

# **Topic 12 – Nonlinear regression**

ENVX1002 Statistics in Life and Environmental Sciences

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## Module overview

- Week

- 9.

- Describing Relationships

- Correlation (calculation, interpretation)
    - Regression (model structure, model fitting)
    - What/when/why/how

- Week

- 10.

- Simple Linear Regression

- Can we use the model? (assumptions, hypothesis testing)
    - How good is the model? (interpretation, model fit)

- Week

- 11.

- Multiple Linear Regression

- Multiple Linear Regression (MLR) modelling
    - Assumptions, interpretation and the principle of parsimony

- **Week 12. Nonlinear Regression**

- Common nonlinear functions
- Transformations

## Regressions

### Simple linear regression

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

Ideal for predicting a continuous response variable from a single predictor variable: “*How does y change as x changes, when the relationship is linear?*”

### Multiple linear regression

$$Y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_k x_{ki} + \epsilon_i$$

“*How does y change as x<sub>1</sub>, x<sub>2</sub>, ..., x<sub>k</sub> change?*”

### Nonlinear regression

$$Y_i = f(x_i, \beta) + \epsilon_i$$

where  $f(x_i, \beta)$  is a nonlinear function of the parameters  $\beta$ : “*How do we model a change in y with x when the relationship is nonlinear?*”

# Nonlinear regression



Carl Friedrich Gauss (1777-1855) and Isaac Newton (1642-1726) Gauss-Newton approach to nonlinear regression is most commonly used

## Nonlinear relationships

Linear relationships are simple to interpret since the rate of change is constant.

**“As one changes, the other changes at a constant rate.”**

Nonlinear relationships often involve exponential, logarithmic, or power functions.

**“As one changes, the other changes at a rate that is *not proportional* to the change in the other.**

## Dealing with nonlinearity

### Transformations

Often, a nonlinear relationship may be transformed into a linear relationship by applying a transformation to the response variable or the predictor variable(s).

- **Logarithmic:**  $y = \log(x)$
- **Exponential:**  $y = e^x$
- **Square-root:**  $y = \sqrt{x}$
- **Inverse:**  $y = \frac{1}{x}$
- Usually works when  $y$  changes **monotonically** with  $x$ .
- More interpretable and easier to fit.

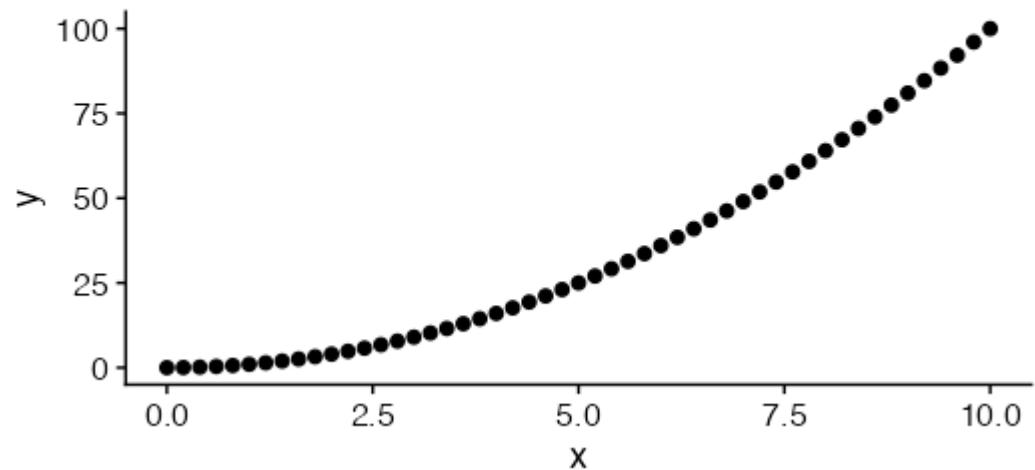
## Nonlinear relationships: exponents

- $x^2$  is the *square* of  $x$ .
- $x^3$  is the *cube* of  $x$ .
- $x^a$  is  $x$  raised to the *power* of  $a$ .

In a relationship where  $y$  is a function of  $x^a$ , as  $x$  increases,  $y$  increases nonlinearly at a rate that depends on the value of  $x$  and  $a$  ( $\frac{dy}{dx} = ax^{a-1}$ ).

```
# Plot a simulation of above in ggplot2
set.seed(123)
tibble(x = seq(0, 10, by = 0.2), y = x^2) %>%
  ggplot(aes(x = x, y = y)) +
  geom_point() +
  labs(x = "x", y = "y") +
  ggtitle(expression(y == x^2)) +
  theme(plot.title = element_text(size = 40, face = "bold"))
```

$$y = x^2$$



## Nonlinear relationships: logarithms

- $\log_e(x)$  is the *natural logarithm* of  $x$ .
- $\log_{10}(x)$  is the *common logarithm* of  $x$ .
- $\log_a(x)$  is the *logarithm* of  $x$  to the base  $a$ .

### Interpretation:

- If  $\log_a(y) = x$ : as  $x$  increases, the value of  $y$  increases by  $y = a^x$ .
- If  $y = \log_a(x)$ : as  $x$  increases, the value of  $y$  increases by  $y = \log_a(x)$ . As  $y$  increases, the value of  $x$  increases by  $x = a^y$ .

## Exponents and logarithms

	Exponents	Logarithms
<b>Definition</b>	If $a^n = b$ , $a$ is the base, $n$ is the exponent, and $b$ is the result.	If $\log_a b = n$ , $a$ is the base, $b$ is the result, and $n$ is the logarithm (or the exponent in the equivalent exponential form).
<b>Example</b>	$2^3 = 8$	$\log_2 8 = 3$
<b>Interpretation</b>	2 raised to the power of 3 equals 8.	The power to which you must raise 2 to get 8 is 3.
<b>Inverse</b>	The logarithm is the inverse operation of exponentiation.	The exponentiation is the inverse operation of logarithm.
<b>Properties</b>	$(a^n)^m = a^{n \cdot m}$ , $a^n \cdot a^m = a^{n+m}$ , $\frac{a^n}{a^m} = a^{n-m}$	$\log_a(b \cdot c) = \log_a b + \log_a c$ , $\log_a\left(\frac{b}{c}\right) = \log_a b - \log_a c$ , $\log_a(b^n) = n \cdot \log_a b$

### i Note

For your understanding, not examinable.

# Common nonlinear functions

$$f(x_i, \beta)$$

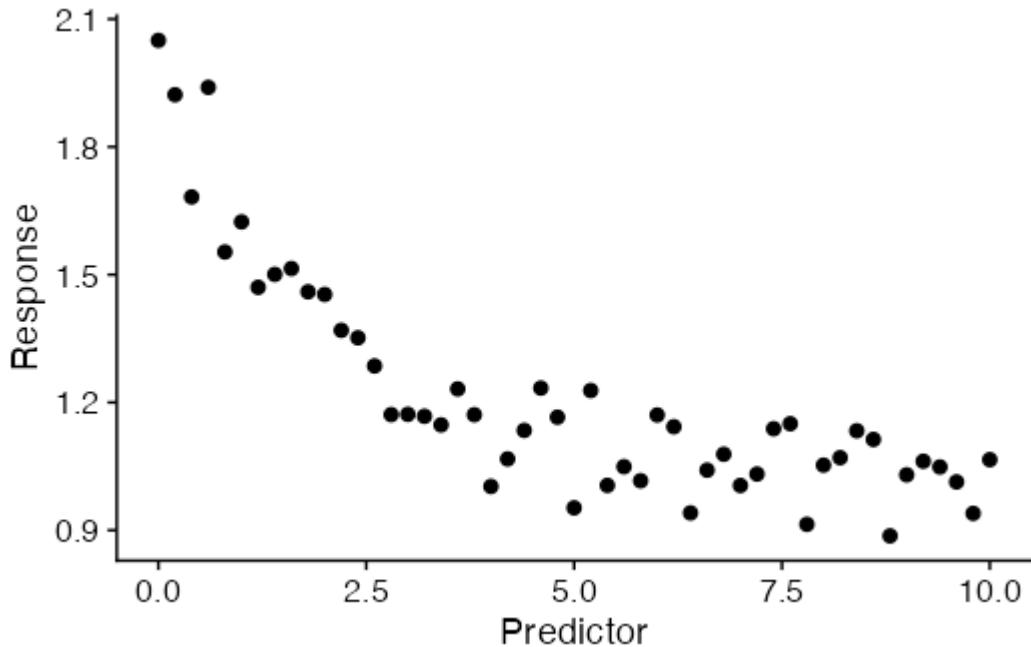
## Exponential decay relationship

Response variable *decreases* and approaches limit as predictor variable increases.

$$y = a \cdot e^{-bx}$$

```
set.seed(429) # set seed
# Simulate data:
decay ← tibble(
  predictor = seq(0,10, by = 0.2),
  response = abs(exp(-0.5*predictor) + rnorm(length(predictor), mean = 1, sd = 0.1)))

ggplot(data = decay, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response")
```



Examples: radioactive decay, population decline, chemical reactions.

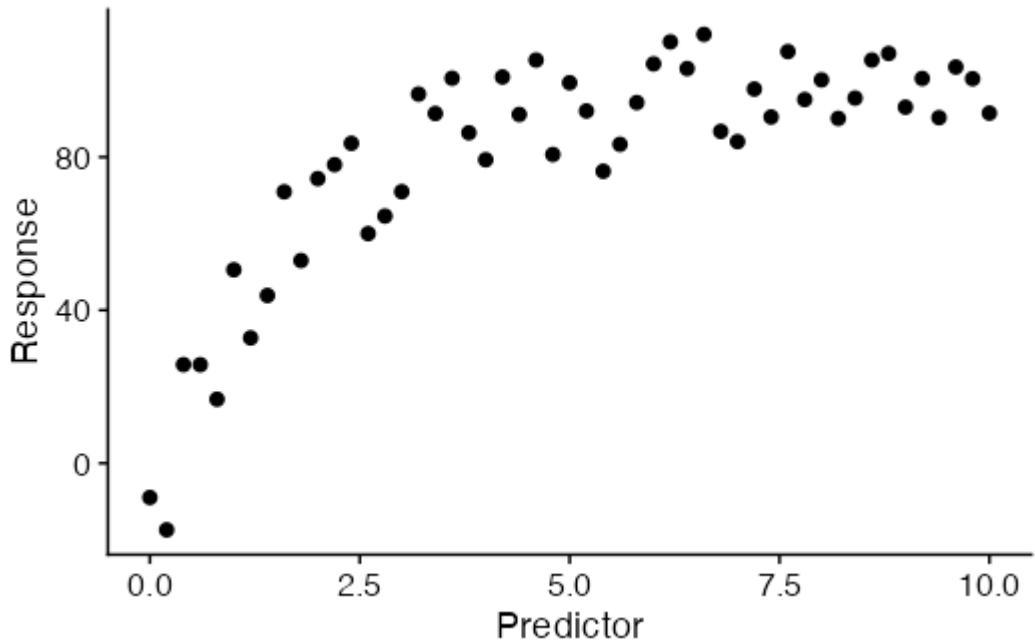
## Asymptotic relationship

Response variable *increases* and approaches a limit as the predictor variable increases.

$$y = a + b(1 - e^{-cx})$$

```
set.seed(442) # set seed
# Simulate data:
asymptotic = tibble(
  predictor = seq(0, 10, by = 0.2),
  response = 100*(1-exp(-0.5*predictor)) + rnorm(length(predictor), mean = 0, sd = 10))

ggplot(data = asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response")
```



Examples: population growth, enzyme kinetics.

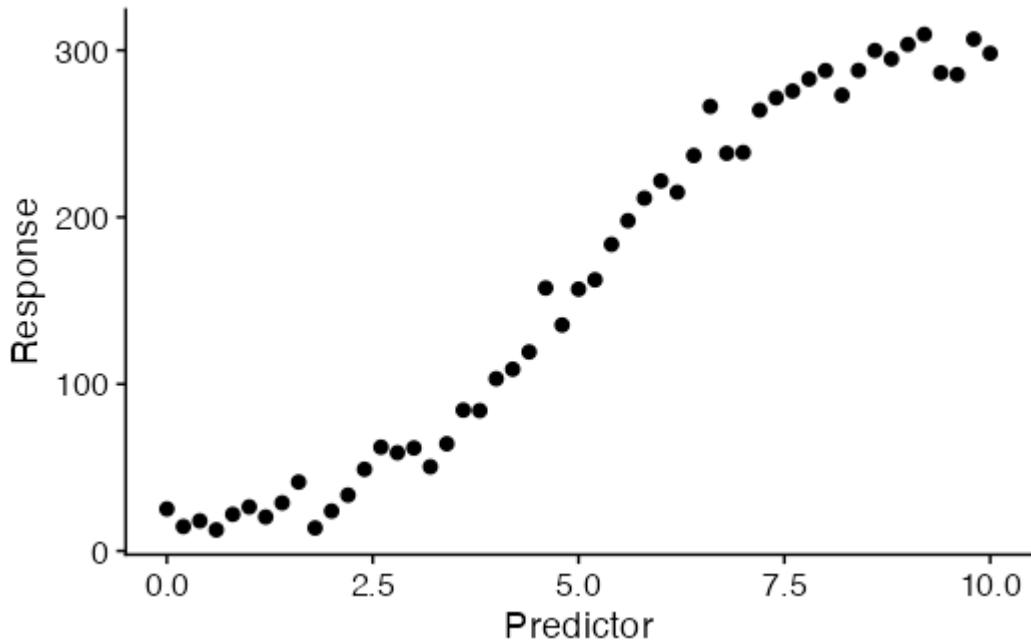
## Logistic relationship

An S-shaped relationship, where the response variable is at first exponential, then asymptotic.

$$y = c + \frac{d - c}{1 + e^{-b(x-a)}}$$

```
set.seed(450)
# Simulate data:
logistic ← tibble(predictor = seq(0, 10, by = 0.2),
  response = 10 + abs(300 * (1 / (1 + exp(-0.8 * (predictor - 5))))) + rnorm(length(predictor), mean
= 0, sd = 10))

ggplot(data = logistic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response")
```



Examples: growth of bacteria, disease spread, species growth.

