

Statistical Eco(-toxico)logy

Improving the Utilisation of Data for
Environmental Risk Assessment

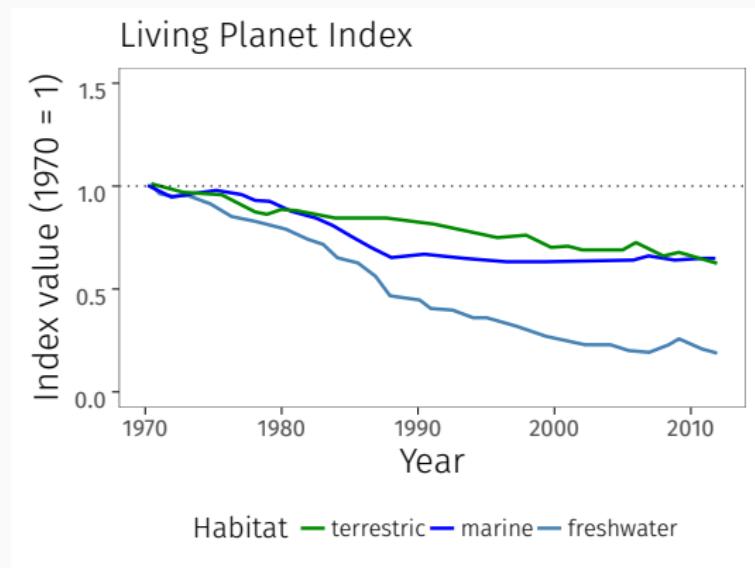
Eduard Szöcs

25th January 2017

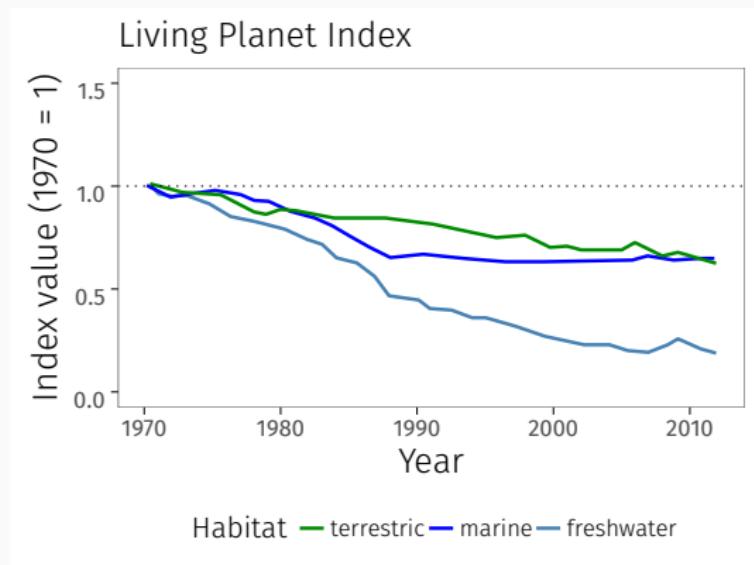
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Freshwater biodiversity is strongly declining



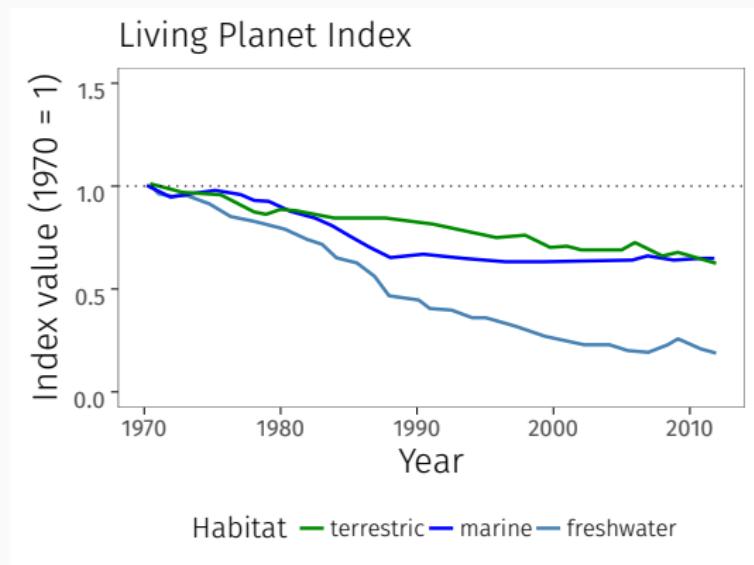
Freshwater biodiversity is strongly declining



Reasons

- Habitat loss
- Overexploitation
- Pollution
- Invasive species

Freshwater biodiversity is strongly declining



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- Habitat loss
- Overexploitation
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Environmental Risk Assessment and Environmental Monitoring

Environmental Risk Assessment and Monitoring

Plant Protection Products
Regulation 1107/2009

Water Framework Directive
2000/60/EC

Environmental
Risk
Assessment

Environmental
Monitoring

Environmental Risk Assessment and Monitoring

Plant Protection Products
Regulation 1107/2009

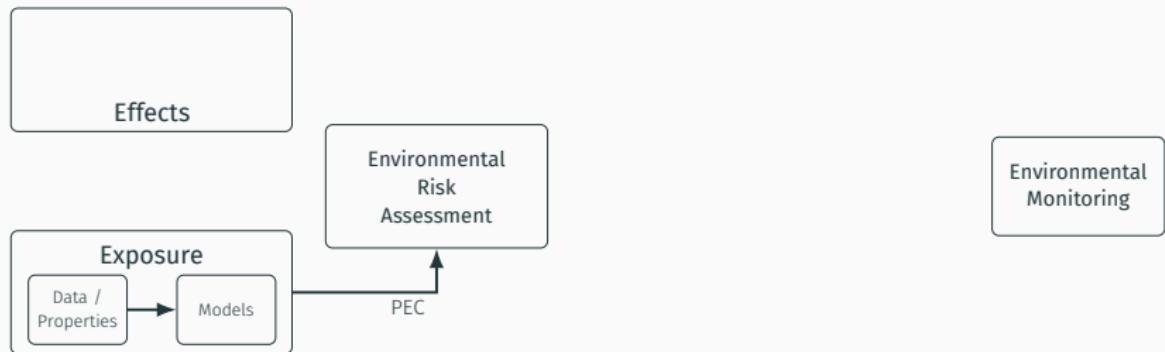
Water Framework Directive
2000/60/EC



Environmental Risk Assessment and Monitoring

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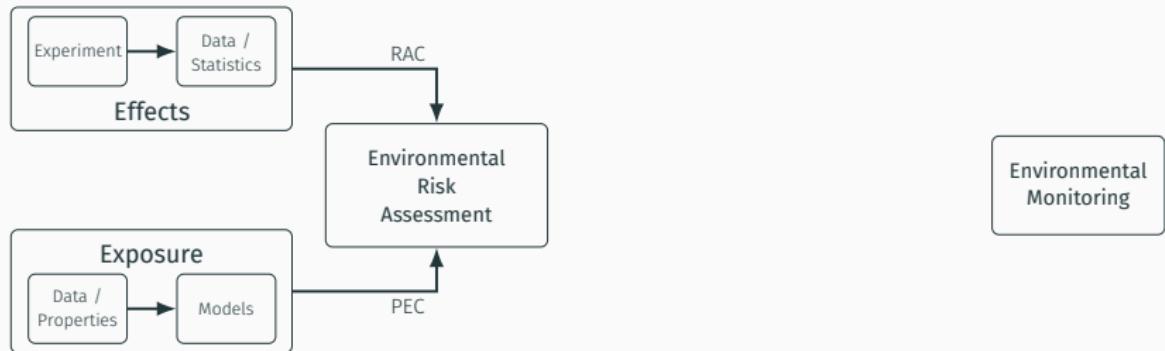
Water Framework Directive
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Environmental Risk Assessment and Monitoring

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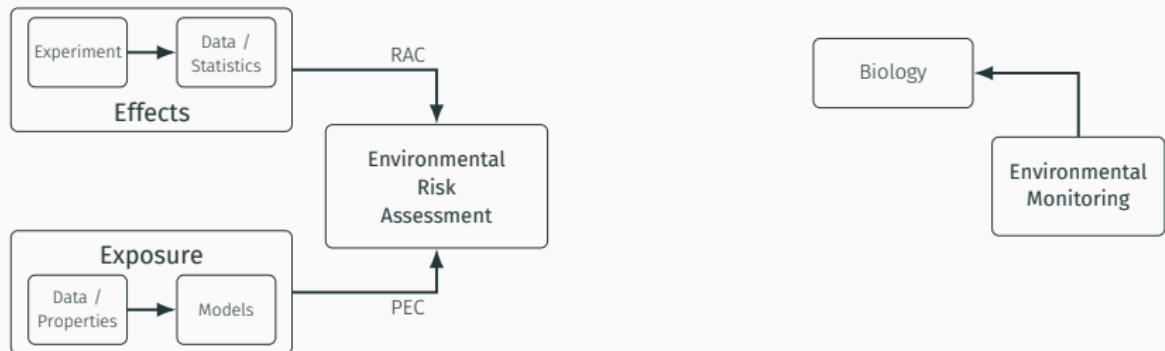
Water Framework Directive
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Environmental Risk Assessment and Monitoring

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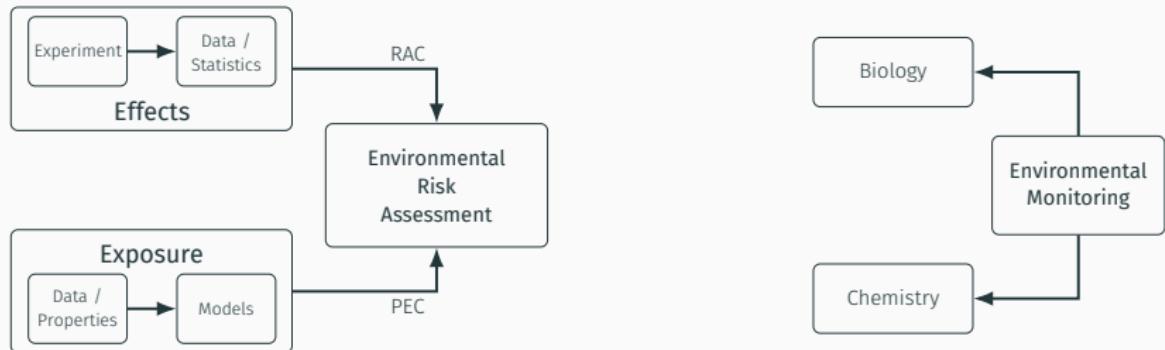
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Environmental Risk Assessment and Monitoring

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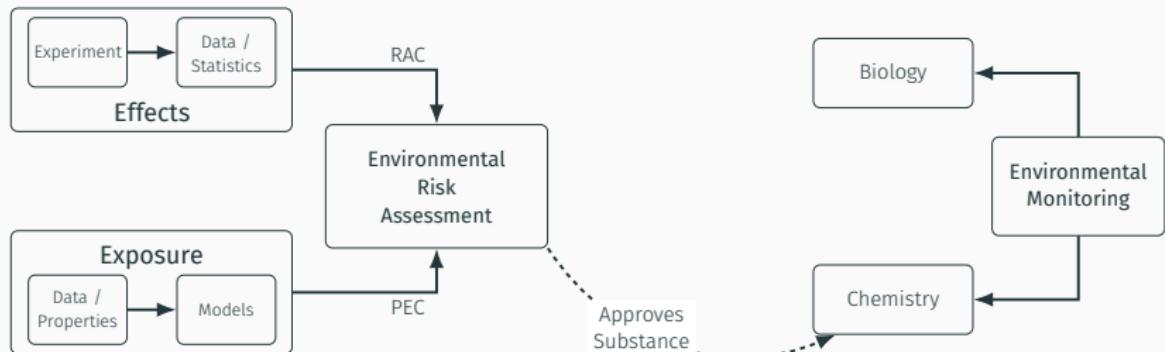
Water Framework Directive
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Environmental Risk Assessment and Monitoring

