Topic 12 – Non-linear regression

ENVX1002 Introduction to Statistical Methods

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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 β: "How do we model a change in y with x wl
relationship is nonlinear?"

Nonlinear regression

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

Non-linear 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 $\boldsymbol{y}$ changes monotically with $\boldsymbol{x}$.
- 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 y increases, x increases at a rate that is equal to x to the power of a.

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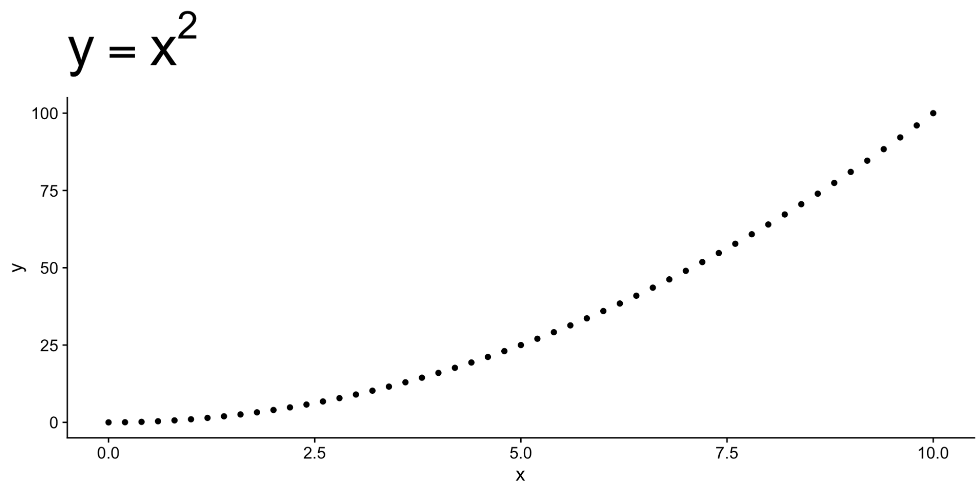

Nonlinear relationships: logarithms

- $log_e(x)$ 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, y increases at a rate of $y = a^x$.
- If $y = \log_a(x)$: as y increases, x also increases, at $x = a^y$.

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	$(a^n)^m = a^{n \cdot m}$, $a^n \cdot a^m = a^{n+m}$, $\frac{a^n}{a^m} = a^{n-m}$	$\log_a(b \cdot c) = \log_a b + \log_a c$, $\log_a\left(\frac{b}{c}\right) = \log_a b - \log_a c$, $\log_a(b^n) = n \cdot \log_a b$

> **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.

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

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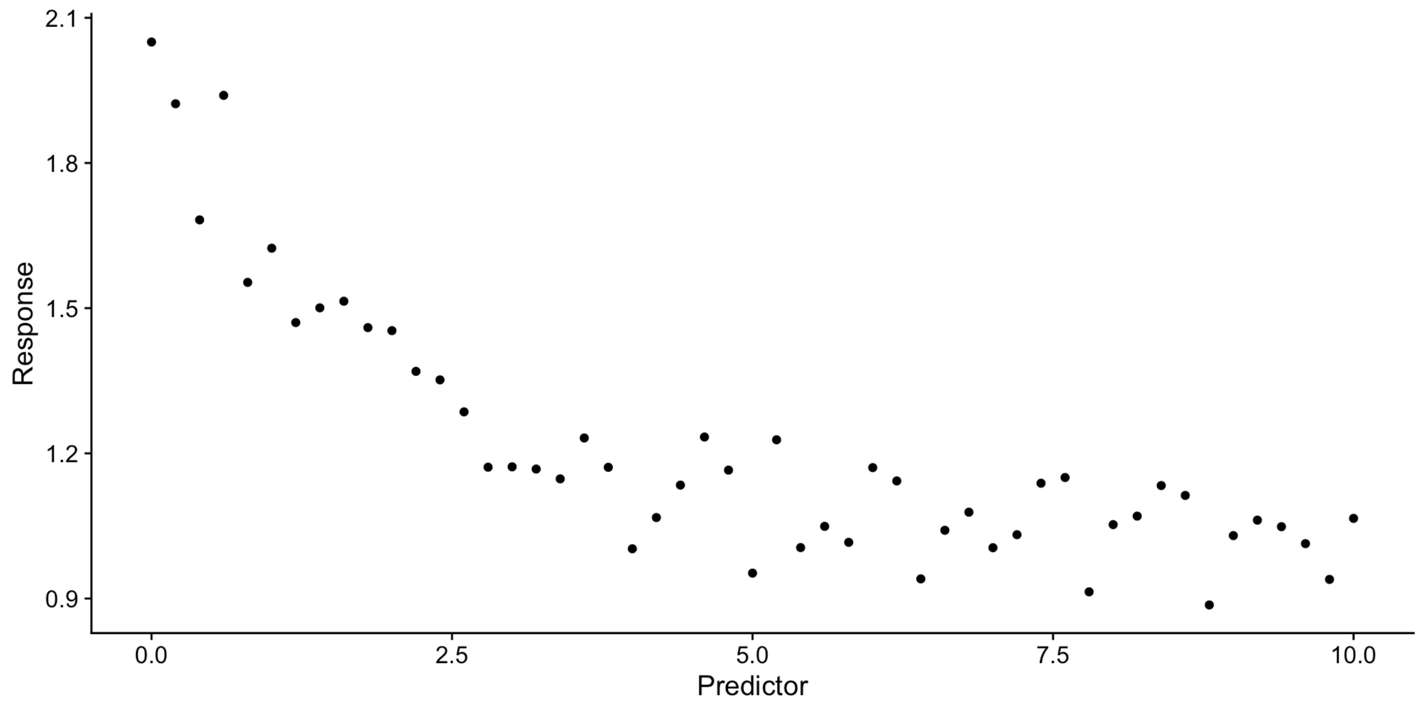

Examples: radioactive decay, population decline, chemical reactions.

Asymptotic relationship

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

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

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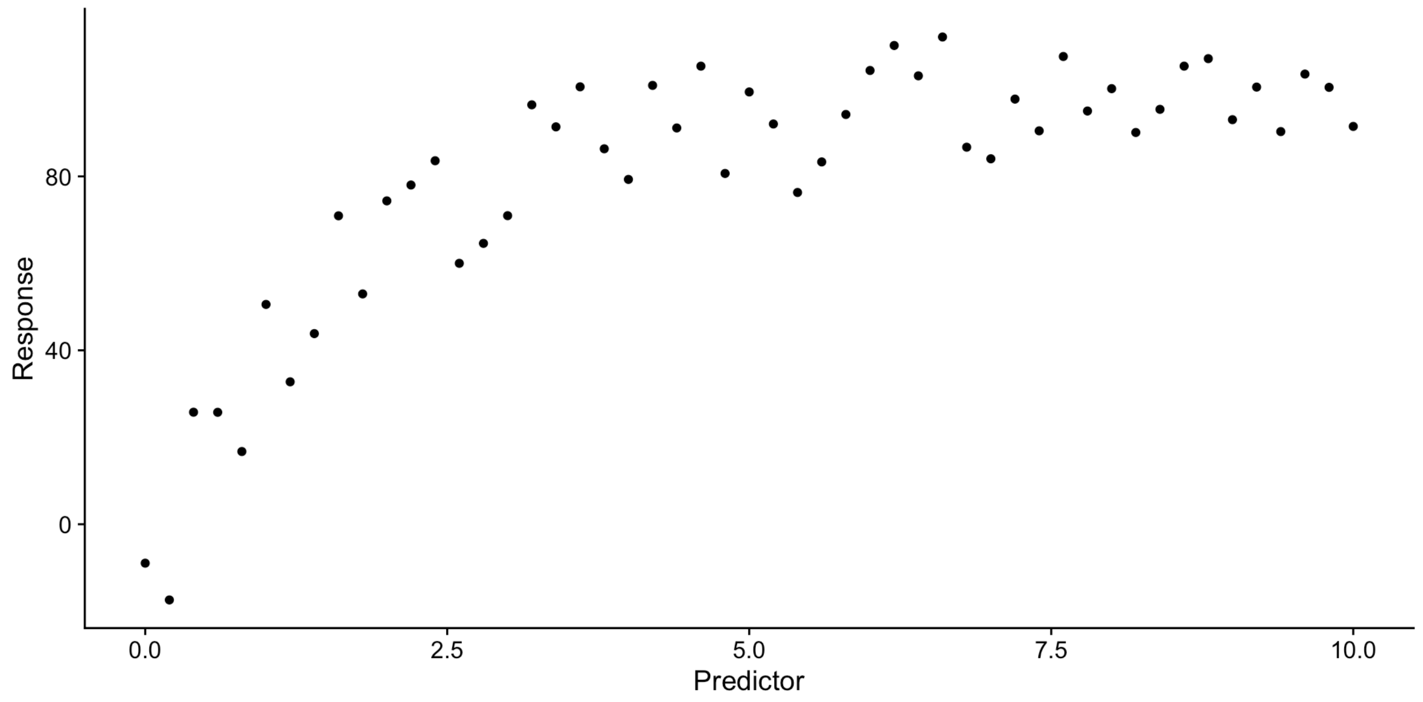

Examples: population growth, enzyme kinetics.

Logistic relationship

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

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

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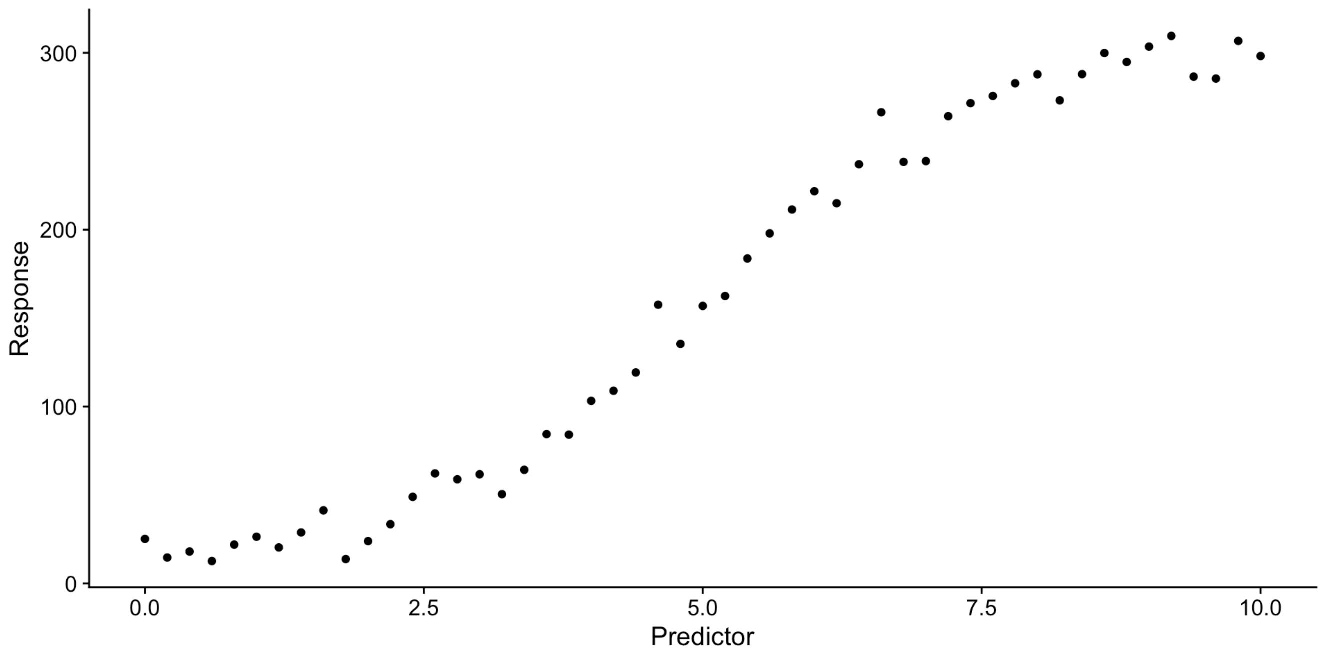

Examples: growth of bacteria, disease spread, species growth.

