

# Using R for scientific computing - ANSWERS

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## Abstract

The answers to the exercises from the document:  
"Using R for scientific computing" (Soetaert 2008).

*Keywords:* scientific computing, lecture notes, R.

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This document gives the answers to the exercises in the lecture notes:

"Using R for scientific computing" (Soetaert 2008).

These notes are an introduction to R - at beginners level. They can be found in package `marelacTeaching`.

In R, write:

```
require(marelacTeaching)

browseURL(paste(system.file(package="marelacTeaching"),
                      "/lecture/R_for_scientific_computing.pdf", sep=""))
```

In order to make this vignette more readable, the questions are repeated.

## Chapter 1

No exercises in this chapter

## Chapter 2 - R as a scientific calculator

```
> (4/6*8-1)^(2/3)
```

```
[1] 2.657958
```

```
> log(20)
```

```
[1] 2.995732
```

```
> log2(4096)
```

```
[1] 12
```

```
> 2*pi*3
```

```
[1] 18.84956
```

```
> exp(2+cos(0.5*pi))
```

```
[1] 7.389056
```

```
> # length of 3rd side of a triangle with size 2.3 and 5.4 and angle pi/8
```

```
> sqrt(2.3^2+5.4^2-2*2.3*5.4*cos(pi/8))
```

```
[1] 3.391288
```

## Chapter 3 - computing with R-variables

### Chapter 3.8.1

Use R-function `mean` to estimate the mean of two numbers, 9 and 17.

```
> mean(c(9,17))
```

```
[1] 13
```

- Create a vector, called V, with even numbers, between 16 and 56. Do not use loops.
- Display this vector
- What is the sum of all elements of V?
- Display the first 4 elements of V
- Calculate the product of the first 4 elements of V
- Display the 4th, 9th and 11th element of V.

```
> (V<-seq(16,56,by=2)) # creates AND displays the vector
```

```
[1] 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 56
```

```
> # or:
```

```
> V <- 16+2*(0:20) ; V
```

```
[1] 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 56
```

```
> sum(V)
```

```
[1] 756
```

```
> V[1:4]
```

```
[1] 16 18 20 22
```

```
> prod(V[1:4])
```

```
[1] 126720
```

```
> V[c(4,9,11)]
```

```
[1] 22 32 36
```

- Create a new vector, W, which equals vector V, multiplied with 3; display its content.
- How many elements of W are smaller than 100?

```
> W<-V*3; W
```

```
[1] 48 54 60 66 72 78 84 90 96 102 108 114 120 126 132 138
[17] 144 150 156 162 168
```

```
> W100<-W[W<100] ; length(W100)
```

```
[1] 9
```

```
> # or
```

```
> length(W[W<100])
```

```
[1] 9
```

- Create a sequence that contains the values  $(1, 1/2, 1/3, 1/4, \dots, 1/10)$
- Compute the square root of each element
- Compute the square ( $^2$ ) of each element
- Create a sequence with values  $(0/1, 1/2, 2/3, 3/4, \dots, 9/10)$

```
> 1/1:10
```

```
[1] 1.0000000 0.5000000 0.3333333 0.2500000 0.2000000 0.1666667
[7] 0.1428571 0.1250000 0.1111111 0.1000000
```

```
> sqrt(1/1:10)
```

```
[1] 1.0000000 0.7071068 0.5773503 0.5000000 0.4472136 0.4082483
[7] 0.3779645 0.3535534 0.3333333 0.3162278
```

```
> (1/1:10)^2
```

```
[1] 1.0000000 0.2500000 0.1111111 0.0625000 0.0400000 0.0277778
[7] 0.02040816 0.0156250 0.01234568 0.0100000
```

```
> (0:9)/(1:10) # or : 0:9/1:10
```

```
[1] 0.0000000 0.5000000 0.6666667 0.7500000 0.8000000 0.8333333
[7] 0.8571429 0.8750000 0.8888889 0.9000000
```

- Create a vector, U, with 100 random numbers, uniformly distributed between -1 and 1.
- Check the range of U; all values should be within -1 and +1.
- Calculate the sum and the product of the elements of U

- How many elements of U are positive?
- Zero all negative values of U.
- Sort U

```
> U <- runif(100,-1,1)
```

```
> range(U)
```

```
[1] -0.9909213  0.9981488
```

```
> sum(U);prod(U)
```

```
[1] -1.218657
```

```
[1] -3.635511e-44
```

```
> length(U[U>0]) # or: sum(U>0)
```

```
[1] 45
```

```
> U[U<0]<-0
```

```
> sort(U)
```

```
[1] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[6] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[11] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[16] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[21] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[26] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[31] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[36] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[41] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[46] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[51] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
[56] 0.02002284 0.04680128 0.05658268 0.11447748 0.11504252
[61] 0.12098049 0.14000587 0.18786472 0.22908129 0.23707964
[66] 0.24404824 0.30910054 0.31237476 0.31647013 0.33722174
[71] 0.39392254 0.39974569 0.44940482 0.48537543 0.50541993
[76] 0.52296326 0.53457159 0.54495527 0.55040841 0.55899920
[81] 0.64158473 0.64706668 0.65104068 0.68341035 0.68511634
[86] 0.76826868 0.78846543 0.79360768 0.79519795 0.79875607
[91] 0.80443442 0.81352619 0.82645501 0.83950564 0.86250425
[96] 0.86841329 0.87070953 0.91567579 0.97224491 0.99814884
```

- Create two vectors: vector x, with the elements: 2,9,0,2,7,4,0 and vector y with the elements 3,5,0,2,5,4,6 (in that order).

- Divide all the elements of y by the elements of x.
- Select all values of y that are larger than the corresponding values of x
- Select all values of y for which the corresponding values of x are 0.
- Remove all values of y for which the corresponding values of x equal 0.
- Zero all elements of x that are larger or equal than 7. Show x.

```
> x<- c(2,9,0,2,7,4,0)
> y<- c(3,5,0,2,5,4,6)
> y/x
```

```
[1] 1.5000000 0.5555556      NaN 1.0000000 0.7142857 1.0000000
[7]          Inf
```

```
> x>y
```

```
[1] FALSE TRUE FALSE FALSE TRUE FALSE FALSE
```

```
> x==0
```

```
[1] FALSE FALSE TRUE FALSE FALSE FALSE TRUE
```

```
> y[y>x]
```

```
[1] 3 6
```

```
> y[x==0]
```

```
[1] 0 6
```

```
> y<-y[x!=0]
```

```
> x[x>=7]<-0 ; x
```

```
[1] 2 0 0 2 0 4 0
```

### Chapter 3.8.2

- Use R-function "matrix" to create a matrix with the following contents:

$$\begin{bmatrix} 3 & 9 \\ 7 & 4 \end{bmatrix}$$

- display it to the screen

- Use R-function "matrix" to create a matrix called "A":

$$\begin{bmatrix} 3 & 9 \\ 7 & 4 \end{bmatrix}$$

- Take the transpose of A.
- Create a new matrix, B, by extracting the first two rows and first two columns of A. Display it to the screen.

```
> A<-matrix(nrow=2,data=c(3,7,9,4)) ; A
```

```
      [,1] [,2]
[1,]    3    9
[2,]    7    4
```

```
> A<-matrix(nrow=3,data=1/1:9,byrow=TRUE) # or: 1/matrix(nrow=3,data=1:9,byrow=TRUE)
> t(A)
```

```
      [,1] [,2] [,3]
[1,] 1.000000 0.250000 0.1428571
[2,] 0.500000 0.200000 0.1250000
[3,] 0.3333333 0.1666667 0.1111111
```

```
> B <- A[1:2,1:2] ; B
```

```
      [,1] [,2]
[1,] 1.00 0.5
[2,] 0.25 0.2
```