Plant Protection Products
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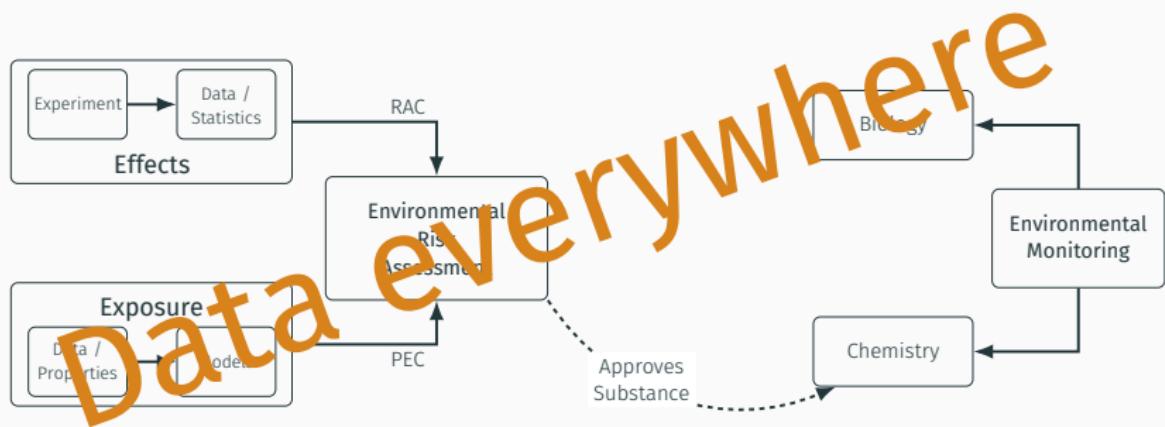
Water Framework Directive
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Environmental Risk Assessment and Monitoring

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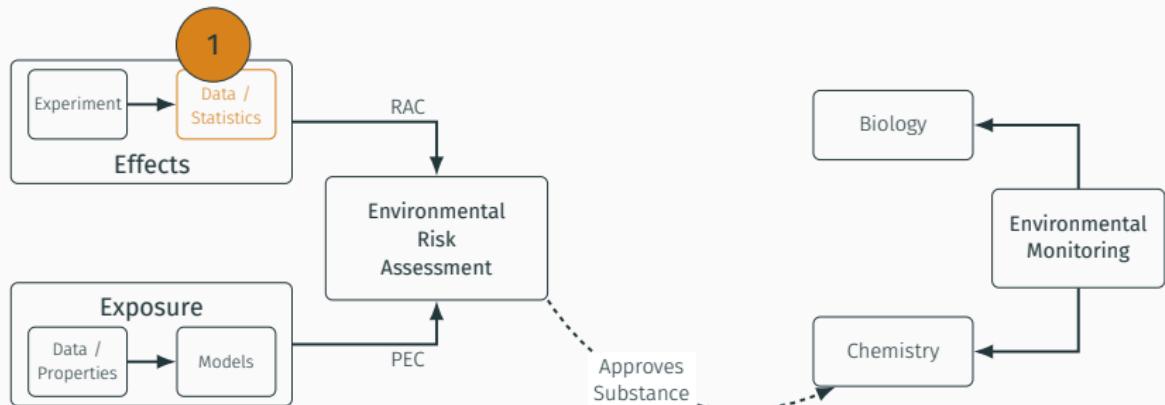
Water Framework Directive
2000/60/EC



Improving Statistics in ERA

Plant Protection Products
Regulation 1107/2009

Water Framework Directive
2000/60/EC



1

Szöcs & Schäfer (2015). "Ecotoxicology is not normal". ESPR 22(18), 13990–13999.

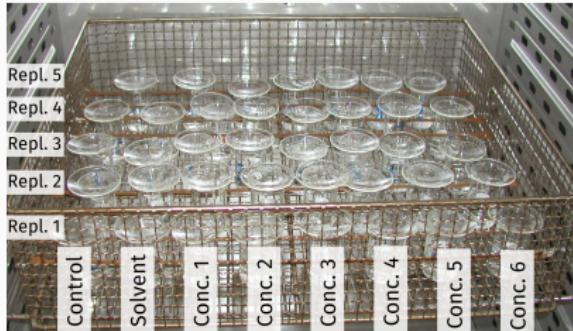
Improving Statistics in ERA

Experiments in Effect Assessment



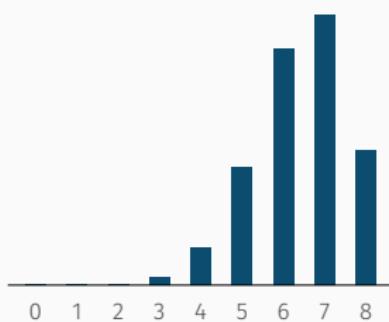
- Daphnia Test
- Lower Tier
- " x out of n survived"

Experiments in Effect Assessment

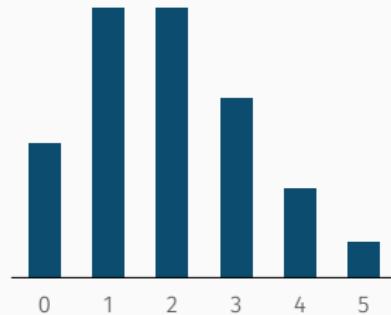


- Daphnia Test
- Lower Tier
- “*x out of n survived*”
- Mesocosm
- Higher Tier
- “*number of animals*”

Ecotoxicology is not normal

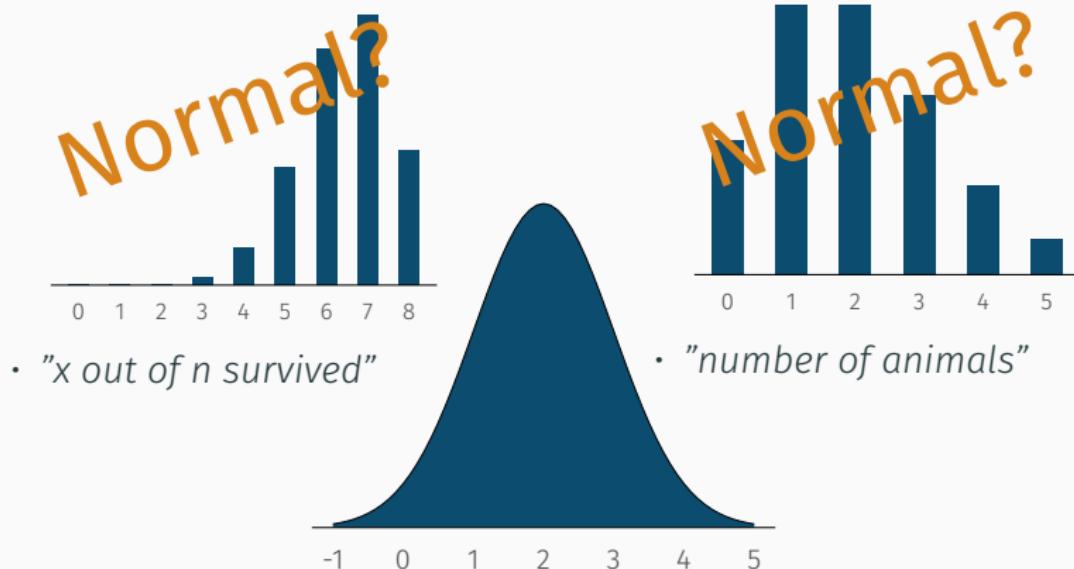


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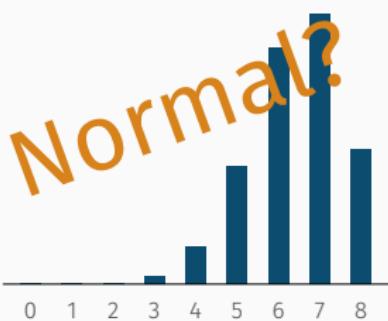


- "number of animals"

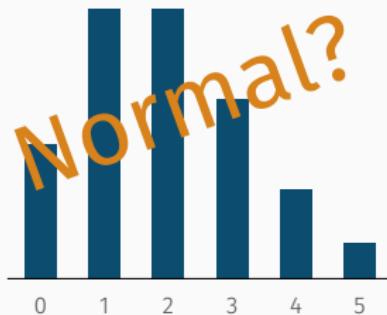
Ecotoxicology is not normal



Ecotoxicology is not normal

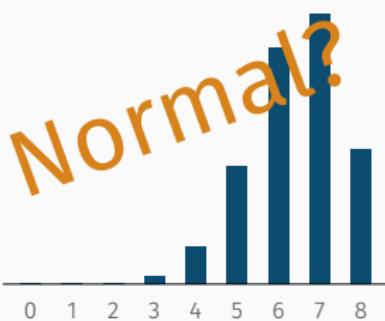


- " x out of n survived"
- binomial data

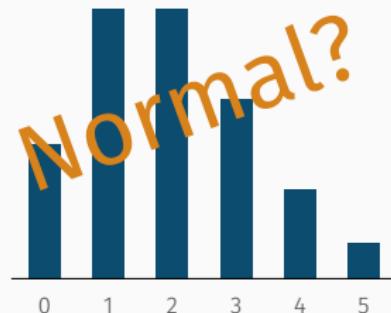


- "number of animals"
- count data

Ecotoxicology is not normal



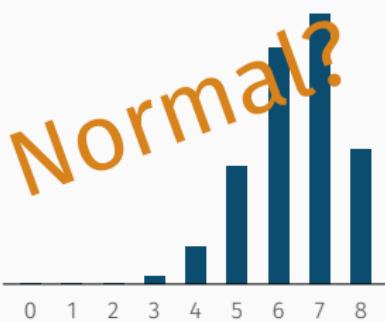
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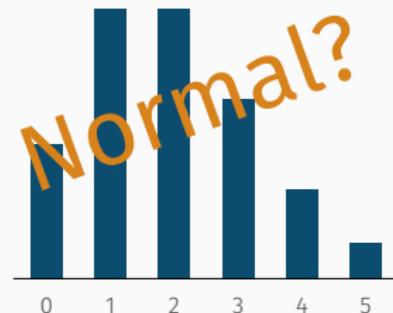
- "number of animals"
- count data

- ignore?

Ecotoxicology is not normal



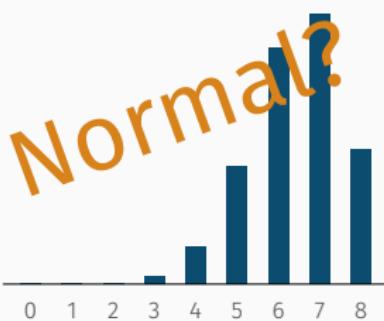
- " x out of n survived"
- binomial data



- "number of animals"
- count data

- ignore?
- transform?

