EDUARD SZÖCS

QUANTITATIVE ECOTOXICOLOGY

WITH R!

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1
Introduction

```
require(devtools)
install_github("qetx", "EDiLD")
```

```
require(qetx)
```

2
The Measurement Process

2.1 Winsorized Mean and Standard Deviation

The following sulfate concentrations (mg/L) were measured during a routine water quality survey of the Savannah River (South Carolina). The data is available in the `qetx` package [1]:

[1] Note that in this case you do not have to assign the data to a name.

```
data(so4)
```

```
so4

##  [1] 1.3 2.3 2.6 3.3 3.5 3.5 3.6 4.0 4.1 4.5 5.2 5.6
## [13] 5.7 6.1 6.2 6.5 6.9 7.1 7.7 7.9 9.9

length(so4)

## [1] 21

mean(so4)

## [1] 5.119

sd(so4)

## [1] 2.137
```

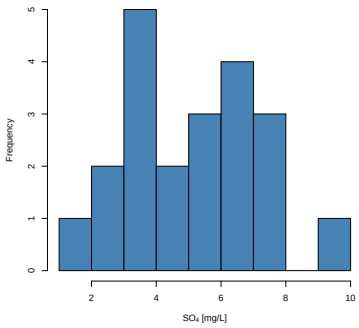

Figure 2.1: A histogramm of the so4 data.

So there are 21 measurements with a mean of 5.12 mg/L and a standard deviation of 2.14 mg/L.

Suppose we have a detection limit of 2.5 mg/L and want to winsorize values below LOD, i.e. replace the two lowest values by 2.6 mg/L and the two highest values by 7.7 mg/L.

Happily there is function in the `qetx` to do this for us: `winsor()`. This function takes a vector of values and a second argument specifying how many values should be winsorized (either by giving a LOD-value or the number of values on each side) [2].

[2] Look at the source of this function - type the function name into the console - to see which computations are done.

```
so4_w <- winsor(so4, lod = 2.5)
so4_w

##  [1] 2.6 2.6 2.6 3.3 3.5 3.5 3.6 4.0 4.1 4.5 5.2 5.6
## [13] 5.7 6.1 6.2 6.9 6.5 7.1 7.7 7.7 7.7
## attr(,"width")
## [1] 2
```

This give the expected results, moreover we see that on each end two observations where modified [3].

[3] stored within the attribute 'width' of the resulting vector. **TODO: verbatim within sidenote.**

```
mean(so4_w)

## [1] 5.081

sd(so4_w)

## [1] 1.792

sd_winsor(so4_w)

## [1] 2.24
```

The Winsorized mean $(\bar{x}_w)$ now is 5.08 mg/L, the standard deviation of the modified data set (s) is 1.79 mg/L and the Winsorized standard deviation (s_w) 2.24 mg/L.

2.2 Probability Plotting

3
Bioaccumulation

4
Tests for Detection of Chronic Lethal and Sub-lethal Stress

5
Lethal and Other Quantal Responses to Stress

5.1 Fitting dose-response models

6
Population and Metapopulation Effects

7
Community Effects

7.1 Species Richness

7.2 Analyzing mesocosm data

Principle Response Curves (PRC)[1] are commonly used for analyzing ecotoxicological mesocosm experiments. PRC is just a special form of Redundancy Analysis (RDA) and analyses the multivariate response to a treatment over time [2].

Here we will analyze the pyrifos data set from the publication[3] which is shipped with the vegan package.

[1] Van den Brink, P. and Ter Braak, C. (1999). Principal response curves: Analysis of time-dependent multivariate responses of biological community to stress. *Environmental Toxicology and Chemistry*, 18(2):138–148