Matrix D

- Use `diag` to create the following matrix, called "D":

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

- Use `cbind` and `rbind` to augment this matrix, such that you obtain:

$$\begin{bmatrix} 1 & 0 & 0 & 4 \\ 0 & 2 & 0 & 4 \\ 0 & 0 & 3 & 4 \\ 5 & 5 & 5 & 5 \end{bmatrix}$$

- Remove the second row and second column of the previous matrix

```
> D <- diag(nrow=3,c(1,2,3))
> DD <- cbind(D,rep(4,3)) # or: cbind(D,4)
> DDD <- rbind(DD,rep(5,4)) # or: rbind(DD,5)
> DDD
```

```
      [,1] [,2] [,3] [,4]
[1,]    1    0    0    4
[2,]    0    2    0    4
[3,]    0    0    3    4
[4,]    5    5    5    5
```

```
> # same, in one sentence
> DD <- rbind(cbind(D,4),5)
> DD[-2,-2]
```

```
      [,1] [,2] [,3]
[1,]    1    0    4
[2,]    0    3    4
[3,]    5    5    5
```

### Chapter 3.8.3 - nematode diversity

- Select the data from station M160b (the 2nd column of Nemaspec); put these data in a vector called "dens".
- Remove from vector dens, the densities that are 0. Display this vector on the screen.
- Calculate N, the total nematode density of this station.
- Divide the values in vector dens by the total nematode density N. Put the results in vector p. The sum of all values in p should equal 1.
- Calculate S, the number of species.
- Estimate the values of diversity indices N1 and N2 and Ni, given by the following formulae:

$$N1 = e^{\sum -p_i \cdot \log_e(p_i)}$$

$$N2 = 1 / (\sum p_i^2)$$

$$Ni = 1 / \max(p_i)$$

- The expected number of species in a sample with size n, drawn from a population which size N, which has S species is given by:

$$ES(n) = \sum_{i=1}^S \left[ 1 - \frac{\binom{N-N_i}{n}}{\binom{N}{n}} \right]$$

What is the expected number of species per 100 individuals ?



- Print all diversity indices to the screen, which should look like:

```
> head(Nemaspec)
```

```

          SPECIES M160a  M160b  M280a  M280b  M530a
1      Acantholaimus    0 6.580261 0.000000 1.120782 1.315487
2 Acantholaimus elegans    0 0.000000 1.439706 0.000000 3.956836
3 Acantholaimus iubilus    0 0.000000 0.000000 0.000000 0.000000
4      Acantholaimus M1    0 5.919719 0.000000 3.628518 0.000000
5      Acantholaimus M10    0 0.000000 0.000000 1.120782 0.000000
6      Acantholaimus M11    0 0.000000 0.000000 0.000000 0.000000
      M530b  M820a  M820b  M990a  M990b  M1220a  M1220b
1 1.727387 3.417313 3.748096 2.447545 3.728838 4.369345 4.787512
2 0.000000 0.000000 2.198407 5.080900 5.330997 3.644567 3.494481
3 1.193131 0.000000 0.000000 1.270450 1.372789 0.000000 0.000000
4 1.193131 1.155307 0.000000 5.052036 6.225598 0.000000 1.166825
5 0.000000 0.000000 0.000000 0.000000 0.000000 1.115981 0.000000
6 0.000000 0.000000 0.000000 0.000000 2.285694 0.000000 0.000000

```

```
> dens <- Nemaspec[,2]
```

```
> dens <- dens[dens>0]
```

```
> N <- sum(dens);
```

```
> p <- dens/N
```

```
> N0 <- length(p)
```

```
> N1 <- exp(sum(-p*log(p)))
```

```
> N2 <- sum(p*p)^(-1)
```

```
> Ni <- 1/max(p)
```

```
> ESS <- N0-1/choose(N,100)*sum(choose(n=(N-dens),k=100))
```

```
> c(N=N,N0=N0,N1=N1,N2=N2,Ni=Ni,ESS=ESS)
```

```

          N          N0          N1          N2          Ni          ESS
576.000000 97.000000 27.782793 8.364525 3.162870 40.502318

```

## Chapter 4 user-defined functions

### Chapter 4.4.1

```
> Sphere <- function(radius)
+ {
+   vol   <- 4/3*pi*radius^3
+   surf  <- 4 *pi*radius^2
+   circ  <- 2*pi*radius
+   return(list(volume=vol,surface=surf,circumference=circ))
+ }
> Sphere(6371)
```

```
$volume
[1] 1.083207e+12
```

```
$surface
[1] 510064472
```

```
$circumference
[1] 40030.17
```

### Chapter 4.4.2

The saturated oxygen concentration in water ( $\text{mol kg}^{-1}$ ), as function of temperature (T), and salinity (S) can be calculated by:  $SatOx = e^A$  where :  $A = -173.9894 + 25559.07/T + 146.4813 * \log(T/100) - 22.204 * T/100 + S * (-0.037362 + 0.016504 * T/100 - 0.0020564 * T/100 * T/100)$  and T is temperature in Kelvin ( $T_{\text{kelvin}} = T_{\text{celsius}} + 273.15$ ).

- Make a function that implements this formula; the default values for temperature and salinity are  $20^\circ\text{C}$  and 35 respectively.
- What is the saturated oxygen concentration at the default conditions?
- Estimate the saturated oxygen concentration for a range of temperatures from 0 to  $30^\circ\text{C}$ , and salinity 35.

```
> SatOx <- function(T=20,S=35)
+ {
+   T <- T+273.15
+   A = -173.9894 + 25559.07/T + 146.4813* log(T/100) -22.204*T/100 + S *
+       (-0.037362+0.016504*T/100-0.0020564 *T/100*T/100)
+   exp(A)
+ }
> SatOx()
```

```
[1] 225.2346
```

```
> SatOx(0:30)
```

```
[1] 349.6542 340.6019 331.9557 323.6924 315.7901 308.2286 300.9890
[8] 294.0533 287.4051 281.0288 274.9098 269.0344 263.3897 257.9638
[15] 252.7452 247.7235 242.8884 238.2306 233.7412 229.4118 225.2346
[22] 221.2020 217.3070 213.5431 209.9038 206.3833 202.9759 199.6764
[29] 196.4796 193.3808 190.3755
```

### Chapter 4.4.3

The Fibonacci numbers are calculated by the following relation:  $F_n = F_{n-1} + F_{n-2}$  With  $F_1 = F_2 = 1$