Ecotoxicology is not normal



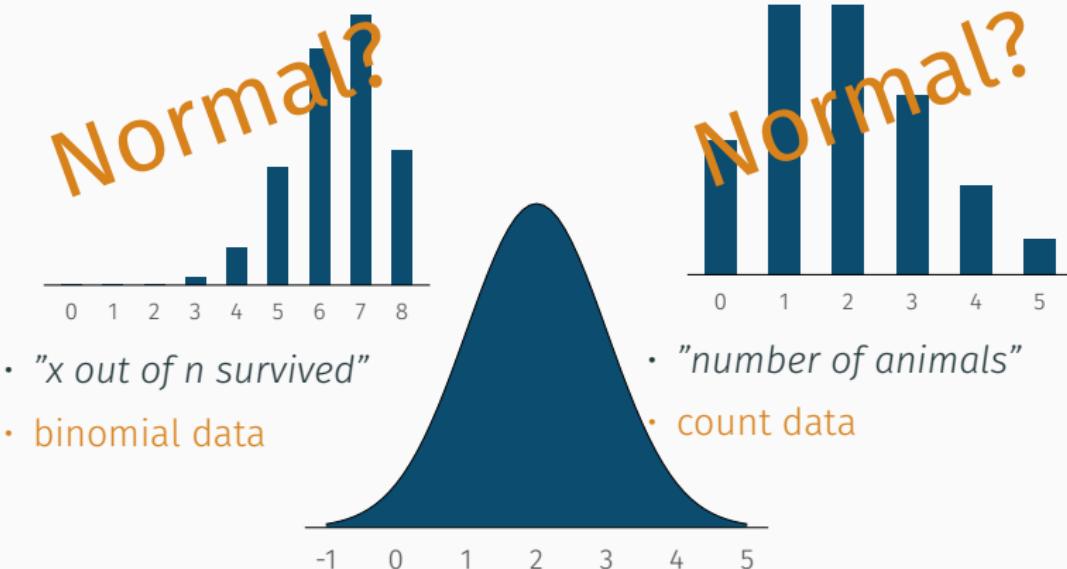
- " x out of n survived"
- binomial data



- "number of animals"
- count data

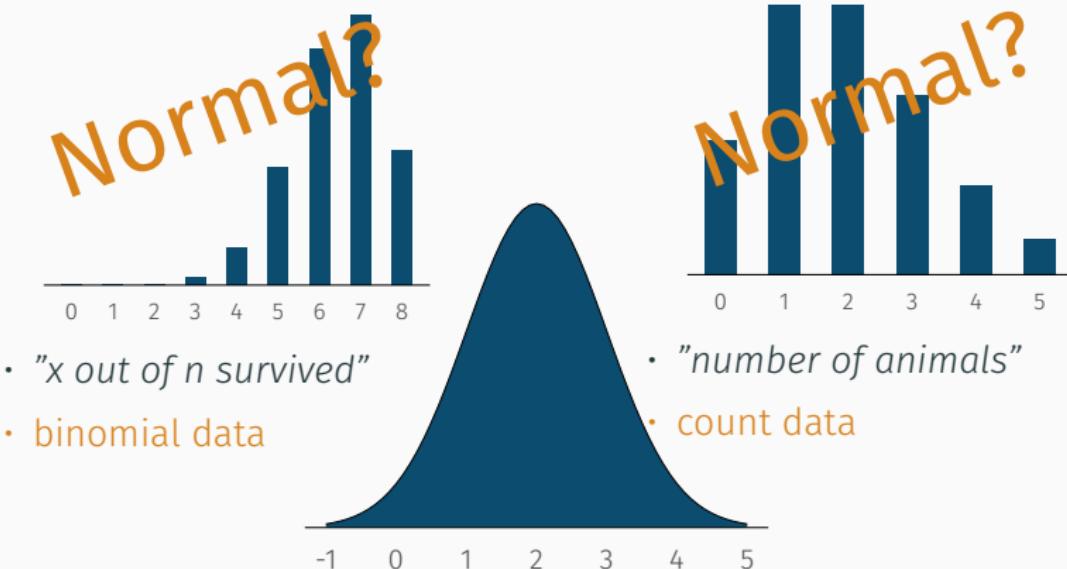
- ignore?
- transform?
- non-parametric?

Ecotoxicology is not normal



- ignore?
- transform?
- non-parametric?
- Generalized Linear Model (GLM)

Ecotoxicology is not normal



- ignore?
- transform?
- non-parametric?
- Generalized Linear Model (GLM)

A recent history of GLM (uncomprehensive) in ecology

J. R. Statist. Soc. A,
(1972), **135**, Part 3, p. 370

370

Generalized Linear Models

By J. A. NELDER and R. W. M. WEDDERBURN

Rothamsted Experimental Station, Harpenden, Herts



Methods in Ecology and Evolution



Methods in Ecology & Evolution

doi: 10.1111/j.2041-210X.2010.00021.x

Do not log-transform count data

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²Department of Environmental Sciences, PO Box 65, University of Helsinki, Helsinki FI-00014, Finland



A recent history of GLM (uncomprehensive) in ecology

Ecology, 92(1), 2011, pp. 3–10
© 2011 by the Ecological Society of America

The arcsine is asinine: the analysis of proportions in ecology

DAVID I. WARTON^{1,2,3} AND FRANCIS K. C. HUI¹

¹*School of Mathematics and Statistics, The University of New South Wales, Sydney, NSW 2052 Australia*
²*Evolution and Ecology Research Centre, The University of New South Wales, Sydney, NSW 2052 Australia*



Methods in Ecology and Evolution



Methods in Ecology and Evolution

doi: 10.1111/j.2041-210X.2011.00127.x

Distance-based multivariate analyses confound location and dispersion effects

David I. Warton^{1*}, Stephen T. Wright¹ and Yi Wang^{1,2}

¹School of Mathematics and Statistics and Evolution & Ecology Research Centre; and ²School of Computer Science and Engineering, The University of New South Wales, NSW 2052, Australia



A recent history of GLM (uncomprehensive) in ecology

Ecotoxicology
DOI 10.1007/s10646-015-1421-0

Analysing chemical-induced changes in macroinvertebrate communities in aquatic mesocosm experiments: a comparison of methods

Eduard Szöcs · Paul J. Van den Brink · Laurent Lagadic · Thierry Caquet ·
Marc Roucaute · Arnaud Auber · Yannick Bayona · Matthias Liess ·
Peter Ebke · Alessio Ippolito · Cajo J. F. ter Braak · Theo C. M. Brock ·
Ralf B. Schäfer



A recent history of GLM (uncomprehensive) in ecology

Environ Sci Pollut Res

DOI 10.1007/s11356-015-4579-3

RESEARCH ARTICLE

Ecotoxicology is not normal

A comparison of statistical approaches for analysis of count
and proportion data in ecotoxicology

Eduard Szöcs¹ · Ralf B. Schäfer¹

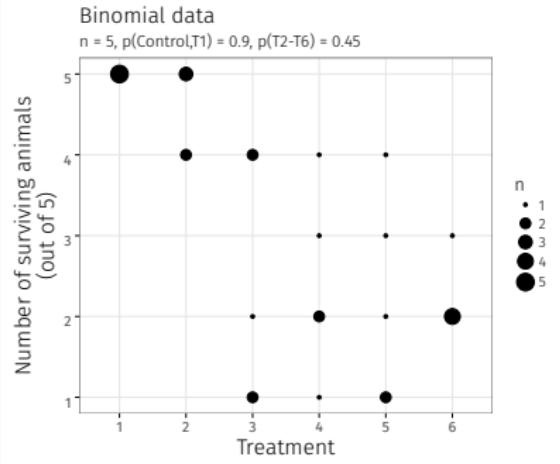


A simulation study



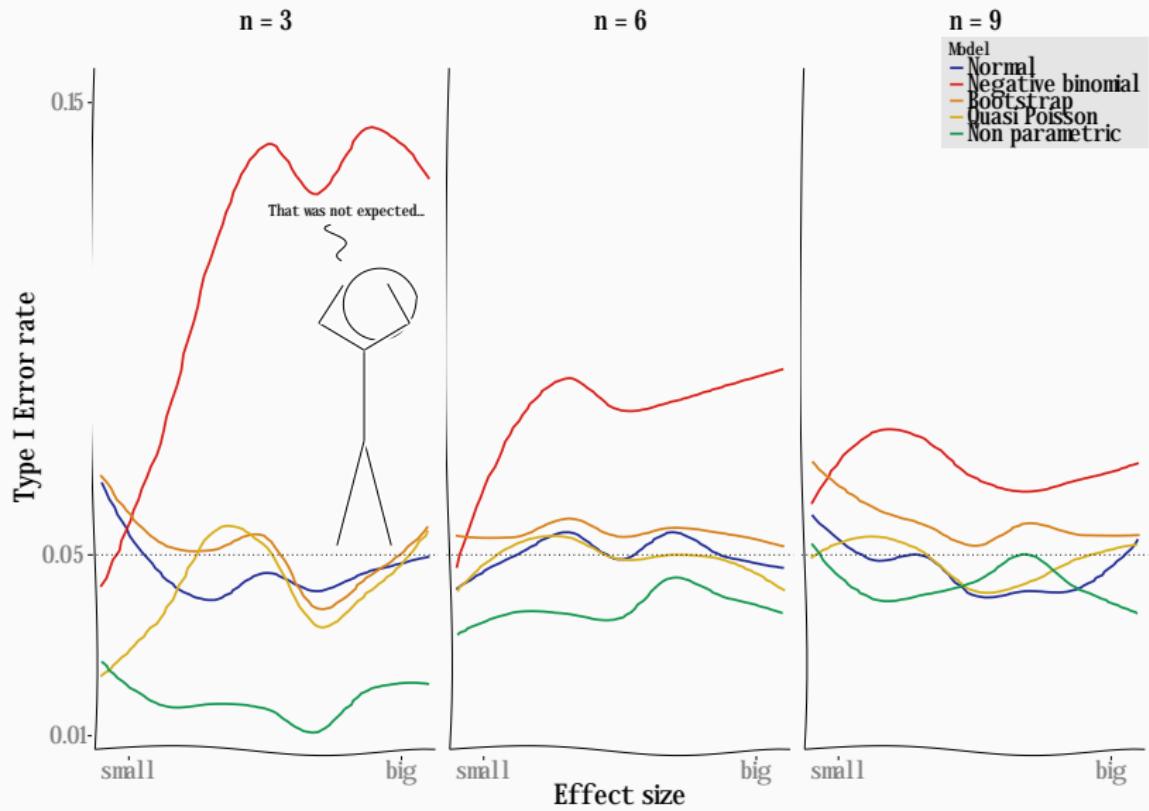
- Count & Binomial data
- Vary replicates & Effect size
- Global test & LOEC

A simulation study

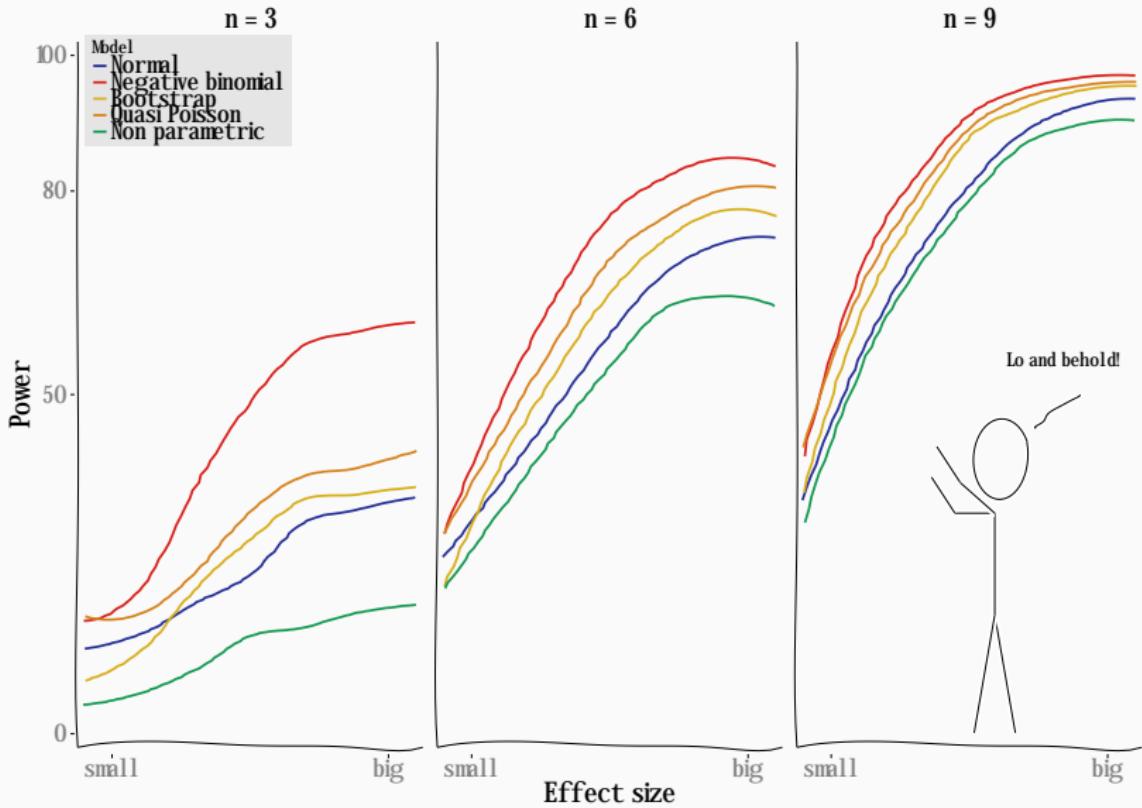


- Count & Binomial data
- Vary replicates & Effect size
- Global test & LOEC
- LM
- GLMs
- Non-parametric

Type I Errors: GLMs can fail



Power: But GLMs can do also better



What we learned from this study

1. Negative-binomial GLM show increased Type I errors
2. Can be fixed via bootstrap
3. Ecotoxicological experiments commonly low power
4. NOECs are not reliable
5. GLMs can increase this power

Where are we today?

