STATISTICAL ECO(-TOXICO)LOGY

IMPROVING THE UTILIZATION OF DATA FOR ECOLOGICAL RISK ASSESSMENT

by

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INTRODUCTION AND OBJECTIVES

1.1 CHEMICAL POLLUTION OF FRESHWATER ECOSYSTEMS

1.2 ECOLOGICAL RISK ASSESSMENT (ERA)

Ecological Risk Assessment is based on two main components: Effects and Exposure Assessment, which are combined in ecological risk assessment. Exposure Assessment aims to derive a predicted environmental concentration (PEC) using mainly modeling techniques. Effect Assessment identifies hazards to the environmental ....

1.3 STATISTICAL ECOTOXICOLOGY

1.4 ENVIRONMENTAL MONITORING

1.5 OBJECTIVES AND OUTLINE OF THE THESIS

This thesis pursues three objectives:

i to scrutinize new methods in statistical ecotoxicology,

ii explore available monitoring data and

iii provide tools to deal with data in ERA

Figure 1.1 provides an overview on the research performed and its relation to ERA as outlined in the previous sections.
The thesis starts with a comparison of statistical methods to analyse ecotoxicological experiments (Chapter **??**). Specific questions addressed were:

- Are newer statistical methods more powerful than currently used methods?
- How much statistical power do current experimental designs in ecotoxicology exhibit?

ERA focuses with its predictions on small streams. Chapter 2 focuses on realised environmental concentrations. Specific goals were:

- Compile all available monitoring data on pesticides in Germany, with a focus on small streams.
- Derive thresholds for agricultural use and catchment size.
- Assess the current pollution in german streams.

The compilation of monitoring data from different data sources, lead to a big inhomogeneous amount of data that first needs to be harmonized. Chapters **??** (chemical data) and **??** (biological data) describe software solutions to simplify and accelerate the workflow of:

- validating and harmonizing chemical and taxonomic names
- link them to other datasets
- search properties and identifiers

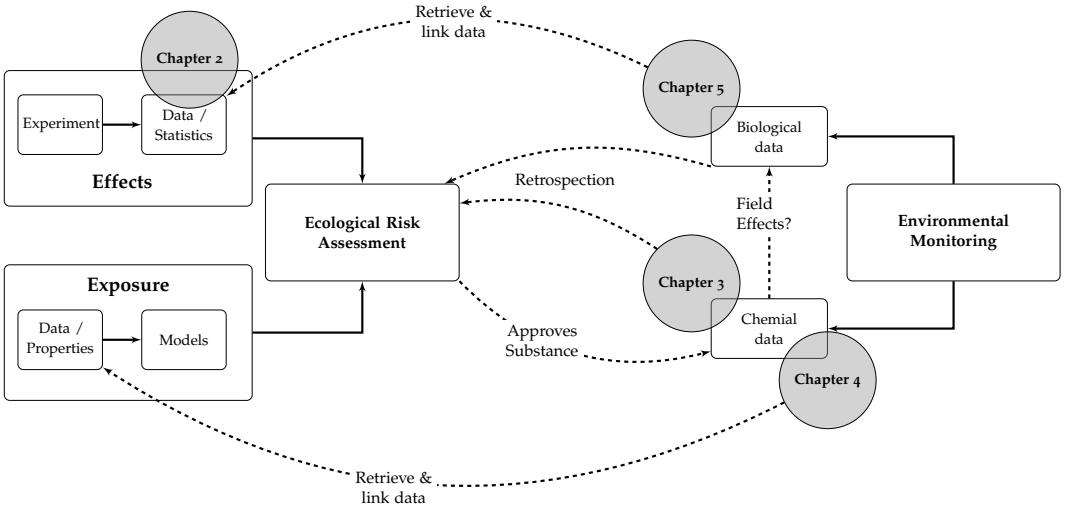

Figure 1.1: Conceptual overview on data in ecological risk assessment and environmental monitoring, as well as parts addressed by this thesis.

1.6 REFERENCES

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LARGE SCALE RISKS FROM PESTICIDES IN SMALL STREAMS

Eduard Szöcs[a], Marvin Brinke[b], Bilgin Karaoglan[c] & Ralf B. Schäfer[a]

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Submitted to *Environmental Science & Technology* in 2016

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DISCUSSION

AUTHOR'S CONTRIBUTIONS

ARTICLE I

TITLE: Ecotoxicology is not normal - A comparison of statistical approaches for analysis of count and proportion data in ecotoxicology

AUTHORS: Eduard Szöcs and Ralf B. Schäfer

STATUS: Published in 2015 in Environmental Science and Pollution Research, Volume 22, Issue 18, pp 13990-13999

CONTRIBUTIONS: Szöcs (85%) Designed research and simulations, analysed data, discussed results, wrote manuscript

Schäfer (15%) Designed research, discussed results, edited manuscript

ARTICLE II

TITLE: Large scale risks from pesticides in small streams

AUTHORS: Eduard Szöcs, Marvin Brinke, Bilgin Karaoglan, and Ralf B. Schäfer

STATUS: Submitted to *Environmental Science & Technology* in 2016

CONTRIBUTIONS: Szöcs (5%) Designed research

Brinke (5%) helped with data, commented on manuscript

Karaoglan (5%) provided data (RACs), commented on manuscript

Schäfer (15%) Designed research, discussed results, edited manuscript

ARTICLE III

TITLE: webchem: An R Package to Retrieve Chemical Information from the Web.