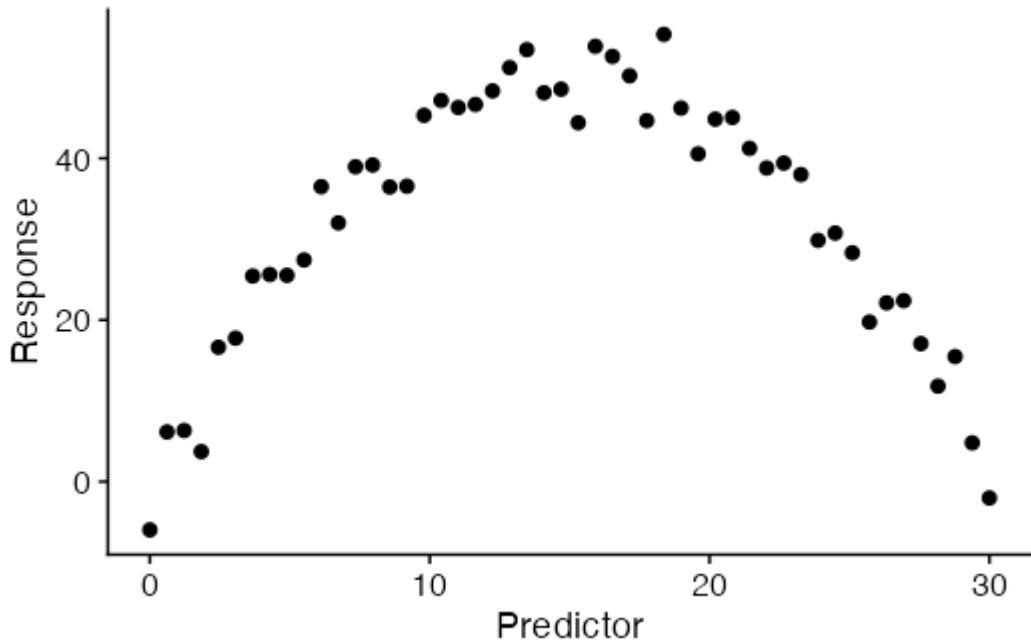
## Polynomial relationship

Response variable changes in a variety of ways as the predictor variable changes. Also known as ‘curvilinear’.

$$y = a + bx + cx^2 + dx^3 + \dots$$

```
# Set seed for reproducibility
set.seed(529)
# Simulate data:
curvilinear ← tibble(predictor = seq(0, 30, length.out = 50),
  response = 50 * (1 - (predictor - 15)^2 / 225) + rnorm(length(predictor), mean = 0, sd = 5))

ggplot(data = curvilinear, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response")
```



Examples: food intake, drug dosage, exercise.

# Transformations

| How far can we go?

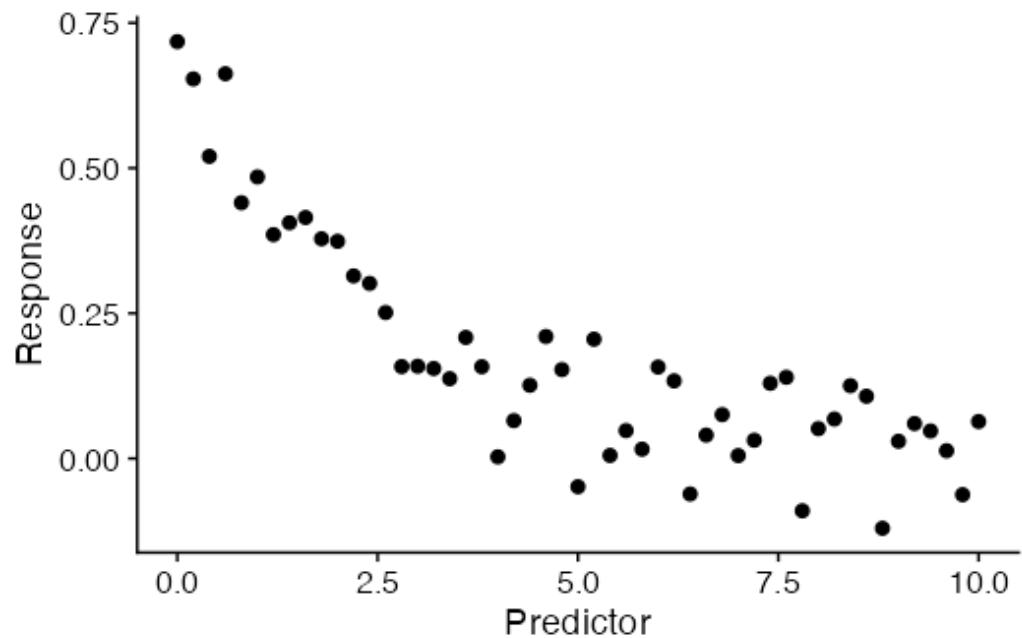
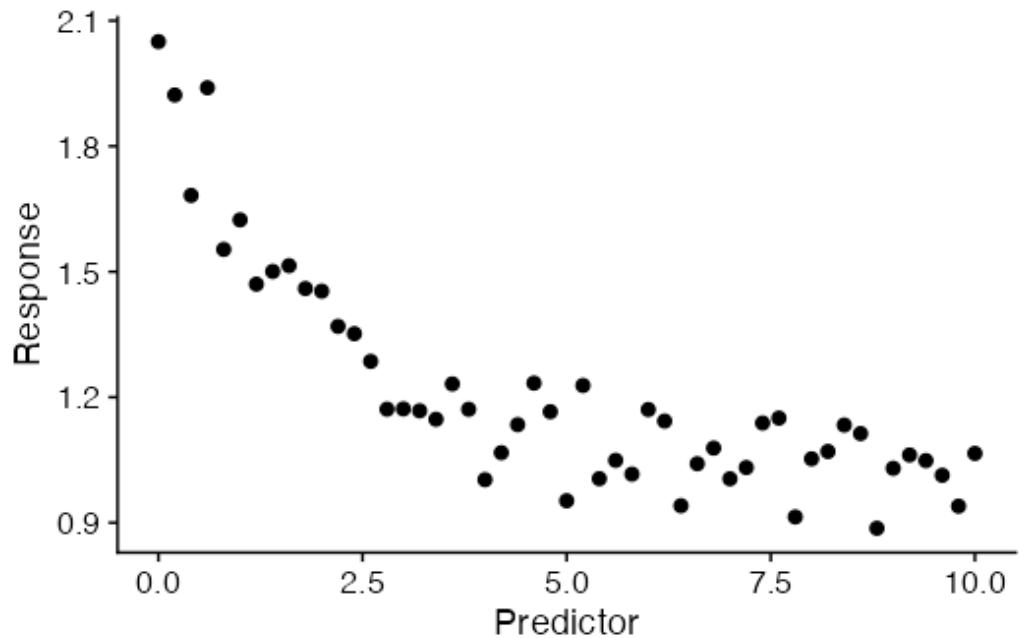
## Transformations: exponential decay

Before transformation

```
ggplot(data = decay,  
       aes(x = predictor, y = response)) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```

After  $\log_e$  transform

```
ggplot(data = decay,  
       aes(x = predictor, y = log(response))) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```



## Transformations: exponential decay

### Before transformation

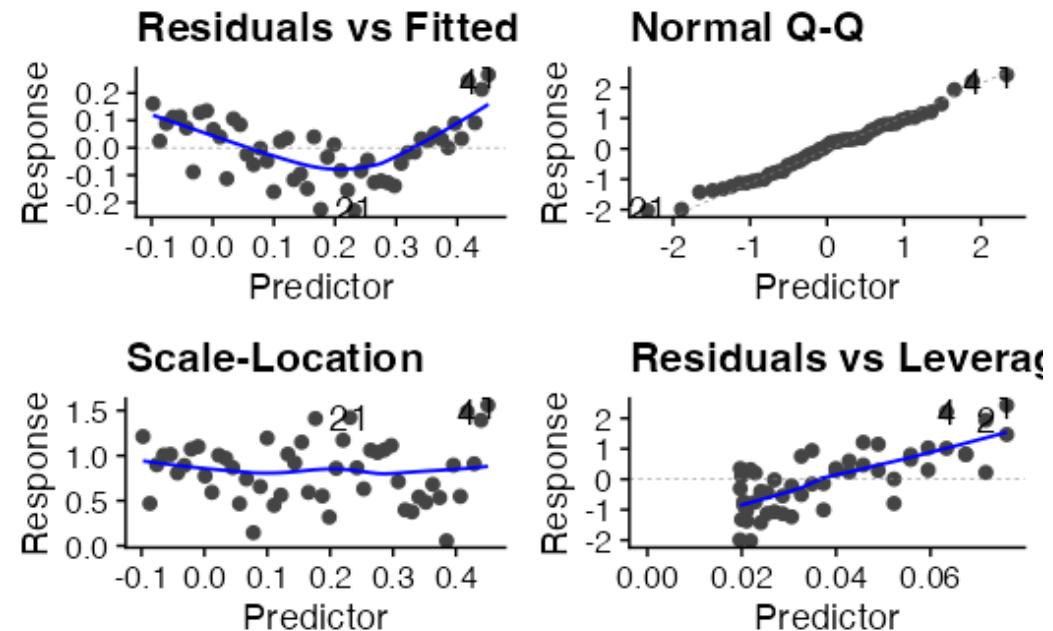
```
autoplot(lm(response ~ predictor, data = decay)) +  
  labs(x = "Predictor", y = "Response")
```

Warning: `fortify(<lm>)` was deprecated in ggplot2 4.0.0.  
i Please use `broom::augment(<lm>)` instead.  
i The deprecated feature was likely used in the ggfortify package.  
Please report the issue at <<https://github.com/sinhrks/ggfortify/issues>>.

Warning: `aes\_string()` was deprecated in ggplot2 3.0.0.  
i Please use tidy evaluation idioms with `aes()`.  
i See also `vignette("ggplot2-in-packages")` for more information.

### After $\log_e$ transform

```
autoplot(lm(log(response) ~ predictor, data = decay)) +  
  labs(x = "Predictor", y = "Response")
```



i The deprecated feature was likely used in the ggfortify package.

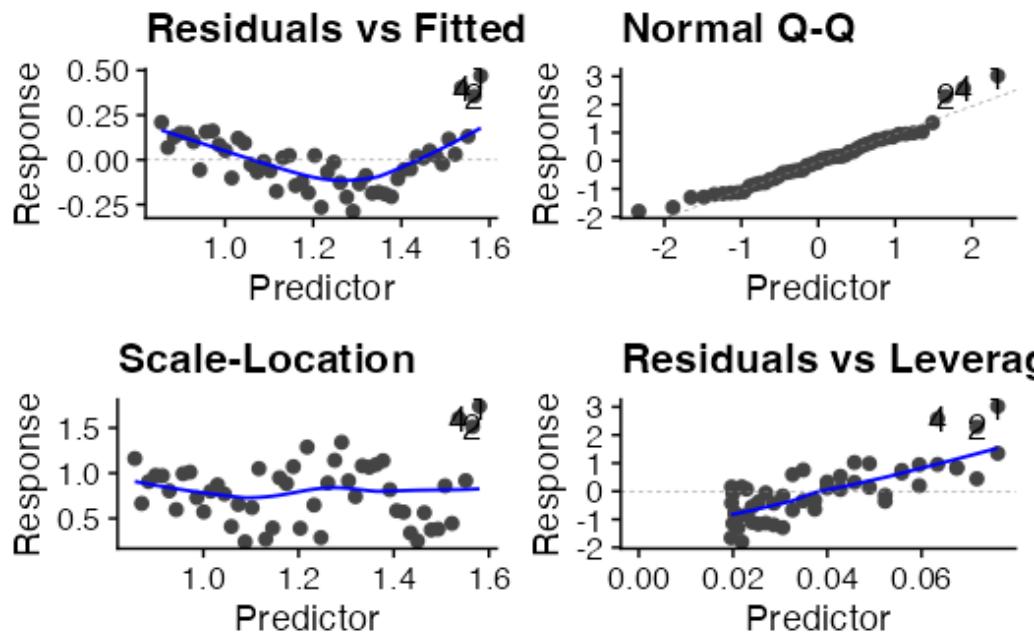
Please report the issue at <<https://github.com/sinhrks/ggfortify/issues>>.

Warning: Using `size` aesthetic for lines was deprecated in ggplot2 3.4.0.

i Please use `linewidth` instead.

i The deprecated feature was likely used in the ggfortify package.

Please report the issue at <<https://github.com/sinhrks/ggfortify/issues>>.