Three days earlier...



Where are we today?

Three days earlier...

Methods in Ecology and Evolution



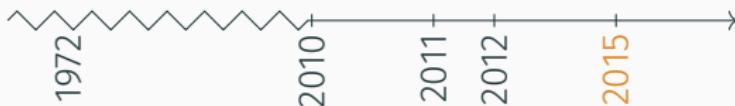
Methods in Ecology and Evolution 2015, **6**, 828–835

doi: 10.1111/2041-210X.12386

For testing the significance of regression coefficients, go ahead and log-transform count data

Anthony R. Ives*

Department of Zoology, University of Wisconsin-Madison, Madison, WI 53706, USA



Methods in Ecology and Evolution



Methods in Ecology and Evolution 2016, 7, 882–890

doi: 10.1111/2041-210X.12552

FORUM

Three points to consider when choosing a LM or GLM test for count data

David I. Warton^{1*}, Mitchell Lyons², Jakub Stoklosa¹ and Anthony R. Ives³

¹School of Mathematics and Statistics and Evolution & Ecology Research Centre, University of New South Wales, NSW 2052, Australia; ²School of Biological, Earth and Environmental Sciences, University of New South Wales, NSW 2052, Australia; and

³Department of Zoology, University of Wisconsin-Madison, Madison, WI 53706, USA



Where are we today?

Three points to consider ...

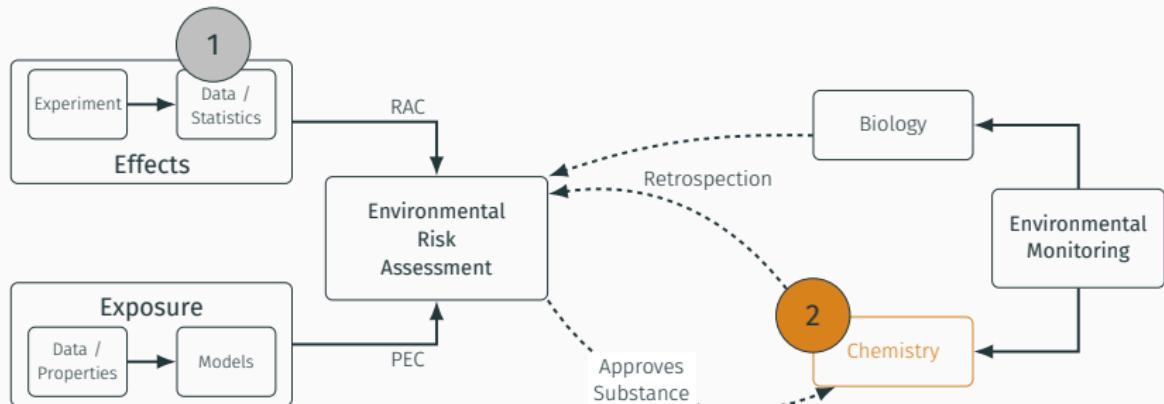
1. Choose your model based on data properties
2. Fix Type I errors by resampling
3. Models that better fit the data have better power properties

Exploring Monitoring Data for ERA

Exploring Monitoring Data for ERA

Plant Protection Products
Regulation 1107/2009

Water Framework Directive
2000/60/EC



2

Szöcs, Brinke, Karaoglan & Schäfer (submitted). "Large scale risks from pesticides in small streams". Environmental Science & Technology.

Exposure Assessment

- prospective

Chemical Monitoring

- retrospective

Exposure Assessment & Environmental Monitoring

Exposure Assessment

- prospective
- Plant Protection Products

Chemical Monitoring

- retrospective
- All chemicals

Exposure Assessment & Environmental Monitoring

Exposure Assessment

- prospective
- Plant Protection Products
- small waters
(1m width, 30cm depth)

Chemical Monitoring

- retrospective
- All chemicals
- large waters
(mainly $>10\text{km}^2$)

Exposure Assessment & Environmental Monitoring

Exposure Assessment

- prospective
- Plant Protection Products
- small waters
(1m width, 30cm depth)
- Regulatory Acceptable concentrations (RAC)

Chemical Monitoring

- retrospective
- All chemicals
- large waters
(mainly $>10\text{km}^2$)
- Environmental Quality Standards (EQS)

Goal: Can monitoring inform ERA?

- Compile nation-wide monitoring data
- Focus on small streams
- Identify risks & influencing factors

Goals & Hypotheses

Goal: Can monitoring inform ERA?

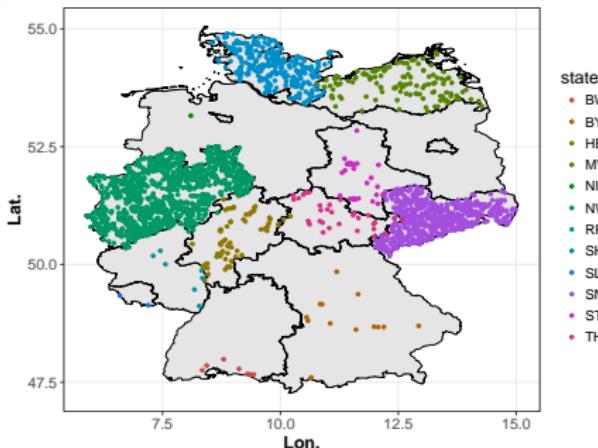
- Compile nation-wide monitoring data
- Focus on small streams
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Hypotheses

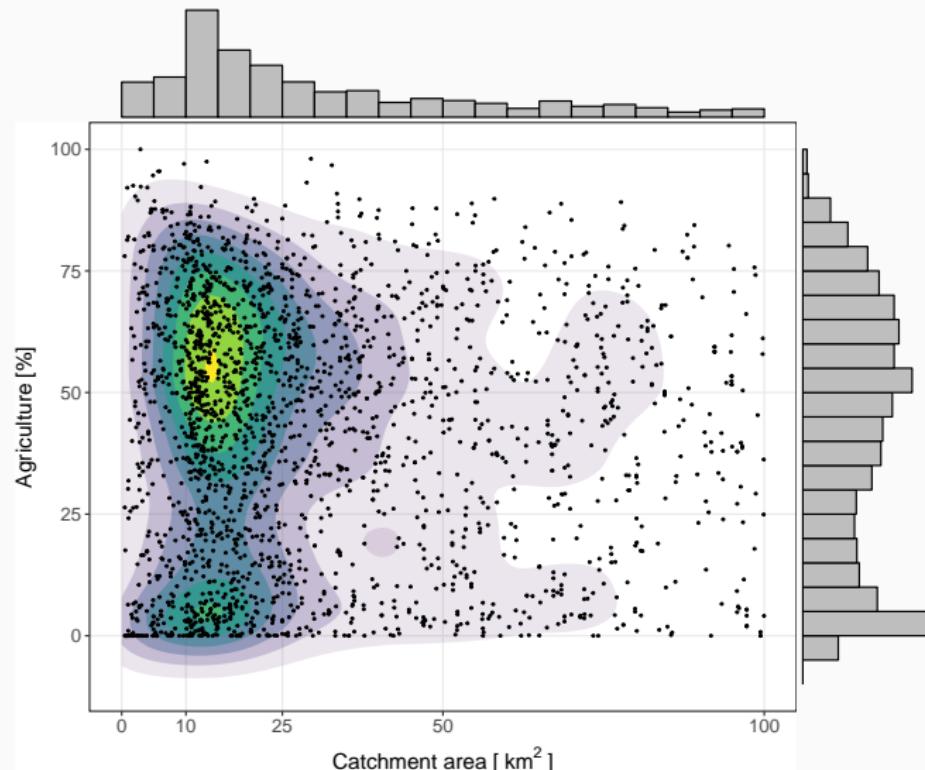
1. Agricultural streams show highest concentrations
2. Small streams show highest concentration
3. Samples at precipitation events show higher concentration
4. Highest concentrations in summer

Compiled data: Big but inhomogeneous

- Federalism
- Compilation & Homogenisation
- 1,766,104 measurements
- 478 pesticides (including metabolites)
- 24,743 samples
- 2,301 sites



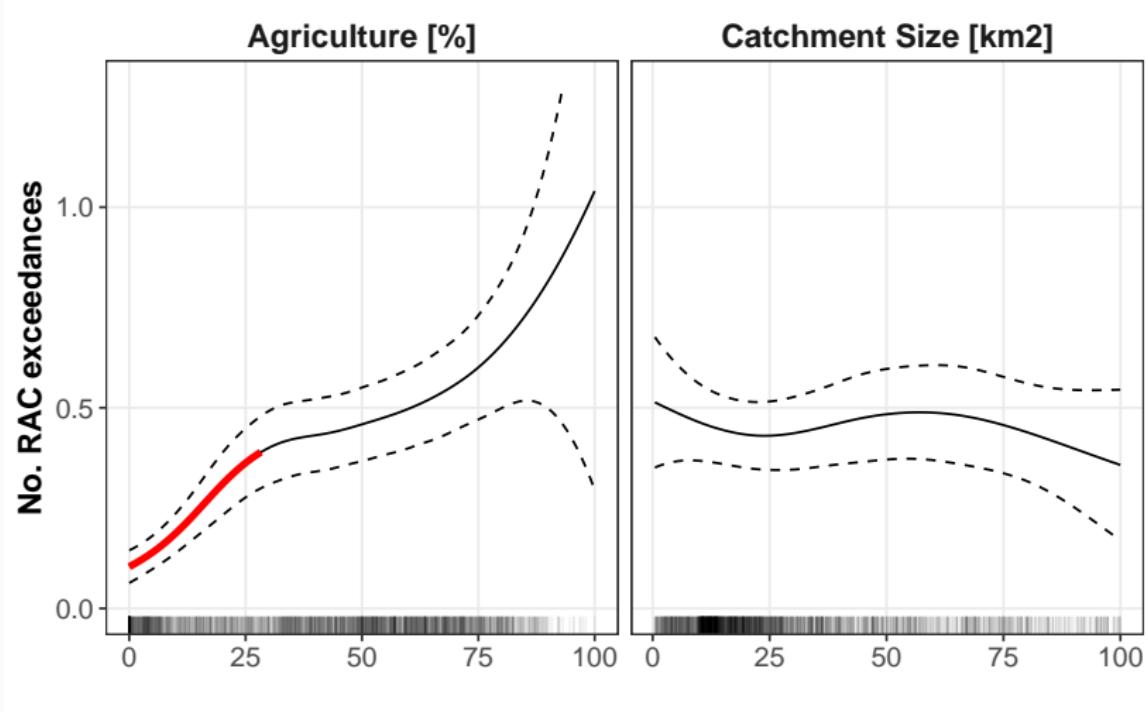
Small streams are underrepresented



Analysing chemical concentrations

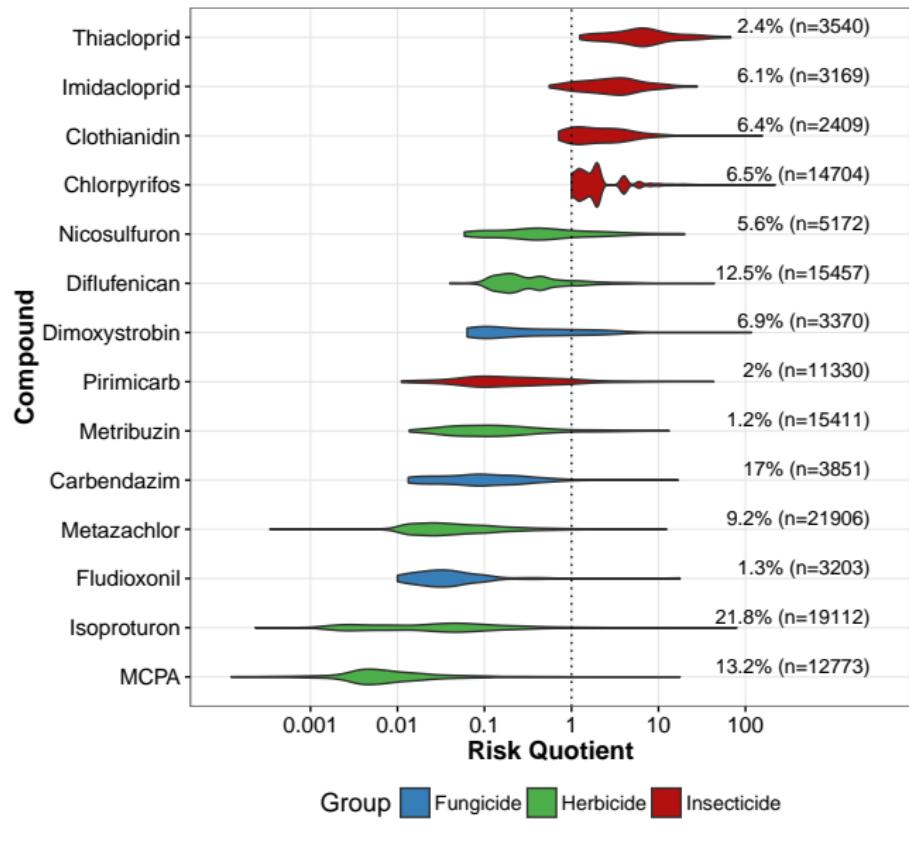
- Risk Quotient: $RQ = \frac{C}{RAC}$
- concentrations < LOQ
-

