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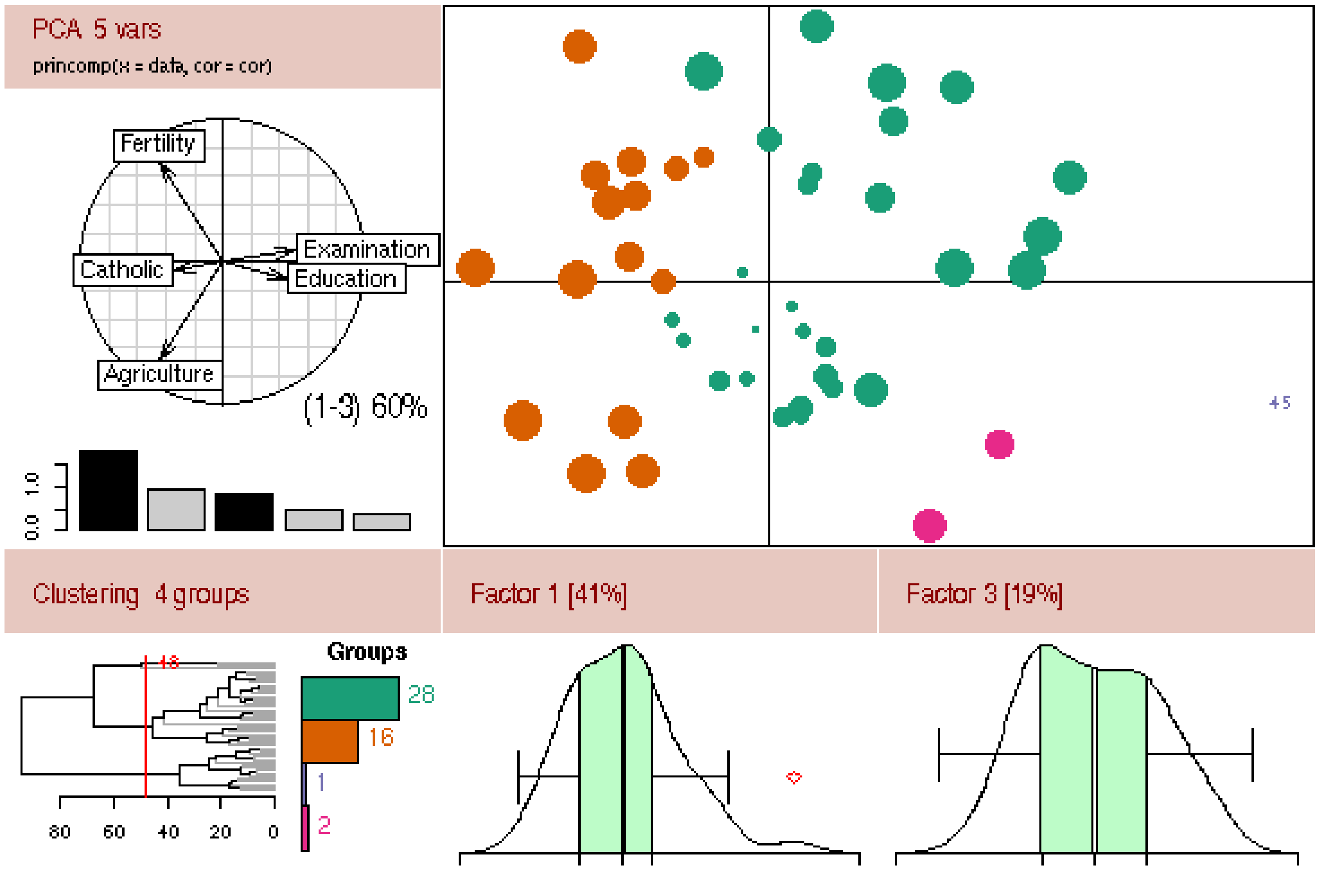
An introduction to the programming language R for environmental reseachers



Norwegian Institute for Water Research

– an institute in the Environmental Research Alliance of Norway

REPORT

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Abstract

The seminar "An introduction to the programming language R for environmental researchers" was arranged at NIVA in 2006. The objective was to help NIVA researchers get familiar with R, because it is freely available, under rapid development, and widely used by environmental scientists world-wide. This report contains the presentations, examples and exercises from the seminar. The main components of the seminar were: (1) Introduction: the R language, scripts, importing data, plotting, etc. (2) From linear models to GAM: linear regression, generalised linear models (GLM), generalised additive models (GAM), model selection. (3) Time series: trends, seasons, autocorrelation, structural changes. (4) Multivariate models: the package "vegan", community analysis, non-metric multidimensional scaling (NMDS), canonical correspondence analysis (CCA), constrained ordination. (5) Data visualization: colour gradients, 3-D GAM plots, lattice. The data and scripts used in the examples are available upon request to the authors.

4 keywords, Norwegian	4 keywords, English
1. Programmeringsverktøy	1. Programming tool
2. Statistisk analyse	2. Statistical analysis
3. Matematisk modellering	3. Mathematical modelling
4. Visualisering	4. Visualization

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An introduction to the programming language R

for environmental researchers

Preface

The seminar "An introduction to the programming language R for environmental researchers" was arranged for researchers at NIVA in 2006. Many types of statistical software are currently in use at NIVA. If more researchers used the same software, we would have a common platform for sharing scripts, data and experiences, which would facilitate collaboration. There are many good types of software available for statistical analysis, but the object-oriented programming software R has three unbeatable benefits.

1) It is freely available and can be downloaded from Internet (http://www.r-project.org), no licence or dongles are required
2) It is under rapid development and the list of available tools ("packages") contributed from users is growing steadily; many cutting-edge methods are available (e.g. GAMs and smoothers, quantile regression, mixed-effect models, community analysis, breakpoint detectors)
3) There is a large and expanding scientific community of R users, with newsletters and web fora for questions and discussions.

Moreover, this software includes all common statistical methods as well as all options for organisation of data. Therefore, all operations from formatting of data to analysis and plotting can be done within one script. This also means that all steps of data treatment and analysis can easily be communicated between researchers via email, which is an enormous benefit when collaborating internationally. However, since R is completely text-based, researchers usually need some introductory training to get familiar with this programme.

The examples given in this report are based on research problems and data provided by participants (Per Stålnacke, Heleen de Wit, and Hilde Trannum). The data and the script files are available upon request (jannicke.moe@niva.no, robert.ptacnik@niva.no).

Oslo, 20.12.2007

Jannicke Moe

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1. INTRODUCTION

Tom Andersen

1.1 The award-winning S language

The origin of **R** is **S**, an object-oriented language for statistical computing. This is used for "Programming with data" - it is thus a whole language, not just a statistical package. S was developed in AT&T labs (now Lucent Technologies) by Richard A. Becker, John M. Chambers, and Allan R. Wilks. The 1998 ACM Software Systems Award was given to John M. Chambers for the S language. The reason was that Chambers's work has "*forever altered the way people analyze, visualize, and manipulate data...*"

S-plus is a value-added version of S sold by Insightful Corporation (formerly MathSoft, Inc.). S-plus has a GUI (graphical user interface) and add-on packages.

1.1.1 The R language and environment

R is a General Public License implementation of S. It was initiated by Ross Ithaka and Robert Gentleman. So R may stand for "Ross & Robert" – supposedly. Or "R is before S" (in the alphabet).

R is freely downloadable and available for several platforms: Unix/Linux, MacOS, Windows. It has an active user community and many add-on packages

1.1.2 Differences between R and S-plus

The rationale behind R is that: "R should make it easier to detect programming errors, while at the same time being as compatible as possible with S".

S-plus stores objects as separate files, whereas R objects are stored internally. R is generally faster than S-plus, especially to load. But - R objects are lost if R crashes! You should save R workspace to avoid this.

It is important to be aware of certain differences: (the meaning will become clear later...):

– Powers in formulae must be in "insulated" in R

S-plus: `y ~ x + x^2`
R: `y ~ x + I(x^2)`

– R uses different default contrasts in (generalized) linear models

S-plus: Helmert contrasts
R: Treatment contrasts

1.1.3 Installing R

R can be installed without administrator privileges! Go to http://cran.r-project.org/ (CRAN = Comprehensive R Archive Network). Select a Precompiled Binary Distribution: Linux, MacOS, or Windows.

Windows installation:
– Select "Windows (95 or later)"
– Select "Base distribution"
– Download and run "rw2011.exe" (or the latest version)

Packages can be installed from the menu *Packages* -> *Install package(s)*. Installation from local zip files is possible, but NOT recommended. When installed, a package can be loaded to the workspace by `require()` or by `library()`.

1.1.4 A first encounter with R

Create a directory (folder) on your home area called “R-seminar” (for example).
Start R.
Select from the menu: *File -> Change dir...*
Select the directory you just created. All files will now be loaded from and saved to this directory.

Type “demo(graphics)” in the “R console” window to see some capabilities of R. Press enter (return) until the demo ends. Notice what happens in the console and graphics windows.

R returns answers to arithmetical expressions typed in the console window.
– Arithmetic operators (+-*/)
– Transcendental functions: sin, cos, exp, log, etc.
– Etc.

Expressions can include named variables.
Expressions can be assigned to variables. R uses a special assignment operator: `"<-"`

Remember:
– R uses Anglo-American decimal separator (period, not comma).
– R is case-sensitive (e.g. ANC ≠ anc)
– Lines starting with # are ignored (comments).

1.2 Object-oriented programming in R

Objects in R can be lists. Lists are in turn ordered collections of objects.
Arrays are lists of objects of a single type: Numerical, character, or logical.
List components can be named:
```
> names(object)
```
How to construct a list:
```
> list(object1, object2, ...)
```
List components can be accessed in different ways:
```
> object$component
> object[index]
> attach(object)
> detach(object)
```

1.2.1 Data frames in R

Data tables are usually arranged as the object type `data.frame`, with different variables in columns and subjects/sites/samples in rows. A data frame is a list of data arrays of same length, but not necessarily of same type (continuous, categorical etc.). Both rows and columns of a data frame can be named. The elements can be accessed by names, or by indexing.
Whole column:
```
> frame$column.name
> frame[, "column.name"]
> frame[, column.number]
```
Single element:
```
> frame[row.number,]$column.name
> frame["row.name", "column.name"]
> frame[row.number, column.number]
```

1.2.2 Importing data into R

In order to read a data file, you need to set the correct search path first. With the command window in front, select from the menu:

File -> Change dir...

and navigate to the directory where your file is located.

Alternatively, you can use the console to tell R where to look for and store files and objects.
Where to look for files:
```
> choose.dir()
```
Where to put objects (optional):
```
> setwd()
```
Within the brackets you must write the whole path with double back-slashes and quotes, e.g.:
```
> choose.dir("C:\\R-seminar\\Day1\\")
```

A data table from an ASCII file or other text can be read into a data frame by `read.table()`:
```
> data.frame <- read.table("datafile.txt", header = TRUE)
```
`header = TRUE`: use first row as variable names.

Alternatively, you can specify the path directly in the read command. This can be useful if you want to read files from different locations in the same script. (NB: this only tells R where to read files from, not where to store files). For example:
```
> DATA <- read.table("C:\\R-seminar\\Day1\\data.txt", header=T)
```
(Here you must write the name of your own path. Note that R uses double backslashes!)
This version can be even further generalised (for easier transfer to new scripts):
```
> path <- "C:\\R-seminar\\Day1\\"
> file <- "data.txt"
> DATA <- read.table(paste(path, file, sep=""), header=T)
```
`paste()` is a useful function for combining text. Here `paste()` is used to combine the path and file names. (`sep=" "` is default, so one must say `sep=""` to avoid the space.)

When using the `read.table()` function, each row in the data table must have the same number of elements. The elements can be separated e.g. by tabs (`sep="\t"`) or by spaces (`sep=" "`). Missing values are coded as “NA” (Not Available).

Proprietary file formats like Excel are not supported. Excel worksheet should be saved as tab-delimited text files, then they can be imported with `read.table()`.

1.2.3 Basic R graphics

Make a scatter plot:
```
> plot(...)
```
Add points to a plot:
```
> points(...)
```
Add lines to a plot:
```
> lines(...)
```
Change plot parameters:
```
> par(...)
```
Add a straight line to a plot:
```
> abline(...)
```
Notice: Smoothing functions (section 2.6) are great to reveal trends in your data. But there are many ways to use them and they can give quite different results, so they should be used with caution.

Make a histogram:
```
> hist(...)
```
Appearance depends on how breaks are set. Again, there are many ways to set them, so be careful.

1.2.4 Scripts in R

A script is a sequence of R commands collected in a text file. There are several benefits of using script files:
– You can build up an analysis
– You can easily change settings and re-run the analysis
– You can make a new analysis or analyse new data by modifying an old analysis
– You can document and recall the steps in your analysis
– You can share models, analyses and plotting routines with colleagues

Make a script file by selecting from the menu: *File* -> *New script*. You can run a script by either:
– Typing `source("scriptfile.R")` in the console window
– Selecting text and right-click: *Run selection*
– Selecting text and pressing ctrl-R

1.2.5 Control structures in R

When you want a part of the script to execute only under certain conditions:

```
if (conditions) {execute commands}
> if (x < 0) {x <- 0}
Other possibilities with if :
       if(test) {yes} else {no}
       ifelse(test, yes, no)
```

When you want a part of the script to execute many times:

```
       for (index) {execute commands}
> for (i in 1:10) {print(10^i)}
```

For larger operations, functions like **`apply()`** are more efficient than `for()` loops (see example p. 67).

Notice: There are different types of brackets:
`()` for grouping expressions
`[]` for indexing
`{}` for grouping statements

1.2.6 User-defined functions in R

When you have a piece of code that you will use repeatedly, you should make a function:

```
       function(input...) {commands... return(output...)}
```

Executing a function script creates a function object. The object is executed when the function is called.

1.2.7 Getting help

R has an extensive set of help files in html format. However, R (and S-plus) help is basically written <u>by</u> programmers <u>for</u> programmers... Manuals are available from inside R:
– Menu *Help* -> *Manuals* (in PDF)
– `help.start()` in console window, opens general HTML help in web browser

Help on commands, functions calls, etc from the console window:

```
> help(plot)  # or
> ?plot  # help window on plot function
```

Syntax, parameters, examples, related topics:

```
> help.search("plot") # all help windows containing "plot"
> help(help.search)  # for options
> help(package = "vegan") # help for an installed package
```

A package must be installed, before you can search for help on the package.

1.3 Example 1: Plot snow cover data

The first example is a time series of snow cover in Asia in the period 1970-1979.

We can specify an integer range by the colon (:) operator
```
> year <- 1970:1979
> year
[1] 1970 1971 1972 1973 1974 1975 1976 1977 1978 1979
```

The `c()` operator constructs a list from its arguments. Arguments can again be lists (lists of lists = matrices, etc)
```
> snow.cover <- c(6.5,12.0,14.9,10.0,10.7,7.9,21.9,12.5,14.5,9.2)
> snow.cover
 [1]  6.5 12.0 14.9 10.0 10.7  7.9 21.9 12.5 14.5  9.2
```

Notice periods (.) are allowed in variable names while e.g. underscores (_) are NOT recommended (cf. MS Access export files). Notice also that variable names are case sensitive
```
> Snow.cover
Error: object "Snow.cover" not found
```

Now let's make a simple plot of the data with the `plot()` command (**Figure 1**, left panel).
```
> plot(year,snow.cover)
```

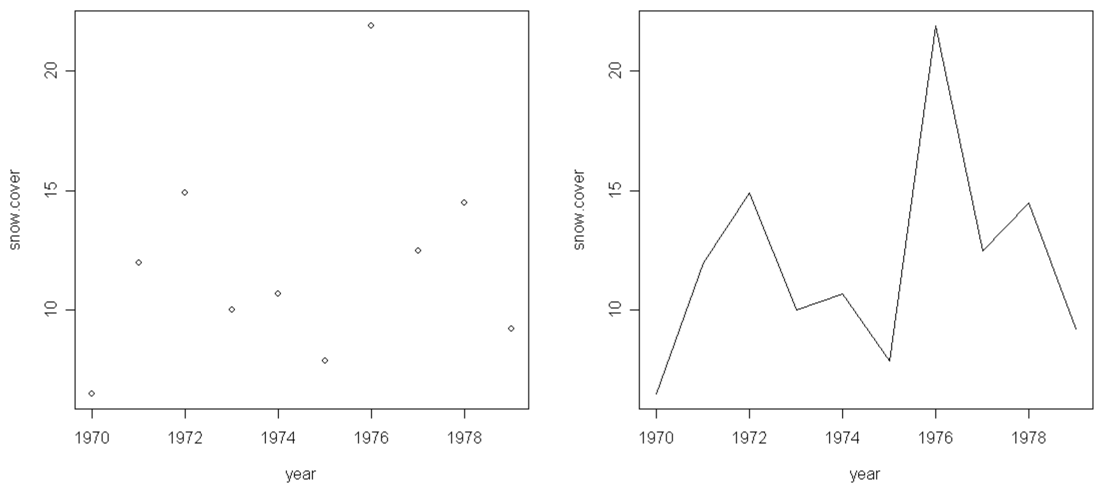


Figure 1. Plots for the data set snow.cover. Left panel: points; right panel: lines.

OK, but kind of dull - aren't there any glitziness-knobs to turn? Let's get some help on this:
```
> help(plot)
```

A line plot would perhaps be more informative? (**Figure 1**, right panel)
```
> plot(year,snow.cover, type = "l")
```

Notice that we use the "<-" operator to assign objects but we use the "=" operator to change function call parameters from default values.

Let's put in some more informative text:
```
> plot(year,snow.cover, type = "l",
+ main = "Asia snow cover 1970-1979",
+ ylab = "Snow cover (mill. sq.km)")
```

Not for the faint of heart: superscripts in legends. Note that the `expression()` function expects individual terms to be separated by asterisks (*)

```
> plot(year,snow.cover, type = "l",
+ main = "Asia snow cover 1970-1979",
+ ylab = expression("Snow cover (" * 10^6 * " " * km^2 * ")"))
```

Check `help(plotmath)` for more info on plotting mathematical symbols.

Now, what about line styles? Nothing about this in the help for `plot()`. Many graphics settings are documented in the catch-all function `par()` even parameters which are normally used in `plot()`...

```
> help(par)
```

Scroll down to the entries for col and lwd

```
        col - set the color of a line (predefined or RGB)
        lwd - set the line width (scaling factor relative to default (1))
> plot(year,snow.cover, type = "l",
+       col = "red", lwd = 4,
+       main = "Asia snow cover 1970-1979",
+       ylab = expression("Snow cover (" * 10^6 * " " * km^2 * ")"))
```

Notice that colors can be specified in several ways

```
#       "red" = "#FF0000" = rgb(255,0,0)
```

The function `colors()` gives a (long) list of predefined colors

Suppose we make many different plot of this type then we could make it into a function `snowplot(t,x,s)` with parameters `t = years`, `x = snow cover`, `s = legend`

```
> snow.plot <- function(t,x,s) {
+ plot(t,x, type = "l", col = "red", lwd = 4, main = s,
+ xlab = "", ylab = expression("Snow cover (" * 10^6 * " " * km^2 * ")"))
+ }
```

The curly brackets {} enclose what the function actually does. Notice that we need to execute the function definition for the snow.plot function to exist in memory. Type the function name in the command window to check that it's there

```
> snow.plot.
```

We can produce the same plot as before by calling our new function:

```
> snow.plot(year,snow.cover,"Asia snow cover 1970-1979")
```

We can add data to an existing plot with functions `points()` and `lines()`
The function `abline()` lets add straight lines to a plot.

```
> help(abline)
```

Let's add a horizontal line for the mean snow cover:

```
> abline(h = mean(snow.cover), lty = 2, lwd = 2, col = "blue")
```

Or maybe we would rather show the snow cover anomalies:

```
> snow.anom <- snow.cover - mean(snow.cover)
> plot(year,snow.anom, type = "l", col = "red", lwd = 4,
+       main = "Asia snow cover 1970-1979",
+       ylab = expression("Snow cover anomaly (" * 10^6 * " " * km^2 * ")"))
+ abline(h = 0, lty = 2, lwd = 2, col = "blue")
```

Maybe it would look better with y axis symmetrical around 0? Parameters settings for axis limits are for some reason not documented in `plot()` but in `plot.default()` ???

```
> help(plot.default)
```

Ahhh... of course, `ylim =` ...
Notice that `xlim` and `ylim` expect 2-element lists as arguments, which we construct with the `c()` operator.

```
> plot(year,snow.anom, type = "l", col = "red", lwd = 4,
+      ylim = c(-11, 11),
+      main = "Asia snow cover 1970-1979",
+      ylab = expression("Snow cover anomaly (" * 10^6 * km^2 * ")"))
> abline(h = 0, lty = 2, lwd = 2, col = "blue")
```

We can make a function for this plot as well. But we should make sure that the function will work with any data set, not just those within the range -11 to 11

```
> snow.anomaly.plot <- function(t,x,s) {
+ z <- x - mean(x)
+ plot(t,z, type = "l", col = "red", lwd = 4, main = s,
+ ylim = c(-1, 1) * (1.05 * max(abs(z))),
+ xlab = "", ylab = expression("Snow cover anomaly (" * 10^6 * " " * km^2 * ")"))
+ abline(h = 0, lty = 2, lwd = 2, col = "blue")
+ }
```

Now check if it works as intended (**Figure 2**):

```
> snow.anomaly.plot(year,snow.cover,"Asia snow cover anomaly 1970-1979")
```

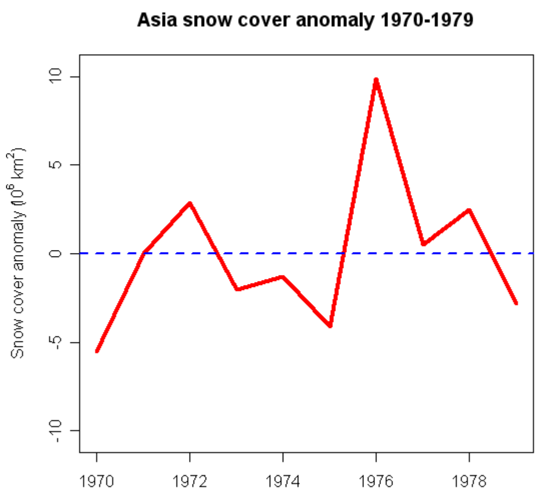


Figure 2. Plots for the data set snow.cover, shown as anomalies (deviations from the mean)

What if we want to have several graphs in the same window?
Again, this is accomplished with the `par()` function
`mfrow` = Multiple figures, row-wise (siebling of `mfcol`)
`mfrow` expects number of rows and columns in a 2-element list

```
> par(mfrow = c(2,1))      # 2 rows of figures with 1 each
```

Now we can plot both absolute snow cover and anomalies below each other (**Figure 3**):

```
> snow.plot(year,snow.cover,"Asia snow cover 1970-1979")
> snow.anomaly.plot(year,snow.cover,"Asia snow cover anomaly 1970-1979")
```

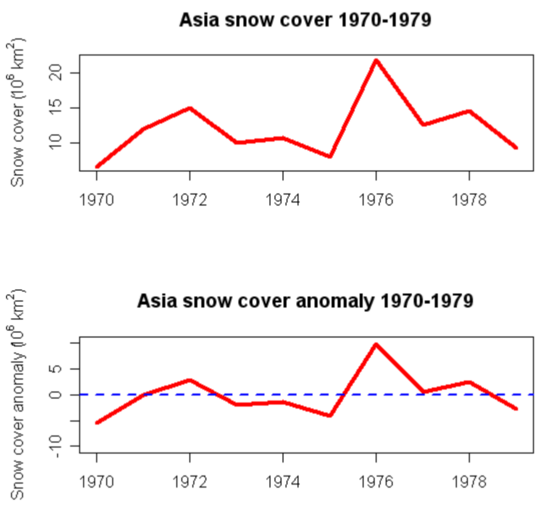


Figure 3. Plots for the data set snow.cover: absolute values (upper) and anomalies (lower).

It is good programming practice to restore default settings:
```
> par(mfrow = c(1,1))
```

We can also save the whole graphics environment and restore it afterwards.
```
> oldpar <- par(mfrow = c(2,1))
> snow.plot(year,snow.cover,"Asia snow cover 1970-1979")
> snow.anomaly.plot(year,snow.cover,"Asia snow cover anomaly 1970-1979")
> par(oldpar)
```

Function `ls()` (unix heritage) gives us a list of the objects that currently exist in the R workspace
```
> ls()
```

If you see more than 5 objects then these are probably leftovers from previous R sessions. Let's continue with a clean slate... We can clear the workspace by either selecting

Misc -> Remove all objects

(you need to have to console window in front for this menu to show), or you can do this mystical incantation:
```
> rm(list=ls(all=TRUE))
```

Remember that R operates exclusively on data structures in memory (while e.g. S-plus operates on files). This means that all our current variables die if R crashes (happens sometimes...). Which is another good reason to work from scripts and save them often!

Entering data in a script with the `c()` function is normally not a good idea except for very small data sets. Typically you will have data in a file of some kind, which you want to read into R.

R does not read propritary file formats like MS Excel directly. This means that data must be exported to a delimited text file first. Select menu *File -> Save as...*, and choose file type Text (Tab delimited)

In order to read a data file, you need to set the correct search path first. With the command window in front, select

File -> Change dir...

and navigate to the directory where your file is located.

To check that you're actually in the right spot, you can view the content of your current working directory by writing (as in ancient DOS):

```
> dir()
```

```
If you see the file name Asia.snow.cover.txt in the working directory you can read
it by using the function read.table()
> asia.snow <- read.table("Asia.snow.cover.txt", header=TRUE)
```

If there is no error message you should see a new object in your workspace:

```
> ls()
[1] "asia.snow"
```

The `asia.snow` object will show its content if we write its name. The generic function `names()` gives a list of an object's attributes:

```
> asia.snow
   year snow.cover
1  1970        6.5
2  1971       12.0
3  1972       14.9
4  1973       10.0
5  1974       10.7
6  1975        7.9
7  1976       21.9
8  1977       12.5
9  1978       14.5
10 1979        9.2

> names(asia.snow)
[1] "year"       "snow.cover"
```

`asia.snow` is an object called a dataframe, which is a rectangular table with individually named columns that can be of different data types. We can inspect a dataframe in a (primitive) spreadsheet view:

```
> fix(asia.snow)
```

We can inspect the contents of any object with the `str()` function. The `summary()` function gives information about the content of an object. An object can also show itself graphically though the `plot()` function. Most objects should have generic functions like `print(), plot(), summary()`

```
> str(asia.snow)
`data.frame':   10 obs. of  2 variables:
 $ year      : int  1970 1971 1972 1973 1974 1975 1976 1977 1978 1979
 $ snow.cover: num  6.5 12 14.9 10 10.7 7.9 21.9 12.5 14.5 9.2
> summary(asia.snow)
      year        snow.cover
 Min.   :1970   Min.   : 6.50
 1st Qu.:1972   1st Qu.: 9.40
 Median :1975   Median :11.35
 Mean   :1975   Mean   :12.01
 3rd Qu.:1977   3rd Qu.:14.00
 Max.   :1979   Max.   :21.90
> plot(asia.snow)
```

The latter gives the same plot as we got earlier from

```
> plot(year,snow.cover)    # (See Figure 1)
```

But what happens if we try this now? We get an error message. This is because the variable "`year`" is currently not visible outside the dataframe "`asia.snow`"

We can make the attributes of a data frame visible in 3 ways:
- Accessing attributes of an object explicitly with the `$` operator
- Accessing individual table columns with the `[[]]` operator
- Make all attributes accessible with the `attach()` function

We can specify a specific attribute with the `$` operator

```
> plot(asia.snow$year, asia.snow$snow.cover)
```

Individual cells in a dataframe can be addressed by bracket indexing `[row,column]`. Entire rows or columns are addressed by `[row, ]` or `[ ,column]`. Double brackets `[[index]]` can be used to access whole columns of a dataframe:

```
> plot(asia.snow[[1]], asia.snow[[2]])
```

We can put all attributes into the search path with `attach()`. It is good programming practice to `detach()` an object when you don't need it anymore (to avoid confusing variables with same name):

```
> attach(asia.snow)
> plot(year,snow.cover)
> detach(asia.snow)
```

In the `read.table()` call we set the parameter `header = TRUE` because we wanted the first row to be treated specially as variable names. What happens if we use the default (`header = FALSE`)?

```
> asia.snow <- read.table("Asia.snow.cover.txt")
> str(asia.snow)
`data.frame':   11 obs. of  2 variables:
 $ V1: Factor w/ 11 levels "1970","1971",..: 11 1 2 3 4 5 6 7 8 9 ...
 $ V2: Factor w/ 11 levels "10.0","10.7",..: 11 8 3 6 1 2 9 7 4 5 ...
```

Now we get 2 variables with generic names V1 and V2, while our variable names appear in the first row of the table. Since there is at least 1 text field in each column, both become factor (nominal) variables. The `summary()` of a factor variable is just an alphabethically sorted list the number of occurrences of each unique string (factor level).

Let's take a closer look at the documentation for `read.table()`

```
> help(read.table)
```

There are actually quite a few knobs to turn in this function. Of particular relevance to non-anglo-americans is the possibility to handle other the default decimal separator dec = "."

The file asia.snow.cover.no.txt uses the official Norwegian decimal separator (,), which the default setting would interpret as text:

```
> asia.snow <- read.table("Asia.snow.cover.no.txt", header = TRUE)
> str(asia.snow)
`data.frame':   10 obs. of  2 variables:
 $ year      : int  1970 1971 1972 1973 1974 1975 1976 1977 1978 1979
 $ snow.cover: Factor w/ 10 levels "10,0","10,7",..: 8 3 6 1 2 9 7 4 5 10
```

The file is read correctly with the setting dec = ",":

```
> asia.snow <- read.table("Asia.snow.cover.no.txt", header = TRUE, dec = ",")
> str(asia.snow)
`data.frame':   10 obs. of  2 variables:
 $ year      : int  1970 1971 1972 1973 1974 1975 1976 1977 1978 1979
 $ snow.cover: num  6.5 12 14.9 10 10.7 7.9 21.9 12.5 14.5 9.2
```

`read.table()` is not very forgiving with empty cells or unequal number of cells per row (remember: no blanks in variable or factor level names, concatenate of pad with periods; e.g. "snow.cover"). Missing values must be flagged with the special symbol "NA" (not applicable). Delete empty rows: they make the table more readable for you, but not for R...

```
> asia.snow <- read.table("Asia.snow.cover.NA.txt", header = TRUE)
> plot(asia.snow, type = "l", col = "red", lwd = 4)
```

We can remove all rows with missing values with the `na.omit()` function:

```
> plot(na.omit(asia.snow), type = "l", col = "red", lwd = 4)
```

We can also assemble a dataframe by hand, from any set of vector objects of the same size. This is most useful for quantities derived from the original input data, e.g. by transformations:

```
> year <- 1970:1979
> snow.cover <- c(6.5,12.0,14.9,10.0,10.7,7.9,21.9,12.5,14.5,9.2)
> asia.snow <- data.frame(year,snow.cover)
> rm(year, snow.cover)
> plot(asia.snow)
```

The Asian snow cover data is more than just a table, it is an ordered table - a time series. So maybe we should have taken this into consideration from the start? R has a particular object class for time series:

```
> help(ts)
Time-Series Objects
Description:
     The function 'ts' is used to create time-series objects.
     'as.ts' and 'is.ts' coerce an object to a time-series and test
     whether an object is a time series.
```

So, let's make a ts object instead. Time series have their own plot method with line as default.

```
> snow.cover <- c(6.5,12.0,14.9,10.0,10.7,7.9,21.9,12.5,14.5,9.2)
> asia.snow <- ts(snow.cover, start = 1970)
> str(asia.snow)
Time-Series [1:10] from 1970 to 1979: 6.5 12 14.9 10 10.7 7.9 21.9 12.5 14.5 9.2
> plot(asia.snow)
```

What more can we do with time series objects?

```
> help.search("time series")
```

`lag.plot()` - that looks interesting? What does it do?

```
> help(lag.plot)
Time Series Lag Plots
Description:
     Plot time series against lagged versions of themselves.
```

OK, let's try it:

```
> lag.plot(asia.snow)
```

Neat, but maybe not too useful for this data set? We will get back to time series objects later in the course, though.

1.4 Example 2: Explore and plot water chemistry data

Water chemistry data from NIVA's national lake survey 1995: subset of 716 lakes from southern Norway.
- Unit for Ca, Mg, Na, K, Cl, SO_4: mg/L
- Unit for HCO_3: meq/L,
- Unit for NO_3: µg/L

```
> ion.data <- read.table("N716ion.txt", header = TRUE)
```

Did we get all the rows and columns that should have been there?

```
> dim(ion.data)
[1] 716  10
```

List variable names to get an overview:

```
> names(ion.data)
 [1] "FYLKE" "K20"    "Ca"     "Mg"     "Na"    "K"      "HCO3"   "Cl"
 [9] "SO4"    "NO3"
```

Show summary statistics:

```
> summary(ion.data)
     FYLKE
 Min.   : 1.000
 1st Qu.: 6.000
 Median : 9.000
 Mean   : 9.356
 3rd Qu.:12.000
 Max.   :16.000
(Etc.)
```

We can use a stem-and-leaf plot get an overview of the distribution of samples among regions (FYLKE)

```
> stem(ion.data$FYLKE)
  The decimal point is at the |

   1 | 000000000000
   2 | 0000000000000
   3 | 000
   4 | 00000000000000000000000000000000000000000000000000
   5 | 00000000000000000000000000000000000000000000000000000000000000000000
   6 | 00000000000000000000000000000000000000000000000000000000000000
   7 | 0000
   8 | 00000000000000000000000000000000000000000000000000000000000000000000
   9 | 0000000000000000000000000000000000000000000000000000000000000000
  10 | 000000000000000000000000000000000000000000000000000000000000
  11 | 00000000000000000000000000000000000000000000000000000000000000000000
  12 | 00000000000000000000000000000000000000000000000000000000000000000000
  13 |
  14 | 00000000000000000000000000000000000000000000000000000000000000000000
  15 | 000000000000000000000000000000000
  16 | 00000000000000000000000000000000000000
```

FYLKE > 16 is missing since this is a S. Norway subset.
FYLKE 13 is missing (used to be Bergen).
FYLKE 3 (Oslo) and 7 (Vestfold) have the lowest number of samples.

How would this work out with a histogram (**Figure 4**)?

```
> hist(ion.data$FYLKE)
```

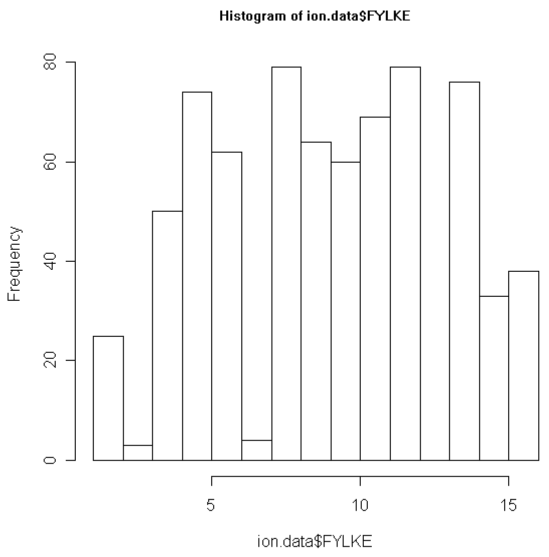


Figure 4. Histogram for NIVA chemistry data: number of observations per Fylke (county).

There's something wrong with the break placement. Maybe we should define the breaks explicitly? Let each bin bracket the integers from 0 to 20 (**Figure 5**):

```
> hist(ion.data$FYLKE,breaks=-0.5:20.5)
```

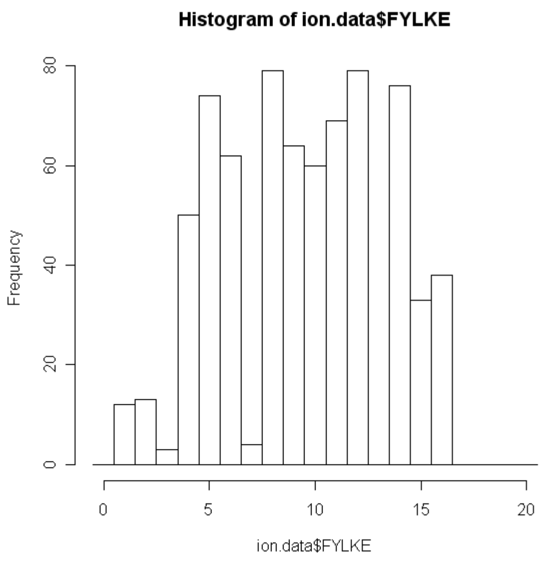


Figure 5. Histogram for NIVA chemistry data: number of observations per Fylke (county), with bins as integers.

What type of variable is FYLKE anyway?

```
> str(ion.data$FYLKE)
int [1:716] 1 1 1 1 1 1 1 1 1 1 ...
```

Maybe FYLKE should be considered a factor variable? Now, how do we make factor variable?

```
> ?factor
```

We overwrite the original with the new factor variable

```
> ion.data$FYLKE <- as.factor(ion.data$FYLKE)
```

Check the result: FYLKE should now be factor

```
> str(ion.data$FYLKE)
Factor w/ 15 levels "1","2","3","4",..: 1 1 1 1 1 1 1 1 1 1 ...
```

Maybe we could change the levels to something more meaningful? What options do we have to do this?

```
> ?levels
```

Ahhh... Of course. We just replace the levels with a list of same length.

```
> levels(ion.data$FYLKE) <-
c("Øf","Ah","Os","He","Op","Bu","Vf","Te","AA","VA","Ro","Ho","SF","MR","ST")
```

Let's see how this worked

```
> summary(ion.data$FYLKE)
Øf Ah Os He Op Bu Vf Te AA VA Ro Ho SF MR ST
12 13  3 50 74 62  4 79 64 60 69 79 76 33 38
```

But what happens if we now want to do the same histogram as before?

```
> hist(ion.data$FYLKE)
Error in hist.default(ion.data$FYLKE) : 'x' must be numeric
```

This gives an error message because FYLKE is no longer numerical.