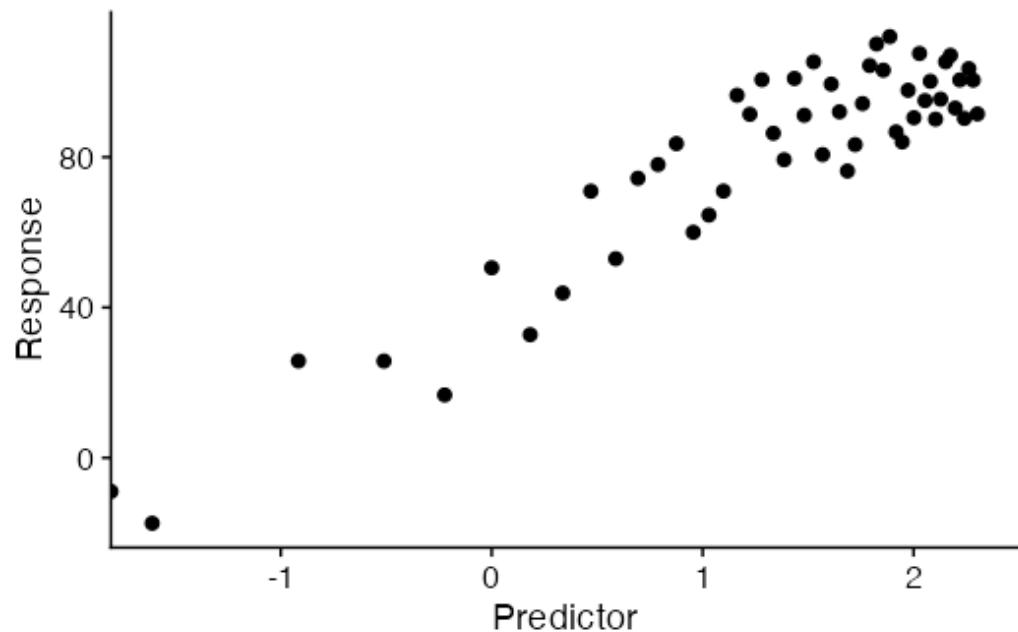
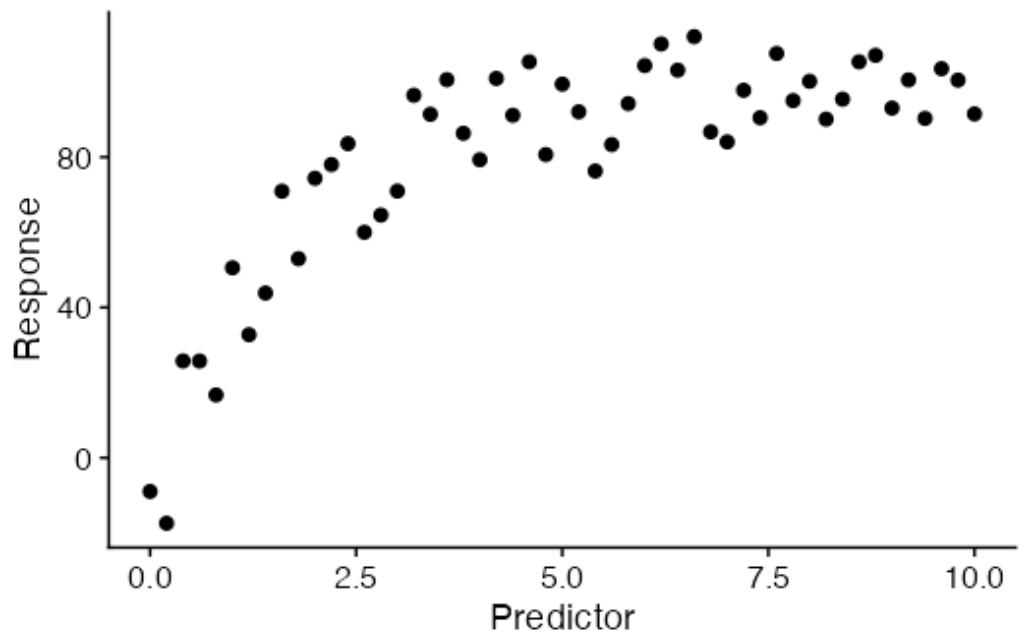
## Transformations: asymptotic relationship

Before transformation

```
ggplot(data = asymptotic,  
       aes(x = predictor, y = response)) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```

After  $\log_e$  transform

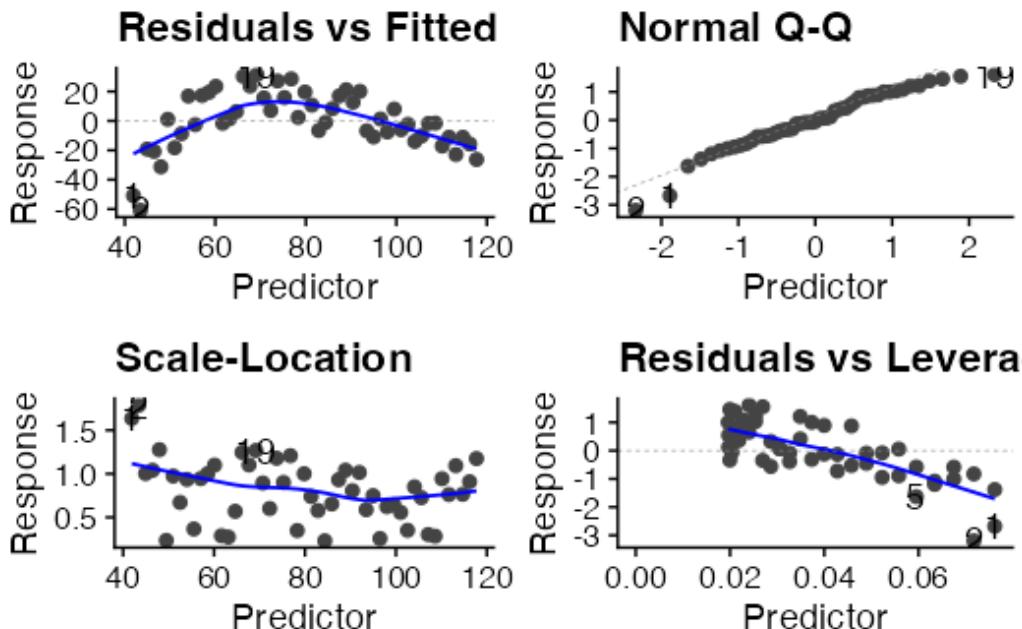
```
ggplot(data = asymptotic,  
       aes(x = log(predictor), y = response)) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```



## Transformations: asymptotic relationship

Before transformation

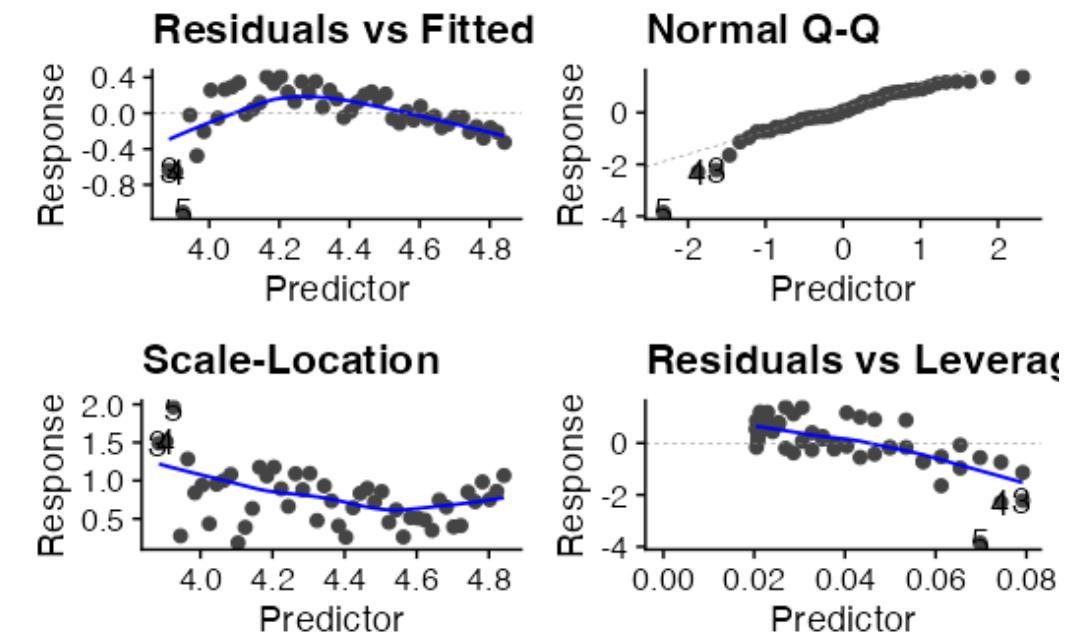
```
autoplot(lm(response ~ predictor, data =  
asymptotic)) +  
  labs(x = "Predictor", y = "Response")
```



After  $\log_e$  transform

```
autoplot(lm(log(response) ~ predictor, data =  
asymptotic)) +  
  labs(x = "Predictor", y = "Response")
```

Warning in log(response): NaNs produced



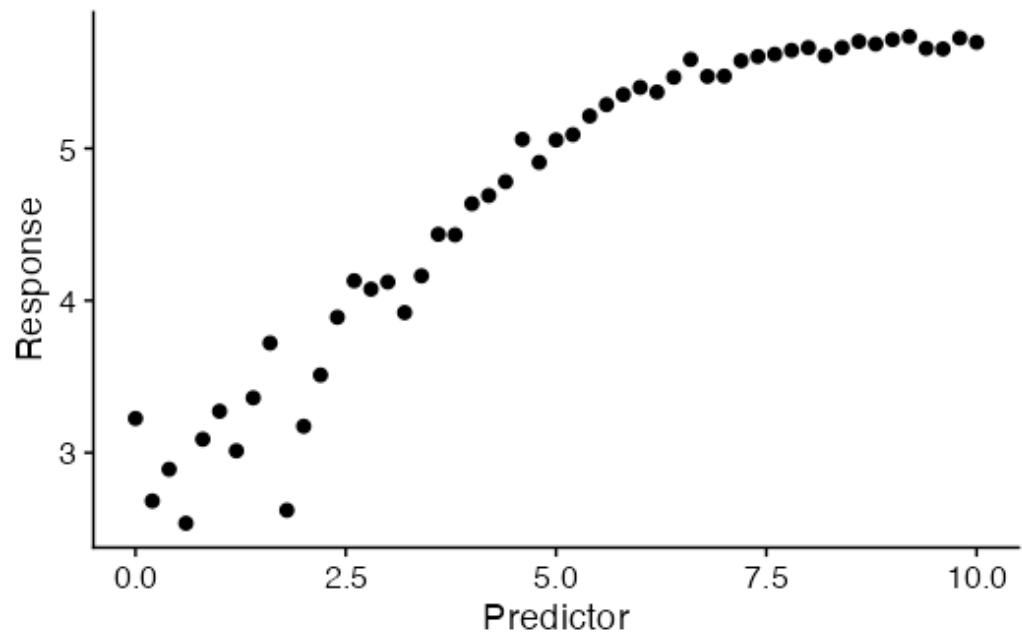
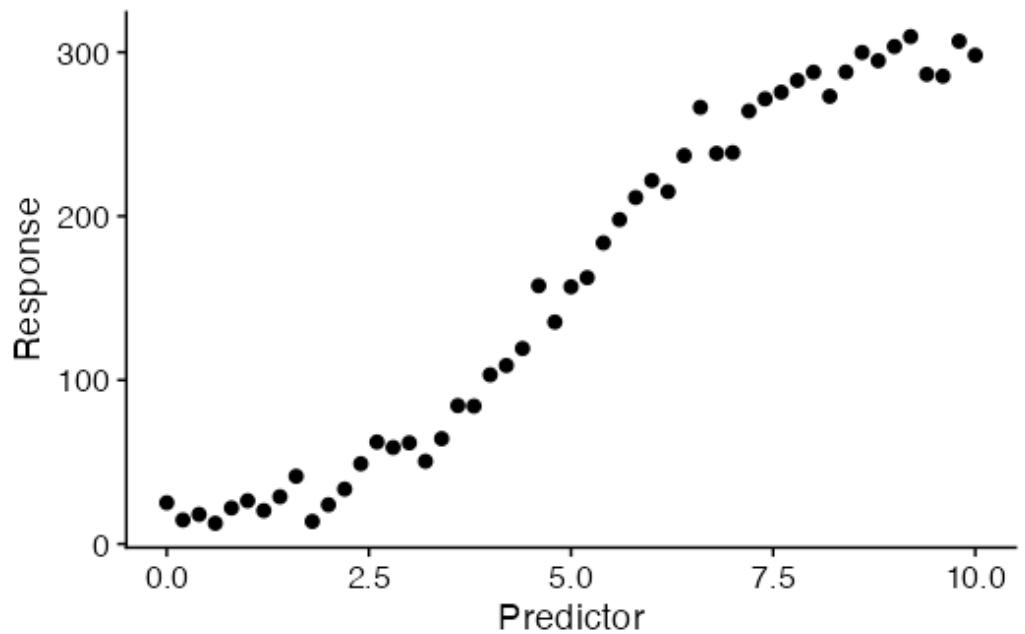
## Transformations: logistic relationship