- Compute the first 50 Fibonacci numbers; store the results in a vector.
- For large n, the ratio  $F_n/F_{n-1}$  approaches the "golden mean"
- What is the value of  $F_{50}/F_{49}$ ; is it equal to the golden mean?
- When is n large enough? (i.e. sufficiently close ( $<1e-6$ ) to the golden mean)

```
> Fibo<-vector()
> Fibo[1:2]<-1
> for (i in 3:50) Fibo[i]<-Fibo[i-1]+Fibo[i-2]
> (1+sqrt(5))/2
```

```
[1] 1.618034
```

```
> Fibo[50]/Fibo[49]
```

```
[1] 1.618034
```

```
> Fibo[2:50]/Fibo[1:49] - (1+sqrt(5))/2
```

```
[1] -6.180340e-01  3.819660e-01 -1.180340e-01  4.863268e-02
[5] -1.803399e-02  6.966011e-03 -2.649373e-03  1.013630e-03
[9] -3.869299e-04  1.478294e-04 -5.646066e-05  2.156681e-05
[13] -8.237677e-06  3.146529e-06 -1.201865e-06  4.590718e-07
[17] -1.753498e-07  6.697766e-08 -2.558319e-08  9.771908e-09
[21] -3.732537e-09  1.425702e-09 -5.445699e-10  2.080072e-10
[25] -7.945178e-11  3.034772e-11 -1.159184e-11  4.427569e-12
[29] -1.691314e-12  6.459278e-13 -2.466916e-13  9.414691e-14
[33] -3.597123e-14  1.376677e-14 -5.329071e-15  1.998401e-15
[37] -8.881784e-16  2.220446e-16 -2.220446e-16  0.000000e+00
[41]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[45]  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
[49]  0.000000e+00
```

### Chapter 4.4.5 - nematode diversity all stations

- Make a function that will calculate the diversity indices for any data matrix.

- Calculate and show diversity on species level

```

> Diversity <- function (Dens, # density, each column a station
+                          S=100) # common number of individuals on which
+                               # to estimate expected number of species
+ {
+
+   nstat <- NCOL(Dens) # number of stations
+   if(is.vector(Dens)) Dens <- matrix(ncol=nstat,Dens)
+   div <- matrix(nrow=nstat,ncol=6,data=NA) # create matrix for results
+   rownames(div) <- colnames(Dens)
+   colnames(div) <- c("N","NO","N1","N2","Ninf",paste("ESS",S,sep=""))
+
+   for (i in 1:nstat)
+   {
+     dens<- Dens[,i]
+     dens<- dens[dens>0] # selection of species present
+     N <- sum(dens) # N, total density
+     p <- dens/N # relative proportion
+     NO <- length(p) # NO = number of species present
+     N1 <- exp(sum(-p*log(p))) # N1 = exp(Shannon-Wiener)
+     N2 <- sum(p*p)^(-1) # Na = sum(sp^a)^(1/(1-a))
+     Ni <- 1/max(p) # Ninf
+     ESS <- NO-1/choose(N,S)*sum(choose(n=(N-dens),k=S))
+     div[i,] <- c(N,NO,N1,N2,Ni,ESS)
+   }
+   return(div)
+ }
> summary(Nemaspec) # calculate summary characteristics

```

	SPECIES	M160a	M160b
Acantholaimus	: 1	Min. : 0.000	Min. : 0.000
Acantholaimus elegans	: 1	1st Qu.: 0.000	1st Qu.: 0.000
Acantholaimus iubilus	: 1	Median : 0.000	Median : 0.000
Acantholaimus M1	: 1	Mean : 1.226	Mean : 1.487
Acantholaimus M10	: 1	3rd Qu.: 0.000	3rd Qu.: 1.341
Acantholaimus M11	: 1	Max. : 182.113	Max. : 30.982
(Other)	:464		
		M530a	M530b
Min. :	0.000	Min. : 0.000	Min. : 0.0000
1st Qu.:	0.000	1st Qu.: 0.000	1st Qu.: 0.0000
Median :	0.000	Median : 0.000	Median : 0.0000
Mean :	1.143	Mean : 0.849	Mean : 0.8553
3rd Qu.:	1.183	3rd Qu.: 0.000	3rd Qu.: 0.0000
Max. :	54.031	Max. : 45.938	Max. : 29.2128
		M820a	M820b
Min. :	0.000	Min. : 0.000	Min. : 0.0000
1st Qu.:	0.000	1st Qu.: 0.000	1st Qu.: 0.0000
Median :	0.000	Median : 0.000	Median : 0.0000
Mean :	1.143	Mean : 1.047	Mean : 0.8553
3rd Qu.:	1.183	3rd Qu.: 1.121	3rd Qu.: 0.0000
Max. :	54.031	Max. : 33.500	Max. : 29.2128
		M990a	

Min. : 0.0000	Min. : 0.0000	Min. : 0.0000
1st Qu.: 0.0000	1st Qu.: 0.0000	1st Qu.: 0.0000
Median : 0.0000	Median : 0.0000	Median : 0.0000
Mean : 0.9234	Mean : 0.9383	Mean : 0.9596
3rd Qu.: 0.0000	3rd Qu.: 0.0000	3rd Qu.: 1.1771
Max. : 78.3521	Max. : 38.0481	Max. : 47.8478

M990b	M1220a	M1220b
Min. : 0.000	Min. : 0.0000	Min. : 0.0000
1st Qu.: 0.000	1st Qu.: 0.0000	1st Qu.: 0.0000
Median : 0.000	Median : 0.0000	Median : 0.0000
Mean : 1.217	Mean : 0.7213	Mean : 0.7085
3rd Qu.: 1.213	3rd Qu.: 0.0000	3rd Qu.: 0.0000
Max. : 51.271	Max. : 37.5895	Max. : 25.6069

```
> # remove species names
> (divspec<-Diversity(Nemaspec[, -1]))
```

	N	NO	N1	N2	Ninf	ESS100
M160a	576	97	27.78279	8.364525	3.162870	40.50232
M160b	699	126	90.15358	66.778414	22.561569	60.68971
M280a	537	148	83.57356	43.779249	9.938717	59.44306
M280b	492	140	87.18598	51.988253	14.686371	61.17590
M530a	399	107	61.03511	29.166239	8.685560	54.97142
M530b	402	105	66.41245	44.308181	13.761081	54.25870
M820a	434	102	47.47238	20.190796	5.539098	48.29562
M820b	441	115	60.48626	33.178177	11.590593	52.14167
M990a	451	121	72.89122	40.725866	9.425726	57.11996
M990b	572	148	88.37314	47.535985	11.156321	61.16281
M1220a	339	106	65.53017	37.188517	9.018488	55.97925
M1220b	333	96	63.58659	41.009214	13.004317	54.90511

*Chapter 4.4.6 - rarefaction diversity* An alternative way of estimating the number of species per 100 individuals is by taking random 'subsamples' of 100 individuals and estimating the number of species from this subsample.

```
> dens <- Nemaspec[, 2]
> dens <- dens[dens>0] # selection of species present
> cs <- round(dens) # rarefaction method can only work with integer numbers
> ind <- NULL # individual organisms; each one belonging to a species
> for (i in 1:length(cs)) ind <- c(ind, rep(i, times=cs[i]))
> ind100 <- sample(ind, size=100) # take 100 random individuals
> Spec <- table(ind100) # table of counts: speciesnr versus nr ind
> ESS100 <- length(Spec) # length of Spec = number of species
> # or, three sentences combined in 1!
> length(table(sample(ind, size=100)))
```

```
[1] 45
```

```
> ESS100 <- vector()  
> for (i in 1:1000) ESS100[i] <- length(table(sample(ind,size=100)))  
> mean (ESS100)
```

```
[1] 40.831
```