Results: Factors influencing risk (landscape)



Results: Factors influencing risk (sampling)

Results: Compounds exceeding risk thresholds

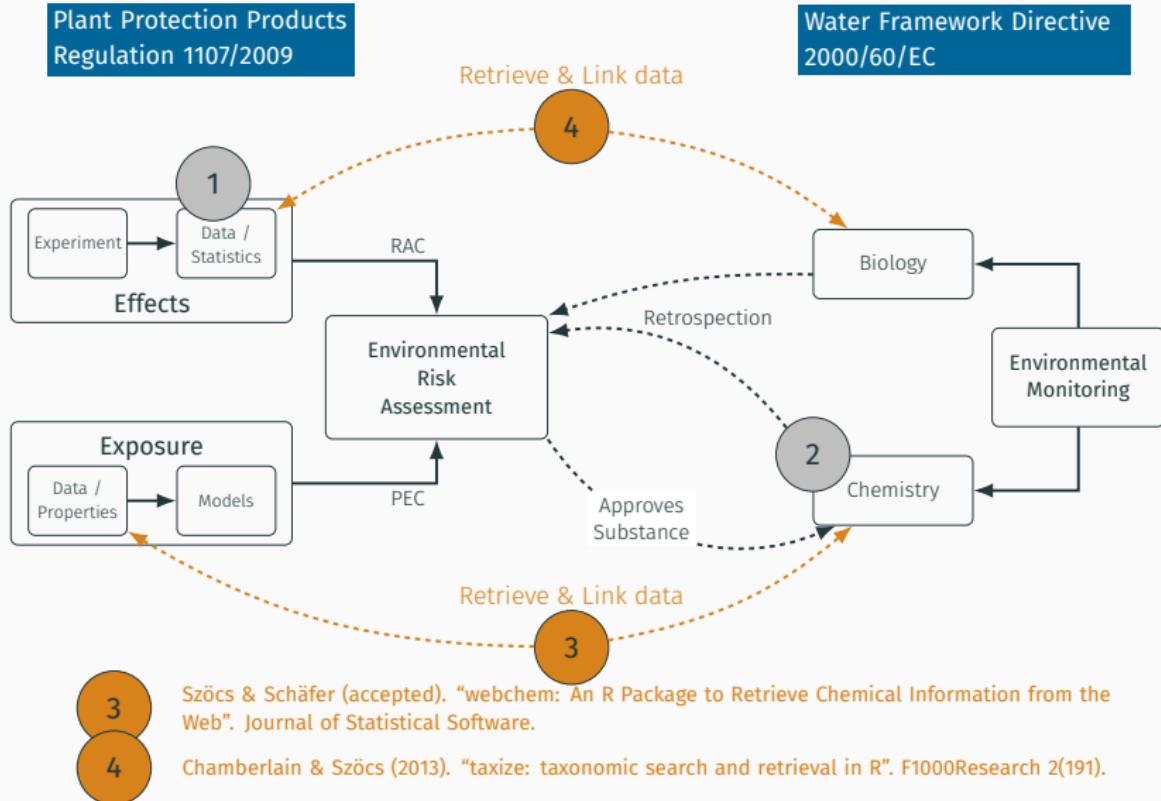


What we learned

1. Huge differences between **states**
2. Small streams currently **underrepresented**
3. **Agriculture** important factor
4. **LOQ** gives additional insights
5. **Underestimated** risk
6. Annual **dynamics**
7. **Neonicotinoids + Chlorpyrifos**

Solutions for Data Handling in ERA

Solutions for Data Handling in ERA



Biologists & Chemists face the same problems

Names

Osmia rufa, *Osmia bicornis*, *Osmia ruffa*, *Osmia unilandauis*, *Osmia spec.*

Chlorpyrifos, Chlorpyriphos,
Chlorphyrifos, Chlorpyrifos-ethyl,
Chlorpypifot

Biologists & Chemists face the same problems

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Hierarchies

Hymenoptera / Apoidea /
Megachilidae / *Osmia* / *rufa*

organophosphate, ester, insecticide

Biologists & Chemists face the same problems

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Hierarchies

Hymenoptera / Apoidea /
Megachilidae / *Osmia / rufa*

organophosphate, ester, insecticide

Traits / Properties

Wing length, Mass, Season

Mass, K_{OW} , LC_{50}

Biologists & Chemists face the same problems

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Identifiers

NCBI, ITIS, EOL, ... 2921-88-2, Clc1c(OP(=S)[...], InChI=1S/C9H11C[...], SBPBAQFW[...], CSID,...

Biologists & Chemists face the same problems

Names

Osmia rufa, *Osmia bicornis*, *Osmia ruffa*, *Osmia unilandauis*, *Osmia spec.* Chlorpyrifos, Chlorpyriphos, Chlorphyrifos, Chlorpyrifos-ethyl, Chlorpypifot

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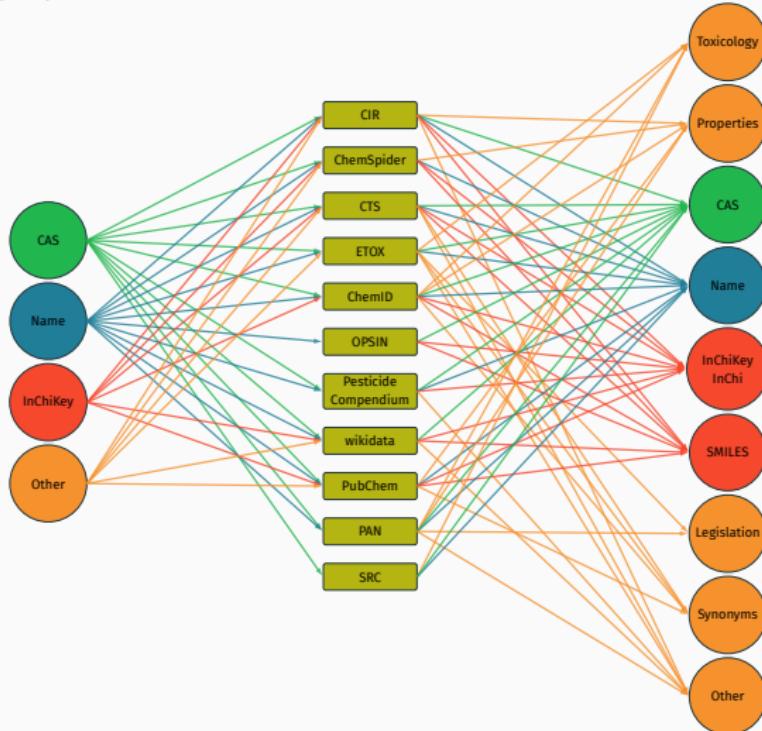
Amount of data

2993 taxa

489 pesticides
(+ 590 other organics)

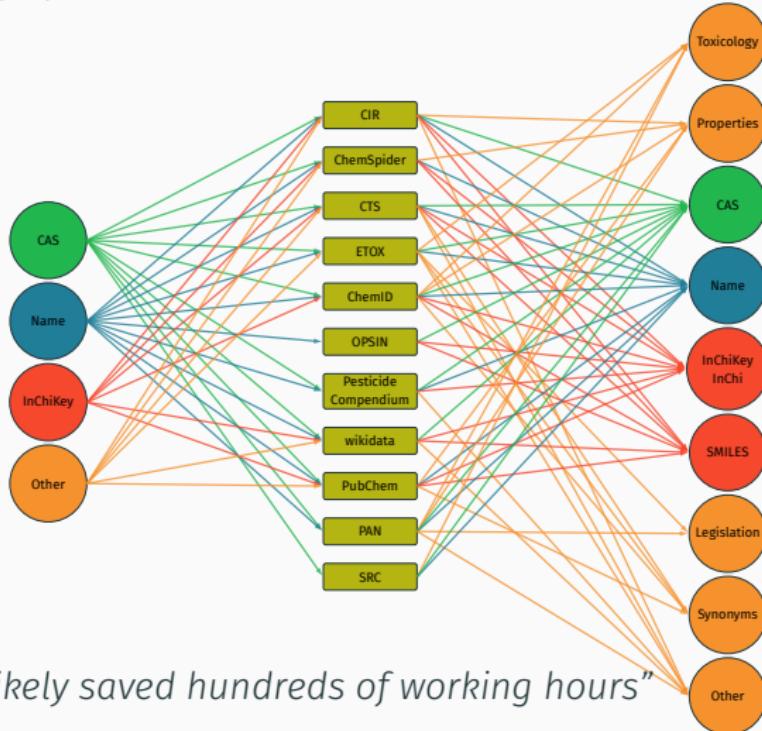
Instead of wasting time...

... use webchem!



Instead of wasting time...

... use webchem!



"webchem ...likely saved hundreds of working hours"

Instead of wasting time...

... use taxize!



Global Invasive Species
Database



ThePlantList

Instead of wasting time...

... use taxize!

The image shows a collection of logos for different biological databases and projects, all related to taxonomy and biodiversity. The logos are arranged in a grid-like fashion within a white rectangular box.