We can recover the numerical ranks of factors with the function `as.integer()`

```
> hist(as.integer(ion.data$FYLKE),breaks=-0.5:20.5)   # Figure 6
```

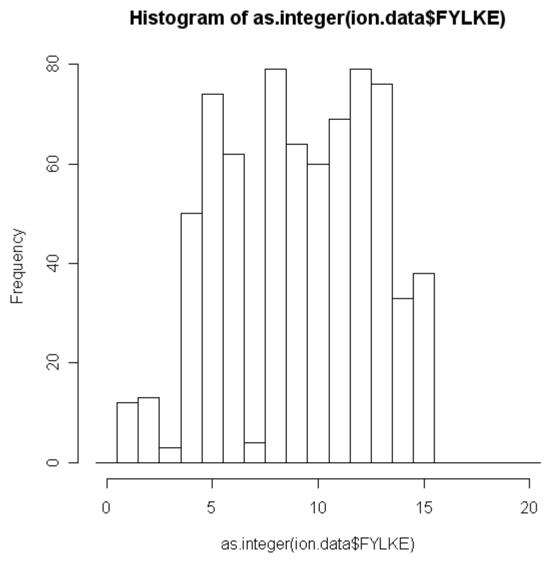


Figure 6. Histogram for NIVA chemistry data: number of observations per Fylke (county), with Fylke as integer.

Ups! - only almost recovered. Notice FYLKE 13 is no longer missing because levels have been remapped from 1,2,..,12,14,15,16 to 1,2,..,12,13,14,15. So maybe this was not the way to do it? Well, what we actually need is to produce bars with values given by `summary(FYLKE)`. Is there something called

```
> ?barplot
```

Yes, that seems to do the job (**Figure 7**).

```
> barplot(summary(ion.data$FYLKE))
```

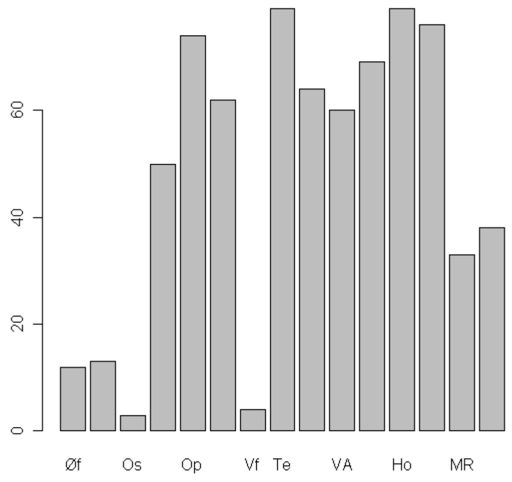


Figure 7. Barplot of NIVA chemistry data: number of observations per Fylke.

Now that we got a regional factor variable, can we then do regional boxplots?

```
> ?boxplot
```

Let's attach the data frame to make the coding more readable

```
> attach(ion.data)
```

Yes, it says we can use a "`y ~ group`" formula to make grouped boxplots. For example chloride grouped by region (expand the windows to all legends)

```
> boxplot(Cl ~ FYLKE)      # Figure 8
```

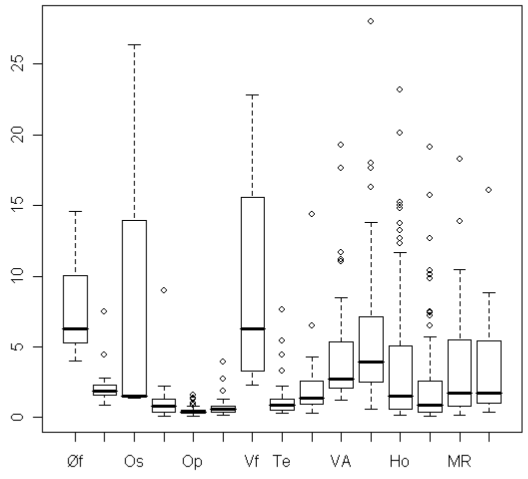


Figure 8. Boxplot of NIVA chemistry data: Chloride per Fylke.

Hmmm... Oslo and Vestfold seems to break a pattern here. These were also the smallest regions with the lowest number of samples. Is there a way to exclude these regions?

```
> ?which
```

So we need a logical statement which is `TRUE` except for Oslo and Vestfold. Remember that R uses the following logical operators: "!" (NOT), "`&`" (AND), "|" (OR). Notice that R uses symbols "`==`" for EQUAL and "`!=`" for NOT EQUAL.

```
> not.Os.Vf <- which((FYLKE != "Os") & (FYLKE != "Vf"))
> boxplot(Cl[not.Os.Vf] ~ FYLKE[not.Os.Vf])
```

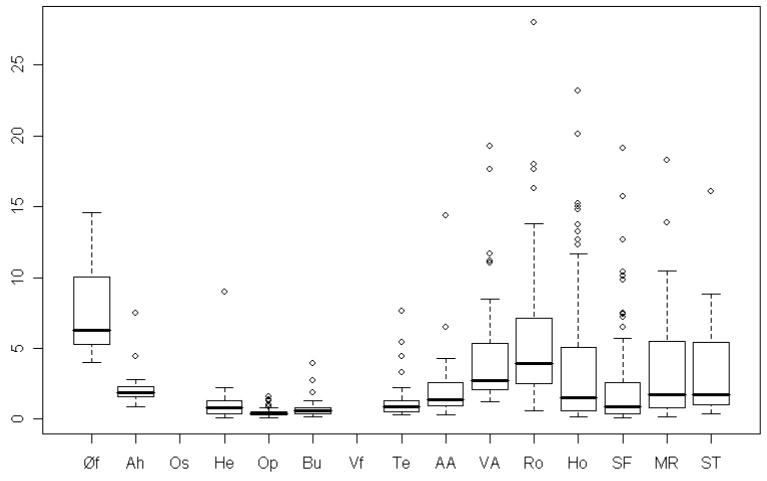


Figure 9. Boxplot of NIVA chemistry data: Chloride per Fylke (excluding Oslo and Vestfold).

Now we see much clearer the contrast between inland and coastal regions. We could also have accomplished this with the subset option in `boxplot()`

```
> boxplot(Cl ~ FYLKE, subset = not.Os.Vf)
```

Now we can get ambitious - Let's make the same regional boxplot for all 9 variables in our data set, arranged in a 3 X 3 matrix.

```
> par(mfrow = c(3,3))
> for (i in 2:10) {
+      boxplot(ion.data[[i]] ~ FYLKE, subset = not.Os.Vf)
+ }
> par(mfrow = c(1,1))  # Reset par()
```

Almost there - except it would be nice to see what plot is which parameter. The function `colnames()` will give us the variable names in a data frame (**Figure 10**).

```
> par(mfrow = c(3,3))
> for (i in 2:10) {
+      boxplot(ion.data[[i]] ~ FYLKE, subset = not.Os.Vf,
+      main = colnames(ion.data)[i])
+ }
> par(mfrow = c(1,1))      # Reset par()
```

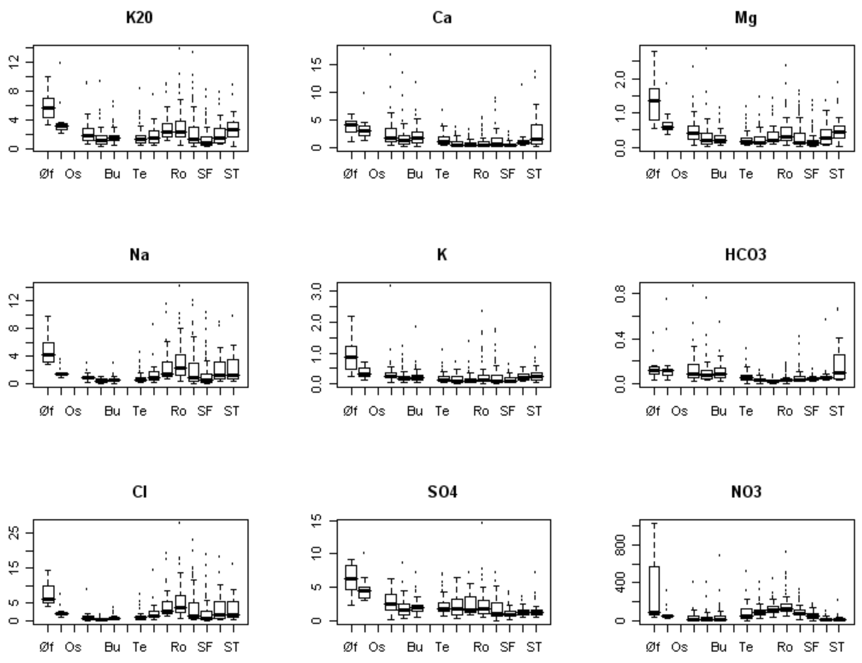


Figure 10. Boxplot for all variables of the NIVA chemistry data.

Water chemistry data are for historical reasons often reported in wildly different units. Let's transform all varables to charge equivalents

```
#    {µeq / L} = {charge} * 1000 * {mg / L} / {mol.weight}
> Ca.eq   <- 2 * 1000 *   Ca / 40.078         # mg/L  -> µeq/L
> Mg.eq   <- 2 * 1000 *   Mg / 24.3050        # mg/L  -> µeq/L
> Na.eq   <- 1 * 1000 *   Na / 22.989770      # mg/L  -> µeq/L
> K.eq    <- 1 * 1000 *    K / 39.0983        # mg/L  -> µeq/L
> HCO3.eq <- 1 * 1000 * HCO3 / 1              # meq/L -> µeq/L
> Cl.eq   <- 1 * 1000 *   Cl / 35.453         # mg/L  -> µeq/L
> SO4.eq  <- 2 * 1000 *  SO4 / 96.0626        # mg/L  -> µeq/L
> NO3.eq  <- 1 *    1 *  NO3 / 14.0067        # µg/L  -> µeq/L
```

# We can then collect all our new variables in a new dataframe

```
> ion.eq <- data.frame(Ca.eq,Mg.eq,Na.eq,K.eq,HCO3.eq,Cl.eq,SO4.eq,NO3.eq)
```

Now can `detach()` the original data and delete intermediate variables. Again, this is good programming practice.

```
> detach(ion.data)
> rm(Ca.eq, Mg.eq, Na.eq, K.eq, HCO3.eq, Cl.eq, SO4.eq, NO3.eq)
```

The default `plot()` method for a dataframe is a scatterplot matrix (**Figure 11**).

```
> plot(ion.eq)
```

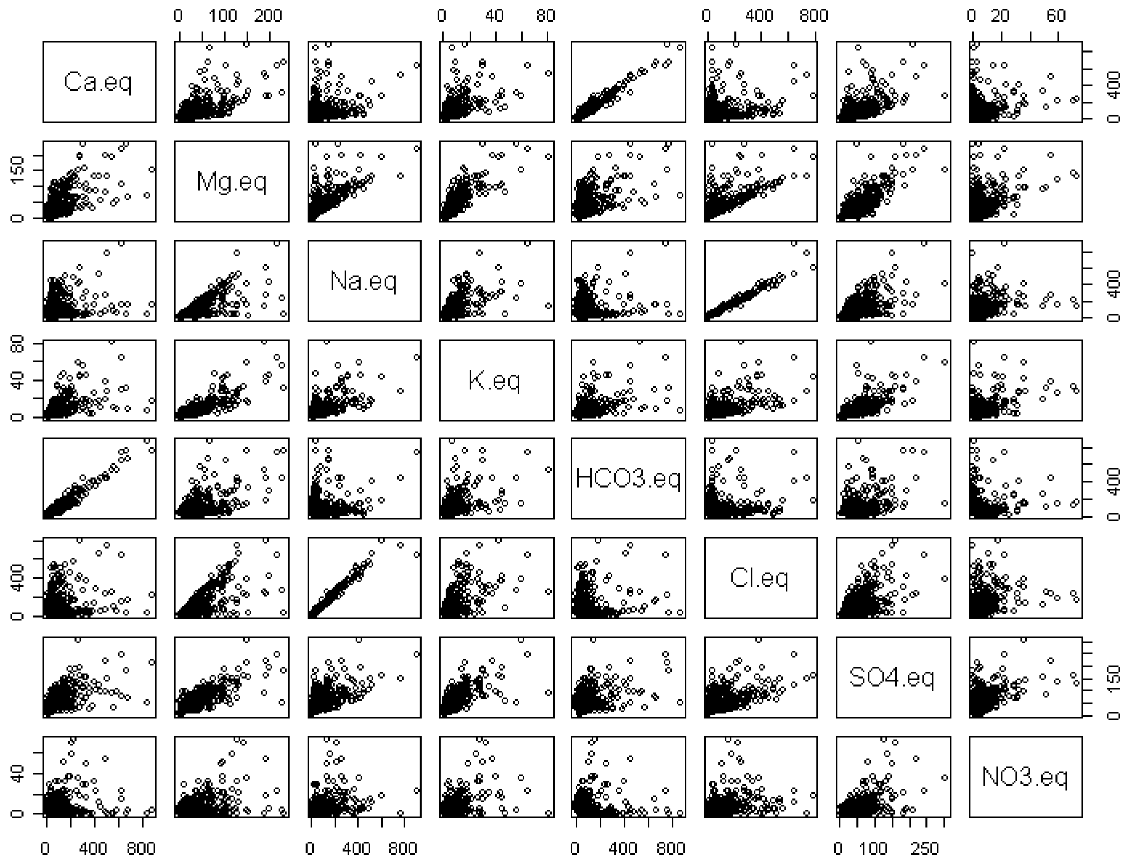


Figure 11. Scatterplot matrix for all variables of the NIVA chemistry data.

The actual function for scatterplot matrices is called `pairs()`

```
> ?pairs
```

The part about panel functions looks interesting. Are there any predefined ones?

```
> help.search("panel")
```

`panel.smooth` looks good, let's try that one (**Figure 12**).

```
> pairs(ion.eq,panel=panel.smooth)
```

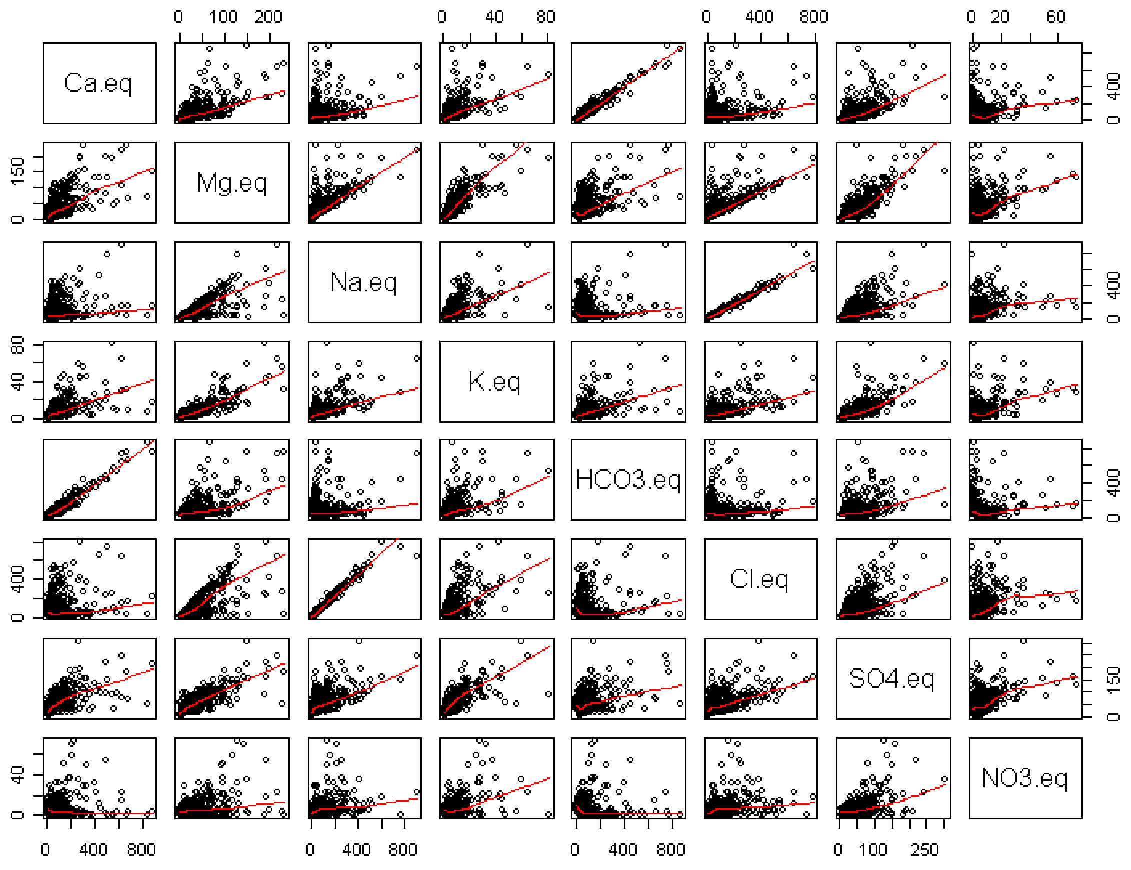


Figure 12. Scatterplot matrix with smoothed functions for all variables of the NIVA chemistry data

Log transformation reveals the chemists' weird ideas about detection limits. Some variables, e.g. HCO3.eq or Cl.eq, show quantization at the detection limit. Notice also that the smooth trend depends on which variable is x and which is y. Compare e.g. `Ca.eq ~ HCO3.eq` and `HCO3.eq ~ Ca.eq`.

There seems to be more correlation structure in this data set than what can be captured by bivariate relations. What options do we have for principal components in R?

```
> help.search("pca")
```

At least 2 different functions: `prcomp()` and `princomp()`. Let's try one of them.

```
> princomp(ion.eq)
Error in cov.wt(z) : 'x' must contain finite values only
```

Which gives an error message, probably because our data has missing values

```
> summary(ion.eq)
     Ca.eq              Mg.eq               Na.eq               K.eq        
 Min.   :  1.996   Min.   :  0.7406   Min.   :  3.045   Min.   : 0.2558  
 1st Qu.: 17.341   1st Qu.:  9.0516   1st Qu.: 21.749   1st Qu.: 2.0461  
 Median : 40.172   Median : 18.1033   Median : 37.843   Median : 3.8365  
 Mean   : 74.952   Mean   : 30.0360   Mean   : 73.860   Mean   : 6.3809  
 3rd Qu.: 92.320   3rd Qu.: 38.6752   3rd Qu.: 82.319   3rd Qu.: 7.4172  
 Max.   :883.278   Max.   :234.5196   Max.   :904.750   Max.   :80.8219  

    HCO3.eq            Cl.eq              SO4.eq             NO3.eq        
 Min.   :  2.00   Min.   :  2.821   Min.   :  2.082   Min.   : 0.00714  
 1st Qu.: 32.00   1st Qu.: 14.103   1st Qu.: 22.902   1st Qu.: 0.92813  
 Median : 48.00   Median : 33.848   Median : 35.394   Median : 4.06948  
 Mean   : 79.35   Mean   : 75.814   Mean   : 46.234   Mean   : 5.72882  
 3rd Qu.: 82.00   3rd Qu.: 85.324   3rd Qu.: 58.295   3rd Qu.: 7.56781  
 Max.   :864.00   Max.   :789.778   Max.   :303.968   Max.   :73.53624  
 NA's   :  5.00                                                          
```

Yes, there's the culprit - HCO3.eq contains 5 missing values. Let's make a selection variable for this subset.

```
> not.missing <- which(!is.na(ion.eq$HCO3.eq))
```

Now try again

```
> p <- princomp(ion.eq, subset = not.missing)
```

Notice that the default for `princomp()` is `cor = FALSE`. That is, principal components on the covariance matrix, which is appropriate in our case since all variables are same unit.

p is now a princomp object which can show itself in various ways

```
> summary(p)
Importance of components:
                            Comp.1      Comp.2      Comp.3       Comp.4
Standard deviation     163.7245863 124.3512080 28.77241113 16.809869114
Proportion of Variance   0.6139391   0.3541584  0.01896051  0.006471816
Cumulative Proportion    0.6139391   0.9680975  0.98705802  0.993529839
                             Comp.5       Comp.6       Comp.7       Comp.8
Standard deviation     13.842010127 6.5386169015 5.6127370499 4.0794439211
Proportion of Variance  0.004388295 0.0009791952 0.0007215176 0.0003811531
Cumulative Proportion   0.997918134 0.9988973294 0.9996188469 1.0000000000
```

So, 97% of the variance is contained in the first 2 PCA axes. Which means we should get a good representation by a biplot of the first 2 axes. Can R do biplots for us?

```
?help.search("biplot")
```

`biplot.princomp()` seems to be what we're looking for...

```
> biplot.princomp(p)
Error: could not find function "biplot.princomp"
```

Which gives an error message on my computer... While the generic `biplot()` seems to work OK (**Figure 13**).

```
> biplot(p)
```

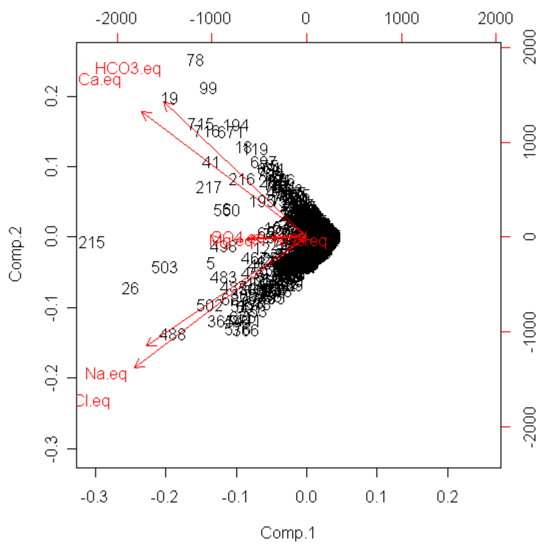


Figure 13. Biplot of principal components of major ions, showing the contribution from sea salts (Na and Cl) and weathering (Ca and HCO_3)

The biplot seems to show very clearly the 2 major sources of ions: Na + Cl from sea salts and Ca + HCO_3 from weathering. We can look in more detail at the sea water contribution under the standard assumption that all chloride is sea salts and that other ions accompany Cl according to the standard composition of sea water (**Figure 14**).

```
> attach(ion.eq)
> par(mfrow=c(2,3))
> plot(Cl.eq,  Ca.eq); abline(0,0.037,col="red")
> plot(Cl.eq,  Mg.eq); abline(0,0.193,col="red")
> plot(Cl.eq,  Na.eq); abline(0,0.852,col="red")
> plot(Cl.eq,   K.eq); abline(0,0.018,col="red")
> plot(Cl.eq,HCO3.eq); abline(0,0.004,col="red")
> plot(Cl.eq, SO4.eq); abline(0,0.103,col="red")
> par(mfrow=c(1,1))
> detach(ion.eq)
```

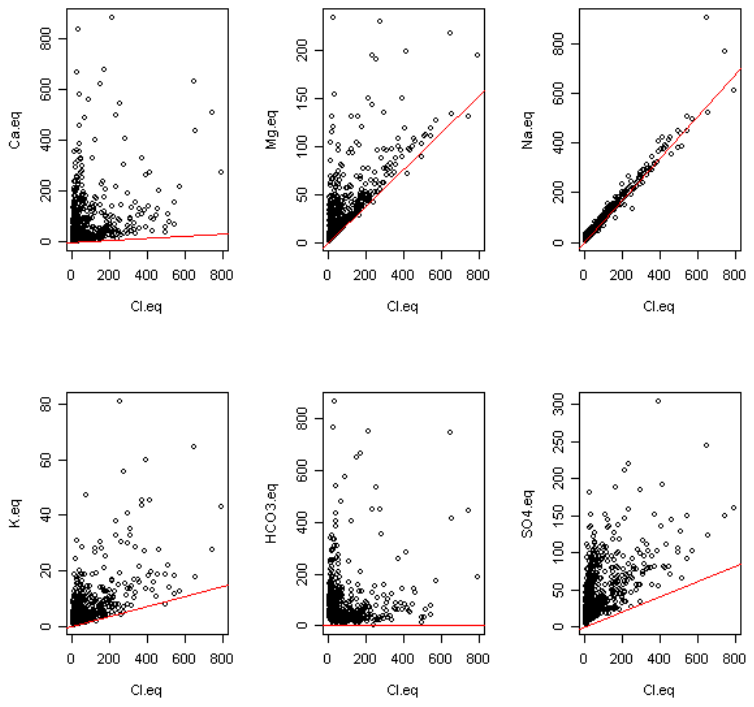


Figure 14. Relations of major ions to chloride, compared to the standard composition of seawater

Since our data are already in charge equivalents, we can easily calculate the acid neutralizing capacity (ANC) as the difference between base cations and strong acid anions. We will expect ANC to be closely related to alkalinity.

```
> attach(ion.eq)
> ANC <- Ca.eq + Mg.eq + Na.eq + K.eq - Cl.eq - SO4.eq - NO3.eq
> plot(ANC,HCO3.eq)
> detach(ion.eq)
```

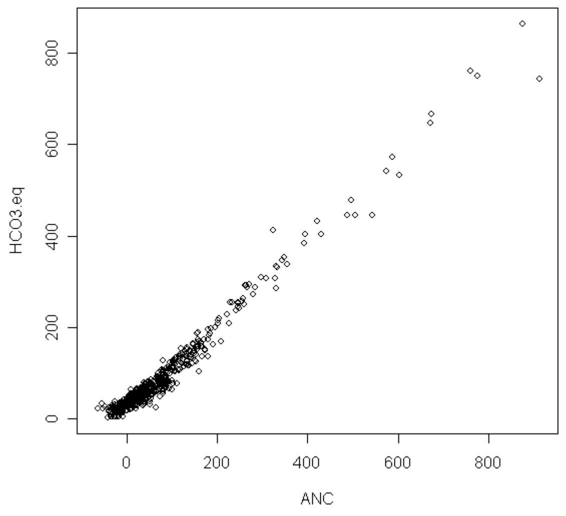


Figure 15. HCO_3 is definitely a major determinant of **ANC.**

Another quantity that is easily calculated from charge equivalents is the equivalent conductivities of individual ions. If molar conductivities are given as (S/m) / (mol/L)) at 20° C then equivalent conductivity = {mol.cond} * {µeq/L} / 1000 = {mS/m}

```
> attach(ion.eq)
> Ca.ec   <- 5.4 *   Ca.eq / 1000# µeq/L -> mS/m
> Mg.ec   <- 4.8 *   Mg.eq / 1000# µeq/L -> mS/m
> Na.ec   <- 4.5 *   Na.eq / 1000# µeq/L -> mS/m
> K.ec    <- 6.7 *    K.eq / 1000# µeq/L -> mS/m
> HCO3.ec <- 4.1 * HCO3.eq / 1000# µeq/L -> mS/m
> Cl.ec   <- 6.8 *   Cl.eq / 1000# µeq/L -> mS/m
> SO4.ec  <- 7.2 *  SO4.eq / 1000# µeq/L -> mS/m
> NO3.ec  <- 8.4 *  NO3.eq / 1000# µeq/L -> mS/m
> detach(ion.eq)
```

Predicted specific conductivity is then just the sum of the equivalent conductivities of the individual major ions (**Figure 16**).

```
K20.pred <- Ca.ec + Mg.ec + Na.ec + K.ec + HCO3.ec + Cl.ec + SO4.ec + NO3.ec
plot(K20.pred,ion.data$K20)
abline(0,1)
```

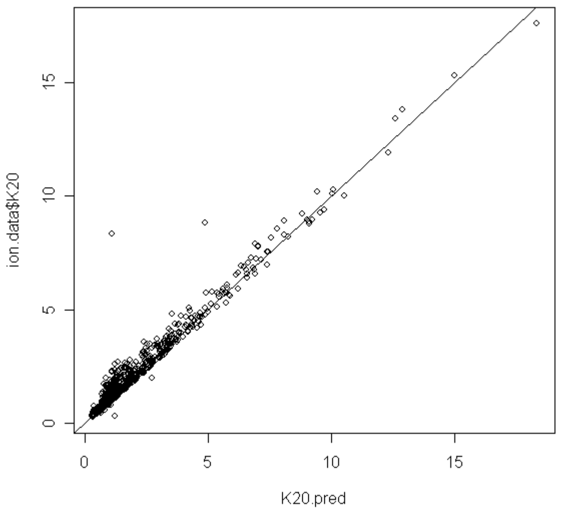


Figure 16. Measured vs. predicted specific conductivity (as the sum of the equivalent conductivities of the individual major ions)

There are at least 4 possible outlier candidates in this plot 2 with much higher measured conductivity than predicted, two of them with somewhat lower conductivity than predicted. Let's look at them in more detail (**Figure 17**).

```
> K20.diff <- ion.data$K20 - K20.pred
> hist(K20.diff, breaks=50)
```

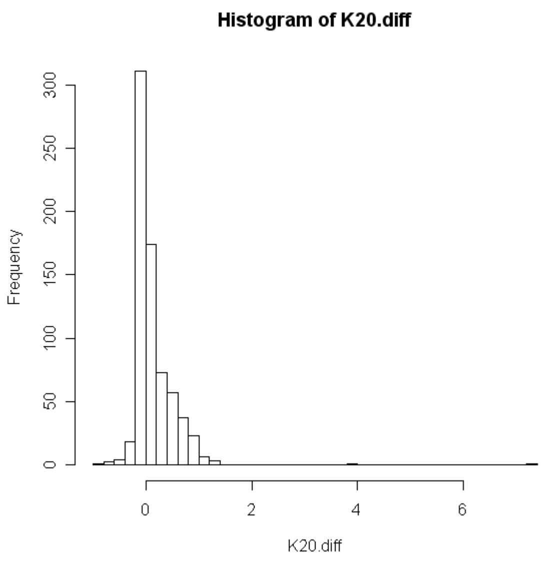


Figure 17. Histogram for of differences between measured and predicted conductivities, showing two possible outliers

Since our data set does not include the cation with the by far highest equivalent conductivity (H+ 32 (S/m)/(mol/L)), we would expect the specific condutivity to be underpredicted in acid lakes (**Figure 18**).

```
> plot(ANC,K20.diff)
```

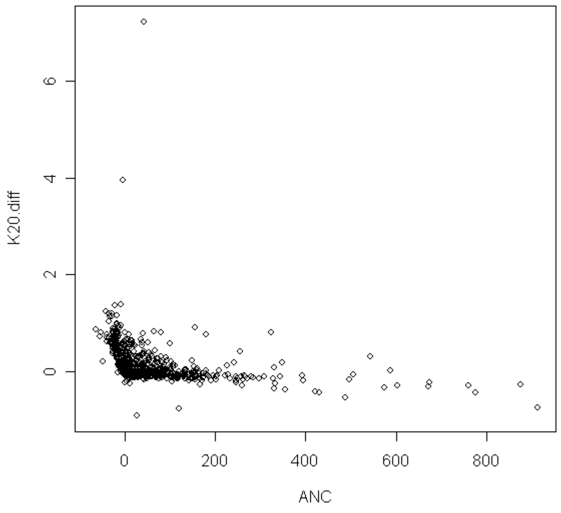


Figure 18. The contribution of H^+ to specific conductivity is highest when ANC is low

2. FROM LINEAR MODELS TO GAM

Jannicke Moe

Topics:
A data import problem: dates format (script: dag2_script1_import_Storgama.txt)
Linear models: regression, ANOVA etc. (script: dag2_script2_LM_Storgama.txt)
Generalised linear models: logistic regression etc. (script: dag2_script3_GLM_Storgama.txt)
Generalised additive models: smooth splines etc. (script: dag2_script4_GAM_Storgama.txt)
Model selection – some issues (no script)

2.1 Linear models: what sort of test should I use?

Let's say you have one response variable (continuous, normally distributed) and various possible predictor variables (**Table 1.** Basic linear models for different combinations of predictor variables, with corresponding model formula in R.). In excel, you must choose the right kind of test from a menu, depending on the type of data you have. I R, on the other hand, you can use a standard test formulation, and the test result will depend of the type of data you put into it. The basic formula is:

```
> lm(y ~ x)
```

This stands for: $y = b_0 + b_1*x$ + residuals

Table 1. Basic linear models for different combinations of predictor variables, with corresponding model formula in R.

Predictor: / **Response:**	**1 predictor variable**	**2 or more predictor variables**
Continuous	Linear regression: `lm(y ~ x)`	Multiple regression `lm(y ~ x1 + x2 + ...)`
Categorical	t-test `lm(y ~ x)`	ANOVA `lm(y ~ x1 + x2 + ...)`
Combination	-	ANCOVA `lm(y ~ x1 + x2 + ...)`

2.2 Linear models in R: some useful commands

```
> fit <- lm(y ~ x1 + x2)  # Store the model as the object "fit"
```

Diagnositic plots (good idea to set `par(mfrow=c(2,3))` !):

```
> plot(fit)
```

What is stored in the fit?

```
> names(fit)
```

The most commonly used info:

```
> summary(fit)
```

Here you find the names that R gives the summary components, so that you can extract them and e.g use them on plots:

```
> names(summaryfit))
```

Examples:
```
> summary(fit)$adj.r.squared   # gives you the R2 value
> summary(fit.1)$coef  # this component turns out to be a matrix
> dimnames(summary(fit.1)$coef) # a matrix has ”dimnames”
             rather than ”names”
> summary(fit)$coef["x1", "t value"]
```

Elements of the fitted object can be accessed just like columns in a dataframe:
```
> fit$coefficients  # gives you the coefficients
> fit$coef   # any unambiguos abbrevation can be used
```

Extractor functions are made to extract certain information, you should use these rather than the object components.
```
> coef(fit)   # same as fit$coef – usually...
> fitted(fit) # fitted values
> resid(fit)  # residuals
> predict(fit)  # predicted values
> predict(fit, se.fit=T)  # ...with standard error
> deviance(fit)
```

Alternative to `lm()` exist for certain types of linear models. For example, comparison of two groups can also be done with the function `t.test(y ~ x)`, but the function `lm(y ~ x)` is simpler. ANOVA can also be done with the function `aov()`:
```
> fit <- aov(y ~ x1 + x2)  # same fit as lm(),
> anova(fit)   # gives you an ANOVA table
```

The function `aov()` seems to do the same as `lm()`, but it is also possible to combine fixed and random effects. This is applicable for balanced design only. For unbalanced design, and for more complicated models, you should use the function `lme()` (linear mixed-effects models, in the package ”nlme”)

2.3 Formula syntax in R – general rules

The following information is extracted from the help file on formulae:
```
> ?formula
```

```
Y ~ F         Response variable Y is modeled as F, where F may include other terms
Fa + Fb       Include both Fa and Fb in the model
Fa - Fb       Include all of Fa in the model, except what is in Fb
Fa : Fb       The interaction between Fa and Fb
Fa * Fb       Fa + Fb +  Fa : Fb
Fb %in% Fa    Fb is nested within Fa
Fa / Fb       Fa + Fb %in% Fa
I(F^m)        All terms in F crossed to order m
.             in update(): the previous set
.             in other formulae: all variables (except the response variable(s) Y)
```

A model with no intercept (going through the origin) can be specified as:
```
      Y ~ F - 1    or
      Y ~ 0 + F
```

While formulae usually involve just variable and factor names, they can also involve arithmetic expressions. The formula `'log(y) ~ a + log(x)'` is quite legal. When such arithmetic expressions involve operators which are also used symbolically in model formulae, there can be confusion between arithmetic and symbolic operator use. To avoid this confusion, the function `'I()'` can be used to bracket those portions of a model formula where the operators are used in their arithmetic sense. For example, in the formula `'y ~ a + I(b+c)'`, the term `'b+c'` is to be interpreted as the sum of `'b'` and `'c'`.

2.4 Generalised linear models (GLM)

What if the y variable is not suitable for linear models? E.g. the y variable is not normally distributed but 0/1, proportions, or Poisson-distributed (e.g. counts). The framework for analysing linear models can be **generalised** using a **link function g()**

```
LM:        y = b0 + b1*x1 + b2*x2 + ...
GLM:    g(y) = b0 + b1*x1 + b2*x2 + ....
```

The link function **transforms the y variable** into something that can be modelled as a **linear combination of predictor variables.** Ordinary linear models are then a ”special case” where the link function = identity.

A typical example of a GLM is **logistic regression**. The y variable is then binary distributed, such as 0/1. A linear model is obviously not appropriate (Figure 19) - a sigmoid curve is better.

We can use the link function "logit" to obtain a linear link between the predictor and response variables:

logit(y) = log(y / (1-y))

logit(y) has range <-Inf, Inf>, and can therefore be modelled as linear combination of the predictor variables.

log(y/(1-y)) = b0 + b1*x

Back-transformation gives:

y = exp(b0 + b1*x)/(1 + exp(b0 + b1*x))

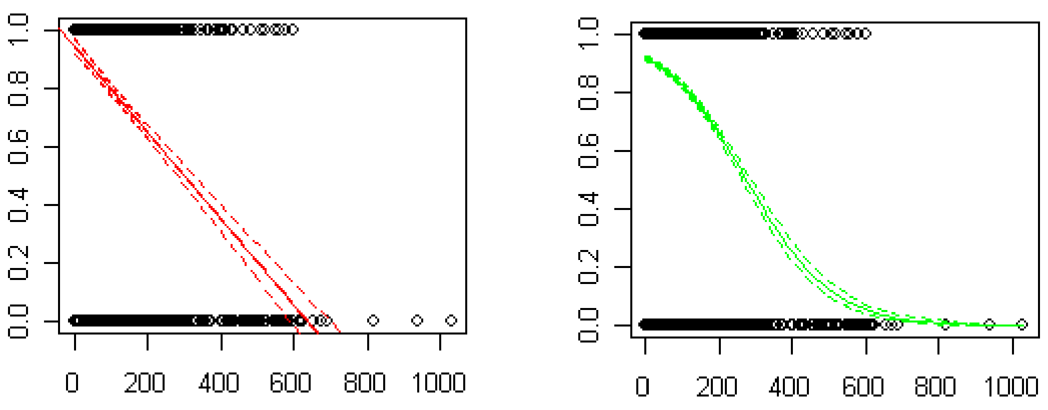


Figure 19. Binary data: linear regression (left panel) versus logistic regression (right panel).

