Assessing Change Over Time

1 Introduction

A **time series** is a sequence of measurements on the same object made over time. For example, we might measure the level of carbon dioxide (CO_2) in a town every day for a year. The purpose of making such measurements is to understand how our variable of interest has changed over time. For example, a government would be keen to know if air pollution levels are getting better or worse, or a conservationist might want to identify declining trends in wildlife populations to better target their conservation objectives.

We can write our set of time series data as $y_1, \ldots, y_T$, where y_i is the observation at time point i, and T is the total number of observations. Time series data are typically **not independent**, since there will often be correlation between consecutive observations. This dependency structure must be taken into account when modelling.

Exercise 1

Can you spot any dependency structure shown in the below plot of log(flow) in the River Dee?

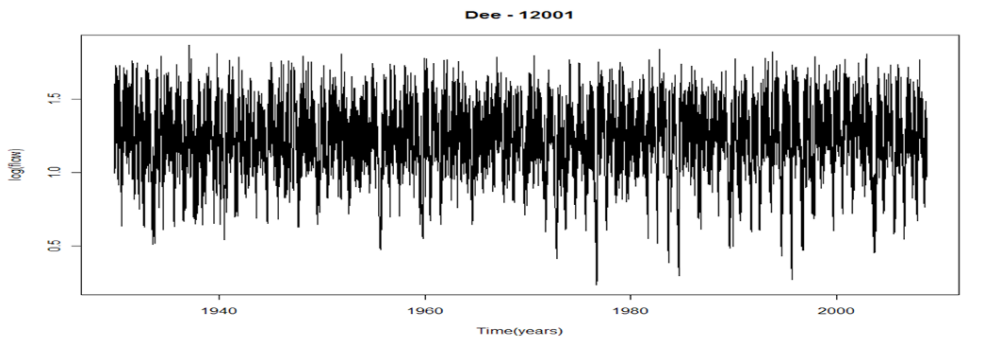


Figure 1: Log(flow) data for River Dee.

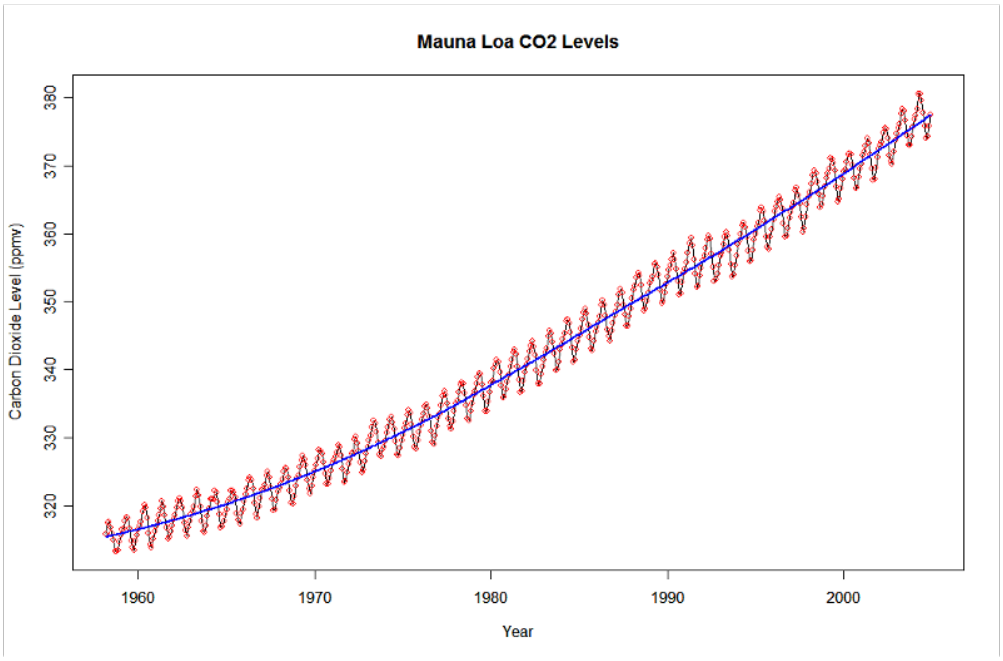
Solution

There is a clear structure to the data. It looks like there is a repeated pattern, once per year. (This is a "seasonal pattern" and we'll go into more details about this later in this section of the course.)

Example: Mauna Loa

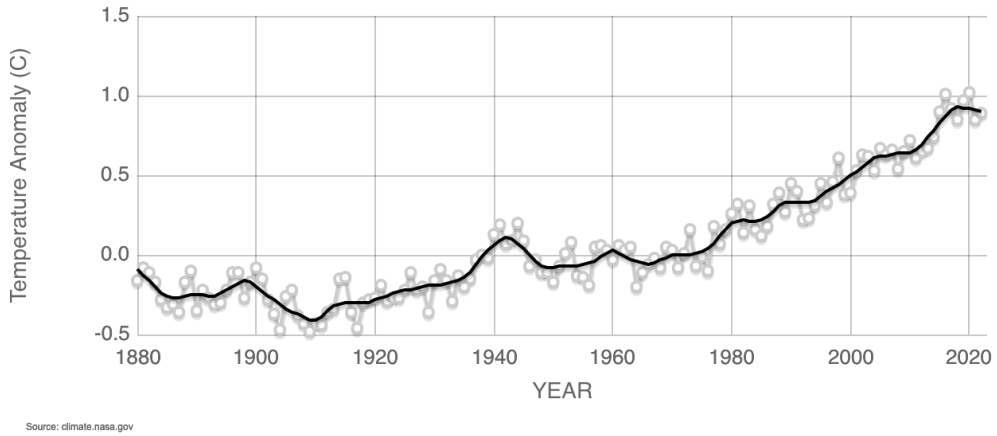
Mauna Loa in Hawaii is one of the biggest and most active volcanoes in the world. CO_2 levels have been monitored since 1958. Mauna Loa is one of the first sites worldwide where increasing CO_2 levels were identified.