Polynomial relationship

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

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

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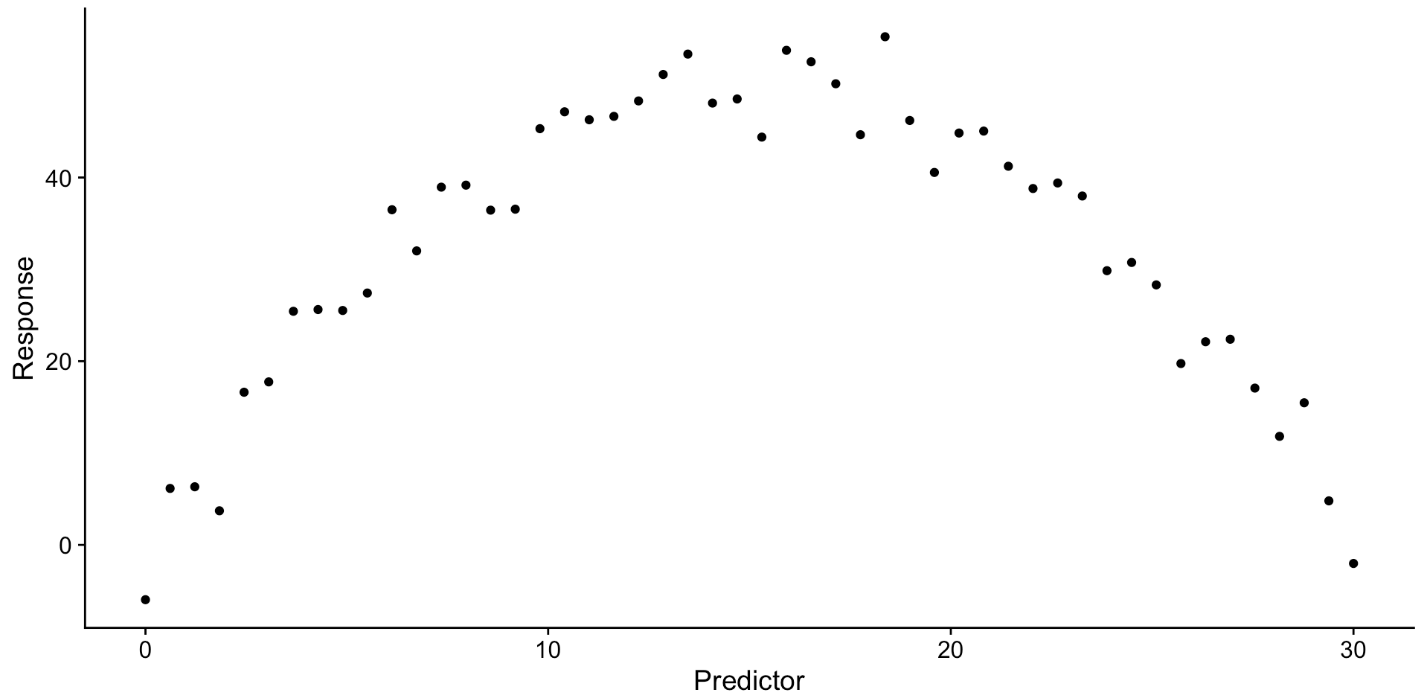

Examples: food intake, drug dosage, exercise.

Transformations

> How far can we go?

Transformations: exponential decay

Before transformation

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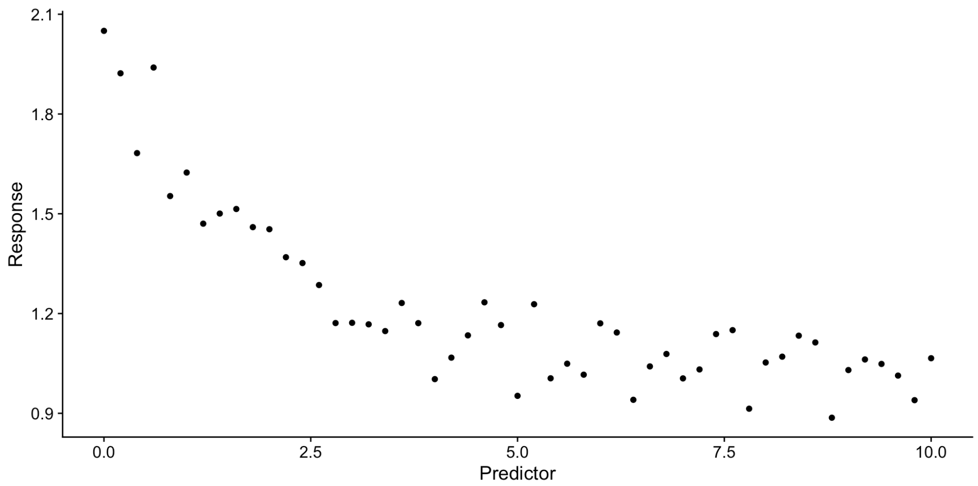
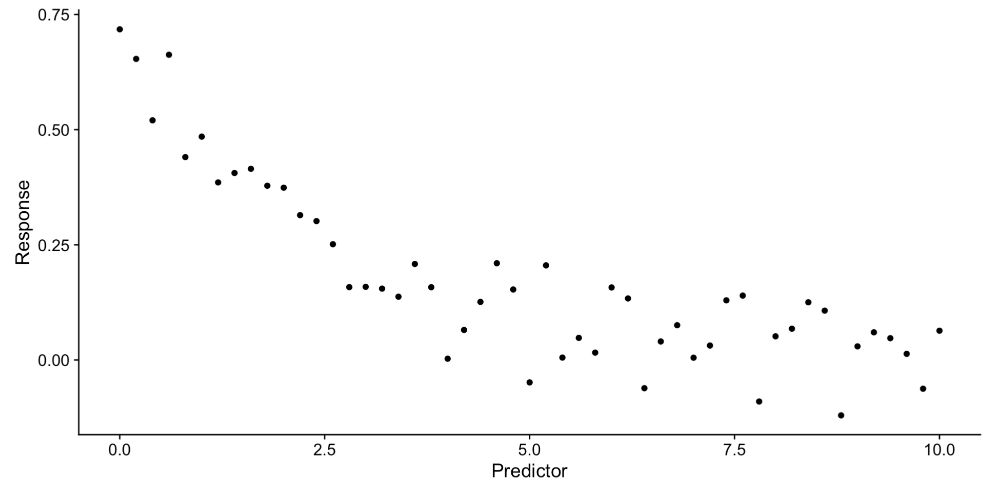


After $\log_e$ transform

▶ Code



Transformations: exponential decay

Before transformation

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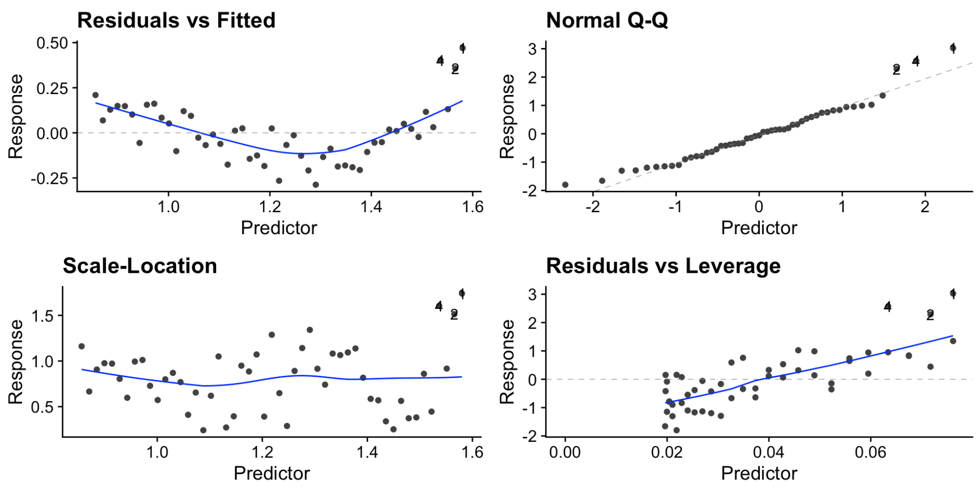

After $\log_e$ transform

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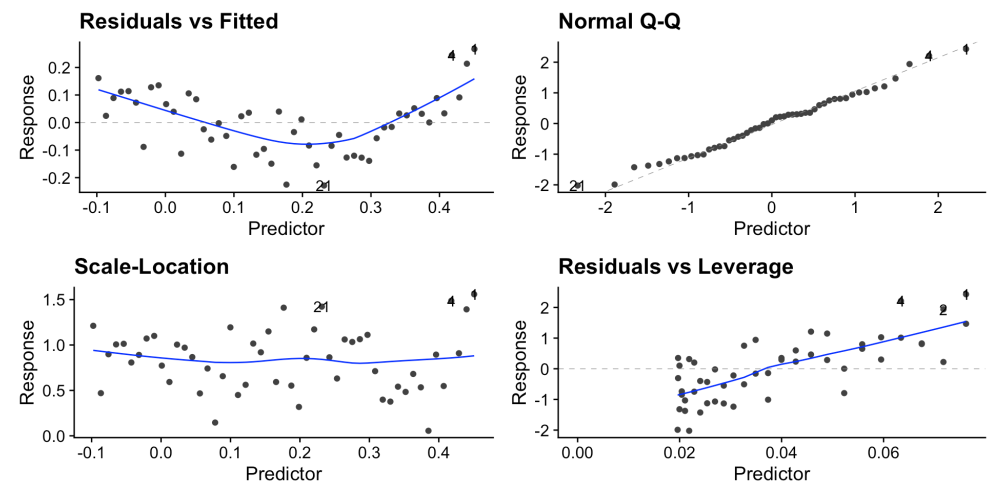
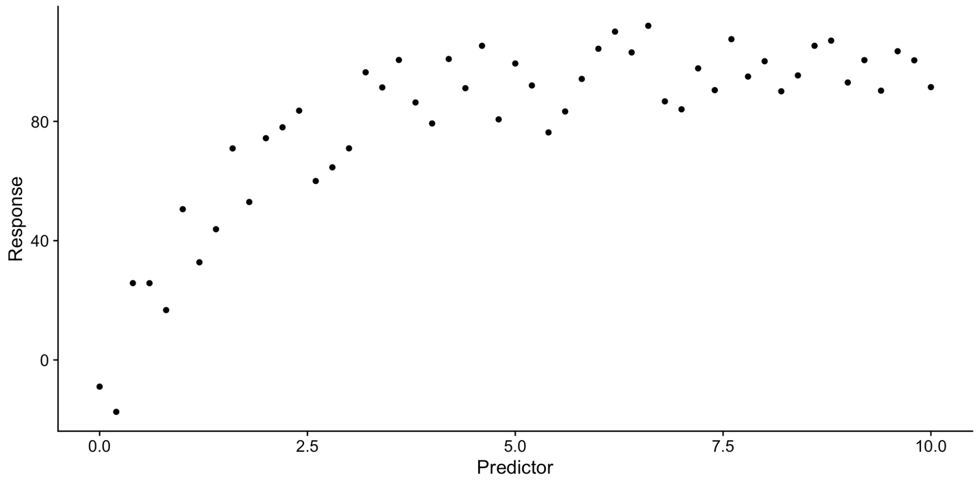