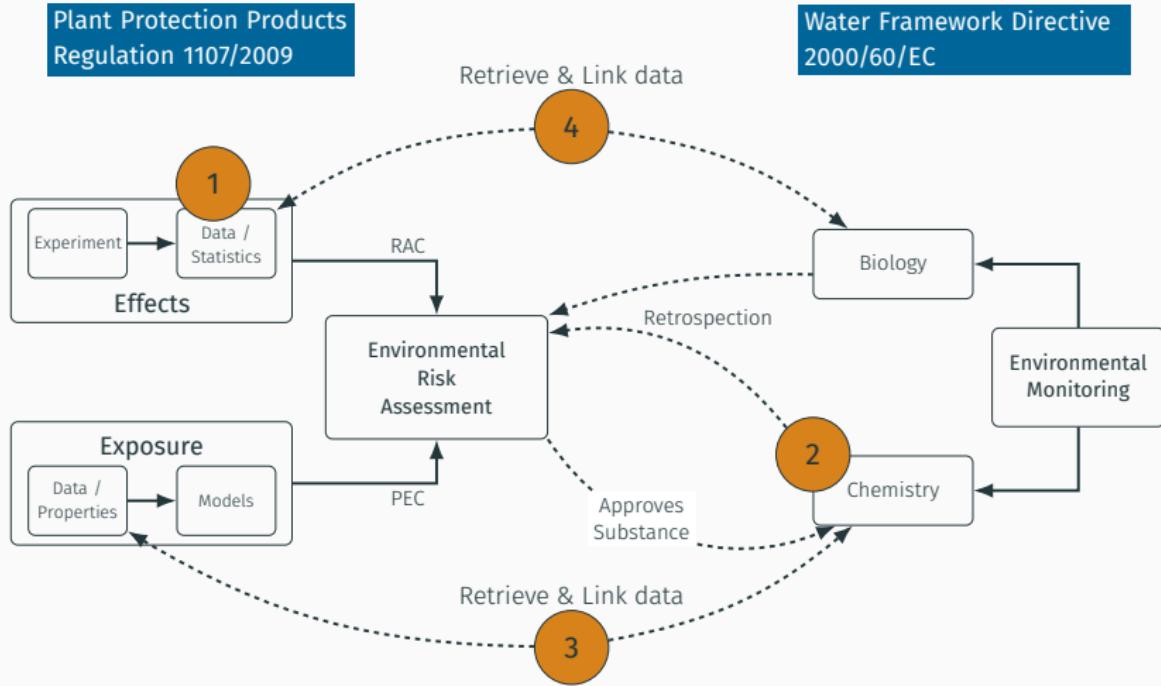
- ITIS**: Logo features a green circular icon with a tree, a bee, and a flower, next to the acronym "ITIS".
- iPlant Collaborative**: Logo features a blue circular icon with a plant, next to the text "iPlant Collaborative™".
- Plantminer**: Logo features a green circular icon with dots connected by lines forming a network, next to the word "Plantminer".
- Catalogue of Life**: Logo features a horizontal bar with blue, yellow, red, and green segments, next to the text "Catalogue of Life".
- Tropicos**: Logo features a green circular icon with a plant, next to the word "Tropicos®".
- Global Invasive Species Database**: Logo features a green circular icon with a plant, next to the text "Global Invasive Species Database".
- gbif**: Logo features a green circular icon with a plant, next to the lowercase letters "gbif".
- NCBI**: Logo features a blue square icon with a white stylized "N" shape, next to the letters "NCBI".
- eOL Encyclopedia of Life**: Logo features a green circular icon with a plant, next to the text "eOL Encyclopedia of Life".
- gnl**: Logo features a green circular icon with colored dots (blue, yellow, red), next to the lowercase letters "gnl".
- RED LIST**: Logo features a red circular icon with a white plant shape, next to the text "RED LIST".
- ubio**: Logo features a green circular icon with a plant, next to the lowercase letters "ubio".
- Canadensys**: Logo features a red circular icon with a white plant shape, next to the lowercase letters "Canadensys".
- ThePlantList**: Logo features a green circular icon with a plant, next to the lowercase letters "ThePlantList".

"Days of searching done during my morning coffee. Amazing. **taxize**."

1. saving of time
2. less errors
3. reproducibility
4. join different data sets
5. easy aggregations

Recap

Recap: What did I look at?



What we learned

✓ Improving Statistics in ERA

- Change your model, not your data
- Ultimately ban NOEC
- Take LOQ into account

What we learned

✓ Improving Statistics in ERA

- Change your model, not your data
- Ultimately ban NOEC
- Take LOQ into account

✓ Exploring Monitoring Data for ERA

- Risk drivers and dynamics
- Agricultural small streams at risk & neglected
- Neonicotinoids
- Feedback for ERA

What we learned

✓ Improving Statistics in ERA

- Change your model, not your data
- Ultimately ban NOEC
- Take LOQ into account

✓ Exploring Monitoring Data for ERA

- Risk drivers and dynamics
- Agricultural small streams at risk & neglected
- Neonicotinoids
- Feedback for ERA

✓ Solutions for Linking Data in ERA

- Handling big eco(toxico-)logical data not easy
- Now easier

Many Thanks To

- My supervisor Prof. Dr. Ralf. B. Schäfer (for his support, openness, opportunities & discussions)
- My colleagues & collaborators (too many to list here)
- German Environment Agency (for funding & collab)
- My parents Anca & Helmut (for their support)
- My girlfriend Anja (for everything)

Statistical Ecotoxicology

Improving the Utilisation of Data for
Environmental Risk Assessment

Eduard Szöcs

💻 <http://edild.github.io/>

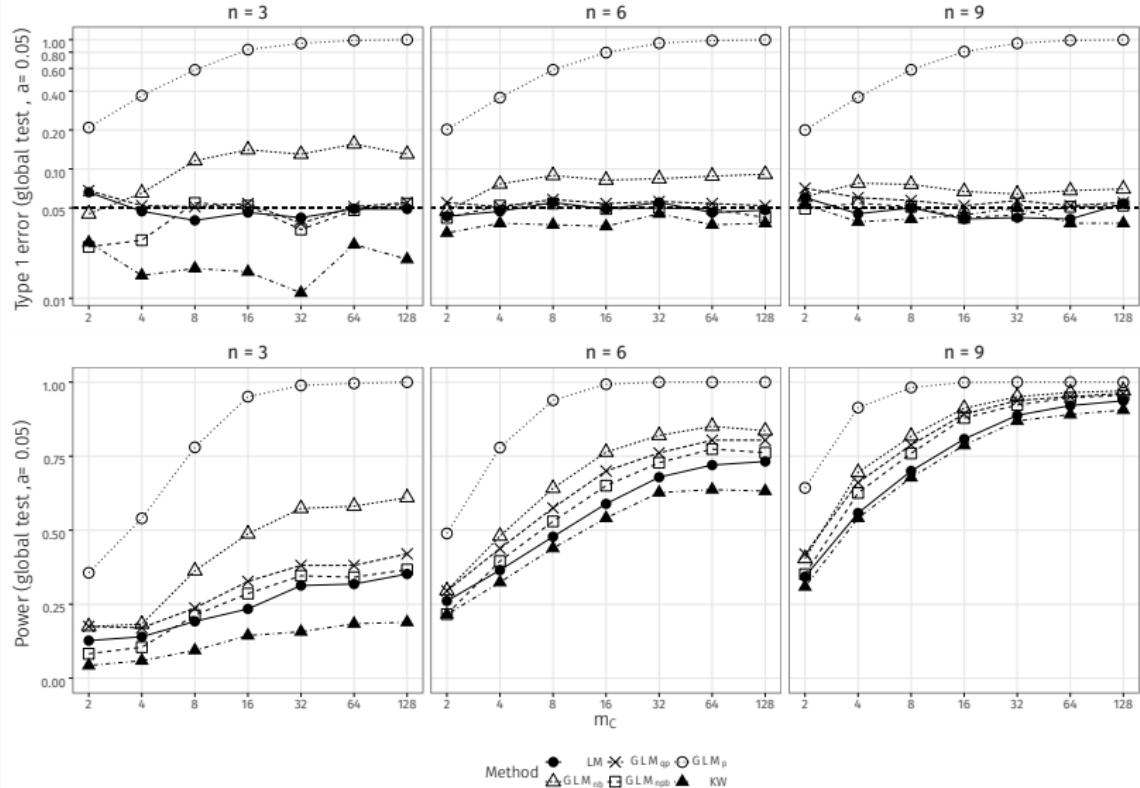
🐦 [@EduardSzoecls](https://twitter.com/EduardSzoecls)

📄 https://github.com/edild/phd_defense

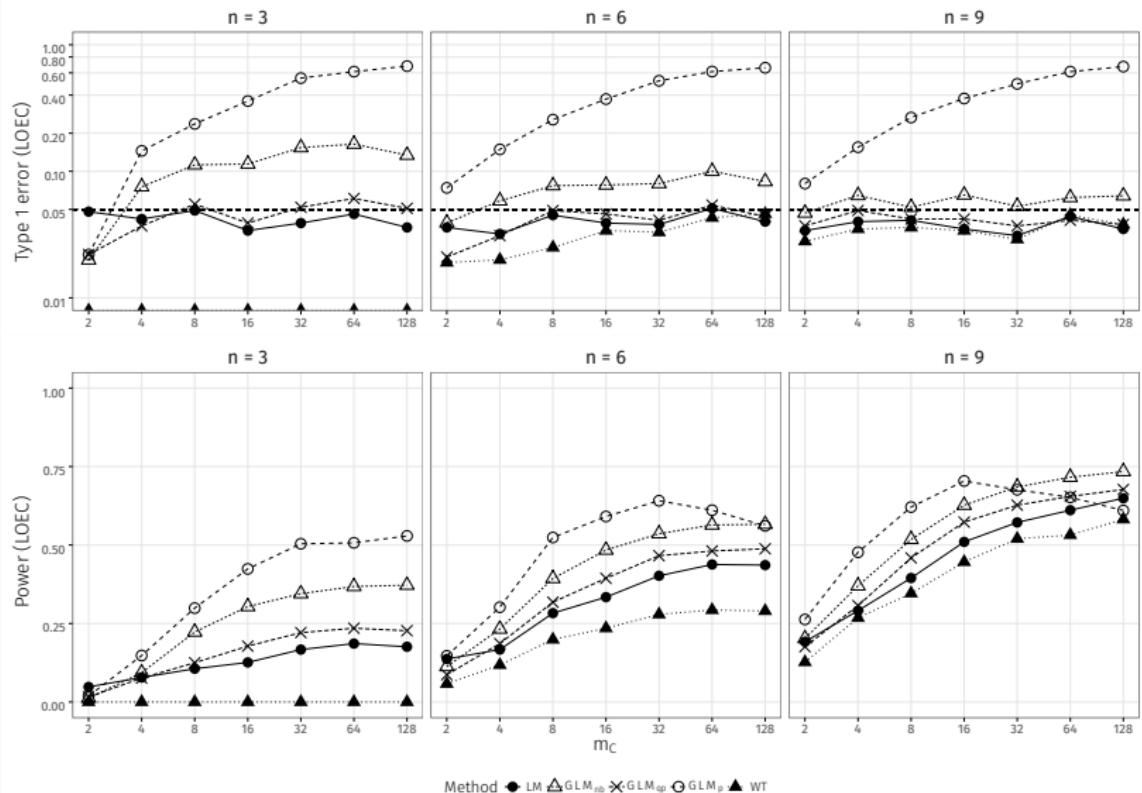
📄 https://github.com/edild/phd_thesis



Power en detail



For LOEC it is even worse



Comparison with Ives...

Szöcs (2015)

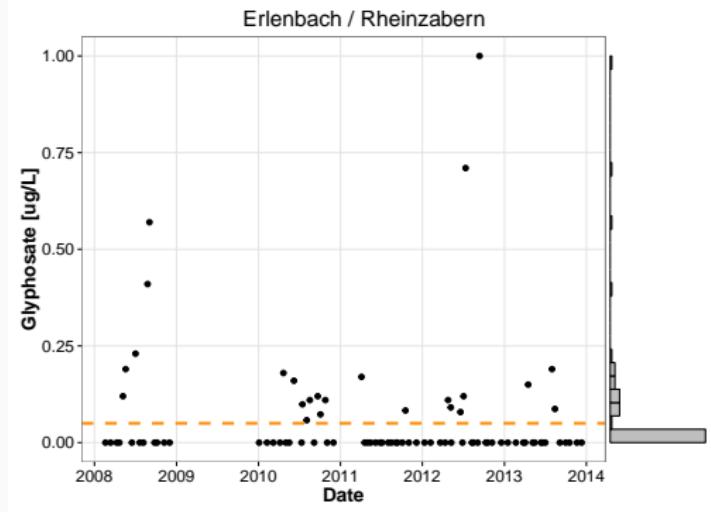
- factorial design
- one predictor
- low replicated
- LM, GLM, bootstrap
- High T1 error of NB
- Quasi-Poisson worked well
- Bootstrap fixes the problems

Ives (2015)

- continuous design
- two predictors
- well replicated
- LM, GLM
- High T1 error of NB
- Quasi-Poisson has problems with multiple predictors
-

