# 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

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

*"How does $y$ change as $x_1$, $x_2$, ..., $x_k$ 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 monotically with $x$.
- More interpretable and easier to fit.

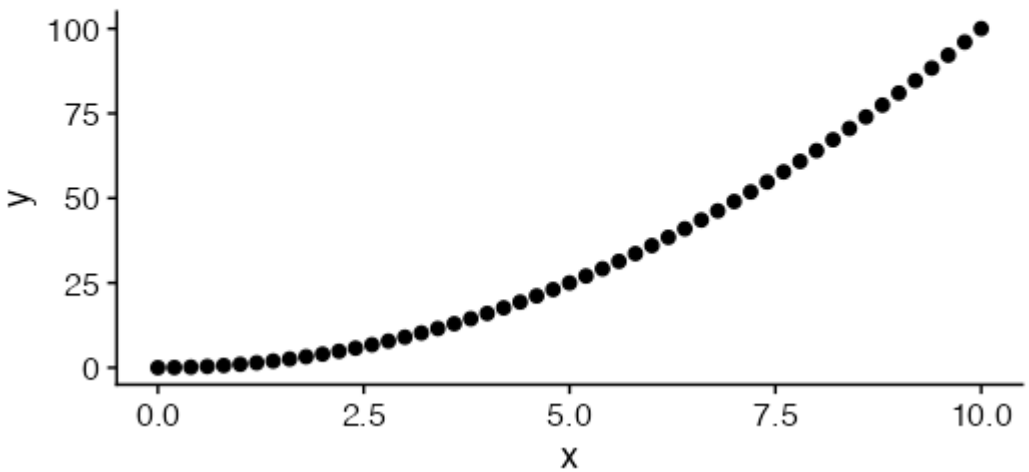
## Nonlinear relationships: exponents

- $x^2$ 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 |
|---|---|---|
| **Definition** | 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). |
| **Example** | $2^3 = 8$ | $\log_2 8 = 3$ |
| **Interpretation** | 2 raised to the power of 3 equals 8. | The power to which you must raise 2 to get 8 is 3. |
| **Inverse** | The logarithm is the inverse operation of exponentiation. | The exponentiation is the inverse operation of logarithm. |
| **Properties** | $(a^n)^m = a^{n \cdot m}, a^n \cdot a^m = a^{n+m}, \frac{a^n}{a^m} = a^{n-m}$ | $\log_a(b \cdot c) = \log_a b + \log_a c, \log_a\left(\frac{b}{c}\right) = \log_a b - \log_a c, \log_a(b^n) = n \cdot \log_a b$ |

**i** Note

For your understanding, not examinable.

# Common nonlinear functions

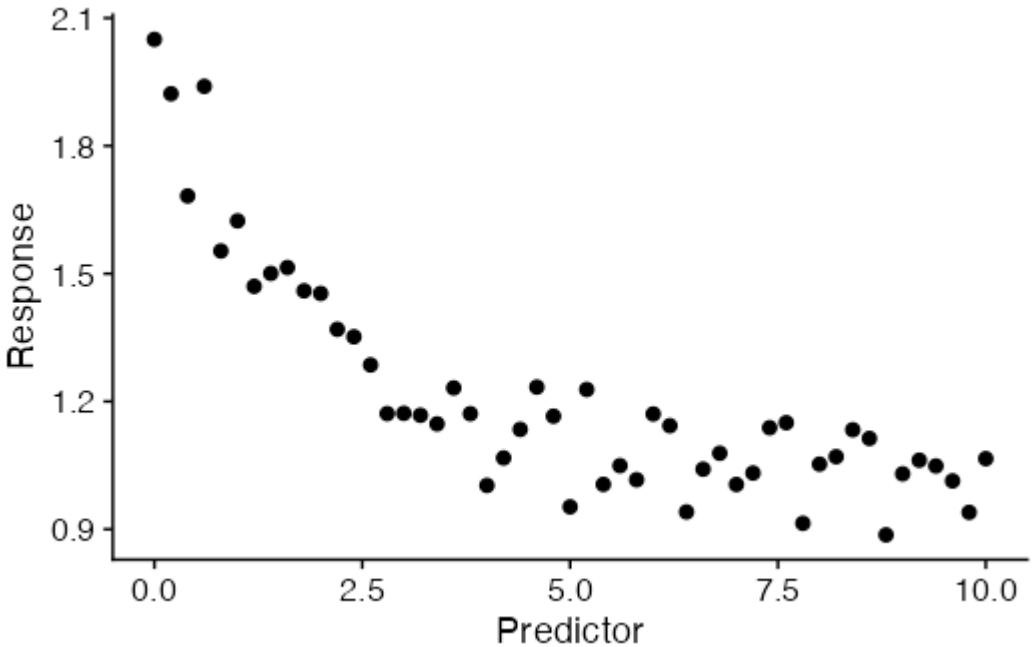
$$f(x_i, \beta)$$

## 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")
```



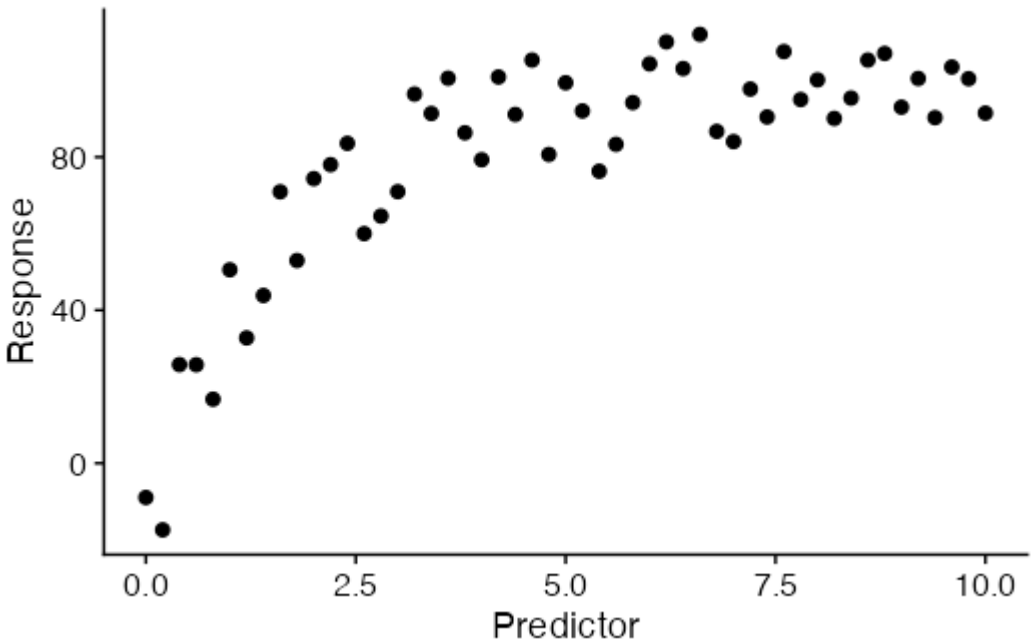

Examples: radioactive decay, population decline, chemical reactions.

## 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")
```



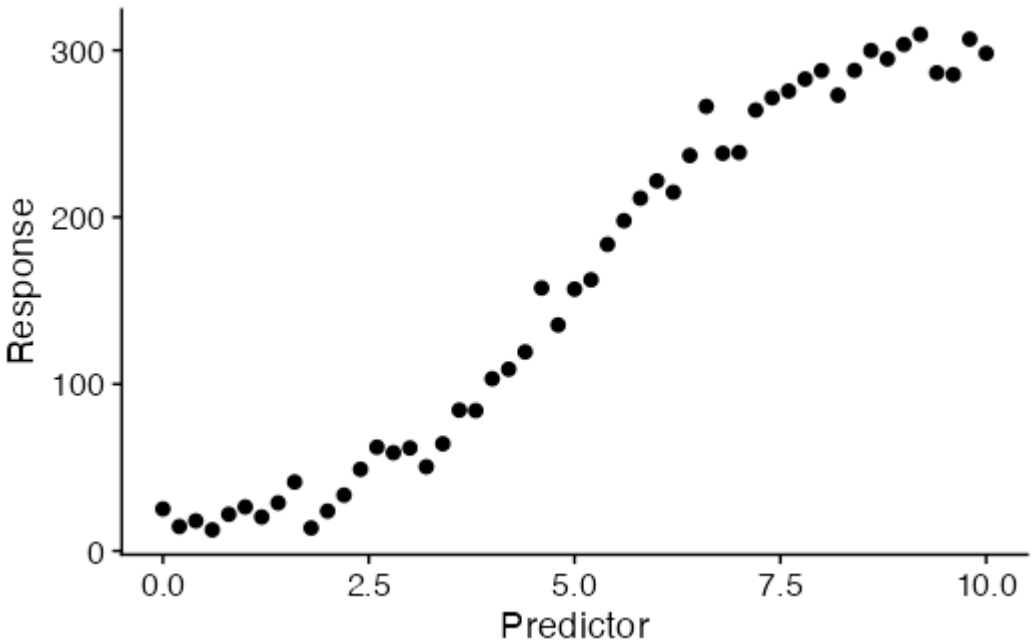

Examples: population growth, enzyme kinetics.

## 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")
```



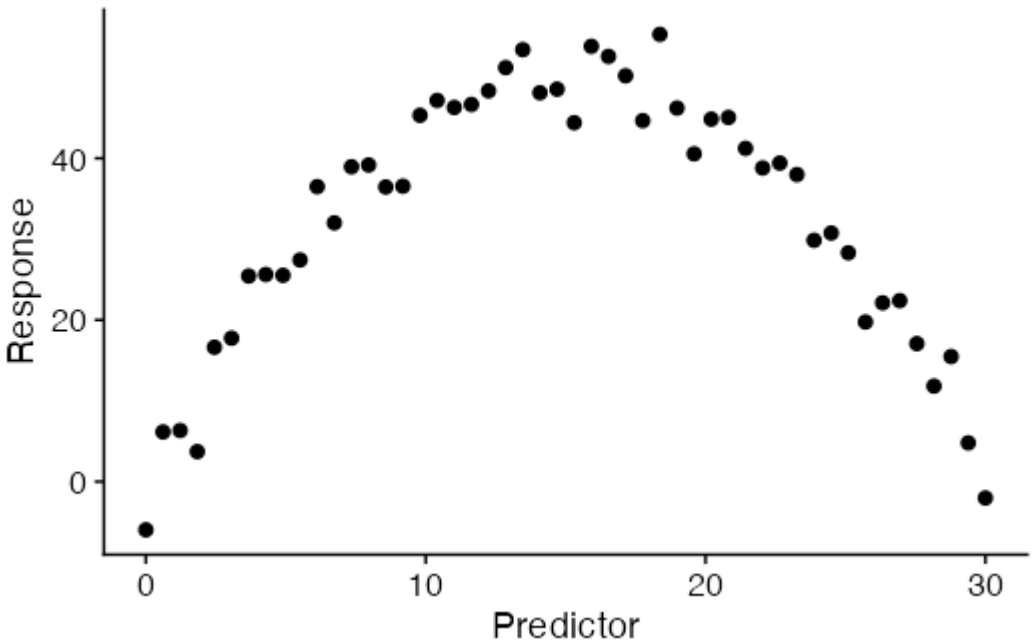

Examples: growth of bacteria, disease spread, species growth.

## Polynomial relationship

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

$$y = a + bx + cx^2 + dx^3 + ...$$

```
# 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?

