

Introduction to Statistical Modeling

Simple Linear Regression

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Introduction

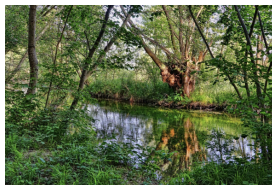
Regression

Goal: describe the relationship between 2 series of observations (X_i, Y_i) , obtained for individual subjects $i = 1, \dots, n$

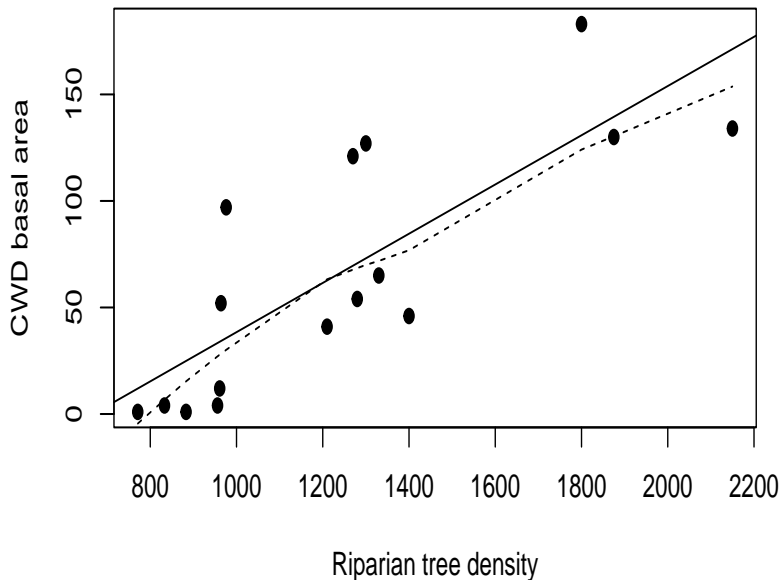
Example:

Basal area of coarse woody debris (CWD) versus tree density along 16 North American lakes

- **Dependent variable, outcome, response Y :** CWD basal area
- **Independent variable, explanatory variable, predictor X :** tree density (in number per km)



CWD versus tree density



Regression

For fixed X , Y will be some function of X plus random noise:

observation = signal + noise

Mathematical modelling of observation:

$$Y_i = f(X_i) + \epsilon_i$$

where $f(x)$ is the expected outcome for subjects with $X_i = x$

$$E(Y_i | X_i = x) = f(x)$$

and ϵ_i is on average 0 for subjects with same X_i :

$$E(\epsilon_i | X_i) = 0.$$

Linear regression

- To obtain accurate and interpretable results, $f(X)$ is often chosen as linear function of unknown parameters
- Use **linear regression model**

$$E(Y|X = x) = \alpha + \beta x$$

with unknown **intercept** α and **slope** β .

- Linear regression model makes assumption on distribution of X and Y , so can be incorrect.

Use of linear regression

- **Prediction:** when Y unknown, but X known, we can predict Y based on X :

$$E(Y|X = x) = \alpha + \beta x.$$

- **Association:** describe biological relation between variable X and continuous measurement Y
 - Slope β : difference in mean outcome between subjects that differ 1 unit in the value of X :

$$\begin{aligned} E(Y|X = x + \delta) - E(Y|X = x) &= \alpha + \beta(x + \delta) - \alpha - \beta x \\ &= \beta\delta. \end{aligned}$$

Least squares estimates

- Least squares (regression) line: line that 'best' fits data.
- Found by choosing values for α and β that minimize sum of squares of **residuals**:

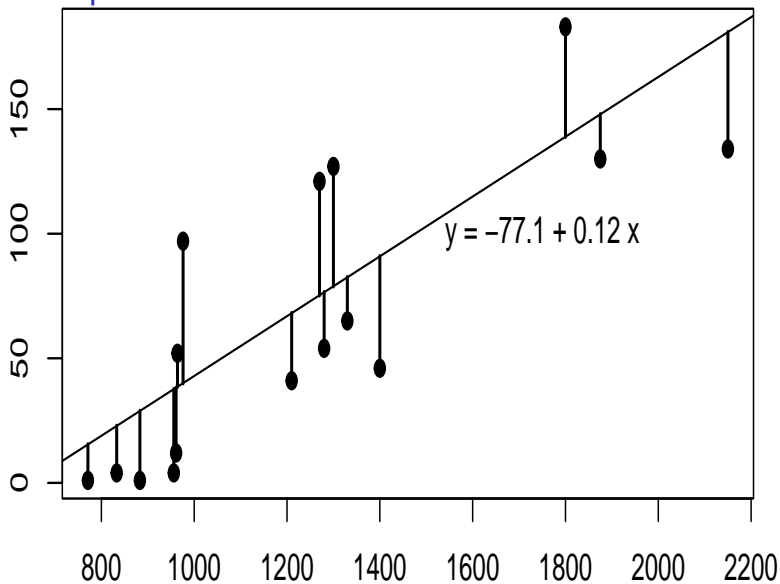
$$\sum_{i=1}^n \underbrace{(Y_i - \alpha - \beta X_i)}_{\text{Residual}}^2$$

