Fachhochschule Südwestfalen
University of Applied Sciences

Statistical Modeling

CH.5 - Transformations

2023 || Prof. Dr. Buchwitz

Wir geben Impulse

Outline

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Outline

Introduction

- Data do not always come in suitable form so that they can be analysed right away and often need to be transformed before carrying out an analysis.
- Transformations are necessary because the original variables of the model using these variables, violates one or more of the standard regression assumptions.
- Transformations are usually applied to accomplish objectives such as to **ensure linearity**, to **achieve normality** or to **stabilize the variance**.
- It is common practice to to fit a linear regression model to the transformed rather than the original variables.

Linearity and Non-Linearity

- As mentioned before we consider a model to be linear when the parameters in the model enter in a linear fashion, even if the predictors occur nonlinearly. **All following models are linear.**

$$
\begin{aligned}
Y &= \beta_0 + \beta_1 X + \epsilon \\
Y &= \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon \\
Y &= \beta_0 + \beta_1 log(X) + \epsilon \\
Y &= \beta_0 + \beta_1 \sqrt{X} + \epsilon
\end{aligned}
$$

- The following model is **non-linear** as the regression parameter β_1 does not enter linearly.

$$Y = \beta_1 + e^{\beta_1 X} + \epsilon$$

Transformations

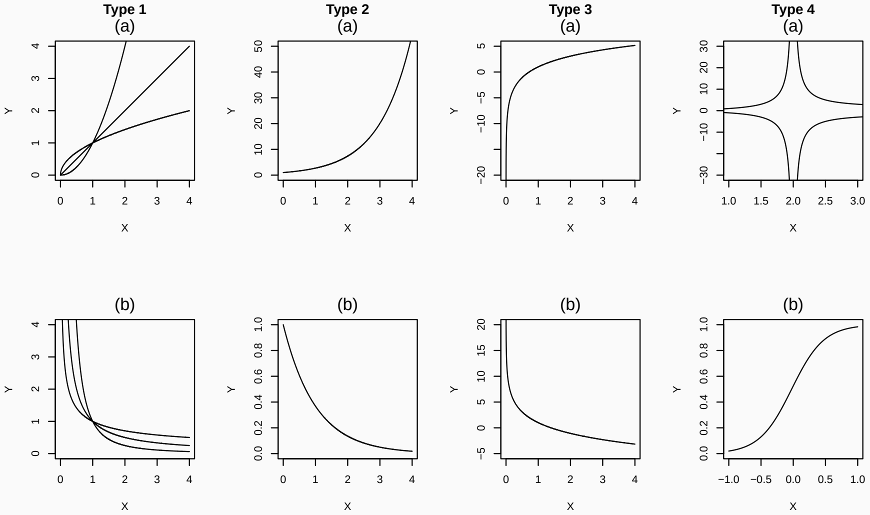
Transformations may be necessary for a variety of reasons:

1. Theoretical considerations may specify that the relationship between two variables is nonlinear.
2. The response variable Y may have a probability distribution whose variance is related to the mean. When relating Y and X, then the variance of Y will change with X. The distribution of Y is often non-normal. This invalidates the standard tests of significance. The unqueal variance also leads to inefficient (not smallest variance) estimates of the error term. Transformations that stabilize variances are coincidentically also good normalizing transforms.
3. When there is no reason to suspect that a transformation is required, the evicence to apply a transformation comes from inspecting the residuals from a fit with the original variables.

Transformations to achieve Linearity

- One of the standard assumptions in regression analysis is the linearity of the formed model.
- When analyzing the scatter plot of Y against X_j data may appear to be nonlinear.
- The following transformations can be chosen based on the pattern of the Y-X-Scatterplot to linearize the realtionship so that linear regression can be applied.