We can observe a clear trend, and also a seasonal pattern. It may be sensible to standardise the data and represent all observations in terms of '**anomalies**', i.e., their deviation from the starting point (1960 mean level).



Example: Global temperature

The plot below shows the global temperature anomaly (the current value compared to the average from 1951–1980).



Source: https://climate.nasa.gov/vital-signs/global-temperature/

Exercise 2

How would you describe the change in global temperature shown in the above plot? We will discuss this in the lecture.

2 Ecological Trend

The purpose of time series modelling is to identify any **trends** which exist in the dataset. But what exactly is a trend? It depends who you ask.

The Joint Nature Conservation Council (JNCC) define it as: *a measurement of change derived from a comparison of the results of two or more statistics.* This is often considered to be the *ecological* definition of trend, i.e., a change (in terms of percentage or some index) between two timepoints.

3 Statistical Trend

In statistics, the definition of a trend is often more wide-ranging:

- A long-term change in the mean level (Chatfield, 1996)
- Long-term movement (Kendall and Ord, 1990)
- Long-term behaviour of the process (Chandler, 2002)
- The non-random function $\mu(t) = E(Y(t))$ (Diggle, 1990)

We may be interested in trends in mean, variance or extreme values. Trends are not limited to linear or monotonic patterns.

3.1 Simple Linear Trend

We can represent a simple linear trend using the standard notation:

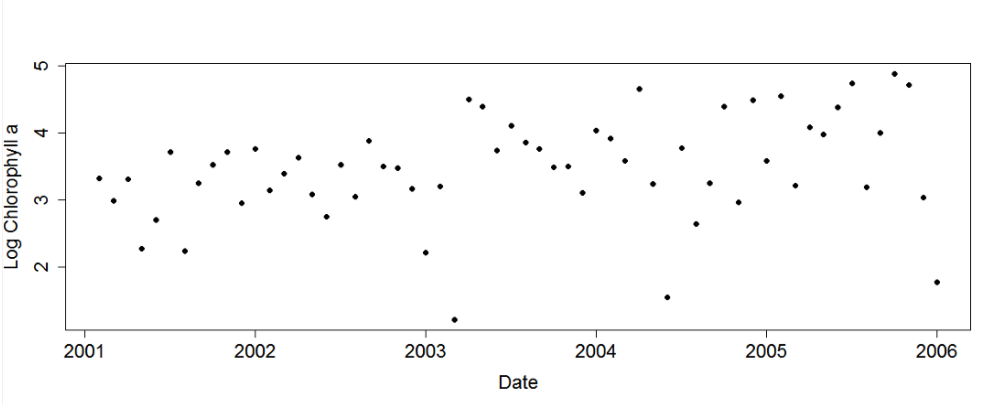
$$Y_t = \beta_0 + \beta_1 x_t + \epsilon_t.$$

Here, β_0 is an intercept and β_1 represents the slope (trend). This is just a standard linear model, with all the usual assumptions (normality, constant variance, independence). This model therefore does not account for any seasonality or autocorrelation in our data.

Example: Chlorophyll levels in a lake

We observe monthly chlorophyll levels in a lake between 2001 and 2006.
We can fit a linear model of the form:

$$\text{Log Chlorophyll} = \beta_0 + \beta_1 \text{ Date} + \text{error}$$



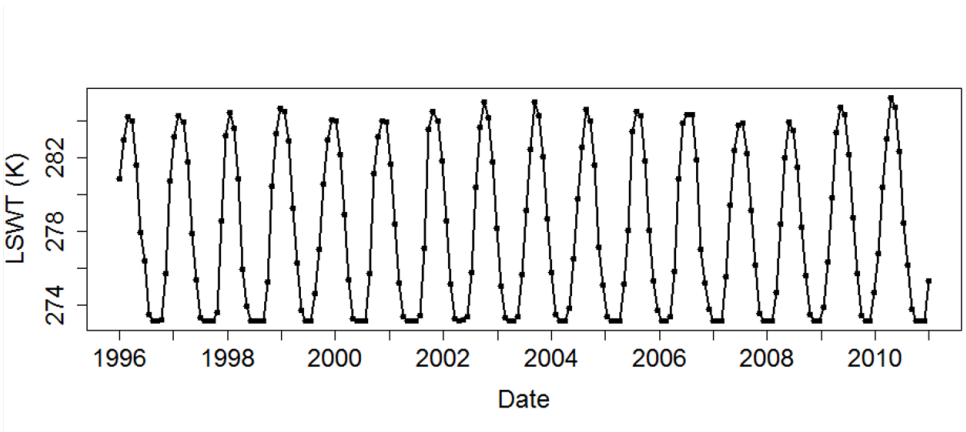
4 Seasonal Patterns

Many environmental time series have some sort of **periodicity** (e.g. a monthly pattern in temperature). We can produce some form of seasonality plot to understand this better. The **period** is the time interval between consecutive peaks or troughs. A **seasonal component** of a dataset is a regular fluctuation with a period of one year or less.