[2] Legendre and Legendre, 2013

[3] Van den Brink and Ter Braak, 1999

```
require(vegan)
data(pyrifos)
head(pyrifos[, c(1:8)])
```

```
##        Simve Daplo Cerpu Alogu Aloco Alore Aloaf Copsp
## w.4.c1 3.951     0     0     0     0     0     0 2.773
## w.4.c2 2.303     0     0     0     0     0     0 2.079
## w.4.c3 4.595     0     0     0     0     0     0 3.761
## w.4.c4 2.398     0     0     0     0     0     0 3.296
## w.4.c5 4.025     0     0     0     0     0     0 3.466
## w.4.c6 2.303     0     0     0     0     0     0 2.197
```

```
dim(pyrifos)
```

```
## [1] 132 178
```

```
ditch <- gl(12, 1, length = 132)
week <- gl(11, 12, labels = c(-4, -1, 0.1, 1, 2, 4, 8, 12,
    15, 19, 24))
dose <- factor(rep(c(0.1, 0, 0, 0.9, 0, 44, 6, 0.1, 44,
    0.9, 0, 6), 11))
```

```
pyrifos_env <- data.frame(ditch, week, dose)
```

```
pyrifos_prc <- prc(response = pyrifos, treatment = dose,
    time = week)
pyrifos_prc_sum <- summary(pyrifos_prc, scaling = 1)
```

```
plot(pyrifos_prc, select = abs(pyrifos_prc_sum$sp) > 1)
```

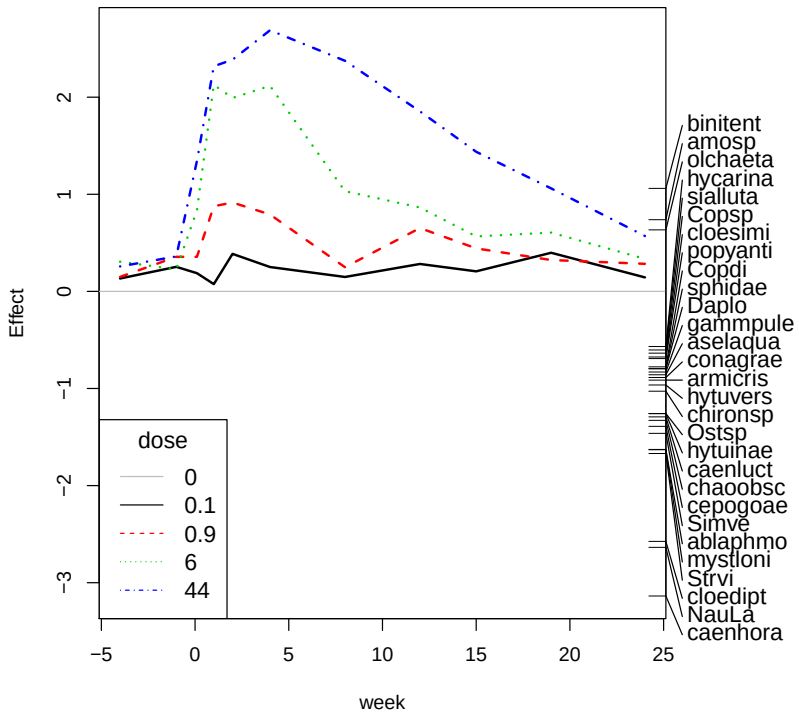

Figure 7.1: Principal response curves (PRC) with species weights for the pyrifos data set indicating the effects of the insecticide on the invertebrate community.

7.3 Species Sensitivity Distributions

R Session Info

```
sessionInfo()

## R version 3.0.2 (2013-09-25)
## Platform: x86_64-pc-linux-gnu (64-bit)
##
## locale:
##  [1] LC_CTYPE=en_US.UTF-8
##  [2] LC_NUMERIC=C
##  [3] LC_TIME=en_US.UTF-8
##  [4] LC_COLLATE=en_US.UTF-8
##  [5] LC_MONETARY=en_US.UTF-8
##  [6] LC_MESSAGES=en_US.UTF-8
##  [7] LC_PAPER=en_US.UTF-8
##  [8] LC_NAME=C
##  [9] LC_ADDRESS=C
## [10] LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_US.UTF-8
## [12] LC_IDENTIFICATION=C
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets
## [6] methods   base
##
## other attached packages:
## [1] vegan_2.1-35    lattice_0.20-23 permute_0.7-4
## [4] qetx_0.0.1      knitr_1.5
##
## loaded via a namespace (and not attached):
## [1] codetools_0.2-8 digest_0.6.3    evaluate_0.5.1
## [4] formatR_0.9     grid_3.0.2      highr_0.2.1
## [7] stringr_0.6.2   tools_3.0.2
```

Bibliography

Legendre, P. and Legendre, L. (2013). *Numerical ecology*. Elsevier, Amsterdam; Boston.

Van den Brink, P. and Ter Braak, C. (1999). Principal response curves: Analysis of time-dependent multivariate responses of biological community to stress. *Environmental Toxicology and Chemistry*, 18(2):138–148.