A logit transformation cannot be done directly on the data, when the response is binary 0/1. In R, the transformation is done implicitly by the function `glm()`. Instead of

```
> lm(y ~ x)
```

we write

```
> glm(y ~ x, family = binomial(link = logit))
```

2.5 ”Families” of distributions in R

What sort link (variance functions) can the different families of distributions use, within the GLM framework? The following table summarises the suitable pairings:

Table 2. Families of distributions applicable for Generalised Linear Models in R.

	binomial	gaussian	Gamma	inverse gaussian	poisson	quasi
logit	x					x
probit	x					x
cloglog	x					x
identity		x	x		x	x
inverse			x			x
log			x		x	x
1/mu^2				x		x
sqrt					x	x

If you have a non-linear relationship for which none of the GLMs seems suitable, then you can specify your own non-linear formula by non-linear least-squares regression, `nls()`. You must specify parameters directly in the formula, and suggest start values (`start=list(...)`).
As an example we can use the backtransformed version of logit(y):

```
> nls(y ~ exp(b0 + b1*x)/(1 + exp(b0 + b1*x)), start=list(b0=0, b1=0) )
```

2.6 Generalised Additive Models (GAM)

GLM allows non-linear models within a linear framework, but we must still specify a parametric model. **Additive Models (AM)**, on the other hand, are not restricted to linear combination of predictor variables. AMs allow you to you can **add** various **functions of predictor variables.**

LM: `y = b0 + b1*x1 + b2*x2 + b3*(x2^2)+ ...`

AM: `y = b0 + f1(x1) + f2(x2) + ...`

Just like linear models, AMs can also be **generalised**, using a link function g():

GAM: `g(y) = b0 + f1(x1) + f2(x2) + ...`

In GAM the functions f() can be **non-parametric,** e.g. loess (locally weighted regression), or so-called splines. In R we can use splines with the function `s()`.

```
> gam(y ~ s(x))
```

Non-parametric regression can give you nice flexible curves, but not conventional parameter estimates. An example of a data set where a GAM may be more suitable than a linear model is shown in Figure 20.

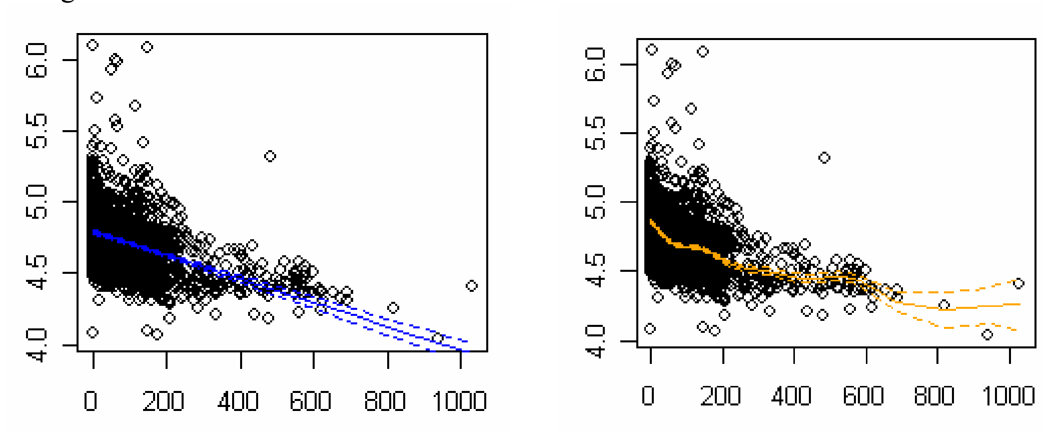


Figure 20. Regression with linear model (LM; left panel) versus generalised additive model (GAM; right panel).

An important consideration when using GAM is how "smooth" your estimated curves should be. If the curves are too smooth, you may lose important details in the data structure. On the other hand, if you allow the curves to get too "wiggly", then the estimated curve may become to specific for your current data set, and be less useful for more general interpretations. The function `gam()` in the package "basis" (and in S-plus) uses 4 degrees of freedom as default. R also has a package "mgcv" with a somewhat different function `gam()`. In this version, degrees of freedom are optimised by cross-validation together with the model fit. We recommend that you use the mgcv version of gam, because of this built-in optimisation of the smoothing.

Figure 21 summarises the relationship between linear models, additive models, and generalised linear and additive models.

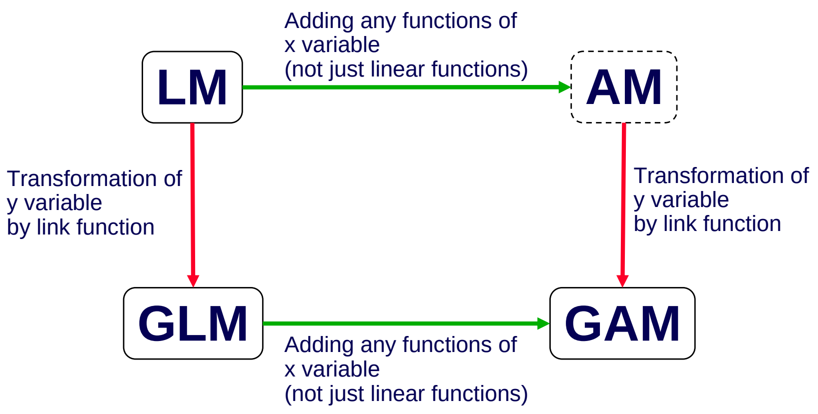

Adding any functions of x variable (not just linear functions)
LM
AM
Transformation of y variable by link function
Transformation of y variable by link function
GLM
GAM
Adding any functions of x variable (not just linear functions)

Figure 21. Relationship between LM, AM, GLM and GAM.

2.7 Model selection

An important consideration for all types of models is how many explanatory variables you should include your model. If there are too few variables, the model will not be able explain much of the variation. On the other hand, if there are too many variables, then the model will be too specific for the current data set. A guideline for model selection is: when is a more complicated model **significantly better** than a simpler model?

Various criteria are developed for model selection, including the following:
- Compare how much variation is explained (R^2)
- Compare how much variation is left (Mallow's Cp, deviance,…)
- Compare criteria based on log-likelihood (AIC, BIC)
- Compare ability to predict new data: cross-validation

In R, some approaches use a mix of criteria. The type of model you have may restrict the choice of approace and criteria. Some examples are given below.

2.7.1 Model selection for LM: ANOVA table

A simple example: Model 1 is a subset of Model 2.

```
> x1 <- 1:10
> y  <- x1^3
> fit.1 <- lm(y ~ x1)            # Adjusted R-squared: 0.8446
> fit.2 <- lm(y ~ x1 + I(x1^2))  # Adjusted R-squared: 0.9963
```

Fit 2 is obviously better than fit 1, but is it significanly better?

```
> anova(fit.1, fit.2)
Analysis of Variance Table
Model 1: y ~ x1
Model 2: y ~ x1 + I(x1^2)
  Res.Df    RSS Df Sum of Sq      F    Pr(>F)
1      8 146837
2      7   3089  1    143748 325.77 3.961e-07 ***
```

The low p-value of this test means that model 2 is signifiantly better.

Model selection by `anova()` is restricted to cases where one or more models are subsets of a more complete model. Note that rows with missing values should be removed before model fitting, to obtain the same number of observations for all models. When applying `anova()` to glm objects, the function does not return p-values directly, but it returns deviances from which a p-value can be calculated.

2.7.2 Model selection for GLM: deviance analysis

We use the same simple example as above.

```
> fit.1 <- glm(y ~ x1)
> fit.2 <- glm(y ~ x1 + I(x1^2))
> deviance(fit.1)
[1] 146836.8
> deviance(fit.2)
[1] 3088.8
```

Again, fit.2 is obviously better than fit 1, but is it significanly better? The difference in deviance is χ^2-distributed with 1 degree of freedom (=difference in number of parameters). Hence, we can test the significance of the difference in deviance with a χ^2 test.

```
> 1 - pchisq(deviance(fit.1) - deviance(fit.2), df=1)
[1] 0
```

The difference is significant ($p < 0.05$).

This kind of test is restricted to cases where deviance can be calculated, and where models are subsets. Deviance is available also for GAMs, but number of parameters is not defined in the same way as for GLMs, so it is not straight-forward to use this test for GAMs.

2.7.3 Akaike's information criterion

Akaike's information criterion (AIC) is calculated as

```
              -2*log-likelihood + k*npar,
```

where npar = the number of parameters in the fitted model, and k = penalty per parameter. The function for AIC in R is

```
> AIC(object, ..., k=2)
```

AIC requires that the log-likelihood function can be easily calculated (which is the case for e.g. GLM, but not for `nls` (non-linear models)), and that the model has parameters in the usual sense (which is not the case for GAM). The models do not have to be subsets of each other, but they must use the same response variable.

2.7.4 Automatic stepwise selection

The function `step()` can help you select the **best model** from a **full model**, by automatically adding or removing terms in a stepwise fashion. This function uses the criteria AIC and Mallow's Cp (the total square errors).

Consider a full model with interactions:
```
> fit <- lm(y ~ (x1 + x2 + x3 + x4)^2)
```

For objects of type lm and glm, you can use
```
> step(fit)
```

For a wider range of object classes (in package ”MASS”), you can use:
```
> stepAIC(fit)
```

2.7.5 Model selection by cross validation

Cross validation is a model selection approach that is applicable for all types of models. The procedure is generally as follows.
1. Specify a model (e.g. full model)
2. Exclude a subset of data (e.g. 1/10): x_{excl}, y_{excl}
3. Estimate the parameters with the remaining data: x_{incl}, y_{incl}
4. Use the x_{excl} as input in the model parameterised by x_{incl}, y_{incl} and predict y_{pred}
5. Compare the y_{pred} with the real $y_{excl\ ,}$: calculate the squared differences
6. Repeat for each subset of the data
7. Sum the calculated squared differences. This gives the CV score for this model
8. Repeat CV calculation for each model

A drawback with this approach is that there is no general rule for defining a significant difference between CV scores.

2.8 Example 3: Nitrate concentrations in the river Storgama

Request from participant (Heleen de Wit): I wish to import a data file so that I can plot different variables versus time, and do time-series analyses. I wish to check if the water nitrate concentration shows a temporal trend, or some pattern, and if there is a relationship with the water TOC (total organic carbon).

2.8.1 Script 1: Import and formatting of dates.

First we try to read the data as they are. I've saved a copy the excel file Storgama_0.xls (first sheet) as a text file "Storgama_0.txt". To tell R where the files are, you can change directory from the menu (*File -> Change dir...*).

```
> DATA <- read.table("Storgama_0.txt", header=T)
```
Why call the object "DATA", not very informative? A benefit is that it's easier to adjust and re-use the script to new datasets.

```
> names(DATA)
 [1] "STID"   "STCOD" "NAME"  "Date"  "pH"    "KOND"  "TOC"   "TOTN"  "NO3.N"
[10] "NH4.N" "ECa"   "ECl"   "ENa"   "EMg"   "ESO4"  "EK"    "ENO3"  "EALK1"
[19] "H."    "ANC1"  "Al.Il" "Al.R"  "LAL"
```

```
> is.factor(DATA$Date) # Dates are formatted as levels - not so useful.
[1] TRUE
```
Can we try to change them into numeric?
```
> as.numeric(DATA$Date)[1:10]# Look at the first 10
 [1]  855 1217 1543  149  149  149  149  149  149  149
```

Even less useful. Let's check helpfiles.

```
> ?date
```

Gives us today's date :-(

```
> help.search("date")
```

format.Date(base) sounds useful

```
> ?format.Date
> as.Date(DATA$Date)[1:10]
 [1] "0017-07-19" "0024-07-19" "0031-07-19" "0003-09-19" "0003-09-19"
 [6] "0003-09-19" "0003-09-19" "0003-09-19" "0003-09-19" "0003-09-19"
```

Totally useless - or something wrong with the format

So maybe we should check what sort of format R actually requires
From helpfile "as.Date":

```
       The default formats follow the rules of the ISO 8601 international
       standard which expresses a day as '"2001-02-03"'.
```

NB: sometimes the most useful information is found not in the description, but in the examples.
I found this at the bottom of the helpfile:

```
    ## read in date/time info in format 'm/d/y'
    dates <- c("02/27/92", "02/27/92", "01/14/92", "02/28/92", "02/01/92")
    as.Date(dates, "%m/%d/%y")
```

HWI has format "%d/%m/%y" - I guess

```
> as.Date(DATA$Date, "%d/%m/%y")[1:10]
 [1] "2019-07-17" "2019-07-24" "2019-07-31" "2019-09-03" "2019-09-03"
 [6] "2019-09-03" "2019-09-03" "2019-09-03" "2019-09-03" "2019-09-03"
```

Now the data series starts in 2020 so either someone has faked these data, or we still have a format problem...

Let's go back to the excel file and see if we find some solution there. It turns out, some of the cells have hidden time values after the date values. Things like this are quite common and can create a lot of trouble when you work with other people's excel files. One solution is to split dates into separate columns for year, month etc. in excel, with these excel function:

=year(), =month(), =day(), =hour(), =minute(), =second().

and combine these together again in R with the function ISOdatetime().
I've done this in "Storgama_1.txt".

```
> file <- "Storgama_1.txt"
> DATA <- read.table(paste(path, file, sep=""), header=T)

> DATA$iso.date <- ISOdate(DATA$year, DATA$month, DATA$day)
```

Why attach the new vector to the dataset, couldn't it just be separate vector?
It can be easier to select rows etc. for all variables if it's in the dataset.

```
> oldpar <- par(mfrow = c(3,2))
> for (i in 18:23) {
+ plot(DATA$iso.date, DATA[[i]], type="l", ylab = names(DATA)[i])
+ }
> par(oldpar)
```

This plot produces **Figure 22**.

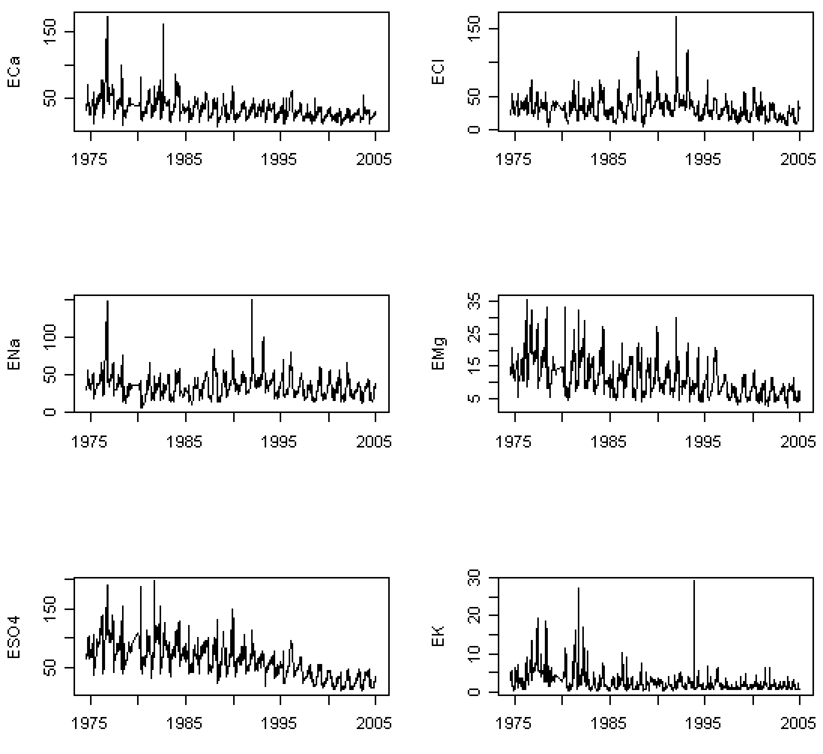


Figure 22. Time-series plots for Storgama.

NB: The rest of the script is optional - not required for subsequent scripts
Alternatively, we can try to import the dates in a date format that R understands.

In "Storgama_1.txt" I've formatted the column "Date": removed everything after the date (replaced " *" by "" in excel), and formattet the date like "%d/%m/%y" (Format cells -> Number -> Date)
Does it now accept the dates as dates? Let's compare with the original version

```
> DATA$Date_original[1:5]
[1] 17/07/1974 24/07/1974 31/07/1974 03/09/1974 03/09/1974
1556 Levels: 01/02/1979 01/02/1993 01/02/1995 01/02/1999 ... 31/12/1985
> DATA$Date[1:5]
[1] 17/07/74 24/07/74 31/07/74 03/09/74 03/09/74
1556 Levels: 01/02/79 01/02/93 01/02/95 01/02/99 01/03/04 01/03/82 ... 31/12/85
```

Both versions are still read as factors

What if we now try to persuade R to read these as numeric dates:

```
> as.Date(DATA$Date_original, "%d/%m/%y")[1:5]
[1] "2019-07-17" "2019-07-24" "2019-07-31" "2019-09-03" "2019-09-03"
> #[1]  "2019-07-17" "2019-07-24" "2019-07-31" "2019-09-03" "2019-09-03"
> as.Date(DATA$Date, "%d/%m/%y")[1:5]
[1] "1974-07-17" "1974-07-24" "1974-07-31" "1974-09-03" "1974-09-03"
> #[1] "1974-07-17" "1974-07-24" "1974-07-31" "1974-09-03" "1974-09-03"
```

Looks much better! But what about those "", is this vector numeric anyway?

```
> is.numeric(as.Date(DATA$Date, "%d/%m/%y"))
[1] TRUE
```

:-)
We'll change this permanently in the dataset

```
> DATA$Date <- as.Date(DATA$Date, "%d/%m/%y")
```

NB: There is a very similar function in another package, which does something slightly different!

```
> ?as.Date (package:base)
   Functions to convert between character representations and objects
   of class '"Date"' representing calendar dates.
> ?as.date  (package:survival)
   Converts any of the following character forms to a Julian date:
    8/31/56, 8-31-1956, 31 8 56, 083156, 31Aug56, or August 31 1956.
```

This does NOT use the standard format "1956-08-31", which the base package uses...

When you search for useful functions, it's proably a good idea to select those from the most common packages, if possible.

Other potentially useful functions for date conversion in package "survival":

```
> library(survival)
Loading required package: splines
>  julian(as.Date("2006-05-02"), origin=as.Date("1960-01-01")) #  Default origin
"1970-01-01"
[1] 16923
attr(,"origin")
[1] "1960-01-01"
>  date.mdy(16923)# uses origin "1960-01-01"
$month
[1] 5

$day
[1] 2

$year
[1] 2006

>  mdy.date(5, 2, 2006)
[1] 2May2006
```

2.8.2 Script 2: Linear models.

Let's look at the data:

```
> plot(DATA[,12:16])
```

This gives pairwise plots of selected parameters (**Figure 23**). (This is not recommended for all parameter columns 12:29 at once).

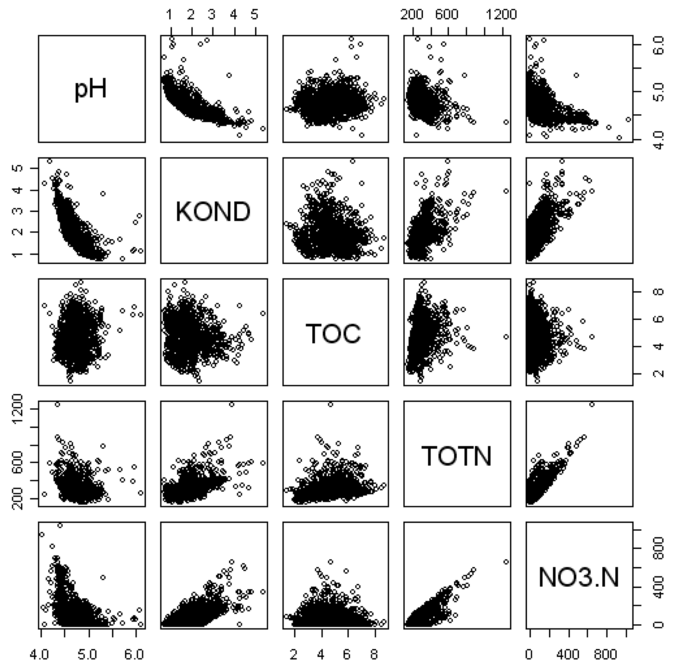


Figure 23. Pairwise plots of parameters from Storgama.

We want to look at certain parameters against time. Make a continuous numeric vector of time, with unit year (with decimals) `as.numeric()` gives date as no. of seconds since 1970-01-01.

```
> DATA$iso.year <- as.numeric(DATA$iso.date)/(365*24*60*60) + 1970
```

"Trend analysis" tries to describe a temporal trend and at the same time account for autocorrelation in the data. "Time-series analysis" in R is a method/framework that requires data with regular intervals (see `?ts`), and which will require some reformatting of the data in this case. We will get back to these issues later. For now, we'll ignore the temporal correlation and treat the data as independent, and start with ordinary regression analyses.

First we can "attach" a dataframe: then the columns of the dataframe will be directly accessible, so that we can skip the "`DATA$`", and wrote "`NO3.N`" instead of "`DATA$NO3.N`"

```
> is.object(NO3.N)# No object with this name
Error: object "NO3.N" not found
> attach(DATA)
> is.object(NO3.N)
[1] FALSE
```

Now the column is "visible" for R, although it's not a proper object.

Does nitrate decrease with time? (**Figure 24**).

```
> windows()
> plot(iso.date, NO3.N, type="l")
```

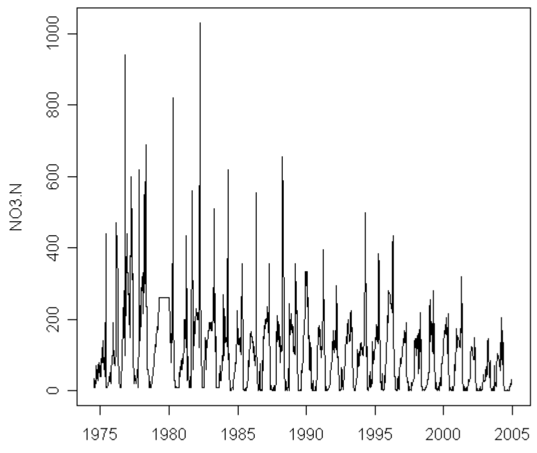


Figure 24. Data series NO3.N from Storgama.

Regression of NO3 against time:
```
> fit.1 <- lm(NO3.N ~ iso.year)
> summary(fit.1)
Call:
lm(formula = NO3.N ~ iso.year)

Residuals:
    Min      1Q  Median      3Q     Max 
-168.17  -78.49  -25.71   47.57  884.64 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 8607.475    680.358   12.65   <2e-16 ***
iso.year      -4.269      0.342  -12.48   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

Residual standard error: 121.2 on 1550 degrees of freedom
Multiple R-Squared: 0.09135,    Adjusted R-squared: 0.09077 
F-statistic: 155.8 on 1 and 1550 DF,  p-value: < 2.2e-16
```
Very significant indeed, but has low adjusted R2 (0.09).

Can seasonal variation explain some of the variation? Use month as a categorical factor. This model is an ANCOVA (Analysis of covariance).
```
> fit.2 <- lm(NO3.N ~ iso.year + as.factor(month))
> summary(fit.2)     # (Only selected lines shown below)
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)    
(Intercept)        7193.1363   519.0880  13.857  < 2e-16 ***
iso.year             -3.5373     0.2609 -13.557  < 2e-16 ***
as.factor(month)2    -0.1264    11.7585  -0.011 0.991423    
as.factor(month)3    35.0309    11.5731   3.027 0.002511 ** 
as.factor(month)4   124.8507    10.9909  11.359  < 2e-16 ***
as.factor(month)5   -60.3850    10.9800  -5.500 4.45e-08 ***
as.factor(month)6  -143.1046    11.5944 -12.343  < 2e-16 ***
as.factor(month)7  -140.2083    12.2217 -11.472  < 2e-16 ***
as.factor(month)8  -131.2791    12.1083 -10.842  < 2e-16 ***
as.factor(month)9  -117.4968    11.5074 -10.211  < 2e-16 ***
as.factor(month)10  -78.3989    11.3861  -6.886 8.36e-12 ***
as.factor(month)11  -42.6922    11.6195  -3.674 0.000247 ***
as.factor(month)12   -2.8566    11.5966  -0.246 0.805462    
```

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

Residual standard error: 91.27 on 1539 degrees of freedom
Multiple R-Squared: 0.4881,     Adjusted R-squared: 0.4842
F-statistic: 122.3 on 12 and 1539 DF,  p-value: < 2.2e-16
```

Adjusted R2 is now much higher (0.48).

Look at coefficients for each month (**Figure 25**). The argument `[-(1:2)]` excludes element 1:2.

```
> barplot(c(0,coef(fit.2)[-(1:2)]), names.arg=1:12)
```

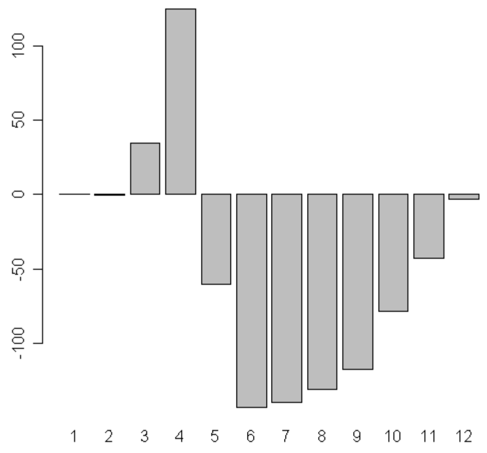


Figure 25. Barplot for estimated coefficients per month for Storgama.

Is there an interaction between year and month? This means that effect of time can be different for each month.

```
> fit.3 <- lm(NO3.N ~ iso.year * as.factor(month))
> summary(fit.3)
Coefficients:
                              Estimate Std. Error t value Pr(>|t|)    
(Intercept)                  4094.0268  1870.6059   2.189   0.0288 *  
iso.year                       -1.9794     0.9404  -2.105   0.0355 *  
as.factor(month)2            -279.6590  2631.3218  -0.106   0.9154    
as.factor(month)3            7380.5148  2600.8831   2.838   0.0046 ** 
as.factor(month)4           15150.6343  2391.2350   6.336 3.10e-10 ***
as.factor(month)5            4852.8377  2383.9214   2.036   0.0420 *  
as.factor(month)6           -2660.6283  2551.1398  -1.043   0.2972    
as.factor(month)7           -3186.2961  2819.9376  -1.130   0.2587    
as.factor(month)8           -2583.3170  2870.0494  -0.900   0.3682    
as.factor(month)9             370.1818  2523.3984   0.147   0.8834    
as.factor(month)10           3715.8048  2483.1261   1.496   0.1348    
as.factor(month)11           1687.2379  2556.7416   0.660   0.5094    
as.factor(month)12           2773.3034  2560.6876   1.083   0.2790    
iso.year:as.factor(month)2      0.1401     1.3226   0.106   0.9156    
iso.year:as.factor(month)3     -3.6920     1.3073  -2.824   0.0048 ** 
iso.year:as.factor(month)4     -7.5590     1.2025  -6.286 4.24e-10 ***
iso.year:as.factor(month)5     -2.4709     1.1989  -2.061   0.0395 *  
iso.year:as.factor(month)6      1.2651     1.2824   0.987   0.3240    
iso.year:as.factor(month)7      1.5273     1.4166   1.078   0.2811    
iso.year:as.factor(month)8      1.2283     1.4415   0.852   0.3943    
iso.year:as.factor(month)9     -0.2452     1.2685  -0.193   0.8468    
iso.year:as.factor(month)10    -1.9073     1.2482  -1.528   0.1267    
iso.year:as.factor(month)11    -0.8700     1.2850  -0.677   0.4985    
iso.year:as.factor(month)12    -1.3957     1.2870  -1.084   0.2783    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 88.58 on 1528 degrees of freedom
```

```
Multiple R-Squared: 0.5213,     Adjusted R-squared: 0.5141
F-statistic: 72.35 on 23 and 1528 DF,  p-value: < 2.2e-16
```

The increased R2 value is probably not worth all the extra parameters.

Does NO_3 have a relationship with TOC?

```
> fit.4 <- lm(NO3.N ~ iso.year + as.factor(month) + TOC)
> summary(fit.4)
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
TOC                   1.0069     1.9195   0.525    0.600
---
Multiple R-Squared: 0.581,      Adjusted R-squared: 0.5755
F-statistic: 105.6 on 13 and 990 DF,  p-value: < 2.2e-16
```

Effect of TOC is not significant (although adjusted R2 is slightly higher).

What if we look at relationship with TOC only?

```
> fit.5 <- lm(NO3.N ~ TOC)
> summary(fit.5)
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  135.487     10.981  12.339  < 2e-16 ***
TOC           -9.680      2.209  -4.382 1.30e-05 ***
---
Multiple R-Squared: 0.01881,    Adjusted R-squared: 0.01783
F-statistic:  19.2 on 1 and 1002 DF,  p-value: 1.298e-05
```

The effect of TOC only is significant, but has a very low R2.

Now what if we try to put year back again:

```
> fit.6 <- lm(NO3.N ~ iso.year + TOC)
> summary(fit.6)
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 6822.1445  1048.2457   6.508 1.20e-10 ***
iso.year      -3.3674     0.5279  -6.379 2.72e-10 ***
TOC           -3.1584     2.3955  -1.318    0.188
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 87.41 on 1001 degrees of freedom
Multiple R-Squared: 0.05714,    Adjusted R-squared: 0.05525
F-statistic: 30.33 on 2 and 1001 DF,  p-value: 1.627e-13
```

Then TOC is no longer significant.

Obviously we need a more systematic way to selecting the best model! We will address this issue later, but now let's look at some alternatives to the linear model.

```
> detach(DATA)      # Good modelling practice to clean up workspace
```

2.8.3 Script 3: Generalised linear models.

We want to describe relationship NO3.N and pH in Storgama (Figure 26). (This relationship is clearer that between TOC and NO3.N)

```
> attach(DATA)
> par(mfrow=c(2,2))       # Make panel for 2x2 plots
> plot(NO3.N, pH, xlab="NO3 (ug/L N)", ylab="pH")
```

First do a linear regression.

```
> fit.lm <- lm(pH ~ NO3.N)
> abline(coef(fit.lm), col="blue")
```

We would like to add some summary stats from `summary(fit.lm)` on the plot: R2, p-value. How do we extract these values?

```
> names(fit.lm)
 [1] "coefficients"  "residuals"     "effects"       "rank"
 [5] "fitted.values" "assign"        "qr"            "df.residual"
 [9] "na.action"     "xlevels"       "call"          "terms"
[13] "model"
> names(summary(fit.lm))
 [1] "call"          "terms"         "residuals"     "coefficients"
 [5] "aliased"       "sigma"         "df"            "r.squared"
 [9] "adj.r.squared" "fstatistic"    "cov.unscaled"
> dimnames(coef(summary(fit.lm)))
[[1]]
[1] "(Intercept)" "NO3.N"
[[2]]
[1] "Estimate"   "Std. Error" "t value"    "Pr(>|t|)"
```

Add title (can also use `main()` for this):

```
> mtext("LM", side=3, line=.5, col="blue")
```

We can use the function `paste()` to combine summary stats values with text on the plot.

```
> mtext(paste("R2=", round(summary(fit.lm)$adj.r.squared,2), sep=""),
+      side=3, line=-2, adj=.5, col="blue")
```

The argument `line=` gives distance from the box, `adj=` gives adjustment left/right.
If the p-value is below 0.001, we'll just write "`p < 0.001`".

```
> pvalue <- coef(summary(fit.lm))[2,"Pr(>|t|)"]      # extract p-value
if (pvalue >= 0.001) {
+      mtext(paste("p=", pvalue, sep=""), side=3, line=-2, adj=1, col="blue")
}
```

The curly brackets mark beginning and end of a statement. This is necessary if the statement is written over more than one line. Here the test failed, therefore nothing happened.

```
> if (pvalue < 0.001)
+      mtext("p<0.001", side=3, line=-2, adj=0.99, col="blue")
```

The test passed, and so the text was added.

PS: It should be possible to write this test more elegantly with the function **`ifelse(test, yes, no)`** or **`if(test) {yes} else {no}`**

We also want to add confidence intervals for the mean. The function

```
       predict.lm(object, interval="confidence")
```

gives a matrix with columns `fit, lwr, upr` (lower and upper confidence intervals) for the mean. Alternatively for the response, see `?predic.lm`.
Make a sequence of x's for which we will predict the response:

```
> new.x  <- data.frame(NO3.N = seq(min(NO3.N, na.rm=T), max(NO3.N, na.rm=T),
+ length=50))
> pred.lm <- predict.lm(fit.lm, interval="confidence", newdata=new.x)
> is.matrix(pred.lm)
[1] TRUE
> is.data.frame(pred.lm)
[1] FALSE
```

Matrices can behave a bit differently from data.frames:
- They don't have "names" for columns, but "`colnames`"
- They also have "`dimnames`", which is a list containing "`rownames`" (= `dimnames[[1]])` and "`colnames`" (= `dimnames[[2]]`)
- Length() for a data.frame is no. of columns, but `length()` for a matrix is no. of elements (=`nrow*ncol`)
- You can't select the columns of a matrix by `DATA$columnname`, but by `DATA[,"columnname"]`
- `dim()`, `nrow()`, `ncol()` work the same way for matrices and data.frames.

```
> lines(new.x$NO3.N, pred.lm[,"fit"], col="blue")
```
This gives the same as line as `abline(coef(fit.lm))`.
```
> lines(new.x$NO3.N, pred.lm[,"lwr"], col="blue", lty=2)
> lines(new.x$NO3.N, pred.lm[,"upr"], col="blue", lty=2)
```

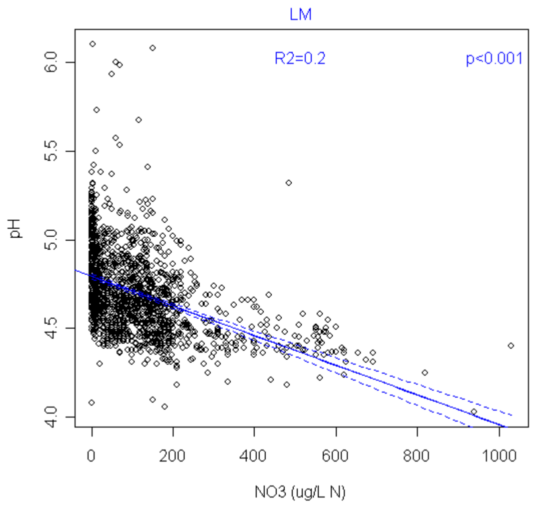


Figure 26. Linear regression of pH vs. NO3 in Storgama

##

Now let's say we're only interested in whether pH is above or below a boundary value of 4.5
```
> boundary    # OK to use this name?
Error: object "boundary" not found
> boundary <- 4.5
```

Change pH data into binary 0/1, below/above boundary. First make empty vector (not really necessary here, but in other cases it's useful).
```
> DATA$pH.bin <- rep(NA, nrow(DATA))
```

Identify those rows with pH above the boundary, with a logical test:
```
test <- DATA$pH > boundary
```
(Why use object "`boundary`" in stead of the value 4.5 directly? - In case we want to change the value later, then it needs to be updated in only one place.)
This gives a vector "`test`" with components `TRUE, FALSE, NA`
```
> DATA$pH.bin <- as.numeric(test)
```
Here, `as.numeric()` translates these components to 1, 0, NA, respectively. We could also make a more compact formulation:
```
> DATA$pH.bin <- as.numeric(DATA$pH > boundary)
```

Note that columns added to a data.frame AFTER it is attached, will not be available directly. So we'll detach and attach the data.frame again.
```
> detach(DATA)
> attach(DATA)

> plot(NO3.N, pH.bin, xlab="NO3 (ug/L N)", ylab=paste("pH >", boundary))
```

How will a linear regression work now (**Figure 27**)?

```
> fit.lm <- lm(pH.bin ~ NO3.N)
> pred.lm <- predict.lm(fit.lm, newdata=new.x, interval="confidence")
> lines(new.x$NO3.N, pred.lm[,"fit"], col="red")
> lines(new.x$NO3.N, pred.lm[,"lwr"], col="red", lty=2)
> lines(new.x$NO3.N, pred.lm[,"upr"], col="red", lty=2)
> mtext(paste("R2=", round(summary(fit.lm)$adj.r.squared,2), sep=""),
+ side=3, line=-2, adj=.5, col="red")
> pvalue <- coef(summary(fit.lm))[2,"Pr(>|t|)"]# extract p-value
> if (pvalue >= 0.001) {
+ mtext(paste("p=", pvalue, sep=""), side=3, line=-2, adj=1, col="red") }
> if (pvalue < 0.001) {
+ mtext("p<0.001", side=3, line=-2, adj=0.99, col="red") }
```

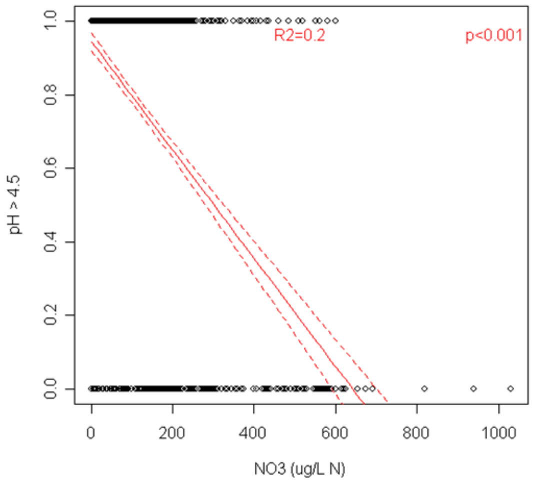


Figure 27. Linear regression of binary transformed pH vs. NO3 in Storgama.

The linear model is significant, but common sense shows that an LM is not appropriate. Look at the range of fitted values compared to the range of original values:

```
> range(pH.bin)
[1] NA NA
> range(pH.bin, na.rm=TRUE)
# na.rm=T can also be used with min(), max(), mean(), stdev(), etc.
[1] 0 1
> range(fitted(fit.lm))
[1] -0.5725272  0.9426986
```

LOGISTIC REGRESSION is the solution here: this method deals with binary response variable. R can also do logistic regression with the response variable in other formats, e.g. proportions. See `?glm`

```
> fit.glm <- glm(pH.bin ~ NO3.N, family=binomial)
```

The default is: `family=binomial(link=logit)`
Note that for GLM, `predict()` or `predict.glm()` gives us predicted y values on the logit-transformed scale (-Inf,Inf)...

```
> range(predict(fit.glm))
[1] -6.536935  2.391123
```

...while `fitted()` gives us fitted y values back-transformed to (0,1) scale.

```
> range(fitted(fit.glm))
[1] 0.001446826 0.916147870
```

The function `predict.glm()` doesn't seemt to give confidence intervals directly, like `predict.lm()` does. But we will still get the standard errors, and can add them ourselves to plot confidence intervals.

```
> pred.glm    <- predict.glm(fit.glm, newdata=new.x, se.fit=T)
> y.lower     <- pred.glm$fit - pred.glm$se.fit
> y.upper     <- pred.glm$fit + pred.glm$se.fit
```

Now we must back-transform the predicted values to (0,1) scale before plotting them (**Figure 28**). We'll make a little function to help us with this.