- Estimates for β and α :

$$\hat{\beta} = \text{Cor}(x, y) \frac{S_y}{S_x} \quad \text{and} \quad \hat{\alpha} = \bar{Y} - \hat{\beta} \bar{X}.$$

with $\text{Cor}(x, y)$ the sample correlation between x and y and S_x , S_y the sample standard deviation.

Residuals plot



See also: residuals animation.

Output linear regression (coefficients only)

```
model <- lm(CWD.BASA ~ RIP.DENS)
summary(model)$coefficients
```

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-77.0990778	30.60800907	-2.518918	0.0245520121
RIP.DENS	0.1155161	0.02343233	4.929772	0.0002216405

Regression line:

$$E(Y|X = x) = -77.10 + 0.12x$$

Output linear regression (full)

```
summary(model)
```

Call:

```
lm(formula = CWD.BASA ~ RIP.DENS)
```

Residuals:

Min	1Q	Median	3Q	Max
-38.62	-22.41	-13.33	26.16	61.35

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-77.09908	30.60801	-2.519	0.024552 *
RIP.DENS	0.11552	0.02343	4.930	0.000222 ***

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

Residual standard error: 36.32 on 14 degrees of freedom

Multiple R-squared: 0.6345, Adjusted R-squared: 0.6084

F-statistic: 24.3 on 1 and 14 DF, p-value: 0.0002216

Interpreting linear regression

- Model: $E(Y|X = x) = -77.10 + 0.12x$
- Expected CWD basal area is 1.2 m^2 larger alongside lakes with 10 more trees per km
- Expected CWD basal area alongside lakes with 1,600 trees per km shoreline:

$$-77.10 + 0.12 \times 1600 = 108 \text{ m}^2$$

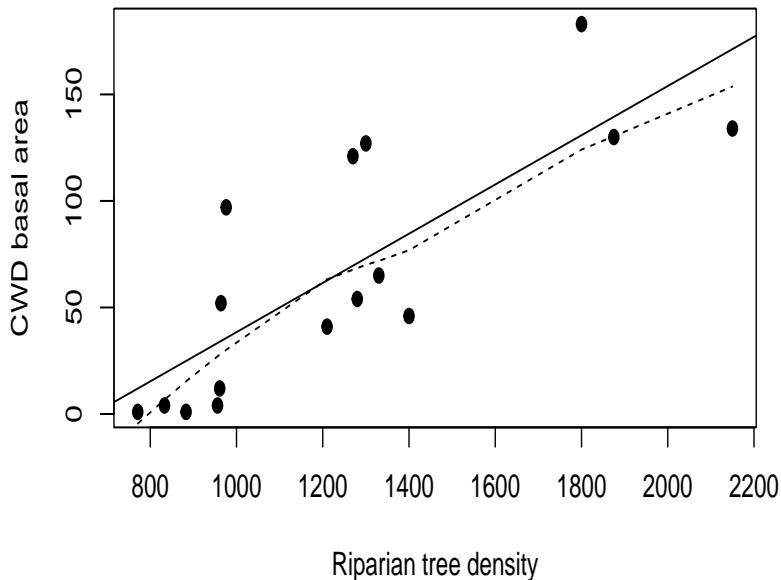
- Expected CWD basal area alongside lakes with 500 trees per km shoreline:

$$-77.10 + 0.12 \times 500 = -17 \text{ m}^2$$

- **Be careful with extrapolation!** (linearity assumption can only be verified within range of data)

Assumptions for linear regression

Verifying linearity assumption



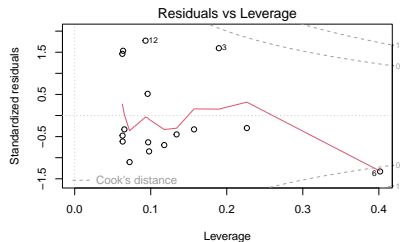
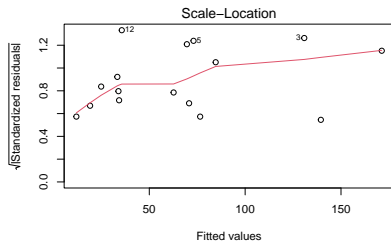
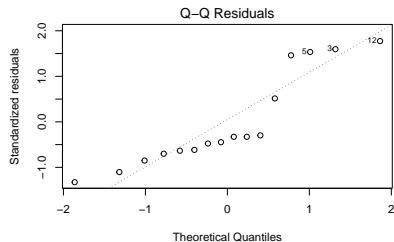
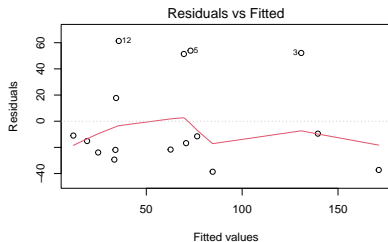
Verifying linearity assumption