Transformations to achieve Linearity



Transformations to achieve Linearity

Function	Transformation	Linear Form	Type
$Y = \alpha X^{\beta}$	$Y' = log(Y),\ X' = log(X)$	$Y' = log(\alpha) + \beta X'$	Type 1
$y = \alpha e^{\beta X}$	$Y' = ln(Y)$	$Y' = ln(\alpha + \beta X)$	Type 2
$Y = \alpha + \beta log(X)$	$X' = log(X)$	$Y = \alpha + \beta X'$	Type 3
$Y = \frac{X}{\alpha X - \beta}$	$Y' = \frac{1}{Y},\ X' = \frac{1}{X}$	$Y' = \alpha - \beta X'$	Type 4 a
$Y = \frac{e^{\alpha+\beta X}}{1+e^{\alpha+\beta X}}$	$Y' = ln(\frac{Y}{1-Y})$	$Y' = \alpha + \beta X$	Type 4 b

Not every curvature is linearizable! Depending on the observed patterns it may be necessary to choose a different estimation method, which we do not discuss here.

Example: Bacteria Data

```
P168
```

```
##     t N_t
## 1   1 355
## 2   2 211
## 3   3 197
## 4   4 166
## 5   5 142
## 6   6 106
## 7   7 104
## 8   8  60
## 9   9  56
## 10 10  38
## 11 11  36
## 12 12  32
## 13 13  21
## 14 14  19
## 15 15  15
```

Your turn

`Nt` Number of surviving bacteria after X-ray exposure of time t.

`t` Exposure time to X-rays in minutes.

Example: Bacteria Data

- The bacteria data was collected to test the "Single-Hit" Hypothesis. The underlying theory (not discussed) states that there is a single vital center in each bacteria that nets to be hit by a X-Ray to inactivate the organism.
- If the theory is applicable the number of surviving bacteria η_t should relate to the exposure time to X-ray t by

$$\eta_t = \eta_0 e^{\beta_1 \cdot t}$$

- The parameters are η_0 and β_1 relate to pyhsical quantities. η_0 is the number of bacteria at the start of tehe experiment and β_1 is the desctruction (decay) rate.

Example: Bacteria Data

- The relation between η_t and t cannot be estimated using OLS directly. Therefore we need to apply a transformation by taking logarithms of both sides

$$ln(\eta_t) = ln(\eta_0 e^{\beta_1 \cdot t}) = ln(\eta_0) + \beta_1 t = \beta_0 + \beta_1 t$$

- The presented equation is deterministic as it contains no error. Introducing the error in the linearized eqaution in an *additive* way, the (transfromed) error must occur in multiplicative form in the original equation ($\epsilon_t = ln(\epsilon'_t)$).

$$ln(\eta_t) = \beta_0 + \beta_1 t + \epsilon_t \quad \rightarrow \quad \eta_t = \eta_0 e^{\beta_1 \cdot t} \epsilon'_t$$

Example: Bacteria Data

```
mod1 <- lm(N_t ~ 1 + t, data = P168)       # Inadequate Model
mod2 <- lm(log(N_t) ~ 1 + t, data = P168) # Adequate Model
```

```
texreg::texreg(list(mod1,mod2), custom.model.names = c("Nt","log(Nt)"))
```

	Nt	log(Nt)
(Intercept)	259.58^{***}	5.97^{***}
	(22.73)	(0.06)
t	-19.46^{***}	-0.22^{***}
	(2.50)	(0.01)
R^2	0.82	0.99
Adj. R^2	0.81	0.99
Num. obs.	15	15

$^{***}p < 0.001$; $^{**}p < 0.01$; $^{*}p < 0.05$

Table 3: Statistical models

Example: Bacteria Data

- The estimate of the intercept in the equation is the best linear unbiased estimate of $ln(\eta_0)$. Given we are interested in $\hat{\beta}_0$, the backtransformation $e^{\hat{\beta}_0}$ **is not an unbiased estimate of η_0!**

```
exp(coef(mod2)[1]) # Not an unbiased estimate!
```