```
> backtrans <- function(x) {
+ exp(x)/(1 + exp(x))# inverse function of logit(y) = log(y)/log(1-y)
+ }
> lines(new.x$NO3.N, backtrans(pred.glm$fit), col="green")
> lines(new.x$NO3.N, backtrans(y.lower), col="green", lty=2)
> lines(new.x$NO3.N, backtrans(y.upper), col="green", lty=2)
> mtext("GLM: Logistic reg.", side=3, line=.5, col="green")
> pvalue <- coef(summary(fit.glm))[2,"Pr(>|z|)"]     # extract p-value
> if (pvalue >= 0.001) {
+     mtext(paste("p=", pvalue, sep=""), side=3, line=-3, adj=1, col="green")
+ }
> if (pvalue < 0.001) {
+     mtext("p<0.001", side=3, line=-3, adj=0.99, col="green")
+ }
```

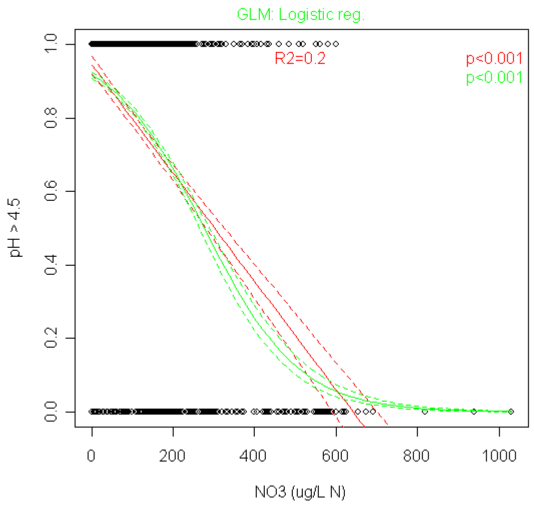


Figure 28. Linear regression (red) and logistic regression (green) of binary transformed pH vs. NO3 in Storgama.

As it turns out, plotting of the logistic regression prediction could be done simpler. The argument `type="response"` gives predicted probabilities p(y) (on scale 0:1), instead of the default log(odds) = log(p(y)/(1-p(y))) (on scale -Inf:Inf)

```
> pred.glm <- predict.glm(fit.glm, newdata=new.x, se.fit=T, type="response")
> y.lower <- pred.glm$fit - pred.glm$se.fit
> y.upper <- pred.glm$fit + pred.glm$se.fit
> lines(new.x$NO3.N, y.lower, col="blue", lty=2)
> lines(new.x$NO3.N, y.upper, col="blue", lty=2)
```

The command `summary(fit.glm)` doesn't give any R2 value for a glm object. But a "pseudo R2" can be calculate from the deviance:

```
> nres <- length(residuals(fit.glm))
> R2 <- (1 - exp((fit.glm$deviance -
+ fit.glm$null.deviance)/nres))/(1 - exp( - fit.glm$null.deviance/nres))
> mtext(paste("R2=", round(R2,2), sep=""), side=3, line=-3, adj=.5, col="green")
```

But for model selection with GLMs we'll use the deviance directly, rather than R2. Compare what you get with `anova(fit.lm)` and `anova(fit.glm)`:

```
> anova(fit.lm)     # gives Analysis of variance
Analysis of Variance Table
Response: pH.bin
            Df  Sum Sq Mean Sq F value    Pr(>F)
NO3.N        1  54.303  54.303  390.28 < 2.2e-16 ***
Residuals 1550 215.666   0.139

> anova(fit.glm)    # gives Analysis of deviance
Analysis of Deviance Table
Model: binomial, link: logit
Response: pH.bin
Terms added sequentially (first to last)
        Df Deviance Resid. Df Resid. Dev
NULL                     1551    1651.97
NO3.N    1   287.28      1550    1364.69
```

A statistical theorem says that we can use the difference in deviance between "null model" and "full model" (given in the the anova table) to test if the parameter(s) in the full model is significant.

```
> dev.null <- anova(fit.glm)["NULL", "Resid. Dev"]
> dev.full <- anova(fit.glm)["NO3.N", "Resid. Dev"]
> 1 - pchisq(dev.null - dev.full, df=1)# df = difference in number of parameters
[1] 0
```

Actually, we can also ask for this test directly within `anova()`:

```
> anova(fit.glm, test="Chi")
Analysis of Deviance Table
Model: binomial, link: logit
Response: pH.bin
Terms added sequentially (first to last)
        Df Deviance Resid. Df Resid. Dev P(>|Chi|)
NULL                     1551    1651.97
NO3.N    1   287.28      1550    1364.69 1.950e-64

> detach(DATA)
```

2.8.4 Script 4: Generalised additive models.

Let's go back to our original y variable.

```
attach(DATA)
plot(NO3.N, pH, xlab="NO3 (ug/L N)", ylab="pH")
fit.lm <- lm(pH ~ NO3.N)
```

Are we certain that a linear model is the best choice? Does pH really decrease lineary with NO3, no lower boundary? We could try various polynomial functions etc., but a more efficient solution is to use GAM for explorative data analysis (when you have "enough" data). See Figure 29.

```
> library(mgcv)
This is mgcv 1.3-16

> fit.gam <- gam(pH ~ s(NO3.N))
```

The argument `s()` is a non-parametric, flexible "spline function"

```
> summary(fit.gam)
Family: gaussian
Link function: identity
Formula:
pH ~ s(NO3.N)
Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 4.698061   0.005334   880.7   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Approximate significance of smooth terms:
            edf Est.rank     F p-value
s(NO3.N) 7.652    9.000 51.89  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.228   Deviance explained = 23.2%
GCV score = 0.044412   Scale est. = 0.044165  n = 1552
> names(summary(fit.gam))
 [1] "p.coeff"       "se"             "p.t"            "p.pv"
 [5] "residual.df"   "m"              "chi.sq"         "s.pv"
 [9] "scale"         "r.sq"           "family"         "formula"
[13] "n"             "dev.expl"       "edf"            "dispersion"
[17] "pTerms.pv"     "pTerms.chi.sq" "pTerms.df"      "cov.unscaled"
[21] "cov.scaled"    "p.table"        "pTerms.table"   "s.table"
[25] "gcv"
```

The command `summary(fit.gam)` gives us R2 and p-value, but with slightly different names than in `summary(fit.lm)`

```
> pred.gam <- predict(fit.gam, newdata=new.x, se.fit=T)
> y.lower <- pred.gam$fit - pred.gam$se.fit
> y.upper <- pred.gam$fit + pred.gam$se.fit
> lines(new.x$NO3.N, pred.gam$fit, col="orange")
> lines(new.x$NO3.N, y.lower, col="orange", lty=2)
> lines(new.x$NO3.N, y.upper, col="orange", lty=2)
> mtext("GAM", side=3, line=.5, col="orange")
> mtext(paste("R2=", round(summary(fit.gam)$r.sq, 2), sep=""),
+ side=3, line=-2, adj=.5, col="orange")
> pvalue <- summary(fit.gam)$s.pv# p-value for spline function
> if (pvalue >= 0.001) {
+ mtext(paste("p=", pvalue, sep=""), side=3, line=-2, adj=1, col="orange")
+ }
> if (pvalue < 0.001) {
+ mtext("p<0.001", side=3, line=-2, adj=0.99, col="orange")
+ }
```

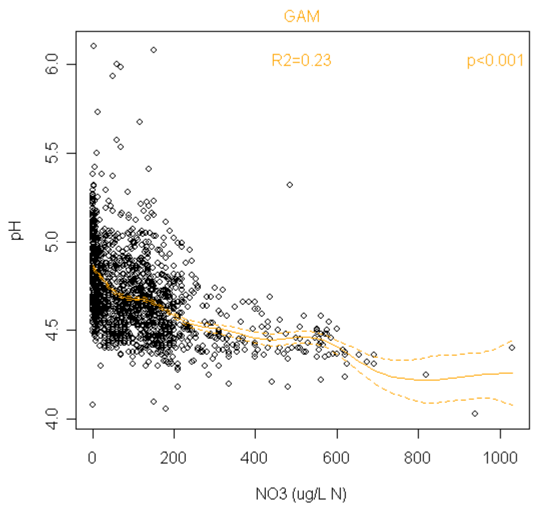


Figure 29. Generalised additive model (GAM) regression of pH vs. NO3 in Storgama.

The GAM curve gives a better description of the relationship between variables (Figure 29). The CI are also more flexible. E.g. for NO3 > 600, you can't really conclude from the data whether pH increases or decreases.

"GCV" stands for generalised cross-validation - a method for automatic optimisation of smoothness together with model fitting. Estimated degrees of freedom is

```
> summary(fit.gam)$edf
[1] 7.651956
```

But we can allow it to be more wiggly or more smooth manually. The `gam()` argument "`gamma=`" multiplies the "penalty" for wigglyness. So lower gamma means more wiggly (**Figure 30**, left panel); higher gamma means more smooth (**Figure 30**, right panel).

```
> plot(NO3.N, pH, xlab="NO3 (ug/L N)", ylab="pH")
> fit.gam.2 <- gam(pH ~ s(NO3.N), gamma=.01)
> pred.gam <- predict(fit.gam.2, newdata=new.x, se.fit=T)
> y.lower <- pred.gam$fit - pred.gam$se.fit
> y.upper <- pred.gam$fit + pred.gam$se.fit
> lines(new.x$NO3.N, pred.gam$fit, col="purple")
> lines(new.x$NO3.N, y.lower, col="purple", lty=2)
> lines(new.x$NO3.N, y.upper, col="purple", lty=2)
```

Not so much difference from the optimised curve

```
> mtext("gamma=.01", side=3, line=.5, col="purple", adj=0)
> mtext(paste("R2=", round(summary(fit.gam.2)$r.sq, 2), sep=""),
+ side=3, line=-2, adj=.5, col="purple")
> pvalue <- summary(fit.gam.2)$s.pv# p-value for spline function
> if (pvalue >= 0.001) {
+ mtext(paste("p=", pvalue, sep=""), side=3, line=-2, adj=1, col="purple")
+ }
> if (pvalue < 0.001) {
+ mtext("p<0.001", side=3, line=-2, adj=0.99, col="purple")
+ }

> fit.gam.3 <- gam(pH ~ s(NO3.N), gamma=100)
> pred.gam<- predict(fit.gam.3, newdata=new.x, se.fit=T)
> y.lower <- pred.gam$fit - pred.gam$se.fit
> y.upper <- pred.gam$fit + pred.gam$se.fit
> lines(new.x$NO3.N, pred.gam$fit, col="turquoise")
> lines(new.x$NO3.N, y.lower, col="turquoise", lty=2)
> lines(new.x$NO3.N, y.upper, col="turquoise", lty=2)
```

Almost linear fit.

```
> mtext("gamma=100", side=3, line=.5, col="turquoise", adj=1)
> mtext(paste("R2=", round(summary(fit.gam.3)$r.sq, 2), sep=""),
+ side=3, line=-3, adj=.5, col="turquoise")
> pvalue <- summary(fit.gam.3)$s.pv# p-value for spline function
> if (pvalue >= 0.001) {
+ mtext(paste("p=", pvalue, sep=""), side=3, line=-3, adj=1, col="turquoise")
+ }
> if (pvalue < 0.001) {
+ mtext("p<0.001", side=3, line=-3, adj=0.99, col="turquoise")
+ }
```

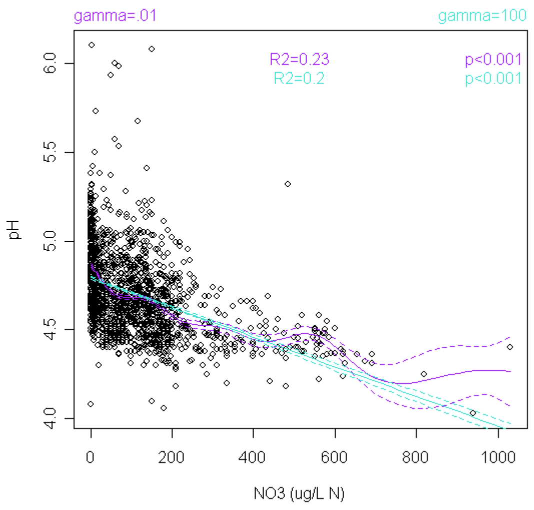


Figure 30. Generalised additive model (GAM) regression of pH vs. NO3 in Storgama, with high and low degree of smoothing.

```
detach(DATA)
```

3. TIME SERIES

3.1 Trends, seasons and autocorrelation

Jannicke Moe

The data are a series on nutrients etc. in River Glomma (from Per G. Stålnacke).

Question: is there a temporal trend in TN (total nitrogen)?

```
> glomma.na <- read.delim("PGS_Glomma_TN.txt")
> names(glomma.na)
[1] "year"  "month" "Q"     "TN"    "SPM"   "TP"    "Cu"    "Pb"
```

The series consists of 13 years x 12 months, with some months lacking observations. Some of the functions we will use do not accept NAs, so we will replace these by other values.

```
> (na.rows <- which(is.na(glomma.na$TN)))
[1]  74 109 124 133 144 152 156
```

Make a new data.frame, where we willl replace NAs with numbers:

```
> glomma <- glomma.na
```

We'll use the mean of all remaining years for that month (assuming there is no long-term trend):

```
> for (i in na.rows) {                  # i runs through rows with NAs
+     for (j in 3:8) {                  # j runs through columns with variables
+           glomma[i,j] <- mean(glomma[glomma$month==glomma$month[i], j], na.rm=T)
+
+     }
+ }
```

For larger operations, functions like `apply()` are more efficient than `for()` loops. Below I will run some functions with both `glomma` and `glomma.na`, to test where NAs are accepted.

```
> plot(glomma)
```

It is hard to spot any trend in Figure 31 (against year or month).

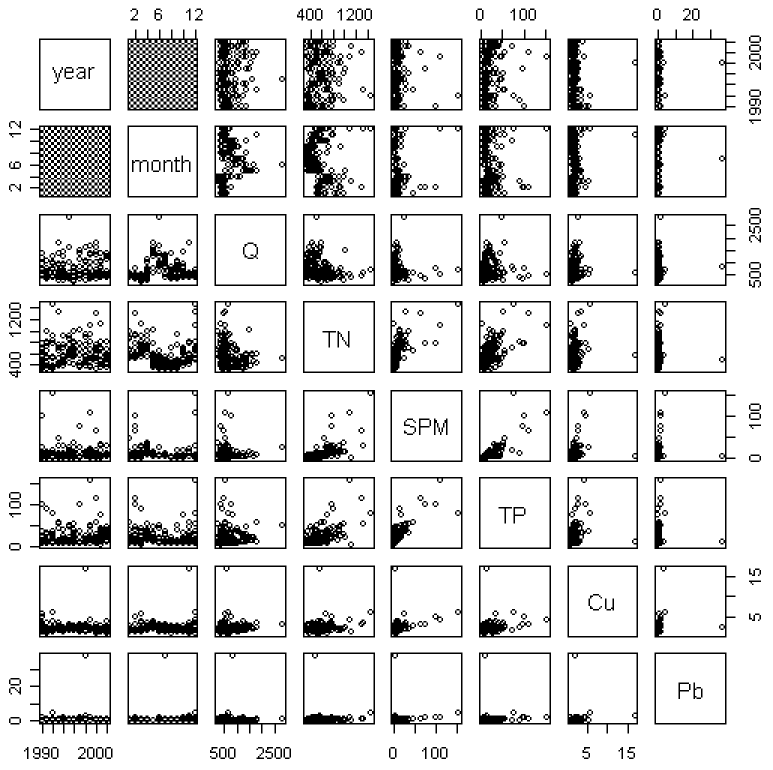


Figure 31. Pair-wise scatterplots for the data set glomma.

To see the trends more clearly, plot each physical/chemical variable (cols 3-8) against time (**Figure 32**).

```
> par(mfrow=c(6,1), oma=c(3,3,2,1), mar=c(1,2,1,1))
> for (i in 3:8) {
+      plot(glomma.na[,i], type="l", col=i)
+ mtext(names(glomma.na)[i], side=2, outer=F, line=3)
+ }
> mtext("Time (months)", side=1, outer=T, line=1)
```

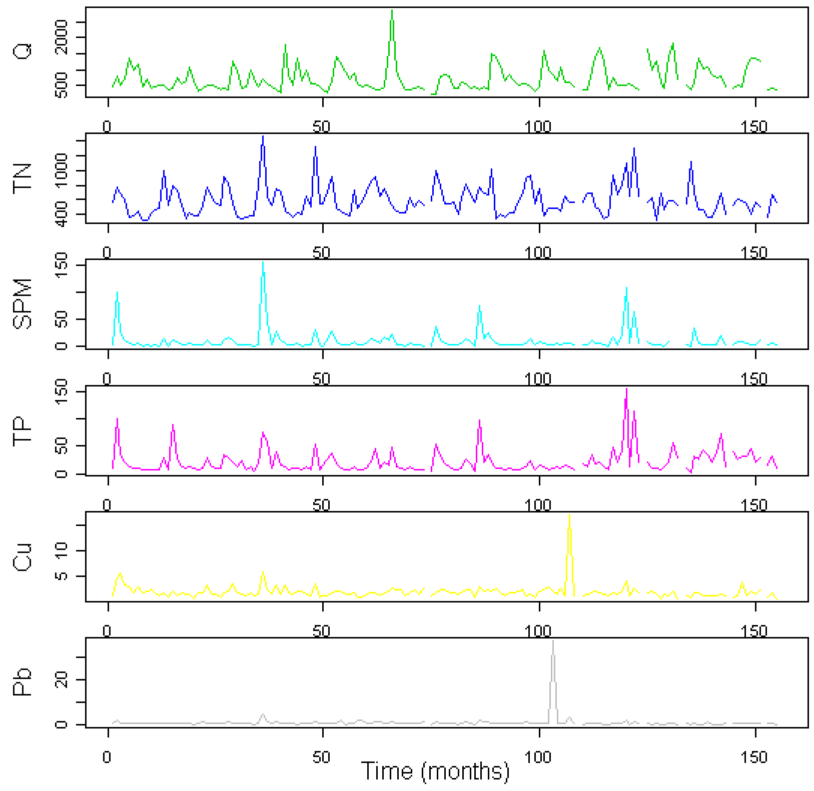


Figure 32. Each chemical variable in the data set glomma plotted against time.

3.1.1 Trend analysis by regression

We can start with a simple regression for TN (although this is not recommended by statisticians, since it invalidates some assumptions).

```
> windows()
> par(mfrow=c(2,1))
```

Fit TN against time sequence counting from 1:end (unit months)

```
> fit.1 <- lm(glomma$TN ~ seq(1:nrow(glomma)))
```

Here I added `seq()` because `lm()` got confused by the ":".

```
> plot(glomma$TN, type="l") # See Figure 33
> abline(coef(fit.1), col="red")
```

We can decompose the model into year and month (month as a categorical covariate), with year.no starting at 1:

```
> glomma$year.no    <- glomma$year - min(glomma$year) + 1
> fit.2 <- lm(glomma$TN ~ glomma$year.no + as.factor(glomma$month))
> summary(fit.2)
Call:
lm(formula = glomma$TN ~ glomma$year.no + as.factor(glomma$month))

Residuals:
    Min      1Q  Median      3Q     Max
-289.92  -95.05  -32.65   64.42  679.93

Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept)                637.253     52.026  12.249  < 2e-16 ***
glomma$year.no               3.574      3.532   1.012 0.313235
```

```
as.factor(glomma$month)2    48.977     64.739   0.757 0.450572
as.factor(glomma$month)3    60.189     64.739   0.930 0.354084
as.factor(glomma$month)4    79.977     64.739   1.235 0.218713
as.factor(glomma$month)5  -118.196     64.739  -1.826 0.069976 .
as.factor(glomma$month)6  -203.811     64.739  -3.148 0.002000 **
as.factor(glomma$month)7  -248.811     64.739  -3.843 0.000182 ***
as.factor(glomma$month)8  -231.606     64.739  -3.578 0.000474 ***
as.factor(glomma$month)9  -185.503     64.739  -2.865 0.004793 **
as.factor(glomma$month)10  -92.427     64.739  -1.428 0.155562
as.factor(glomma$month)11  -51.119     64.739  -0.790 0.431058
as.factor(glomma$month)12  132.091     64.739   2.040 0.043154 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 165.1 on 143 degrees of freedom
Multiple R-Squared: 0.3929,     Adjusted R-squared: 0.3419
F-statistic: 7.712 on 12 and 143 DF,  p-value: 6.364e-11
```

Summer months give strongest seasonal effect, as could be expected.

We obtain the slope per year from `coef(fit.2)[2]`. Divide this by 12 to get the slope per month, as in the plot.

```
> abline(a=coef(fit.2)[1], b=coef(fit.2)[2]/12, col="green")
```

This gives a much better fit (check R2 and p values), but there is still no significant trend per year.

In stead of having 12 different parameter estimates for the months, we can use a non-linear fit with splines in GAM.

```
> library(mgcv)
> fit.3 <- gam(glomma$TN ~ glomma$year.no + s(glomma$month))
> windows()
> par(mfrow=c(3,1))
```

Look at the effect of months (Figure 33, upper panel). Note that this plot is centered around zero on y-axis.

```
> plot(fit.3)
```

Also look at the linear trend (Figure 33, middle panel). Here the unit is years.

```
> plot(unique(glomma$year.no), coef(fit.3)[2]*unique(glomma$year.no), type="l",
+ ylim=c(-200,200))
```

Standard deviations can be added in a cumbersome way:

```
> lines(unique(glomma$year.no),
+ (coef(fit.3)[2] + summary(fit.3)$se[2])*unique(glomma$year.no), lty=2)
> lines(unique(glomma$year.no),
+ (coef(fit.3)[2] - summary(fit.3)$se[2])*unique(glomma$year.no), lty=2)
```

Compare the fitted model with the data (Figure 33, lower panel):

```
> plot(glomma$TN, type="l")
> lines(fitted(fit.3), type="l", col="red")
```

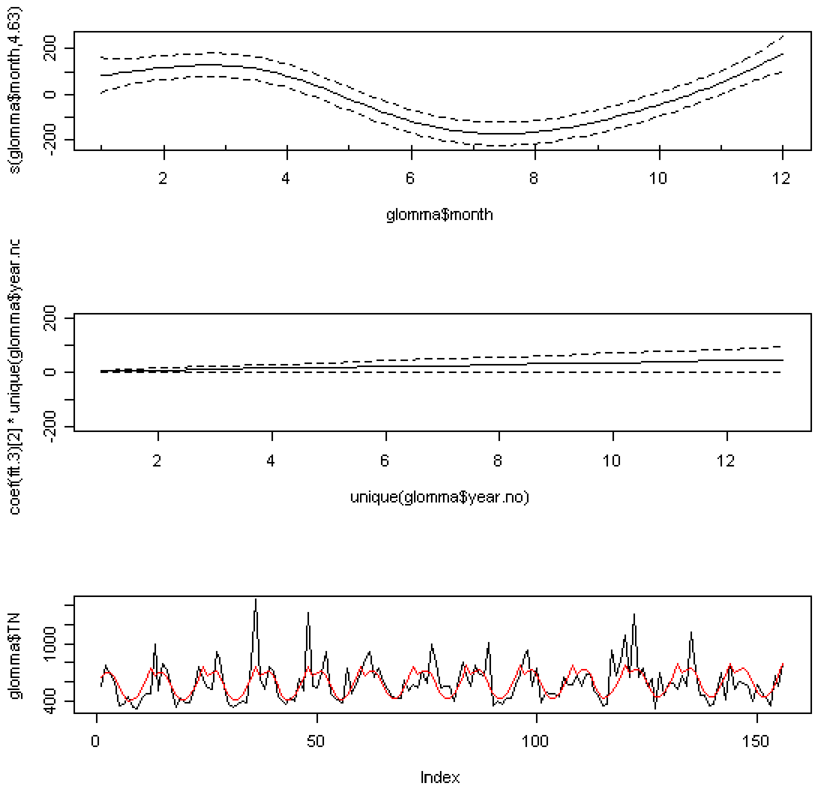


Figure 33. Trend estimations for TN from Glomma. Upper panel: Effect of month on TN, estimated by GAM. Middle panel: linear effect of year on TN. Lower panel: comparison of data and model prediction.

Of course, the trend can also be modelled as splines instead of as a line (Figure 34).

```
> fit.4 <- gam(glomma$TN ~  s(glomma$month) + s(glomma$year.no))
> windows()
> par(mfrow=c(3,1))
> plot(fit.4)  # Plots estimate for each predictor variable in separate plots
>      # NB: Here R asks for a "return", therefore I've added an empty line.
> plot(glomma$TN, type="l")
> lines(fitted(fit.4), col="red")
```

The trend is not significantly non-linear, and not significantly != zero, according to this plot.

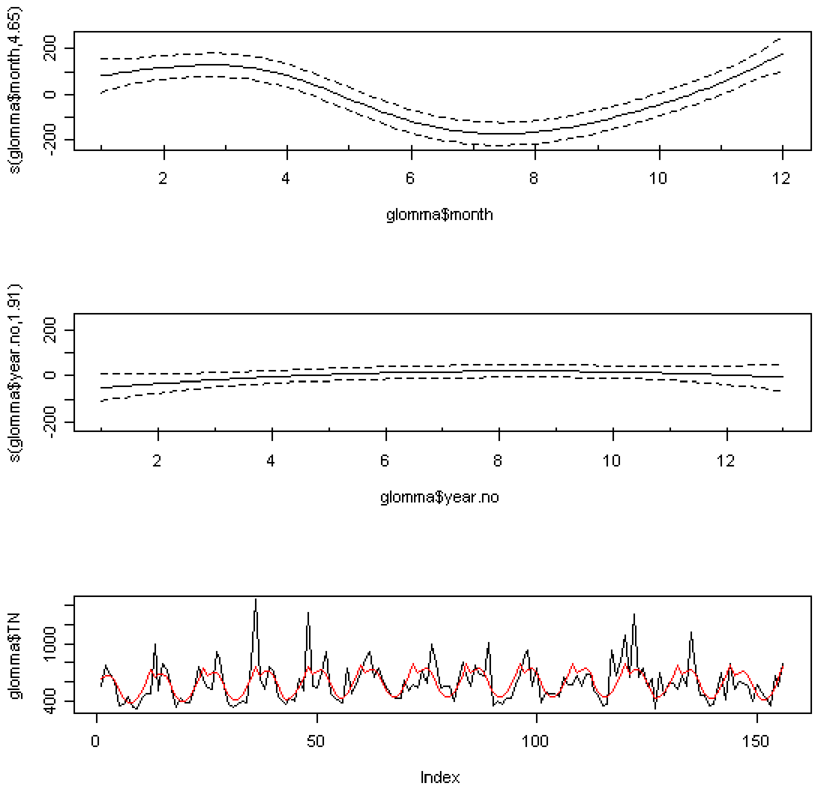


Figure 34. Trend estimations for TN from Glomma. Upper panel: Effect of month on TN, estimated by GAM. Middle panel: effect of year on TN, estimated by GAM. Lower panel: comparison of data and model prediction.

Next we'll make a so-called time-series object, which enables us to do some "proper" time-series analyses. These methods accept serial correlation, and can do operations like decomposition into trend and season more efficiently than regression. In return they demand strictly regular series (equal time intervals), and can be unfriendly towards NAs.

3.1.2 Make time-series object

Time-series plot (Figure 35):

```
> plot.ts(glomma[,3:8], nc=1)    # PS. Note difference from the command plot()
> plot.ts(glomma.na[,3:8], nc=1) # Here NAs are accepted
```

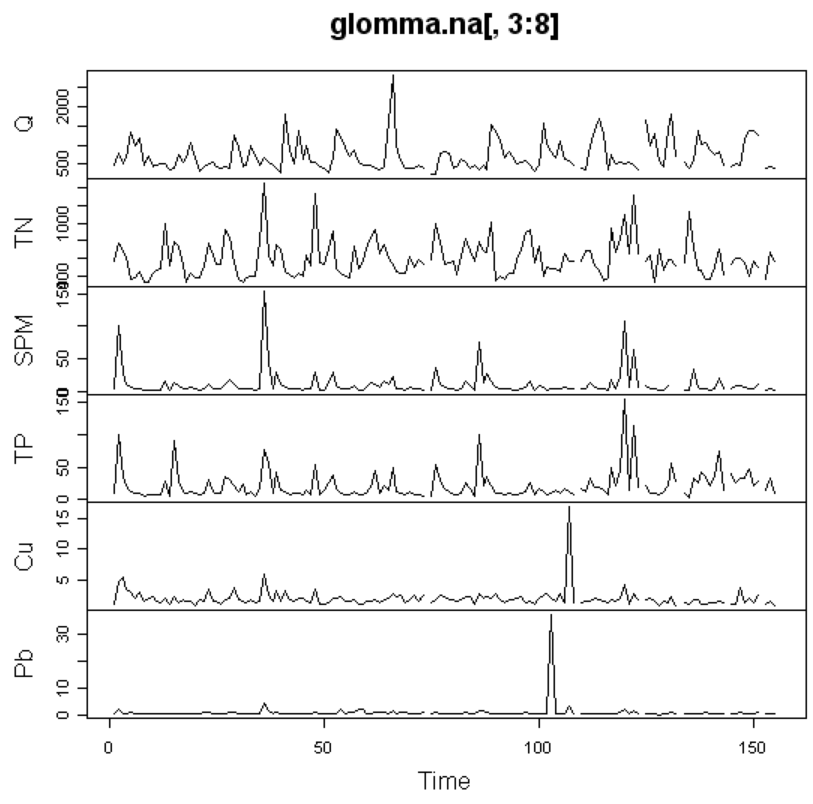


Figure 35. Time-series plot for the data set glomma.

But R doesn't know yet that `glomma` is a time series:

```
> is.ts(glomma)
[1] FALSE
```

… so we'll make it into a time series.

```
> glomma.ts <- ts(glomma[,3:8], start=c(1990, 1), frequency=12,
+      names=names(glomma[3:8]))
```

The time variables are now defined by `start=` and `frequency=` . R assumes that `frequency=12` means months. Here: `start=c(year, month)`, but could be defined with other time units. NB: the time series must have regular intervals! (We can add NAs to obtain this.)

```
> glomma.na.ts <- ts(glomma.na[,3:8], start=c(1990, 1), frequency=12,
+      names=names(glomma.na[3:8]))
> is.ts(glomma.ts)
[1] TRUE
```

Now glomma.ts is no longer a data.frame but a matrix (unfortunately),

```
> is.data.frame(glomma.ts)
[1] FALSE
> is.matrix(glomma.ts)
[1] TRUE
```

… so glomma.ts doesn't have "names" (`$col.name`), but "dimnames" `[,"col.name"]`.

```
> glomma.ts$TN
NULL
```

```
> glomma.ts[,"TN"]
Time Series:
Start = 1
End = 156
Frequency = 1
  [1]  564.0000  774.0000  680.0000  610.0000  355.0000  374.0000  444.0000
  [8]  329.0000  321.0000  431.0000  471.0000  483.0000  991.0000  517.0000
 [15]  796.0000  730.0000  528.0000  333.0000  428.0000  381.0000  378.0000
 [etc.]
```

The rownames and colnames of `glomma.ts[,"TN"]` are not readily available. Note that time variables are not columns in the matrix `glomma.ts`, they are just stored as the time series' attributes

```
> attributes(glomma.ts)          # tsp gives start, end, frequency
$dim
[1] 156   6

$dimnames
$dimnames[[1]]
NULL
$dimnames[[2]]
[1] "Q"    "TN"   "SPM" "TP"   "Cu"   "Pb"

$tsp
[1]   1 156   1

$class
[1] "mts" "ts"
```

Plot the time-series object (Figure 36):

```
> plot.ts(glomma.ts, nc=1)
```

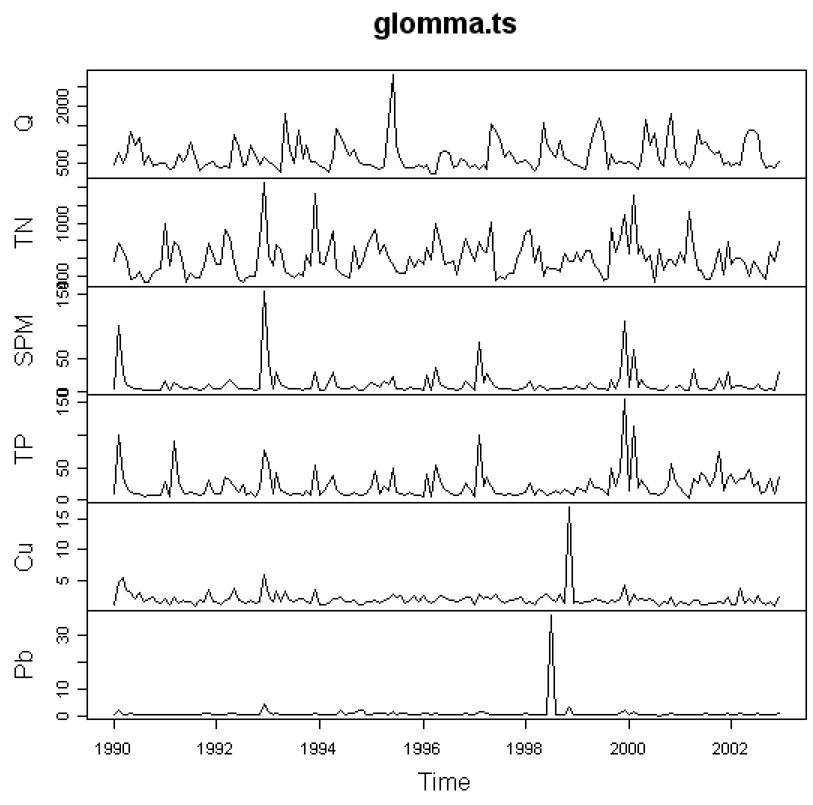


Figure 36. Time-series plot of time-series object glomma.ts.

Notice difference on x-axis compared to Figure 35, where we have used the same function `plot.ts()` but plotted the data frame `glomma` rather than the time-series object `glomma.ts`. On the other hand, the ordinary `plot()` function used on a ts object will also behave like the function `plot.ts()`.

```
> plot(glomma.ts, nc=1)
```

3.1.3 Trend analysis by non-parametric trend test

Mann-Kendall is a simple non-parametric test (not making assumptions about data distribution), checking whether there is a monotonous trend (not necessarily linear).

```
> library(Kendall)
> MannKendall(glomma$TN)
tau = 0.0662, 2-sided pvalue =0.22136
```

We can try to account for seasonal variation. This test requires a time-series object. Here, seasons are implicit (given by the time series' frequency).

```
> SeasonalMannKendall(glomma.ts[,"TN"])
tau = 0.140, 2-sided pvalue =0.020947
```

Now it's significant, but less significant than the regression test (compare with `summary(fit.2)`), as it should be.

3.1.4 Trend analysis by seasonal decomposition

Now that we have a ts object, we can decompose it into trend, season, and residuals. The function `stl()` does this with loess smoothing. Let's try this decomposition with TN.

```
> TN.stl <- stl(glomma.ts[,"TN"], s.window="periodic")
```

`s.window` = span for seasonal extraction,

`t.window` = for trend extraction, set by R if not given

```
> plot(TN.stl, col.range="yellow", main=paste("Seasonal decomposition, t.window=",
+ TN.stl$win[2]))
```

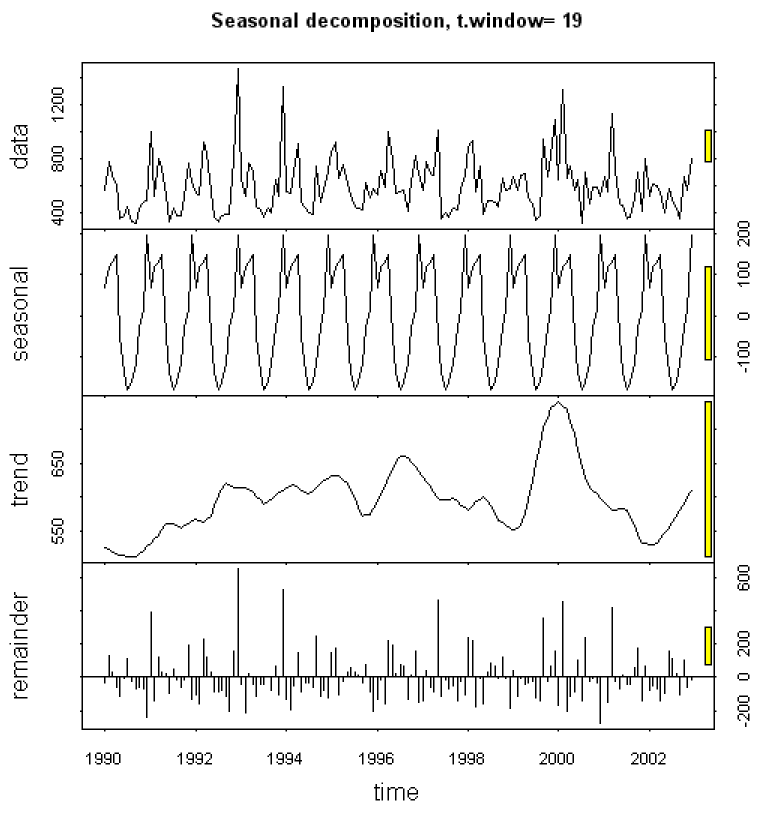


Figure 37. Seasonal decomposition of time-series object glomma.ts.

The yellow bars indicate the difference in scale for the different components. NAs are apparently not welcome here:

```
> TN.stl <- stl(glomma.na.ts[,"TN"], s.window="periodic", na.action=na.exclude)
Error in stl(glomma.na.ts[, "TN"], s.window = "periodic", na.action = na.exclude) :
        series is not periodic or has less than two periods
> TN.stl <- stl(glomma.na.ts[,"TN"], s.window="periodic", na.action=na.omit)
Error in na.omit.ts(as.ts(x)) : time series contains internal NAs
> TN.stl <- stl(glomma.na.ts[,"TN"], s.window="periodic", na.action=na.pass)
Error in stl(glomma.na.ts[, "TN"], s.window = "periodic", na.action = na.pass) :
        NA/NaN/Inf in foreign function call (arg 1)
```

We can make the the trend estimation more smooth or less smooth (Figure 38)

```
windows()
plot(stl(glomma.ts[,"TN"], s.window="periodic", t.window=35), col.range="yellow",
       main="Seasonal decomposition, t.window=35")
windows()
plot(stl(glomma.ts[,"TN"], s.window="periodic", t.window=7), col.range="yellow",
       main="Seasonal decomposition, t.window=7")
```

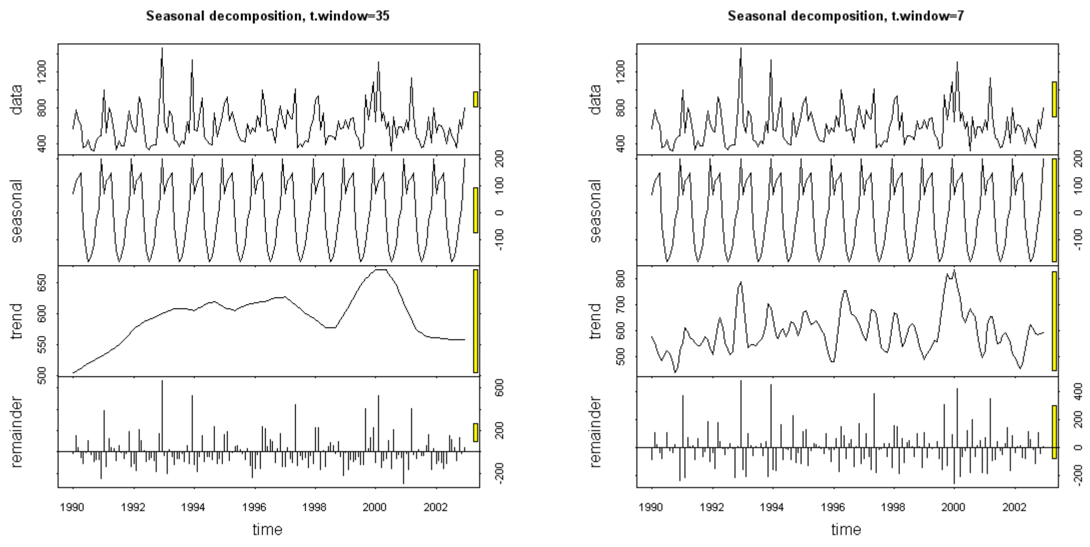


Figure 38. Seasonal decomposition of time-series object glomma.ts, with more smoothing (left panel) and less smoothing (right panel).

Which month gives peak TN, according to our seasonal decomposition?