## Chapter 5 - statistics

- Perform a hierarchic clustering of the Nemaspec dataset and plot the dendrogram
- Perform a principal component analysis (PCA) and plot the results
- repeat the PCA analysis, with the first two stations removed

```
> nemaspec <- Nemaspec[,-1]
> hc <- hclust(dist(t(nemaspec)), "ave")
> par(mfrow=c(2,2))
> plot(hc)
> plot(hc, hang = -1)
> x <- prcomp(t(nemaspec))
> biplot(x)
> x2 <- prcomp(t(nemaspec[-(1:2)]))
> biplot(x2)
> par(mfrow=c(1,1))
```

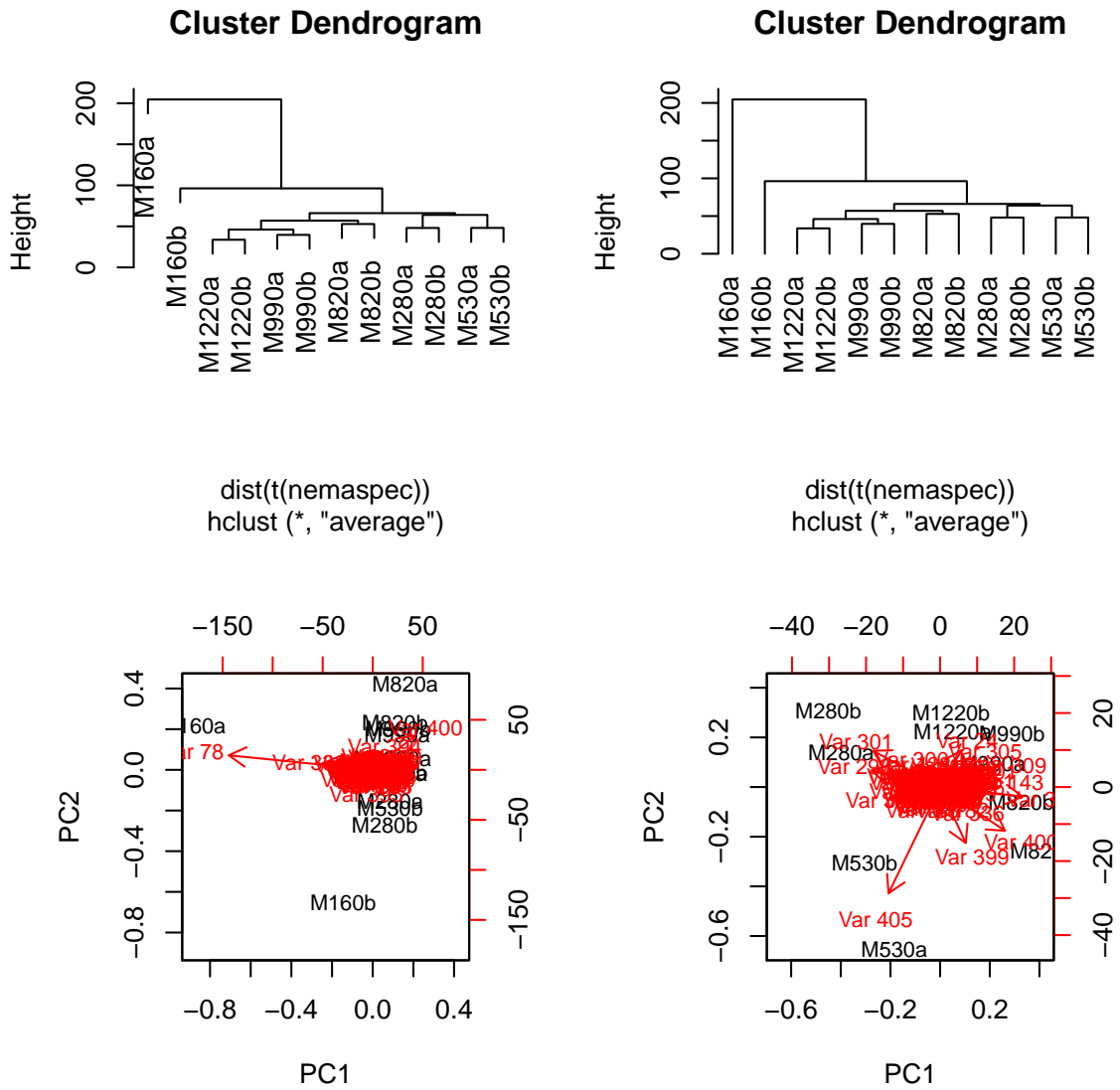


Figure 1: Cluster analysis and PCA of nematode data



## Chapter 6 - graphics

- Create a script file which draws a curve of the function  $y = x^3 \sin^2(3\pi x)$  in the interval  $[-2, 2]$ .
- Make a curve of the function  $y = 1/\cos(1 + x^2)$  in the interval  $[-5, 5]$ .
- The relative importance of ammonia

$$P_{[NH_3]} = \frac{K_N}{K_N + [H^+]}$$

- Plot the relative fraction of toxic ammonia to the total ammonia concentration as a function of pH, where  $\text{pH} = -\log_{10}([H^+])$  and for a temperature of  $30^\circ\text{C}$ . Use a range of pH from 4 to 9. The value of  $K_N$  is  $8 \cdot 10^{-10}$  at a temperature of  $30^\circ\text{C}$ .
- Add to this plot the relative fraction of ammonia at  $0^\circ\text{C}$ ; the value of  $K_N$  at that temperature is  $8 \cdot 10^{-11} \text{ mol kg}^{-1}$ .
- For the US, the population density in 1900 ( $N_0$ ) was 76.1 million; the population growth can be described as:

$$N(t) = \frac{K}{1 + \left[\frac{K - N_{t0}}{N_{t0}}\right] e^{-a \cdot (t - t_0)}}$$

$a = 0.02 \text{ yr}^{-1}$ ,  $K = 500$  million of people.

Actual population values are:

1900	1910	1920	1930	1940	1950	1960	1970	1980
76.1	92.4	106.5	123.1	132.6	152.3	180.7	204.9	226.5

- Plot the population density curve as a thick line, using the US parameter values.
- Add the measured population values as points. Finish the graph with titles, labels etc. . .

```
> par(mfrow=c(2,2))
> # simple curves
> curve(x^3*sin(3*pi*x)^2,-2,2)
> curve(1/cos(1+x^2),-5,5)
> # ammonia
> pN <- function(pH,Kn=8*10^-10) Kn/(Kn+10^-pH)
> curve(pN(x),4,9,main="fraction toxic ammonium")
> curve(pN(x,Kn=8*10^-11),4,9,add=TRUE,col="red")
> legend("topleft",lty=1,col=c("black","red"),c("30 dg","0 dg"))
> # US population
> K <- 500
> N0 <- 76.1
> a <- 0.02
> curve(K/(1+((K-N0)/N0*exp(-a*(x-1900))))),1900,1980,main="US population",
+       xlab="year",ylab="million",lwd=2)
> N <- matrix(ncol=2,data=c(
```

```
+ seq(1900,1980,by=10), 76.1,92.4,106.5,123.1,132.6,152.3,180.7,204.9,226.5
+
+ ) )
> points(N)
```