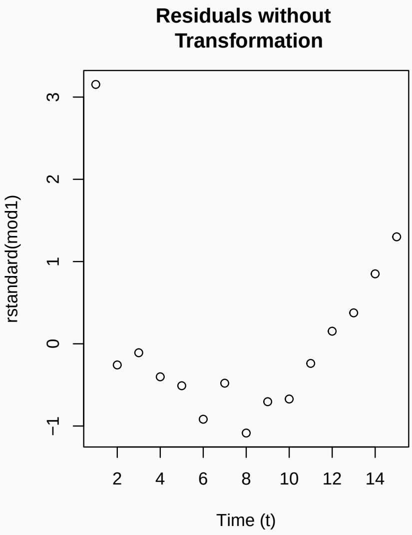
```
## (Intercept)
##       392.7
```

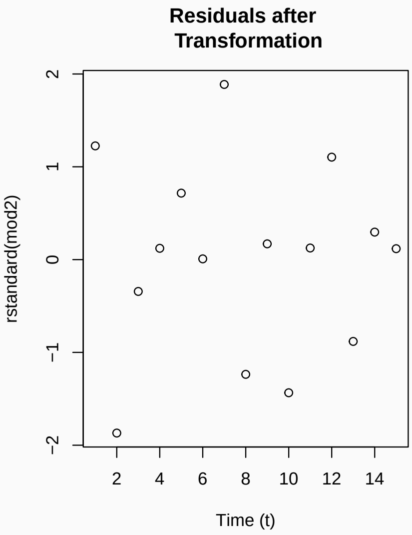
- To obtain a (nearly) unbiased estimate the correction $\hat{\eta}_0 = exp(\hat{\beta}_0 - \frac{1}{2}Var(\hat{\beta}_0))$ can be applied.

```
exp(coef(mod2)[1] - 0.5 * coef(summary(mod2))[,"Std. Error"][1]^2)
```

```
## (Intercept)
##         392
```

Example: Bacteria Data



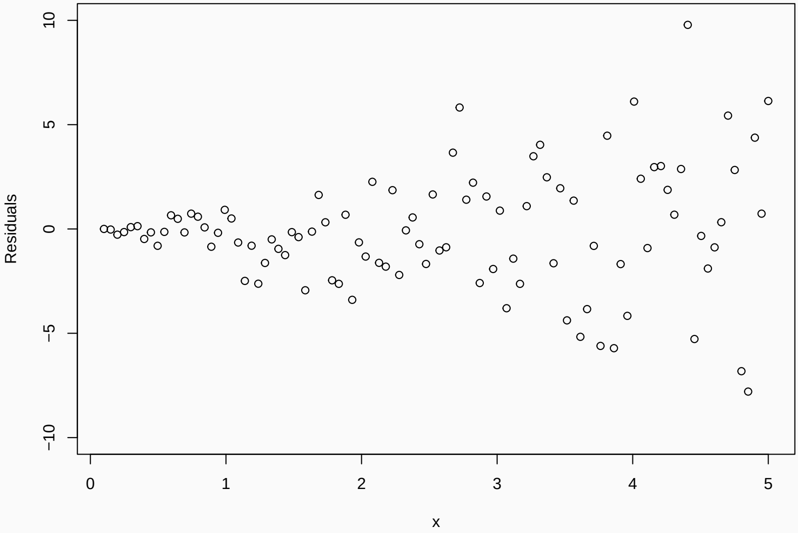


Heteroscedasticity

Heteroscedasticity

Constancy of error variance is one of the assumptions of least squares theory. If the error variance is not constant the error is said to be **heteroscedastic**. It is detected by graphs of the residuals against **all** predictors, which usually show a funnel (increase or decrease with X).