Transformations: asymptotic relationship

Before transformation

▶ Code



After $\log_e$ transform

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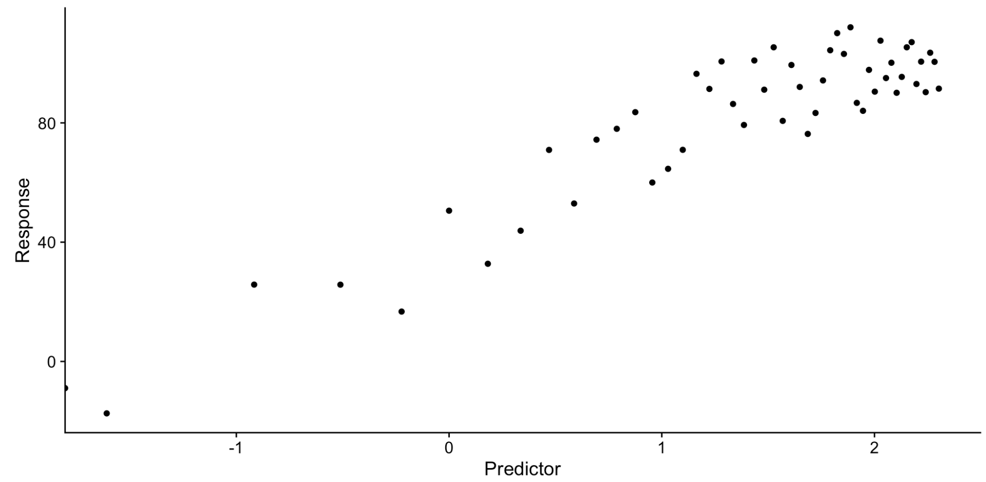

Transformations: asymptotic relationship

Before transformation

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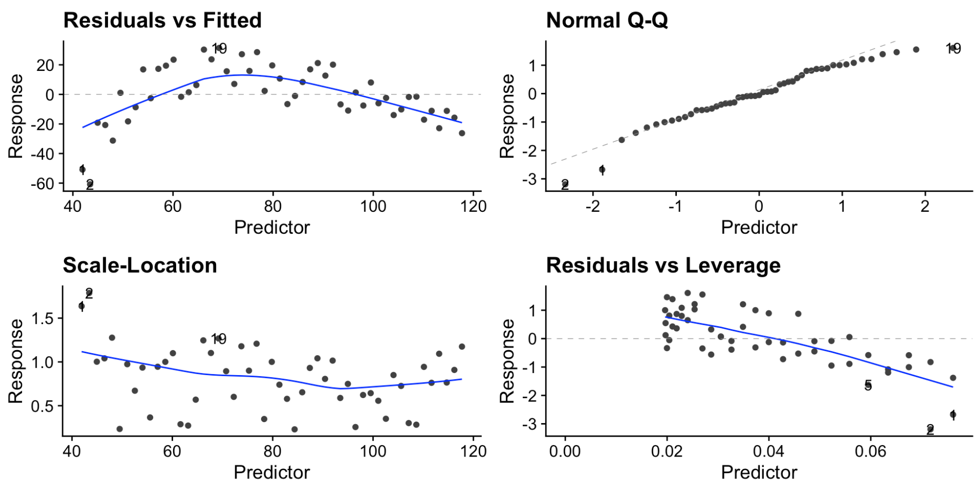

After $\log_e$ transform

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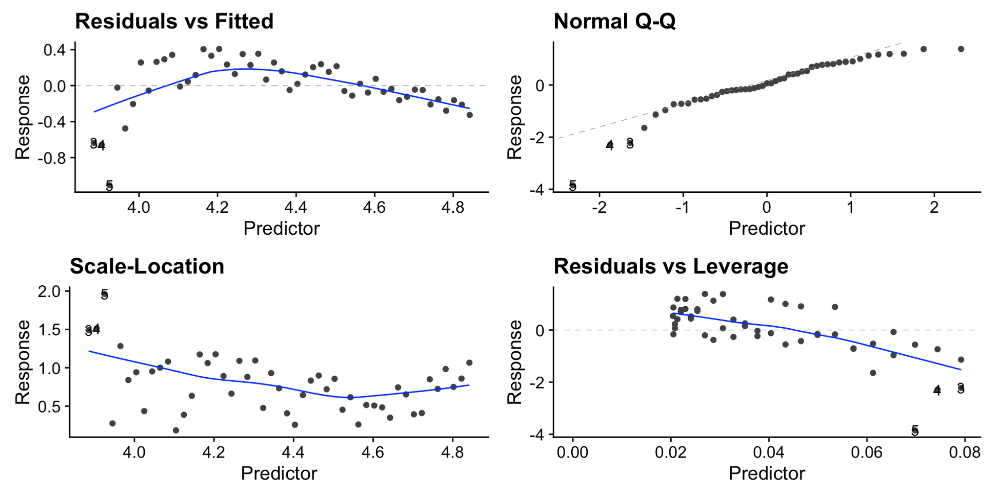
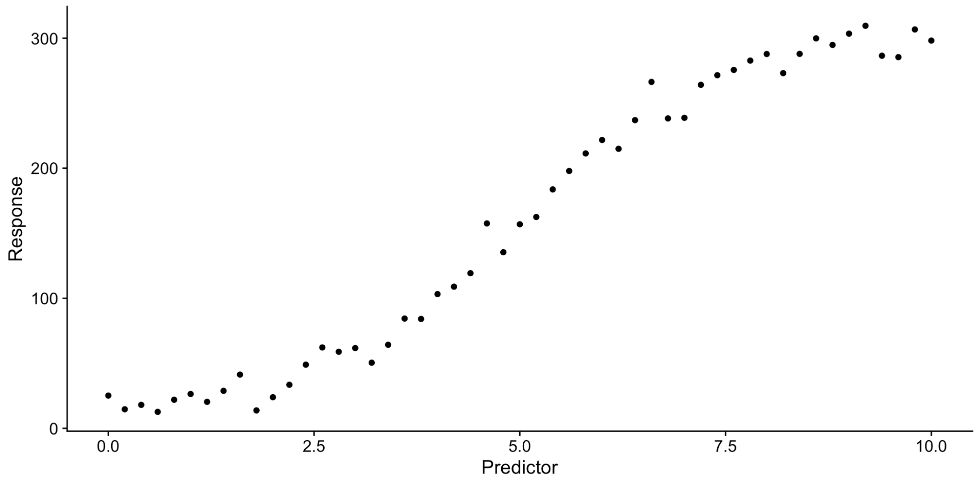


Transformations: logistic relationship

Before transformation

▶ Code



After $\log_e$ transform

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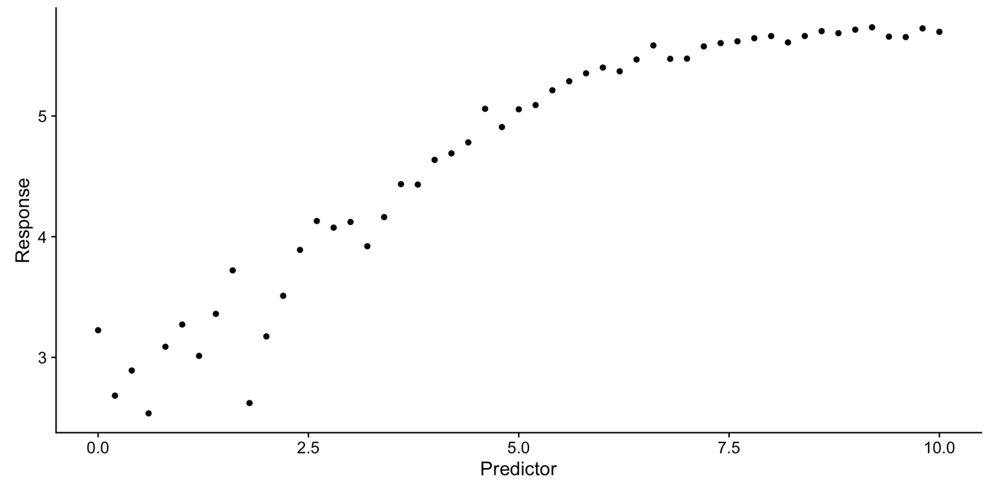

Transformations: logistic relationship

Before transformation

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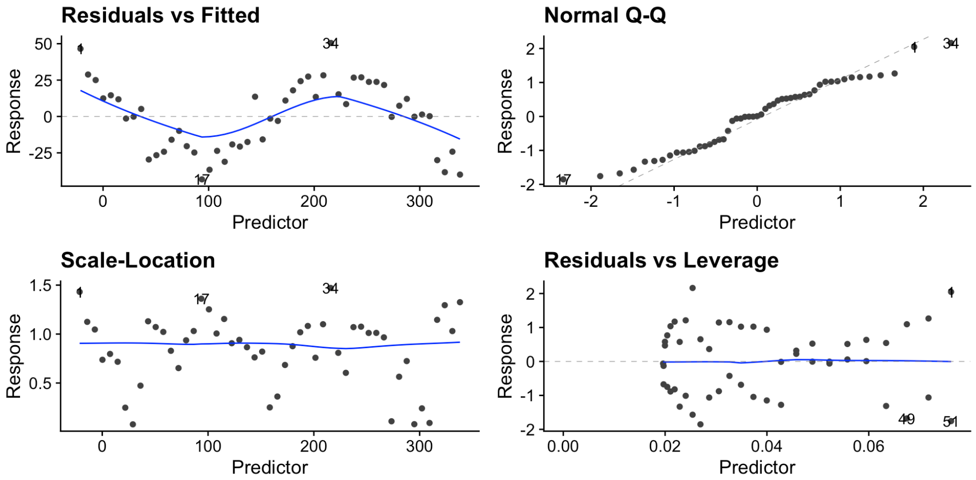