Before transformation

```
ggplot(data = logistic,  
       aes(x = predictor, y = response)) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```

After  $\log_e$  transform

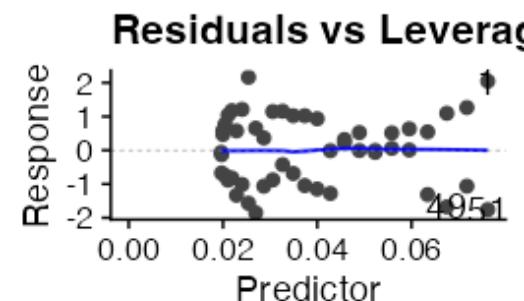
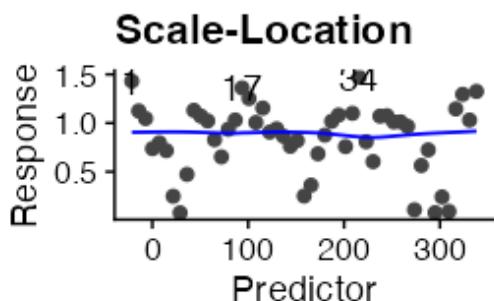
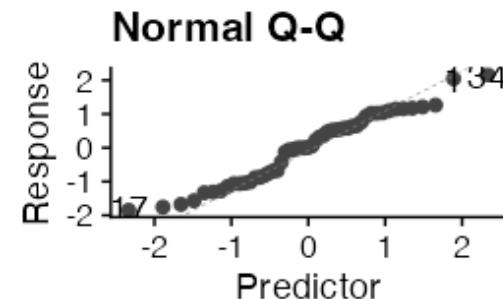
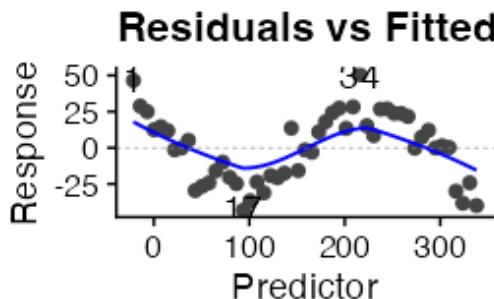
```
ggplot(data = logistic,  
       aes(x = predictor, y = log(response))) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```



## Transformations: logistic relationship

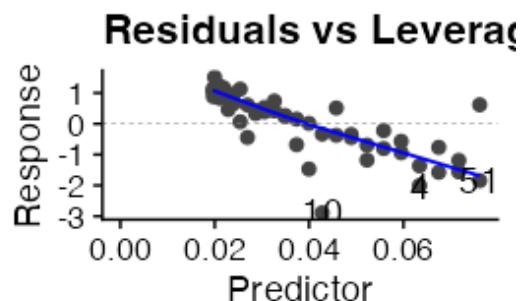
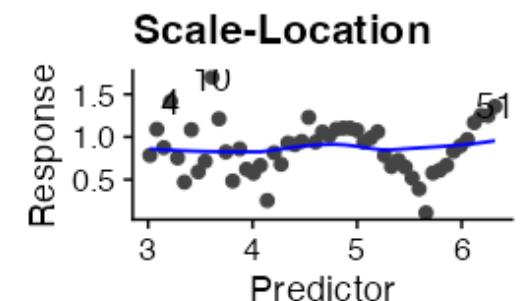
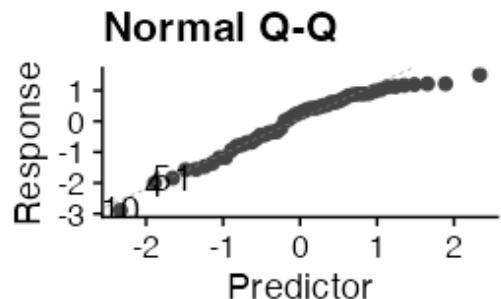
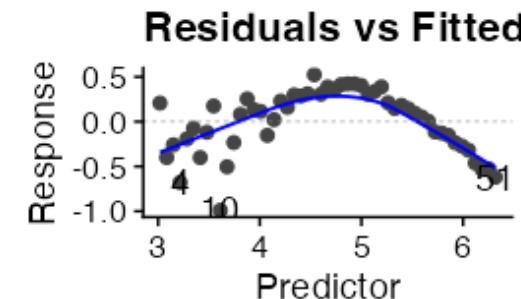
### Before transformation

```
autoplplot(lm(response ~ predictor, data =  
logistic)) +  
  labs(x = "Predictor", y = "Response")
```



### After $\log_e$ transform

```
autoplplot(lm(log(response) ~ predictor, data =  
logistic)) +  
  labs(x = "Predictor", y = "Response")
```



## Transformations: polynomial relationship

### Before transformation

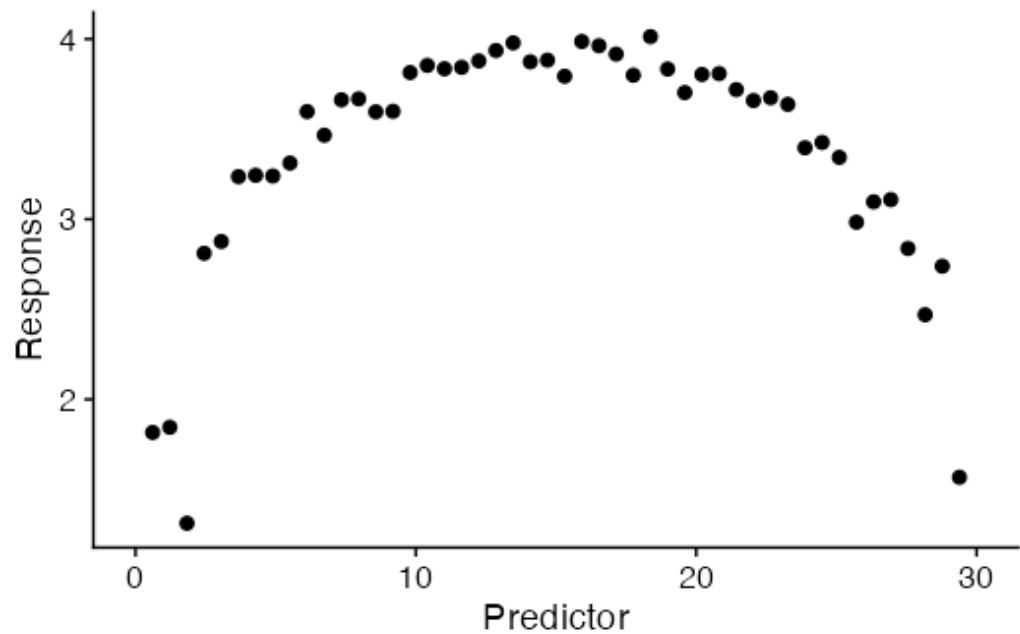
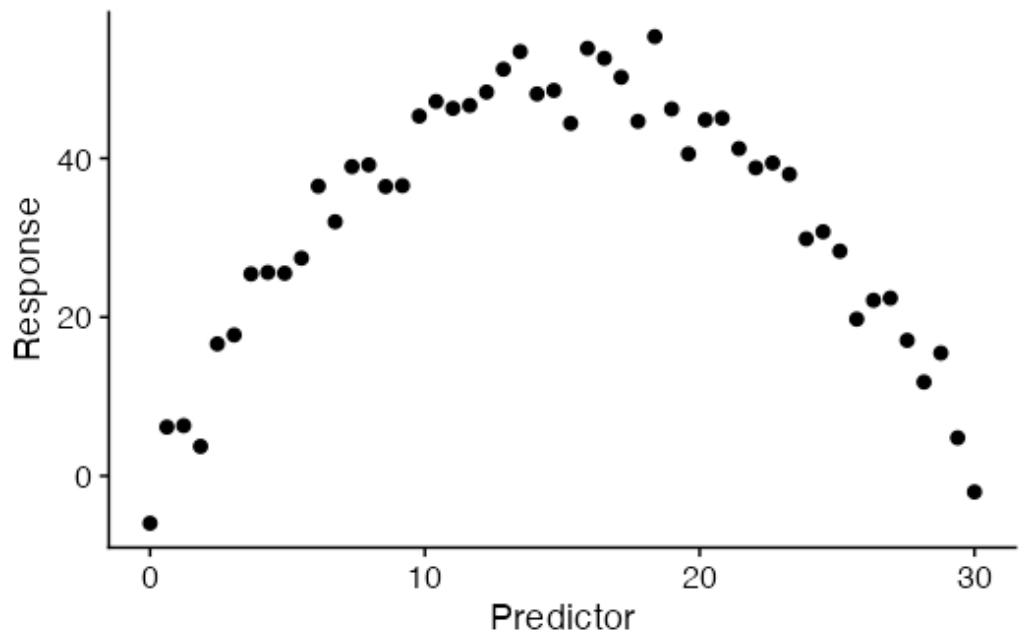
```
ggplot(data = curvilinear,  
       aes(x = predictor, y = response)) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```

### After $\log_e$ transform

```
ggplot(data = curvilinear,  
       aes(x = predictor, y = log(response))) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```

Warning in log(response): NaNs produced

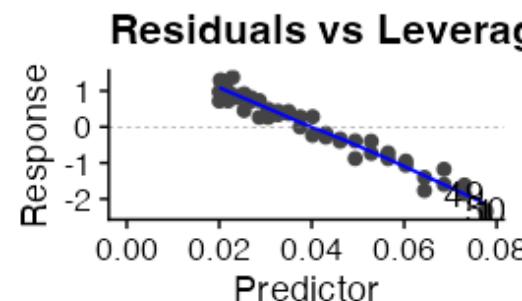
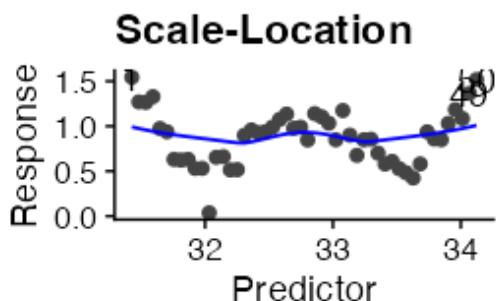
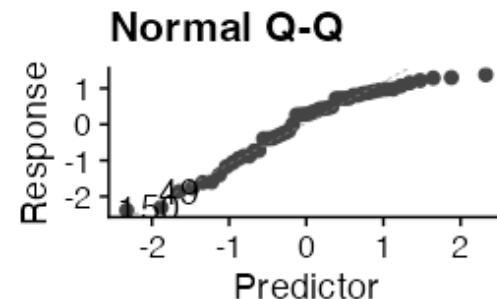
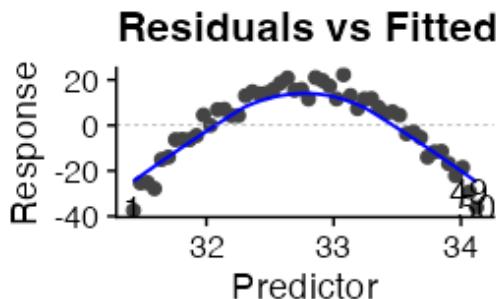
Warning: Removed 2 rows containing missing  
values or values outside the scale range  
(`geom\_point()`).



## Transformations: polynomial relationship

Before transformation

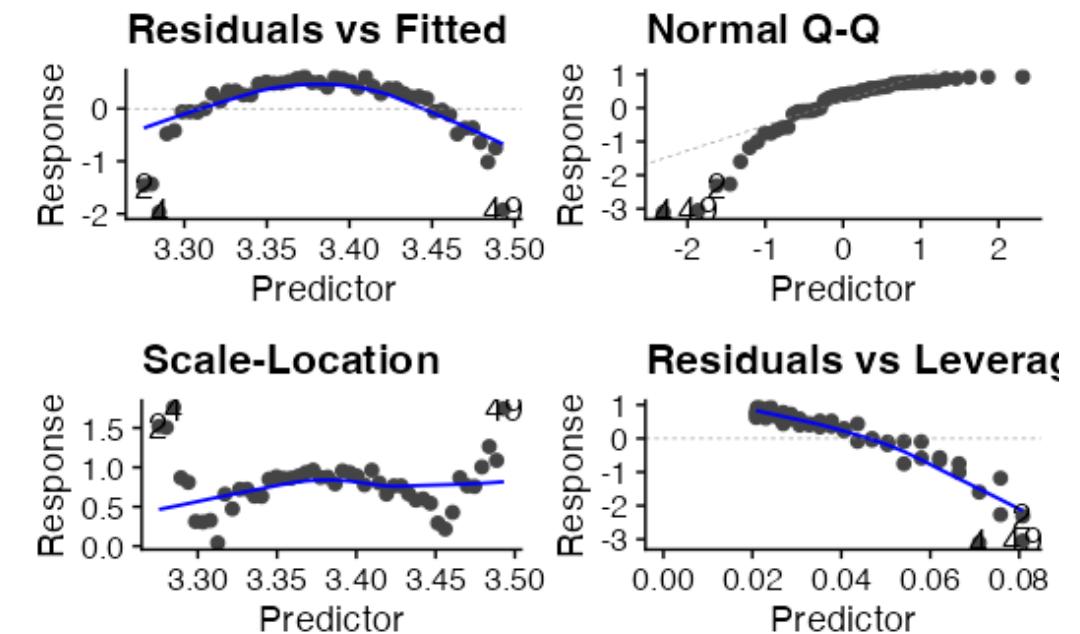
```
autoplot(lm(response ~ predictor, data =  
curvilinear)) +  
  labs(x = "Predictor", y = "Response")
```