- Have a look at the `iris` data; What is the class and dimension of the data set?
- Produce a scatter plot of petal length against petal width
- Repeat the same graph, using different symbol colours for the three species.
- Create a box-and whisker plot for sepal length where the data values are split into species groups
- Now produce a similar box-and whisker plot for all four morphological measurements, arranged in two rows and two columns.

```
> head(iris)
```

```
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1          5.1          3.5          1.4          0.2  setosa
2          4.9          3.0          1.4          0.2  setosa
3          4.7          3.2          1.3          0.2  setosa
4          4.6          3.1          1.5          0.2  setosa
5          5.0          3.6          1.4          0.2  setosa
6          5.4          3.9          1.7          0.4  setosa
```

```
> class(iris)
```

```
[1] "data.frame"
```

```
> dim(iris)
```

```
[1] 150  5
```

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

```
> plot(iris$Petal.Length,iris$Petal.Width,cex=1.5,pch=15,
+       xlab="Petal length", ylab=" Petal width")
```

```
> plot(iris$Petal.Length,iris$Petal.Width,cex=1.5,pch=15,
+       xlab="Petal length", ylab=" Petal width",
+       col=c("red","blue","green")[iris$Species])
```

```
> legend("bottomright",pch=15,col=c("red","blue","green"),
+       legend=levels(iris$Species))
```

```
> boxplot(Petal.Width~Species,data=iris)
```

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

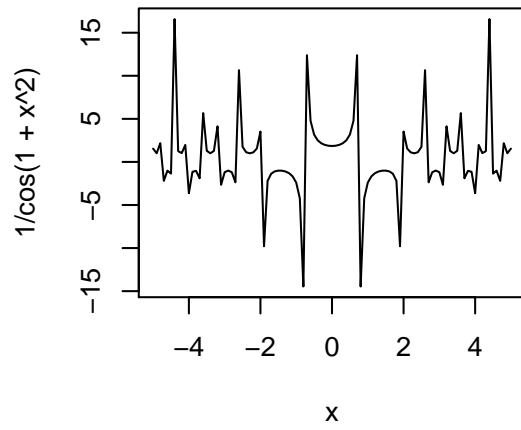
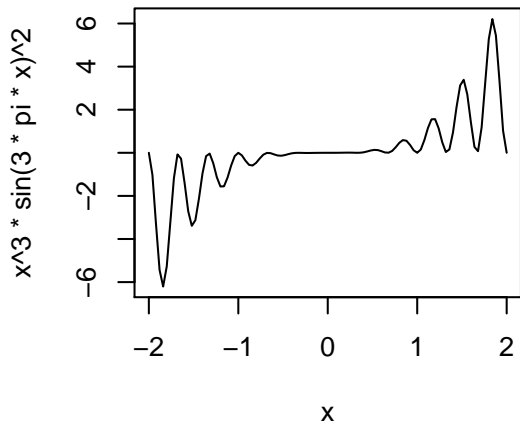
```
> boxplot(Sepal.Length~Species, data=iris,main="sepal length")
```

```
> boxplot(Sepal.Width~Species, data=iris,main="sepal width")
```

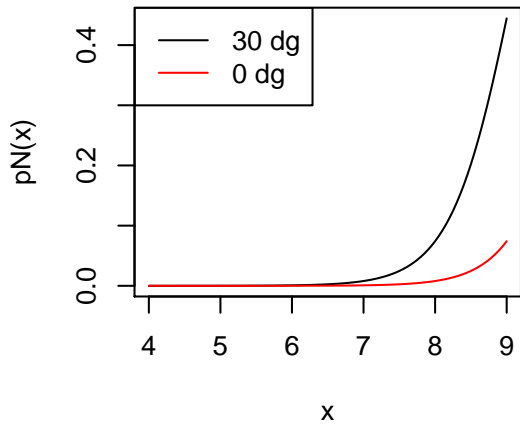
```
> boxplot(Petal.Length~Species, data=iris,main="petal length")
```

```
> boxplot(Petal.Width~Species, data=iris,main="petal width")
```

```
> mtext(outer=TRUE,side=3,line=-2,"Iris data set",cex=1.5)
```