After $\log_e$ transform

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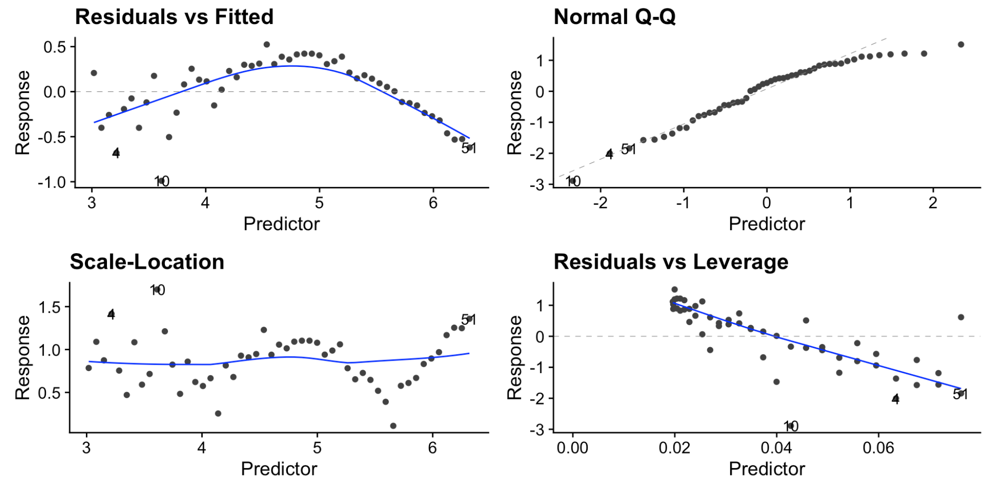
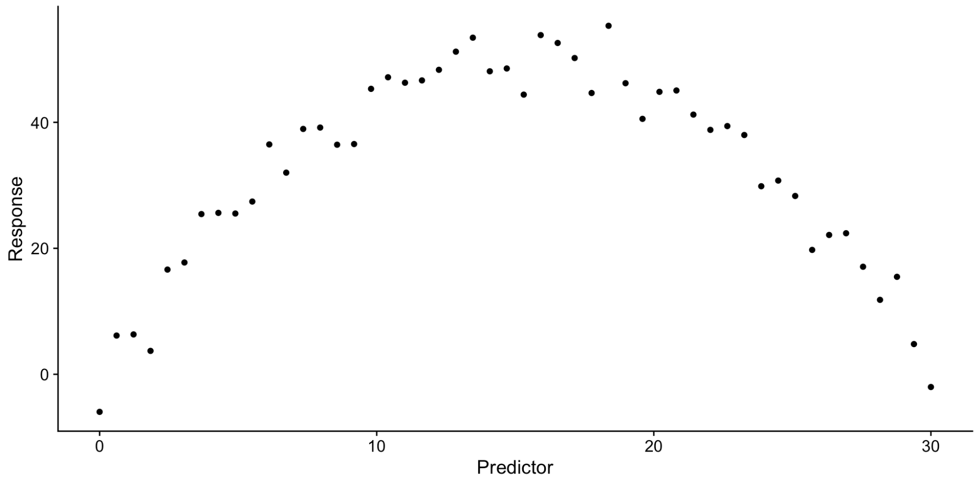


Transformations: polynomial relationship

Before transformation

▶ Code



After $\log_e$ transform

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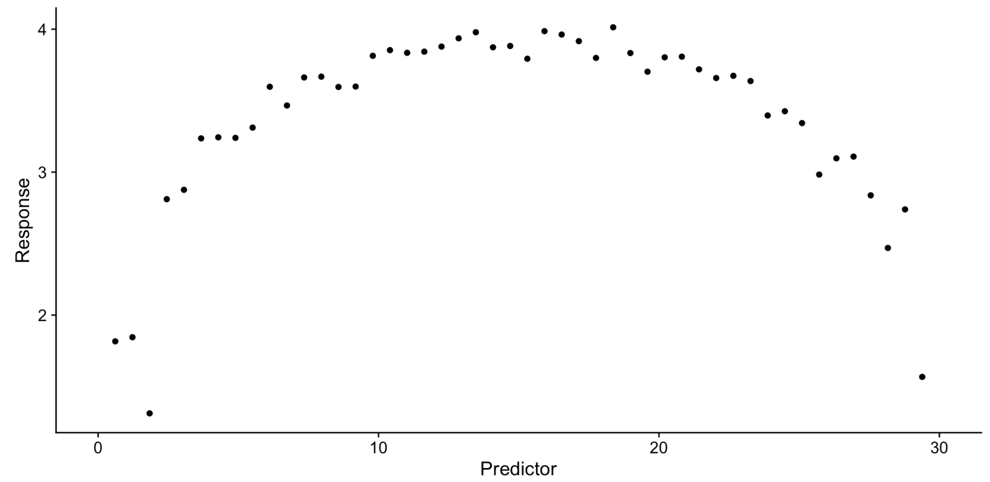
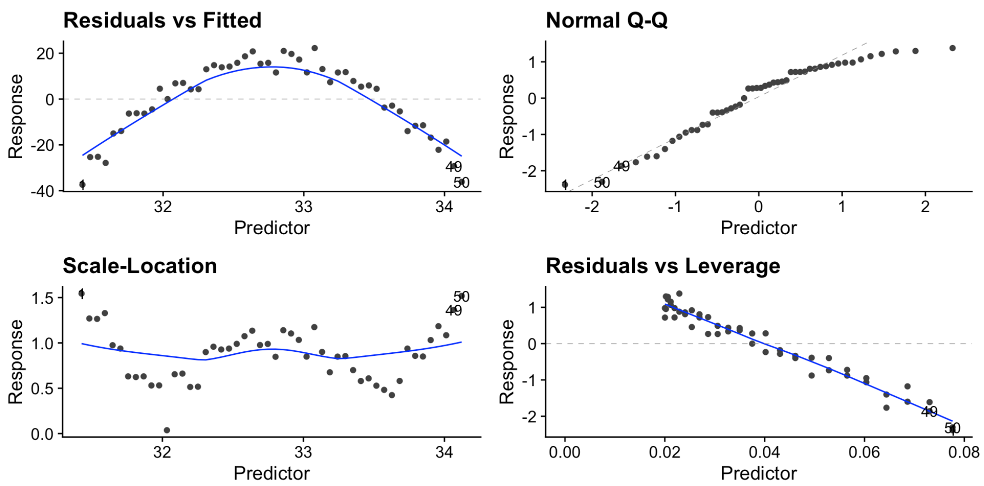


Transformations: polynomial relationship

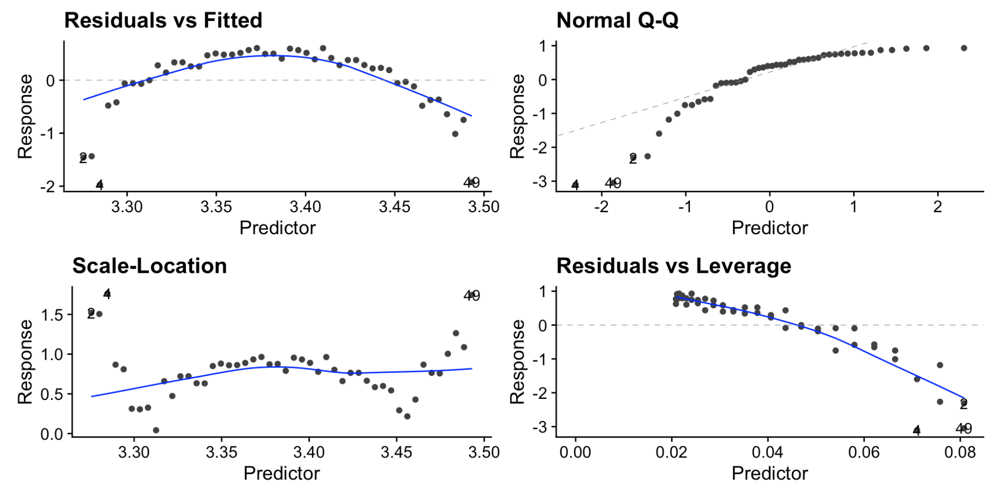
Before transformation

▶ Code



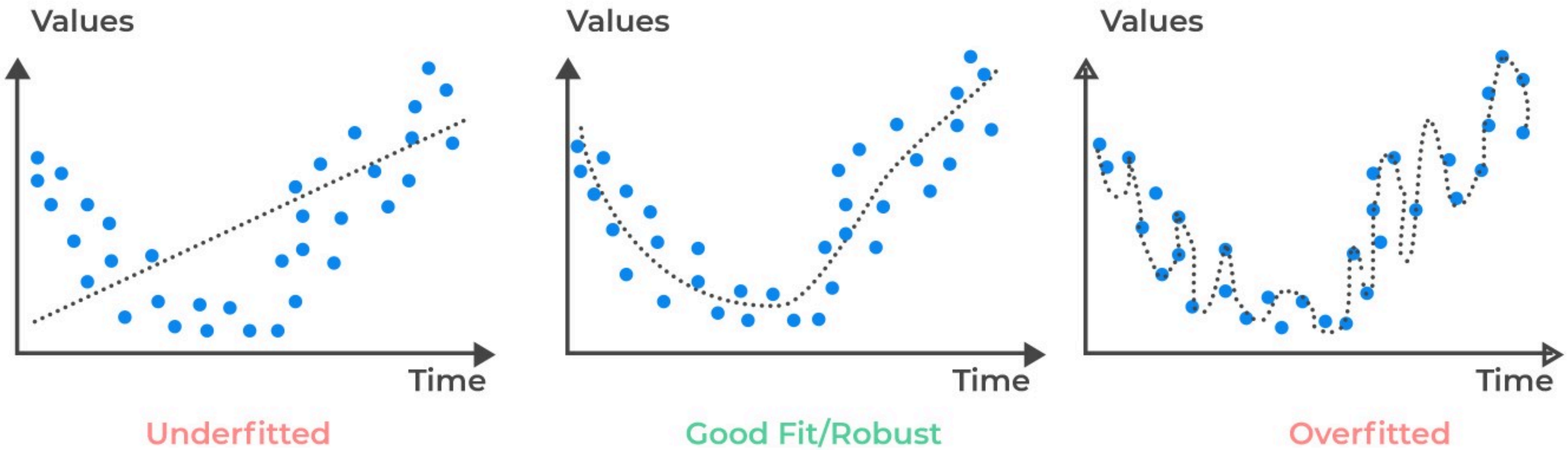
After $\log_e$ transform

▶ Code



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 β 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