- An alternative (more convenient when there are multiple predictors) is a **residual plot**.
- Note: residuals are prediction errors:

$$e_i = y_i - \hat{\alpha} - \hat{\beta}x_i$$

- If linear model correct, then scatterplot of e_i versus x_i or predictions $\hat{\alpha} + \hat{\beta}x_i$ shows no pattern

Verifying linearity assumption



Inference for simple linear regression

To be able to draw conclusions about the linear regression model

$$E(Y|X) = \alpha + \beta X$$

we need extra assumptions:

- **Homoscedasticity:** for fixed X , Y has constant variance

$$\text{Var}(Y|X) = \sigma^2,$$

estimated by the residual mean square error:

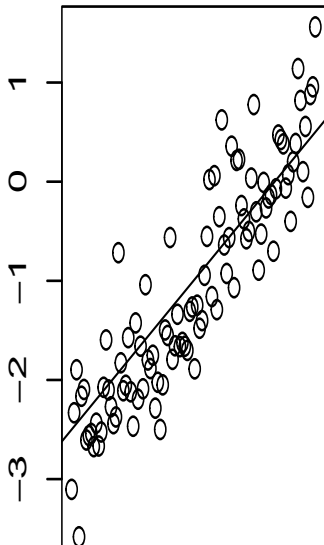
$$\text{MSE} = \sum_{i=1}^n e_i^2 / (n - 2)$$

- **Normality:** for fixed X , Y is normally distributed

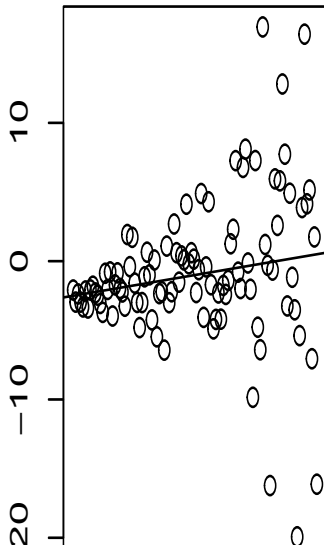
$$Y|X \sim N(\alpha + \beta X, \sigma^2)$$