Heteroscedasticity



Heteroscedasticity

- Heteroscedasticity causes parameter estimates which lack precision in a theoretical sense. The estimated standard errors of the coefficients are often understated, giving a false sense of accuracy.
- The assumed normal distribution has the property that its mean and variance independent in the sense that one is not a function of the other. This is not the case for e.g. the Binomial or Poisson distributions.
- Heteroscedasticity can easily be removed by means of suitable transformations, given that the probability distribution of the response is known.
- The discussed transformations **stabilize the variance** and make the distribution of the transformed variable **closer to the normal distribution**.

Example: Detection of heteroscedastic Errors

```
P176
```

```
##       X   Y
## 1   294  30
## 2   247  32
## 3   267  37
## 4   358  44
## 5   423  47
## 6   311  49
## 7   450  56
## 8   534  62
## 9   438  68
## 10  697  78
## 11  688  80
## 12  630  84
## 13  709  88
## 14  627  97
## 15  615 100
## 16  999 109
## 17 1022 114
## 18 1015 117
## 19  700 106
## 20  850 128
## 21  980 130
## 22 1025 160
## 23 1021  97
## 24 1200 180
## 25 1250 112
## 26 1500 210
## 27 1650 135
```

Your turn

- X Number of supervised workers.
- Y Number of Supvervisors.

Example: Detection of heteroscedastic Errors

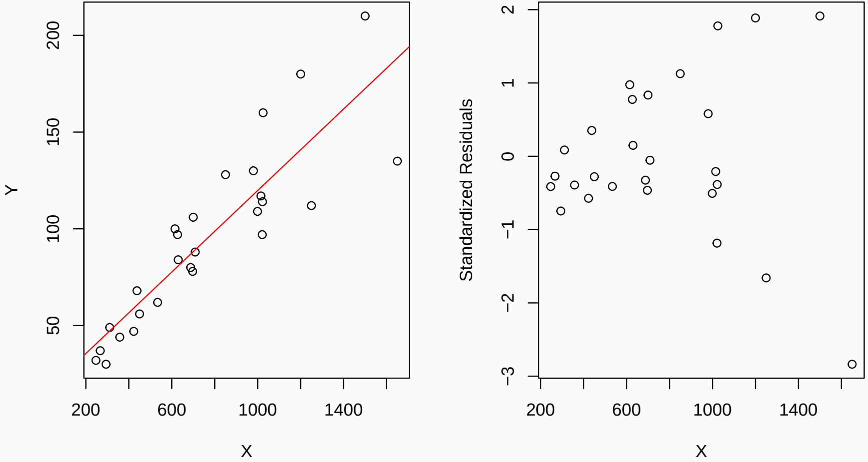
```r
mod <- lm(Y ~ 1 + X, data=P176)
texreg::texreg(mod)
```

	Model 1
(Intercept)	14.45
	(9.56)
X	0.11^{***}
	(0.01)
R^2	0.78
Adj. R^2	0.77
Num. obs.	27

$^{***}p < 0.001$; $^{**}p < 0.01$; $^{*}p < 0.05$

Table 4: Statistical models

Example: Detection of heteroscedastic Errors



Removal of heteroscedastic Errors

- In many applications unequal error variance is observed in a for where the variance increses when the predictor variable increases.
- Based on this empirical observation, we can hypothesize that the standard deviation of the residuals is **proportional** to X.

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

$$\text{with} \quad Var(\epsilon_i) = k^2 x_i^2 \quad \text{and} \quad k > 0$$

Removal of heteroscedastic Errors

- Given a proportional relationship between the standard deviation and the predictor indicates that it is beneficial to divide both sides of the regression equation by x_i:

$$\frac{y_i}{x_i} = \frac{\beta_0}{x_i} + \beta_1 + \frac{\epsilon_i}{x_i}$$

- Defining a new set of variables and coefficients

$$Y' = \frac{Y}{X}, \quad X' = \frac{1}{X}, \quad \beta_0' = \beta_1, \quad \epsilon' = \frac{\epsilon}{X}$$

  yields the new following form:

$$y_i' = \beta_0' + \beta_1' x_i' + \epsilon_i'$$

Removal of heteroscedastic Errors

- For the transformde model the $Var(\epsilon_i') = k^2$. If our assumption about the error term fits the model properly, we must work with the transformed variables Y/X (response) and $1/X$ (predictor).