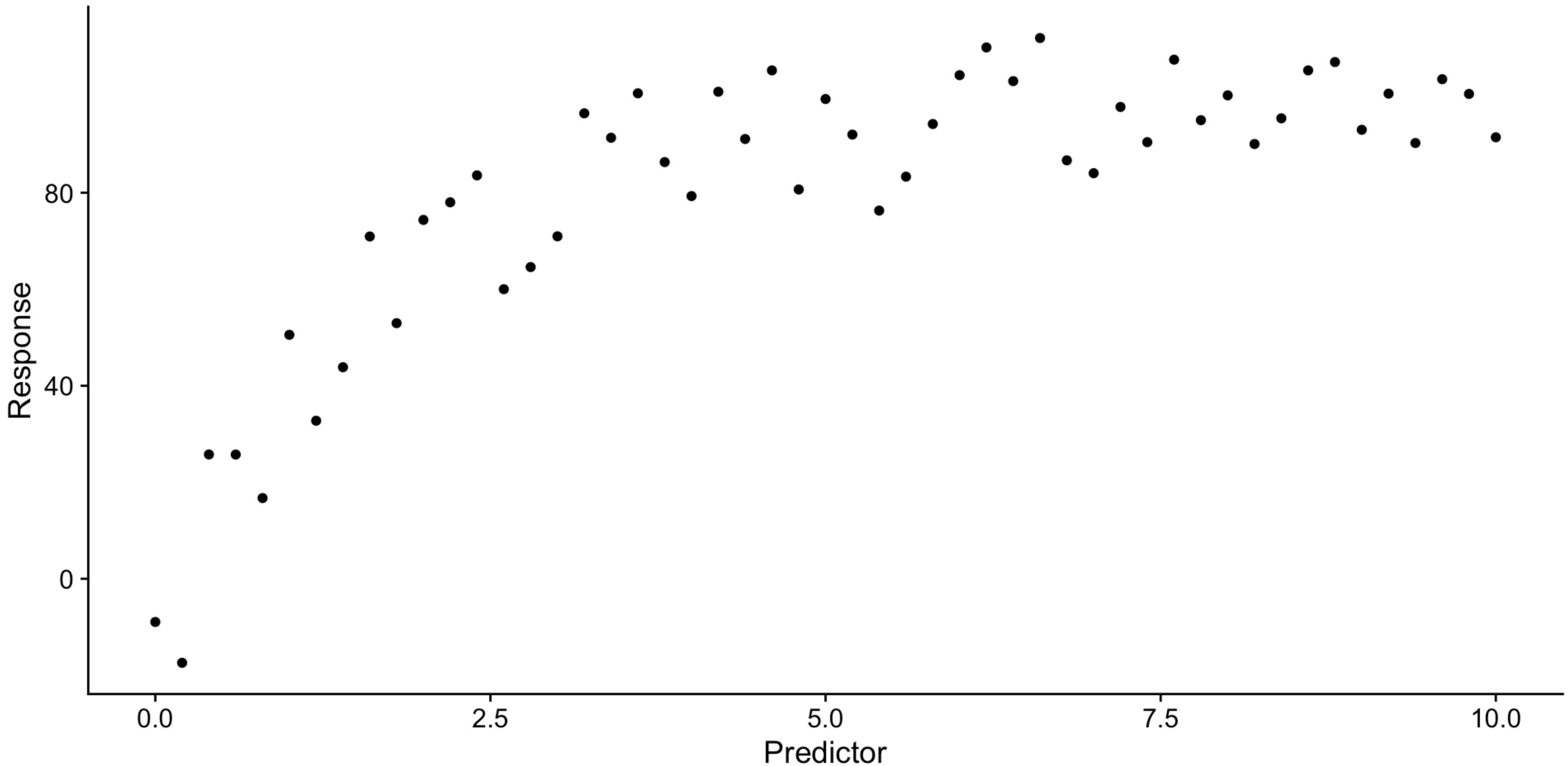
Polynomial fitting

Using the `asymptotic` data

The data

See Slide 11 for the relationship and mathematical expression.

▶ Code

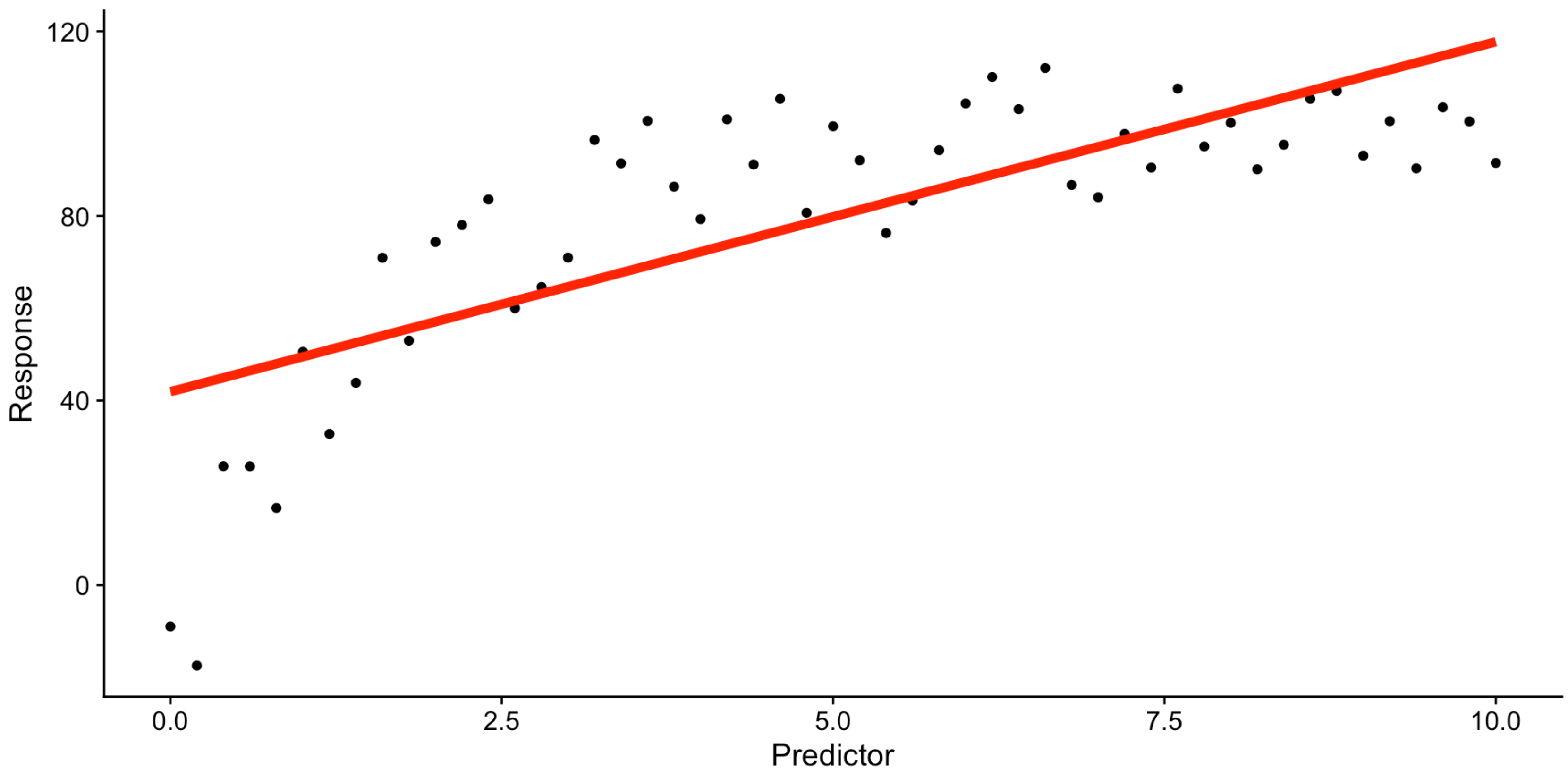


Fitting the model (linear)

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

▶ Code

▶ Code

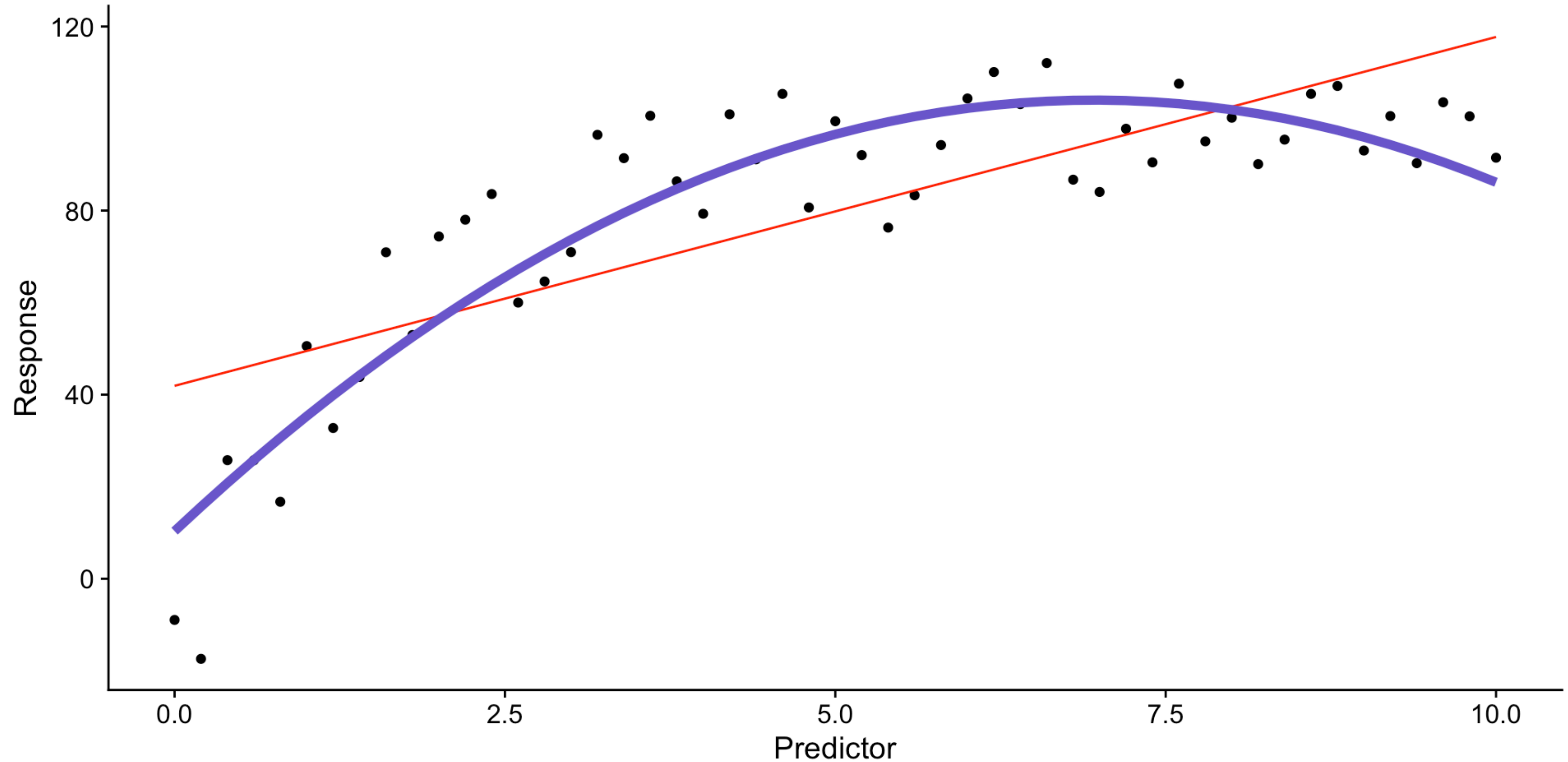


Fitting the model (`poly(degree = 2)`)