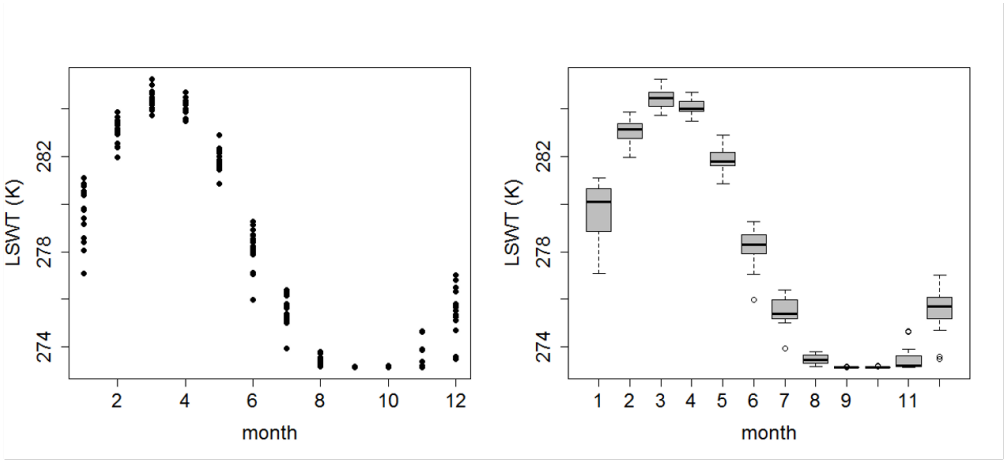
Example: Mean surface water temperature in Lake Nam

Lake Nam (Namtso) is a mountain lake in Tibet. The mean surface water temperature was measured monthly between 1996 and 2011.

We can plot the data over time, showing clear pattern in the data:

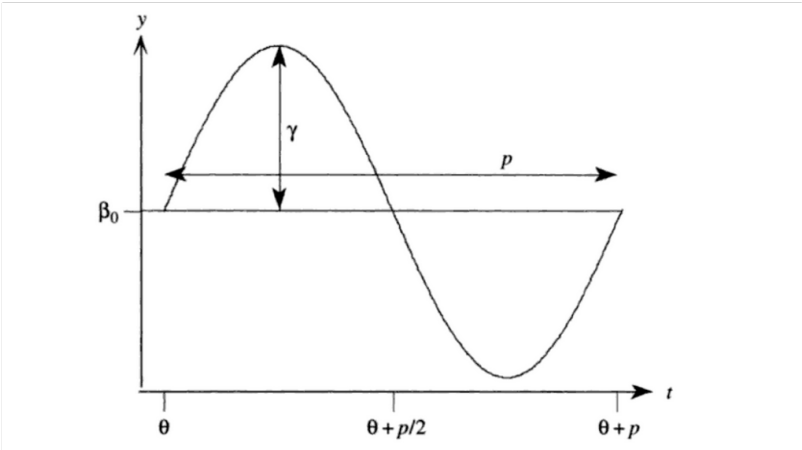


We should therefore plot the data by month. Doing so indicates a clear seasonal pattern. There is a peak in Month 3 and a trough in Months 9/10:



5 Harmonic Regression

The monthly pattern is very similar to a sine wave, and we can use this feature in our modelling. This is known as harmonic regression, and is suitable when we have a regular seasonal trend (as we just saw in the Lake Nam example).



Harmonic regression is based on an equation of the form

$$Y_t = \beta_0 + \gamma \sin\left(\frac{2\pi[u_t - \theta]}{p}\right) + \epsilon_t$$

Here, γ is the amplitude of the wave, p is the period of the wave, and θ represents the 'position' on the wave (in radians). However, it can often be more convenient to rewrite this in the form of a simple multiple regression model, taking advantage of the double angle formula.

Given that $\sin(a-b) = \sin(a)\cos(b) - \cos(a)\sin(b)$, we can show that:

$$\begin{aligned}\gamma \sin\left(\frac{2\pi[u_t - \theta]}{p}\right) &= \gamma \sin\left(\frac{2\pi u_t}{p} - \frac{2\pi\theta}{p}\right) \\ &= \gamma\left[\sin\left(\frac{2\pi u_t}{p}\right)\cos\left(\frac{2\pi\theta}{p}\right) - \cos\left(\frac{2\pi u_t}{p}\right)\sin\left(\frac{2\pi\theta}{p}\right)\right]\end{aligned}$$

Since π, θ and p are known, we can create new regression parameters $\gamma_1 = \gamma\cos\left(\frac{2\pi\theta}{p}\right)$ and $\gamma_2 = -\gamma\sin\left(\frac{2\pi\theta}{p}\right)$

The final harmonic regression model can thus be written:

$$Y_t = \beta_0 + \gamma_1 \sin\left(\frac{2\pi u_t}{p}\right) + \gamma_2 \cos\left(\frac{2\pi u_t}{p}\right) + \epsilon_t$$

Our new parameters γ_1 and γ_2 control the seasonal trends, with p representing the period. β_0 is still the intercept term, which can also be interpreted as the overall mean. Note that this is still a linear model, since it is linear in the coefficients.