```
> which.max(TN.stl$time.series[1:12])  # Which month during first 12 months?
[1] 12
```

Which are the first and second highest peak?

```
> rev(order(TN.stl$time.series[1:12]))[1:2]
[1] 12  4
```

Consider: is the double peak in seasonal effect reasonable?

3.1.5 Autocorrelation

Time-series data are often correlated in time (a reason why regression should not be used). We can check the autocorrelation as a function of number of lags (here: months)

```
> windows()
> par(mfrow=c(3,1))
> acf(glomma[,"TN"])# Original data.frame: unit is months
> acf(glomma.ts[,"TN"])# Time-series object: unit is years
```

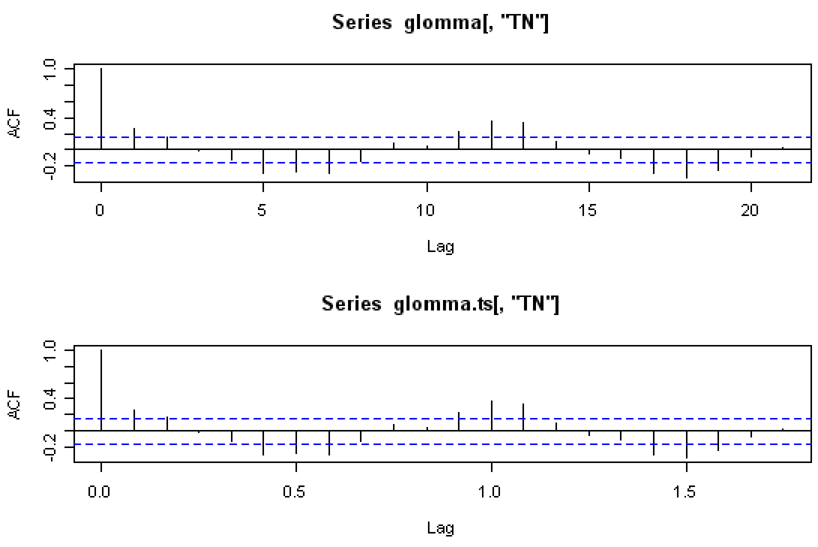


Figure 39. Autocorrelation plots for dataset glomma (upper panel) and for time-series object glomma.ts.

The ACF plot (Figure 39) indicates significant autocorrelation for lag around 11-13 months, which should not be a surprise.

Autocorrelation can also be tested with an autoregressive model `ar()`, which uses AIC to select number of significant lags

```
> ar(glomma.ts[,"TN"])
Call:
ar(x = glomma.ts[, "TN"])

Coefficients:
      1        2        3        4        5        6        7        8  
 0.1018   0.0847  -0.0421  -0.0393  -0.1454  -0.0476  -0.1188  -0.0045  
      9       10       11       12       13  
 0.1404  -0.1090   0.0524   0.2029   0.1704  

Order selected 13  sigma^2 estimated as  32336
```

Here, the estimated order of 13 lags corresponds to 13 months. Let's try also the time series with NA's.

```
> ar(glomma.na.ts[,"TN"], na.action=na.exclude)
Call:
ar(x = glomma.na.ts[, "TN"], na.action = na.exclude)

Coefficients:
      1        2        3        4        5        6        7  
 0.1738   0.0041   0.0175  -0.1133  -0.1111  -0.1777  -0.1500  

Order selected 7  sigma^2 estimated as  36083
```

The NA version gives a different result, so the function `ar()` does not seem robust to missing values...

We can also test the residuals from the seasonal decomposition. We have seen the residuals in the `stl` plot so we know they exist, but how do we get the numbers?

```
> names(TN.stl)
[1] "time.series" "weights"     "call"        "win"         "deg"        
[6] "jump"        "inner"       "outer"      
```

Check what "time.series" contains:
```
> names(TN.stl$time.series)
NULL
```
When `names()` does not work, it can be useful to try `dimnames()`
```
> dimnames(TN.stl$time.series)
[[1]]
NULL
[[2]]
[1] "seasonal"  "trend"     "remainder"

> windows()
> par(mfrow=c(3,1))
> acf(glomma.ts[,"TN"])
> acf(TN.stl$time.series[,"remainder"]) # (unit is years)
> ar(TN.stl$time.series[,"remainder"])
Call:
ar(x = TN.stl$time.series[, "remainder"])

Coefficients:
      1        2        3        4        5        6        7        8
-0.3867  -0.3873  -0.4804  -0.4980  -0.5335  -0.4663  -0.5522  -0.4707
      9       10       11       12       13       14       15       16
-0.2449  -0.5266  -0.4503  -0.3780  -0.2023  -0.2896  -0.2729  -0.0976
     17       18
-0.1862  -0.2192

Order selected 18  sigma^2 estimated as  16490
```

Now there is not much autocorrelation left, as expected (Figure 40, upper panel).

What about the trend?
```
> acf(TN.stl$time.series[,"trend"])
> ar(TN.stl$time.series[,"trend"])

Call:
ar(x = TN.stl$time.series[, "trend"])

Coefficients:
      1        2        3
 1.4052  -0.1569  -0.2988

Order selected 3  sigma^2 estimated as  59.95
```

There is strong autocorrelation is in the trend (Figure 40, middle panel), as expected.

The estimated seasonal effect will of course also have a strong autocorrelation (Figure 40, lower panel).
```
> acf(TN.stl$time.series[,"seasonal"])
```

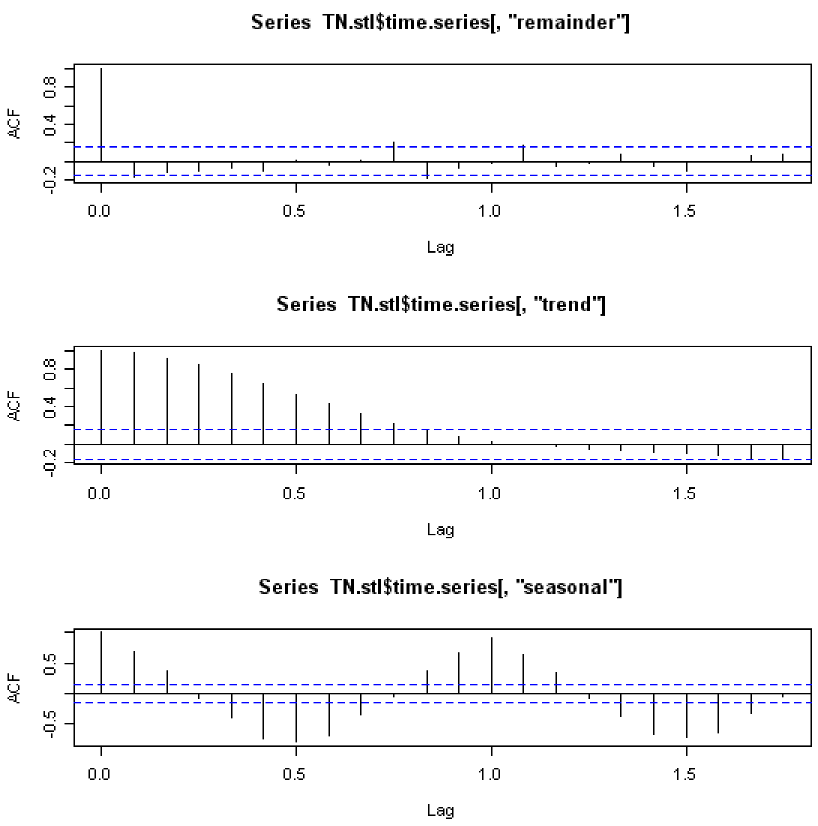


Figure 40. Autocorrelation plots for remainders (residuals) from AR-model of dataset glomma (upper panel); for the estimated temporal trend (middle panel); and for the seasonal effect (lower panel).

There is a large framework for time-series analysis called ARIMA, if interested see `?arima`

3.2 Structural changes in time series

Tom Andersen

Data set from Ringkøbing fjord, Denmark (DMU). The data are from 1980-2004, averaged to monthly means.

```
> ring1 <- read.table("Ringkøbing monthly TS.txt", header=TRUE)
> names(ring1)
 [1] "Year"    "Month"   "Nsamp"   "Temp"    "Sal"     "Transp" "Chla"    "TotP"
 [9] "PO4"     "TotN"    "NO3"
> summary(ring1)
      Year          Month            Nsamp           Temp
 Min.   :1980   Min.   : 1.000   Min.   :0.000   Min.   : 0.000
 1st Qu.:1986   1st Qu.: 4.000   1st Qu.:1.000   1st Qu.: 4.200
 Median :1992   Median : 7.000   Median :2.000   Median : 9.800
 Mean   :1992   Mean   : 6.561   Mean   :2.139   Mean   : 9.984
 3rd Qu.:1998   3rd Qu.:10.000   3rd Qu.:3.000   3rd Qu.:15.300
 Max.   :2004   Max.   :12.000   Max.   :5.000   Max.   :22.030
 (etc.)
```

There are a lot of missing values, especially for Chla. Where are they? Let's make a function to count missing values

```
> count.na <- function(x) { sum(is.na(x)) }
```

Let's test our function, first columnwise.

```
> apply(ring1,2,count.na)
  Year  Month  Nsamp    Temp     Sal Transp    Chla    TotP     PO4    TotN     NO3
     0      0      0      33      32     31      64      26      45      26      26
```

OK, this gives the same results as `summary()`.

```
> attach(ring1)
> TotP.missing <- tapply(TotP, Year, count.na)
> plot(1980:2004,TotP.missing)   # Figure 41
```

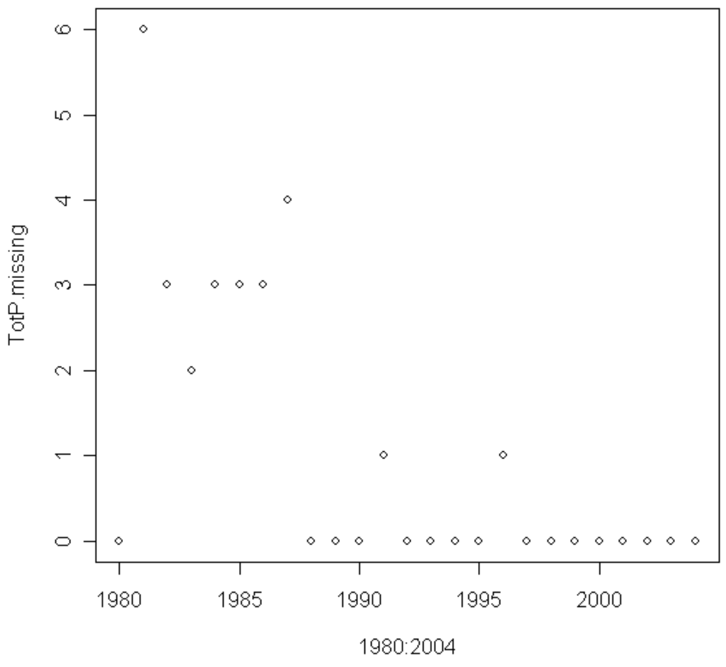


Figure 41. Number of missing TotP values per year, in the data from Ringkøbingfjord.

Notice the difference between `apply()` and `tapply()` (as commented below):

```
> apply(ring1, 2, count.na)      # = number of missing in each column of ring1
  Year  Month  Nsamp    Temp     Sal Transp    Chla    TotP     PO4    TotN     NO3
     0      0      0      33      32     31      64      26      45      26      26
> tapply(TotP, Year,count.na)    # = number of missing TotP in each year
1980 1981 1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
   0    6    3    2    3    3    3    4    0    0    0    1    0    0    0    0
1996 1997 1998 1999 2000 2001 2002 2003 2004
   1    0    0    0    0    0    0    0    0

> detach(ring1)
```

Most missing values are in the years before 1988. Let's make a subset of the years 1988-2004:

```
> ring1.1988 <- subset(ring1, Year > 1987)
```

Now, let's make a time-series (ts) object out of this. We skip the first 3 columns containing time information, since time is implicit in the ts object definition.

```
> ring1.ts <- ts(ring1.1988[4:11], frequency=12, start=c(1988,1))
> plot(ring1.ts)    # Figure 42
```

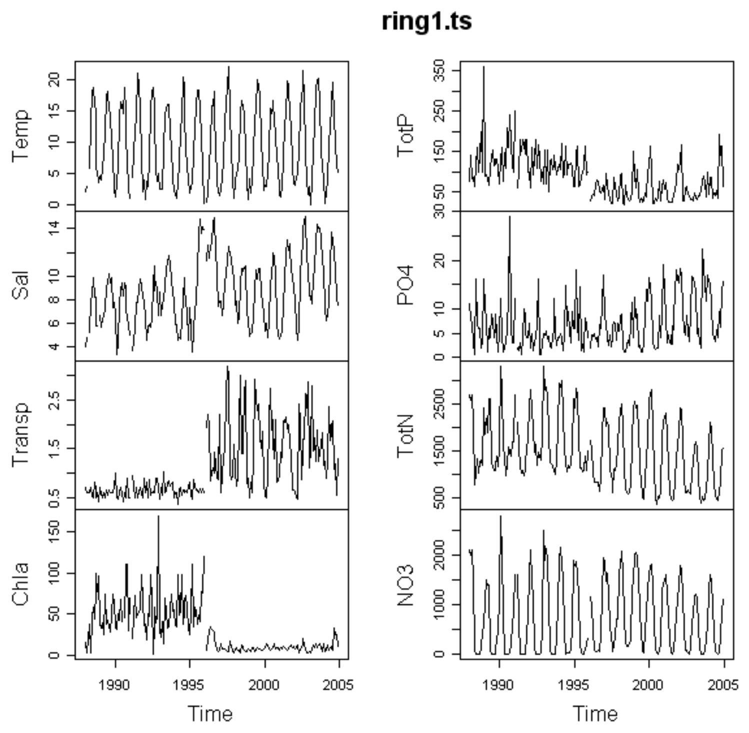


Figure 42. Time-series plot of data from Ringkøbingfjord.

Something very special seems to have happened in 1995! In the summer of 1995 the outlet of Ringkøbing fjord was widened so that the seawater exchange increased. The resulting increase in salinity allowed filter-feeding clams to establish, leading to a fast decrease in chlorophyll.

Let's use the `strucchange` package to investigate this regime shift. (Notice that `strucchange` depends on other packages, therefore installation from local zip file is not recommended.)

```
> require(strucchange)
Loading required package: strucchange
Loading required package: zoo
Loading required package: sandwich
[1] TRUE
```

`Fstats()` calculates the F-statistic for all possible breakpoints of a linear model. This significance of the identified breakpoint(s) can be tested with `sctest()`.
Let's test if there is a change in the mean of some variables. The model formula for x = constant is
`x ~ 1`.

```
> par(mfrow=c(2,2)) # Figure 43
```

Temperature:

```
> fs.temp <- Fstats(Temp ~ 1, data=ring1.ts)
> plot(fs.temp, main="Temperature")
> lines(breakpoints(fs.temp))
> sctest(fs.temp)
sup.F = 1.1378, p-value = 0.982
```

Breakpoint(s) are detected, but not significant.

Salinity:

```
> fs.Sal <- Fstats(Sal  ~ 1, data=ring1.ts)
> plot(fs.Sal, main="Salinity")
> lines(breakpoints(fs.Sal))
> sctest(fs.Sal)
sup.F = 47.0139, p-value = 3.677e-10
```

Highly significant breakpoint in March 1995

Chlorophyll a:

```
> fs.Chla <- Fstats(Chla ~ 1,data=ring1.ts)
> plot(fs.Chla, main="Chlorophyll")
> lines(breakpoints(fs.Chla))
> sctest(fs.Chla)
sup.F = 240.5308, p-value < 2.2e-16
```

Highly significant breakpoint in October 1995

```
> fs.TotP <- Fstats(TotP ~ 1,data=ring1.ts)
> plot(fs.TotP, main="Total P")
> lines(breakpoints(fs.TotP))
> sctest(fs.TotP)
sup.F = 122.1825, p-value < 2.2e-16
```

# Highly significant breakpoint in November 1995

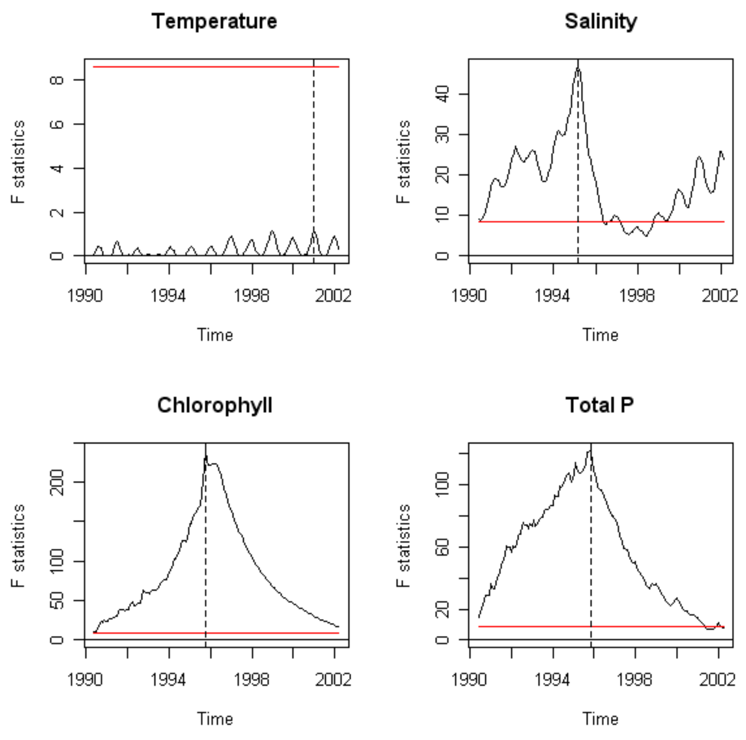


Figure 43. Breakpoint analyses for data from Ringkøbingfjord.

Now let's try a more complicated model: There were significant breakpoints in both the Chla and TotP time series. Was there also a change in the relationship between them? (**Figure 44**)

```
> fs.Chla.TotP <- Fstats(log10(Chla) ~ log10(TotP),data=ring1.ts)
> plot(fs.Chla.TotP, main="Chlorophyll vs. Total P")
> lines(breakpoints(fs.Chla.TotP))
> sctest(fs.Chla.TotP)
sup.F = 148.9023, p-value < 2.2e-16
```

Yes, highly significant, but half a year later (July 1996).

We can visualize the two regression lines in a plot (**Figure 44**):

```
> bp <- fs.Chla.TotP$breakpoint
> plot(log10(Chla) ~ log10(TotP), data = ring1)
> points(log10(Chla) ~ log10(TotP), data = ring1, subset = 1:bp, col = 2, pch = 19)
> abline(lm(log10(Chla) ~ log10(TotP), data = ring1, subset = 1:bp), col = 2)
> abline(lm(log10(Chla) ~ log10(TotP), data = ring1, subset = -(1:bp)))
```

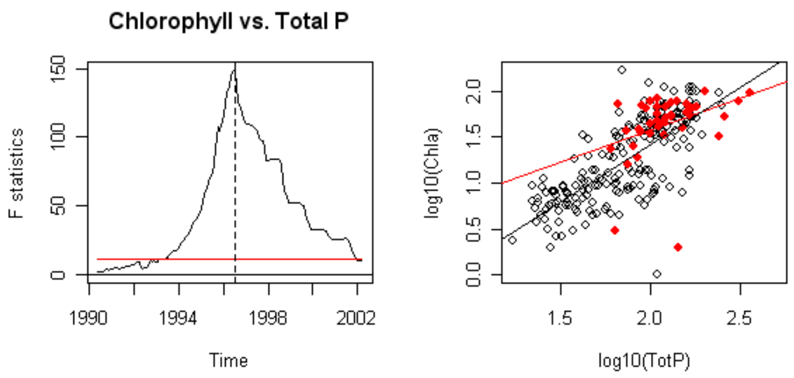
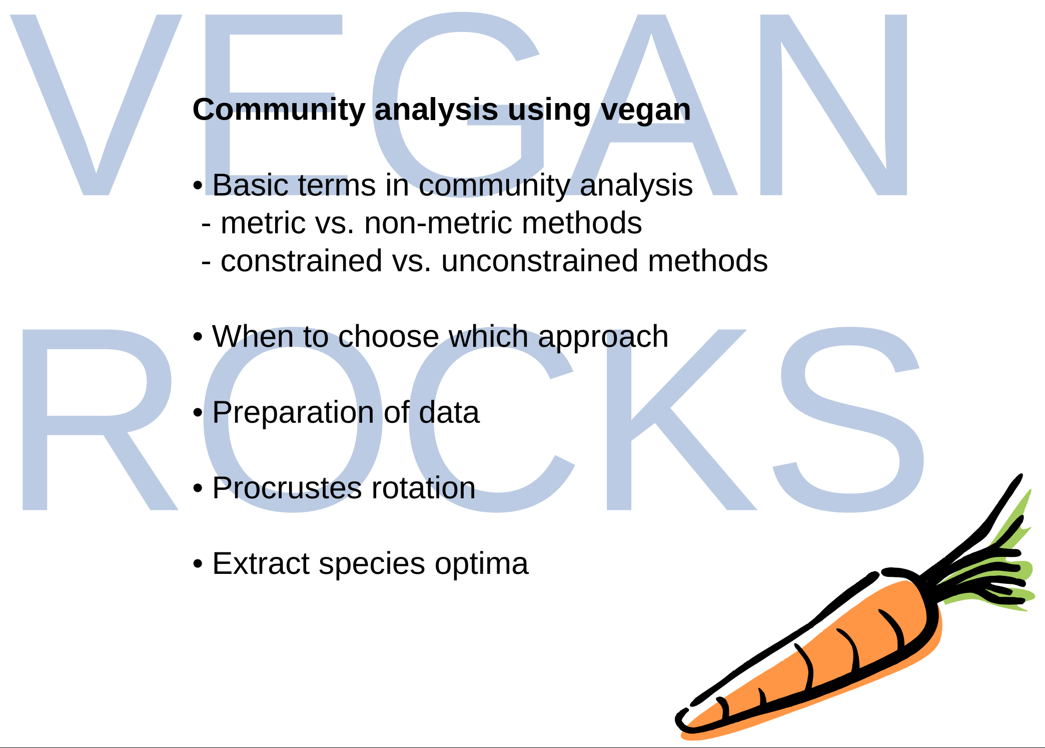


Figure 44. Breakpoint analysis for relationship between Total P and chlorophyll from Ringkøbingfjord.

So, the relationship between Chla and TotP became stronger after the establishment of benthic filter feeders. The reason is possibly that Chla yield per unit TotP was light limited before mussel invasion, and because mussel removal of TotP makes the TotP gradient longer. The 3 outliers (2 before, 1 after) are probably winter values. Maybe the next step would be to look for a seasonal component?

4. MULTIVARIATE MODELS IN VEGAN

Robert Ptacnik



VEGAN ROCKS

Community analysis using vegan

• Basic terms in community analysis
 - metric vs. non-metric methods
 - constrained vs. unconstrained methods

• When to choose which approach

• Preparation of data

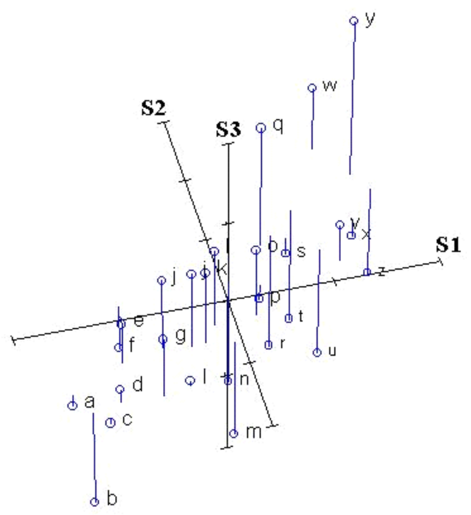
• Procrustes rotation

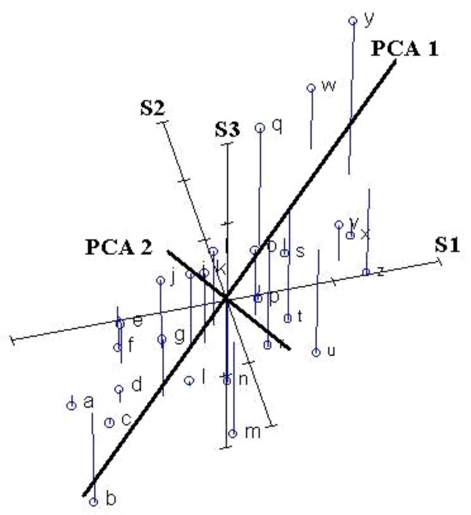
• Extract species optima

What is ordination?

Reduce dimensionality in multivariate data

-> organize your data such that overriding gradients become visible ('gradient analysis')





(from http://ordination.okstate.edu/index.html)

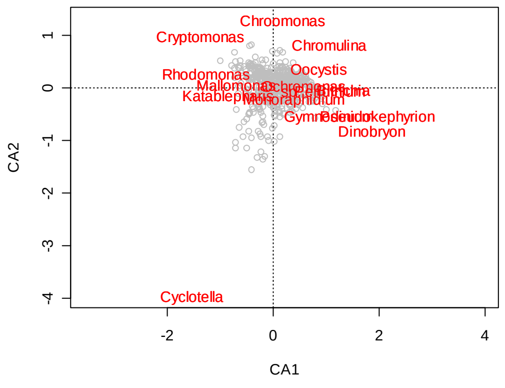
Constrained vs. unconstrained ordination

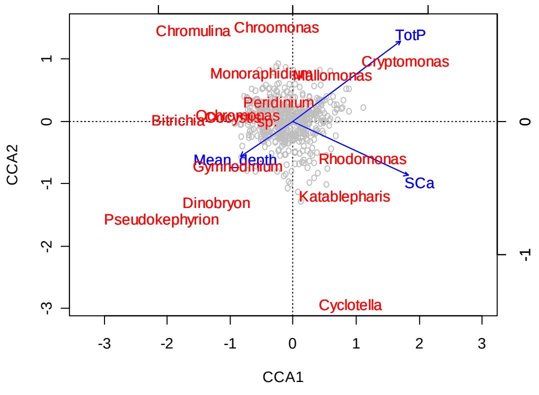
Unconstrained: Obtain distribution from species' information.

-> Find best ordination with respect to community data.

Constrained: Force analysis to build axes based on environmental variables.

-> See how data can be organized based on environmental data.





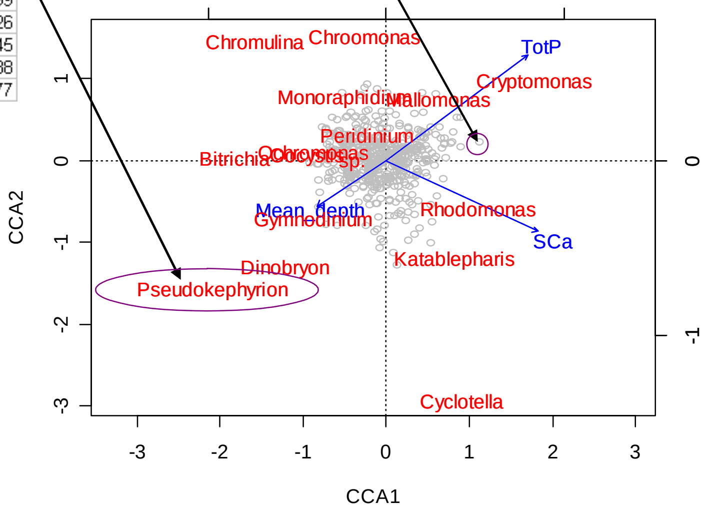
Ordination results: 2 types of scores

species scores

	CCA1	CA1
Pseudokephyrion	-0.5561	0.082183
Cyclotella	0.049147	-1.48453
Bitrichia	-0.39666	0.15183
Mallomonas	0.21791	-0.07886
Peridinium	0.056283	0.23534
Oocystis	-0.19935	0.207644
Chromulina	-0.32073	0.375428
Monoraphidium	-0.04596	-0.04793
Dinobryon	-0.26226	0.013498
Gymnodinium	-0.15816	-0.01474
Chroomonas	-0.03809	0.42882
Katablepharis	0.112105	-0.17599
Rhodomonas	0.165267	-0.08726
Cryptomonas	0.475516	0.160345
Ochromonas	-0.25158	0.079738
sp.	-0.1061	0.01077

site scores

	CCA1	CA1
NO_1886	-2.65402	0.068088
NO_3230	-2.75736	0.176683
NO_1517	-0.72284	0.140024
NO_3231	-3.04971	-0.0638
NO_702	-0.33638	-0.6654
NO_2009	-1.34894	-3.74242
NO_4460	-1.14975	-1.48201
NO_4498	-2.84753	0.898243
NO_4518	-2.39425	0.824404
NO_5083	-1.85829	0.80939



In the process of ordination, axes are calculated which represent the (dis-) similarity of samples and species, with most similar observations most close to each other.
The maximum variation that can be explained in a one-dimensional space is translated into the first ordination axis (CCA1 below). Next, as much of the remaining variation that can be explained (again in a one-dimensional space) is being projected onto the second axis, and so on.

How much of the variability can be explained by the 1st, 2nd, 3rd... axis? ->'inertia'.

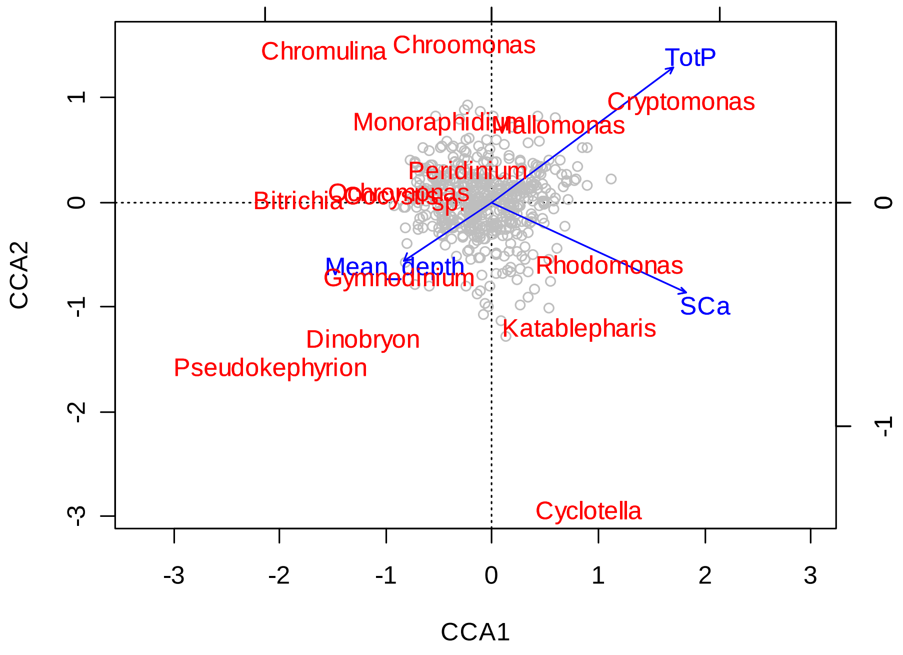
In case of constrained ordination the inertia is split into constrained and unconstrained component.

```
Inertia Rank
Total         0.80328
Constrained   0.05322    1
Unconstrained 0.75006   15
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
   CCA1
0.05322