Homoscedasticity versus heteroscedasticity

Homoscedasticity

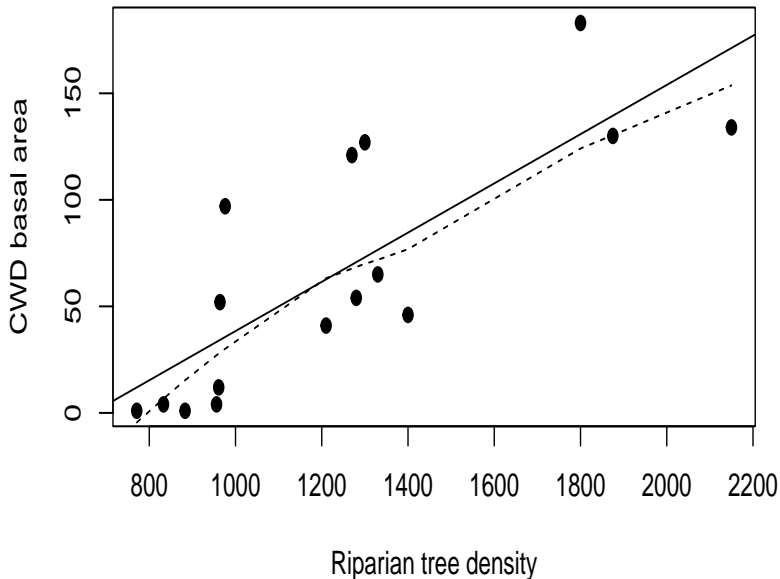


Heteroscedasticity



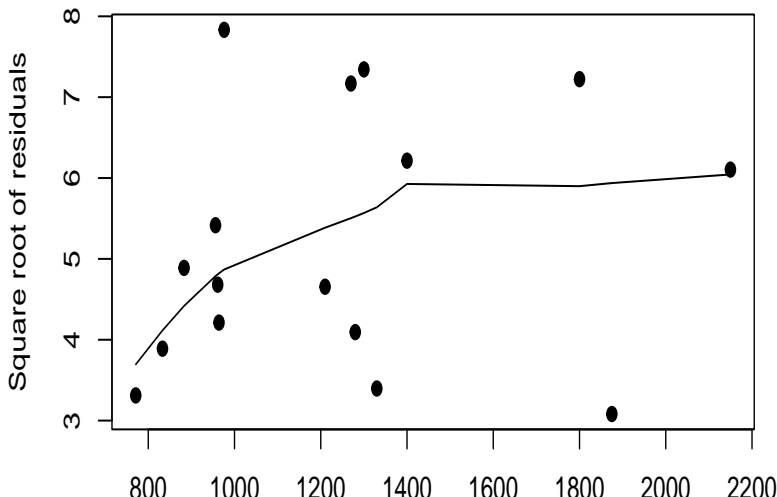
Homoscedasticity?

Hard to check on regression plot directly!

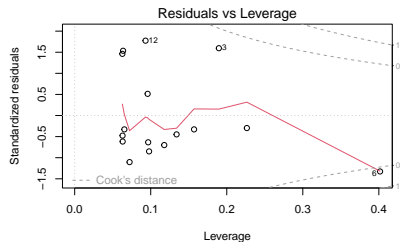
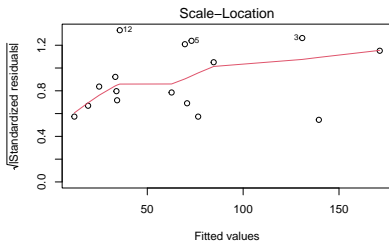
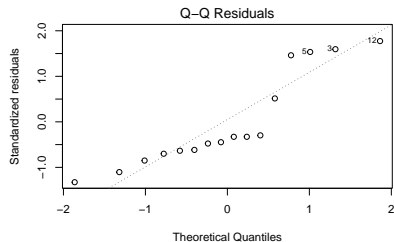
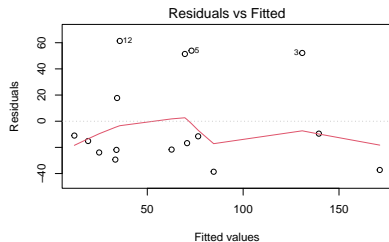


Assumption of homoscedasticity

- Squared residuals carry information on residual variability.
- If these are associated with explanatory variable, then indication of **heteroscedasticity**.
- Scatterplot of e_i^2 or $\sqrt{|e_i|}$ versus x_i or predictions.



Assumption of homoscedasticity



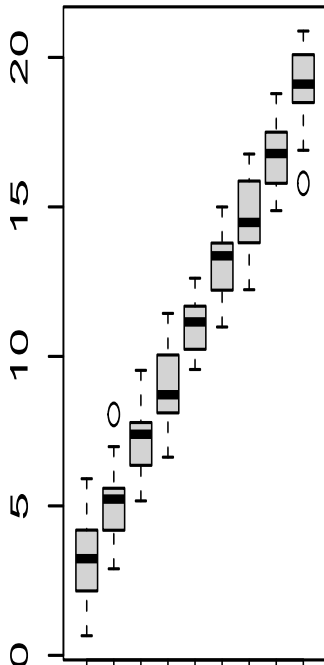
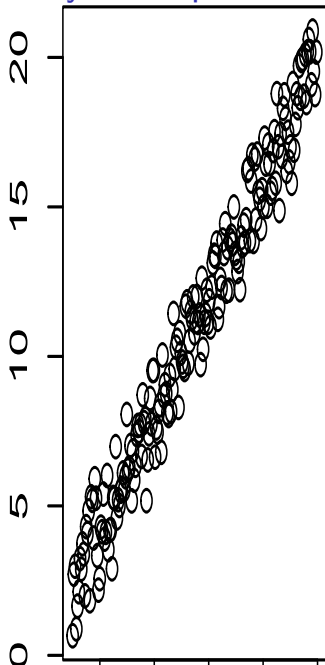
Normality assumption

- Assumption: outcomes normally distributed **for fixed values of explanatory variable**:

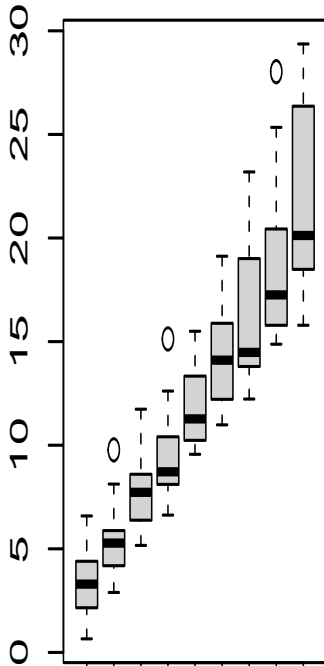
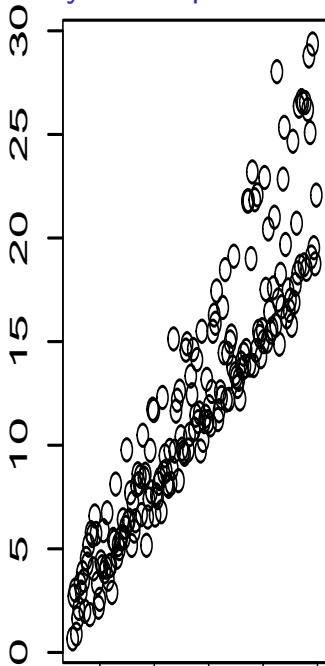
$$Y|X \sim N(a + bX, \sigma^2).$$

- Can be checked using QQ-plot of the residuals.

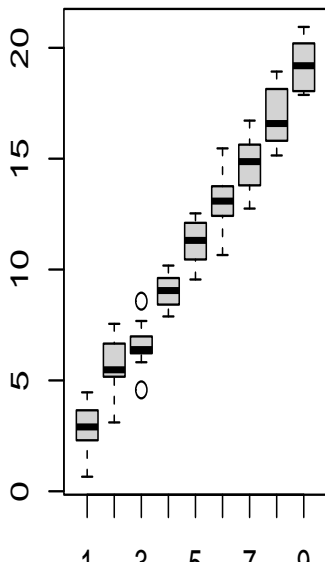
Normality assumption valid



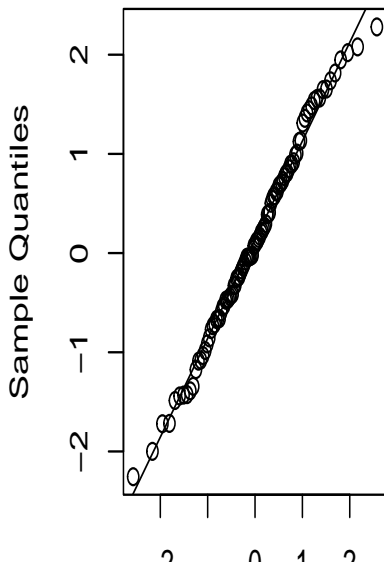
Normality assumption not valid



QQ plot of residuals ($Y|X$ normal)

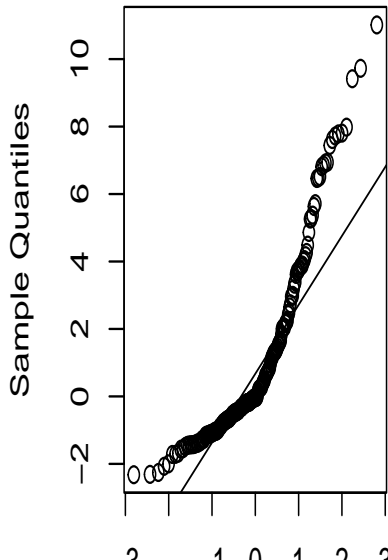
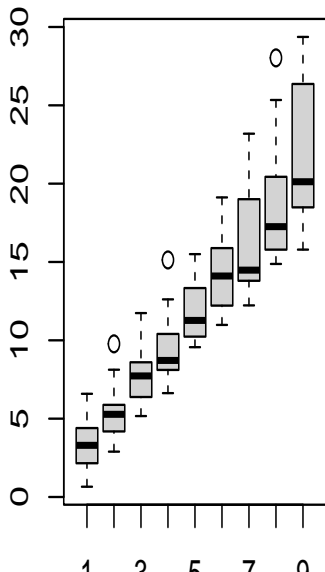


Q-Q plot of $Y|X$

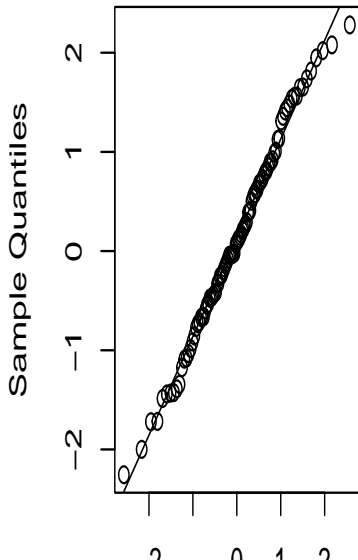


QQ plot of residuals ($Y|X$ not normal)