After  $\log_e$  transform

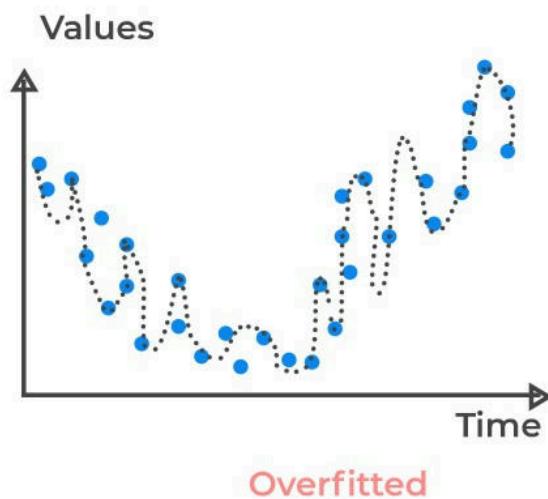
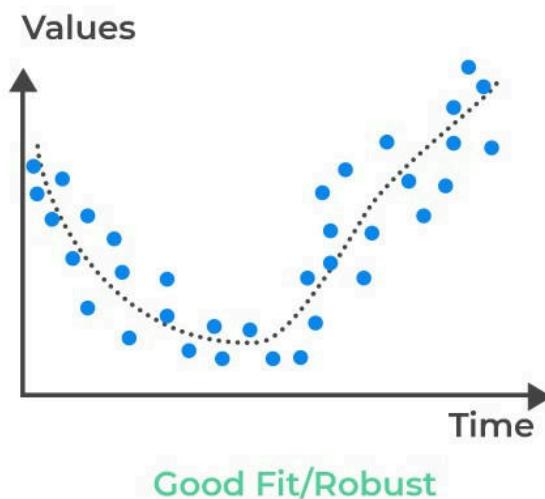
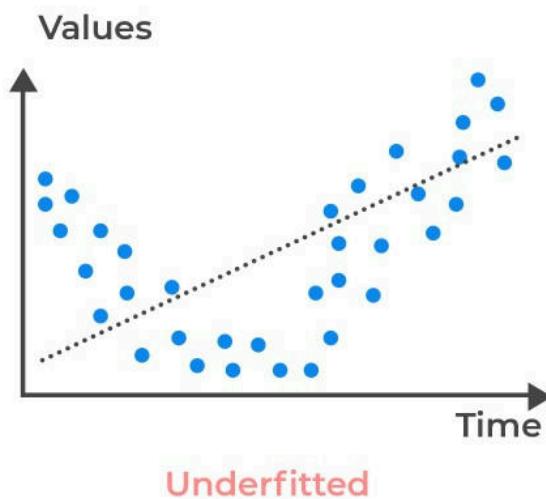
```
autoplot(lm(log(response) ~ predictor, data =  
curvilinear)) +  
  labs(x = "Predictor", y = "Response")
```

Warning in log(response): NaNs produced



## Did the transformations work?

- To a *certain* extent...
- **Problems:**
  - Relationships typically do not meet the linear assumption, but seem “ok” for other assumptions.
  - Poor fit to the data (over or underfitting in some areas).
  - Difficult to interpret the results.



## Nonlinear regression

- A way to model complex (nonlinear) relationships.
  - ▶ i.e. phenomena that arise in the natural and physical sciences e.g. biology, chemistry, physics, engineering.
- At least *one* predictor is not linearly related to the response variable.
- Unique/specific shape - apply only if you are sure of the relationship, e.g. asymptotic, quadratic.

## Performing nonlinear regression

- **Polynomial regression:** still linear in the parameters and a good place to start.
- **Nonlinear regression:** use the `nls()` function to fit the following nonlinear models:
  - ▶ Exponential growth
  - ▶ Exponential decay
  - ▶ Logistic

# Polynomial regression

| A special case of multiple linear regression used to model nonlinear relationships.

## Model

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \dots + \beta_k x_i^k + \epsilon_i$$

where  $k$  is the degree of the polynomial.

- The model is still linear in the parameters  $\beta$  and can be fitted using least squares.
- Instead of multiple predictors, we have multiple *terms* of the same predictor (same  $x$ ).
- Only the *highest-order term* is tested for significance.
- Can still be fit using `lm()`.
- The more complex, the less likely it follows a true biological relationship...

...

## Adding polynomial terms

- Linear:  $y = \beta_0 + \beta_1 x$
- Quadratic:  $y = \beta_0 + \beta_1 x + \beta_2 x^2$
- Cubic:  $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$
- Each level increases the power of the predictor by 1.

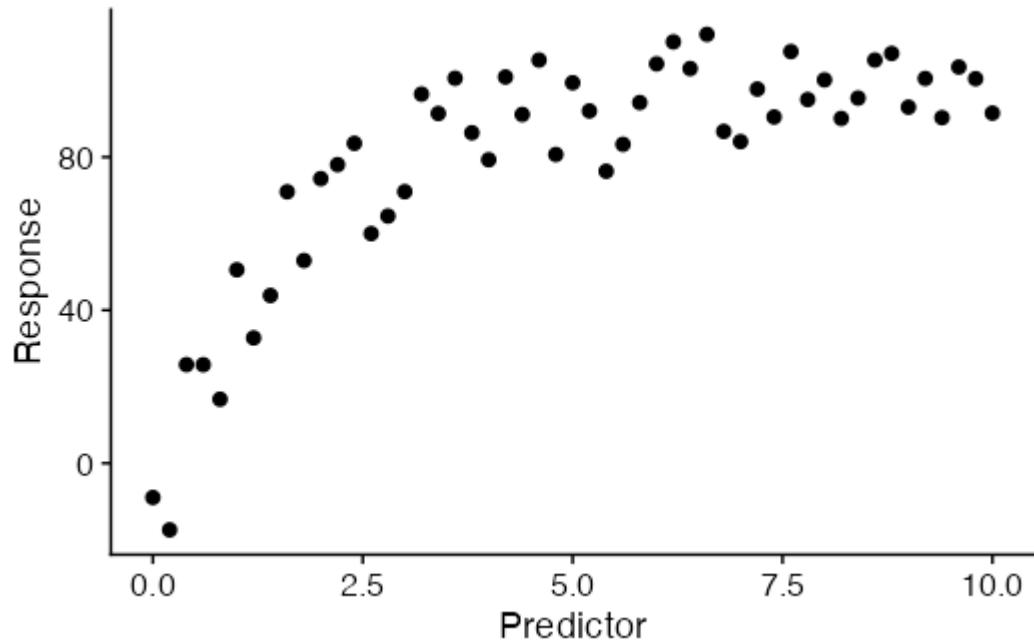
# Polynomial fitting

Using the `asymptotic` data

## The data

See Slide 11 for the relationship and mathematical expression.

```
ggplot(asymptotic, aes(x = predictor, y = response)) +  
  geom_point() +  
  labs(x = "Predictor", y = "Response")
```

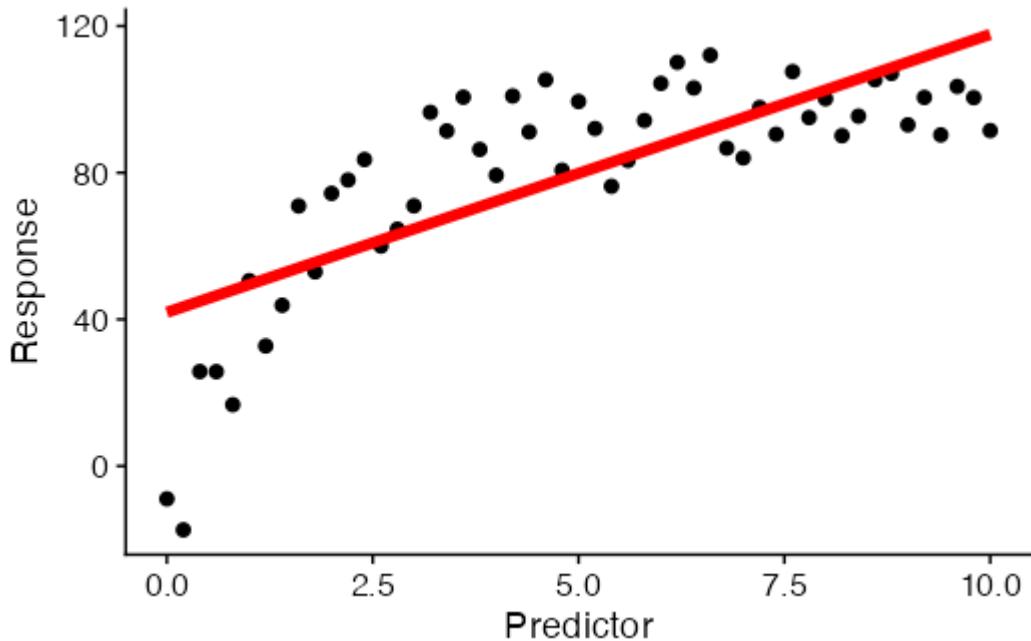


## Fitting the model (linear)

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

```
lin_fit ← lm(response ~ predictor, asymptotic)
```

```
ggplot(asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response") +
  geom_line(aes(y = predict(lin_fit)), color = "red", size = 2)
```

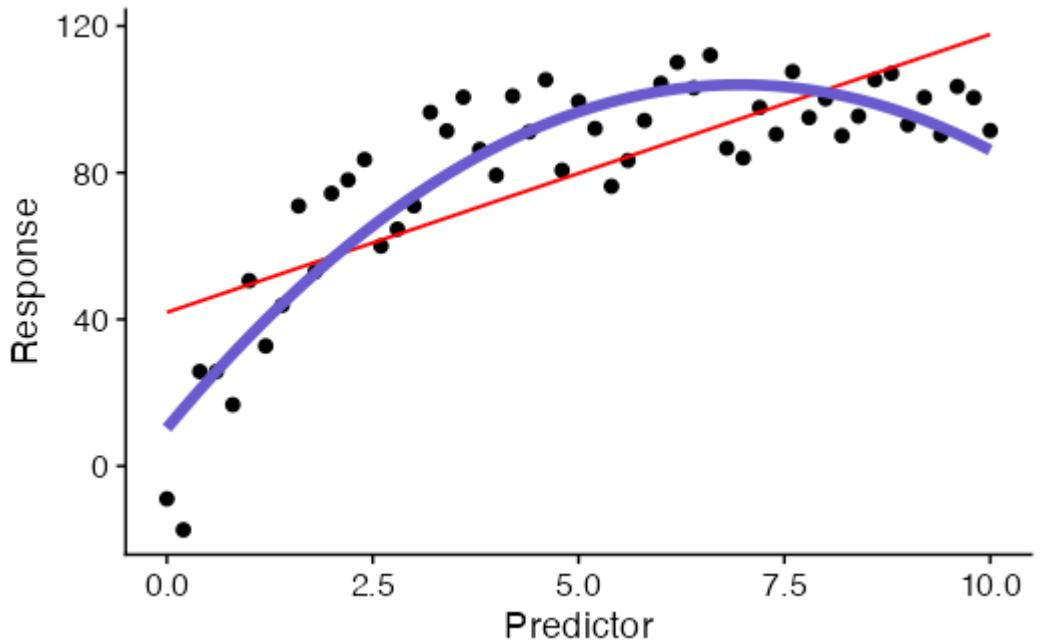


## Fitting the model (`poly(degree = 2)`)

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i$$

```
poly2_fit ← lm(response ~ poly(predictor, 2), asymptotic)
```

```
ggplot(asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response") +
  geom_line(aes(y = predict(lin_fit)), color = "red") +
  geom_line(aes(y = predict(poly2_fit)), color = "slateblue", size = 2)
```

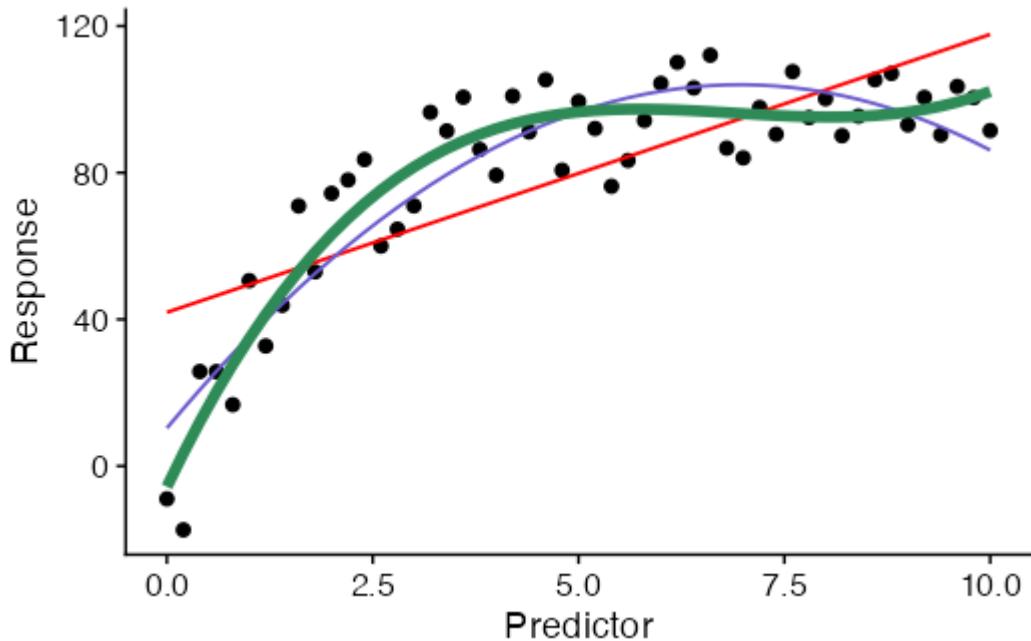


## Fitting the model (`poly(degree = 3)`)

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \epsilon_i$$

```
poly3_fit ← lm(response ~ poly(predictor, 3), asymptotic)
```

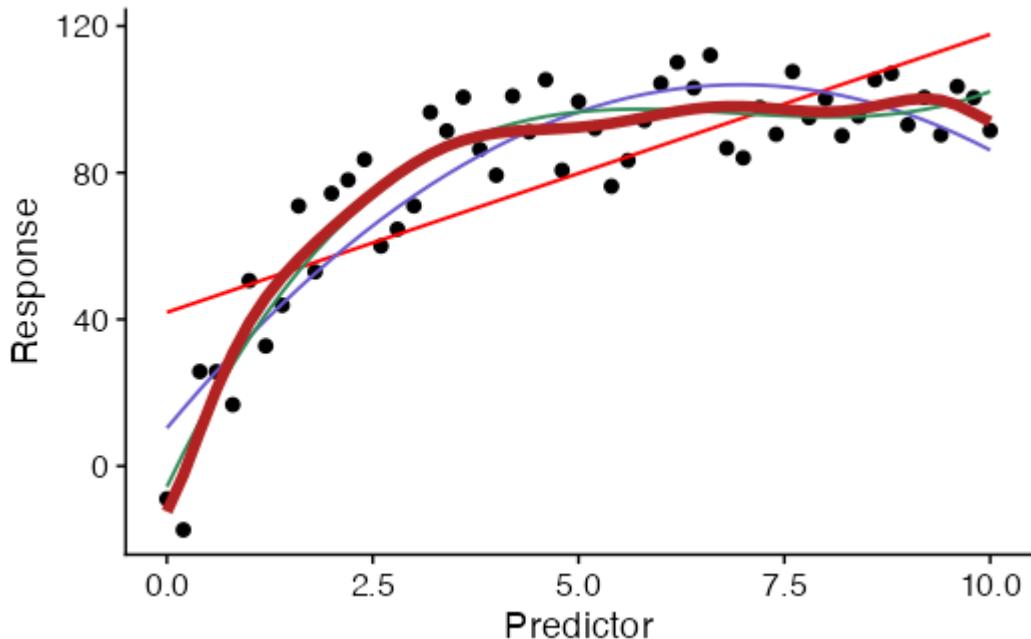
```
ggplot(asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response") +
  geom_line(aes(y = predict(lin_fit)), color = "red") +
  geom_line(aes(y = predict(poly2_fit)), color = "slateblue") +
  geom_line(aes(y = predict(poly3_fit)), color = "seagreen", size = 2)
```



## Fitting the model (`poly(degree = 10)`)

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \dots + \beta_{10} x_i^{10} + \epsilon_i$$

```
poly10_fit ← lm(response ~ poly(predictor, 10), asymptotic)
```



Model	R2
Linear	0.570
Poly2	0.820
Poly3	0.872
Poly10	0.862

**i** Note

We use adjusted R<sup>2</sup> for polynomials - extra terms, extra complexity, so extra penalty.