The standard harmonic regression assumes we have the **same seasonal pattern** each year, but this may not always be appropriate. There are many more sophisticated models available if this assumption does not hold. Some are still based on sine and cosine waves, while others may use autocorrelation functions or a form of semiparametric smoothing.

6 Time Series Model

The seasonal variation can sometimes be so strong that it obscures the overall trend (or any other patterns). In most cases, we are not actually particularly interested in actually knowing about the seasonal trend. In these cases, it is simply a nuisance factor that we need to account for in our model. Our primary interest is usually in understanding the longer term trends in our data.

We often try to remove or separate out this seasonal pattern when analysing time series. We can therefore think of our overall time series model in the following form:

$$X = \text{trend} + \text{seasonal component} + \text{error}$$

In terms of mathematical notation, we can write this as

$$X_t = m_t + s_t + \epsilon_t.$$

Our error, ϵ_t is assumed to be random, and follows the distribution $\epsilon_t \sim \text{Normal}(0, \sigma^2)$.

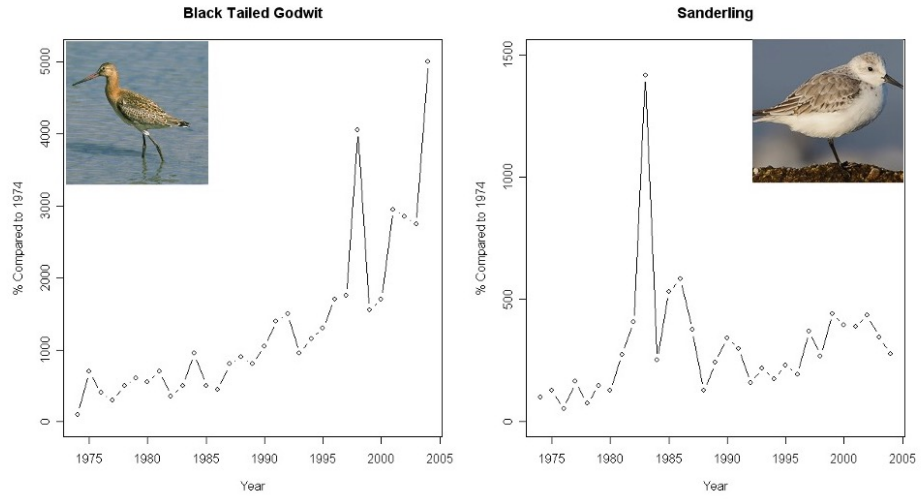
7 Estimating Trend

We have now identified a method for isolating the trend in our model. However, we still have to work out the best way to explore and understand this trend. We want to know the size of the trend, but also have to assess whether it is linear, and also test for statistical significance.

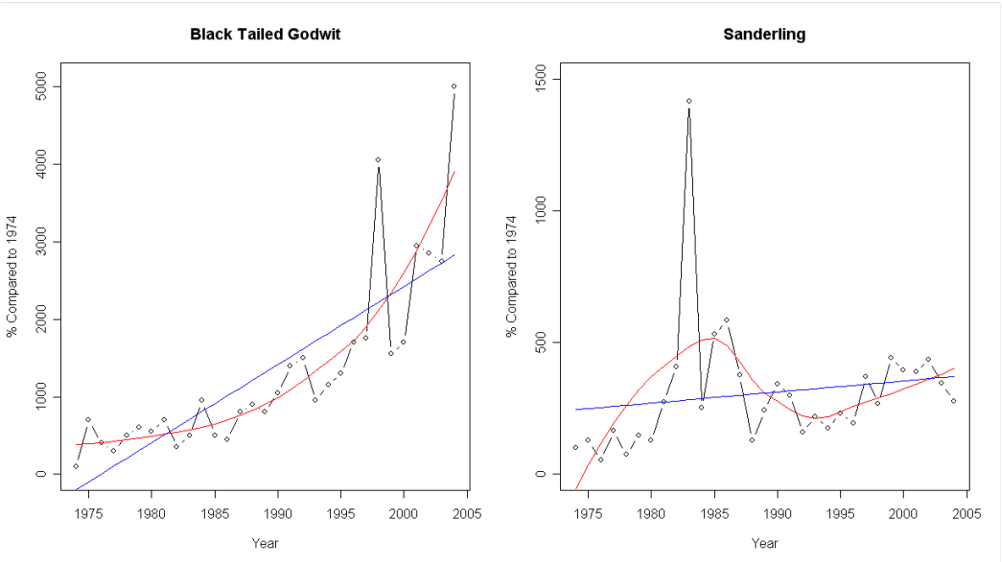
A variety of models and techniques exist for exploring our trend.

Example: Bird populations

We have collected annual data on the population of two birds between 1975 and 2005. What are the trends? Are they significantly different from zero?



We have fitted two models to attempt to assess the trends for each bird. The blue line is a linear regression, while the red line is a more flexible additive model.



