Lab 12 - Non-linear models

ENVX1002 Handbook

Semester 1, 2025

💡 Learning outcomes

- Calculate "by hand" the initial estimates of the parameters of a non-linear model
- Interpret tables of regression coefficients for polynomials to perform hypothesis testing
- Fit polynomials and non-linear models to data using least-squares fitting using the SOLVER add-in in Excel
- Fit polynomials and non-linear models to data in R, and interpret the outputs

Before we begin

Create your Quarto document and save it as `Lab-12.qmd` or similar.

The following data files are required:

1) east_creek.csv

Over the past few weeks you have explored linear models and how to interpret model summary output. Again we have stepped up the complexity, now venturing into the world of non-linear models.

This practical focuses on fitting non-linear models to data with an emphasis on 3 important classes of functions that all budding biologists and environmental scientists should know

- polynomials,
- exponential models, and
- logistic models.

A question before we begin:

What are some advantages and disadvantages of non-linear models as compared to polynomials?

Polynomials

Quadratic

$y = \beta_0 + \beta_1 x + \beta_2 x^2$

where the parameters are the y-intercept (b_0), the linear component (b_1) and the quadratic component (b_2).

If b_2 is negative then the shape of the function is convex upwards, i.e. y increases with x until reaches a peak and then y decreases.

It is easy to understand so it has been commonly used for modelling the response of yield to inputs such as fertiliser, seeding rates. This is despite much criticism for being unrealistic.

Limitations:

(i) rate of increase to peak is same as rate of decrease past peak

(ii) does not level off as x becomes small or very large, y just keeps increasing or decreasing.

Cubic

$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

Compared to the quadratic model which has 1 turning point, a cubic model has 2 turning points.

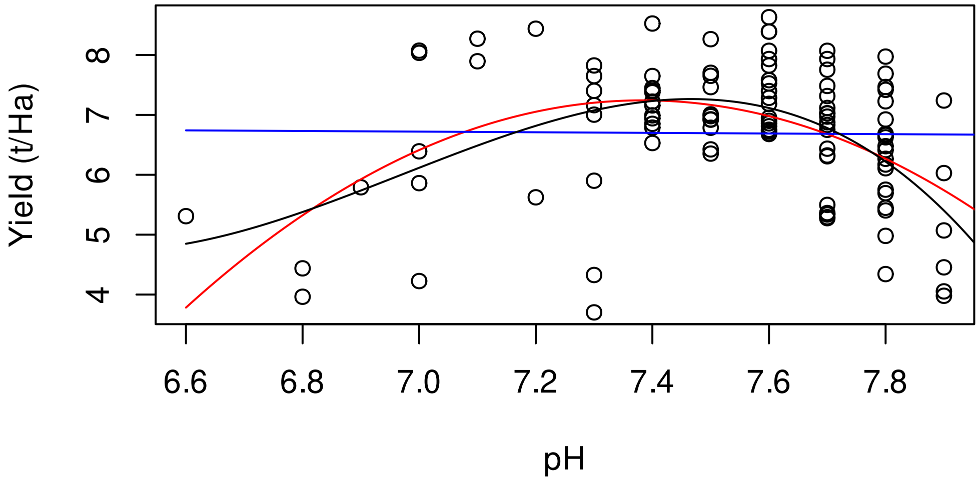
Exercise 1: Interpreting polynomials

A study was performed to examine the soil properties that control the within-field variation in crop yield. The focus of this question is on soil pH which among other things controls the availability of nutrients to plants.

This exercise does not require you to read in any data, but rather focus on interpreting the model output and comparing the models.

The figure below shows the raw observations of yield plotted against pH with three models fitted; a linear model, quadratic polynomial and a cubic polynomial.

a) which line corresponds to which model?



b) based on the output from the 3 models below, which model fits the data best? Note: no hypothesis testing yet, just how well the model fits the data (r^2).