$$\text{Transformed:} \quad \frac{\hat{Y}}{X} = \hat{\beta}_0' + \frac{\hat{\beta}_1'}{X} \qquad \text{Original:} \quad \hat{Y} = \hat{\beta}_1' + \hat{\beta}_0' X$$

Removal of heteroscedastic Errors

Removal of heteroscedastic Errors

```
mod2 <- lm(I(Y/X) ~ 1 + I(1/X), data=P176)
summary(mod2)
```

```
##
## Call:
## lm(formula = I(Y/X) ~ 1 + I(1/X), data = P176)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -0.0415 -0.0138 -0.0050  0.0247  0.0354
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    0.121      0.009   13.45    6e-13 ***
## I(1/X)         3.803      4.570    0.83     0.41
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0227 on 25 degrees of freedom
## Multiple R-squared:  0.027,  Adjusted R-squared:  -0.012
## F-statistic: 0.693 on 1 and 25 DF,  p-value: 0.413
```

Note

The results here are expressed in terms of the transfromed variables () so measures except the coefficient estimates (their SD, t-values, ...) like R^2 cannot simply be interpreted.

Weighted Least Squares

- Linear regression models with heteroscedastic erros can also be fitted by a method called teh *weighted least squares* (WLS), ehtere parameter estimates are obtained by minimizing **weighted sum of squares** of residuals.
- The weights in that case are chosen to be inversely proportional to the variance of the errors. In the discussed example, this means

$$\text{WLS:} \quad \sum \frac{1}{x_i^2}(y_i - \beta_0 - \beta_1 x_i)^2 \qquad \text{OLS:} \quad \sum (y_i - \beta_0 - \beta_1 x_i)^2$$

Weighted Least Squares

```
mod.wls <- lm(Y ~ 1 + X, weights = 1/X^2, data=P176)
summary(mod.wls)
```

```
##
## Call:
## lm(formula = Y ~ 1 + X, data = P176, weights = 1/X^2)
##
## Weighted Residuals:
##     Min      1Q  Median      3Q     Max
## -0.0415 -0.0138 -0.0050  0.0247  0.0354
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    3.803      4.570    0.83     0.41
## X              0.121      0.009   13.45    6e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0227 on 25 degrees of freedom
## Multiple R-squared:  0.879,  Adjusted R-squared:  0.874
## F-statistic:  181 on 1 and 25 DF,  p-value: 6.04e-13
```

Note

Performing OLS on the transformed variables Y/X and $1/X$ is equivalent to the shown WLS Model.

Logarithmic Transformation

- The most widely used transformation is the logarithmic transformation, where $ln(Y)$ is used as response instead of Y.

$$ln(y_i) = \beta_0 + \beta_1 x_i + \epsilon_i$$

- This transformation is particularly useful for variables, where the standard deviation is large compared to the mean.
- Working on a **log scale** has the effect of dampening variability and reducing asymmetry and also reduces heteroskedasticity.
- Results obtained on a log scale are sometimes **harder to interpret** than on the original scale and original variables.