Exercise 3

Which of the models are more appropriate? Have we adequately captured the patterns in the data?

Solution

Neither relationship appears to be linear, so that the additive models are more appropriate than the linear regression models here. However, both models fail to capture the peaks in the data well, so that we could consider whether other models are more appropriate. E.g., models for extremes may be more appropriate if we are interested in the peaks.

In our bird population example, both models indicate the overall trend, but they do not test for significance. We therefore cannot be sure whether the changes are 'genuine' or are simply down to random variation. We can use non-parametric approaches (e.g., Mann-Kendall test and the Seasonal Kendall) to assess the trend in our data.

7.1 Mann-Kendall test

The **Mann-Kendall test** is commonly used to detect trends in environmental, climate, and hydrological data. It looks for a consistent increase or decrease in a trend over time (not necessarily linear). It is commonly used for short time series, where we may not have sufficient data for more sophisticated approaches.

Assume we have an ordered dataset $z_1, \dots, z_T$

1. Compute ALL possible differences $d = z_j - z_k$ where $j > k$.
2. Create an indicator function sign$(z_j - z_k)$ such that:

$$\text{sign}(z_j - z_k) = \begin{cases} 1 & \text{if } z_j - z_k > 0 \\ 0 & \text{if } z_j - z_k = 0 \\ -1 & \text{if } z_j - z_k < 0 \end{cases}$$

3. The Mann-Kendall statistic, S, is given by

$$S = \sum_{k=1}^{n-1} \sum_{j=k+1}^{n} \text{sign}(z_j - z_k)$$

Our test statistic measures the size and direction of the trend:

- A positive value of S suggests the data are increasing over time (an upward trend).
- A negative value of S suggests a downward trend.
- $S = 0$ implies no trend.

We can carry out a hypothesis test to assess whether S is significantly different from zero:

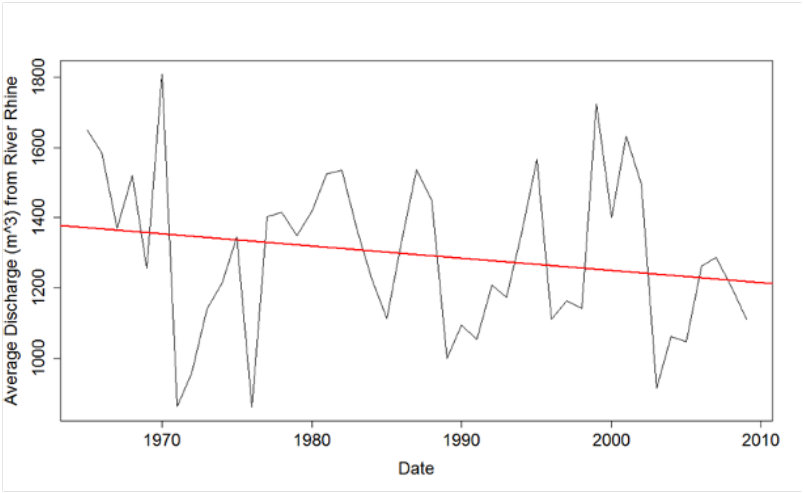
$$H_0 : \text{our data are independent random realisations (no trend)}$$
$$H_1 : \text{there is a significant trend in our data}$$

We compare the test statistic to a standard normal distribution $Z_{(1-\alpha/2)}$.

We can use the `mk.test` function in the `trend` R package, to carry out the Mann-Kendall test.

Exercise

Below, we have plotted the average discharge (m^3) from the River Rhine over many years (black line), with the overall trend line added (red line).



We carry out the Mann-Kandall test in R as follows, where the vector `Q` contains the average discharge data:

```
mk.test(Q)
```

```
Mann-Kendall Test two-sided homogeneity test
Statistics for total series

H0: S = 0 (no trend)
HA: S != 0 (monotonic trend)

Statistics for total series
      S  varS    Z    tau  pvalue
 1 -144 10450 -1.4 -0.145 0.16185
```

Given these results, what can we say in terms of the hypotheses of the test?

Solution

Here we see a p-value of 0.16, which means that there is no evidence to reject H_0 and therefore we believe that it is possible that there is no trend present.

7.2 Kendall rank correlation coefficient

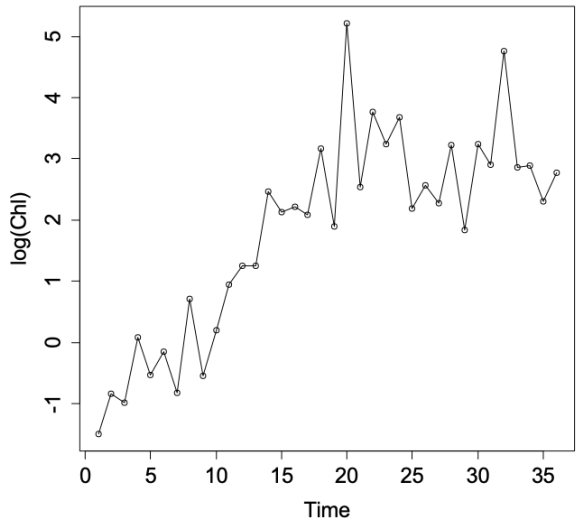
We can also compute a rank correlation coefficient, τ, which measures the strength of our trend,

$$\tau = \frac{S}{D}.$$

Here, $D = \frac{n(n-1)}{2}$, the number of pairwise comparisons used in the calculation of S. τ has a range $(-1, 1)$, similar to the standard correlation used in regression modelling.