1. Linear model:

```

Call:
lm(formula = yield ~ ph, data = soil)

Residuals:
    Min      1Q  Median      3Q     Max 
-3.0027 -0.5540  0.2189  0.7643  1.9424 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)  
(Intercept)  7.08842    3.05279   2.322   0.0221 *
ph          -0.05249    0.40438  -0.130   0.8970  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.137 on 108 degrees of freedom
Multiple R-squared:  0.000156,  Adjusted R-squared:  -0.009102 
F-statistic: 0.01685 on 1 and 108 DF,  p-value: 0.897
```

2. Quadratic model:

```

Call:
lm(formula = yield ~ ph + I(ph^2), data = soil)

Residuals:
    Min      1Q  Median      3Q     Max 
-3.5010 -0.4380 -0.0099  0.5871  1.7064 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept) -299.9031    54.2430  -5.529 2.30e-07 ***
ph            83.1948    14.6954   5.661 1.27e-07 ***
I(ph^2)       -5.6336     0.9942  -5.667 1.24e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.002 on 107 degrees of freedom
Multiple R-squared:  0.2309,    Adjusted R-squared:  0.2166 
F-statistic: 16.07 on 2 and 107 DF,  p-value: 7.921e-07
```

3. Cubic model:

```

Call:
lm(formula = yield ~ ph + I(ph^2) + I(ph^3), data = soil)

Residuals:
    Min      1Q  Median      3Q     Max 
-3.3734 -0.4540  0.0526  0.5171  1.9561 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)  
(Intercept) 1719.020   1082.451   1.588   0.1152  
ph          -745.066    443.767  -1.679   0.0961 .
I(ph^2)      107.461     60.570   1.774   0.0789 .
I(ph^3)       -5.140      2.752  -1.867   0.0646 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.9908 on 106 degrees of freedom
Multiple R-squared:  0.2554,	Adjusted R-squared:  0.2344 
F-statistic: 12.12 on 3 and 106 DF,  p-value: 6.971e-07
```

c) Use the R output to perform hypothesis testing to find the best model. Write out the hypotheses you are testing.

Exercise 2: Fitting polynomials in R

This exercise will use real data from a yield-fertiliser trial in Bedfordshire, United Kingdom.

First thing we can do is fit a linear model to the fertiliser data:

```r
# create fertiliser and yield objects
fert <- c(0, 100, 170, 225)
yield <- c(3.32, 5.23, 5.41, 5.02)

# Fits a linear model and saves it to an object called lin.mod
lin.mod <- lm(yield ~ fert)

# Summarises key features of model
summary(lin.mod)
```

```

Call:
lm(formula = yield ~ fert)

Residuals:
      1       2       3       4 
-0.4469  0.6727  0.2995 -0.5252 

```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 3.766929   0.634765   5.934   0.0272 *
fert        0.007904   0.004243   1.863   0.2035
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.7134 on 2 degrees of freedom
Multiple R-squared:  0.6344,    Adjusted R-squared:  0.4515
F-statistic:  3.47 on 1 and 2 DF,  p-value: 0.2035
```

a) What is the model fit like in this model?

Fit and plot a quadratic polynomial in R. In R a quadratic polynomial can be fitted using the following lines of code:

```
# create a new variable which is the square of the fertilizer rates
fert2 <- fert^2

# fit the quadratic model incorporating fert2
quad.mod <- lm(yield ~ fert + fert2)

summary(quad.mod)
```

```

Call:
lm(formula = yield ~ fert + fert2)

Residuals:
        1         2         3         4
-0.005611  0.024528 -0.032791  0.013874

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.326e+00  4.324e-02   76.92  0.00828 **
fert         2.786e-02  9.014e-04   30.91  0.02059 *
fert2       -9.064e-05  3.921e-06  -23.12  0.02752 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.0436 on 1 degrees of freedom
Multiple R-squared:  0.9993,    Adjusted R-squared:  0.998
F-statistic: 731.7 on 2 and 1 DF,  p-value: 0.02613
```

b) What is the fit like for our quadratic model? is it better than our linear model?

In Excel it is easy to fit a line, by creating a scatterplot, then **add Trendline...** and selecting **Polynomial** (2nd order).

To fit our polynomial line in R, we need to obtain model predictions first.

To plot model predictions you first need to predict at fine intervals of the predictor to make a continuous plot that is not jagged or stepped. To create a new prediction dataset you can use the following code:

```
# creates a sequence of numbers from 0 to 225 going up in increments of 1
new.fert <- seq(0, 225, 1)
```

We can use our model to predict at the values in the new prediction dataset, in this case `new.fert`.

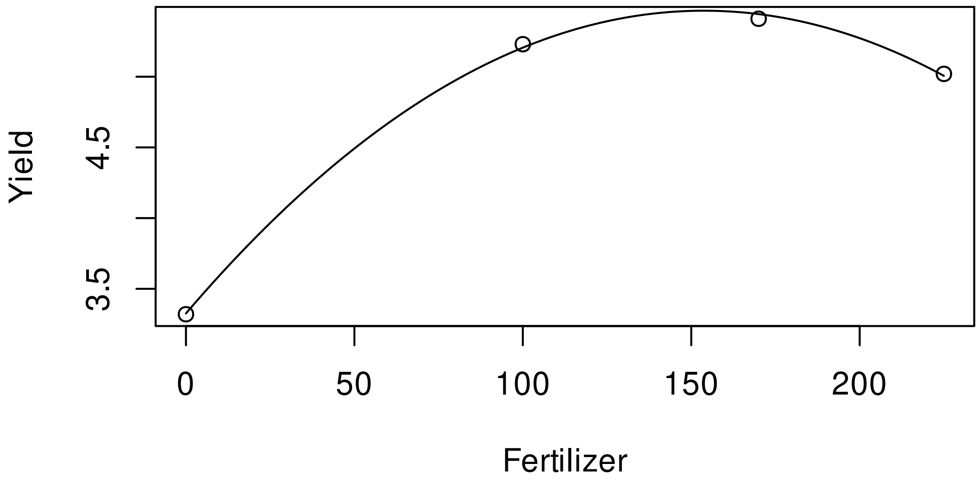
```
new.pred <- predict(quad.mod, list(fert = new.fert, fert2 = new.fert^2))
```

The general form of the `predict` function is `predict(model object, list object)`.

The list object tells R what object contains the data we will use to predict. For example in our case the model was built on fert and fert2 so we have to tell the predict function what object contains the new values for each of these, in our case new.fert.

Now we plot the raw observation as points and add an overlay of the model fit as lines:

```
plot(fert, yield, xlab = "Fertilizer", ylab = "Yield")
lines(new.fert, new.pred) # Adds lines to original plot
```



Exponential function

$y = y_0 e^{kx}$

where the parameters are y_0 which is the multiplier which expresses the starting or final value, and k which is negative for exponential decay and positive for the exponential growth.

The half life (for decay) or doubling time (for growth) can be calculated as

$\frac{log_e 2}{k}$

Limitations:

(i) harder to fit than polynomials

(ii) exponential growth has no horizontal asymptote; keeps going up.

Exercise 3: Initial estimates for exponential growth function

In this exercise we will find initial estimates of the parameters of an exponential growth model by visual assessment of plots of the data and/or rough calculations. The initial estimates of the parameters are needed as starting points for the iterative fitting methods we will use in the practicals, e.g. SOLVER in Excel and the `nls()` function in R.

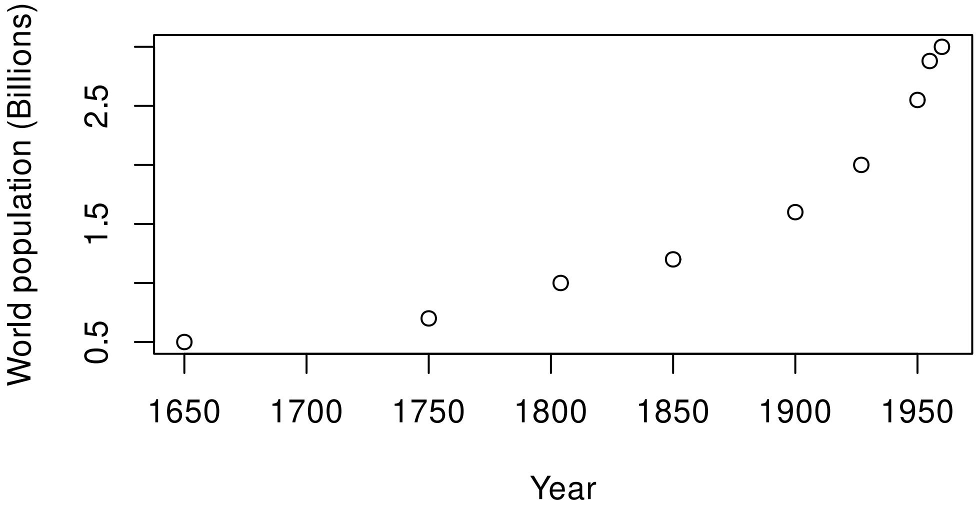
The plot and table below presents the population of the world from 1650-1965.

We wish to model the data with an exponential growth function of the form;

$y = y_0 e^{kx}$

where

- y is the population in the year x,
- y_0 is the population in 1650 and
- k is the rate constant.



Year	1650	1750	1804	1850	1900	1927	1950	1955	1960
Pop (billions)	0.5	0.7	1	1.2	1.6	2	2.55	2.88	3

a) Provide an initial estimate of y_0.

The parameter k can be estimated from a linear model fitted to $\log_e$ population against year.

Rather than formally fitting a linear model you could estimate the slope approximately by using the smallest and largest value to estimate the slope and therefore k.

b) Use this approach to estimate k.

Hint:

$$slope = k = \frac{log_e y_{max} - log_e y_{min}}{x_{max} - x_{min}}$$

c) For an exponential growth model the doubling time of a population can be estimated by $\log_e 2$ / k.

Examine the graph and/or table to estimate the doubling time and use this to estimate k. You will have to make k the subject in the equation for estimating the doubling time.

d) How similar were the estimates of k?

Exercise 4 : Exponential growth models

This data is from Jenkins & Adams (2010) who studied soil respiration rates against temperature for different vegetation communities in the Snowy Mountains. They fitted an exponential growth model to the data.

The purpose of this exercise is to illustrate the dangers of using Excel's in-built functions for statistics more complex than calculating means and fitting simple models.

Plot the data in Excel and using the **Add Trendline…** option. Make sure tick the option for displaying the equation in the graph.

a) The researchers performed the experiment up to a temperature of 40 degrees C, would you expect exponential growth in the respiration rate to continue if high temperatures were considered? Is there a better model?

Now fit the same model in R using the nls function. Code to get you started is:

```
temp<-c(5,10,20,25,30,35,40)
respiration<-c(1,2,4,6,8,11,18)

##Initial parameters
exp.mod<-c(Bp=1.0,Cp=0.1)

##Fits exponential model
res.exp<-nls(respiration~Bp * exp(temp*Cp),start=exp.mod,trace=T)
```

```
2025.224    (3.23e+01): par = (1 0.1)
90.64319    (7.34e+00): par = (0.6559559 0.09162898)
2.841421    (9.49e-01): par = (0.7302258 0.08091595)
1.488431    (5.63e-02): par = (0.7944381 0.07731867)
1.483685    (1.52e-03): par = (0.8033809 0.07707711)
1.483681    (4.12e-05): par = (0.8036903 0.07706805)
1.483681    (1.71e-06): par = (0.8037011 0.07706768)
```

```
##Summarise model
summary(res.exp)
```

```

Formula: respiration ~ Bp * exp(temp * Cp)

Parameters:
   Estimate Std. Error t value Pr(>|t|)
Bp 0.803701   0.118632   6.775  0.00107 **
Cp 0.077068   0.004048  19.037 7.37e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```

Residual standard error: 0.5447 on 5 degrees of freedom

Number of iterations to convergence: 6
Achieved convergence tolerance: 1.71e-06
```

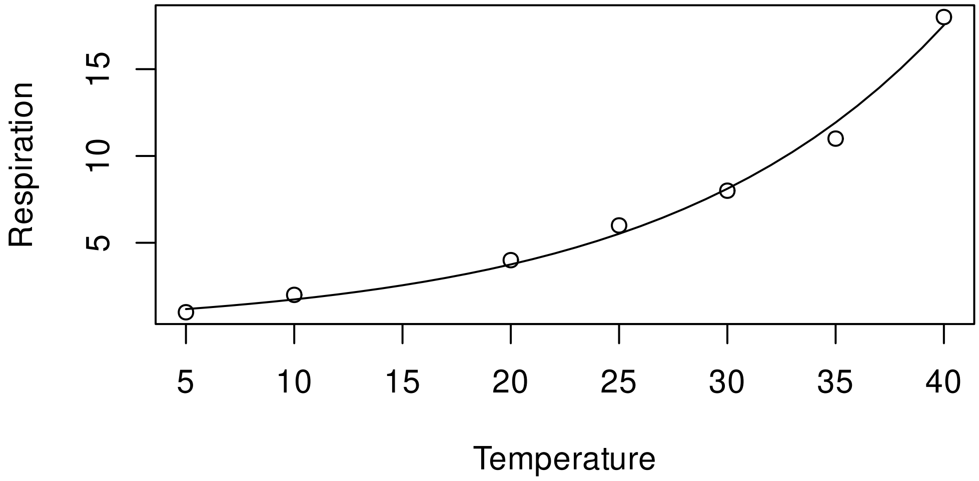
b) Now you can fit a line to the plot. Does this look similar to your trendline in Excel?