**fraction toxic ammonium**



**US population**

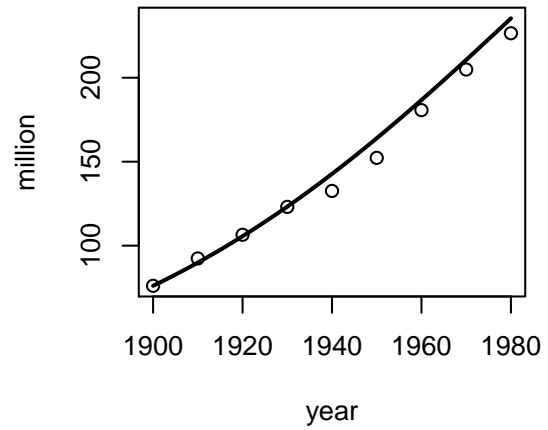


Figure 2: Use of R-function curve to plot simple functions

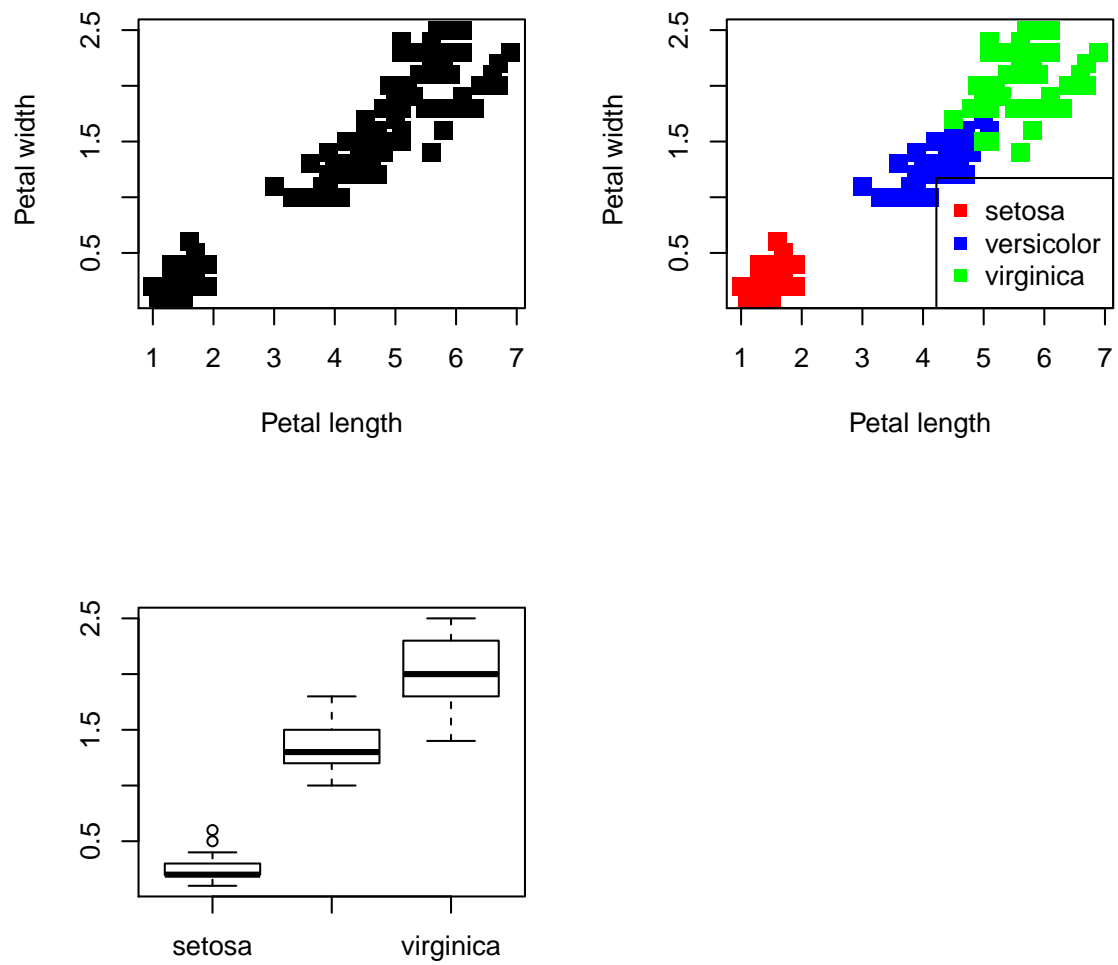


Figure 3: The iris data set

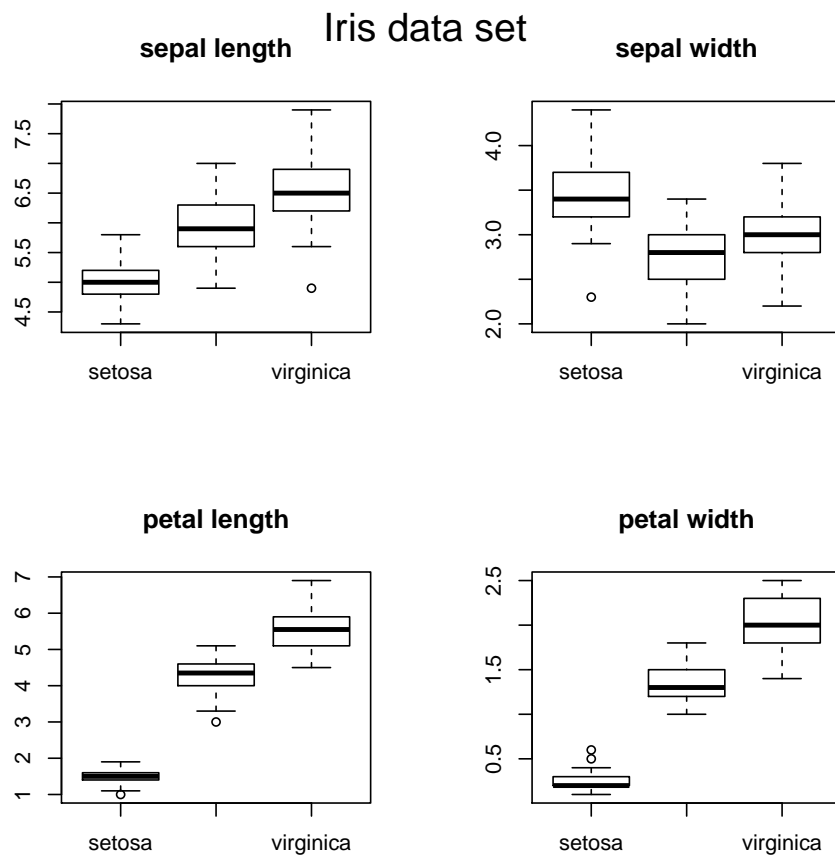


Figure 4: The iris data set

## Chapter 7 - matrix algebra

### Chapter 7.1.1

- Create matrices called "A" and "B":

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 6 & 4 & 1 \\ -2 & 1 & -1 \end{bmatrix}$$

$$B = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix}$$

- Take the inverse of A and the transpose of A.
- Multiply A with B.
- Estimate the eigenvalues and eigenvectors of A.
- For a matrix A, x is an eigenvector, and  $\mu$  the eigenvalue of a matrix A, if  $Ax = \mu x$ . Test it!

```
> A <- matrix(nrow=3, data=c(1,6,-2,2,4,1,3,1,-1))
> B <- matrix(nrow=3, data=1:9)
> solve(A); t(A)
```

```
      [,1]      [,2]      [,3]
[1,] -0.1111111  0.1111111 -0.2222222
[2,]  0.08888889 0.1111111  0.3777778
[3,]  0.31111111 -0.1111111 -0.1777778
```

```
      [,1] [,2] [,3]
[1,]    1    6   -2
[2,]    2    4    1
[3,]    3    1   -1
```

```
> A%*%B
```

```
      [,1] [,2] [,3]
[1,]   14   32   50
[2,]   17   50   83
[3,]   -3   -9  -15
```

```
> eigen(A)
```

```
$values
```

```
[1]  6.366696+0.000000i -1.183348+2.380697i -1.183348-2.380697i
```

```

$eigen
      [,1]      [,2]      [,3]
[1,] -0.36275602+0i -0.0725936-0.5240033i -0.0725936+0.5240033i
[2,] -0.93146469+0i -0.2632991+0.4856291i -0.2632991-0.4856291i
[3,] -0.02795726+0i  0.6441961+0.0000000i  0.6441961+0.0000000i

> ee<-eigen(A)
> A%%ee$eigen[,1]

      [,1]
[1,] -2.3095572+0i
[2,] -5.9303521+0i
[3,] -0.1779954+0i

> ee$values[1]*ee$eigen[,1]

[1] -2.3095572+0i -5.9303521+0i -0.1779954+0i

```

### Chapter 7.1.2 killer whale model

- Create a matrix, called P:

$$\begin{bmatrix}
 0 & 0.0043 & 0.1132 & 0 \\
 0.9775 & 0.9111 & 0 & 0 \\
 0 & 0.0736 & 0.9534 & 0 \\
 0 & 0 & 0.0452 & 0.9804
 \end{bmatrix}$$

- What is the value of the largest eigenvalue (the so-called dominant eigenvalue) and the corresponding eigenvector?.
- Create a new matrix, T, which equals P, except for the first row, where the elements are 0.
- Now estimate  $N = (I - T)^{-1}$ , where I is the identity matrix.

```

> A<- matrix (nrow=4,data=c(0,      0.9775,0,      0,
+                          0.0043,0.9111,0.0736,0,
+                          0.1132,0,      0.9534,0.0452,
+                          0,0,0,0.9804))
> eigen(A)

```

```

$values
[1] 1.025441326 0.980400000 0.834222976 0.004835698

```

```

$eigen
      [,1] [,2]      [,3]      [,4]
[1,] 0.06634512  0 -0.0659050  0.678780909
[2,] 0.56718211  0  0.8379894 -0.732135578
[3,] 0.57945357  0 -0.5175160  0.056807091
[4,] 0.58149491  1  0.1600233 -0.002631995