Eigenvalues for unconstrained axes:
     CA1      CA2
0.122600 0.111737
```

Significance of results can be tested with permutation test.



Types of ordination

axes are... / method for scores..	unconstrained	constrained
Chi^2 distances weighted averaging	**CA (DCA)** correspondence analysis	**CCA** canonical correspondence analysis
euclidean distances least squares	**PCA** principal components analysis	**RDA** redundancy analysis
dissimilarity matrix rank-based	**NMDS** non-metric multidimensional scaling	-

Constrained vs. unconstrained ordination

Pros and Cons

Unconstrained: Obtain distribution from species' information

Advantage: 'let the community tell you how sites are related to each other' The sites are grouped based on their true variation

Disadvantage: Analysis more time-consuming; potential problems with large datasets (NMDS);

Constrained: Force analysis to build axes based on environmental variables

Advantage: Species can be more easily associated with environmental data

Disadvantage: Only the variation that can be related to env. variables will be visible

Types of ordination - when to choose which

	unconstrained	constrained
weighted averaging	CA many species have zero observations	CCA -/-
least squares	PCA gradual differences in community	RDA -/-
rank-based	NMDS binary data (pres./abs.)	-

Types of ordination - commands in vegan

`spec: species matrix`
`env: environmental predictors`
	unconstrained	constrained

weighted averaging	CA `cca(spec)`	CCA `cca(spec, env)`
least squares	PCA `rda(spec)`	RDA `rda(spec, env)`
rank-based	NMDS `metaMDS(spec)`	-

Constrained vs. unconstrained ordination

Two approaches

start with unconstrained analysis
(NMDS, CA, PCA)
`ordi <- cca(resp)`

↓

fit environmental variables to ordination
(incl. permutation test)
`envfit(ordi, env, perm=1000)`

↓

select most relevant variables
and plot them into ordination

start with constrained analysis
(CCA, RDA)
`cca(resp, env)`

↓

improve model with formula interface
`cca(resp~Fac1+Fac2*(Fac3+Fac4)..)`

↓

test variables by permutation test

run reduced model

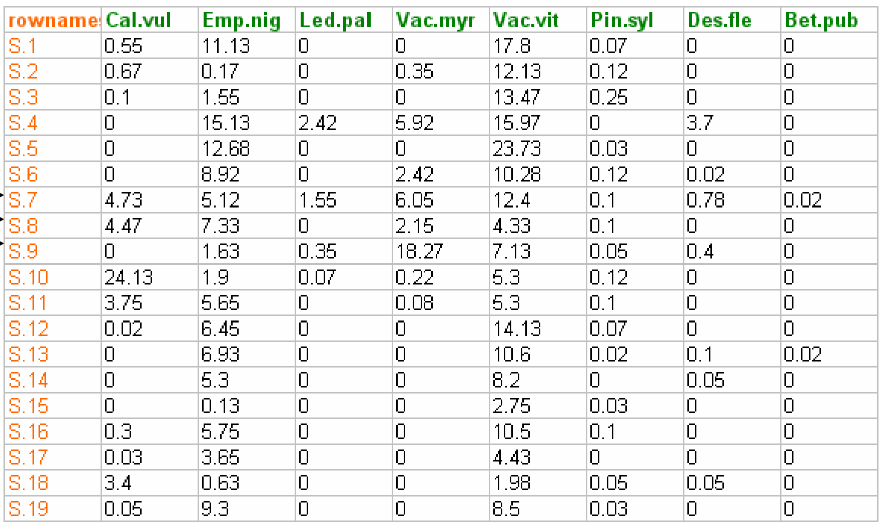
Structure of data

- no missing values accepted
- sums of each single row and column must be >0 (species)
- factors can be used (environ. variables)

Use short identifiers (e.g. *TP* instead of *Total Phosphorus (µg/L)*)
>> easier to read on plot

column = species

row =
observation



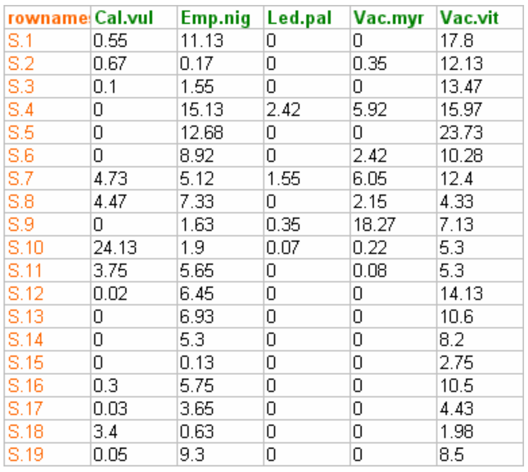
rowname	Cal.vul	Emp.nig	Led.pal	Vac.myr	Vac.vit	Pin.syl	Des.fle	Bet.pub
S.1	0.55	11.13	0	0	17.8	0.07	0	0
S.2	0.67	0.17	0	0.35	12.13	0.12	0	0
S.3	0.1	1.55	0	0	13.47	0.25	0	0
S.4	0	15.13	2.42	5.92	15.97	0	3.7	0
S.5	0	12.68	0	0	23.73	0.03	0	0
S.6	0	8.92	0	2.42	10.28	0.12	0.02	0
S.7	4.73	5.12	1.55	6.05	12.4	0.1	0.78	0.02
S.8	4.47	7.33	0	2.15	4.33	0.1	0	0
S.9	0	1.63	0.35	18.27	7.13	0.05	0.4	0
S.10	24.13	1.9	0.07	0.22	5.3	0.12	0	0
S.11	3.75	5.65	0	0.08	5.3	0.1	0	0
S.12	0.02	6.45	0	0	14.13	0.07	0	0
S.13	0	6.93	0	0	10.6	0.02	0.1	0.02
S.14	0	5.3	0	0	8.2	0	0.05	0
S.15	0	0.13	0	0	2.75	0.03	0	0
S.16	0.3	5.75	0	0	10.5	0.1	0	0
S.17	0.03	3.65	0	0	4.43	0	0	0
S.18	3.4	0.63	0	0	1.98	0.05	0.05	0
S.19	0.05	9.3	0	0	8.5	0.03	0	0

Structure of data: usually 2 matrices with matching rows

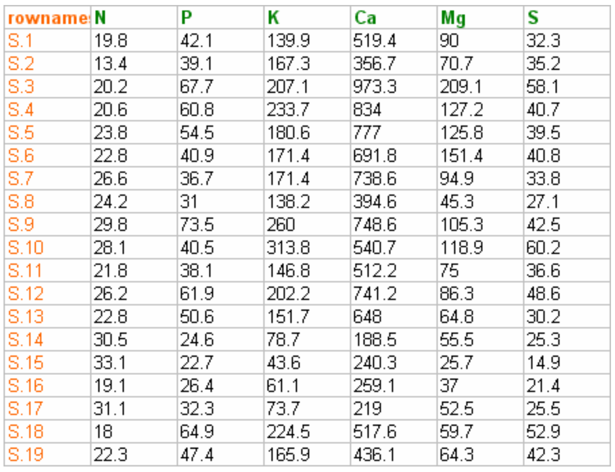
dependent matrix (community)

independent matrix (env. parameters)

rows must match



rowname	Cal.vul	Emp.nig	Led.pal	Vac.myr	Vac.vit
S.1	0.55	11.13	0	0	17.8
S.2	0.67	0.17	0	0.35	12.13
S.3	0.1	1.55	0	0	13.47
S.4	0	15.13	2.42	5.92	15.97
S.5	0	12.68	0	0	23.73
S.6	0	8.92	0	2.42	10.28
S.7	4.73	5.12	1.55	6.05	12.4
S.8	4.47	7.33	0	2.15	4.33
S.9	0	1.63	0.35	18.27	7.13
S.10	24.13	1.9	0.07	0.22	5.3
S.11	3.75	5.65	0	0.08	5.3
S.12	0.02	6.45	0	0	14.13
S.13	0	6.93	0	0	10.6
S.14	0	5.3	0	0	8.2
S.15	0	0.13	0	0	2.75
S.16	0.3	5.75	0	0	10.5
S.17	0.03	3.65	0	0	4.43
S.18	3.4	0.63	0	0	1.98
S.19	0.05	9.3	0	0	8.5

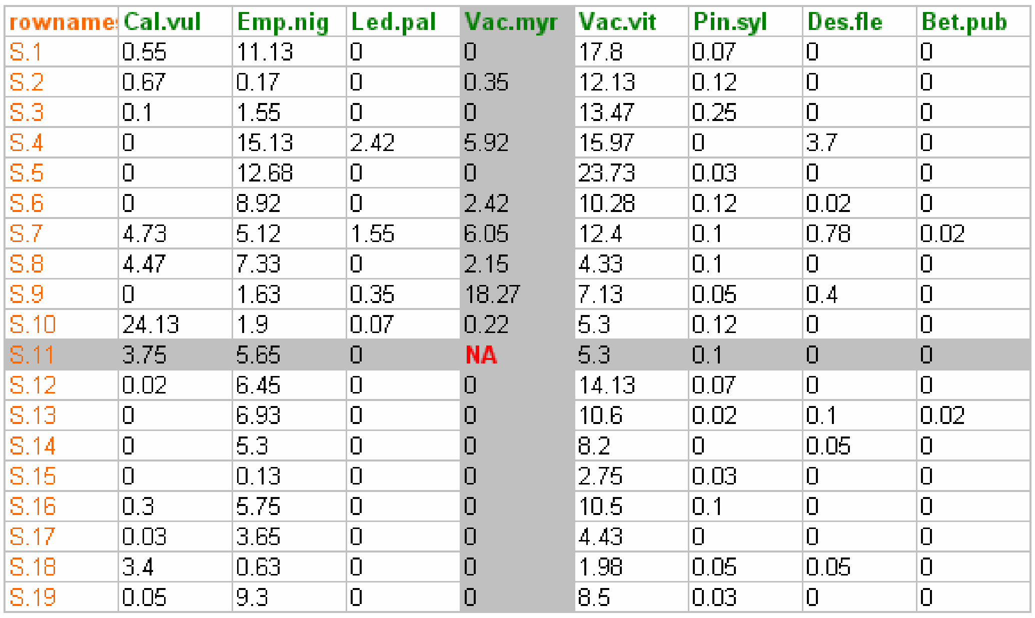


rowname	N	P	K	Ca	Mg	S
S.1	19.8	42.1	139.9	519.4	90	32.3
S.2	13.4	39.1	167.3	356.7	70.7	35.2
S.3	20.2	67.7	207.1	973.3	209.1	58.1
S.4	20.6	60.8	233.7	834	127.2	40.7
S.5	23.8	54.5	180.6	777	125.8	39.5
S.6	22.8	40.9	171.4	691.8	151.4	40.8
S.7	26.6	36.7	171.4	738.6	94.9	33.8
S.8	24.2	31	138.2	394.6	45.3	27.1
S.9	29.8	73.5	260	748.6	105.3	42.5
S.10	28.1	40.5	313.8	540.7	118.9	60.2
S.11	21.8	38.1	146.8	512.2	75	36.6
S.12	26.2	61.9	202.2	741.2	86.3	48.6
S.13	22.8	50.6	151.7	648	64.8	30.2
S.14	30.5	24.6	78.7	188.5	55.5	25.3
S.15	33.1	22.7	43.6	240.3	25.7	14.9
S.16	19.1	26.4	61.1	259.1	37	21.4
S.17	31.1	32.3	73.7	219	52.5	25.5
S.18	18	64.9	224.5	517.6	59.7	52.9
S.19	22.3	47.4	165.9	436.1	64.3	42.3

Structure of data

what to do with missing values?

- delete column (loose species/predictor)
- delete row (delete observation)
- fill gap with predicted value (requires some consideration)

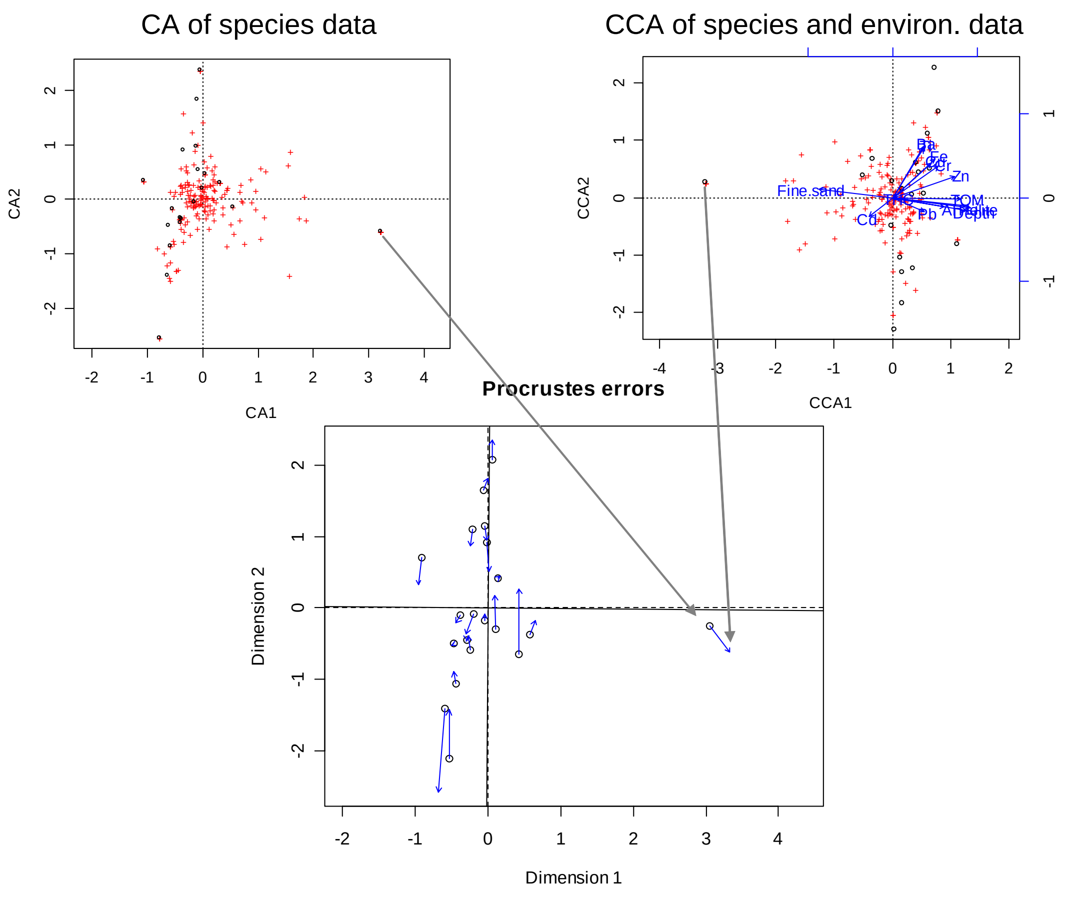


rowname	Cal.vul	Emp.nig	Led.pal	Vac.myr	Vac.vit	Pin.syl	Des.fle	Bet.pub
S.1	0.55	11.13	0	0	17.8	0.07	0	0
S.2	0.67	0.17	0	0.35	12.13	0.12	0	0
S.3	0.1	1.55	0	0	13.47	0.25	0	0
S.4	0	15.13	2.42	5.92	15.97	0	3.7	0
S.5	0	12.68	0	0	23.73	0.03	0	0
S.6	0	8.92	0	2.42	10.28	0.12	0.02	0
S.7	4.73	5.12	1.55	6.05	12.4	0.1	0.78	0.02
S.8	4.47	7.33	0	2.15	4.33	0.1	0	0
S.9	0	1.63	0.35	18.27	7.13	0.05	0.4	0
S.10	24.13	1.9	0.07	0.22	5.3	0.12	0	0
S.11	3.75	5.65	0	NA	5.3	0.1	0	0
S.12	0.02	6.45	0	0	14.13	0.07	0	0
S.13	0	6.93	0	0	10.6	0.02	0.1	0.02
S.14	0	5.3	0	0	8.2	0	0.05	0
S.15	0	0.13	0	0	2.75	0.03	0	0
S.16	0.3	5.75	0	0	10.5	0.1	0	0
S.17	0.03	3.65	0	0	4.43	0	0	0
S.18	3.4	0.63	0	0	1.98	0.05	0.05	0
S.19	0.05	9.3	0	0	8.5	0.03	0	0

Comparing ordinations - Procrustes rotation

```
Procrustes analysis determines a **linear
transformation** (translation, reflection,
orthogonal rotation, and scaling) of the
points in matrix Y to best conform them to
the points in matrix X.
```

*(...) Theseus "**fitted**" Procrustes to his own bed and cut off his head and feet. (...) Killing Procrustes was the last adventure of Theseus on his journey from Troezen to Athens. (from Wikipedia)*



4.1 Multivariate analyses: Examples

4.1.1 Example 4: Basics in vegan

```
>
> rm(list=ls())     #clean workspace
> require(vegan)    # load vegan
Loading required package: vegan
[1] TRUE
```

Let's start with an example dataset from Jari Oksanen.

```
> data(varespec) # data on distribution of 44 understorey plant species on 24 sites
> data(varechem) # environmental data for the sampling sites
```

First we use Nonmetric Multidimensional Scaling (NMDS)

```
> x11(10,5)  # set size of window: x11(width, height)
> par(mfrow=c(1, 2)) # split into two panels
> nm1 <- metaMDS(varespec)
Square root transformation
Wisconsin double standardization
Loading required package: MASS
Run 0 stress 18.44915
Run 1 stress 23.60978
Run 2 stress 21.43612
Run 3 stress 22.97361
Run 4 stress 19.82376
Run 5 stress 19.48413
Run 6 stress 22.81606
Run 7 stress 21.37383
Run 8 stress 19.5049
Run 9 stress 18.25658
... New best solution
... rmse 0.04516871   max residual 0.1694442
Run 10 stress 20.4831
Run 11 stress 26.25915
Run 12 stress 19.69805
Run 13 stress 18.25658
... New best solution
... rmse 4.832084e-05   max residual 0.0001559065
*** Solution reached

> nm1 # inspect result

Call:
metaMDS(comm = varespec)

Nonmetric Multidimensional Scaling using isoMDS (MASS package)

Data:     wisconsin(sqrt(varespec))
Distance: bray

Dimensions: 2
Stress:     18.25658
Two convergent solutions found after 13 tries
Score scaling: centring, PC rotation, halfchange scaling

> plot(nm1)
```

R doesn't want to show us the species. OK, plot in two steps:

```
> plot(nm1, type="n") # empty plot
> text(nm1, "species", col=2) # the species
> text(nm1, "sites",  col=1)
```

Fitting environmental data to the NMDS:
`envfit()` fits environmental variables into existing ordination.
If 'perm=xxx' is given, the fit is testen with xxx permutations and statistics are returned

```
> (ef.nm1 <- envfit(nm1, varechem, perm = 1000))

***VECTORS
              NMDS1     NMDS2     r2 Pr(>r)
N         -0.057241 -0.998360 0.2536  0.043 *
P          0.619606  0.784913 0.1938  0.100 .
K          0.766361  0.642411 0.1809  0.135
Ca         0.685118  0.728432 0.4119  0.003 **
Mg         0.632459  0.774594 0.4270  0.001 ***
S          0.191286  0.981534 0.1752  0.139
Al        -0.871651  0.490127 0.5269 <0.001 ***
Fe        -0.936054  0.351857 0.4450  0.005 **
Mn         0.798774 -0.601632 0.5231  0.001 ***
Zn         0.617446  0.786613 0.1879  0.122
Mo        -0.903091  0.429449 0.0610  0.510
Baresoil   0.924936 -0.380124 0.2508  0.043 *
Humdepth   0.932874 -0.360203 0.5200  0.001 ***
pH        -0.648097  0.761558 0.2308  0.077 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
P values based on 1000 permutations.
```

Note that when commands are written in parantheses, the results are written in the console.

Add environmental gradients:

```
> plot(ef.nm1) # note: plot.envfit draws into existing ordination
> plot(ef.nm1, p.max = 0.05, col = "red") # highlight the significant variables
```

Arrows and names look a bit messy together (not shown) - why not split into two plots (Figure 45):

```
> par(mfrow=c(1, 2))
> plot(nm1) #
```

Note that this plot may look slightly different on your pc, because `nmds()` starts with arbitrary initial values and converges to an optimal solution from these initial values.

```
> plot(ef.nm1) # add environmental gradients
> plot(ef.nm1, p.max = 0.05, col = "red") # highlight the significant ones
> plot(nm1, type="n") # empty plot
> text(nm1, "species", col=2) # the species
> text(nm1, "sites",  col=1)
```

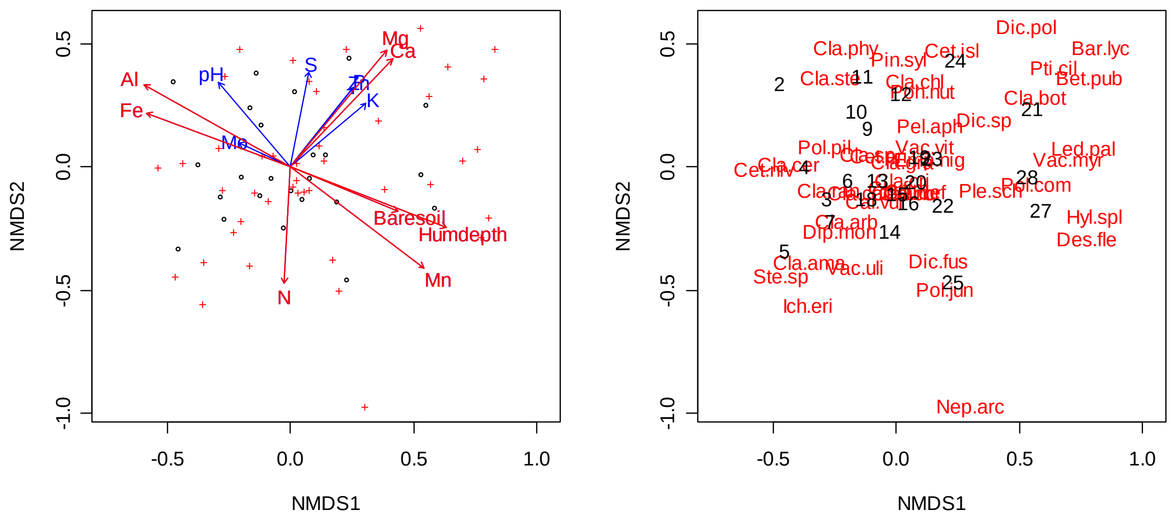


Figure 45. Non-metric multidimensional scaling (NMDS) for the `varespec`-data.

Compare with PCA (Figure 46):

```
> x11(6, 6)
> ca1 <- cca(varespec)
> plot(ca1)
```

Note that `pca()` shows the species names. There are different settings for default plot function.

```
> (ef.ca1 <- envfit(ca1, varechem, perm = 1000))

***VECTORS

               CA1       CA2     r2 Pr(>r)
N         0.474695 -0.880150 0.2196  0.086 .
P         0.448265  0.893901 0.3054  0.020 *
K         0.736164  0.676803 0.1773  0.140
Ca        0.697240  0.716838 0.3064  0.025 *
Mg        0.773175  0.634192 0.2466  0.057 .
S         0.051368  0.998680 0.0902  0.389
Al       -0.974910 -0.222600 0.4995  0.001 ***
Fe       -0.963899 -0.266270 0.3682  0.011 *
Mn        0.914437  0.404729 0.4750  0.001 ***
Zn        0.770385  0.637578 0.1766  0.133
Mo       -0.638085 -0.769966 0.0539  0.588
Baresoil  0.979466 -0.201608 0.2533  0.058 .
Humdepth  0.916024  0.401123 0.4524  0.002 **
pH       -0.998306  0.058180 0.2187  0.106
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
P values based on 1000 permutations.
> plot(ef.ca1) # note: this plotting method requires existing plot
> plot(ef.ca1, p.max = 0.05, col = "red") # as above
```

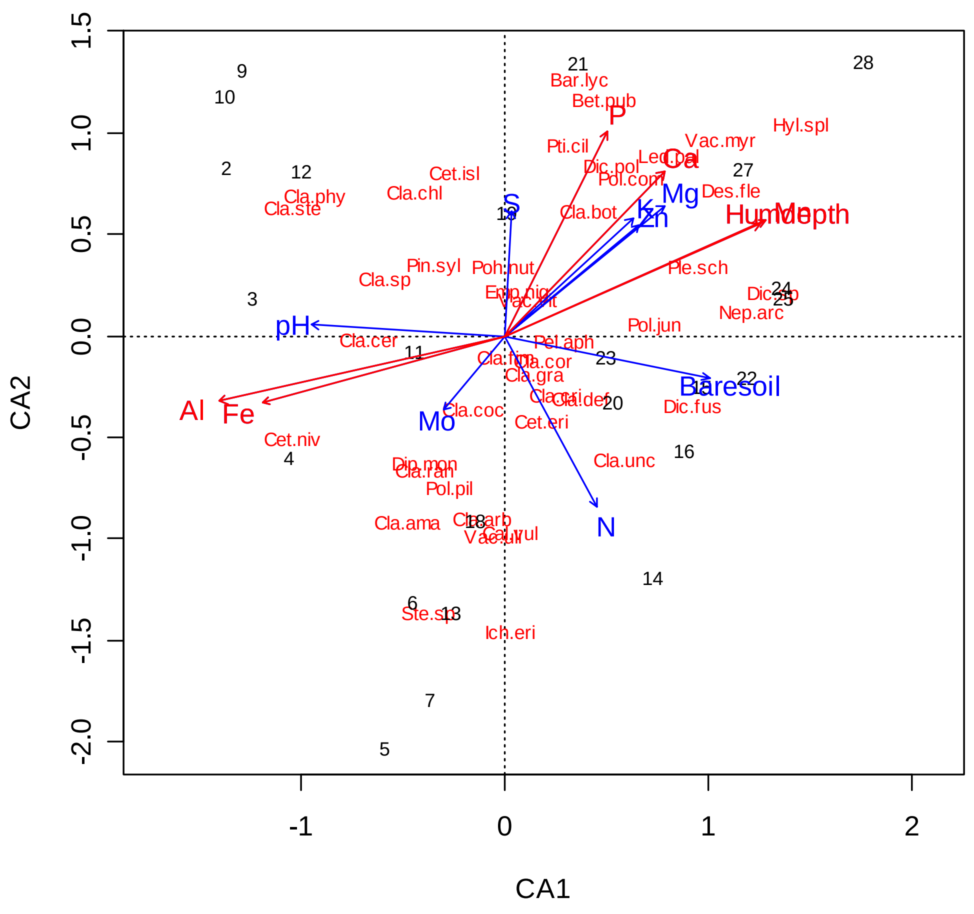


Figure 46. PCA of same data as in Figure 45.

Compare how well environmental variables could be fit into the two different ordinations. Discuss differences; which method works better with this dataset?

Illustrate major gradients (Figure 47):

```
> x11()
> plot(nm1); plot(ef.nm1)
> ordisurf(nm1, varechem$Al, add=T, col=2) # fit surface (GAM) over ordination
Loading required package: mgcv
This is mgcv 1.3-13
Loading required package: akima

Family: gaussian
Link function: identity

Formula:
y ~ s(x1, x2, k = knots)

Estimated degrees of freedom:
 5.087141   total =  6.08714

GCV score:  8798.657
```

```
> ordisurf(nm1, varechem$Humdepth, add=T, col=3)

Family: gaussian
Link function: identity

Formula:
y ~ s(x1, x2, k = knots)

Estimated degrees of freedom:
 5.481066   total =  6.481066

GCV score:  0.2213074
```

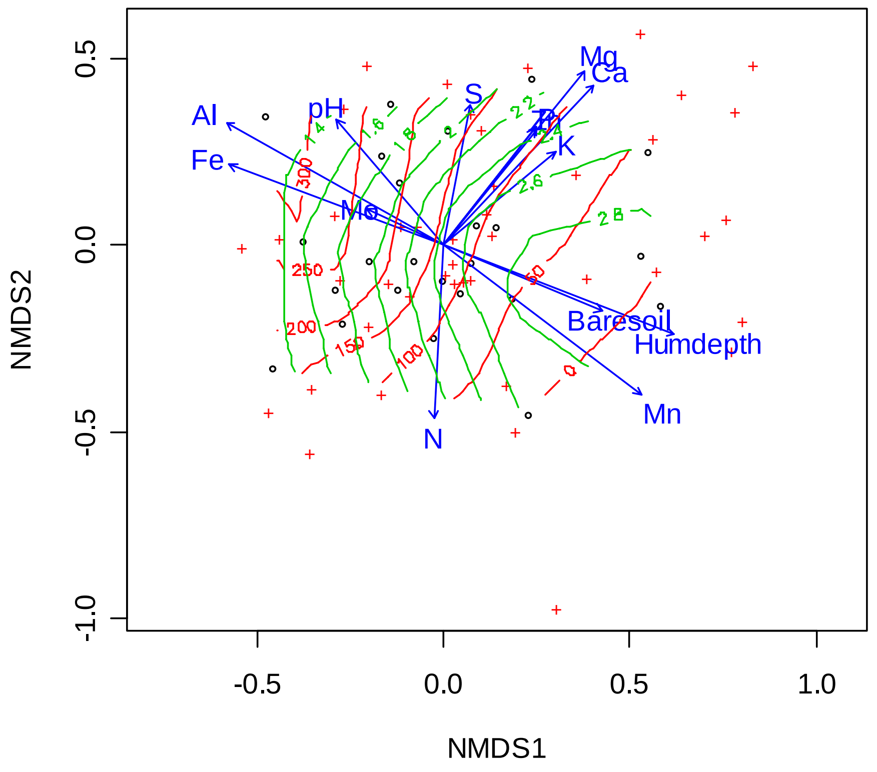


Figure 47. NMDS with suface fits for the environmental variables ‘Al’ (red) and ‘Humdepth’ (green).

```
> #              ((
> # C O F F E E   ))
> #  B R E A K   |   |o)
> #              |___|
```

4.1.2 Example 5: Applications of non-metric multidimensional scaling (NMDS) & canonical correspondence analysis (CCA) to benthos data

Unless we restarted R we don't have to reload vegan.

```
> rm(list=ls()) #clean workspace
```

Load data from Hilde Trannum: open EXCEL-sheet, highlight the data in sheet 'speci' and copy table to the clipboard (= press 'ctrl'+'C'). Then return to R and run

```
> traspe <- read.delim(file="clipboard", row.names=1) # '..., header=T' redundant,
is the default
```

Now go again to EXCEL and copy the environmental data in the same way, then run

```
> traenv <- read.delim(file="clipboard", row.names=1)
```

If this doesn't work, load these files instead

```
> load("traspe.bin")
> load("traenv.bin")
```

We can save these tables for further use in R (open with `load("file.bin")`)

```
> save(traspe, file="traspe.bin")
> save(traenv, file="traenv.bin")
```

It is useful to have separate identifier for binary files.
Function `file.bin()` stores data in binary format. This can only be opened within R. Advantage: easier to open: `load("file.bin")`, instead of `read.table("file.txt", header=T, row.names=T)`.

I want to check if the rows match; the function `match(x,y)` finds matching objects among two vectors.

```
> match(rownames(traspe), rownames(traenv))
 [1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20
> match(rownames(traspe), rownames(traenv))/1:20
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

The species list is very long. Problem: many taxa occur only at one site. Should we exclude taxa occuring below a minimum number? This depends on the focus of the analysis. If the focus is on the sites, these taxa give still info on species richness, but if focus is on the species and their distribution, we should exclude rare taxa (stochastic occurence). First let's see how the data are distributed.

Visualize number of sites per taxon. The `apply()` function is useful for aggregation of arrays/matrices:

`apply(array, margin, function):` `margin=1` -> by row; `margin=2` -> by column

An example for usage of `apply()`:

```
> mat <- traspe[1:3, 1:3]
> mat
        Abra.sp Abys.sp Agla.mal
GOL1-1        0      28        5
GOL1-10       0      41        7
GOL1-11       0      20        9
> apply(mat, 1, sum)
 GOL1-1 GOL1-10 GOL1-11
     33      48      29
> apply(mat, 2, sum)
 Abra.sp  Abys.sp Agla.mal
       0       89       21
> apply(mat>0, 1, sum) # row-sums = sums per site
 GOL1-1 GOL1-10 GOL1-11
      2       2       2
> apply(mat>0, 2, sum) # column-sums = sums per taxon
 Abra.sp  Abys.sp Agla.mal
       0        3        3
> x11(6, 6)
> hist(apply(traspe>0, 2, sum), xlab="Nr. sites per taxon")
```

This gives too few breaks. We can increase the number of breaks (Figure 48):

```
> hist(apply(traspe>0, 2, sum), breaks=20, xlab="Nr. sites per taxon")
```

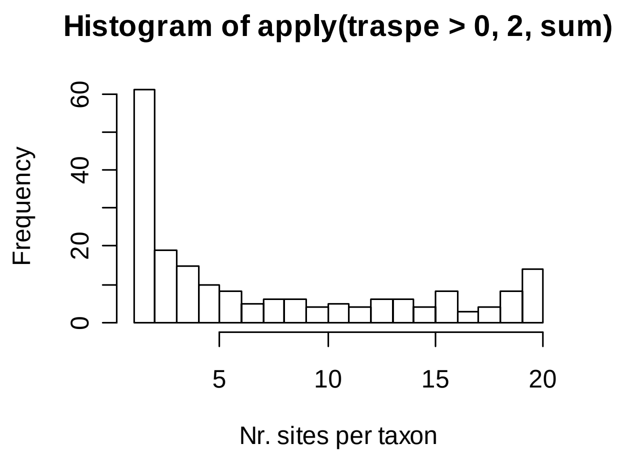


Figure 48. Histogram of no. of sites per taxon.

You can abbreviate command within function: 'bre=..' instead of 'breaks=' (or any non-ambiguous abbrevation).
So let's exclude taxa with less than 5 occurences:

```
> sel <- which(apply(traspe>0, 2, sum)>4)
```

Check if this works (**Figure 49)**:

```
> hist(apply(traspe[sel]>0, 2, sum), breaks=20, xlab="Nr. sites per taxon")
```

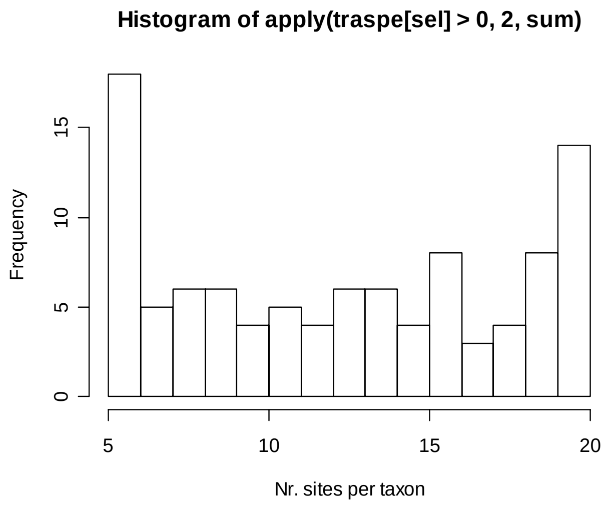


Figure 49. Histogram of no. of sites per taxon.

Should these taxa be excluded? If yes:

```
# > traspe<-traspe[sel] # below, we continue with the full dataset
```

Check environmental variable for their distribution

```
> x11()
> pairs(traenv) # not shown
```

There are too many at once; focus on metals:

```
> pairs(traenv[1:11])
```

Let's see log-transformed data now (Figure 50):

```
> pairs(log(traenv[1:11]))
```

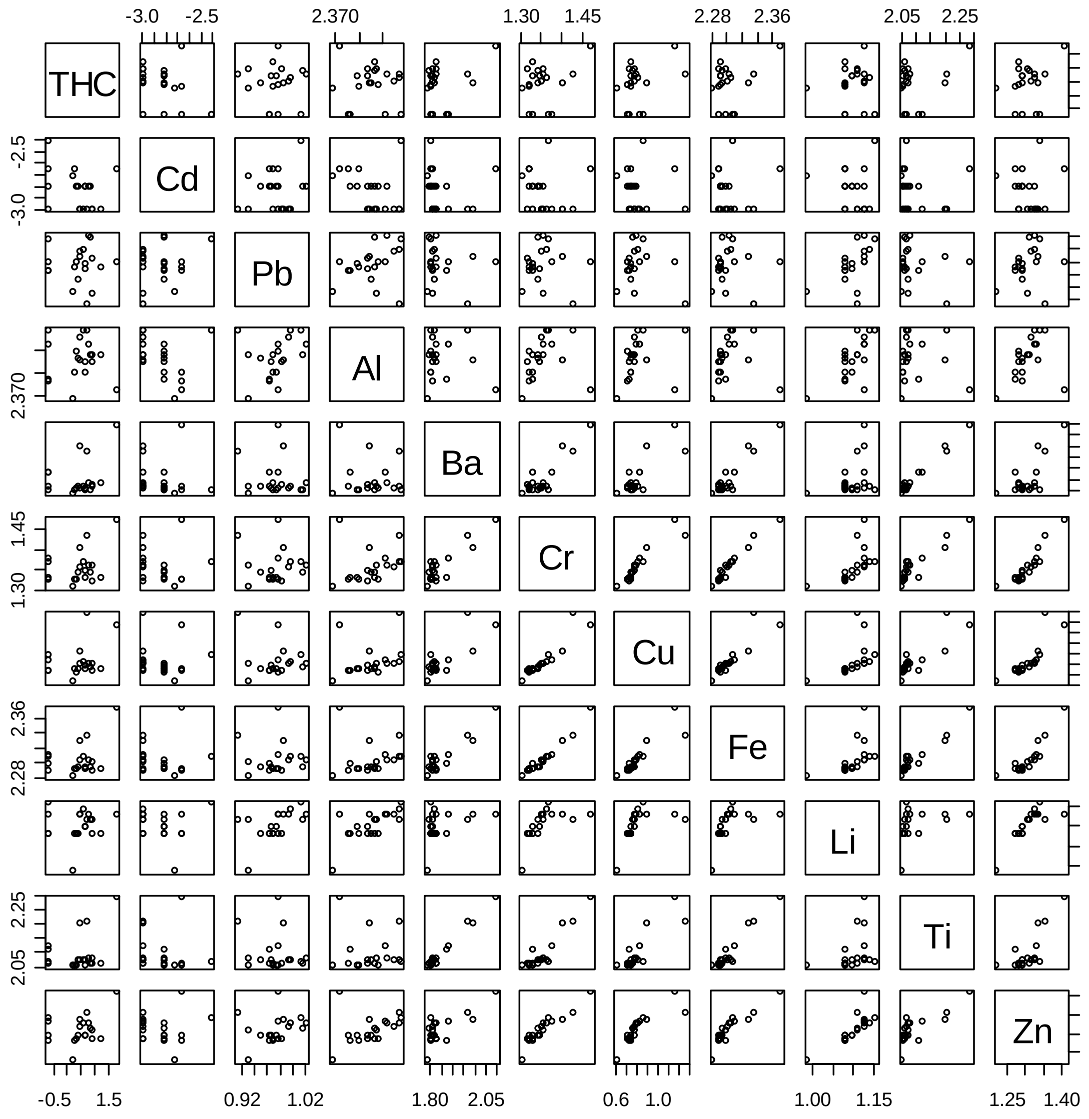


Figure 50. Command `pairs`: pair wise scatterplots of environmental variables.

Log-transformed values are not better. Log-transformation of THC and Cd would yield negative values. This can avoid by multiplying by 1000.

```
> traenv[, 1:2] <- log10(1000*traenv[, 1:2])
```

Check correlations among environmental variables. The function `cor(x)` gives a correlation matrix.

```
> round(cor(traenv),2) # not so clear to read, try:
            THC    Cd    Pb    Al    Ba    Cr    Cu    Fe    Li    Ti    Zn
THC        1.00 -0.33 -0.04 -0.05  0.33  0.34  0.33  0.35  0.04  0.31  0.29
Cd        -0.33  1.00  0.21 -0.32 -0.09 -0.05 -0.07  0.00 -0.08 -0.07  0.02
Pb        -0.04  0.21  1.00  0.32 -0.13 -0.02 -0.22 -0.01  0.55 -0.16  0.27
Al        -0.05 -0.32  0.32  1.00 -0.15  0.19  0.24  0.06  0.69 -0.10  0.35
Ba         0.33 -0.09 -0.13 -0.15  1.00  0.89  0.81  0.94  0.31  0.99  0.76
Cr         0.34 -0.05 -0.02  0.19  0.89  1.00  0.91  0.98  0.60  0.93  0.93
Cu         0.33 -0.07 -0.22  0.24  0.81  0.91  1.00  0.88  0.45  0.85  0.81
Fe         0.35  0.00 -0.01  0.06  0.94  0.98  0.88  1.00  0.53  0.96  0.91
Li         0.04 -0.08  0.55  0.69  0.31  0.60  0.45  0.53  1.00  0.34  0.80
```

```
Ti          0.31 -0.07 -0.16 -0.10  0.99  0.93  0.85  0.96  0.34  1.00  0.78
Zn          0.29  0.02  0.27  0.35  0.76  0.93  0.81  0.91  0.80  0.78  1.00
TOM         0.11 -0.17  0.46  0.41  0.28  0.43  0.32  0.37  0.74  0.27  0.60
Depth      -0.06  0.05  0.50  0.50  0.07  0.25  0.19  0.21  0.78  0.06  0.52
Fine.sand   0.01 -0.01 -0.36 -0.55 -0.26 -0.50 -0.47 -0.40 -0.82 -0.28 -0.68
Pelite      0.03 -0.06  0.38  0.58  0.26  0.50  0.45  0.41  0.86  0.28  0.69
             TOM Depth Fine.sand Pelite
THC         0.11 -0.06      0.01   0.03
Cd         -0.17  0.05     -0.01  -0.06
Pb          0.46  0.50     -0.36   0.38
Al          0.41  0.50     -0.55   0.58
Ba          0.28  0.07     -0.26   0.26
Cr          0.43  0.25     -0.50   0.50
Cu          0.32  0.19     -0.47   0.45
Fe          0.37  0.21     -0.40   0.41
Li          0.74  0.78     -0.82   0.86
Ti          0.27  0.06     -0.28   0.28
Zn          0.60  0.52     -0.68   0.69
TOM         1.00  0.69     -0.82   0.82
Depth       0.69  1.00     -0.85   0.89
Fine.sand  -0.82 -0.85      1.00  -0.99
Pelite      0.82  0.89     -0.99   1.00
```

The function `symnum(x)` gives a symbolic representation of numbers:

```
> symnum(cor(traenv))  # 'symnum' symbolizes the matrix produced by 'cor'
          TH Cd Pb A B Cr Cu Fe L Ti Z TO D F. Pl
THC       1
Cd        .  1
Pb              1
Al           .  .  1
Ba        .          1
Cr        .          + 1
Cu        .          + *  1
Fe        .          * B  +  1
Li              .  , . .  .  .  1
Ti        .          B *  +  B  . 1
Zn                 . , *  +  *  , ,  1
TOM             .  .   .  .  .  ,    . 1
Depth           .  .            ,    . ,  1
Fine.sand       .  .   .  .  .  +    , +  + 1
Pelite          .  .   .  .  .  +    , +  + B  1
attr(,"legend")
[1] 0 ' ' 0.3 '.' 0.6 ',' 0.8 '+' 0.9 '*' 0.95 'B' 1
```

Let's see how the distribution of metals is related to the morphology of the sites:

```
> nm.env <- metaMDS(traenv[1:11])
Wisconsin double standardization
Run 0 stress 6.960043
Run 1 stress 6.954604
... New best solution
... rmse 0.001560382   max residual 0.002971707
*** Solution reached

> x11()
> plot(nm.env, type="n",  main="NMDS of contaminants")  # Gives Figure 51
```

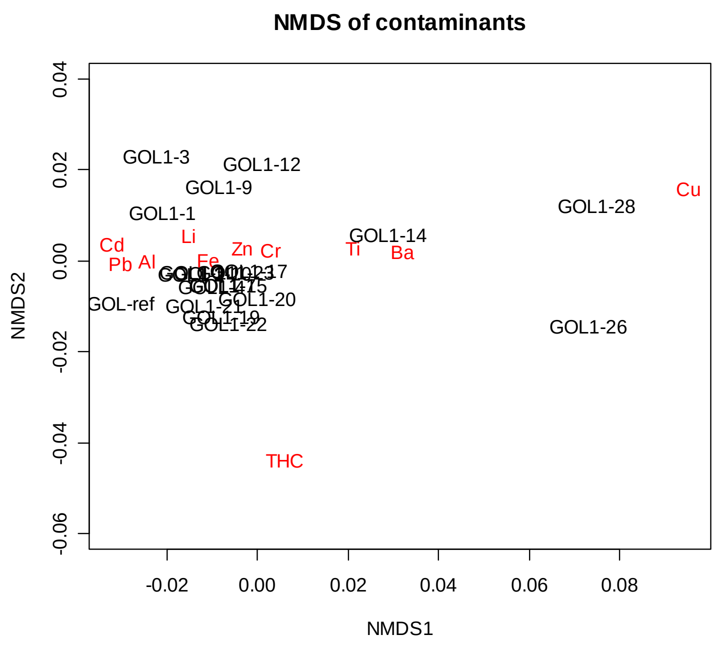


Figure 51. NMDS of contaminants.

```
> text(nm.env, "species", col=2) # the species
> text(nm.env, "sites",  col=1)
> (ef.nm.env<-envfit(nm.env, traenv[12:15], perm=1000))

***VECTORS

             NMDS1    NMDS2     r2 Pr(>r)
TOM        0.60443  0.79666 0.1239  0.326
Depth      0.19037  0.98171 0.0857  0.382
Fine.sand -0.37688 -0.92626 0.2647  0.106
Pelite     0.41919  0.90790 0.2409  0.135
P values based on 1000 permutations.
> # only weak effects
>
> # NMDS of sqrt-transformed species data
> nm.sp<-metaMDS(sqrt(traspe))
Run 0 stress 13.99375
Run 1 stress 13.97234
... New best solution
... rmse 0.006179893   max residual 0.01612660
Run 2 stress 14.42431
Run 3 stress 13.9723
... New best solution
... rmse 0.0004250777   max residual 0.001250656
*** Solution reached

> x11()
> plot(nm.sp, main="all species") # Figure 52
```

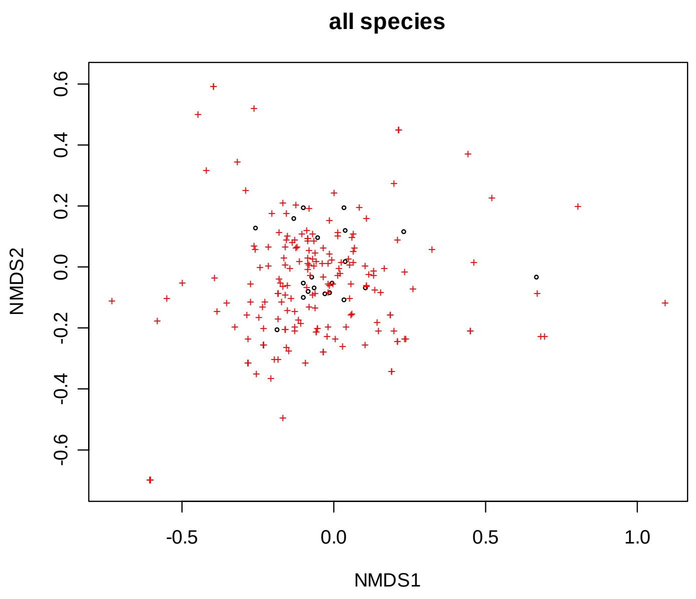


Figure 52. NMDS for all species.