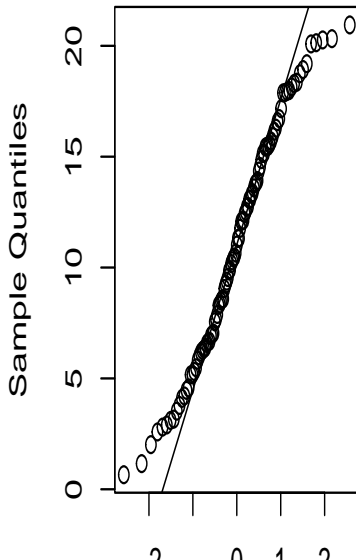
Q-Q plot of $Y|X$



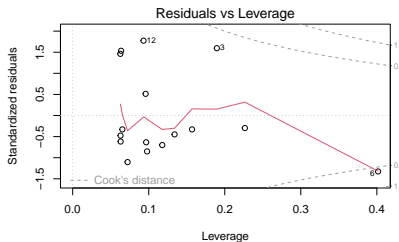
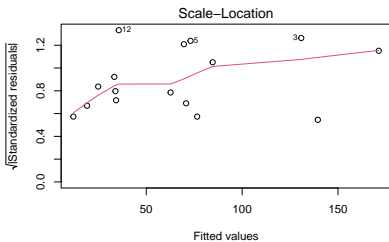
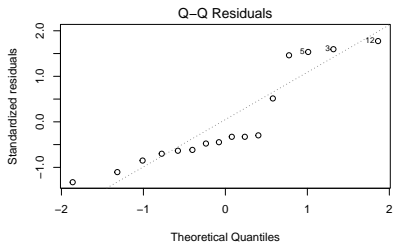
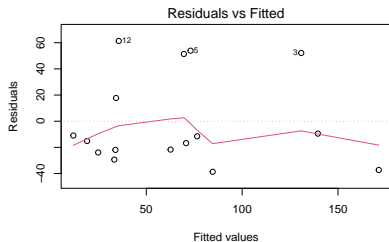
Do not use QQ-plot of Y !
Q-Q plot of $Y|X$



Q-Q plot of Y



Checking for normality with R diagnostic plots



What if homoscedasticity or normality false?

- Transformation of **dependent variable** can help to obtain normality and homoscedasticity.
- Example transformations:
 $\sqrt{Y}, Y^2, 1/Y, \exp Y, \exp(-Y), \ln Y$.
- Transformation of **independent variable** does not change distribution of Y for given X :
 - does not help in obtaining normality or homoscedasticity.
 - does help to obtain linearity if normality and homoscedasticity are ok.

What if homoscedasticity or normality false?

- Often because outcome can only take on values in certain interval (e.g. $[0, 1]$, positive numbers, ...)
- **Solution:** transform outcome such that it can take on all real values
- Example: CWD.BASA is always positive: take \ln to make outcome real-valued:

Transforming the outcome

```
model2 <- lm(log(CWD.BASA) ~ RIP.DENS)
summary(model2)
```

Call:

```
lm(formula = log(CWD.BASA) ~ RIP.DENS)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-2.23086	-0.78379	0.04559	0.72335	2.05022

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-0.5570100	1.0739690	-0.519	0.6121
RIP.DENS	0.0031573	0.0008222	3.840	0.0018 **

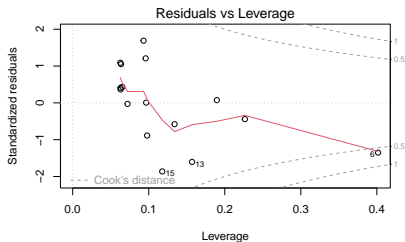
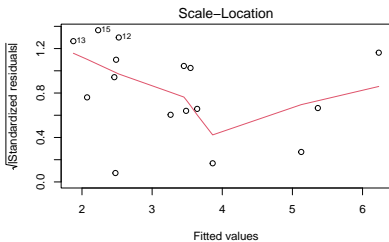
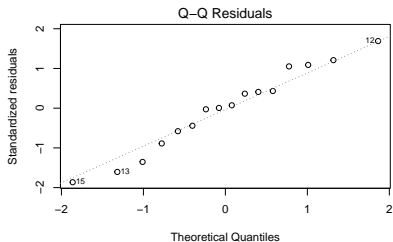
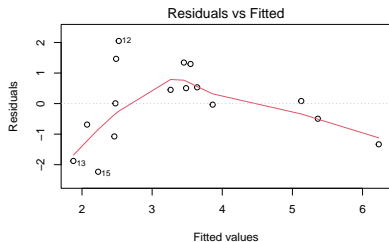
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Residual standard error: 1.274 on 14 degrees of freedom

Multiple R-squared: 0.513, Adjusted R-squared: 0.4782

F-statistic: 14.75 on 1 and 14 DF, p-value: 0.001802

Residual plots



Higher-order regression

What if linearity assumption is false?

- Transformation of dependent variable
- Transformation of independent variable
- If residuals reveal **quadratic association**, such that

$$e_i \approx \delta_0 + \delta_1 x_i + \delta_2 x_i^2$$

then

$$y_i = \hat{\alpha} + \hat{\beta}x_i + e_i \approx (\hat{\alpha} + \delta_0) + (\hat{\beta} + \delta_1)x_i + \delta_2 x_i^2$$

Quadratic regression

- We assume

$$E(Y|X) = \alpha + \beta X + \gamma X^2$$

- Unknown parameters estimated by **least squares method**:
minimize

$$\sum_{i=1}^n (Y_i - \alpha - \beta X_i - \gamma X_i^2)^2$$

Quadratic regression

Call:

```
lm(formula = log(CWD.BASA) ~ RIP.DENS + I(RIP.DENS^2))
```

Residuals:

	Min	1Q	Median	3Q	Max
	-1.6872	-0.4462	-0.1621	0.4214	2.1399

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-9.686e+00	3.114e+00	-3.110	0.00828	**
RIP.DENS	1.726e-02	4.673e-03	3.693	0.00270	**
I(RIP.DENS^2)	-4.960e-06	1.628e-06	-3.047	0.00935	**

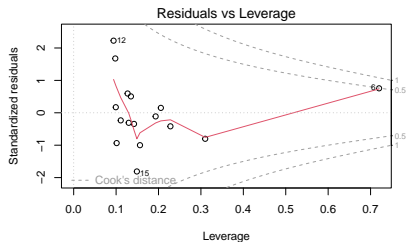
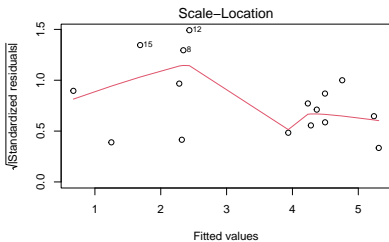
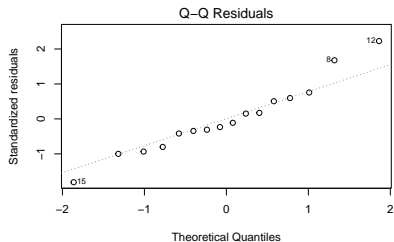
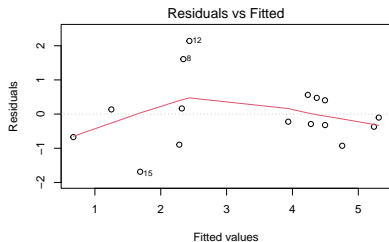
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.01 on 13 degrees of freedom

Multiple R-squared: 0.7159, Adjusted R-squared: 0.6722

F-statistic: 16.38 on 2 and 13 DF, p-value: 0.0002801

Residual plots



Building model proceeds hierarchically

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-9.686141e+00	3.114228e+00	-3.110287	0.008281158
RIP.DENS	1.726034e-02	4.673452e-03	3.693275	0.002704501
I(RIP.DENS^2)	-4.960374e-06	1.627703e-06	-3.047469	0.009345380

- Add terms to model and keep those as long as they are significantly associated with outcome
- Example: adding third order term is not significant contribution (p-value 0.26)
- Adding proceeds **hierarchically**: lower order terms are kept as long as higher order terms are in model

Results

- We conclude

$$E\{\ln(Y)|X\} = -9.69 + 0.017X - 4.96 \cdot 10^{-6}X^2$$

or equivalently that geometric mean CWD basal area for given tree density X is equal to

$$\exp(-9.69 + 0.017X - 4.96 \cdot 10^{-6}X^2)$$

- For $X = 500$ we now find 0.086 m^2 (previously: -17 m^2)
- **How precise is this?**

Interpreting the results of a regression model

Inference for mean outcome

Given an input $X = x_h$, what do we expect the outcome Y to be on average?

Use the regression equation:

- $\hat{y}_h = \hat{\alpha} + \hat{\beta}x_h$ is unbiased estimator of $E(Y|X = x_h) = \alpha + \beta x_h$.

What is the uncertainty of this estimator?

For this we need the standard error of \hat{Y}_h .

Inference for mean outcome: uncertainty

- Standard error of \hat{Y}_h is

$$SE(\hat{Y}_h) = \sqrt{MSE \left\{ \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum_i (X_i - \bar{X})^2} \right\}}.$$

- Tests and CI for $E(Y|X_h)$ based on

$$\frac{\hat{Y}_h - E(Y|X_h)}{SE(\hat{Y}_h)} \sim t_{n-p}$$

with p number of unknown parameters in model.

Inference for mean outcome: intuition

- Highest precision for predictions in $X_h = \bar{X}$: relative confidence in predictions for X **close to mean**.
- Lower precision as predictions have X further **away from the mean**.

Prediction in R