```

```

> T <- A
> T[1,] <- 0
> N <- solve(diag(4)-T) ; N

      [,1] [,2] [,3] [,4]
[1,] 1.00000 0.00000 0.00000 0.00000
[2,] 10.99550 11.24859 0.00000 0.00000
[3,] 17.36628 17.76602 21.45923 0.00000
[4,] 40.04878 40.97062 49.48761 51.02041

```

### *Chapter 7.1.3. System of equations*

Solve the following system of linear equations for the unknown xi:

$$3x_1 + 4x_2 + 5x_3 = 0$$

$$6x_1 + 2x_2 + 7x_3 = 5$$

$$7x_1 + x_2 = 6$$

Check the results

```

> A <- matrix(nrow=3,data=c(3,6,7,4,2,1,5,7,0))
> B <- c(0,5,6)
> x <- solve(A,B)
> A %*% x - B

```

```

      [,1]
[1,] 2.498002e-16
[2,] 0.000000e+00
[3,] 0.000000e+00

```



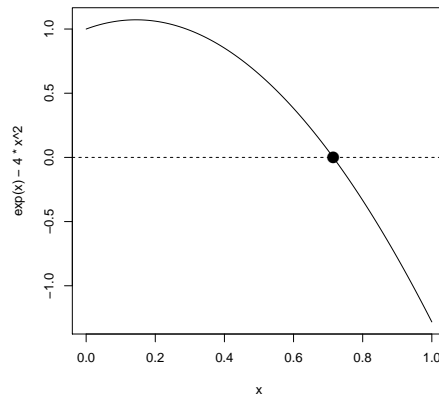


Figure 5: The root of a simple function

## Chapter 8 - roots of functions

### Chapter 8.3.1 simple root of equations

- Find the root of the equation  $e^x = 4x^2$  in the interval  $[0,1]$ . First draw the function curve.
- Solve the equation  $1000 = y * (3 + x) * (1 + y)^4$  for  $y$  and with  $x$  varying over the range from 1 to 100. Plot the root as a function of  $x$ .

```
> root<-uniroot(f=function(x) exp(x)-4*x^2,interval=c(0,1))

> curve(exp(x)-4*x^2,0,1)
> abline(h=0,lty=2)
> points(root$root,0,pch=16,cex=2)

> res<-vector()
> for (x in 1:100)
+ res[x]<-uniroot (f=function(y) y*(3+x)*(1+y)^4-1000,c(-1000,1000))$root

> plot(1:100,res)
```

### Chapter 8.3.2. $pCO_2$ rises increase acidity

- Estimate the pH at equilibrium with alkalinity  $2300 \text{ mol kg}^{-1}$  and the current  $pCO_2$  of 360 ppm.
- Use package seacarb to estimate the dissociation constants and Henry's constants at temperature  $20^\circ C$ , salinity 0, and pressure 0.
- Estimate pH as a function of  $pco_2$ , varying between 200 and 1250

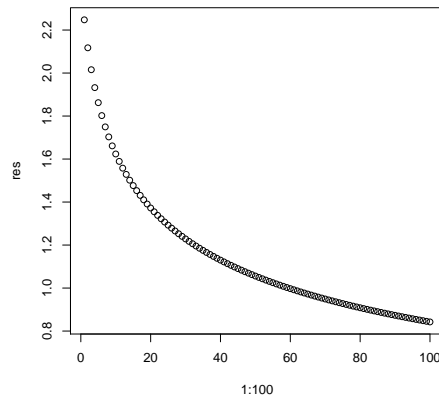


Figure 6: Roots of an equation  $y=f(x)$  for a sequence of  $x$ -values

- What is the value of pH at  $p\text{CO}_2 = 1250$

(see lecture notes for formulae)

```
> require(seacarb)
> k1 <- K1(S=0,T=20,P=0)
> k2 <- K2(S=0,T=20,P=0)
> kh <- Kh(S=0,T=20,P=0)
> nonlinfun <- function(pH,pco2=360,alk=2300e-6)
+ {
+   H <- 10^(-pH)
+   CO2 <- pco2*kh
+   HCO3 <- k1*CO2/H
+   CO3 <- k2*HCO3/H
+   return( HCO3+2*CO3-H*1.e6 - alk)
+ }
> uniroot(nonlinfun,interval=c(2,12),pco2=360,alk=2300,tol=1e-30)

$root
[1] 8.581004

$f.root
[1] -4.547474e-12
attr(,"unit")
[1] "mol/kg-soln"
attr(,"pH scale")
[1] "total scale"
attr(,"method")
[1] "Millero (2010)"

$iter
```

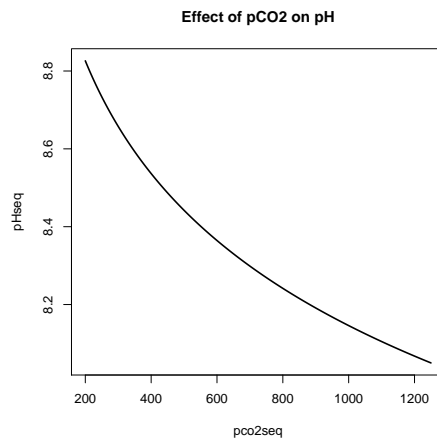


Figure 7: pH as a function of pCO2

```
[1] 15
```

```
$estim.prec
```

```
[1] 3.552714e-15
```

```
> pHseq <- vector()
> pco2seq <- 200:1250
> for (i in 1:length(pco2seq))
+   pHseq[i] <- uniroot(nonlinfun, interval=c(2, 12),
+                       pco2=pco2seq[i], alk=2300, tol=1e-30)$root
> # max drop of pH
> pHseq[length(pHseq)]
```

```
[1] 8.050006
```

```
> plot(pco2seq, pHseq, type="l", lwd=2, main="Effect of pCO2 on pH")
```

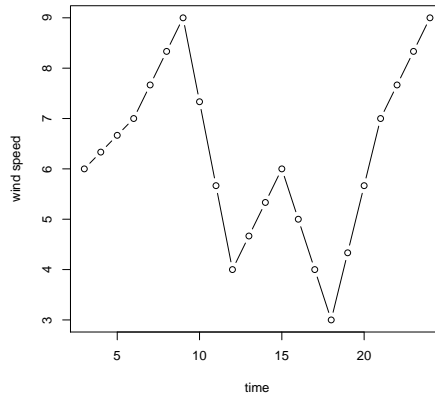


Figure 8: The interpolated wind data

## Chapter 9 - interpolating, smoothing, curve fitting

*Chapter 9.1 interpolating wind data* Wind velocities are: 5,6,7,9,4,6,3,7,9 at time 0, 3, ..., 24 o'clock respectively.

- Interpolate the three-hourly measurements to hourly measurements.
- Make a plot of the interpolated values

```
> t3    <- seq(3,24,by=3)
> wind3 <- c(6,7,9,4,6,3,7,9)
> plot(approx(t3,wind3,xout=3:24),type="b" ,xlab="time",ylab="wind speed")
```

### *Chapter 9.2 Fitting primary production data*

Primary production (pp) at different light intensities are given; Fit the resulting production estimates (pp), as a function of light intensity (ll) with the 3-parameter Eilers-Peeters equation. The primary production is calculated as:

$$pp = p_{\max} \cdot \frac{2 \cdot (1 + \beta) \cdot I/I_{\text{opt}}}{(I/I_{\text{opt}})^2 + 2 \cdot \beta \cdot I/I_{\text{opt}} + 1}$$

where I is light and pmax,  $\beta$  and Iopt are parameters.