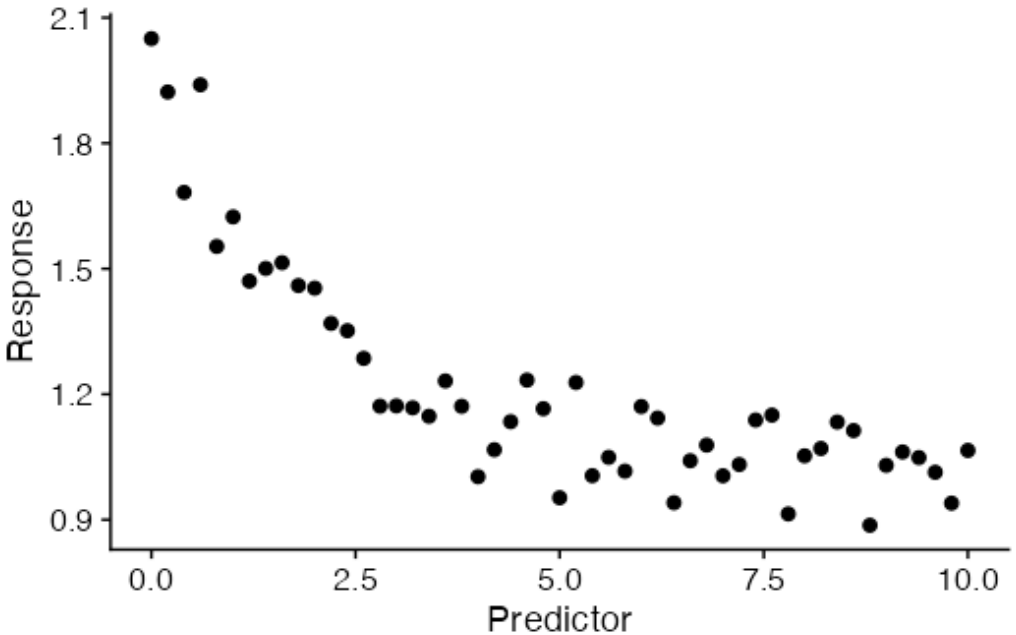
# Transformations: exponential decay

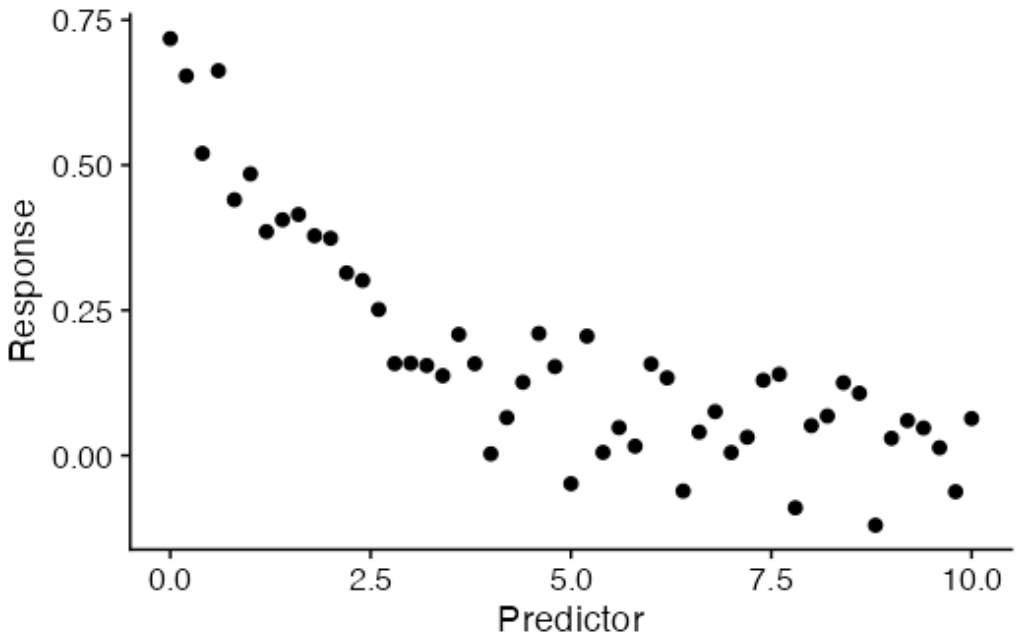
## Before transformation

```
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")
```


2.1
1.8
1.5
1.2
0.9
Response
0.0
2.5
5.0
7.5
10.0
Predictor


0.75
0.50
0.25
0.00
Response
0.0
2.5
5.0
7.5
10.0
Predictor

# Transformations: exponential decay

## Before transformation

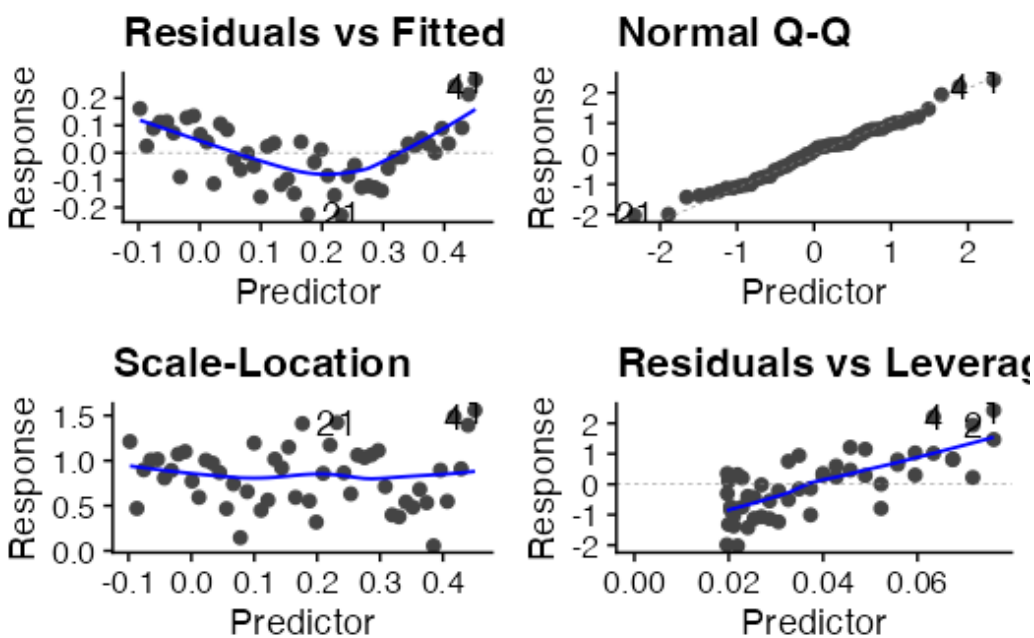
```
autoplot(lm(response ~ predictor, data = decay))
+
  labs(x = "Predictor", y = "Response")
```

```
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.
```

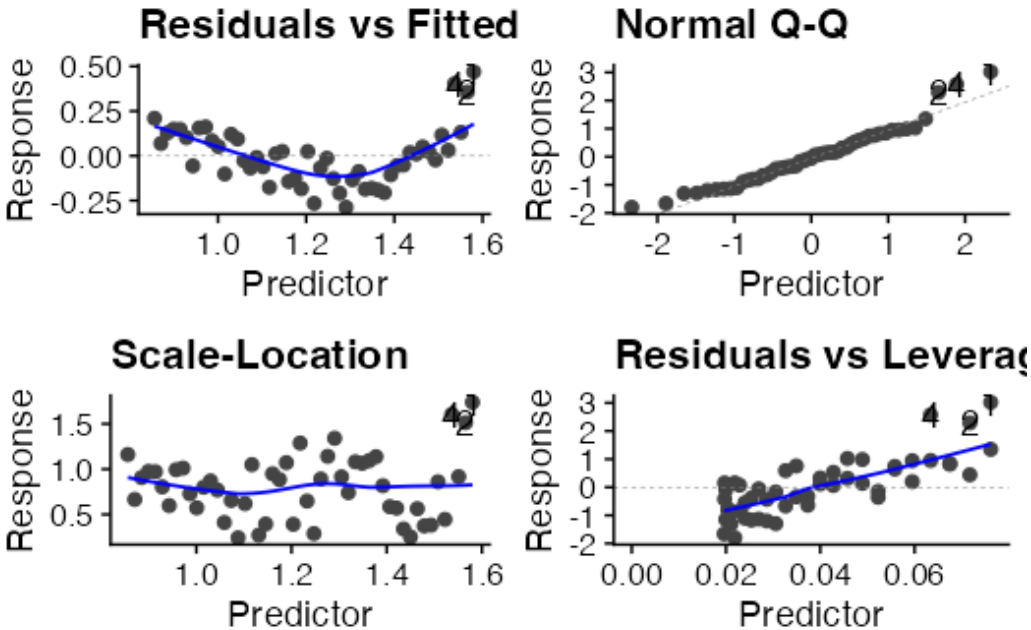
## After $\log_e$ transform

```
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>.
```


Residuals vs Fitted
Response
0.50
0.25
0.00
-0.25
1.0
1.2
1.4
1.6
Predictor
Normal Q-Q
Response
3
2
1
0
-1
-2
-2
-1
0
1
2
Predictor
Scale-Location
Response
1.5
1.0
0.5
1.0
1.2
1.4
1.6
Predictor
Residuals vs Leverag
Response
3
2
1
0
-1
-2
0.00
0.02
0.04
0.06
Predictor