Logarithmic Transformation

```
mod1 <- lm(log(Y) ~ 1 + X, data=P176)
texreg::texreg(mod1, digits = 8,
               custom.model.names = "log(Y)")
```

	log(Y)
(Intercept)	3.51502316***
	(0.11106702)
X	0.00120408***
	(0.00013155)
R^2	0.77016652
Adj. R^2	0.76097318
Num. obs.	27

$^{***}p < 0.001$; $^{**}p < 0.01$; $^{*}p < 0.05$

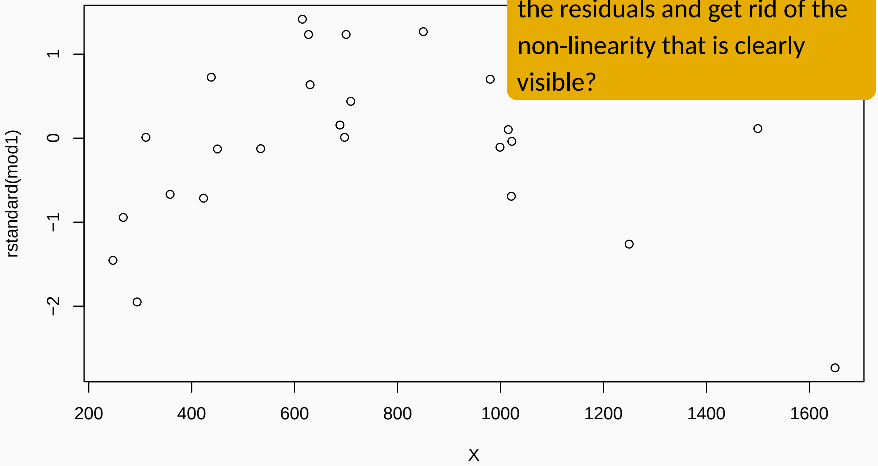
Table 5: Statistical models

Logarithmic Transformation

```
plot(P176$X, rstandard(mod1), xlab="X")
```

Your turn

What could you do to improve the residuals and get rid of the non-linearity that is clearly visible?



Logarithmic Transformation

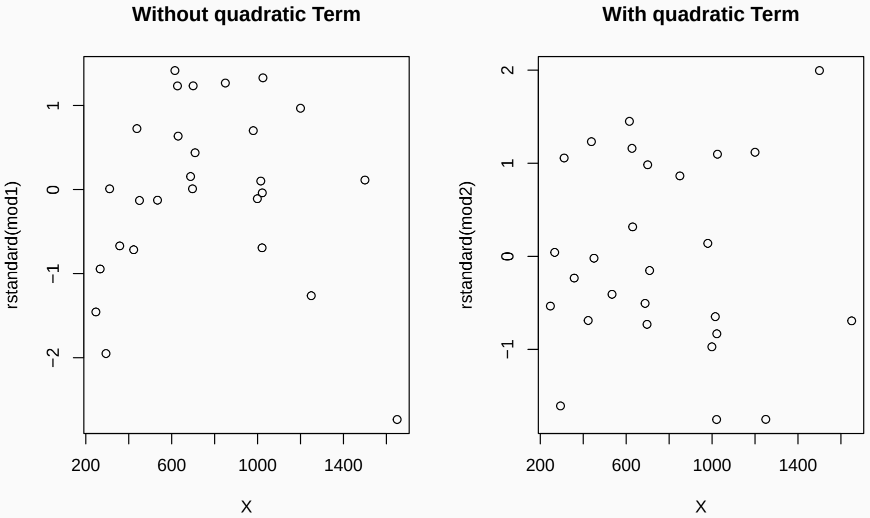
```
mod1 <- lm(log(Y) ~ 1 + X, data=P176)
mod2 <- lm(log(Y) ~ 1 + X + I(X^2), data=P176)
texreg::texreg(list(mod1,mod2), digits = 8,
               custom.model.names = c("log(Y)","log(Y)"))
```

	log(Y)	log(Y)
(Intercept)	3.51502316***	2.85160036***
	(0.11106702)	(0.15664013)
X	0.00120408***	0.00311267***
	(0.00013155)	(0.00039893)
X^2		−0.00000110***
		(0.00000022)
R^2	0.77016652	0.88569267
Adj. R^2	0.76097318	0.87616706
Num. obs.	27	27