AUTHORS: Eduard Szöcs and Ralf B. Schäfer

STATUS: Accepted in 2016 in *Journal of Statistical Software*

CONTRIBUTIONS: Szöcs (90%) Designed, programmed and tested software, wrote manuscript

Schäfer (10%) discussed results, edited manuscript

ARTICLE IV

TITLE: taxize: taxonomic search and retrieval in R

AUTHORS: Scott A. Chamberlain and Eduard Szöcs

STATUS: Published in 2013 in *F1000Research, Volume 2, Issue 191*

CONTRIBUTIONS: Chamberlain (50%) Designed, programmed and tested software, wrote manuscript

Szöcs (50%) Designed, programmed and tested software, wrote manuscript

DECLARATION

I, the author of this work, certify that this work contains no material which has been accepted or submitted for the award of any other degree at any university or other tertiary institution. The work has been interdependently prepared. All aids and sources have been clearly specified and the contribution of other authors have been documented and reference lists given.

Neustadt a.d. Weinstraße,
25th October, 2016

Eduard Szöcs

CURRICULUM VITAE

Eduard Szöcs

Personal

Date of birth	16.06.1987
Nationality	german
Marital Status	single
Languages	German (native), English (very good), Romanian (good)

Education

04.2014–present **Ph.D. Environmental Sciences**, *University of Koblenz-Landau*, Landau.
Statistical Ecotoxicology - Improving the utilization of data for ecological risk assessment.

04.2012–03.2014 **M. Sc. Ecotoxicology**, *University of Koblenz-Landau*, Landau.
Thesis: Analysing mesocosm experiments: Principal Response Curves vs. Multivariate Generalized Linear Models.

11.2011 **B. Sc. Umweltwissenschaften**, *University of Koblenz-Landau*, Landau.
Thesis: Effects of salinity and pesticides on community structure of macroinvertebrates in Australian streams.

09.2007–11.2011 **Dipl. Umweltwissenschaften**, *University of Koblenz-Landau*, Landau.

Work Experience and Teaching

02.2016 – present **Research Assistant**, *University of Koblenz-Landau*, Landau.
Field Study in Romania, Data analyses, maintenance of databases and servers, PhD research.

11.2015 – present **Freelance Scientist & Consultant**.
Data sourcing, cleaning and analysis with specialization in Environmental & Ecological data. Courses in ecological statistics with the software *"R"*.

04.2015 – 01.2016 **Research Assistant**, *University of Koblenz-Landau*, Landau.
UBA Project: "PSM in Kleingewässern" (FKZ 3714674040/1). Building, maintaining and analysing a nation-wide german pesticide monitoring database.

05.2014 – 04.2015 **Research Assistant**, *University of Koblenz-Landau*, Landau.
Data analyses, maintenance of databases and servers, PhD research.

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12.2014 – 02.2015 **Teaching Assistant**, *University of Koblenz-Landau*, Landau.
Multivariate Statistics Course.

12.2013 – 02.2014 **Teaching Assistant**, *University of Koblenz-Landau*, Landau.
Multivariate Statistics Course.

12.2013 **Research Assistant**, *University of Koblenz-Landau*, Landau.
Development of a PostgreSQL-database of german physico-chemical data.

12.2012 – 02.2013 **Teaching Assistant**, *University of Koblenz-Landau*, Landau.
Multivariate Statistics Course.

12.2012 **Research Assistant**, *Department System Ecotoxicology, UFZ – Helmholtz Centre for Environmental Research*, Leipzig.
Development of rspear R-package.

05.2012 – 07.2012 **Internship**, *Department System Ecotoxicology, UFZ – Helmholtz Centre for Environmental Research*, Leipzig.
Field Study on the effects of pesticides on macroinvertebrates.

12.2011 – 02.2012 **Teaching Assistant**, *University of Koblenz-Landau*, Landau.
Multivariate Statistics Course.

07.2010 **Teaching Assistant**, *University of Koblenz-Landau*, Landau.
Aquatic Field Course.

06.2006 – 07.2007 **Internship**, *Landschaftspflegeverband Südpfalz e. V.*, Landau.
Freiwilliges Ökologisches Jahr.