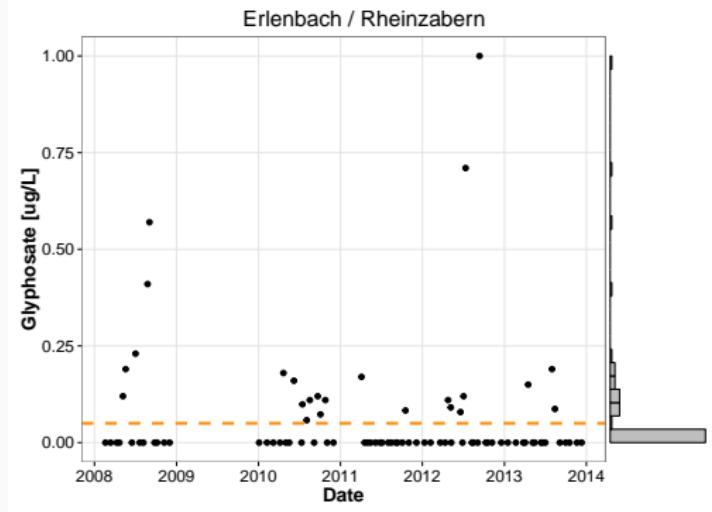
Idiosyncrasies of chemical concentrations

- continuous distribution in \mathbb{R}_0^+
 - censoring
($x < \text{LOQ}$)



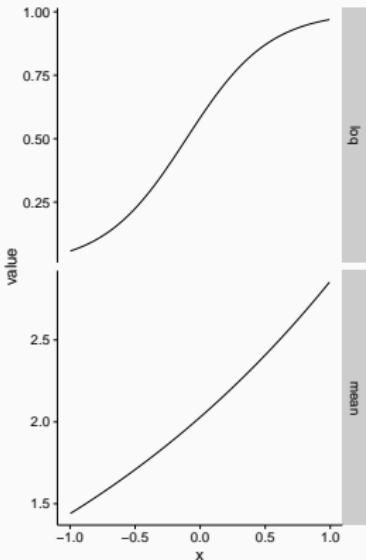
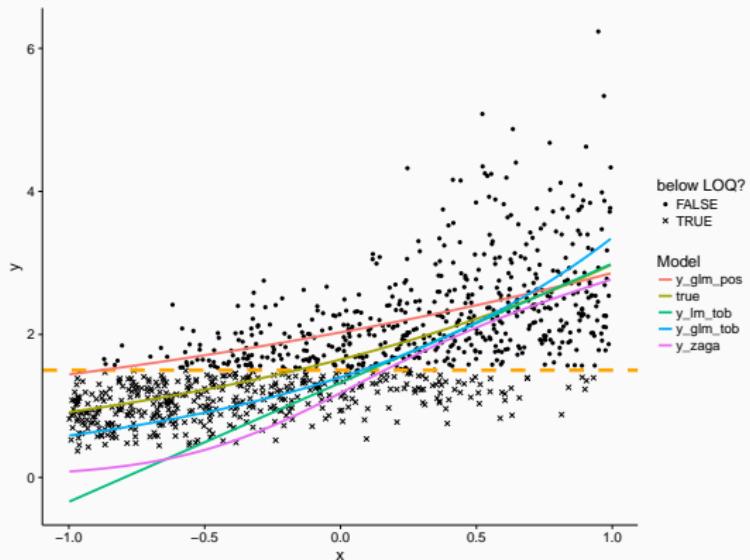
Idiosyncrasies of chemical concentrations

- continuous distribution in \mathbb{R}_0^+
 - censoring ($x < \text{LOQ}$)
 - non-linearity (season, trends)
 - dependency (spatial, temporal)
 - missing data

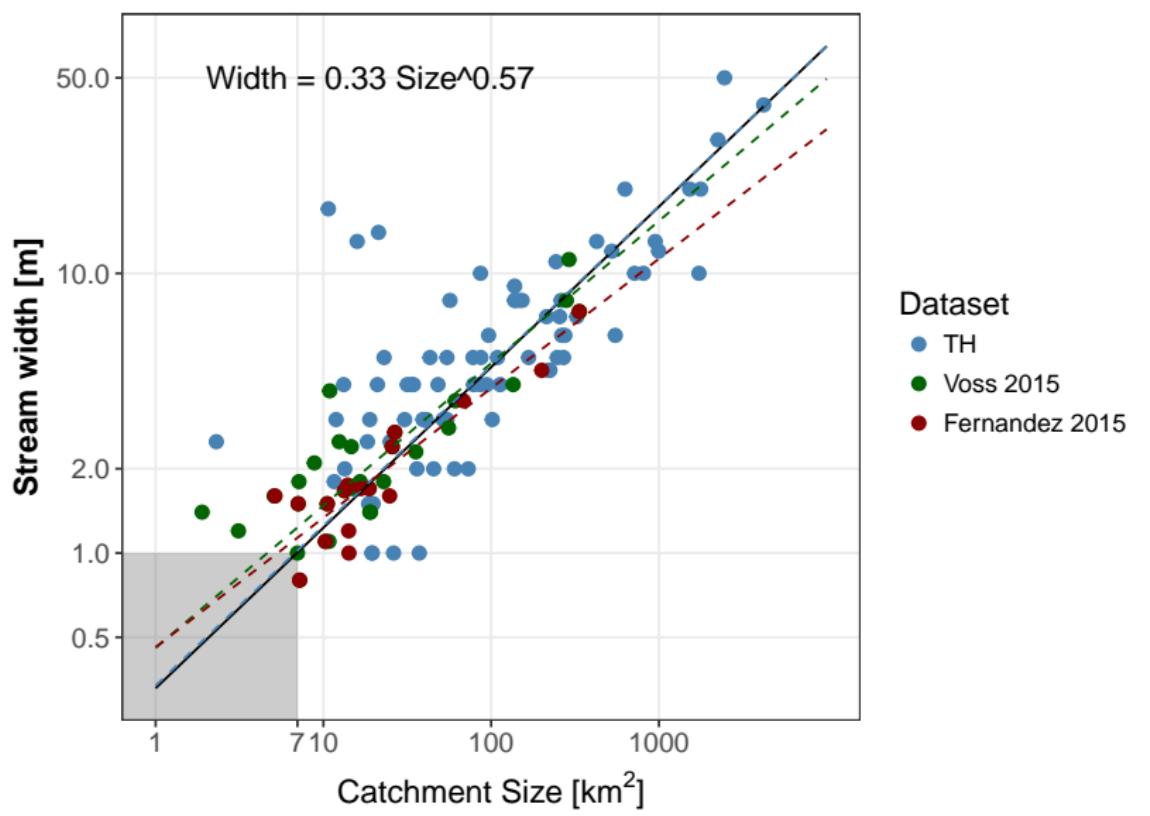


ZAGA what...?

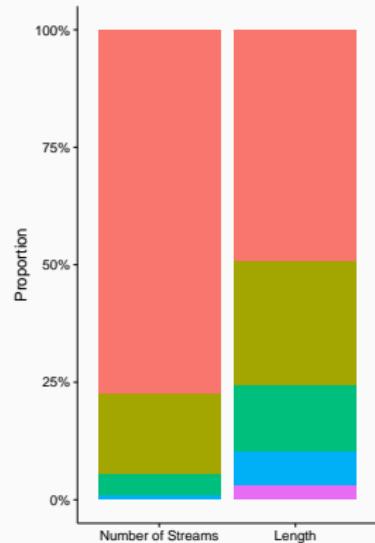
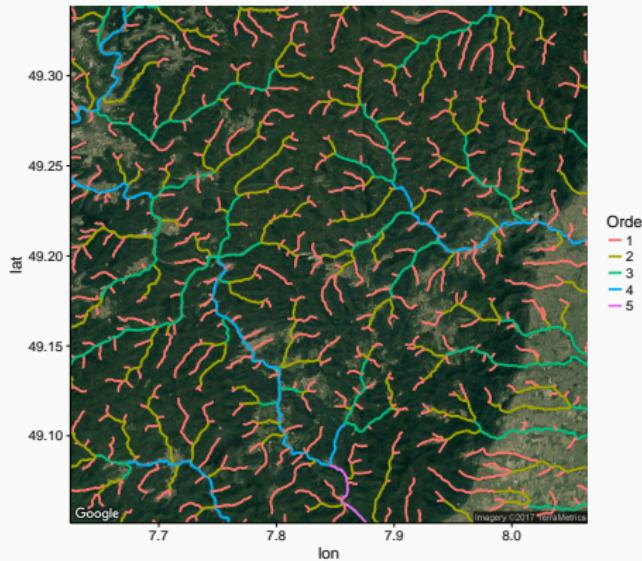
shiny app: <http://uni-ko-ld.de/g4>



Stream size / width



Importance of small streams



- Biodiversity
- Refuge for re-colonisation

Dynamics

Comparison with other studies

Szöcs (2016)

- Germany
- Monitoring
- Grab sampling
- Pesticides
- Neonics + Chlorpyrifos (OP)
- ZAGA (<LOQ)

Stehle (2015)

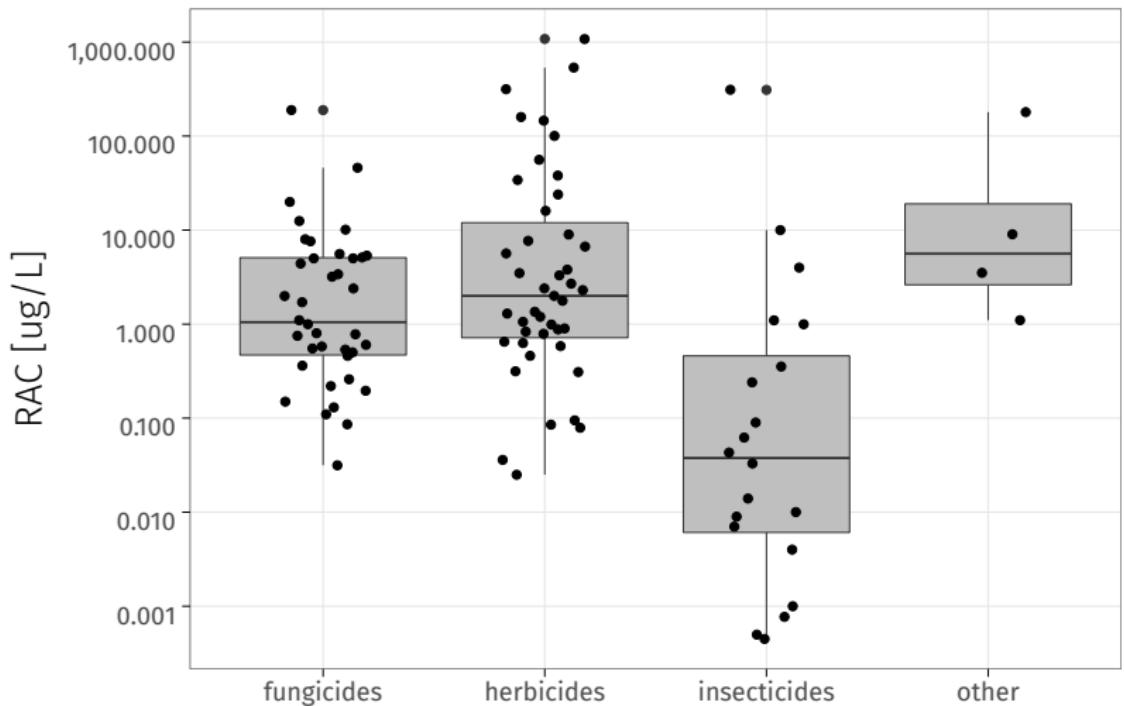
- Europe / Global
- Publications
- Grab & Event driven sampling
- Insecticides
- Organophos.+ Pyrethroids
- LM for >LOQ

Knauer (2016)

- Switzerland
- Monitoring
- Grab sampling
- Pesticides
- Chlorpyrifos + Herb + Fung
- no model