Are the ordinations for contaminants and species similar? We can test by procrustes rotation

```
> (pro<-protest(nm.env, nm.sp))

Call:
protest(X = nm.env, Y = nm.sp)

Correlation in a symmetric Procrustes rotation:  0.6625
Significance:  < 0.001
Based on 1000 permutations.
```

The two ordinations are correlated (Figure 53), which is not a surprise if the contaminants have an effect.

```
> x11()
> plot(pro)
```

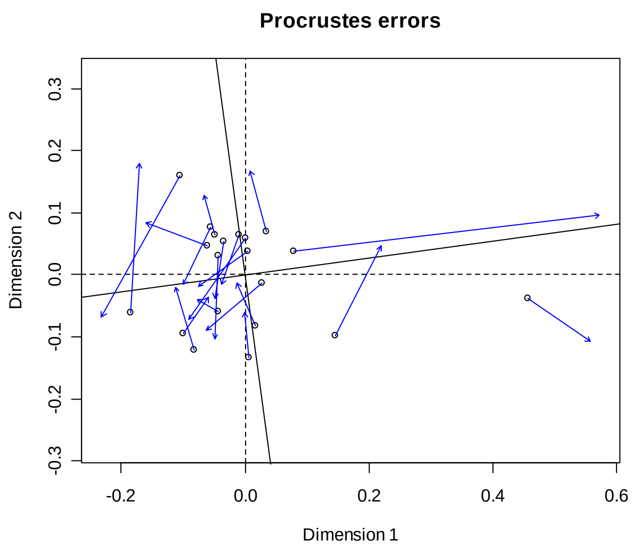


Figure 53. Procrustes rotation comparing the NMDS of species and contaminants.

We assume that both site morphology and heavy metals influence species distribution, so we first test all parameters in the ordination.

```
> (ef.nm.sp<-envfit(nm.sp, traenv, perm=1000))

***VECTORS

              NMDS1     NMDS2     r2 Pr(>r)
THC        0.943970  0.330030 0.3357  0.030 *
Cd        -0.894964  0.446138 0.0469  0.689
Pb        -0.347455  0.937697 0.0094  0.916
Al        -0.547694  0.836679 0.0630  0.580
Ba         0.992854 -0.119331 0.7945 <0.001 ***
Cr         0.989163  0.146824 0.6686  0.001 ***
Cu         0.999901  0.014096 0.4370  0.023 *
Fe         0.998195  0.060055 0.7562 <0.001 ***
Li         0.443578  0.896236 0.2674  0.080 .
Ti         0.994916 -0.100706 0.7655 <0.001 ***
Zn         0.958421  0.285358 0.5642 <0.001 ***
TOM        0.614459  0.788948 0.1607  0.217
Depth      0.169195  0.985583 0.2600  0.079 .
Fine.sand -0.344508 -0.938783 0.2034  0.124
Pelite     0.340739  0.940158 0.2668  0.071 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
P values based on 1000 permutations.
```

Well, many relationships, but hard to interpret (overfitting! – remember we have only 19 sites!)
A better way with constrained ordination?

```
> x11(); par(mfrow=c(2, 2))
> plot(nm.sp, main="metaMDS traspe")    # Figure 54, upper left
> plot(ef.nm.sp)
> plot(ef.nm.sp, p.max = 0.05, col = "red")
> (cca1<-cca(sqrt(traspe)~., traenv))   # Figure 54, upper right

Call:
cca(formula = sqrt(traspe) ~ THC + Cd + Pb + Al + Ba + Cr + Cu +      Fe + Li + Ti
+ Zn + TOM + Depth + Fine.sand + Pelite, data = traenv)

              Inertia Rank
Total          1.0304
Constrained    0.8433   15
Unconstrained  0.1871    4
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
   CCA1    CCA2    CCA3    CCA4    CCA5    CCA6    CCA7    CCA8    CCA9   CCA10
0.11174 0.08121 0.07868 0.07037 0.06634 0.06042 0.05543 0.05044 0.04818 0.04759
  CCA11   CCA12   CCA13   CCA14   CCA15
0.03975 0.03756 0.03396 0.03195 0.02966

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4
0.05270 0.05043 0.04377 0.04020

> plot(cca1, main="CCA traspe with traenv")
```

A high amount of variability is explained; this is expected with high number of explanatory variables. However, does this help?

```
> ca1 <- cca(sqrt(traspe))
> plot(ca1, main="CA traspe")    # Figure 54, lower left
> (pro <- protest(ca1, cca1))
```

```
Call:
protest(X = ca1, Y = cca1)

Correlation in a symmetric Procrustes rotation:  0.9455
Significance:  < 0.001
Based on 1000 permutations.

> plot(pro) # Figure 54, lower right
```

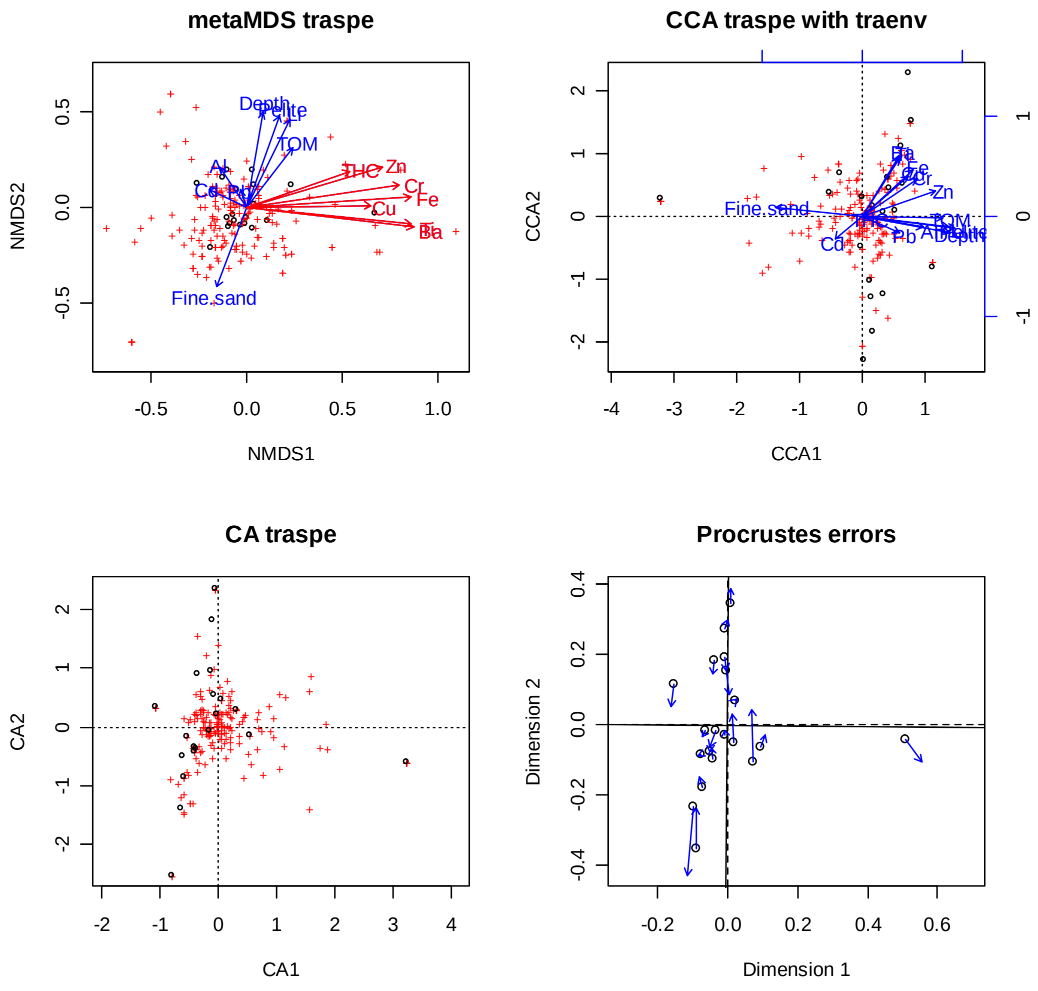


Figure 54. Various ordinations and procrustes errors between overfitted CCA and unconstrained PCA (lower left).

'Unconstrained' CCA (practically identical to CA, see Figure 54) has too many variables, and is hard to interpret. We should therefore build a better (restricted) model.

```
> mod0 <- cca(sqrt(traspe) ~ 1, traenv)
> mod1 <- cca(sqrt(traspe) ~ ., traenv)
> mod <- step(mod0, scope=list(lower = ~1, upper=formula(mod1)))
```

```
Start:  AIC= 101.6
 sqrt(traspe) ~ 1

            Df    AIC
+ Pelite     1 101.52
+ Depth      1 101.60
<none>         101.61
+ Fine.sand  1 101.64
+ Li         1 101.64
+ Zn         1 101.78
+ TOM        1 101.81
+ Cr         1 102.00
+ Cu         1 102.01
+ Fe         1 102.01
+ Al         1 102.11
+ Ti         1 102.13
+ Ba         1 102.15
+ Cd         1 102.23
+ Pb         1 102.32
+ THC        1 102.48

Step:  AIC= 101.52
 sqrt(traspe) ~ Pelite

            Df    AIC
<none>         101.52
- Pelite     1 101.61
+ Cu         1 101.91
+ Fe         1 102.00
+ Zn         1 102.00
+ Ti         1 102.01
+ Ba         1 102.02
+ Cr         1 102.03
+ Cd         1 102.05
+ Pb         1 102.25
+ Depth      1 102.27
+ THC        1 102.28
+ Al         1 102.35
+ Li         1 102.39
+ Fine.sand  1 102.41
+ TOM        1 102.45

> mod

Call:
cca(formula = sqrt(traspe) ~ Pelite, data = traenv)

              Inertia Rank
Total          1.0304
Constrained    0.1019    1
Unconstrained  0.9285   18
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
  CCA1
0.1019

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4     CA5     CA6     CA7     CA8
0.08413 0.08018 0.07580 0.07199 0.06573 0.05875 0.05716 0.05520
(Showed only 8 of all 18 unconstrained eigenvalues)
```

Stepwise selection does not work well (all exc. Pelite removed).
Pelite seems to be a major, overriding factor. We can ‘partial out’ the effect of Pelite in order to make a potential effect of the heavy metals more visible.

```
> (cca.Ba <- cca(sqrt(traspe) ~ Ba + Condition(Pelite), traenv))
              Inertia Rank
Total         1.03038
Conditional   0.10190    1
Constrained   0.06715    1
Unconstrained 0.86133   17
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
   CCA1
0.06715

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4     CA5     CA6     CA7     CA8
0.08046 0.07678 0.07357 0.06791 0.06356 0.05731 0.05522 0.05381
(Showed only 8 of all 17 unconstrained eigenvalues)

> anova(cca.Ba) # permutation test on effect of Ba
Permutation test for cca under direct model

Model: cca(formula = sqrt(traspe) ~ Ba + Condition(Pelite), data = traenv)
         Df  Chisq      F N.Perm Pr(>F)
Model     1 0.0672 1.3254   1200 0.0675 .
Residual 17 0.8613
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Number of 'Ba' after removing the effect of 'Pelite' is marginally significant.
We can perform this test with all potential candidates

```
> (cca.Zn <- cca(sqrt(traspe) ~ Zn + Condition(Pelite), traenv)) # same for Zn
              Inertia Rank
Total         1.03038
Conditional   0.10190    1
Constrained   0.06792    1
Unconstrained 0.86056   17
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
   CCA1
0.06792

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4     CA5     CA6     CA7     CA8
0.08193 0.07850 0.07254 0.06574 0.06157 0.05723 0.05582 0.05399
(Showed only 8 of all 17 unconstrained eigenvalues)

> anova(cca.Zn)
Permutation test for cca under direct model

Model: cca(formula = sqrt(traspe) ~ Zn + Condition(Pelite), data = traenv)
         Df  Chisq      F N.Perm  Pr(>F)
Model     1 0.0679 1.3417   2300 0.06391 .
Residual 17 0.8606
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Is species richness related to the environmental variables? We need a non-parametric test as data are clearly non-normally distributed.

```
> require(Hmisc)
[1] TRUE
> nspe <- as.numeric(apply(traspe >0, 1, sum))
> x11()

> par(mfrow=c(2, 2)) # Figure 55
> plot(nspe ~ Depth, data=traenv)
> plot(nspe ~ Pelite, data=traenv)
> plot(nspe ~ Ba, data=traenv)
> plot(nspe ~ Zn, data=traenv)
```

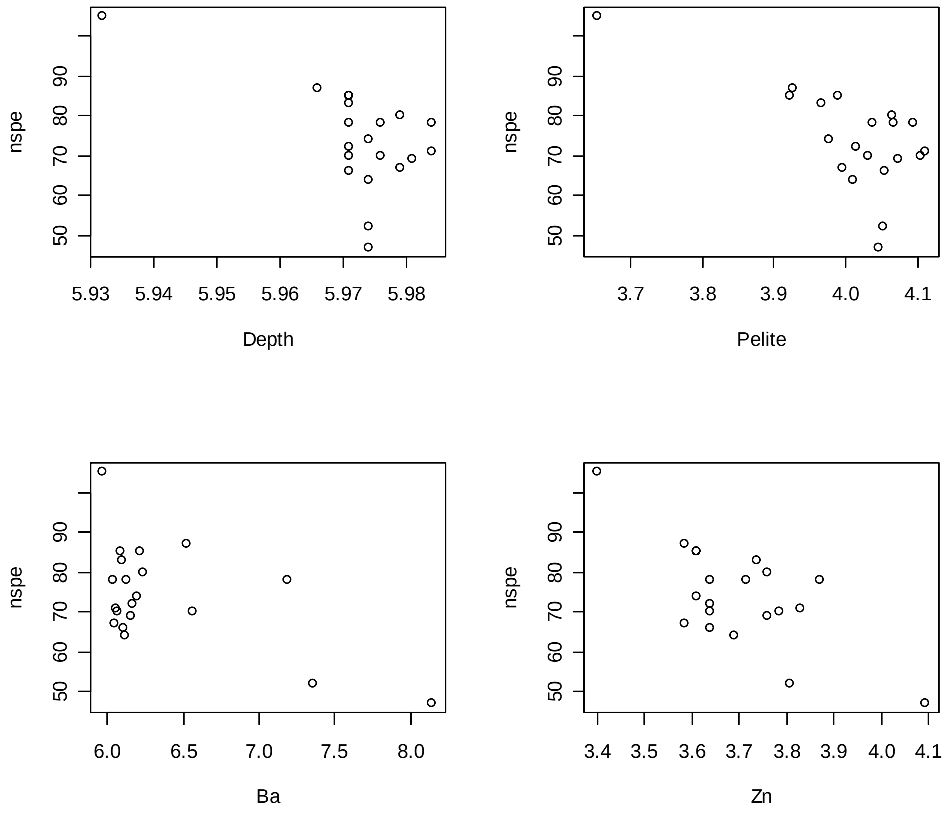


Figure 55. Number of species per site plotted against different environmental factors.

```
> spearman.test(nspe, traenv$Zn) # and same way for other variables
    Rsquare           F         df1         df2      pvalue           n
 0.23140882  5.41947241  1.00000000 18.00000000  0.03177332 20.00000000
```

Alternatively:

```
> cor.test(nspe, traenv$Zn, method="spearman")
```

For more than 1 parameter, we can use 2-dimensional GAM (Section 5).

```
> #
> #   L U N C H
> #   B R E A K  ><(((*>
> #
```

4.1.3 Example 6: constrained ordination. Extracting indicator values from an ordination.

```
> rm(list=ls())
> load("NOgen.bin") # phytoplankton composition data from Norwegian lakes (genus
level)
> load("NOenv.bin") # corresponding chemistry and lake morphometry
```

NMDS cannot be used with such large dataset (R will get stuck).
The genus data are very skewed, with many zeros. We will therefore apply a square-root-transformation when performing ordinations (`sqrt(data)`, see below).
Some species may be very rare or absent.

```
> sel.gen <- which(apply(NOgen>0, 2, sum)>10)
> NOgen <- NOgen[sel.gen]
```

Environmental variables - should we apply log-transformation?

```
> pairs(NOenv[3:9])
> pairs(log10(NOenv[3:9]))
> lNOenv <- log10(NOenv)
> symnum(cor(lNOenv))
              sy sm M A S_ SC C TN TP
syear         1
smonth           1
Mean_depth          1
Altitude              1
Surface_area        .   1
SCa                 .      1
Chlorophyll.a       .      .  1
TotN                       .  . 1
TotP                .      .  , ,  1
attr(,"legend")
[1] 0 ' ' 0.3 '.' 0.6 ',' 0.8 '+' 0.9 '*' 0.95 'B' 1
```

It doesn't look too bad (**Figure 56**).

```
> (ca1 <- cca(sqrt(NOgen)))

Call:
cca(X = sqrt(NOgen))

              Inertia Rank
Total           5.405
Unconstrained   5.405   82
Inertia is mean squared contingency coefficient

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8
0.4318 0.3338 0.2828 0.2740 0.2440 0.2327 0.2060 0.2040
(Showed only 8 of all 82 unconstrained eigenvalues)

> x11()
> plot(ca1) # Figure 57.
```

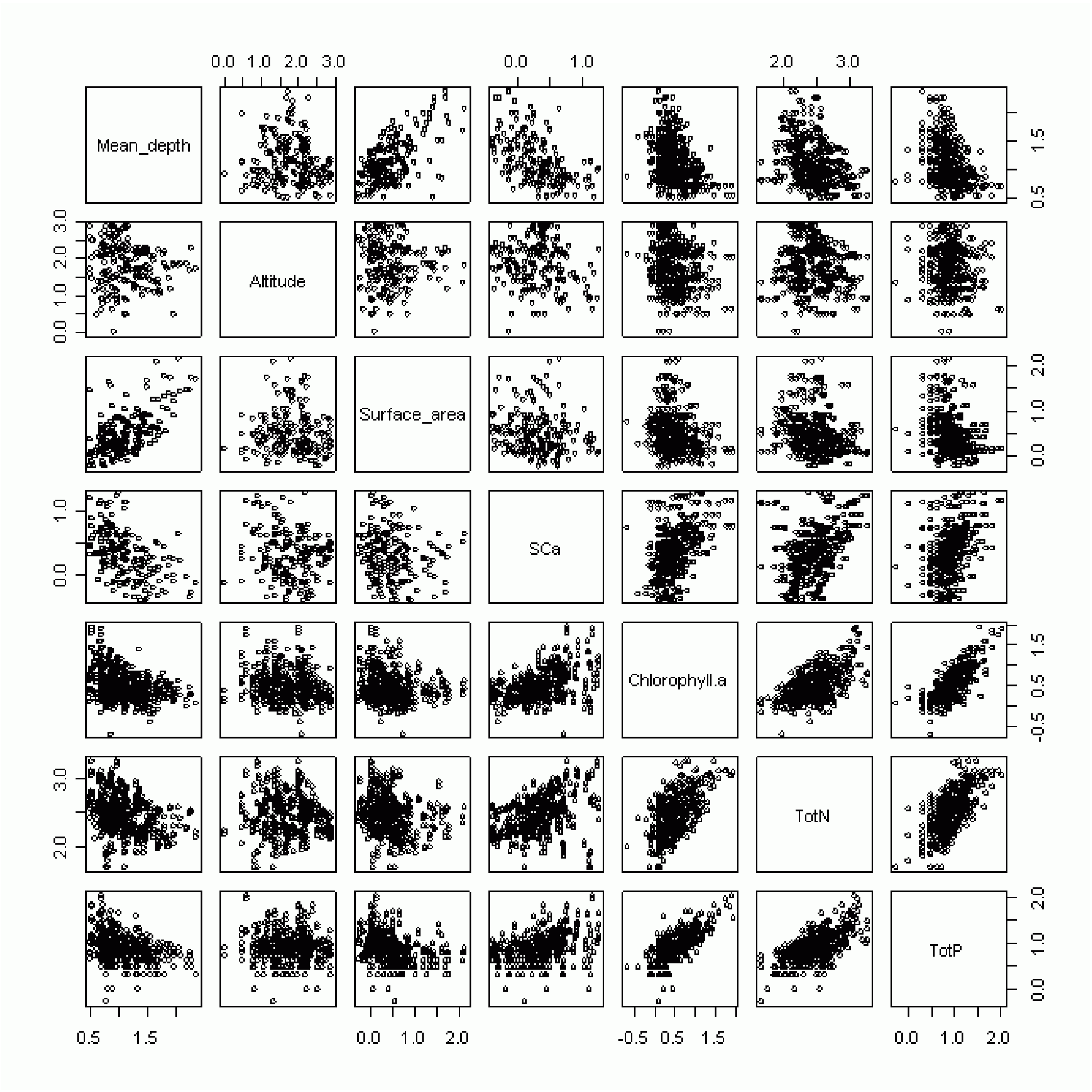


Figure 56. Pair-wise scatterplots of environmental variables.

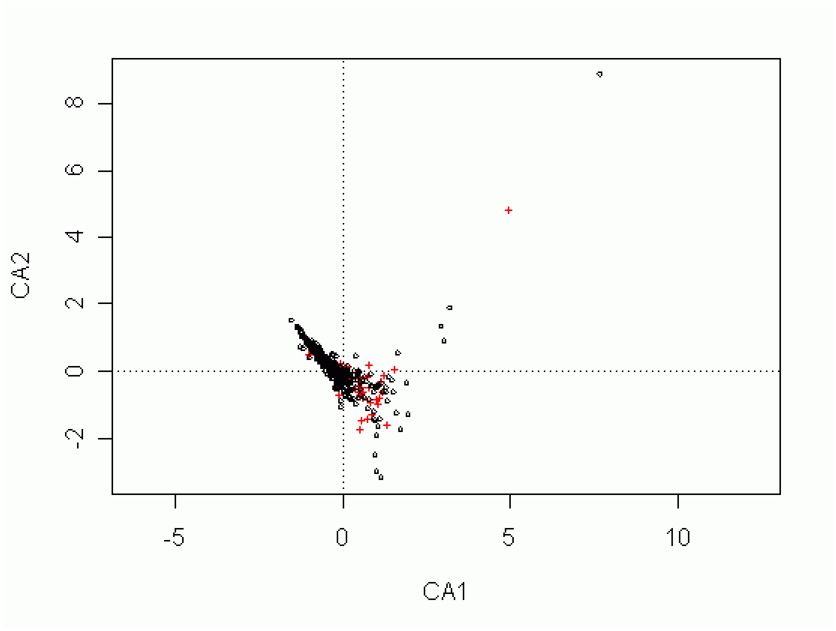


Figure 57. PCA of the phytoplankton matrix.

```
> (ef.ca1 < -envfit(ca1, lNOenv, perm=1000))

***VECTORS

                    CA1       CA2     r2 Pr(>r)
syear          0.584072 -0.811702 0.1367  0.003 **
smonth         0.765518 -0.643414 0.0007  0.948
Mean_depth    -0.831706  0.555216 0.2036 <0.001 ***
Altitude      -0.999551  0.029968 0.1096 <0.001 ***
Surface_area  -0.888171  0.459514 0.0184  0.140
SCa            0.899901 -0.436093 0.3687 <0.001 ***
Chlorophyll.a  0.887499 -0.460809 0.6504 <0.001 ***
TotN           0.882269 -0.470746 0.3658 <0.001 ***
TotP           0.923900 -0.382634 0.5109 <0.001 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
P values based on 1000 permutations.
```

We may suspect that the main gradient is eutrophication. Thus it would be nice to illustrate role of Chlorophyll (i.e. eutrophication).
The function `cut(x, nbreaks,...)` breaks vector into pieces of even intervals.

```
> chl.code <- cut(lNOenv$Chlorophyll.a, 30, labels=F) # (see part 6. for details)
> x11(); par(bg="darkgrey")
> plot(scores(ca1)$sites, pch=20,  col=heat.colors(30)[chl.code])
```

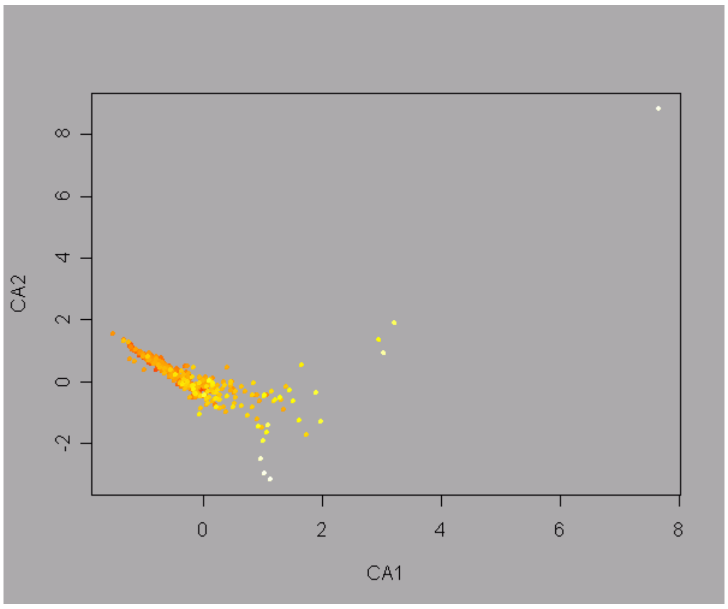


Figure 58. PCA of the phytoplankton matrix. The colorcode illustrates the Chlorophyll-a concentration (dark=low, light=high).

Figure 58 illustrates that communities become more different as Chl-a increases. From previous analyses we know that in addition to eutrophication, lake depth and alkalinity (Ca, here SCa) are important variables.

```
> (cca1<-cca(sqrt(NOgen)~Chlorophyll.a+Mean_depth+SCa, data=lNOenv))

Call:
cca(formula = sqrt(NOgen) ~ Chlorophyll.a + Mean_depth + SCa,      data = lNOenv)

              Inertia Rank
Total           5.405
Constrained     0.401    3
Unconstrained   5.004   82
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
   CCA1    CCA2    CCA3
0.31334 0.06839 0.01925

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8
0.3551 0.2723 0.2665 0.2452 0.2335 0.2111 0.2007 0.1780
(Showed only 8 of all 82 unconstrained eigenvalues)
```

Note the difference between inertia of first and second constrained axes.

```
> x11()
> par(bg="grey")
> plot(cca1)
> points(cca1, pch=20, col=heat.colors(30)[chl.code])
```

The first axis is mainly eutrophication (**Figure 59**).

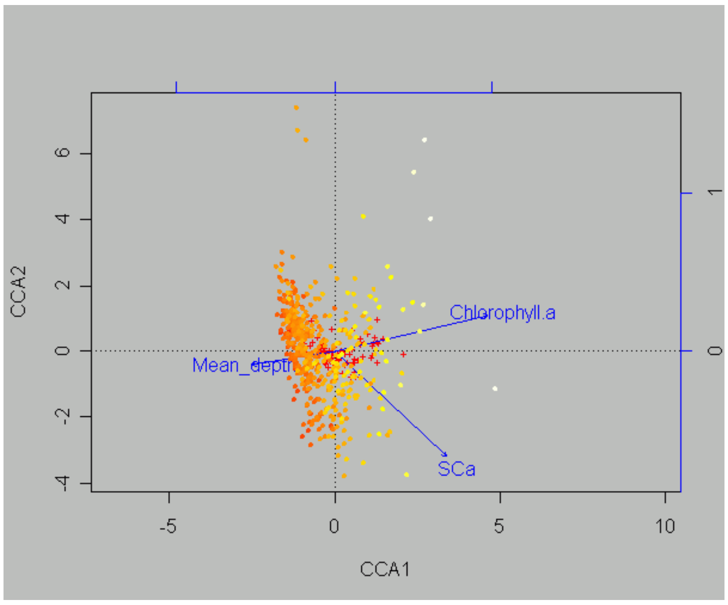


Figure 59. CCA of the phytoplankton data with three predictors.

For extracting indicator values, we need to extract the optima of the genera on the eutrophication gradient. We could directly use the species scores from the first axis, but there is obvioulsy correlation with the other variables. Let's partial out SCa first.

```
> (cca2<-cca(sqrt(NOgen)~Chlorophyll.a+Condition(Mean_depth+SCa), data=lNOenv))

Call:
cca(formula = sqrt(NOgen) ~ Chlorophyll.a + Condition(Mean_depth +      SCa), data
= lNOenv)

              Inertia Rank
Total          5.4054     
Conditional    0.2346    2
Constrained    0.1664    1
Unconstrained  5.0044   82
Inertia is mean squared contingency coefficient 

Eigenvalues for constrained axes:
  CCA1 
0.1664 

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8 
0.3551 0.2723 0.2665 0.2452 0.2335 0.2111 0.2007 0.1780 
(Showed only 8 of all 82 unconstrained eigenvalues)
```

Now the first axis explains much less than before.

```
> x11()
> plot(cca2) # Figure 60
> points(cca2, pch=20, col=heat.colors(30)[chl.code])
```

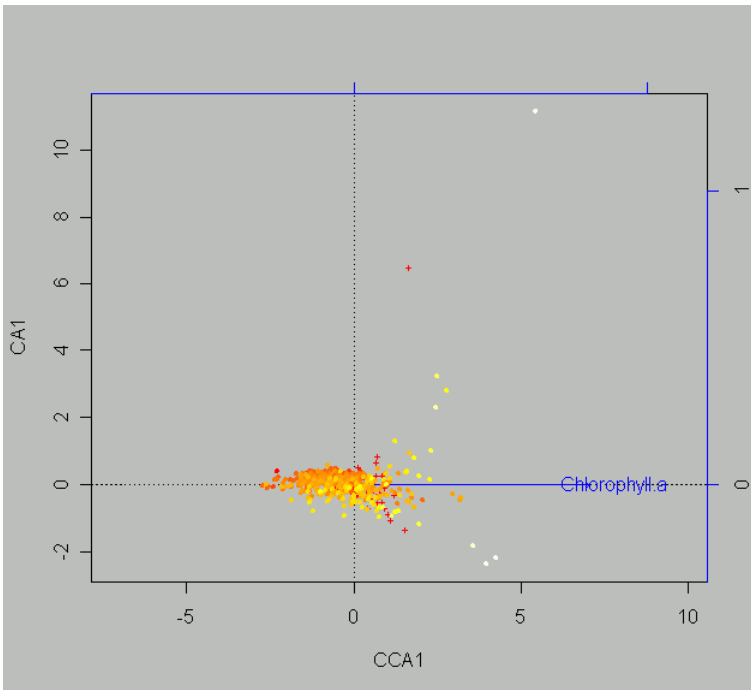


Figure 60. CCA against Chlorophyll-a where the effects of CA and Depth are partialled out.

Re-inferring the lake trophic status from the optima of the species: we can use the optima derived from the CCA for predicting lake trophic status. This is a way to test if the species are useful indicators. We want to avoid circularity and will therfore splite the data into training and predicting dataset. We divide into two random groups using the `sample()` function.

```
       sample(x, y, replace=T): select randomly y elements from vector x
```

```
> set1 <- sort(sample(1:501, 250, replace=F))
> set2 <- (1:501)[-set1]
> (cca.set1 <- cca(sqrt(NOgen[set1, ]) ~ Chlorophyll.a + Condition(Mean_depth+SCa),
+ data=lNOenv[set1, ]))

Call:
cca(formula = sqrt(NOgen[set1, ]) ~ Chlorophyll.a + Condition(Mean_depth +
SCa), data = lNOenv[set1, ])

              Inertia Rank
Total          4.9851
Conditional    0.2683    2
Constrained    0.1945    1
Unconstrained  4.5223   82
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
  CCA1
0.1945

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8
0.3373 0.3126 0.2525 0.2300 0.2209 0.2023 0.1945 0.1807
(Showed only 8 of all 82 unconstrained eigenvalues)
```

The output is comparable to the output of total data set (above). Species optima for Chl-a correspond to the first ordination axis.

```
> specopt <- scores(cca.set1)$species[, 1]
```

Plot species-optima with function `dotchart()`

```
> par(mfrow=c(1, 2))
> dotchart((sort(specopt))[1:41], xlim=range(specopt))  (Figure 61).
> dotchart((sort(specopt))[42:83], xlim=range(specopt))
```

Both plots should have same x-scale, though showing different optima. The function `range()` extracts min and max of the optima, and can be used to set the scale for the x-axis.

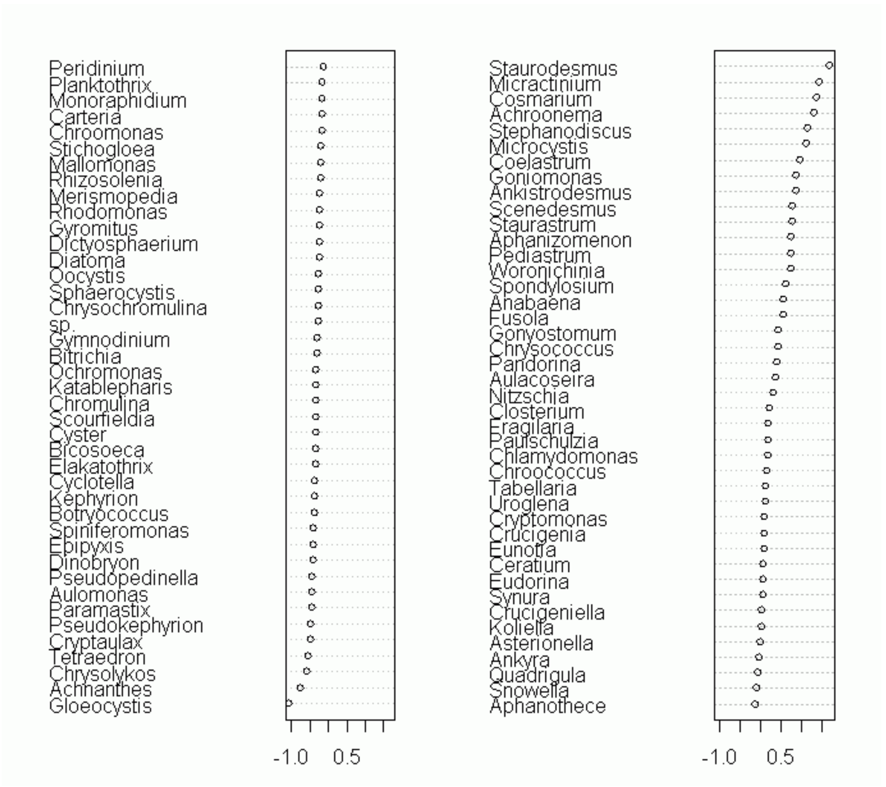


Figure 61. Dotchart illustrating the species optima.