Exercise

Chlorophyll levels in a lake have been measured over 36 years, as shown in the plot below.



Given that $S = 384$, compute τ to measure the strength of the trend.
Answer (to 2 decimal places): ____
Solution

$$\begin{aligned} D &= \frac{n(n-1)}{2} \\ &= \frac{35 \times 36}{2} \\ &= 680 \end{aligned}$$

$$\tau = \frac{S}{D} = \frac{384}{680} = 0.61$$

8 Seasonal Kendall test

The *seasonal* Kendall test accounts for seasonality by computing S for each of M seasons separately, then combining the results. For example, if we had monthly data, we might compute S separately for each month. Let S_j be the Kendall statistic for season j, then the overall statistic is given by:

$$S_k = \sum_{j=1}^{M} S_j$$

Again, this can be compared to a standard normal distribution $Z_{(1-\alpha/2)}$.

9 Smoothing in Time Series

Environmental time series data are often complex and traditional parametric methods are difficult to implement. The relationship between our parameter of interest and time may not follow a linear pattern. We could simply keep adding polynomial functions, but this may become inefficient and lead to a model with too many parameters. It is often more elegant to consider an approach which uses **smoothing**.

We can express the relationship between any response and explanatory variable as

$$y = f(x).$$

Here y is the response, x is our explanatory variable and $f()$ is a function which describes their relationship. Smoothing techniques are used to model $f()$ without specifying any specific statistical form of the underlying function.

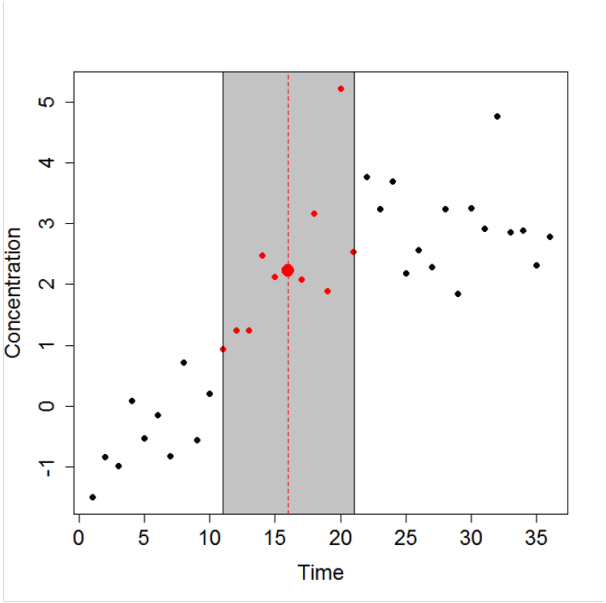
There is a whole course on smoothing methods (Flexible Regression), and many of you will already have taken this. Therefore we will simply focus briefly on a couple of key methods which are used for environmental data. We will look at one method mainly used for descriptive purposes (LOWESS) and one which is used for estimation (penalised splines).

9.1 LOWESS

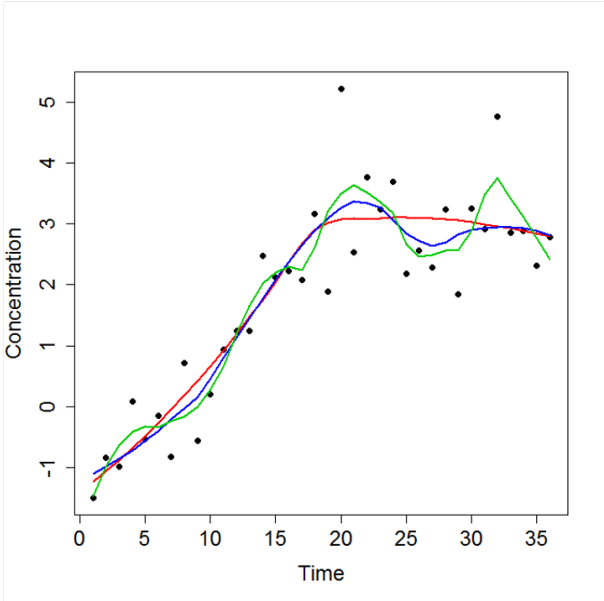
LOWESS (LOcally WEighted Scatterplot Smoothing) is an approach which is often used to obtain a graphical illustration of our data. It involves carrying out a series of polynomial regressions on small regions of the data, and then combining them. The more datapoints we have in a region, the smoother our curve will be. This can be somewhat computationally intensive compared to simple moving average methods, but generally produces a smoother function.

LOWESS involves carrying out the following steps:

- Identify a target point, x.
- Construct a 'window' containing its k nearest neighbours.
- Fit a weighted polynomial to these k datapoints.
- We then choose a new target point and repeat until we have covered all timepoints.

