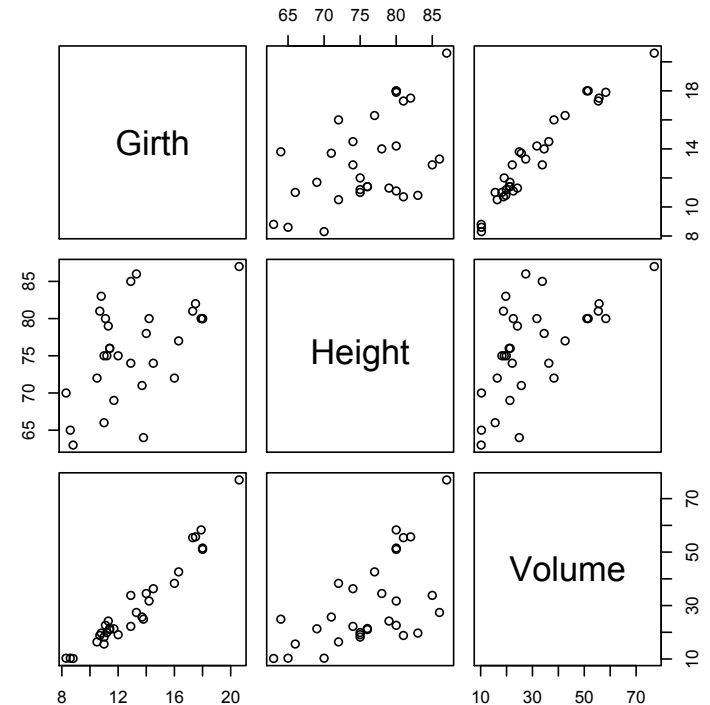
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```

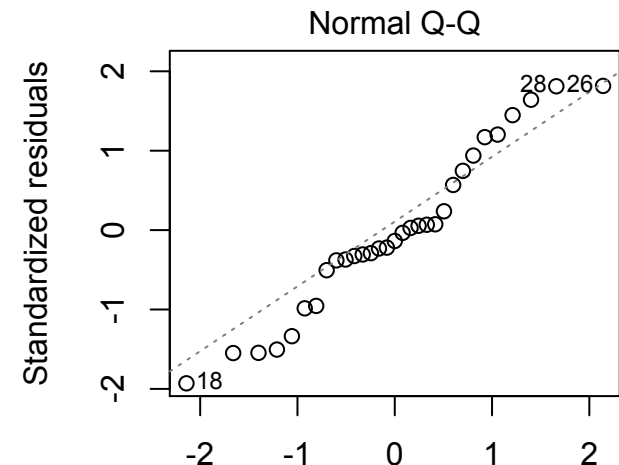
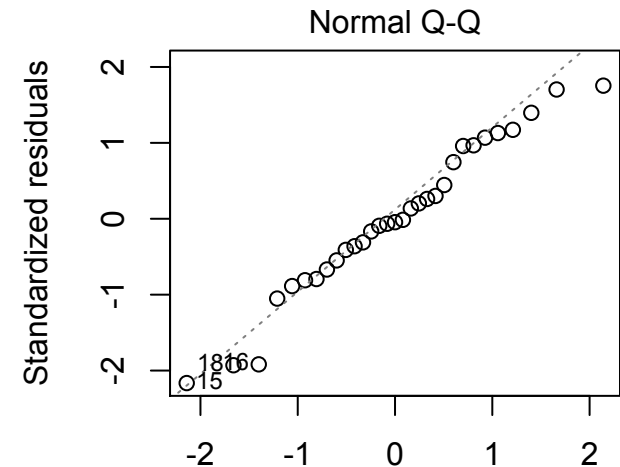
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```



Multiple Regression:

Shapiro-Wilk test p-value: 0.5225

Example: *Predicting timber volume of cherry trees*

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

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```

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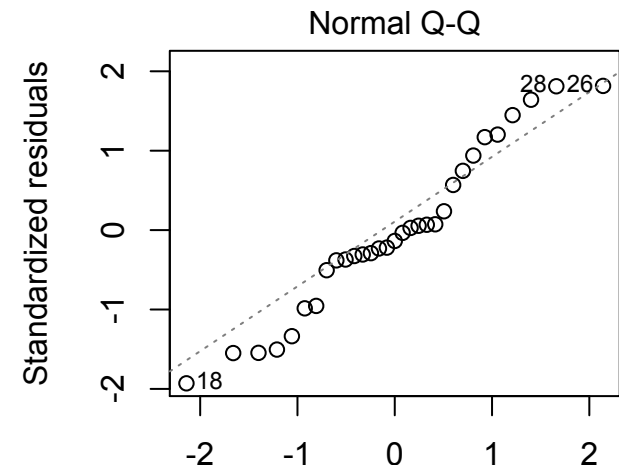
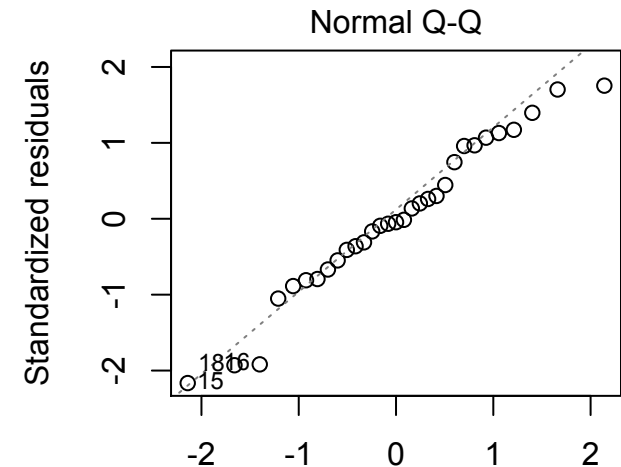
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```