Using weighted averaging, we calculate a trophic score as predicted from the species. The function `wascores(x, y)` calculates weighted averages for sites from species optima(x) and the transposed composition matrix (`t(y)`). See **Figure 62.**

```
> wascr <- wascores(specopt, t(sqrt(NOgen[set2, ])))
> x11(6, 6)
> plot(lNOenv$Chlorophyll.a[set2], wascr, xlab="log(Chlrophyll-a)",
+ ylab="trophic score")
> plot(NOenv$Chlorophyll.a[set2], wascr, log="x", xlab="Chlrophyll-a",
+ ylab="trophic score", main="all species")
```

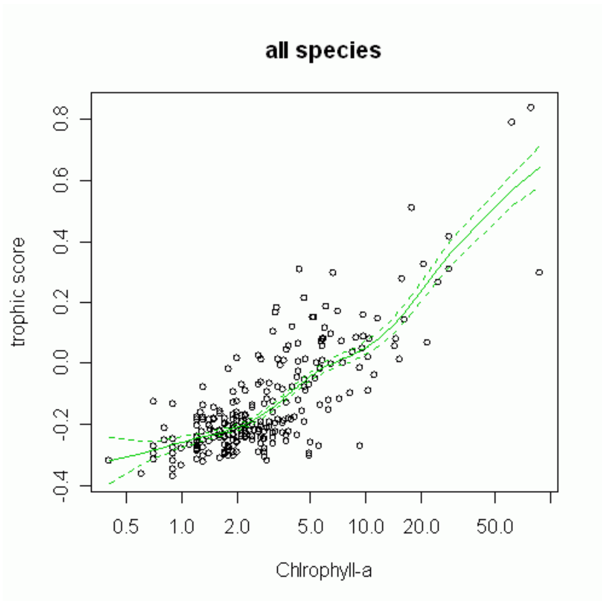


Figure 62. The calculated trophic scores plotted against the chlorophyll-a concentration.

```
> require(mgcv)
[1] TRUE
> gmod<-gam(wascr~s(lNOenv$Chlorophyll.a[set2]))
> gpred<-predict(gmod, se.fit=T)
> lines(NOenv$Chlorophyll.a[set2], gpred$fit, col=3)
> lines(NOenv$Chlorophyll.a[set2], gpred$fit+gpred$se.fit, col=3, lty=2)
> lines(NOenv$Chlorophyll.a[set2], gpred$fit-gpred$se.fit, col=3, lty=2)
```

Now we used all genera, but we can also select those with best fit.
```
> x11(6, 4)
```
The function `goodness()` extracts value for how well a site or species fits in the ordination (**Figure 63**). The larger the better, low goodness implies that species are randomly distributed.
```
> hist(goodness(cca.set1, "species"), bre=30)
> abline(v=0.05, col=2)
```
The red line in the histogram indicates the cut-off level for weak fit.

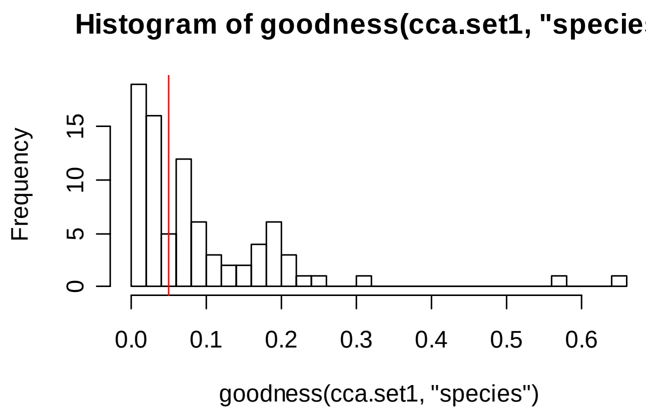


Figure 63. Histogram of the species' 'goodness' in the CCA.

```
> sel.ind <- which(goodness(cca2, "species")>0.05)
> wascr <- wascores(specopt[sel.ind], t(sqrt(NOgen[set2, sel.ind])))
> x11(6, 6) # Figure 64
> plot(NOenv$Chlorophyll.a[set2], wascr, log="x", xlab="Chlrophyll-a",
+ ylab="trophic score", main="selected species")
```

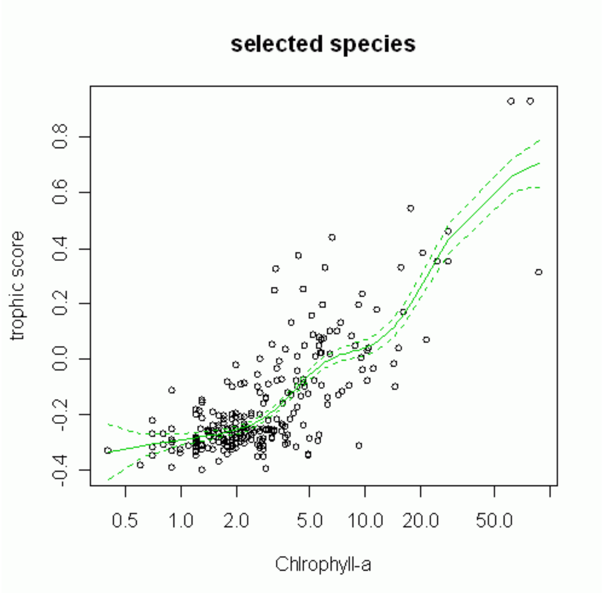


Figure 64. As Figure above, but for selected species only.

```
> gfit<-gam(wascr~s(lNOenv$Chlorophyll.a[set2]))
> gpred<-predict(gfit, se.fit=T)
> lines(NOenv$Chlorophyll.a[set2], gpred$fit, col=3)
> lines(NOenv$Chlorophyll.a[set2], gpred$fit+gpred$se.fit, col=3, lty=2)
> lines(NOenv$Chlorophyll.a[set2], gpred$fit-gpred$se.fit, col=3, lty=2)
```

> # - optional for ### P A R T T H R E E ###
Is there another way to obtain species optima? Can we use median of all the sites where a species occurs? How do we get the Chl-values of the sites where species 1 occurs?

```
> NOgen[, 1]>0
  [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
 [13] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
(…)
```

This function returns `TRUE` for all sites, so that we can get the corresponding Chl-values:

```
> lNOenv$Chlorophyll.a[NOgen[, 1]>0]
 [1] -0.09691001 -0.04575749  0.00000000  0.11394335  0.11394335  0.20411998
 [7]  0.23044892  0.23044892  0.23044892  0.25527251  0.30103000  0.30103000
[13]  0.38021124  0.43136376  0.44715803  0.58433122  0.59106461  0.65321251
```

…and the median

```
> median(lNOenv$Chlorophyll.a[NOgen[, 1]>0])
[1] 0.2428607
```

OK, now let's produce a vector with all genus optima

```
> meds <- NA
> for(i in 1:length(NOgen)) {
+ meds[i] <- median(lNOenv$Chlorophyll.a[NOgen[, i]>0])     }
> wascr <- wascores(meds, t(sqrt(NOgen)))
> x11()
> plot(NOenv$Chlorophyll.a, wascr, log="x", main="median optima - all species")
> gmod <- gam(wascr ~ s(lNOenv$Chlorophyll.a))
> gpred <- predict(gmod, se.fit=T)
> lines(NOenv$Chlorophyll.a, gpred$fit, col=3)
> lines(NOenv$Chlorophyll.a, gpred$fit+gpred$se.fit, col=3, lty=2)
> lines(NOenv$Chlorophyll.a, gpred$fit-gpred$se.fit, col=3, lty=2)
```

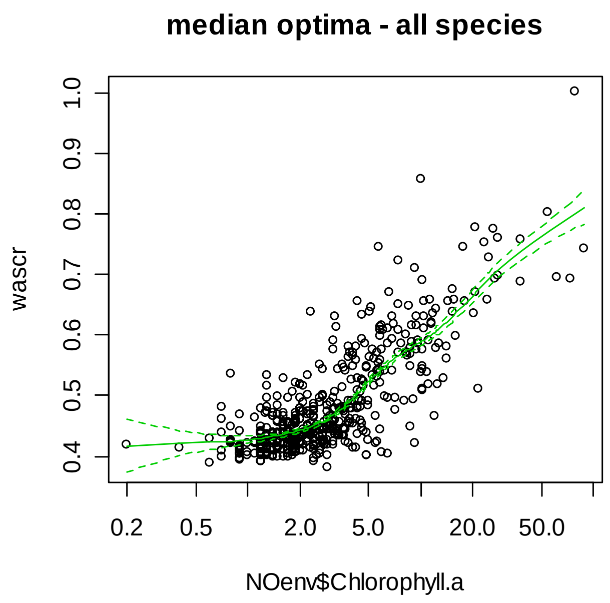


Figure 26. Predicted trophic scores from the species' medians using weighted averaging. The figure is very similar compared to the figure produced from the CCA scores (Fig. 26). The reason is that also the CCA uses weighted averaging for finding species scores, and because we had only one conbstraining variable (chlorophyll-*a*) in the CCA.

```
> #  F I N I  :-)
```

5. DATA VISUALIZATION AND LATTICE

(Robert Ptacnik)

TOPIC: create color-gradients; 3-dim GAM; Lattice

5.1 Colour gradients and 3-D GAM plots

```
> rm(list=ls())
```

Defining colorcodes

```
> load("Nstati7-9.bin") #  North-European lake data, samples jul-sept (REBECCA DB)
> attach(Nstati)
```

The following object(s) are masked from Nstati (position 3) :

```
         Alkalinity Alkalinity_type Altitude Altitude_type Ca Chlorophyll.a Colour
country_code entry_code entry_no GIG GIG_type Humic_type lake_code Mean_depth
Mean_depth_Type Nsamp pH Reference_lake SCa SColour sday site_code site_nr smonth
Surface_area Surface_area_type syear Temperature tot.biov TotN TotP Transparency
```

```
> chl.code<-cut(log(Chlorophyll.a), 30, labels=F)
> x11(8,4)
> par(mfrow=c(1, 2)) # 'par(mfrow=c(X,Y))':split plotting window by X x Y rows x
columns)
> plot(Chlorophyll.a, chl.code, log="x")
```

See Figure 65, left panel.

```
> plot(Chlorophyll.a, chl.code, log="x", col=cm.colors(30)[chl.code], pch=19)
```

See Figure 65, right panel.

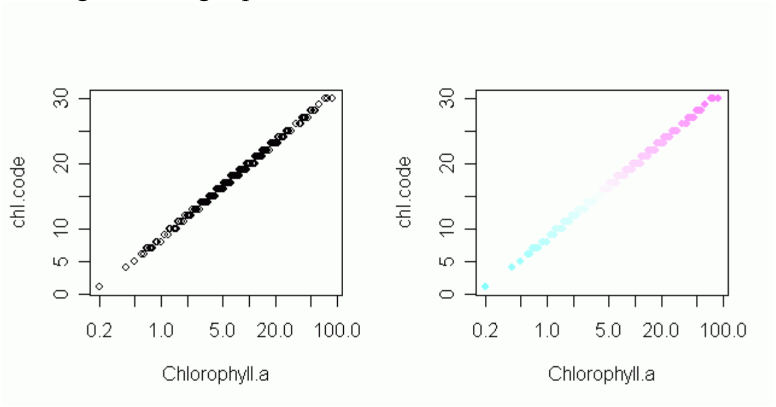


Figure 65. Example for how to code a color gradient. The y-values range from 0-30 and code the corresponding cyan-magenta colors: `cm.colors(30)`.

Colors are hard to see; change background (**Figure 66**).

```
> x11(12,4)
> par(bg="dark grey")
> par(mfrow=c(1, 3))
> plot(Chlorophyll.a, chl.code, log="x", col=cm.colors(30)[chl.code], pch=19,
main="cm.colors")
> plot(Chlorophyll.a, chl.code, log="x", col=heat.colors(30)[chl.code], pch=19,
main="heat.colors")
> plot(Chlorophyll.a, chl.code, log="x", col=rainbow(30)[chl.code], pch=19,
main="rainbow")
```

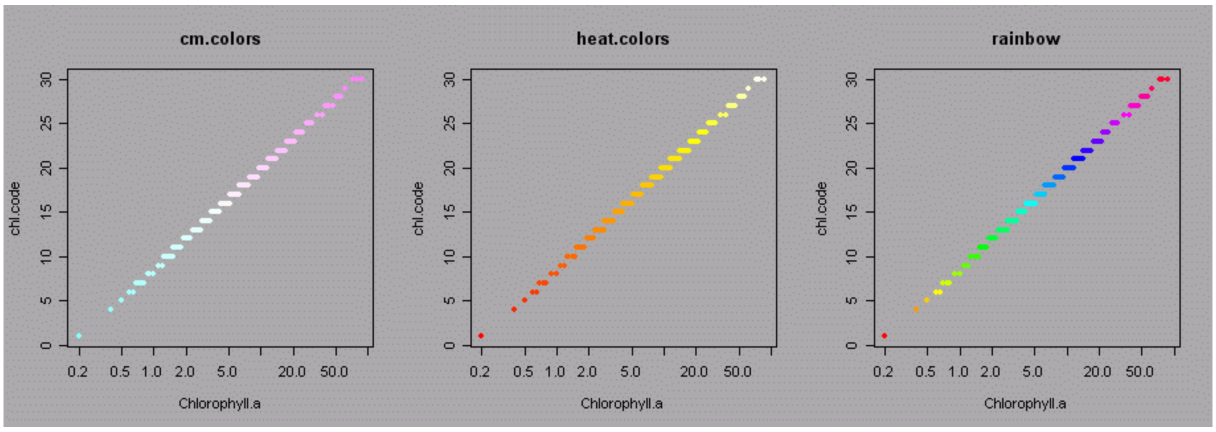


Figure 66. Different default color gradients on grey background. (`cm.colors(), heat.colors(), rainbow()`).

function 'identify':

'identify(x,y,labels=...)' identify dots in scatterplot (works also e.g. within vegan-objects)

```
> x11(5,5)
> plot(TotP, Mean_depth, log="xy", col=heat.colors(30)[chl.code], pch=19)
```

See Figure 67

```
> identify(TotP, Mean_depth)
[1] 498 798
```

Right-mouse click 'stop' to interrupt

```
> identify(TotP, Mean_depth, labels=rownames(Nstati)) #specify labels
[1] 708 997
```

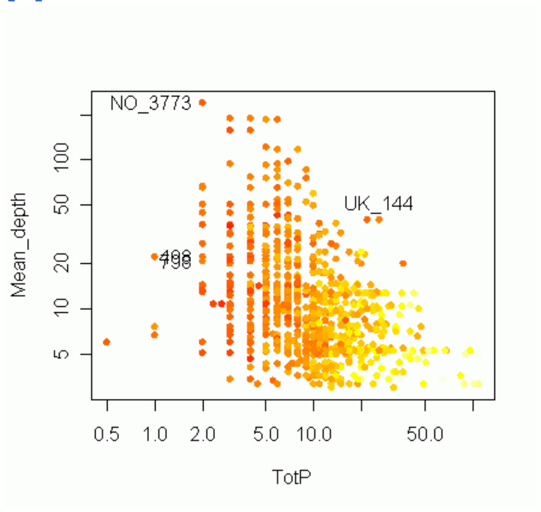


Figure 67. Mean depth plotted against total phosphorus, and showing chlorophyll-a as color gradient. The labels were produced using the 'identify' function.

Interpolate and visualize areas

```
> require(mgcv)
[1] TRUE
> require(akima) # interpolation applications
[1] TRUE
```

Nstati contains missing values; for GAM analysis need datamatrix without missing values

```
> mat <- data.frame(TP=TotP, MD=Mean_depth, Chl.a=Chlorophyll.a)
> detach(Nstati)
> wh <- which(apply(mat, 1, sum)>0) #which rowsums are positive (i.e. have no NA)
> mat <- mat[wh, ]
> gmod <- gam(log(Chl.a)~s(log(TP), k=4)+s(log(MD),k=4), data=mat)
> summary(gmod)

Family: gaussian
Link function: identity

Formula:
log(Chl.a) ~ s(log(TP), k = 4) + s(log(MD), k = 4)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.28410    0.01689   76.02   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
             edf Est.rank       F  p-value
s(log(TP)) 2.928    3.000 460.651  < 2e-16 ***
s(log(MD)) 2.149    3.000   6.812 0.000152 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.646   Deviance explained = 64.8%
GCV score = 0.2742   Scale est. = 0.27246   n = 955

> gpred <- predict(gmod)
```

interp(x, y, z) interpolates between three vectors of equal length such that they can e.g. be plotted by surface plot `contour()` (**Figure 68**)

```
> ip <- interp(log(mat$TP), log(mat$MD), gpred, duplicate="mean")
> x11(5,5)
> contour(ip, xlab="TP", ylab="Mean Depth", nlevels=15)
```

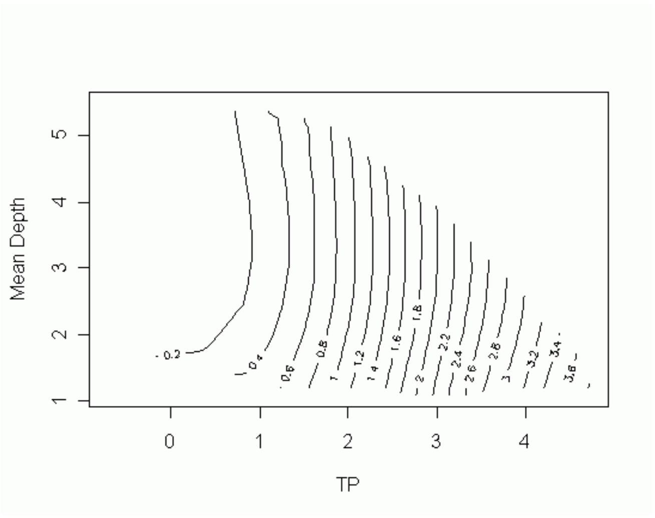


Figure 68. 3-dimentional interpolation of the data shown in **Figure 67**, showing the third variable (here chl-a) as contour lines (function contour()).

```
> x11(5,5)
> filled.contour(ip, xlab="TP", ylab="Mean Depth",
+ plot.axes={axis(1);axis(2);points(log(mat$TP), log(mat$MD), col="grey")}) ## [not
shown]
```

Filled contour doesn't accept the `log()` function; we have to define desired axis-ticks manually

```
> xtick<-log(c(0.5, 1:10, seq(10, 100, 10)))
> ytick<-log(c(3:10, seq(20, 100, 20), 150, 200))
> x11(5,5)
> filled.contour(ip, xlab="TP", ylab="Mean Depth", color.palette=rainbow,
+ plot.axes={axis(1, at=xtick, labels=exp(xtick));
+ axis(2, at=ytick, labels=exp(ytick));points(log(mat$TP), log(mat$MD),
col="grey")})
```

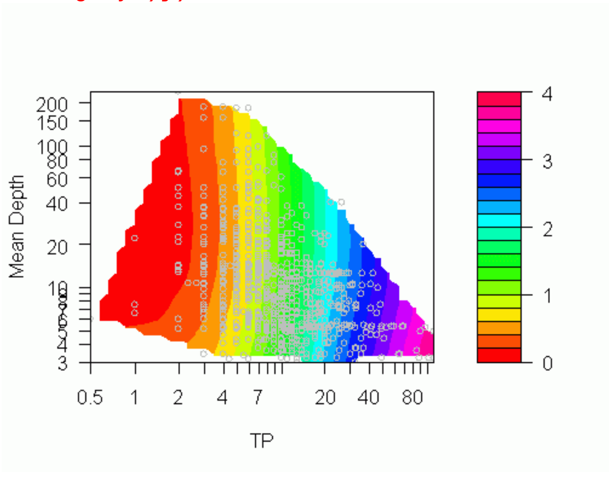


Figure 69. Example for the `filled.contour()` function.

Wonderful colors (**Figure 69**)...
Overlay of datapoints:

```
> require(MASS)
[1] TRUE
> x11(5,5)
> plot(Chlorophyll.a~TotP, log="xy", data=Nstati)
```

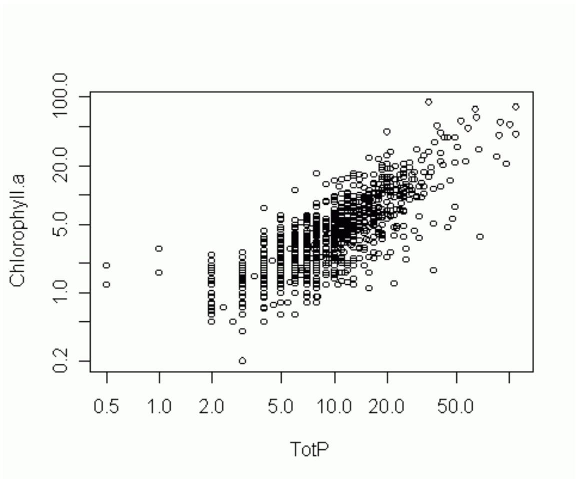


Figure 70. A scatterplot can be difficult to read when too many dots are plotted together.

Overlay of datapoints - high density blurrs trends in data (**Figure 70**)
-> 2-dim density estimation (**Figure 71**).

```
> ip<-kde2d(log(Nstati$TotP), log(Nstati$Chlorophyll.a))
> x11(5,5)
> filled.contour(ip)  # [not shown]
> xtick<-log(c(0.5, 1:10, seq(10, 100, 10)))
> ytick<-log(c(0.5, 1:10, seq(20, 100, 20), 150, 200))
> filled.contour(ip, plot.axes={axis(1, at=xtick, labels=exp(xtick));
+ axis(2, at=ytick, labels=exp(ytick))})
```

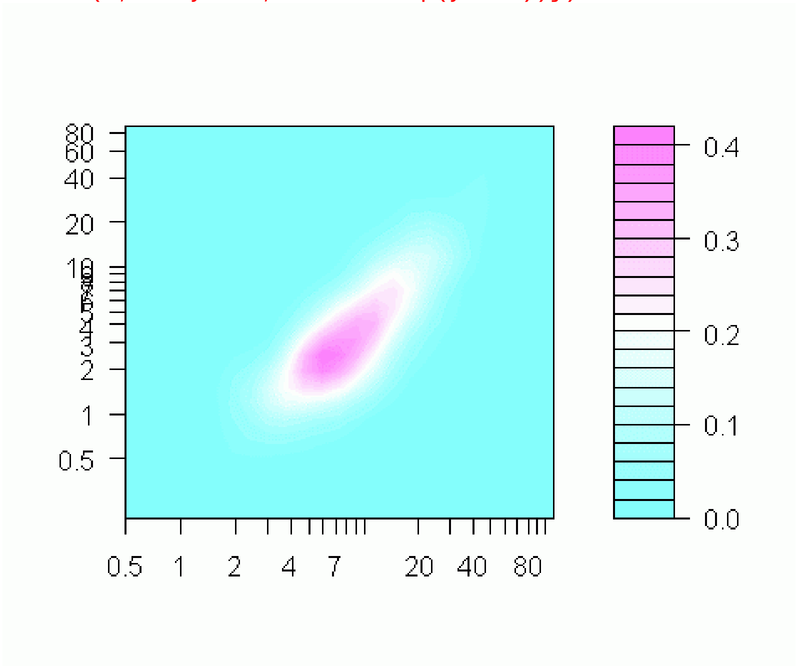


Figure 71. 2-dim density estimation of the data shown in **Figure 70**.

Compare **Figure 71** with scatterplot (**Figure 69**) – density plot shows better where data centers.

5.2 Lattice

What mean 'lattice' and 'trellis' in R...

```
Trellis Graphics is a framework for data visualization developed
at the Bell Labs by Rick Becker, Bill Cleveland et al, extending
ideas presented in Bill Cleveland's 1993 book _Visualizing Data_.

Lattice is best thought of as an implementation of Trellis
Graphics for R.

(from the R help menue - '?lattice')
```

.. and elsewhere?

"**Lattice** is suitable for **trellis** or as decorative sections in fences, handrails, arbors, pergolas, garden or deck privacy screens, windbreaks etc. ..."

So it is some kind of geometric arrangement of data? read further...

```
> require(lattice)
[1] TRUE
```

Simple density estimation (**Figure 72**):

```
> x11(5,5)
> plot(density(log10(Nstati$Chlorophyll.a)))
```

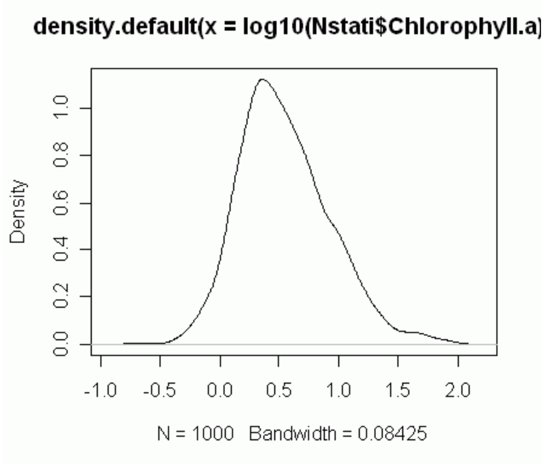


Figure 72. A density plot, indicating the number of observations along a gradient

In lattice, we can split by any factor, e.g. country (**Figure 73**):

```
> x11(5,5)
> densityplot(log10(Nstati$Chlorophyll.a), groups=Nstati$country_code, auto.key=T)
```

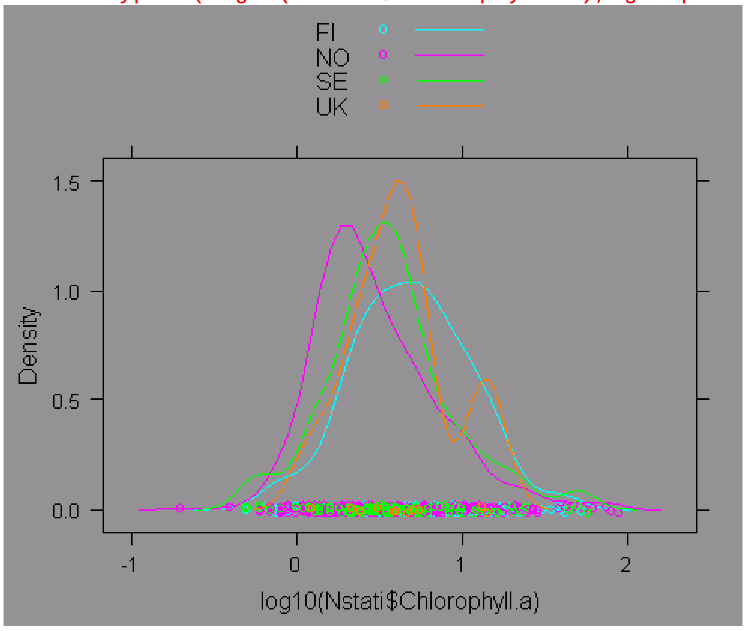


Figure 73. Implementation of the density function in the `lattice` package. The data are split by countries.

```
> x11(5,5)
> boxplot(log10(Chlorophyll.a)~country_code, data=Nstati) # standard boxplot, not
shown
> x11(5,5)
> bwplot(log10(Chlorophyll.a)~country_code, data=Nstati)  # lattice version...
> x11(5,5)
> bwplot(log10(Chlorophyll.a)~country_code|GIG_type, data=Nstati) # ...allows split
by factors (Figure 74).
```

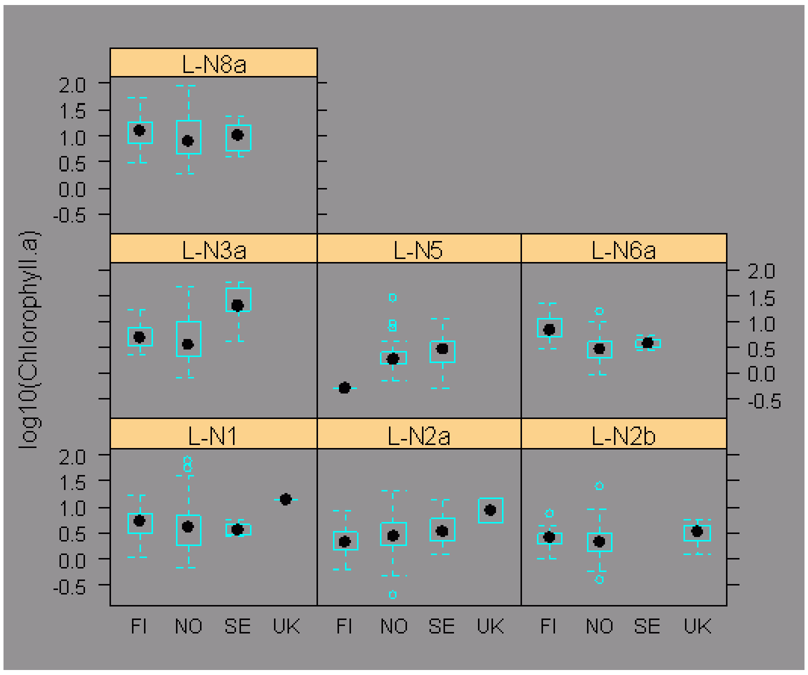


Figure 74. A boxplot produced with the `lattice` command `bwplot`.

Ordinary scatterplot (**Figure 75**):

```
> x11(5,5)
> plot(Chlorophyll.a~TotP, log="xy", data=Nstati, pch=as.numeric(country_code))
```

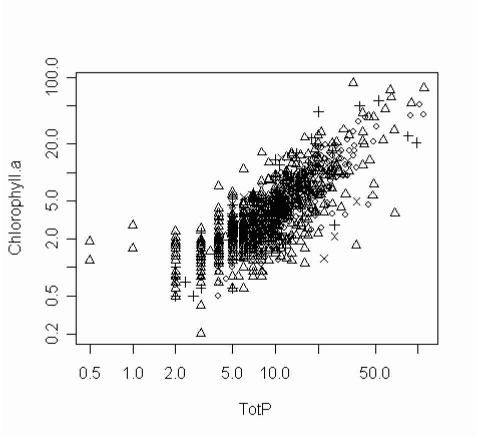


Figure 75. Standard scatterplot

Countries are not really separated; try lattice scatterplot `xyplot()` (**Figure 76**):

```
> x11(5,5)
> xyplot(log10(Chlorophyll.a)~log(TotP), groups=country_code, data=Nstati,
auto.key=T)
```

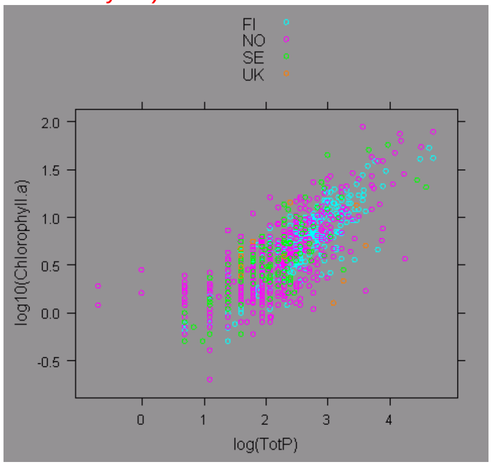


Figure 76. `xyplot` produces scatterplots (and others, see `?xyplot`). Countries are grouped by a color-code.

Split by country (**Figure 77**):

```
> x11(5,5)
> xyplot(log10(Chlorophyll.a)~log(TotP)|country_code, data=Nstati)
```

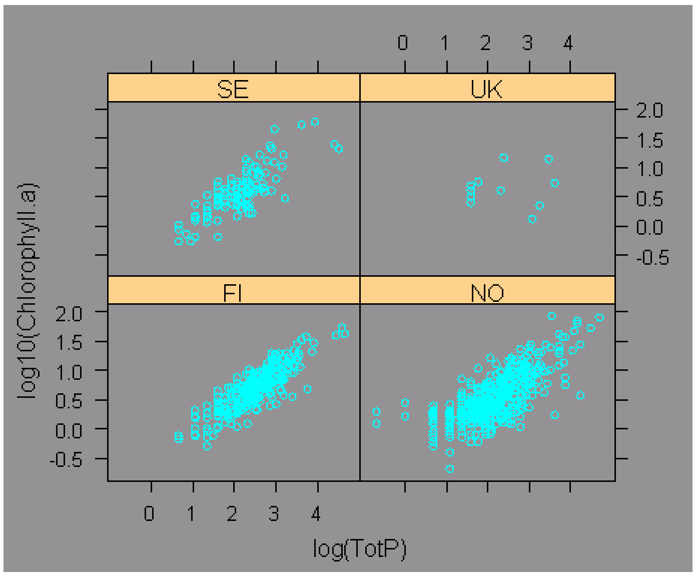


Figure 77. `xyplot`. Data split by countries into sub-panels.

Split by lake types (**Figure 78**):

```
> xyplot(log10(Chlorophyll.a)~log(TotP)|GIG_type, groups=country_code, data=Nstati,
auto.key=T)
```

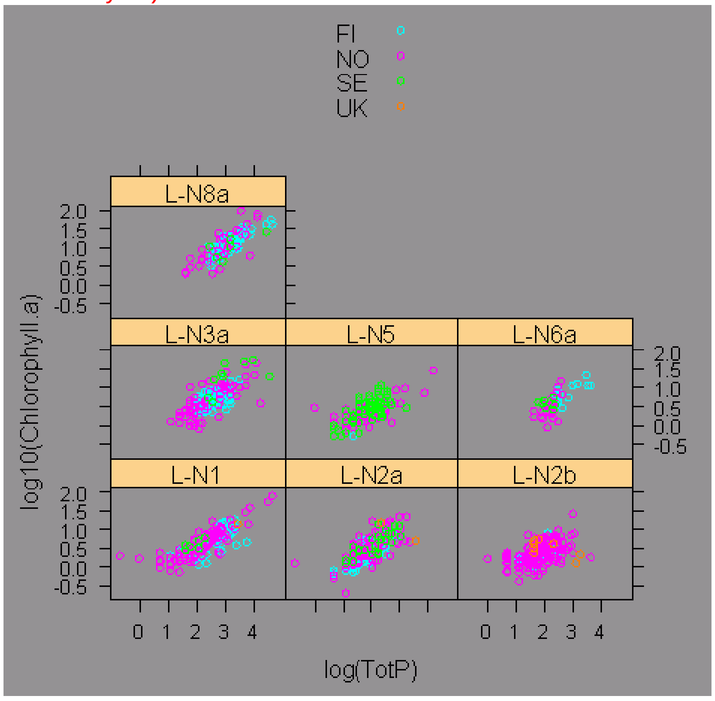


Figure 78. `xyplot`. Combining split-and group function.

Illustrate y against two or more x variables (makes sense only if they have same unit; **Figure 79**):

```
> xyplot(log10(Chlorophyll.a)~log10(TotN)+log10(TotP)|country_code, data=Nstati,
auto.key=T)
```

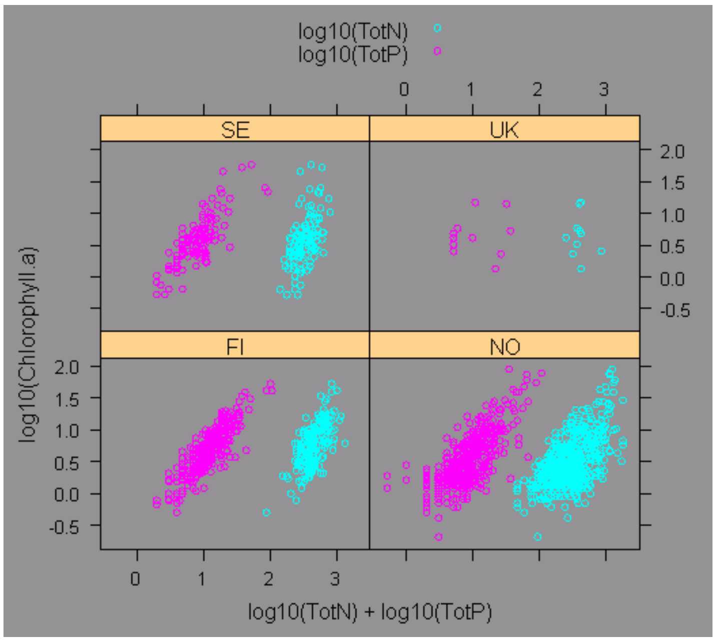


Figure 79. `xyplot`. Two or more variables can be plotted together using a function argument in the command.

Visualize aggregated information of the Nstati table (**Figure 80**). Make an aggregated table first.
'x' in `aggregate(x, list(y), func)` will be aggregated by function `func()`.

```
> agg.Nstati<-aggregate(Nstati$TotP>0, list(country=Nstati$country_code,
+  GIG_type=Nstati$GIG_type), sum)
> x11(5,5)
> barchart(x~GIG_type|country, data=agg.Nstati, ylab="nr. of lakes")
```

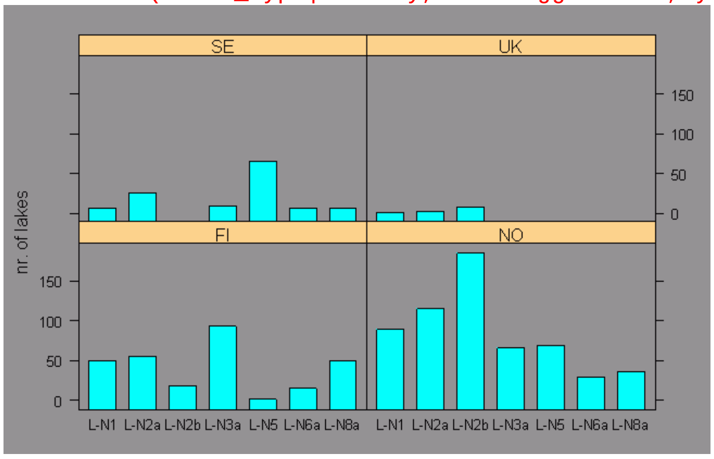


Figure 80. Example of a `barchart` plot.

```
> x11(5,5)
> dotplot(GIG_type~x|country, data=agg.Nstati, xlab="nr. of lakes")
```

See Figure 81.

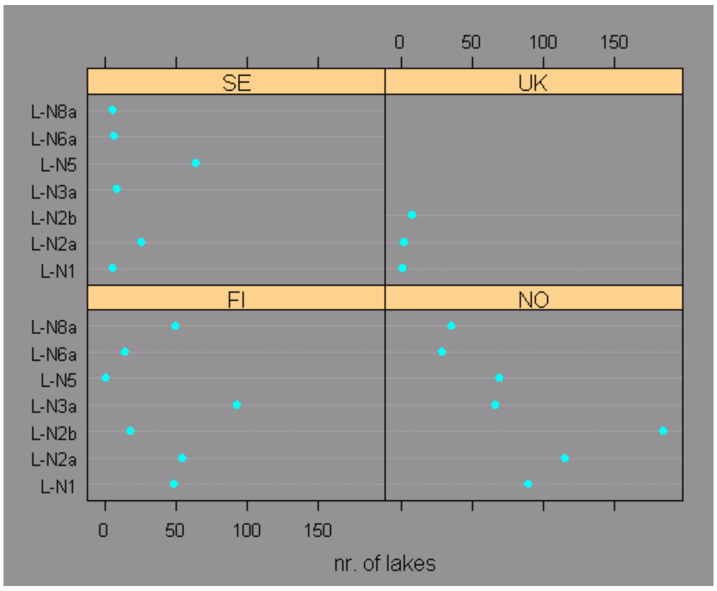


Figure 81. The `dotplot` function.

```
> #################
> # T H E   E N D #
> #################
```

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