$^{***}p < 0.001$; $^{**}p < 0.01$; $^{*}p < 0.05$

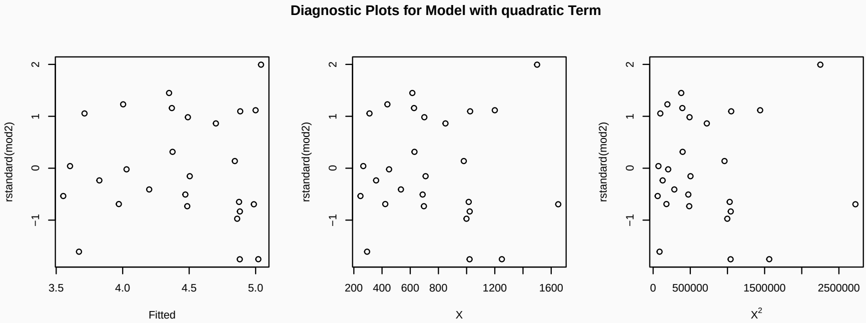
Table 6: Statistical models

Logarithmic Transformation



Logarithmic Transformation

- Residuals for the model $ln(y_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i$ appear satisfactory. There is no appreance of heteroscedasticity or non-linearity in the residuals.



Applying different transformation may yield mulitple acceptable candidates, which all may be used as final models.

Power Transformation

- The common transformations $ln(Y)$, $1/Y$ and $\sqrt{Y}$ can be seen as special cases of the so called **power transformation**.

$$Y^{\lambda}$$

- It is also common to use the Box-Cox-Transformation $(Y^{\lambda} - 1)/\lambda$ which approaches $log(Y)$ as λ approaches 0.
- Reciprocal ($\lambda = -1$), square root ($\lambda = 0.5$) and logarithmic transformation ($\lambda = 0$) can all be modeled within this framework.
- Choosing transformations based on empirical evidence to achieve normality and/or to stabilize the error variance may require **experimentation** with different power transforms.
- Typical values for λ are between -2 and 2 and should be sufficient for most practical use cases.

Example: Brain Data

```
P184
```

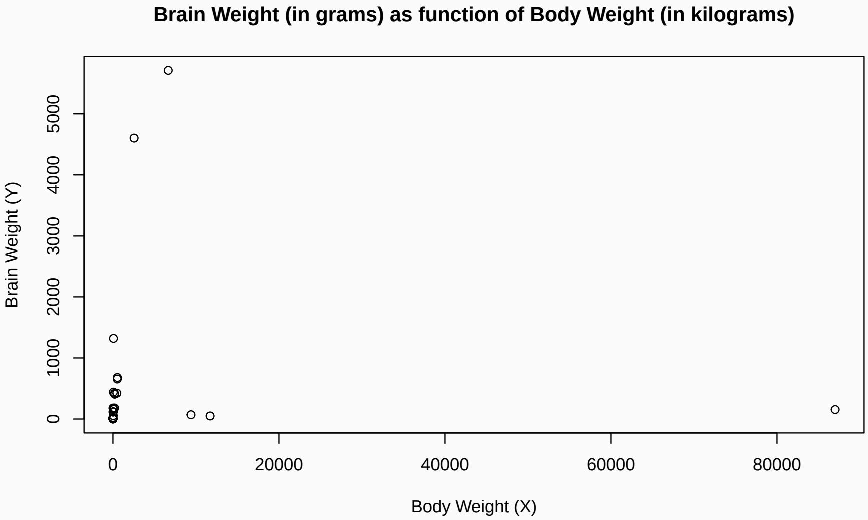
```
##                   BrainWeight BodyWeight
## Mountain beaver           8.1      1.350
## Cow                     423.0    465.000
## Graywolf                119.5     36.330
## Goat                    115.0     27.660
## Guineapig                 5.5      1.040
## Diplodocus               50.0  11700.000
## Asian elephant         4603.0   2547.000
## Donkey                  419.0    187.100
## Horse                   655.0    521.000
## Potar monkey            115.0     10.000
## Cat                      25.6      3.300
## Giraffe                 680.0    529.000
## Gorilla                 406.0    207.000
## Human                  1320.0     62.000
## African elephant       5712.0   6654.000
## Triceratops              70.0   9400.000
## Rhesus monkey           179.0      6.800
## Kangaroo                 56.0     35.000
## Hamster                   1.0      0.120
## Mouse                     0.4      0.023
## Rabbit                   12.1      2.500
## Sheep                   175.0     55.500
## Jaguar                  157.0    100.000
## Chimpanzee              440.0     52.160
## Brachiosaurus           154.5  87000.000
## Rat                       1.9      0.280
## Mole                      3.0      0.122
## Pig                     180.0    192.000
```