Add the best-fit line to the graph. (note: use coef to retrieve the best parameter values).

```
> ll <- c(0.,1,10,20,40,80,120,160,300,480,700)
> pp <- c(0.,1,3,4,6,8,10,11,10,9,8)
> plot(ll,pp,xlab= expression("light, \u03c4Einst" ~ m^{-2} ~ s^{-1}),
+      ylab="production",pch=15,cex=1.5)
> fit<-nls(pp ~pmax*2*(1+b)*(ll/iopt)/
+          ((ll/iopt)^2+2*b*ll/iopt+1),
+          start=c(pmax=max(pp),b=0.005,iopt=ll[which.max(pp)]))
> summary(fit)
```

Formula:  $pp \sim pmax * 2 * (1 + b) * (ll/iopt) / ((ll/iopt)^2 + 2 * b * ll/iopt + 1)$

Parameters:

	Estimate	Std. Error	t value	Pr(> t )	
pmax	10.4351	0.3171	32.909	7.93e-10	***
b	1.5998	0.4353	3.676	0.00626	**
iopt	209.6324	15.8051	13.264	9.96e-07	***

---

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

Residual standard error: 0.5445 on 8 degrees of freedom

Number of iterations to convergence: 7

Achieved convergence tolerance: 9.994e-06

```
> pars <- as.list(coef(fit))
> with(pars,
+ curve(pmax*2*(1+b)*(x/iopt)/((x/iopt)^2+2*b*x/iopt+1),
+       add=TRUE,lwd=2)
> title(expression (frac(pmax**2**%(1+beta)**%I/Iopt,
+ (I/Iopt)^2+2**%beta**%I/Iopt+1)),cex.main=0.8)
```

Formula:  $pp \sim pmax * 2 * (1 + b) * (1/iopt) / ((1/iopt)^2 + 2 * b * 1/iopt + 1)$

Parameters:

	Estimate	Std. Error	t value	Pr(> t )	
pmax	10.4351	0.3171	32.909	7.93e-10	***
b	1.5998	0.4353	3.676	0.00626	**
iopt	209.6324	15.8051	13.264	9.96e-07	***

---

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

Residual standard error: 0.5445 on 8 degrees of freedom

Number of iterations to convergence: 7

Achieved convergence tolerance: 9.994e-06

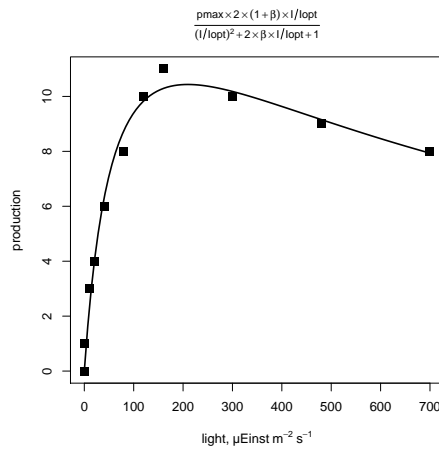


Figure 9: Primary production data with fit

## Chapter 10 differential equations

### Chapter 10.1 Lotka-Volterra model

- Solves the following system of ODEs

$$\begin{aligned}\frac{dx}{dt} &= a \cdot x \cdot \left(1 - \frac{x}{K}\right) - b \cdot x \cdot y \\ \frac{dy}{dt} &= g \cdot b \cdot x \cdot y - e \cdot y\end{aligned}$$

for initial values  $x=300, y=10$  and parameter values:  $a=0.05, K=500, b=0.0002, g=0.8, e=0.03$

- Make three plots, one for  $x$  and one for  $y$  as a function of time, and one plot expressing  $y$  as a function of  $x$ . Arrange these plots in 2 rows and 2 columns.
- run the model with other initial values ( $x=200, y=50$ ); add the  $(x,y)$  trajectories to the phase-plane plot

```
> require(deSolve)
> model <- function (time,VAR,pars)
+ {
+   with (as.list(c(VAR,pars)), {
+     # the rate of change of the state variables
+     dx      <- a*x*(1-x/K)-b*x*y
+     dy      <- g*b*x*y      - e*y
+
+     return(list(c(dx,dy)))
+   })
+ }
> pars  <- c(a=0.05,b=0.0002,K=500,g=0.8,e=0.03)
> VAR   <- c(x=300,y=10)
> times <- seq(0,1000,1)
> out   <- as.data.frame(lsoda(VAR,times,model,pars))
> plot(out$x,out$y,type="l")
> VAR   <- c(x=200,y=50)
> out2  <- as.data.frame(lsoda(VAR,times,model,pars))
> lines(out2$x,out2$y,lty=2)
```

### Chapter 10.2 Lorenz Butterfly

Solve the Lorenz equations:

$$\begin{aligned}\frac{dx}{dt} &= -\frac{8}{3} \cdot x + y \cdot z \\ \frac{dy}{dt} &= -10 \cdot (y - z) \\ \frac{dz}{dt} &= -x \cdot y + 28y - z\end{aligned}$$

Use as initial conditions  $x=y=z=1$ ; create output for a time sequence ranging from 0 to 100, and with a time step of 0.005.

```
> require(scatterplot3d)
> model<-function(t,state,parameters)
```

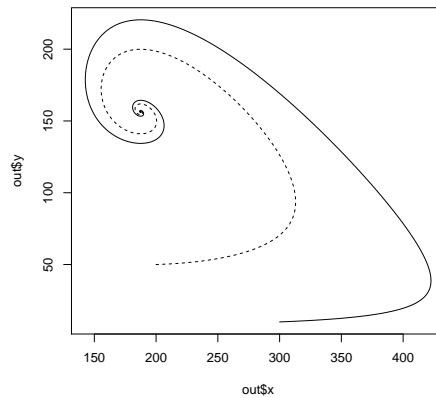


Figure 10: Result of the lotka-volterra model

```

+ {
+   with(as.list(c(state)),{
+
+     dx    <- -8/3*x+y*z
+     dy    <- -10*(y-z)
+     dz    <- -x*y+28*y-z
+
+     list(c(dx,dy,dz))      })
+
+ } # end of model
> state <-c(x=1, y=1, z=1)
> times <-seq(0,100,0.005)
> out   <-as.data.frame(lsoda(state,times,model,0))
> scatterplot3d(out$x,out$y,out$z,type="l",
+               main="Lorenz butterfly",ylab="",grid=FALSE,box=FALSE)

```



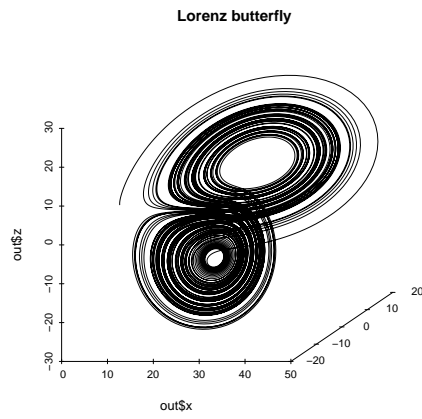


Figure 11: Results of the Lorenz model

## References

Soetaert K (2008). *using R for scientific computing*. NIOO-CEME, Yerseke.

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