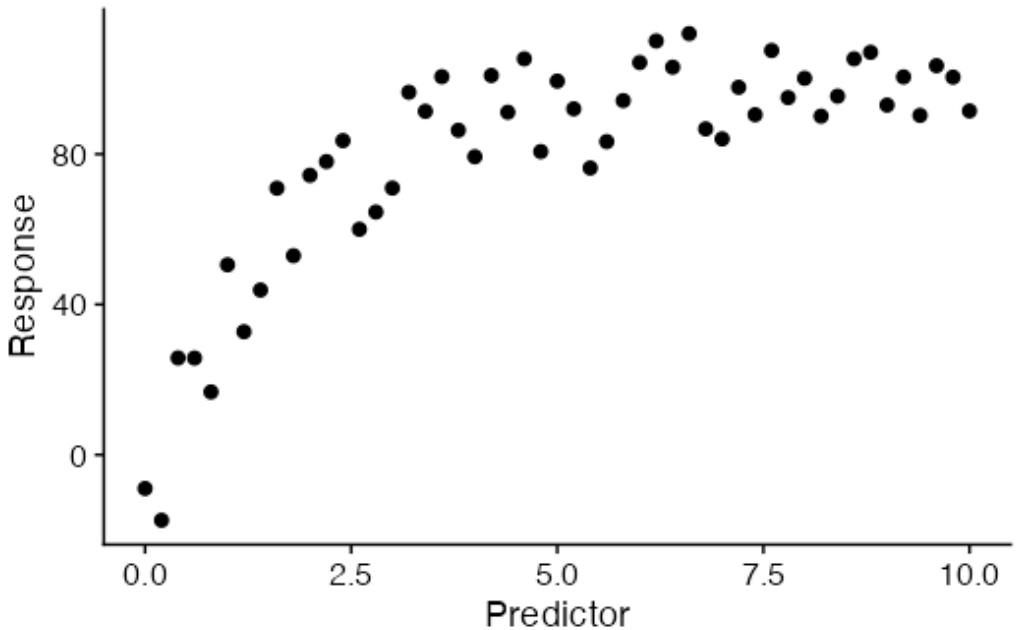
# Transformations: asymptotic relationship

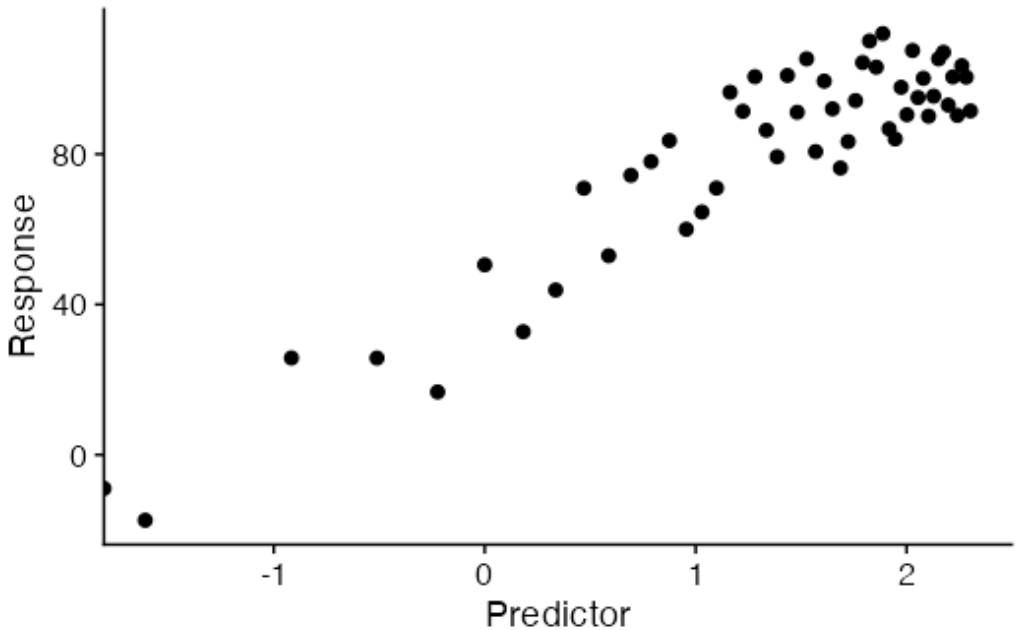
## Before transformation

```
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")
```

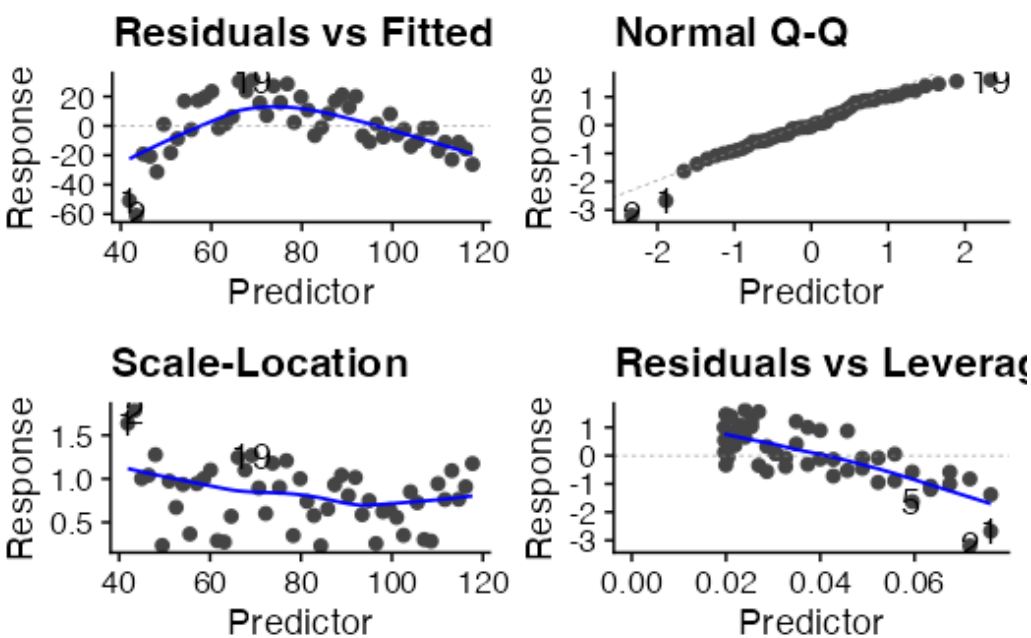

Response
80
40
0
0.0
2.5
5.0
7.5
10.0
Predictor


Response
80
40
0
-1
0
1
2
Predictor

# Transformations: asymptotic relationship

## Before transformation

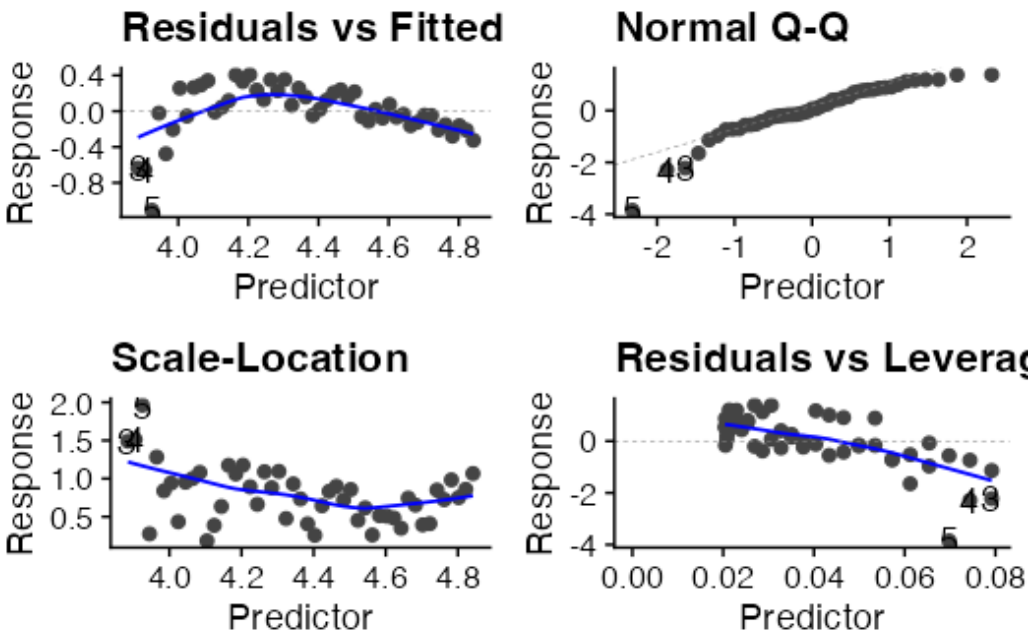
```
autoplot(lm(response ~ predictor, data =
asymptotic)) +
  labs(x = "Predictor", y = "Response")
```




## After $\log_e$ transform

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

```
Warning in log(response): NaNs produced
```


Residuals vs Fitted
Response
Predictor
0.4
0.0
-0.4
-0.8
4.0
4.2
4.4
4.6
4.8
Normal Q-Q
Response
Predictor
0
-2
-4
-2
-1
0
1
2
Scale-Location
Response
Predictor
2.0
1.5
1.0
0.5
4.0
4.2
4.4
4.6
4.8
Residuals vs Leverag
Response
Predictor
0
-2
-4
0.00
0.02
0.04
0.06
0.08

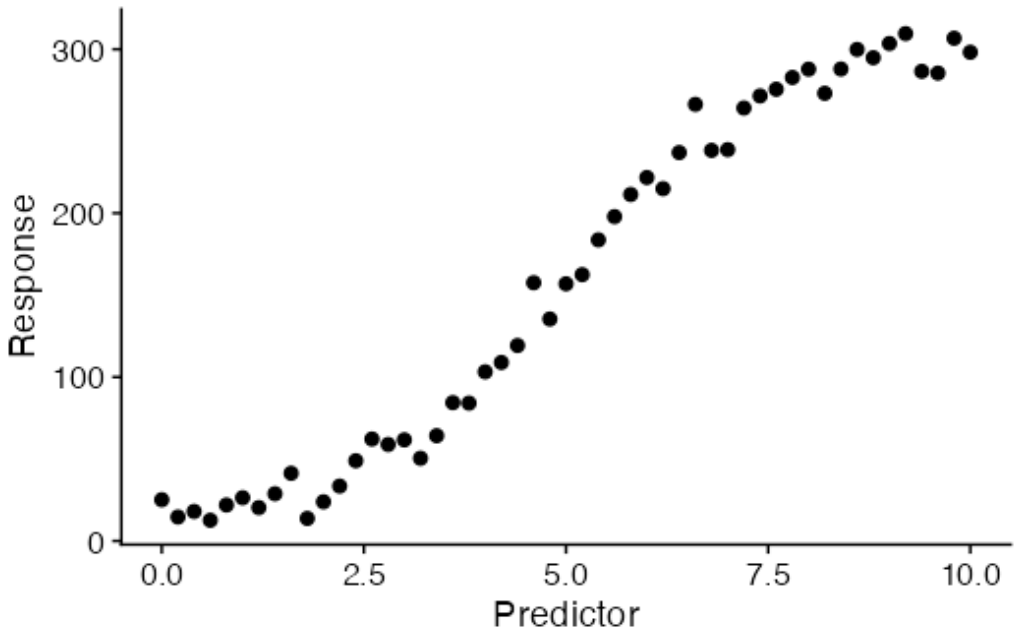
# Transformations: logistic relationship