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

▶ Code

▶ Code

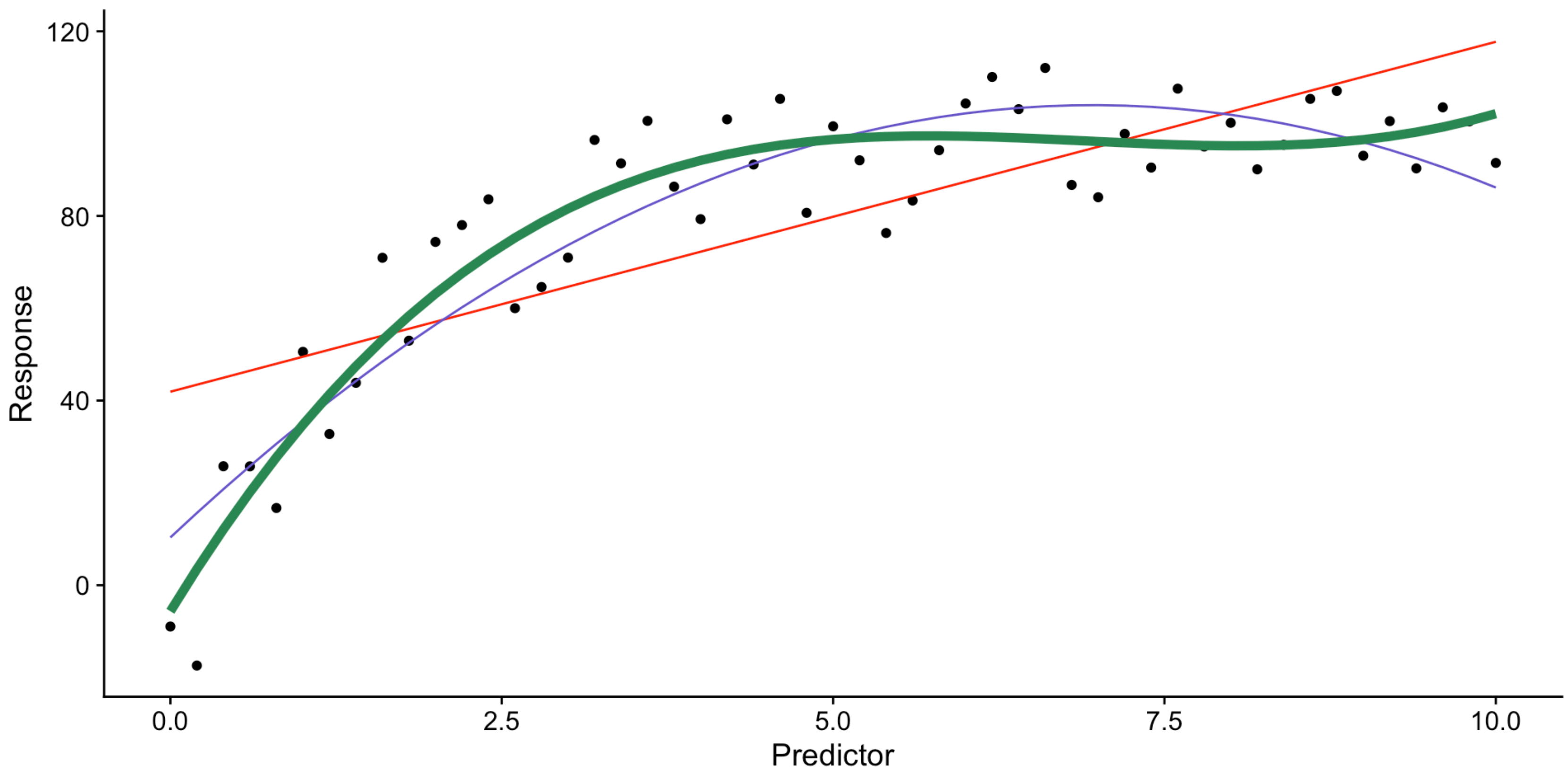


Fitting the model (`poly(degree = 3)`)

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

▶ Code

▶ Code



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

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \ldots + \beta_1 0 x_i^{10} + \epsilon_i$$

▶ Code

▶ Code

▶ Code

Comparison of R^2 of Polynomial Models

Model	R2
Linear	0.570
Poly2	0.820
Poly3	0.872
Poly10	0.862

ⓘ **Note**

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.

▶ Code

```
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    
```

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 β.

- Y_i is the continuous response variable.
- x_i is the vector of predictor variables.
- β is the vector of unknown parameters.
- ϵ_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**).

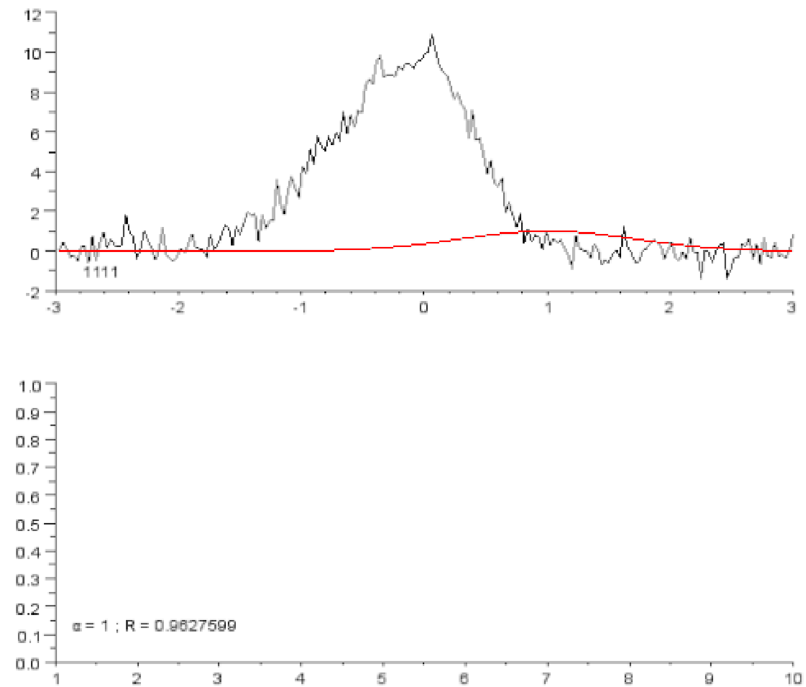
Basically:

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

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.

▶ Code

- `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()`

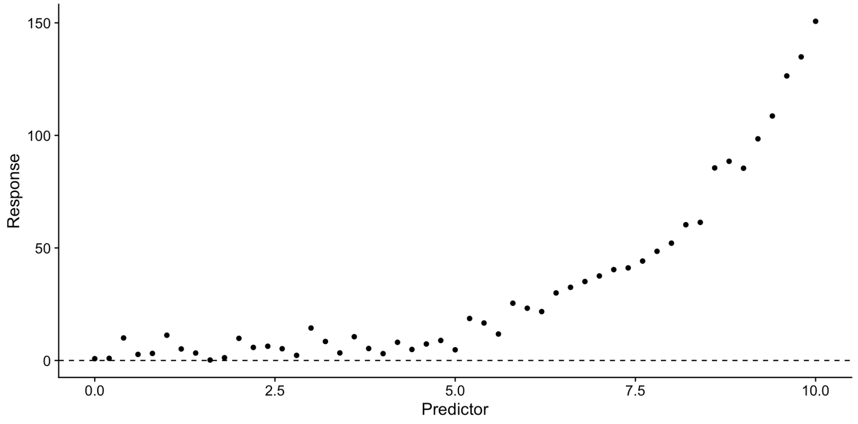
$y = y_0 e^{kx}$

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.

▶ Code



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!