```
#Plots raw data
plot(temp,respiration,xlab='Temperature',ylab='Respiration')

#Creates new dataset for predictions ( 5 to 40 at an interval of 1)
temp.new<-seq(5,40,1)

#Makes predictions onto temp.new
pred.exp<-predict(res.exp,list(temp=temp.new))

#Adds model fit to existing plots
lines (temp.new,pred.exp)
```



Compare the parameters values between Excel and R. You can extract the RSS value from an `nls` object by using the code below:

```
deviance(res.exp)
```

```
[1] 1.483681
```

c) Calculate the RSS value for the Excel exponential model. Based on this, which is the better model?

When faced with the need to fit an exponential function, one approach that was used before computing power became readily accessible was to log the y values which linearises the relationship with x, enabling the modeller to use a simple linear model.

If we linearise, model would be $log_e(y) = b_0 + b_1 x$, where e^{b_0} is the y_0 parameter in an exponential model, and b_1 is the k parameter in the exponential model. This is similar to what was demonstrated in the lecture this week.

In Excel, log the soil respiration data and fit a linear model. You will see that the fitted model gives the same values as the exponential model fitted to the untransformed data.

If you compare the r^2 values for both you will see they are the same. This means that Excel reports the r^2 of the linear model fitted to logged respiration as the r^2 of the exponential model fitted to the raw data. This is naughty of Excel.

For the dataset used here the exponential model fits it so well the Excel approach is only slightly different to the correct approach used in R.

In cases where the model does not fit the data so well the differences would be larger. Logarithm makes smaller values larger and larger values smaller.

WHY IS THIS SUB-OPTIMAL?

- Regression modelling assumes that the residuals are normally distributed so logging normally distributed data will change the distribution to a non-normal one – it is best to analyse the data without transformation.
- Modelling data on the logged scale reduces the impact that larger values have on minimising the RSS but when you plot the fitted model with the original data you may observe large discrepancies for larger values. In other words, using a linear model on the log(data) can result in a higher discrepancy for larger values when plotting the fitted model on the original data. Therefore, the model fitted to the logged data is not necessarily the best on the original data.
- The reporting of the R-squared on the logged data on a model purported to be fitted to untransformed data is just wrong as the R-squared on the log scale will be better as the variation in the data has been reduced but we really want to know how well an exponential model fits the raw data.

Logistic function

$$y = A + \frac{C}{1+e^{-B(t-M)}}$$

where the parameters are A which is the starting point or initial condition, C which is the value of y where the functions flattens out (the horizontal asymptote), M which is the value of x where the change in y is largest (always occurs at y = A + 0.5C), and 0.5B is growth rate of individual when t = M.

Commonly used to model growth that has a sigmoid shape, i.e. where growth is initially slow, then picks up to a maximum, then slows down again as the system reaches a maximum.

Limitations:

Harder to fit than polynomials.

Exercise 5: Logistic models

In this exercise you will model the yield of pasture over time (since sowing) using a logistic function. Since the yield at sowing = 0, the A parameter will be set to 0 and the form of the logistic function that you will use is:

$y = A + \frac{C}{1+e^{-B(t-M)}}$

a) Fit the model in Excel using SOLVER and in R using the `nls` function. Refer to previous exercises for `nls` function structure and implement the logistic function. You will need to specify credible starting values for the parameters (see Box below).

b) Plot the fitted model with the observations.

c) Compare the parameters estimated by R and Excel.

STARTING VALUES

When fitting non-linear functions (i.e. logistic or exponential) using iterative procedures such as `nls` or SOLVER the starting estimates of the parameters have to be approximately correct to find a solution.

The best way to ensure that you have suitable starting values is to plot the data with the predictions overlaid for your starting parameters. You can then see how close your initial model is to the data.

For the logistic model the parameters have clear meanings so suitable starting values are:

(i) C is the maximum value of y so just use the maximum value of y in the raw data as the starting value.

(ii) M is the value of t when y = 0.5C, this can be read approximately off the graph.

(iii) B is harder to estimate but good starting point is 0.1.

That's it for Module 3! Great work exploring non-linear models!

Thank you all (students and demonstrators!) for your hard work and enthusiasm throughout this Module. Good luck with Project 3 and the final exam!