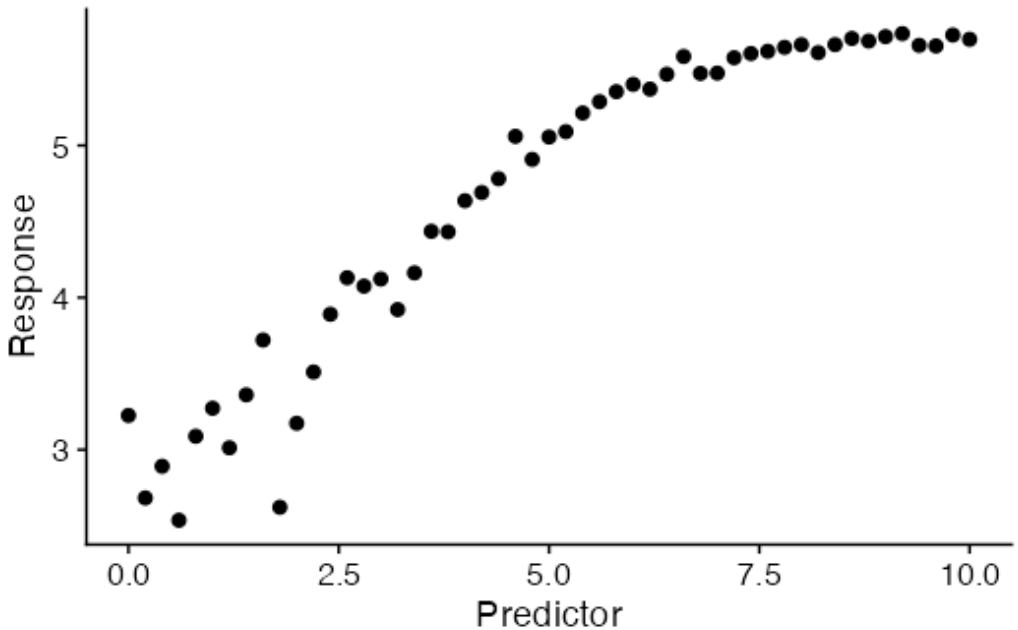
## Before transformation

```
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")
```

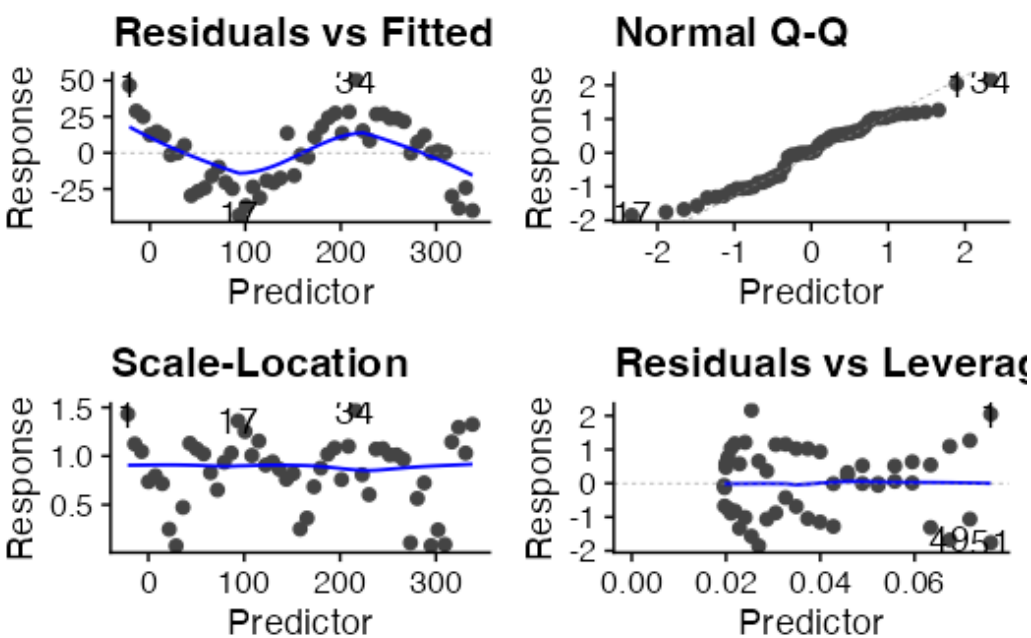

Response
300
200
100
0
0.0
2.5
5.0
7.5
10.0
Predictor


Response
5
4
3
0.0
2.5
5.0
7.5
10.0
Predictor

# Transformations: logistic relationship

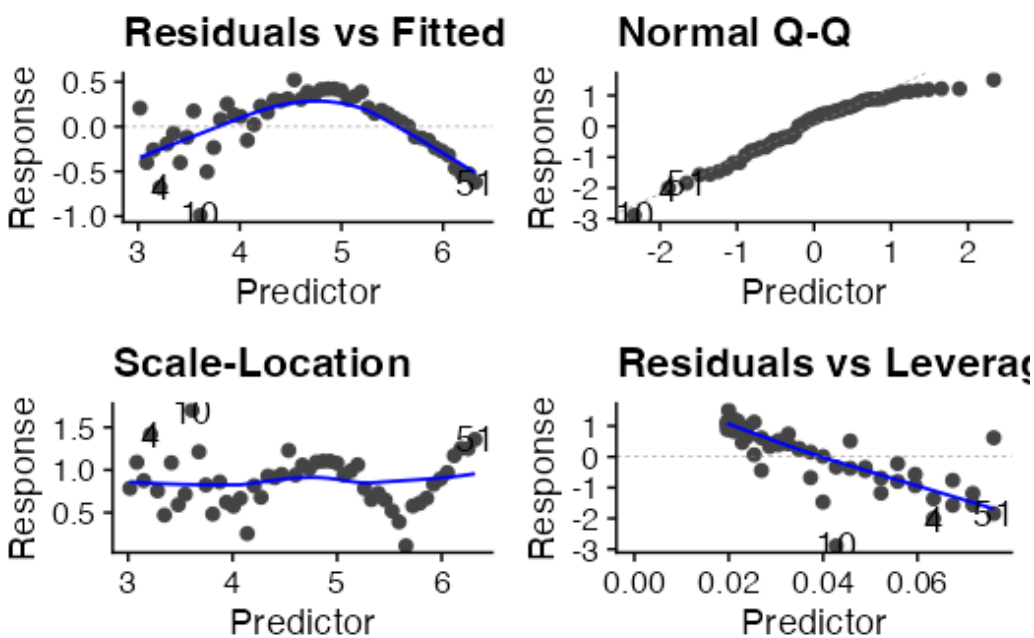
## Before transformation

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




## After $\log_e$ transform

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



# Transformations: polynomial relationship

## Before transformation

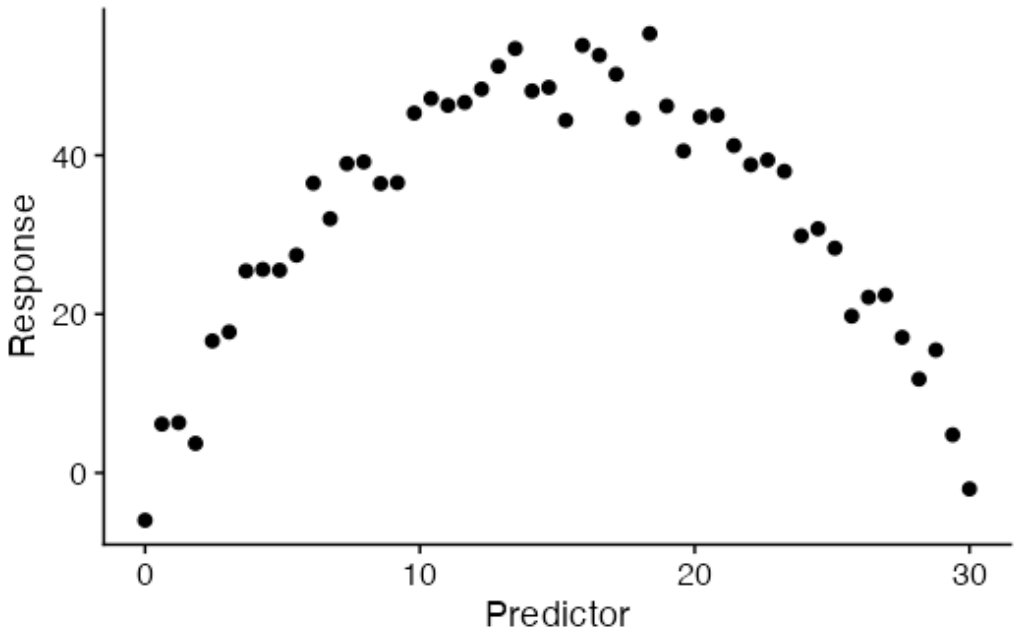
```
ggplot(data = curvilinear,
       aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response")
```

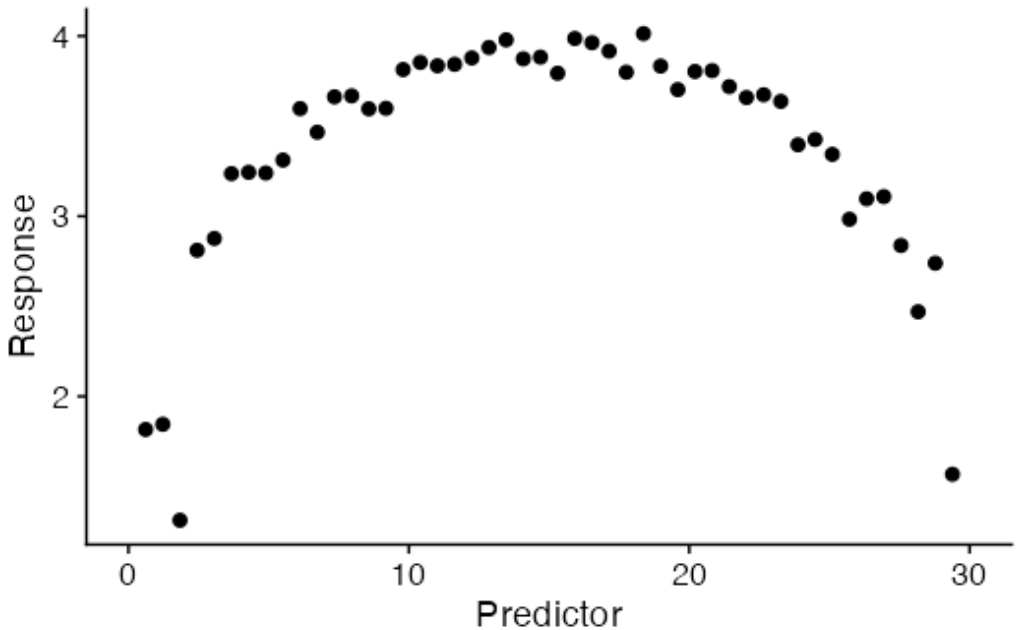
## After $\log_e$ transform

```
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()`).
```