## Limitations

- Meaning of the coefficients is not always clear.
- Extrapolation can be *dangerous*.
- Extra terms can lead to overfitting and are difficult to interpret:
- Parsimony: is the most complex term (highest power) significant? If not, use a lower power.

```
summary(poly10_fit)
```

Call:

```
lm(formula = response ~ poly(predictor, 10), data = asymptotic)
```

Residuals:

Min	1Q	Median	3Q	Max
-17.1659	-8.6908	-0.0494	8.8003	16.4012

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	79.818	1.552	51.426	< 2e-16 ***

```

poly(predictor, 10)1  159.368    11.084   14.378 < 2e-16 ***
poly(predictor, 10)2 -106.939    11.084  -9.648 5.37e-12 ***
poly(predictor, 10)3  48.570    11.084   4.382 8.28e-05 ***
poly(predictor, 10)4 -19.411    11.084  -1.751  0.0876 .
poly(predictor, 10)5  1.193     11.084   0.108  0.9148
poly(predictor, 10)6 -2.769     11.084  -0.250  0.8040
poly(predictor, 10)7 -1.343     11.084  -0.121  0.9042
poly(predictor, 10)8 -4.009     11.084  -0.362  0.7195
poly(predictor, 10)9 -2.851     11.084  -0.257  0.7984
poly(predictor, 10)10 5.769     11.084   0.520  0.6056
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

Residual standard error: 11.08 on 40 degrees of freedom  
 Multiple R-squared: 0.8897, Adjusted R-squared: 0.8621  
 F-statistic: 32.26 on 10 and 40 DF, p-value: 4.846e-16

## Still:

- Easy to fit: just add polynomial terms to the model.
- Simple to perform: use `lm()`.

# **Nonlinear fitting**

## Fitting a nonlinear model

If you have some understanding of the underlying relationship (e.g. mechanistic process) between the variables, you can fit a nonlinear model.

### Mathematical expression

$$Y_i = f(x_i, \beta) + \epsilon_i$$

where  $f(x_i, \beta)$  is a nonlinear function of the parameters  $\beta$ .

- $Y_i$  is the continuous response variable.
- $x_i$  is the vector of predictor variables.
- $\beta$  is the vector of unknown parameters.
- $\epsilon_i$  is the random error term (residual error).

## Assumptions

Like the linear model, the nonlinear model assumes *INE*:

- Error terms are independent (**Independence**).
- Error terms are normally distributed (**Normality**).
- Error terms have equal/constant variance (**Homoscedasticity**).

Basically:

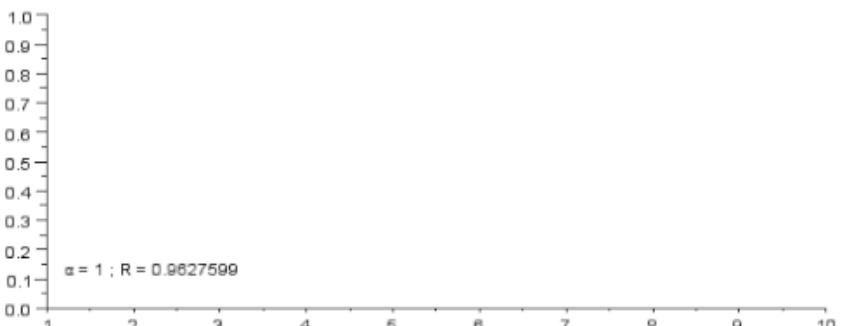
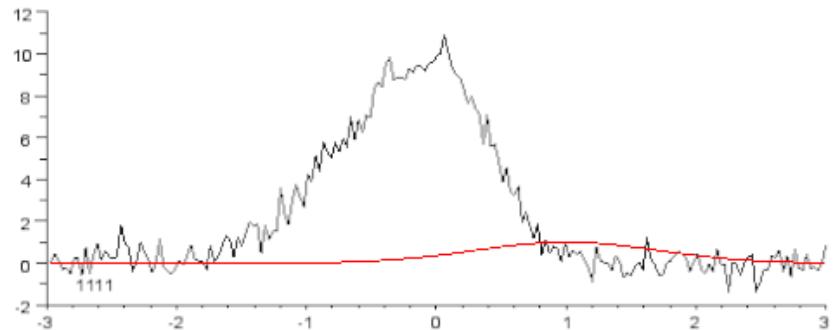
$$\epsilon_i \sim N(0, \sigma^2)$$

...

Like all other models we have seen, we focus on the residuals to assess the model fit, since the residuals are the only part of the model that is random.

## Estimating the model parameters

- The parameters are estimated using the **method of least squares**.
- For nonlinear models, a nonlinear optimization algorithm is used to find the best fit, rather than ordinary least squares:
  - ▶ **Gauss-Newton algorithm**
  - ▶ **Levenberg-Marquardt algorithm**
- This can only be performed iteratively and depends on a “best guess” of the parameters *as a start*.
  - ▶ **i.e. we need to provide a starting point for a nonlinear least squares algorithm to begin.**



Source: [Wikipedia](#)

## Two methods in R

Use `nls()` function in R.

```
nls(formula, data, start)
```

- `formula`: a formula object, response variable ~ predictor variable(s).
- `data`: a data frame containing the variables in the model (response, predictor).
- `start`: a named list of starting values for the parameters in the model.

Self-starting functions: `SSexpf()`, `SSasymp()`, `SSlogis()`, etc.

- Self-starting functions estimate the starting values for you.
- Named after the models they fit.
- Existing functions have pre-set formulas.
- Can define own functions but more complex than `nls()`.

## **Example: Fitting an exponential model**

## With `nls()`

$$y = y_0 e^{kx}$$

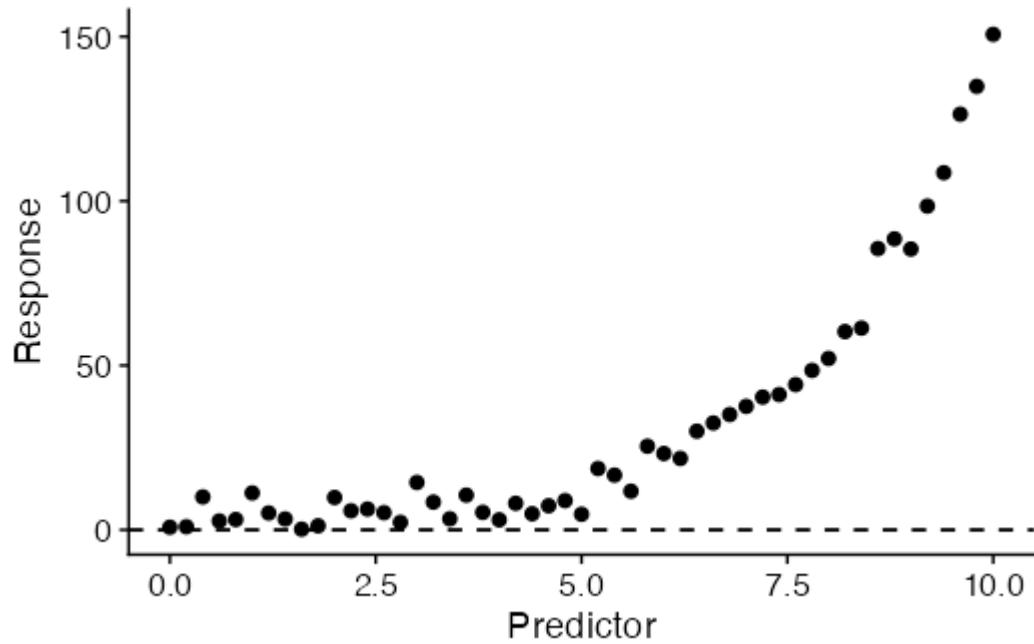
where

- $y$  is the response and  $x$  is the predictor
- $y_0$  is the value of  $y$  when  $x = 0$
- $k$  is the rate of change

$k$  can be estimated with the equation  $slope = k = \frac{\log_e y_{max} - \log_e y_{min}}{x_{max} - x_{min}}$ , but usually a value of 1 is a good starting point.

```
set.seed(123)
growth ← tibble(
  predictor = seq(0, 10, by = 0.2),
  response = abs(exp(0.5*predictor) + rnorm(length(predictor), mean = 1, sd = 5)))

ggplot(data = growth, aes(x = predictor, y = response)) +
  geom_point() +
  geom_hline(yintercept = 0, linetype = "dashed") +
  labs(x = "Predictor", y = "Response")
```

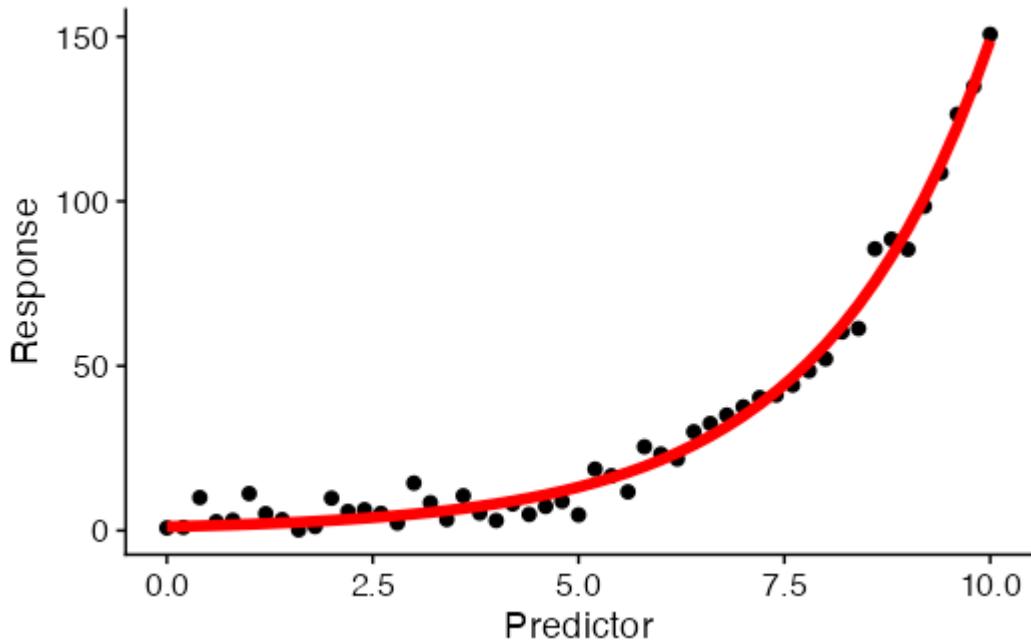


## First guess

Based on the plot, we can estimate  $y_0 \neq 0$  and  $k = 1$ . Because of the equation,  $y = y_0 e^{kx}$ ,  $y_0$  cannot be 0!

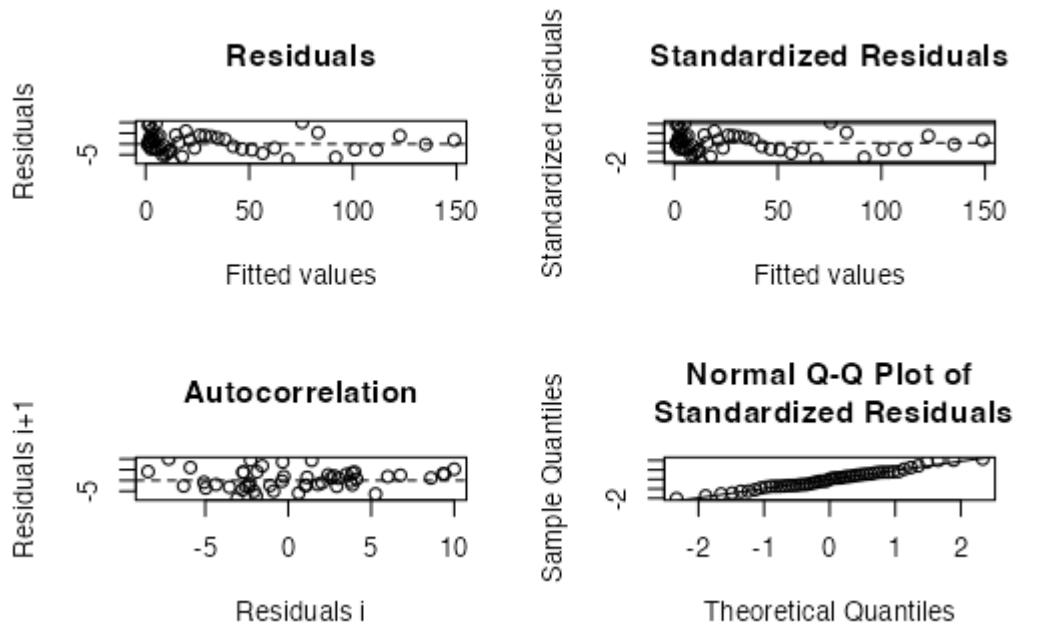
```
fit_exponential ← nls(response ~ y0*exp(k*predictor), data = growth,
  start = list(y0 = 0.1, k = 1))
```