▶ Code

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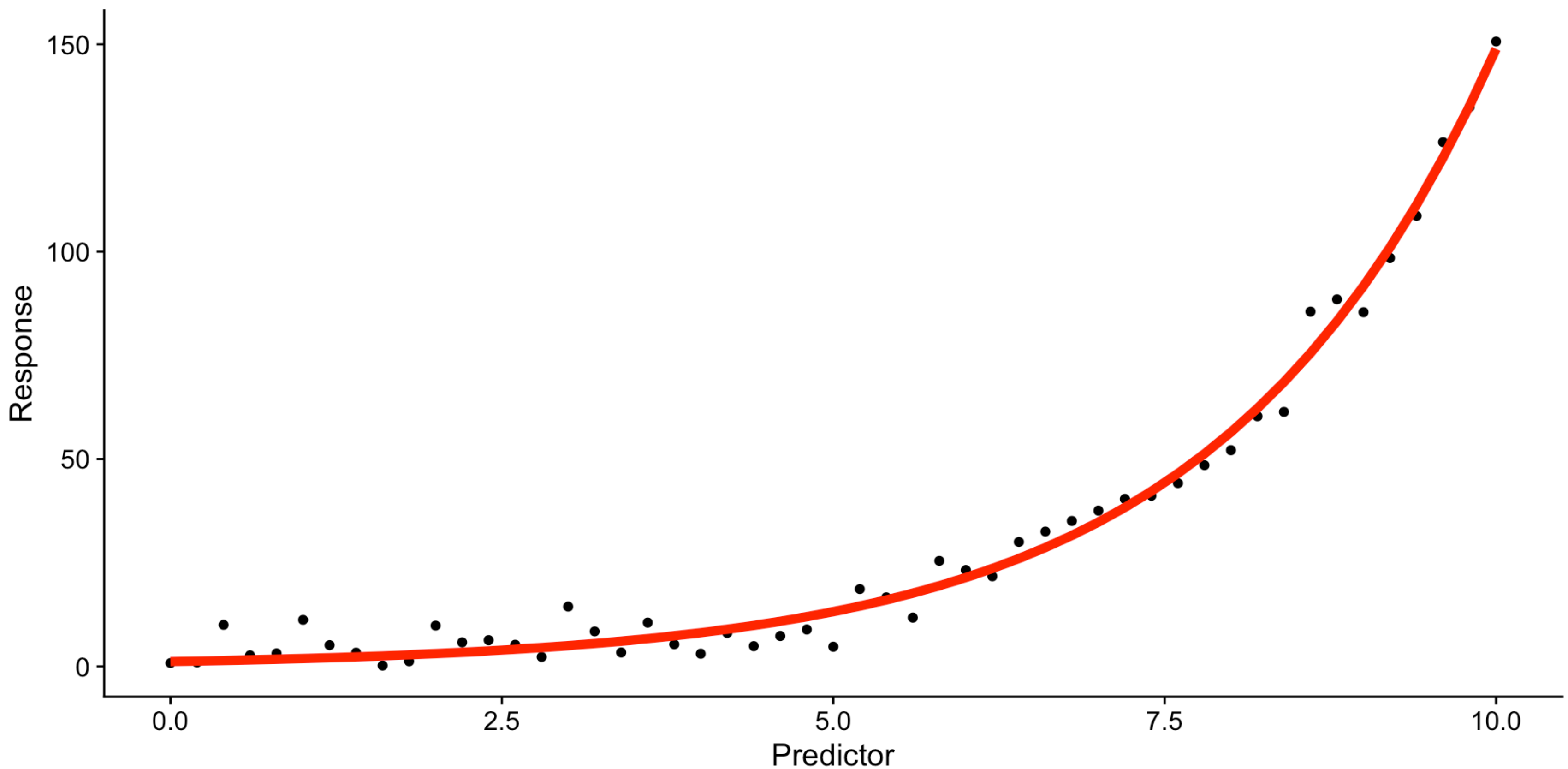
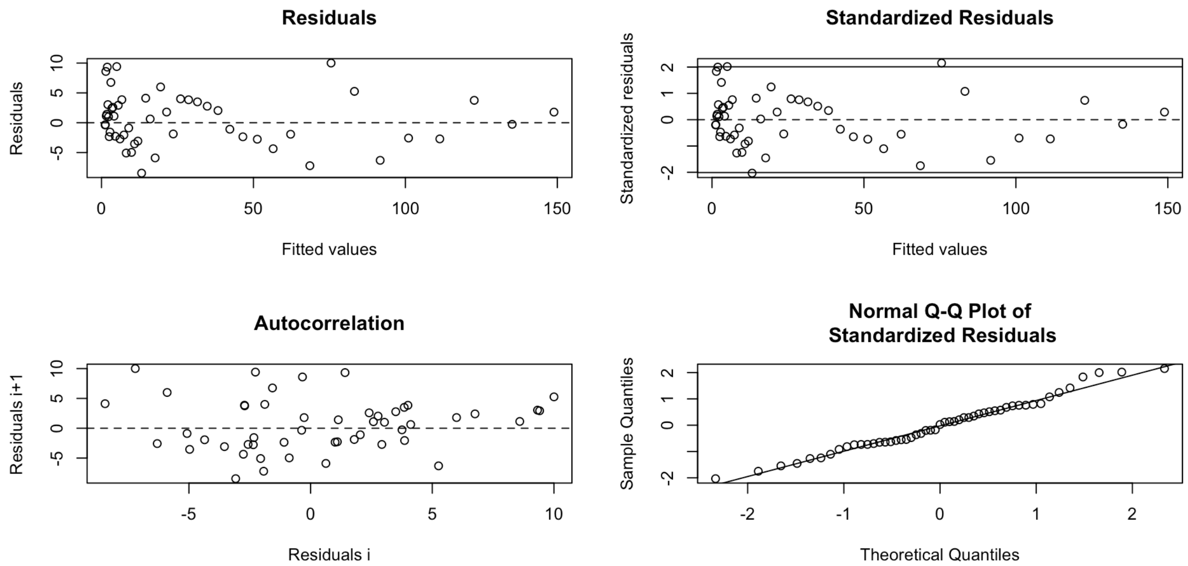


Check assumptions

- ▶ Code



- 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.
- Non-linear models typically should meet assumptions because they are fitted specifically to the dat

Interpretation

▶ Code

```
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: 1.204e-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 c 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.

▶ Code

```
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: 1.982e-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.

▶ Code

```

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

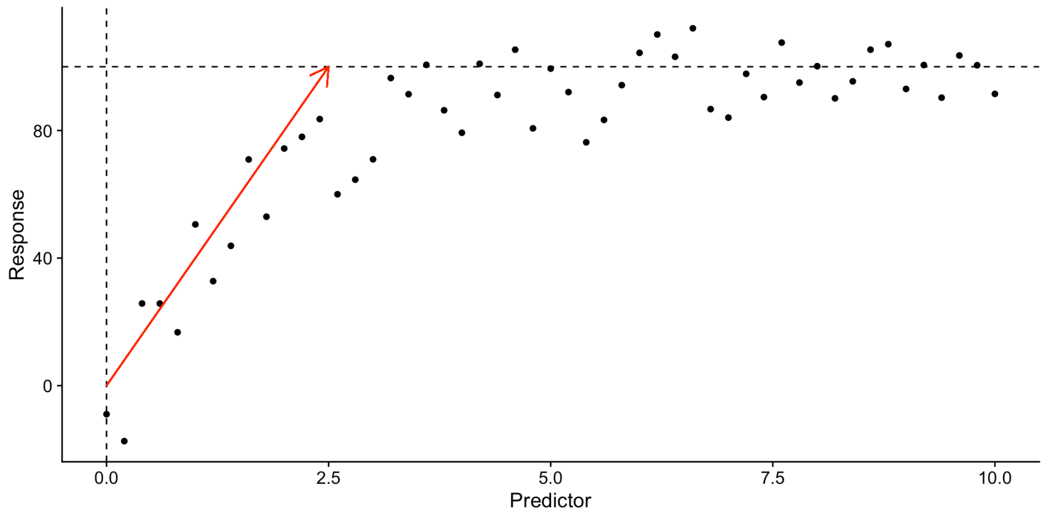
The equation

- 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.

▶ Code

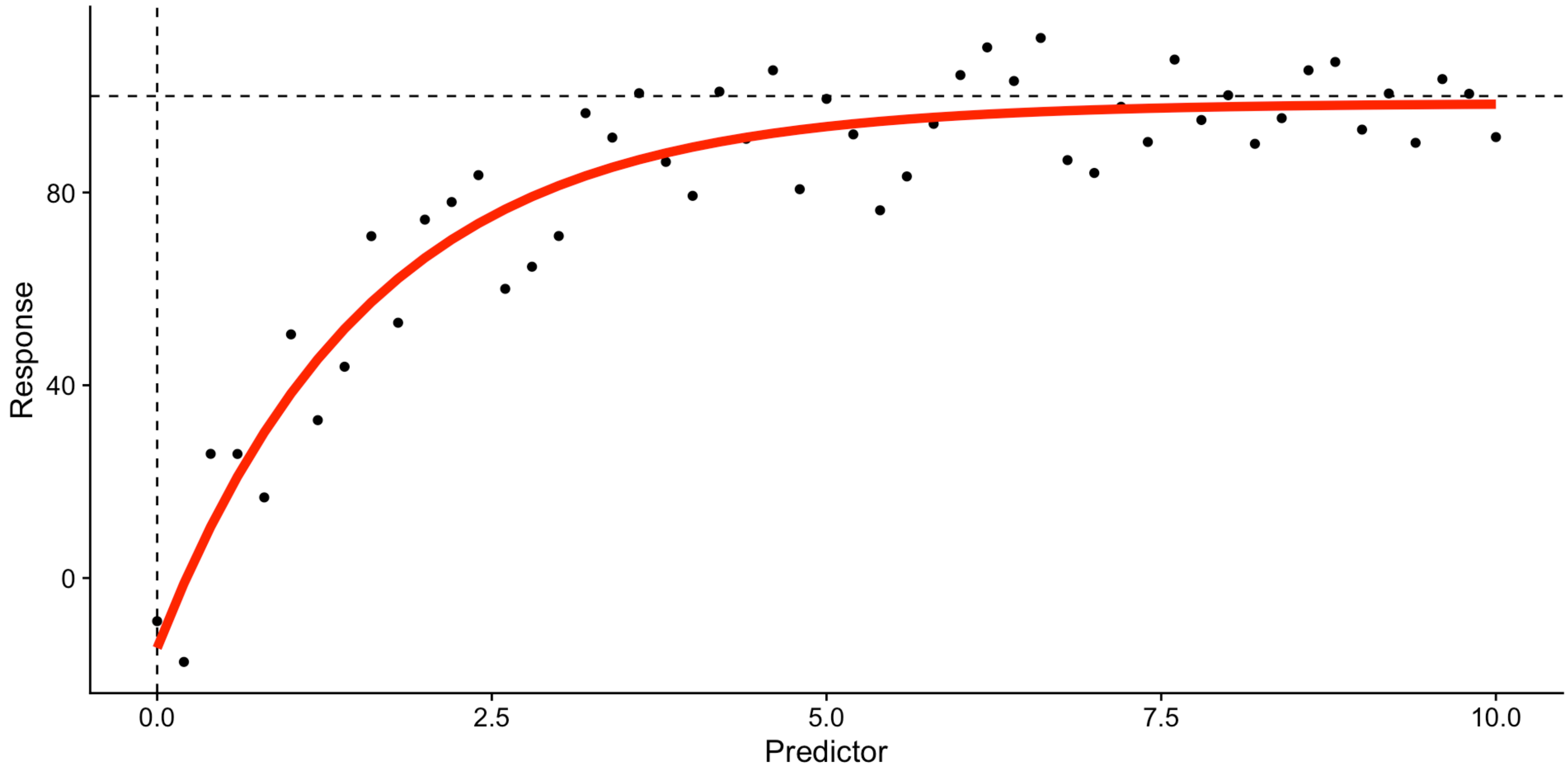


Some plausible estimates – $R_0 = 0$, $Asym = 100$, $lrc = 0.8$.

Fit model

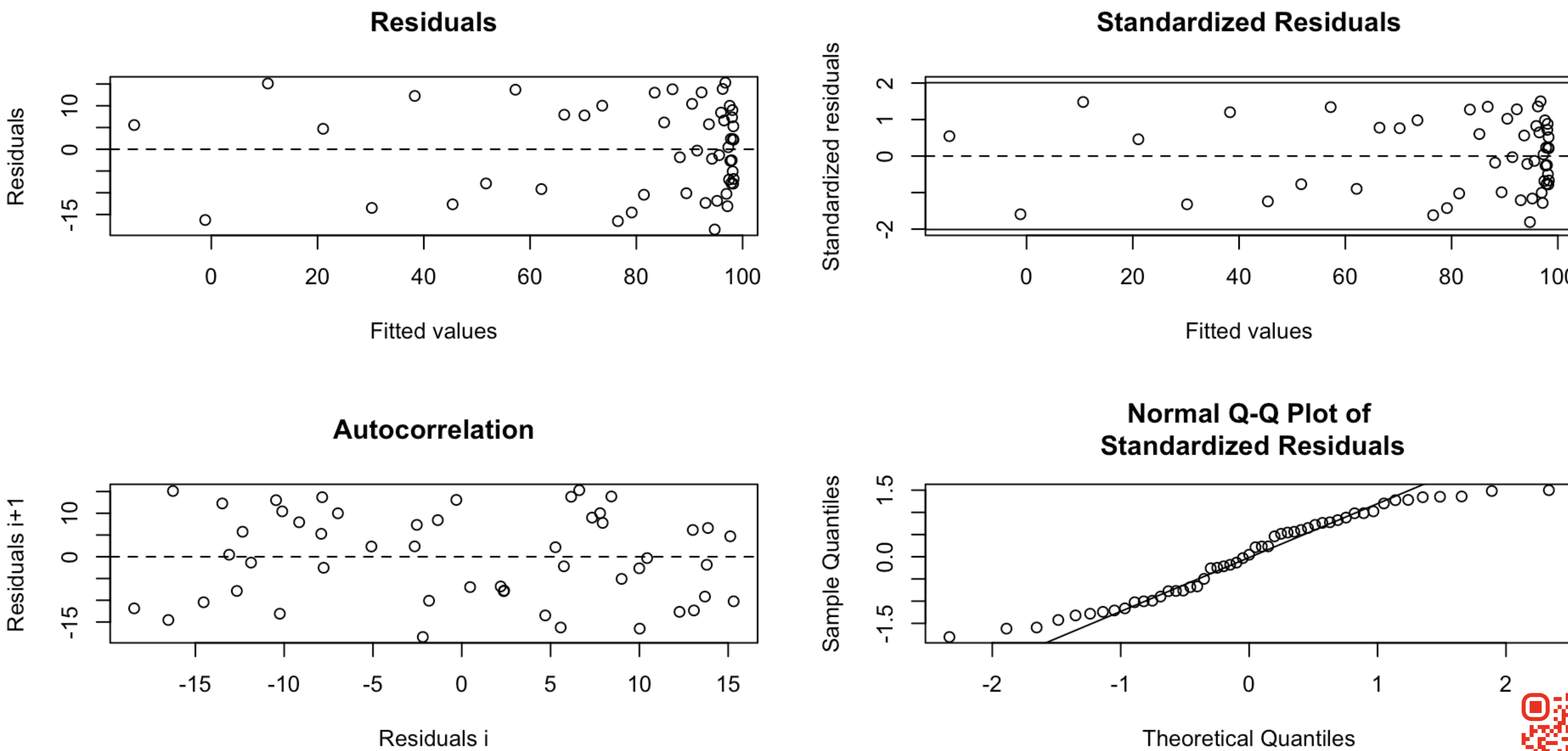
▶ Code

▶ Code



Check assumptions

▶ Code



Interpretation

▶ Code