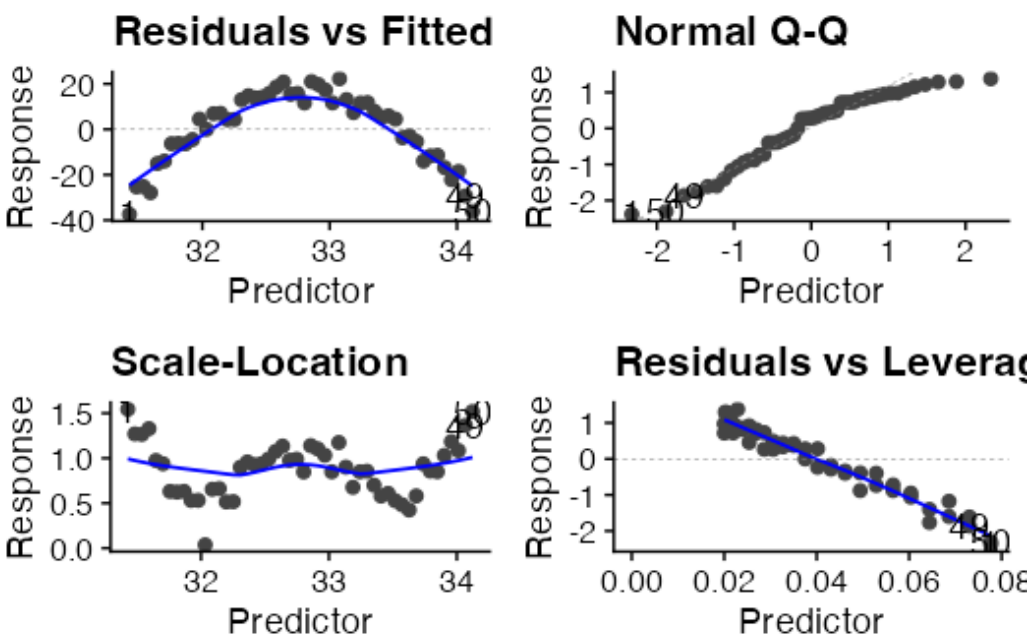

Response
40
20
0
0
10
20
30
Predictor


Response
4
3
2
0
10
20
30
Predictor

# Transformations: polynomial relationship

## Before transformation

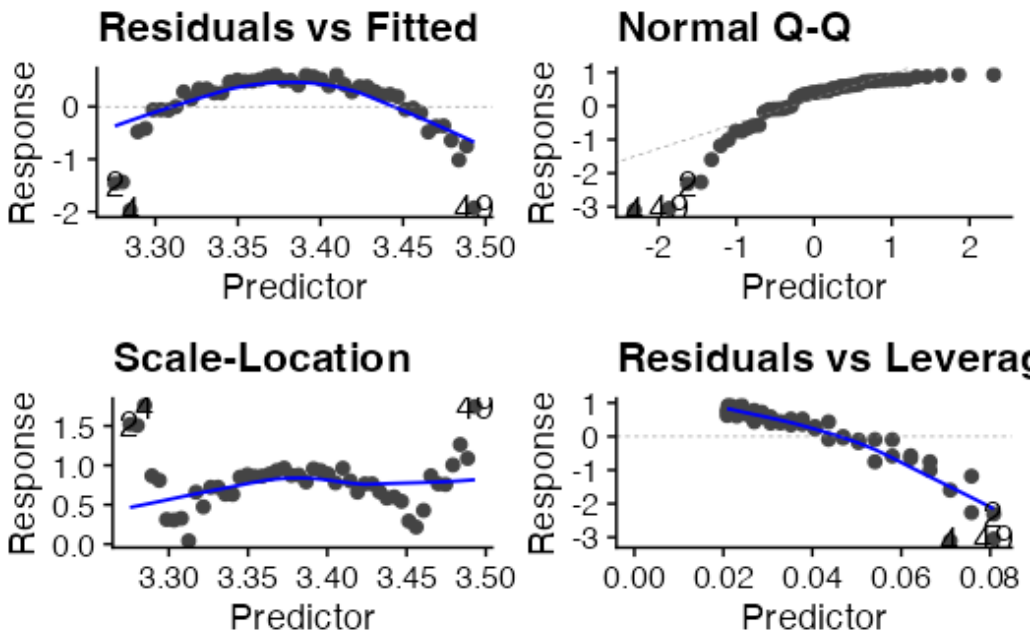
```
autoplot(lm(response ~ predictor, data =
curvilinear)) +
  labs(x = "Predictor", y = "Response")
```




## After $\log_e$ transform

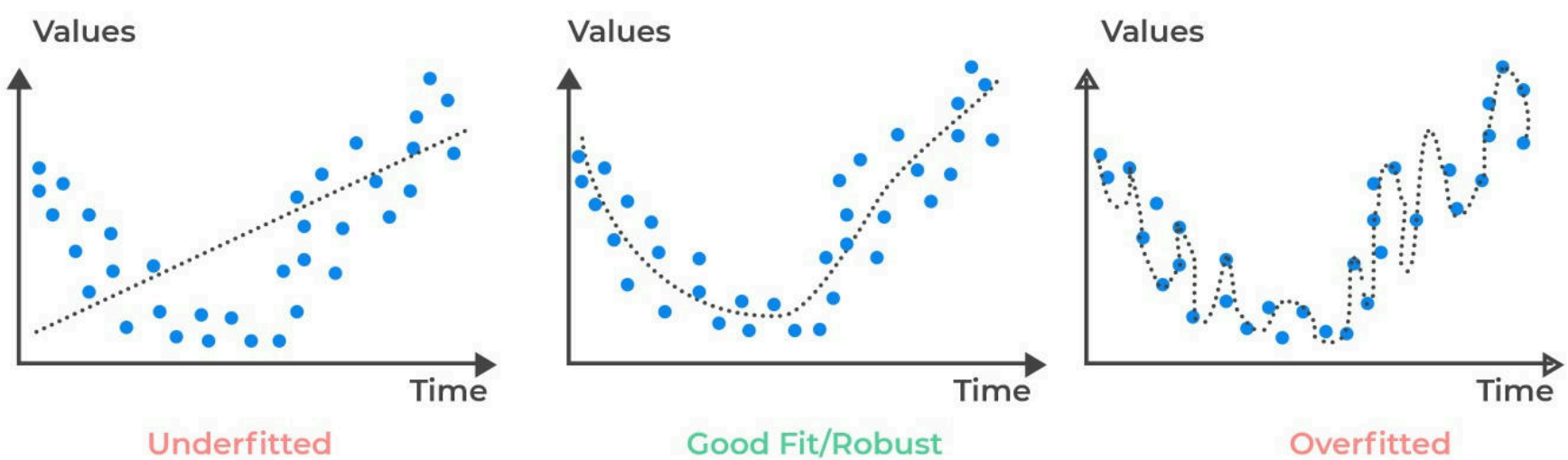
```
autoplot(lm(log(response) ~ predictor, data =
curvilinear)) +
  labs(x = "Predictor", y = "Response")
```

```
Warning in log(response): NaNs produced
```


Residuals vs Fitted
Response
Predictor
3.30 3.35 3.40 3.45 3.50
0
-1
-2
Normal Q-Q
Response
Predictor
-2 -1 0 1 2
1
0
-1
-2
-3
Scale-Location
Response
Predictor
3.30 3.35 3.40 3.45 3.50
1.5
1.0
0.5
0.0
Residuals vs Leverag
Response
Predictor
0.00 0.02 0.04 0.06 0.08
1
0
-1
-2
-3

## 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

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

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.