```
ggplot(data = growth, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response") +
  geom_line(aes(y = predict(fit_exponential)), color = "red", size = 2)
```



## Check assumptions

```
library(nlstools)
resids ← nlsResiduals(fit_exponential)
plot(resids)
```



- These plots determine if the residuals are normally distributed and have equal variance
- *Normal QQ* looks good
- *Residuals vs fitted* and *Standardized Residuals* even spread but slight fanning.
- With *Autocorrelation* we want random scatter around 0 – this indicates independence. Harder to meet with time-series data.
- Nonlinear models typically should meet assumptions because they are fitted specifically to the data.

## Interpretation

```
summary(fit_exponential)
```

Formula: response ~ y0 \* exp(k \* predictor)

Parameters:

	Estimate	Std. Error	t value	Pr(> t )
y0	1.1694	0.1291	9.059	4.82e-12 ***
k	0.4847	0.0121	40.057	< 2e-16 ***

---

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

Residual standard error: 4.409 on 49 degrees of freedom

Number of iterations to convergence: 8

Achieved convergence tolerance: 1.192e-06

- The model is significant since the p-value is less than 0.05 for all parameters.
- If this were real data (e.g. population growth), the parameters themselves e.g. rate of change, are useful

- The parameterised model is:

$$y = 1.17 \cdot e^{-0.484x}$$

The R-squared value is not reported for nonlinear models as the sum of squares is not partitioned into explained and unexplained components. You can use the **residual standard error** and plots instead to compare between models.

## A really bad guess

What if we don't estimate our parameters very well? R will either give an error or get there eventually.

Note the parameters and residual standard error are the same as the previous slide - but the  
Number of iterations to convergence is higher.

```
fit_exponential ← nls(response ~ y0*exp(k*predictor), data = growth,  
start = list(y0 = 50, k = 1.5)) # totally bogus numbers  
  
summary(fit_exponential)
```

Formula: response ~ y0 \* exp(k \* predictor)

Parameters:

	Estimate	Std. Error	t value	Pr(> t )
y0	1.1694	0.1291	9.059	4.82e-12 ***
k	0.4847	0.0121	40.057	< 2e-16 ***

---

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

Residual standard error: 4.409 on 49 degrees of freedom

Number of iterations to convergence: 28

Achieved convergence tolerance: 2.003e-06



Tip

If an error pops up, try different starting values - the **rate of change** is most likely the problem.

## Fitting the model with `SSexpf()`

- `SSexpf()` is from the `nltraa` package.
- It has the same formula as above – different names for parameters ( $y_0 = a$ ,  $k = c$ ) but we can re-define them to anything we want
- Reaches the same result but with less effort.

```
library(nltraa)
```

```
Attaching package: 'nltraa'
```

```
The following object is masked from 'package:lattice':
```

```
barley
```

```
fit_exponential_ss ← nls(response ~ SSexpf(predictor, y0, k), data = decay)
summary(fit_exponential_ss)
```

Formula: response ~ SSexpf(predictor, y0, k)

Parameters:

	Estimate	Std. Error	t value	Pr(> t )
y0	1.65486	0.04699	35.22	< 2e-16 ***
k	-0.06527	0.00590	-11.06	6.33e-15 ***

---

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

Residual standard error: 0.1471 on 49 degrees of freedom

Number of iterations to convergence: 5

Achieved convergence tolerance: 1.048e-06

## **Example: Fitting an asymptotic model**

## The equation

- There are multiple equations for asymptotic models, this is the equation that `SSasymp()` (base R) uses:

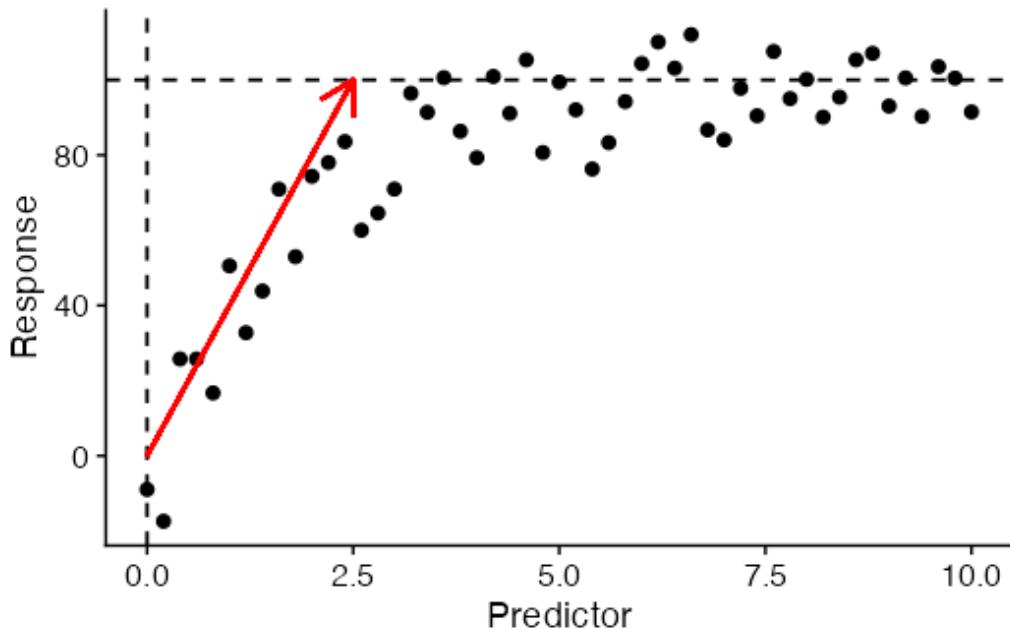
$$y = Asym + (R_0 - Asym) \cdot e^{-e^{lrc} \cdot x}$$

- $R_0$  is value of  $y$  when  $x = 0$ .
- $Asym$  is the upper limit: the maximum value of  $y$ .
- $lrc$  is the rate of change: the rate at which  $y$  approaches the upper limit.

...

```
ggplot(data = asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  geom_hline(yintercept = 100, linetype = "dashed") +
  geom_vline(xintercept = 0, linetype = "dashed") +
  ## plot the rate
  geom_segment(aes(x = 0, y = 0, xend = 2.5, yend = 100),
               arrow = arrow(length = unit(0.5, "cm")),
               color = "red") +
  labs(x = "Predictor", y = "Response")
```

```
Warning in geom_segment(aes(x = 0, y = 0, xend = 2.5, yend = 100), arrow = arrow(length =  
unit(0.5, : All aesthetics have length 1, but the data has 51 rows.  
i Please consider using `annotate()` or provide this layer with data containing  
a single row.
```



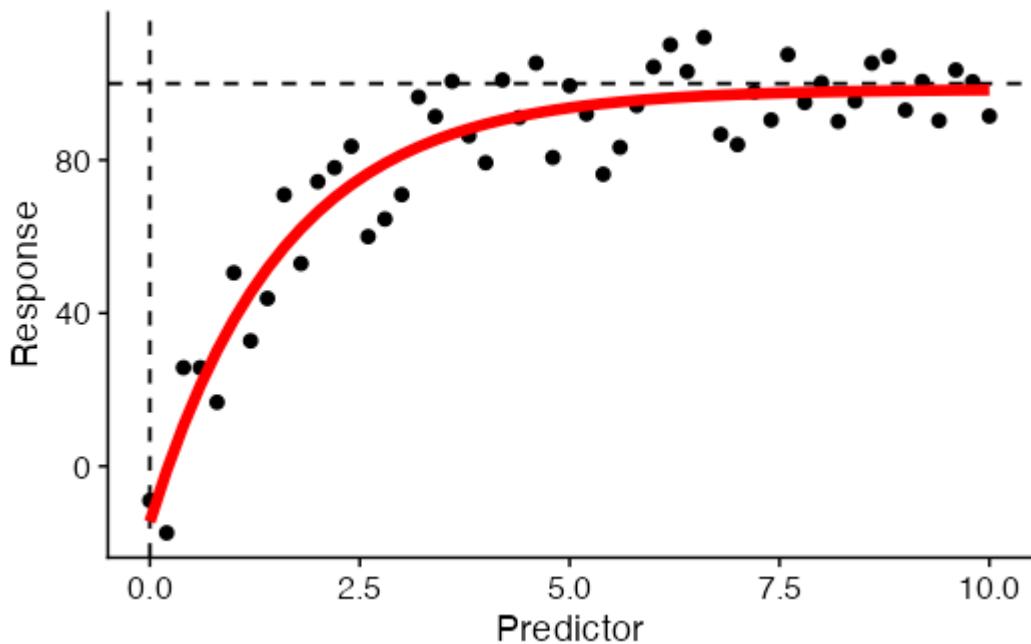
Some plausible estimates –  $R_0 = 0$ ,  $Asym = 100$ ,  $lrc = 0.8$ .

## Fit model

```
# fit_asymptotic ← nls(response ~ Asym + (R0-Asym)*(exp(-exp(lrc)*predictor)), data = asymptotic,
#   start = list(R0 = 0, Asym = 100, lrc = 0.8))

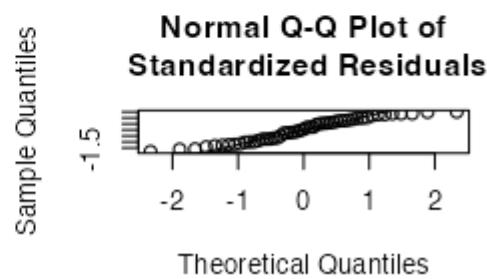
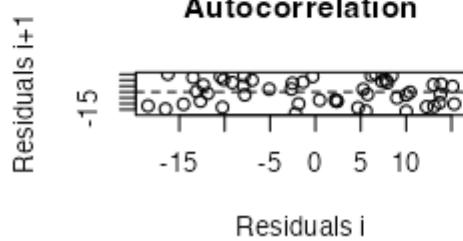
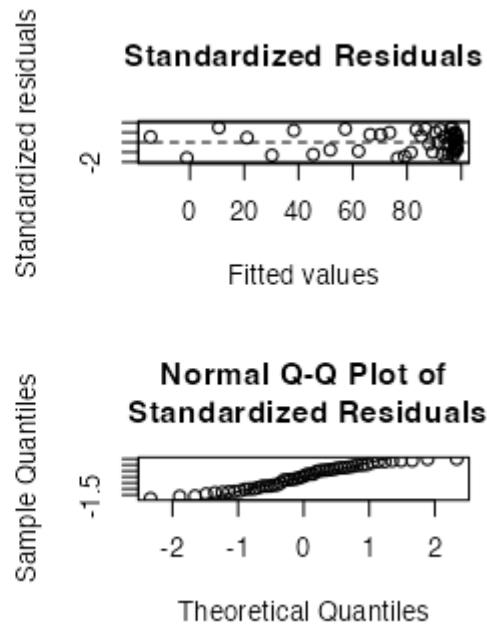
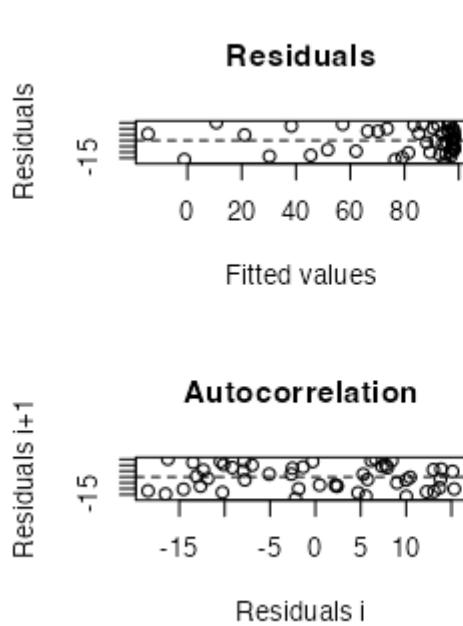
fit_asymptotic ← nls(response ~ SSasymp(predictor, Asym, R0, lrc), data = asymptotic)

ggplot(data = asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  geom_hline(yintercept = 100, linetype = "dashed") +
  geom_vline(xintercept = 0, linetype = "dashed") +
  labs(x = "Predictor", y = "Response") +
  geom_line(aes(y = predict(fit_asymptotic)), color = "red", size = 2)
```



## Check assumptions

```
library(nlstools)
resids ← nlsResiduals(fit_asymptotic)
plot(resids)
```



## Interpretation