Programming Skills

Expert R

Intermediate LaTeX, git, PostgreSQL, GrassGIS, PostGIS, shell, regex, xml, xpath, html, cloud computing

Beginner CDK, openbabel, NetLogo, Python, C++

(Beginner = *"I know the basics and can get the job done"*; Intermediate = *"I can effectively apply these tools"*; Expert = *"I can develop and expand these tools."*)

Software

I have developed or contributed to the following open source software for the R computing environment:

- The **webchem** package to retrieve chemical information from the web.
- The **taxize** package (together with Scott Chamberlain) allows taxonomic search, retrieval and handling in R.
- Contributions to the **vegan** package.
- The **rspear** package calculates $\text{SPEAR}_{\text{pesticides}}$ in R (deprecated).
- A web application to calculate statistical power for population endpoints in mesocosm experiments (currently offline / deprecated).
- Various other R packages and functions related to eco(toxico-)logy and environmental sciences.

All software is freely available from my github account (`https://github.com/EDiLD`), homepage (`https://edild.github.io`) or The Comprehensive R Archive Network (CRAN) (`https://edild.github.io`).

Publications and Conference contributions

Articles

[1] L. Lagadic, R. B. Schäfer, M. Roucaute, **E. Szöcs**, S. Chouin, J. de Maupeou, C. Duchet, E. Franquet, B. Le Hunsec, C. Bertrand, and et al. (2016). "No association between the use of Bti for mosquito control and the dynamics of non-target aquatic invertebrates in French coastal and continental wetlands". *Science of The Total Environment* 553, 486–494.

[2] V. C. Schreiner, **E. Szöcs**, A. K. Bhowmik, M. G. Vijver, and R. B. Schäfer (2016). "Pesticide mixtures in streams of several European countries and the USA". *Science of The Total Environment* 573, 680–689.

[3] **E. Szöcs** and R. B. Schäfer (2016). "Statistical hypothesis testing—To transform or not to transform?" *Integrated Environmental Assessment and Management* 12 (2), 398–400.

[4] J. G. Mbaka, **E. Szöcs**, and R. B. Schäfer (2015). "Meta-analysis on the responses of traits of different taxonomic groups to global and local stressors". *Acta Oecologica* 69, 65–70.

[5] **E. Szöcs** and R. B. Schäfer (2015). "Ecotoxicology is not normal: A comparison of statistical approaches for analysis of count and proportion data in ecotoxicology". *Environmental Science and Pollution Research* 22 (18), 13990–13999.

[6] **E. Szöcs**, P. J. v. d. Brink, L. Lagadic, T. Caquet, M. Roucaute, A. Auber, Y. Bayona, M. Liess, P. Ebke, A. Ippolito, C. J. F. t. Braak, T. C. M. Brock, and R. B. Schäfer (2015). "Analysing chemical-induced changes in macroinvertebrate communities in aquatic mesocosm experiments: a comparison of methods". *Ecotoxicology* 24 (4), 760–769.

[7] **E. Szöcs**, E. Coring, J. Bäthe, and R. B. Schäfer (2014). "Effects of anthropogenic salinization on biological traits and community composition of stream macroinvertebrates". *Science of The Total Environment* 468–469, 943–949.

[8] S. A. Chamberlain and **E. Szöcs** (2013). "taxize: taxonomic search and retrieval in R [v2; ref status: indexed, http://f1000r.es/24v]". *F1000Research* 2 (191).

[9] R. B. Schäfer, M. Bundschuh, D. A. Rouch, **E. Szöcs**, P. C. von der Ohe, V. Pettigrove, R. Schulz, D. Nugegoda, and B. J. Kefford (2012). "Effects of pesticide toxicity, salinity and other environmental variables on selected ecosystem functions in streams and the relevance for ecosystem services". *Science of the Total Environment* 415 (1), 69–78.

[10] **E. Szöcs**, B. J. Kefford, and R. B. Schäfer (2012). "Is there an interaction of the effects of salinity and pesticides on the community structure of macroinvertebrates?" *Science of the Total Environment* 437 (1), 121–126.

Poster

[1] **E. Szöcs** and R. B. Schäfer (2015). "Ecotoxicology is not normal". SETAC Europe; Barcelona.

[2] **E. Szöcs** and S. A. Chamberlain (2014). "taxize: taxonomic search and retrieval in R". International Statistical Ecology Conference; Montpellier.

[3] **E. Szöcs**, B. J. Kefford, V. Pettigrove, and R. B. Schäfer (2011). "Einfluss von Pestiziden und Salinität auf Makroinvertebratengemeinschaften". SETAC GLB; Landau.

As a service to the scientific community I performed a total of 4 reviews for the journals *Proceedings*

of the Royal Society B, PhytoKeys, Zookeys and *Environmental Toxicology and Chemistry*.

Workshops held

07.2015 **Data analysis in freshwater ecology using R**, *9th Symposium for European Freshwater Sciences*, Geneva.
Workshop held together with Dr. Ralf B. Schäfer and Avit Kumar Bhowmik.
Workshop homepage: `https://github.com/EDiLD/sefs9_Rworkshop`

11.2015 **Data Visualization with ggplot2**, *Workshop held at Young Academics Conference 2015 - Land-Water-Interactions*, Klingenmünster.
Workshop homepage: `https://github.com/EDiLD/r_landau_2015`

Neustadt a.d. Weinstraße, September 19, 2016