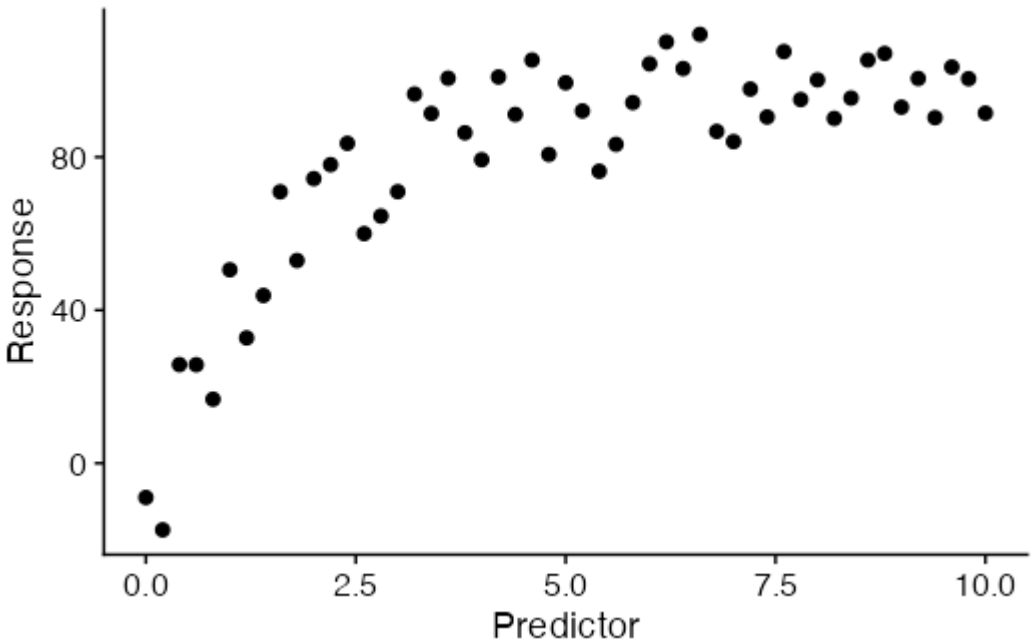
# Polynomial fitting

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")
```

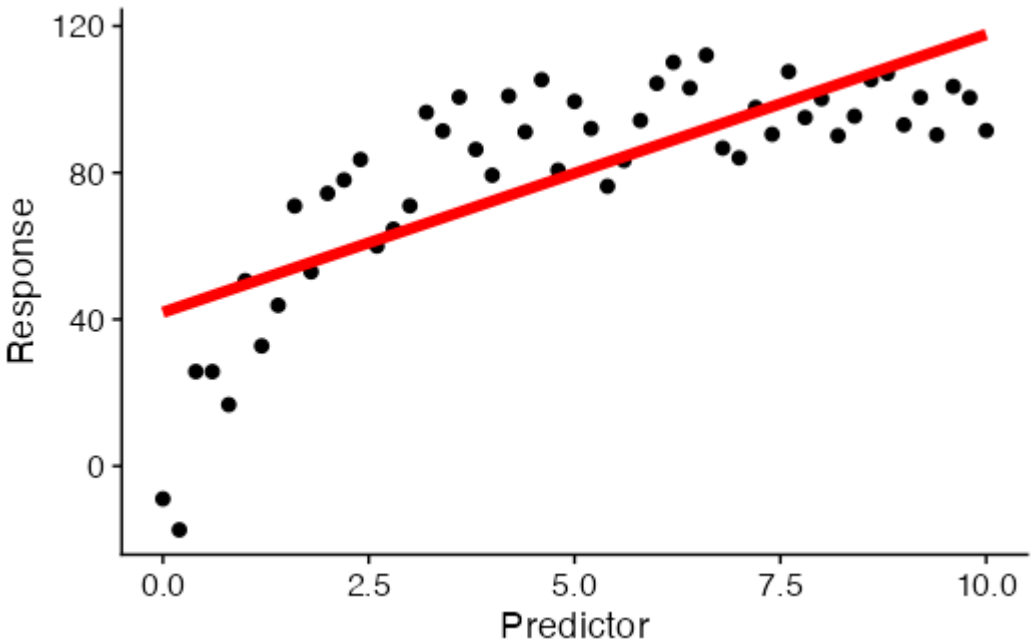

Response
80
40
0
0.0
2.5
5.0
7.5
10.0
Predictor

## 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)
```

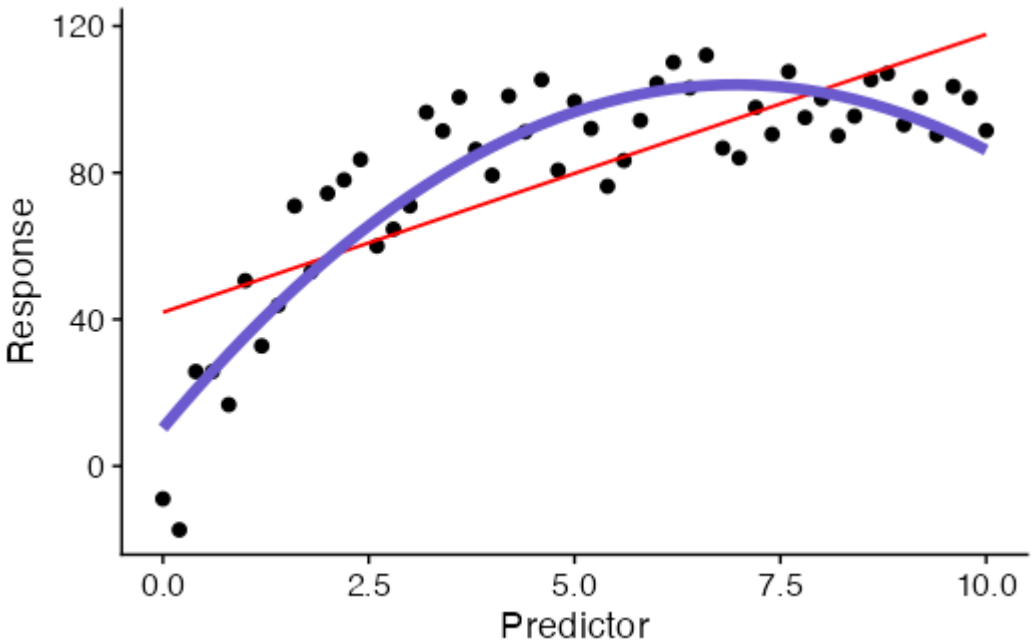

120
80
40
0
Response
0.0
2.5
5.0
7.5
10.0
Predictor

## 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)
```

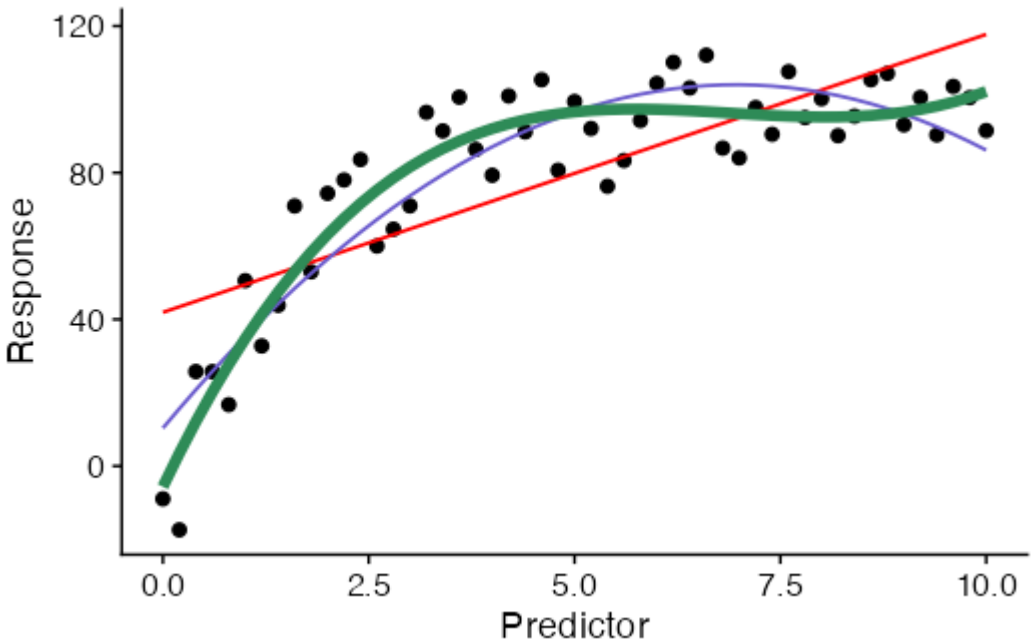

120
80
40
0
Response
0.0
2.5
5.0
7.5
10.0
Predictor

## 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)
```

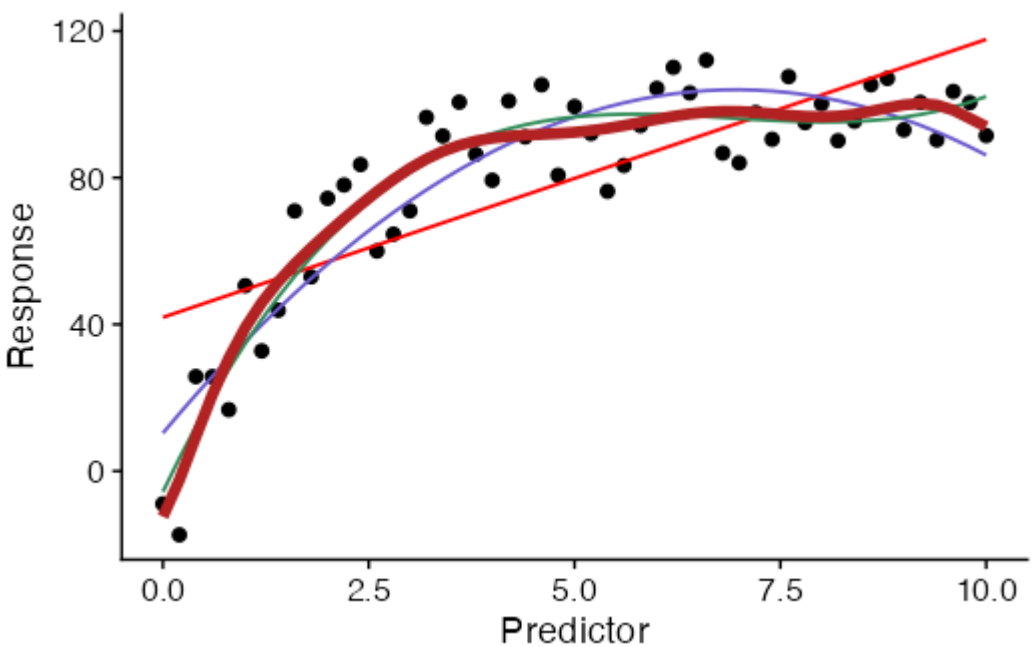
```
ggplot(asymptotic, aes(x = predictor, y = response)) +
  geom_point() +
  labs(x = "Predictor", y = "Response") +
  geom_line(aes(y = predict(lin_fit)), color = "red") +
  geom_line(aes(y = predict(poly2_fit)), color = "slateblue") +
  geom_line(aes(y = predict(poly3_fit)), color = "seagreen", size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


120
80
40
0
Response
0.0
2.5
5.0
7.5
10.0
Predictor

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

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

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



| Model | R2 |
|---|---|
| Linear | 0.570 |
| Poly2 | 0.820 |
| Poly3 | 0.872 |
| Poly10 | 0.862 |

> **Note**
>
> We use adjusted $R^2$ 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:

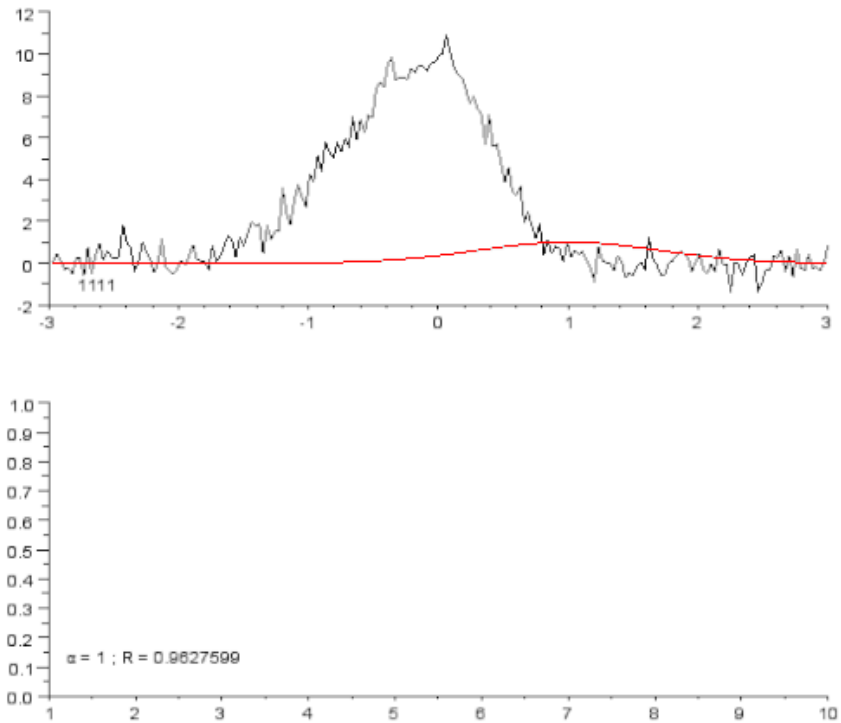
$$\epsilon_i \sim N(0, \sigma^2)$$

. . .

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()`

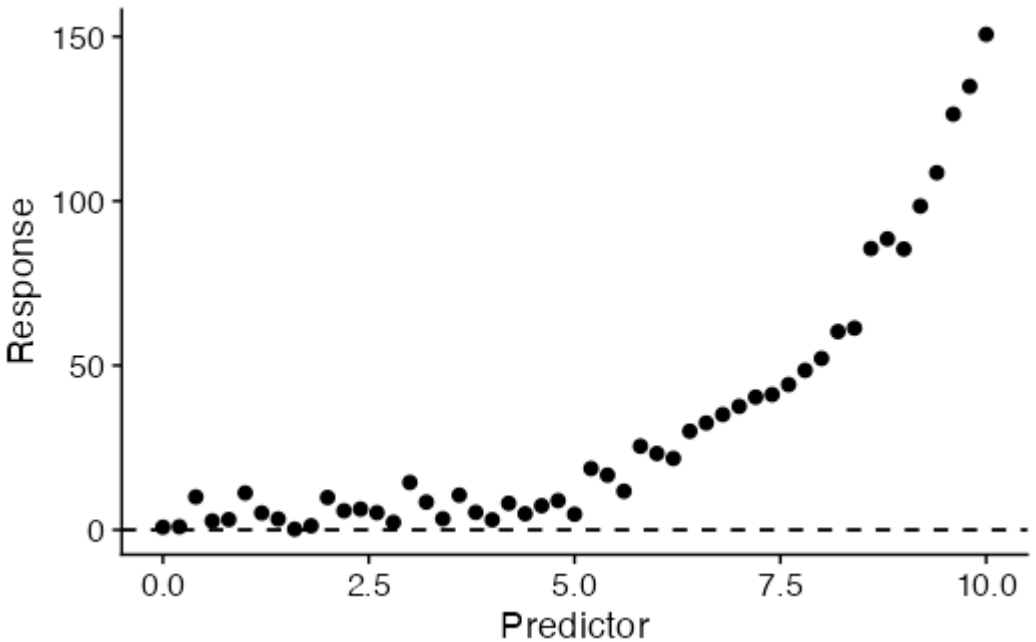
$y = y_0 e^{kx}$

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")
```