```
summary(fit_asymptotic)
```

Formula: response ~ SSasymp(predictor, Asym, R0, lrc)

Parameters:

	Estimate	Std. Error	t value	Pr(> t )
Asym	98.5204	2.2852	43.113	< 2e-16 ***
R0	-14.5176	6.6416	-2.186	0.03374 *
lrc	-0.4626	0.1134	-4.079	0.00017 ***

---

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

Residual standard error: 10.21 on 48 degrees of freedom

Number of iterations to convergence: 0

Achieved convergence tolerance: 3.341e-07

- The model is significant since the p-value is less than 0.05 for all parameters.

- If this were real data (e.g. population growth), the parameters themselves e.g. rate of change, are useful
- The parameterised model is:

$$y = 98.5 + (-14.5 - 98.5) \cdot e^{-e^{-0.463} \cdot x}$$

# Example: fitting a logistic model

## The equation

There are multiple equations for logistic models, but they all have an ‘S’ or sigmoid shape. The equation that `SSlogis()` (base R) assumes  $y$  is positive and uses:

$$y = \frac{Asym}{1 + e^{\frac{xmid-x}{scal}}}$$

where

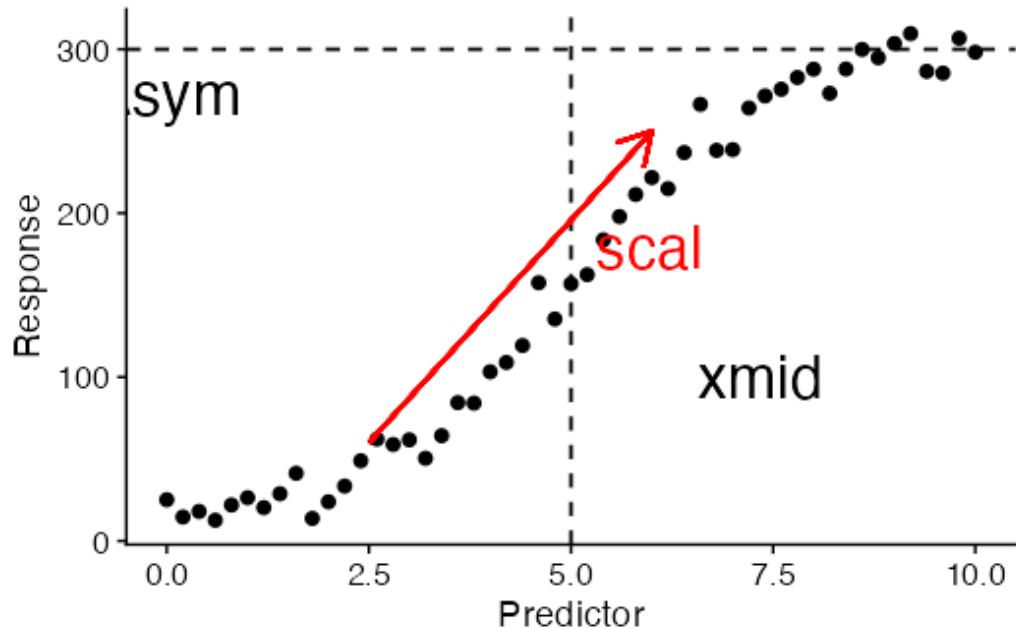
- $Asym$  is the upper limit: the maximum value of  $y$ .
- $xmid$  is the value of  $x$  when  $y$  is halfway between the lower and upper limits.
- $scal$  is the rate of change: the rate at which  $y$  approaches the upper limit.

```
ggplot(data = logistic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response") +
  geom_hline(yintercept = 300, linetype = "dashed") +
  geom_vline(xintercept = 5, linetype = "dashed") +
  # label the lines above
  annotate("text", x = 0, y = 300, label = "Asym", size = 8, vjust = 1.5) +
```

```
annotate("text", x = 5, y = 100, label = "xmid", size = 8, hjust = -1) +
## plot the rate
geom_segment(aes(x = 2.5, y = 60, xend = 6, yend = 250),
             arrow = arrow(length = unit(0.5, "cm")),
             color = "red") +
# label the rate
annotate("text", x = 4, y = 180, label = "scal", size = 8, colour = "red", hjust = -1)
```

Warning in geom\_segment(aes(x = 2.5, y = 60, xend = 6, yend = 250), arrow = arrow(length =  
unit(0.5, : All aesthetics have length 1, but the data has 51 rows.

i Please consider using `annotate()` or provide this layer with data containing  
a single row.



Some starting values would be  $Asym = 300$ ,  $xmid = 5$ ,  $scal = 1$ .

## Fit model

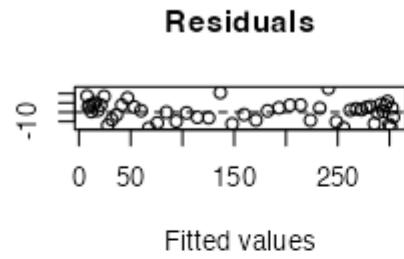
Estimating the parameters or using the self-starting function `SSlogis()` gives a near-identical result.

```
# fit_logistic ← nls(response ~ Asym/(1+exp((xmid-predictor)/scal)), data = logistic,
#   start = list(Asym = 300, xmid = 5, scal = 1))

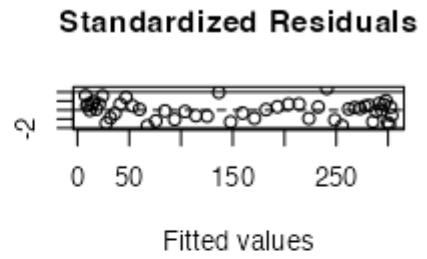
fit_logistic ← nls(response ~ SSlogis(predictor, Asym, xmid, scal), data = logistic)

resids ← nlsResiduals(fit_logistic)
plot(resids)
```

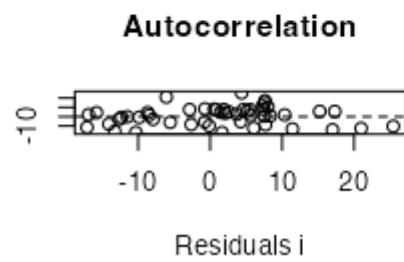
Residuals



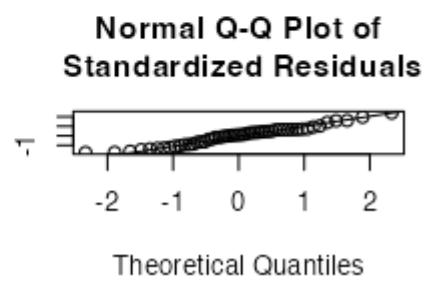
Standardized residuals



Residuals  $i+1$



Sample Quantiles



## Interpretation

`SSlogis()` guessed the parameters on the first try.

```
summary(fit_logistic)
```

Formula: response ~ SSlogis(predictor, Asym, xmid, scal)

Parameters:

	Estimate	Std. Error	t value	Pr(> t )
Asym	310.64727	4.62579	67.16	<2e-16 ***
xmid	4.92715	0.07142	68.99	<2e-16 ***
scal	1.34877	0.05418	24.90	<2e-16 ***

---

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

Residual standard error: 10.22 on 48 degrees of freedom

Number of iterations to convergence: 1

Achieved convergence tolerance: 6.632e-07

- The model is significant since the p-value is less than 0.05 for all parameters.
- If the model visually fits well and relationship has reasoning (parameter significance not always important).
- The parameterised model is:

$$y = \frac{310}{1 + e^{\frac{4.93-x}{1.35}}}$$

## **How do we know which model is better? (Advanced)**

Note: this is non-examinable content but might be useful for your project.

## Example: polynomial regression

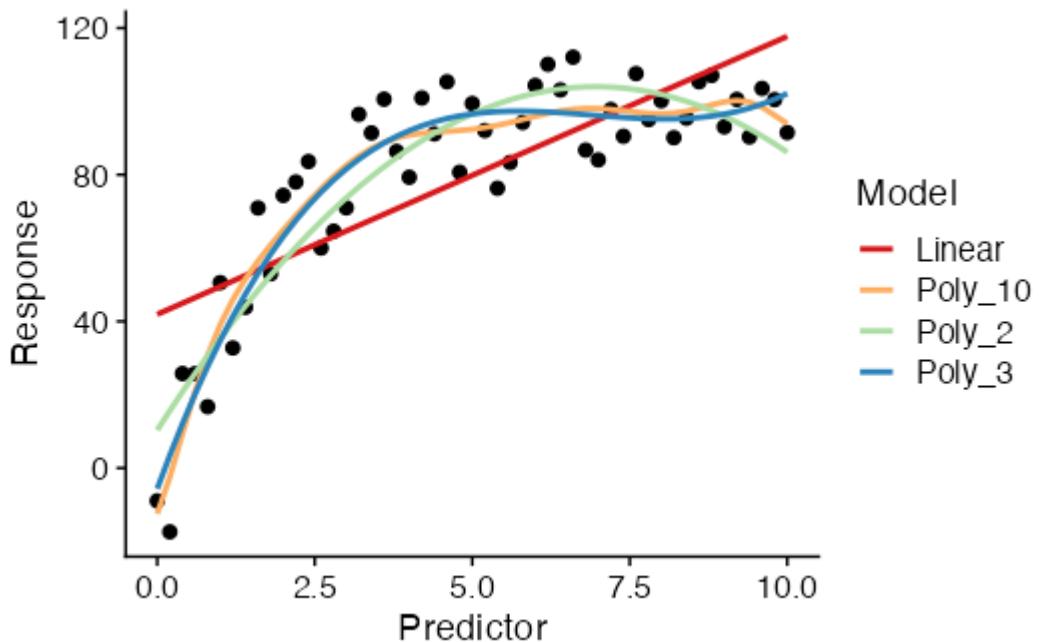
```
library(tidyr)

# Create a new data frame with predictor values and model predictions
predictions ← data.frame(
  predictor = asymptotic$predictor,
  Linear = predict(lin_fit),
  Poly_2 = predict(poly2_fit),
  Poly_3 = predict(poly3_fit),
  Poly_10 = predict(poly10_fit)
)

# Reshape the data to long format
predictions_long ← predictions %>%
  pivot_longer(cols = -predictor, names_to = "Model", values_to = "response")

# Plot the data
ggplot(predictions_long, aes(x = predictor, y = response, color = Model)) +
  geom_point(data = asymptotic, aes(x = predictor, y = response), inherit.aes = FALSE) +
  geom_line(linewidth = 1) +
```

```
labs(x = "Predictor", y = "Response") +  
  scale_color_brewer(palette = "Spectral")
```



## Prediction quality

We can use prediction quality metrics to compare the fits.

- Akaike information criterion (AIC) and Bayesian information criterion (BIC).
  - ▶ Useful for comparing model fits.
  - ▶ Has a penalty for more predictors
- Residual standard error, residual sum of squares (`deviance(mod)`), root mean squared error (RMSE) and mean absolute error (MAE).
  - ▶ Essentially the difference between observed and predicted (residuals).
  - ▶ RMSE penalises larger residuals.

## AIC and BIC

Use the `broom` package to extract the AIC and BIC values from the model fits.

```
library(broom)
# collect all polynomial fits into a single tibble using glance
poly_fits ← tibble(
  model = c("linear", "poly2", "poly3", "poly10"),
  fit = list(lin_fit, poly2_fit, poly3_fit, poly10_fit)) %>%
  mutate(glance = map(fit, glance)) %>%
  unnest(glance) %>%
  select(model, AIC, BIC)
poly_fits
```

```
# A tibble: 4 × 3
  model     AIC     BIC
  <chr>   <dbl>   <dbl>
1 linear   453.   459.
2 poly2    409.   416.
3 poly3    392.   402.
4 poly10   402.   425.
```

- The smaller the AIC or BIC, the better the fit compared to other models.

## Calculate RMSE and MAE

```
predictions ← data.frame(  
  observed = asymptotic$response,  
  Linear = predict(lin_fit),  
  Poly_2 = predict(poly2_fit),  
  Poly_3 = predict(poly3_fit),  
  Poly_10 = predict(poly10_fit)  
)  
  
errors ← predictions %>%  
  pivot_longer(cols = -observed, names_to = "Model", values_to = "Predicted") %>%  
  group_by(Model) %>%  
  summarise(  
    RMSE = sqrt(mean((observed - Predicted)^2)),  
    MAE = mean(abs(observed - Predicted)))  
)  
  
knitr::kable(errors, digits=2, caption = "Comparison of RMSE and MAE for different models")
```

Model	RMSE	MAE
Linear	19.38	15.17
Poly_10	9.82	8.57
Poly_2	12.30	9.88
Poly_3	10.25	8.83

- From the results, the polynomial to the degree of 10 has the lowest error - but visually we know it is overfitting, and the cubic polynomial is more parsimonious.
- We can say the model has a prediction error of 10.25 units (RMSE) and 8.83 units (MAE).

**i** Note

Both the RMSE and MAE measure error on the same scale as the response variable. e.g. if the response variable is in kg, the error will be in kg.

## Summary

- With nonlinear relationships, there are three possible approaches:
  1. **Linearise** the relationship by transforming:
    - Fit: easy
    - Interpret: difficult
  2. Add **polynomial** terms:
    - Fit: easy
    - Interpret: difficult
  3. Fit the model using a **nonlinear** algorithm:
    - Fit: difficult
    - Interpret: easy



...

- Nonlinear models:
  - Useful for modelling more complex relationships. Require some understanding of the underlying relationship and equations.

- ▶ Mainly for prediction rather than interpreting relationships.
- ▶ Self-starting functions have limited pre-defined formulas.
- ▶ Assumptions **INE**.

# Thanks!

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