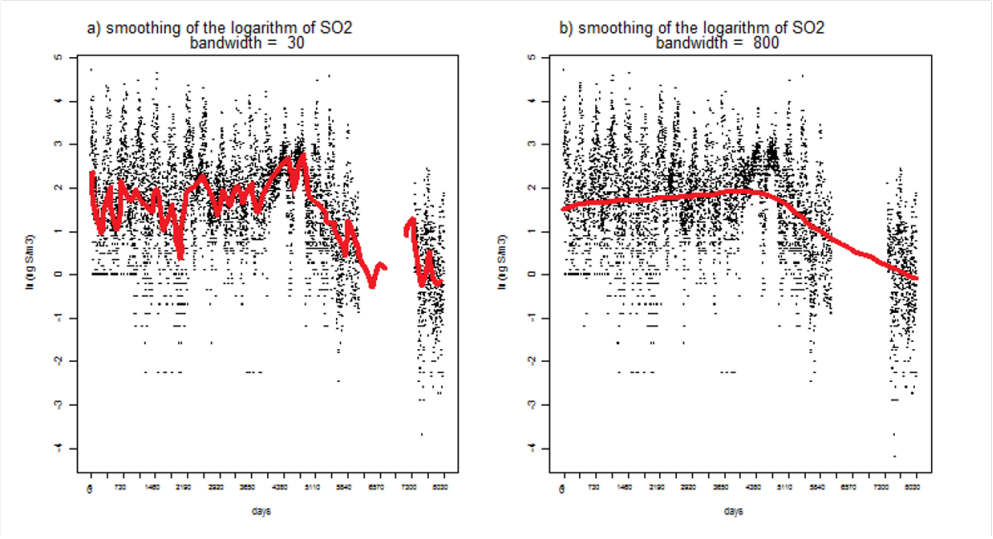


We have to decide on the size of the window. In R, the default is that each window contains two-thirds of the data. We can fit these models in R using the `scatter.smooth` or `loess` functions. The different colours in the plot below show different sizes of windows. The wider the window, the smoother the function (green narrowest, red widest).



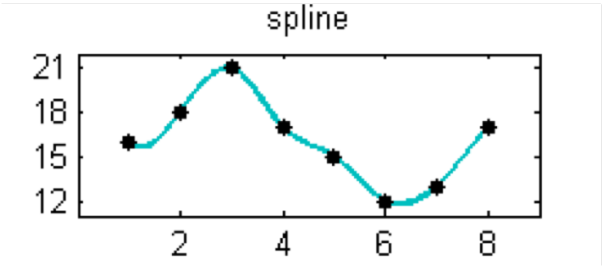
Example: SO_2 levels

Air quality SO_2 levels are measured daily over 30 years. The right plot with a wider window (higher bandwidth) is smoother (maybe too smooth?). The narrower bandwidth on the left leads to a gap where there are missing values.



9.2 Splines

Splines are an alternative approach to constructing a smooth function. This approach uses piecewise polynomials to estimate the function $f(x)$. Spline functions are polynomial segments which are joined together smoothly at predefined subintervals. The points where the functions join together are known as **knots**.



Our model takes the form:

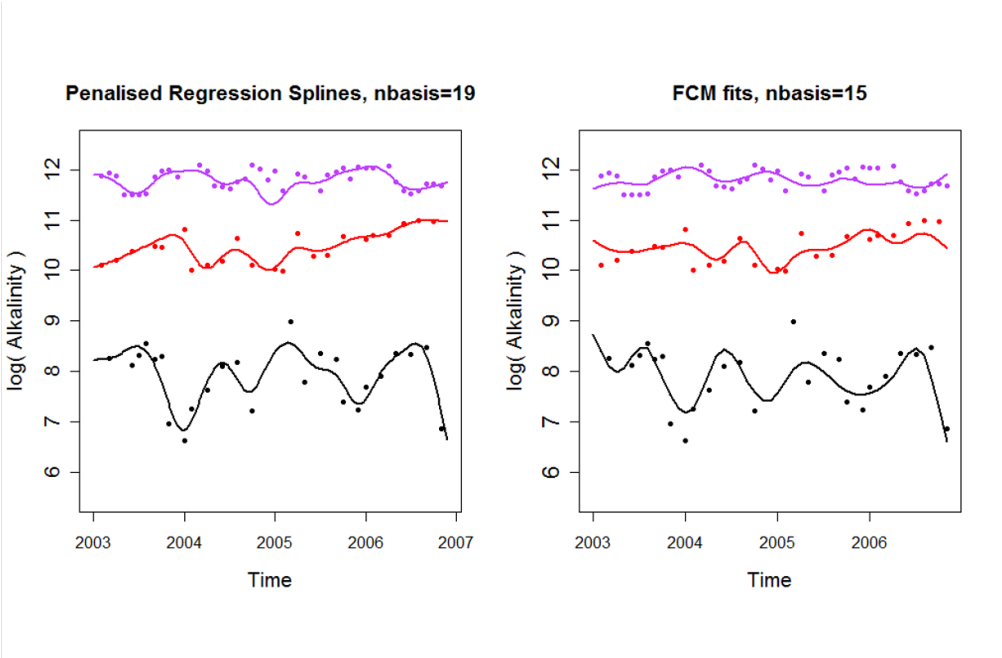
$$Y_i = f(x_i) + \epsilon_i$$

We estimate the function $f()$ as

$$\hat{f}(x_i) = \sum_{k=0}^{p} \beta_k b_k(x_i)$$

Here, $b_k()$ is a set of polynomial functions known as *basis functions* and β_k are their coefficients. We must decide in advance the value of k, which defines the number of basis functions used.