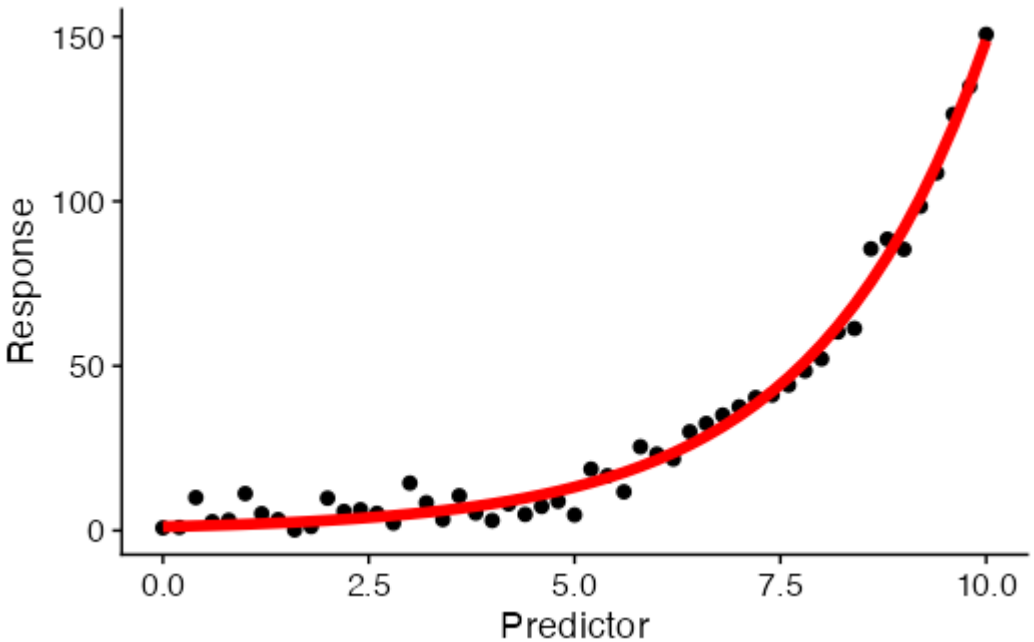

150
100
50
0
Response
0.0
2.5
5.0
7.5
10.0
Predictor

## First guess

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

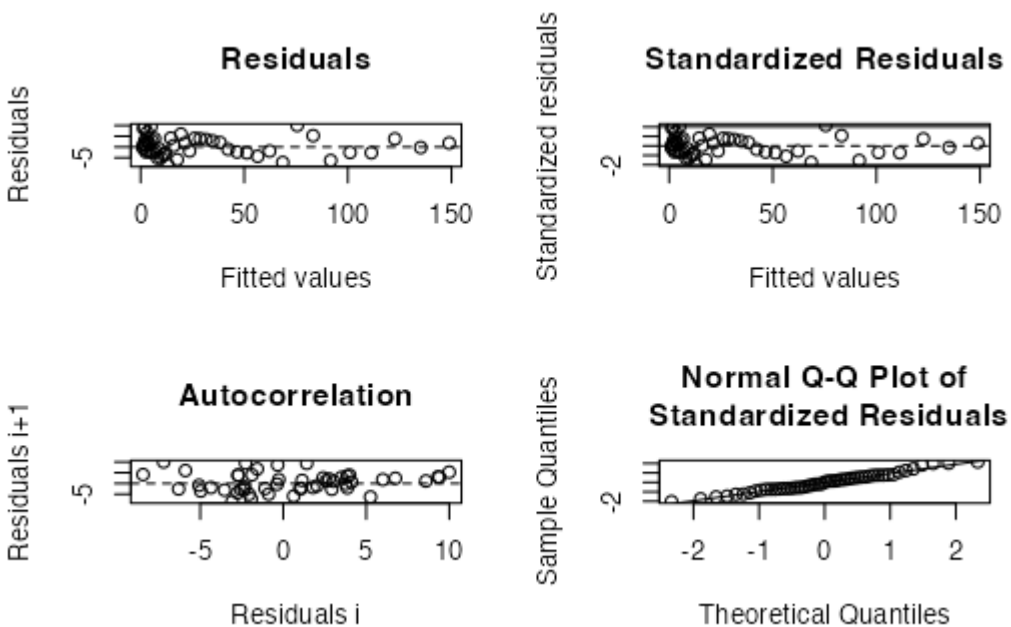
```
fit_exponential ← nls(response ~ y0*exp(k*predictor), data = growth,
  start = list(y0 = 0.1, k = 1))
```

```
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)
```


150
100
50
0
Response
0.0
2.5
5.0
7.5
10.0
Predictor

# 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 `nlraa` 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(nlraa)
```

```

Attaching package: 'nlraa'
```

```
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:

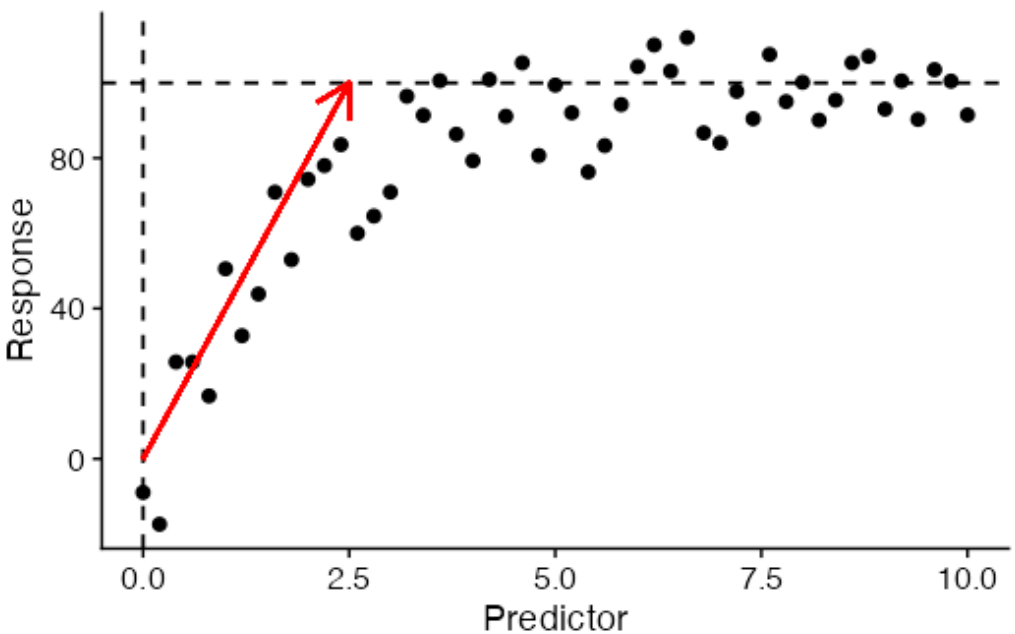
$$y = Asym + (R_0 - Asym) \cdot e^{-e^{lrc} \cdot x}$$