Your turn

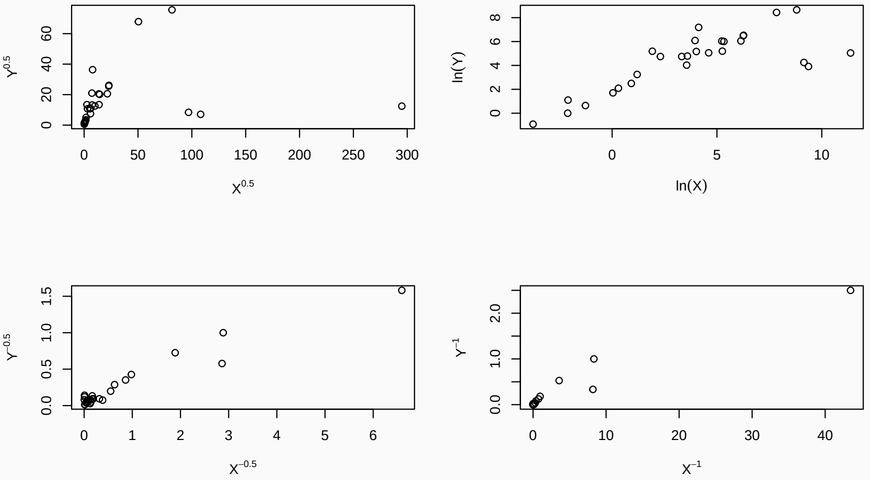
`BrainWeight` Brain Weight of the animal in grams.

`BodyWeight` Body Weight of the respective animal in kilograms.

Example: Brain Data



Power Transformation



Power Transformation

- The logarithmic transformation ($\lambda = 0$) is the most appropriate one for the data.
- In the case of $\lambda = 0$ the relationship looks linear, but three data points (dinosaurs) deviate from the other observations.
- In the example the power tranformation has been applied to X and Y simultaneously and with the same value of λ. In practice it may be more appropriate to raise each value to a different power, choose tha values **independelty** or transform only a single variable.
- Heteroscedasticity and non-linearity can be diagnsoed by checking the residuals of the model. The final model (with applied transformations) should not show evidence of heteroscedasticity or deterministic patterns.

Model

```r
data <- P184[-c(6,16,25), ]
mod1 <- lm(BrainWeight ~  1 + BodyWeight, data = data)
mod2 <- lm(BrainWeight ~ -1 + BodyWeight, data = data)
texreg::texreg(list(mod1, mod2), digits = 4,
               custom.model.names = c("BrainWeight","BrainWeight"))
```

	BrainWeight	BrainWeight
(Intercept)	191.2226	
	(110.0878)	
BodyWeight	0.9432***	0.9865***
	(0.0766)	(0.0754)
R^2	0.8683	0.8771
Adj. R^2	0.8626	0.8719
Num. obs.	25	25

$^{***}p < 0.001$; $^{**}p < 0.01$; $^{*}p < 0.05$

Table 7: Statistical models