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I(Girth^2):Height 2.108e-03  2.722e-05   77.44   <2e-16 ***
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Multiple R-squared:  0.995,    Adjusted R-squared:  0.9949
F-statistic: 5996 on 1 and 30 DF,  p-value: < 2.2e-16

```



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:

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

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

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

Response: y = Volume

Predictor: x₁ = Girth

Predictor: x₂ = 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

Non-linear models:

Motivating example: *Predicting timber volume of cherry trees*

$$y = \beta_0 x_1^{\beta_1} x_2^{\beta_2} + \epsilon$$

Response: y = Volume

Predictor: x_1 = Girth

Predictor: x_2 = Height

Can't solve using standard regression approaches.

Instead, use a library that can estimate parameters for non-linear models, e.g. “nls” in R.

Con's:

- May require initial parameter estimates
- May not find globally optimal solution – depends on initial parameter estimates
- May not converge at all
- Slower – iterative approach
- Becomes slower and less reliable as the function becomes more complex

Pro's:

- Allows dealing with a wider class of model functional forms

Non-linear models:

Motivating example: *Predicting timber volume of cherry trees*

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

Response: y = Volume
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Predictor: x_2 = Height

Can't solve using standard regression approaches.

Instead, use a library that can estimate parameters for non-linear models, e.g. “nls” in R.

Parameters:

	Estimate	Std. Error	t value	Pr(> t)
beta0	0.001449	0.001367	1.060	0.298264
beta1	1.996921	0.082077	24.330	< 2e-16 ***
beta2	1.087647	0.242159	4.491	0.000111 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.533 on 28 degrees of freedom

Number of iterations to convergence: 5

Achieved convergence tolerance: 8.255e-07

AIC = 150.4

Parameters:

	Estimate	Std. Error	t value	Pr(> t)
beta1	2.27405	0.12967	17.54	< 2e-16 ***
beta2	-0.58432	0.08242	-7.09	8.44e-08 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.216 on 29 degrees of freedom

Number of iterations to convergence: 10

Achieved convergence tolerance: 8.673e-06

AIC = 181.1

Note: poor parameter interpretation

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.

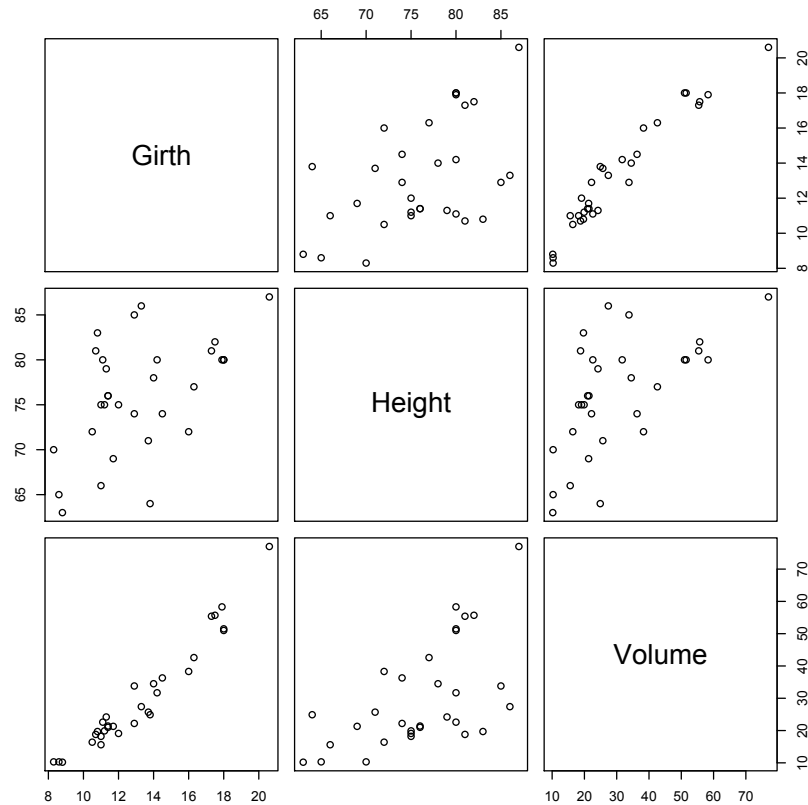
What to use and when:

	Multiple regressors	Non-Gaussian error model	Non-linear model	Autocorrelated data
Simple regression				
Multiple regression	✓			
Generalised linear model	✓	✓		
Non-linear model	✓	✓	✓	
Time series analysis				✓

Multiple Regression in R:

R functions:

`plot(x,y)`



Multiple Regression in R:

R functions:

plot(x,y)

m1 = lm(y~x)

summary(m1)

confint(m1)

Call:

```
lm(formula = log(Volume) ~ log(Girth) + log(Height), data = trees)
```

Residuals:

Min	1Q	Median	3Q	Max
-0.168561	-0.048488	0.002431	0.063637	0.129223

Coefficients:

	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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Multiple R-squared: 0.9777, Adjusted R-squared: 0.9761

F-statistic: 613.2 on 2 and 28 DF, p-value: < 2.2e-16

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

Multiple Regression in R:

R functions:

plot(x,y)

m1 = lm(y~x)

summary(m1)

##

Shapiro-Wilk normality test

confint(m1)

##

data: residuals(m1)

shapiro.test(residuals(m1))

W = 0.97013, p-value = 0.5225

Multiple Regression in R:

R functions:

`plot(x,y)`

`m1 = lm(y~x)`

`summary(m1)`

`confint(m1)`

`shapiro.test(residuals(m1))`

`AIC(m1)`

`stepAIC(m1)`

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
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- Catholic	1	956.57	3114.6	205.10
- Education	1	2249.97	4408.0	221.43

Call:

lm(formula = Fertility ~ Agriculture + Education + Catholic +
Infant.Mortality, data = swiss)

Residuals:

Min	1Q	Median	3Q	Max
-14.6765	-6.0522	0.7514	3.1664	16.1422

Coefficients:

	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 *
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`shapiro.test(residuals(m1))`

`AIC(m1)`

`stepAIC(m1)`

`nls(volume~beta0*girth^beta1*height^beta2, start=list(beta0=1,beta1=2,beta2=1))`