- $R_0$ 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.
```

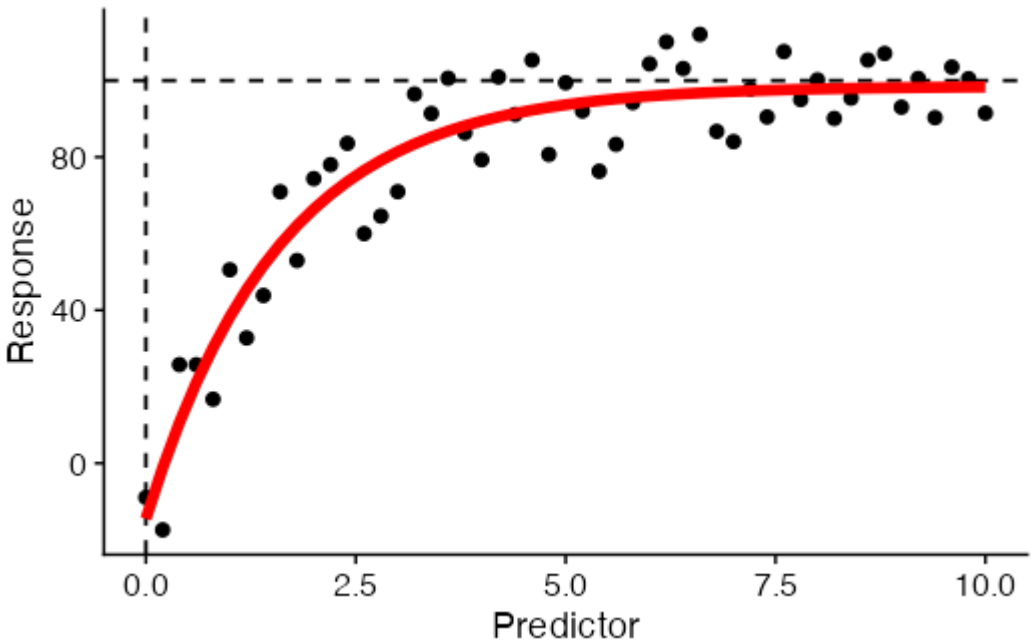



Some plausible estimates – $R_0 = 0, Asym = 100, lrc = 0.8$.

## Fit model

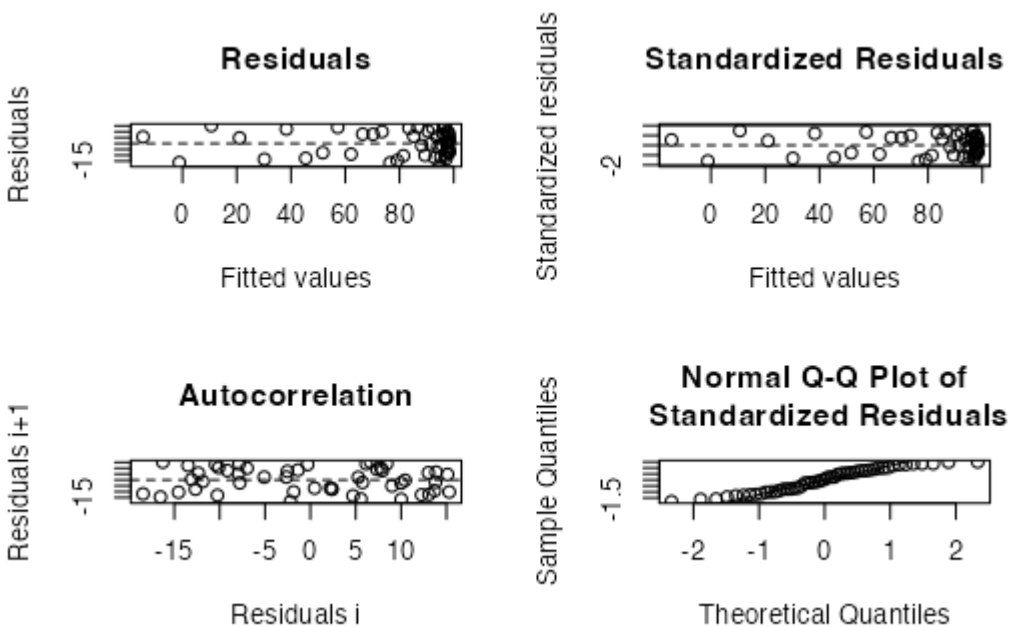
```
# fit_asymptotic ← nls(response ~ Asym + (R0-Asym)*(exp(-exp(lrc)*predictor)), data = asymptotic,
#   start = list(R0 = 0, Asym = 100, lrc = 0.8))

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)
```


Response
80
40
0
0.0
2.5
5.0
7.5
10.0
Predictor

# 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:

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

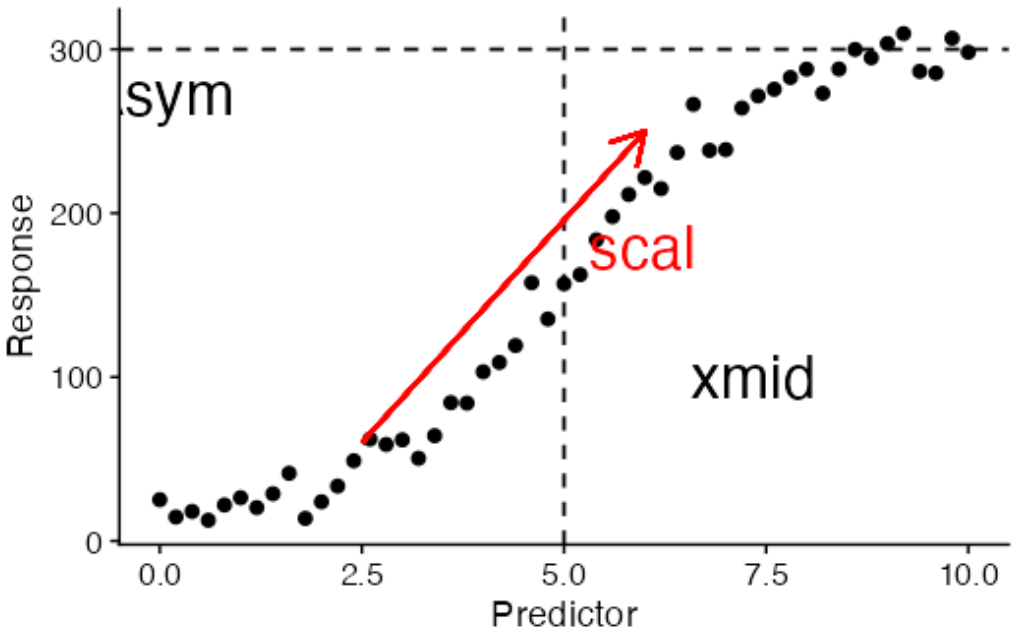
where

- $Asym$ 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.
```

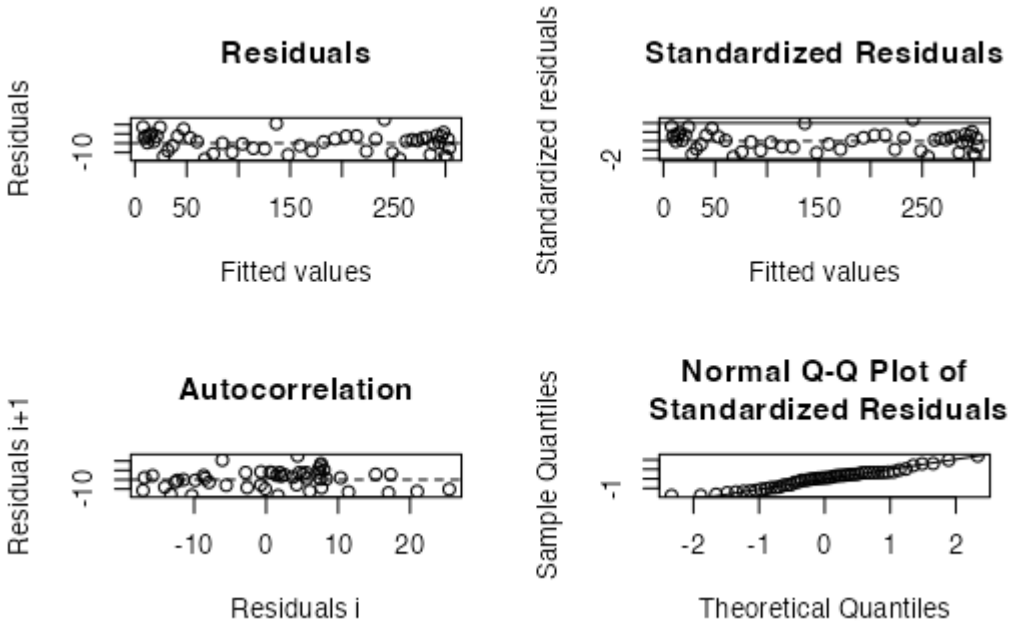



Some starting values would be $Asym = 300$, $xmid = 5$, $scal = 1$.

## 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
Residuals
-10
0
50
150
250
Fitted values
Standardized Residuals
Standardized residuals
-2
0
50
150
250
Fitted values
Autocorrelation
Residuals i+1
-10
-10
0
10
20
Residuals i
Normal Q-Q Plot of
Standardized Residuals
Sample Quantiles
-1
-2
-1
0
1
2
Theoretical 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:

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

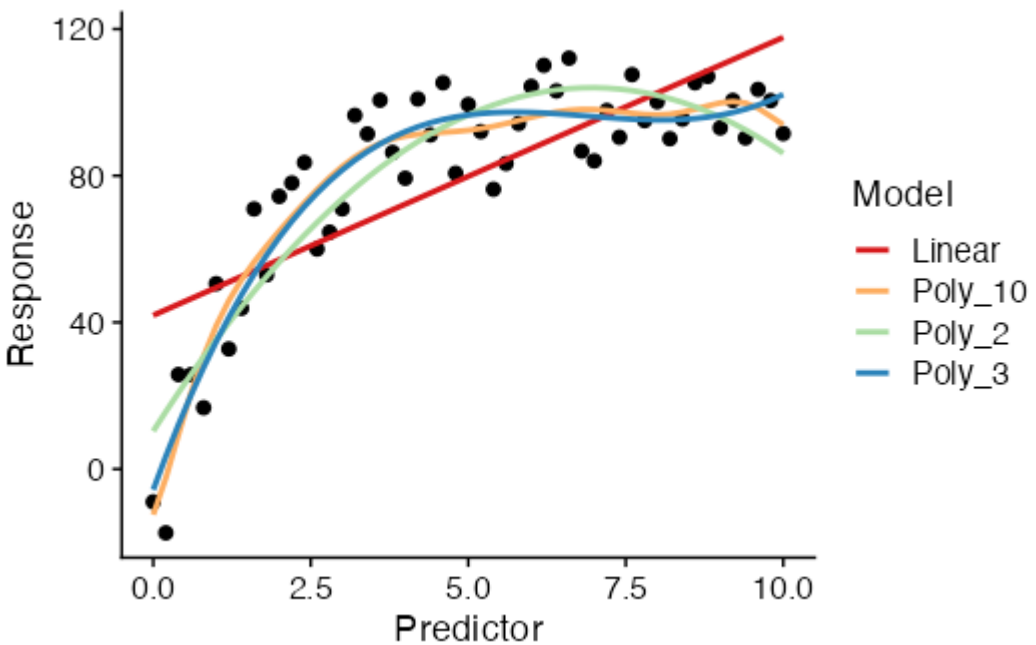
# How do we know which model is better? (Advanced)

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 parsimonius.
- We can say the model has a prediction error of 10.25 units (RMSE) and 8.83 units (MAE).

> **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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