Increasing the number of basis functions leads to a more "wiggly" line. Too few basis functions might make the line too smooth, too many might lead to overfitting.



Choosing the correct number of basis functions can be difficult. Penalised splines (p-splines) avoid this issue. Using penalised splines, we can set a large number of basis functions, but then penalise the coefficients to encourage smoothness. This is a modified form of a standard linear regression, with a parameter λ which controls the smoothness of the estimator.

9.3 Additive Models

Developing methods for estimating smooth functions is only one part of the process. We must also work out how to include these in our models. Additive models are a general form of statistical model which allows us to incorporate smooth functions alongside linear terms.

$$y_i = \alpha + \sum_{j=1}^{k} g_j(x_{ij}) + \epsilon_{ij}$$

Here $g_j()$ is a smooth function for the jth explanatory variable and α is the overall mean. Note that $g_j()$ could simply be a linear function for one or more variables.

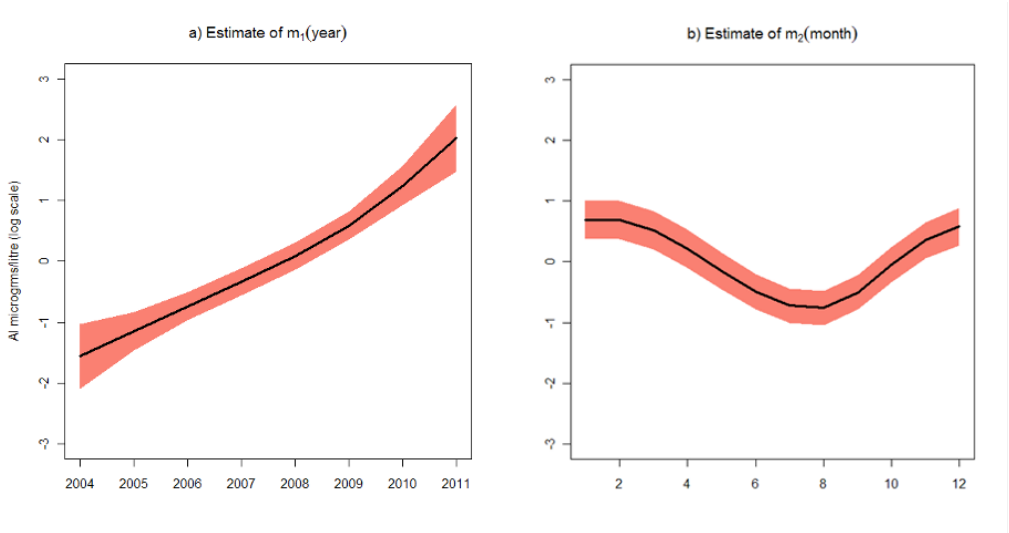
Suppose that we have a variable that exhibits a long-term trend and a seasonal pattern (like we saw in the Mauna Loa example). There are two main ways that we can incorporate this: via a separable structure, or via a non-separable structure.

9.3.1 Separable trend and seasonality

We could fit a model with smooth terms for both year (top plot) and month (bottom plot). We assume that the seasonal pattern does not change from year to year (i.e., no interaction). This can be written in the form

$$y = f_1(x_1) + f_2(x_2) + \epsilon$$

We can observe a roughly linear increasing trend, but with a seasonal pattern featuring a peak in the winter.

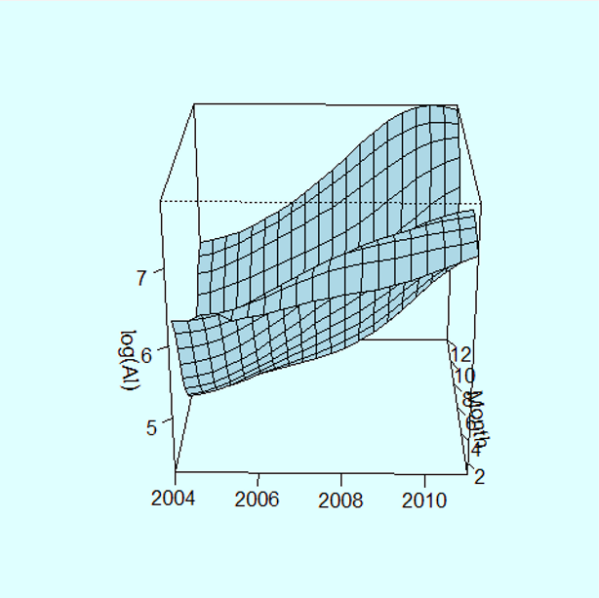


9.3.2 Non-separable trend and seasonality

Suppose we decided there was a month by year interaction (i.e., the seasonal pattern may differ by year, or the long-tern trend over the years may differ by month). We would incorporate this via a bivariate term. This can be written in the form

$$y = f(x_1, x_2) + \epsilon$$

This can be harder to interpret visually, but we can still see a similar pattern.



Note that this non-separable structure also introduces additional computation complexity (i.e., we have lots more parameters to estimate), so that it may be much slower to fit such a model, or it may require additional computational resources, compared to fitting a model with a separable structure.