```
model3 <- lm(I(log(CWD.BASA)) ~ RIP.DENS + I(RIP.DENS^2))
p <- predict(model3,
              newdata = data.frame(RIP.DENS=c(1000, 1500)),
              interval = "confidence")
p
```

	fit	lwr	upr
1	2.613829	1.966541	3.261118
2	5.043534	4.149293	5.937775

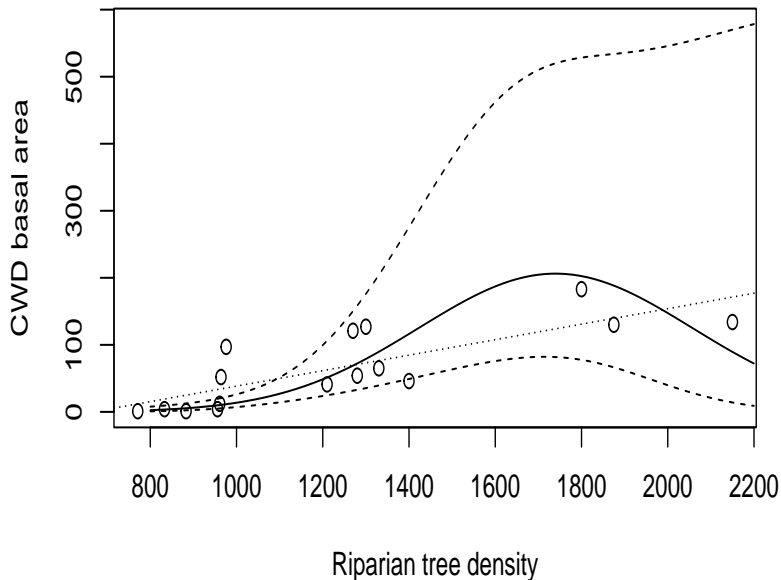
Prediction in R

Predictions and lower/upper bound of the CI are for `log(CWD.BASA)` and need to be transformed back:

```
exp(p)
```

	fit	lwr	upr
1	13.65123	7.145917	26.07867
2	155.01687	63.389137	379.09068

Expected outcome with 95% CI



Inference for slope β

- The regression coefficient $\hat{\beta}$ is an (unbiased) estimator of β , the population regression coefficient.
- It comes with a measure of uncertainty: standard error of $\hat{\beta}$:

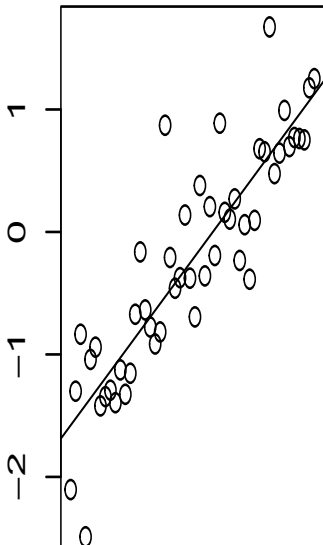
$$SE(\hat{\beta}) = \sqrt{\frac{MSE}{\sum_i (X_i - \bar{X})^2}}.$$

with $MSE = \frac{1}{n-2} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$

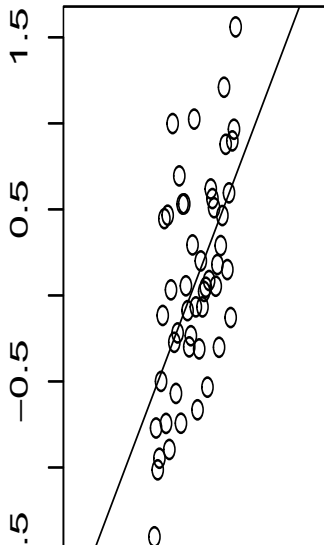
- Large spread on X improves precision.

Spread and precision

$$SE(\beta) = 0.04$$



$$SE(\beta) = 0.12$$



Association tree density vs. CWD

Tests and confidence intervals for β are based on

$$\frac{\hat{\beta} - \beta}{SE(\hat{\beta})} \sim t_{n-2}$$

```
summary(model)$coefficients
```

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-77.0990778	30.60800907	-2.518918	0.0245520121
RIP.DENS	0.1155161	0.02343233	4.929772	0.0002216405

Association tree density vs. CWD

- 95% CI for β needs $t_{14,0.975} = 2.14$
- CI is given by

$$[0.116 - 2.14 \times 0.0234, 0.116 + 2.14 \times 0.0234] = [0.066, 0.166]$$

```
confint(model)
```

	2.5 %	97.5 %
(Intercept)	-142.74672817	-11.4514274
RIP.DENS	0.06525871	0.1657734