```
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: 3.197e-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

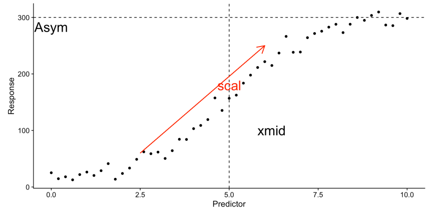
There are multiple equations for logistic models, but they all have an ‘S’ or sigmoid shape. The equation that `SSlogis()` (base R) assumes y is positive and uses:

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

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.

▶ Code

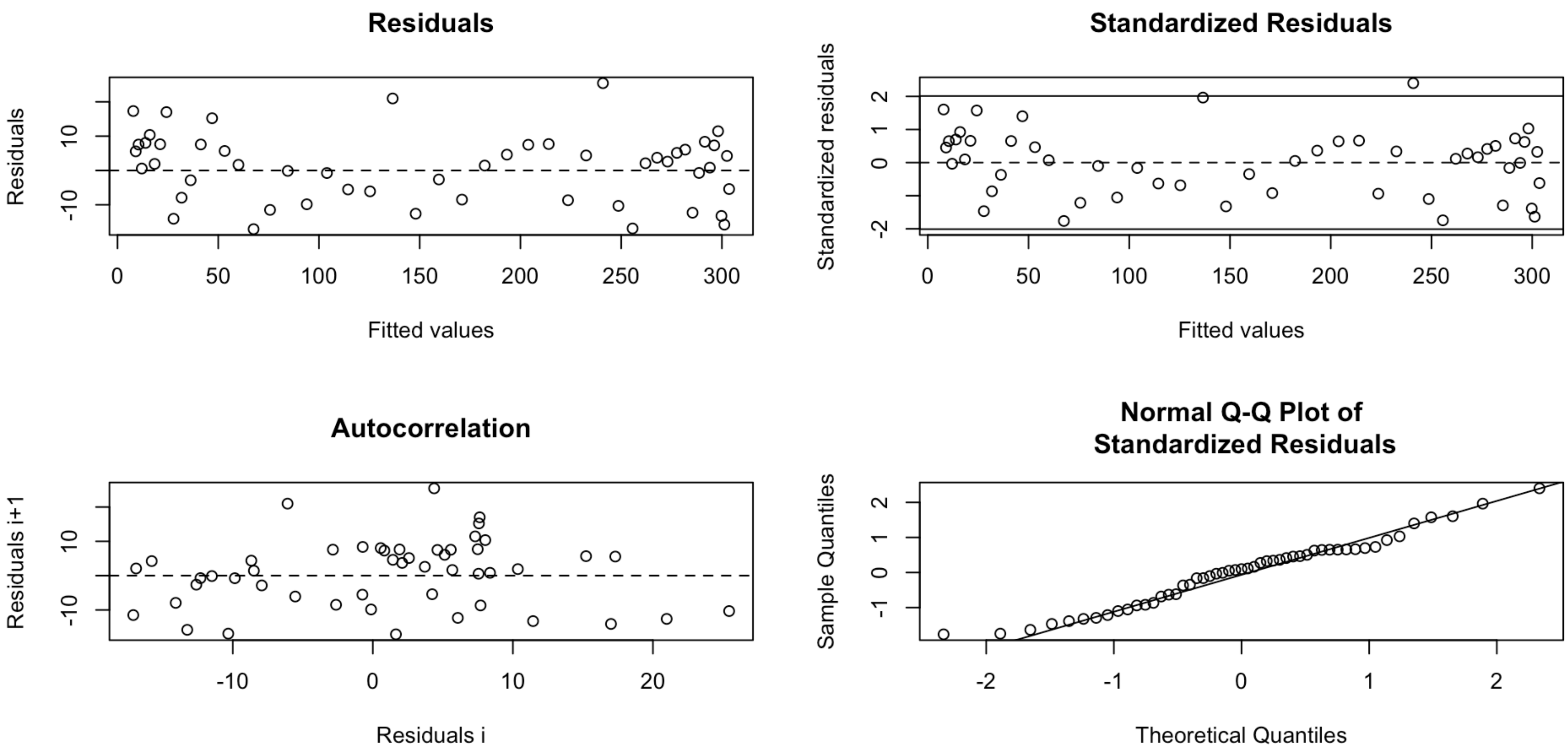


Some starting values would be $Asym = 300$, $xmid = 5$, $scal = 1$.

Fit model

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

▶ Code



Interpretation

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

▶ Code

```
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: 6.626e-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 but not all parameters are significant – that is fine.
- The parameterised model is:

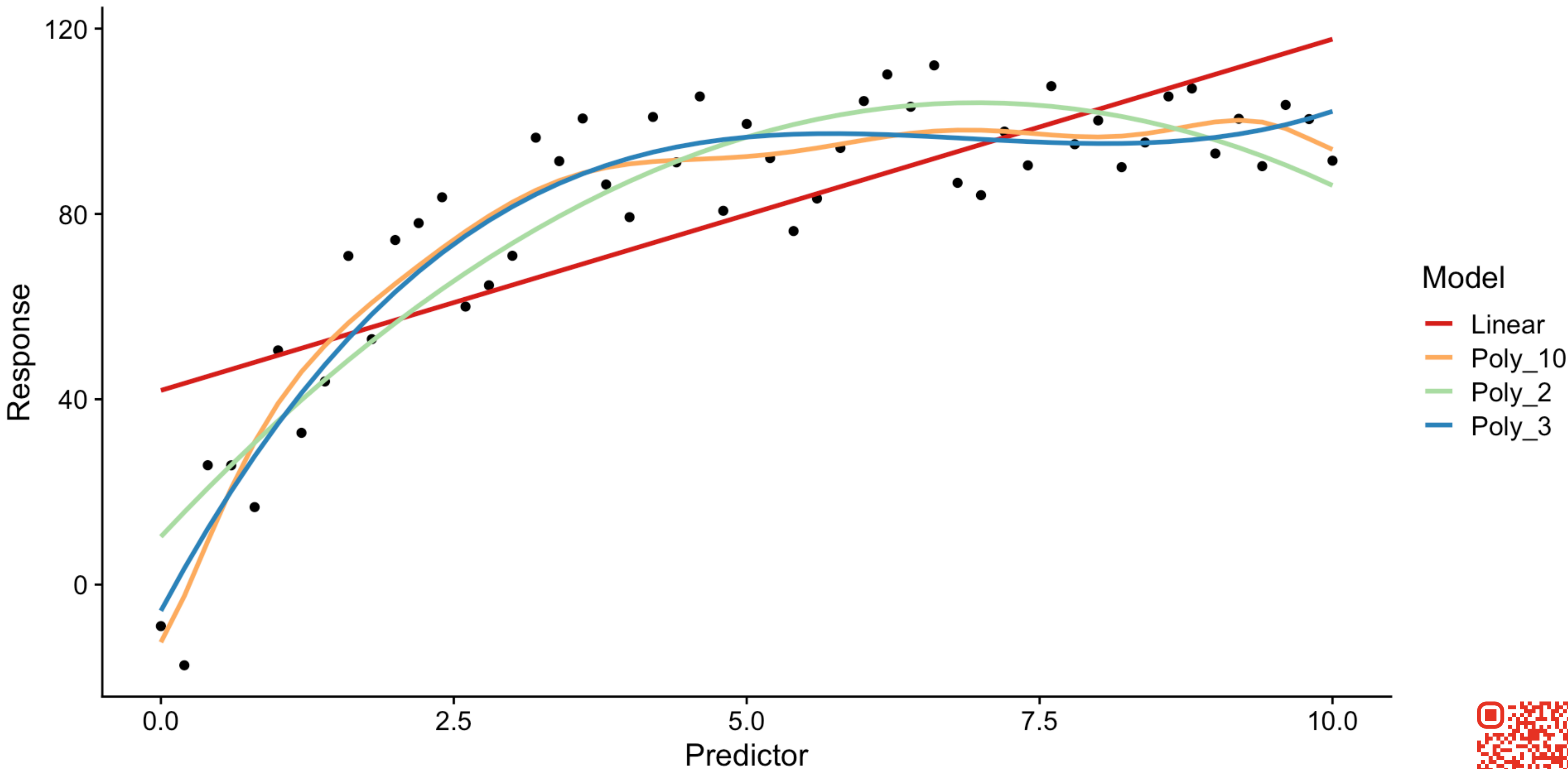
$$y = \frac{310}{1 + e^{\frac{4.93 - x}{1.35}}}$$

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

▶ Code



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.

▶ Code

```
# 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

▶ Code

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!