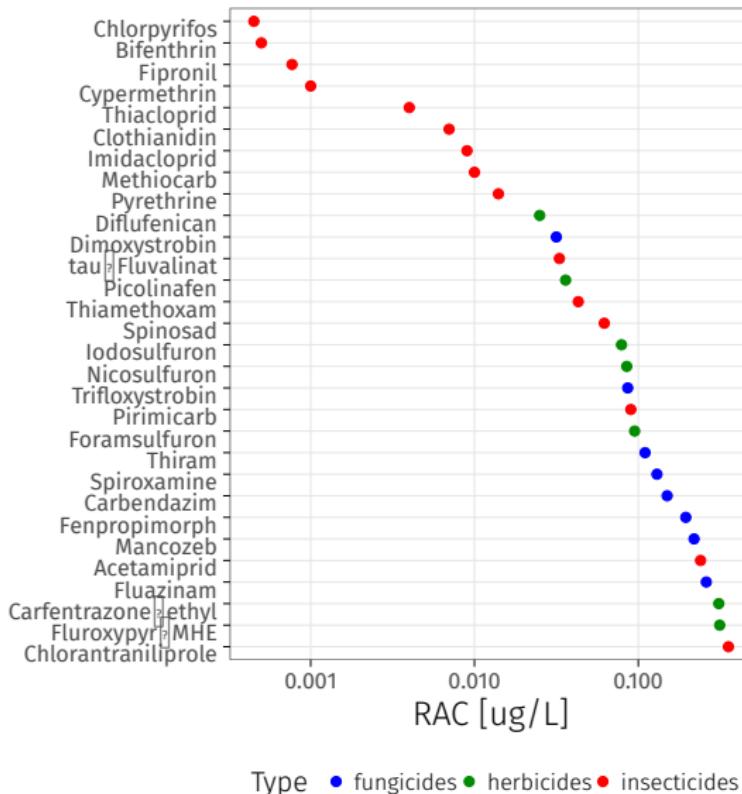
RACs by Type

105 RACs provided by UBA splitted by group

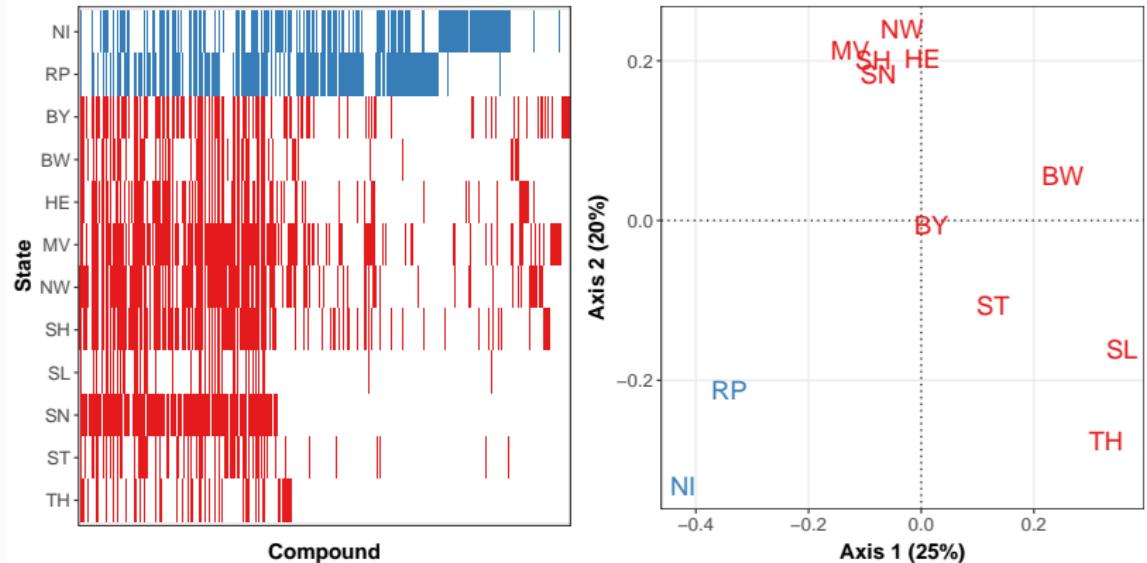


RACs by Compound (Add Stehle to plot...)

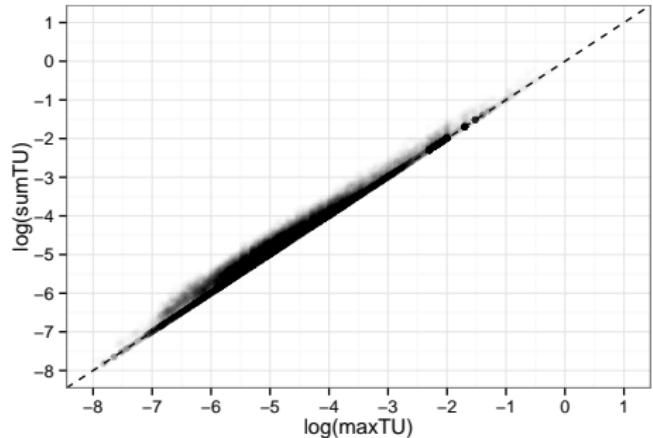
30 lowest RACs



Analysed compound spectra by state



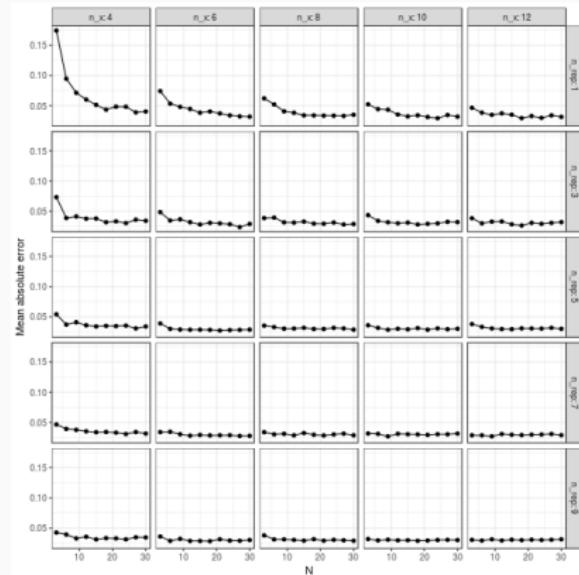
Mixtures are common, but one compound dominates the risk



- up to 50 compounds in one sample
- high correlation
- ~ 0.5 TU increase
- mainly one compound responsible for risk

Simulations are worth their work, use them *a priori*!

Experimental design for dose-response experiments - a simulation
http://edild.github.io/lc50_bias_sim/



GLM-Explorer: <http://uni-ko-lid.de/g3>

Reasons for observed RAC exceedances

- Risk Mitigation fails
 - Risk mitigation measures (erosion rills, wind)
 - Farmer do not adhere (GAP, no spray zones)
- Risk Assessment fails
 - Exposure Assessment
 - Models not working (Knäbel et al.)
 - Effect Assessment
 - Missed sensitive species
 - New document asks also for insects

Risk Mitigation Measures

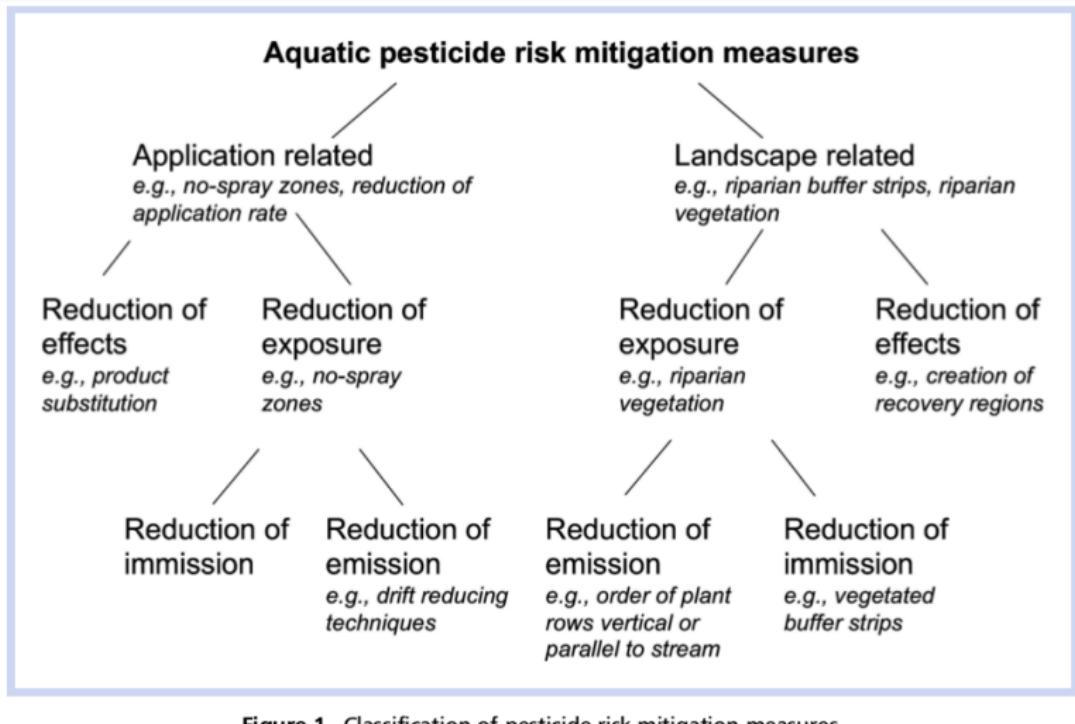
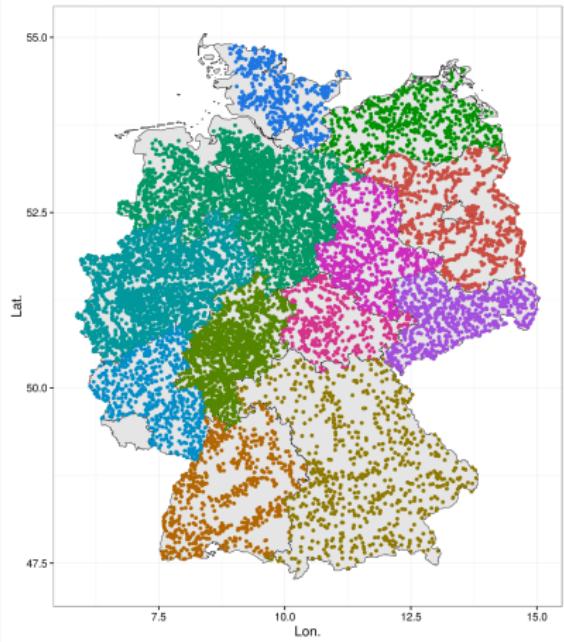


Figure 1. Classification of pesticide risk mitigation measures.

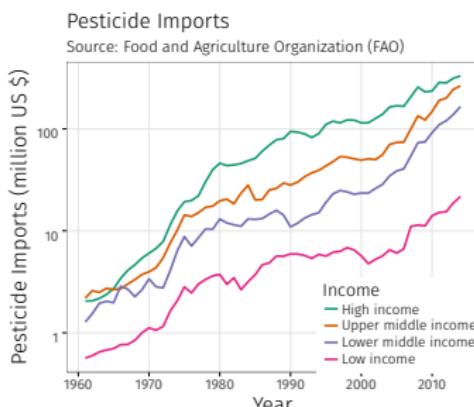
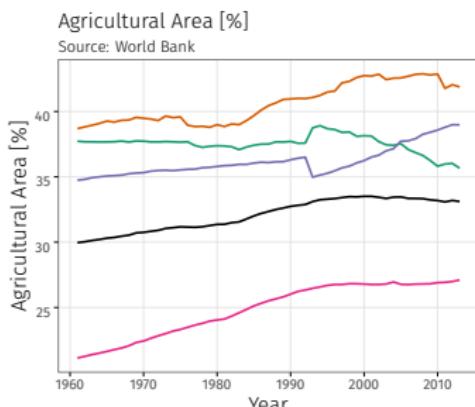
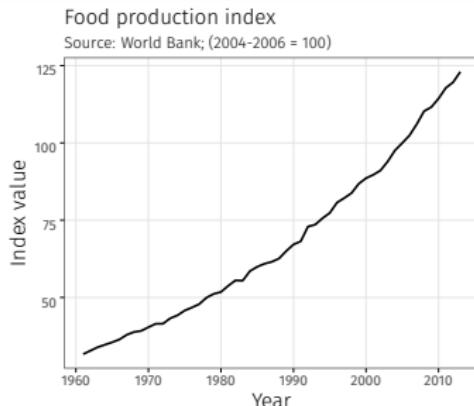
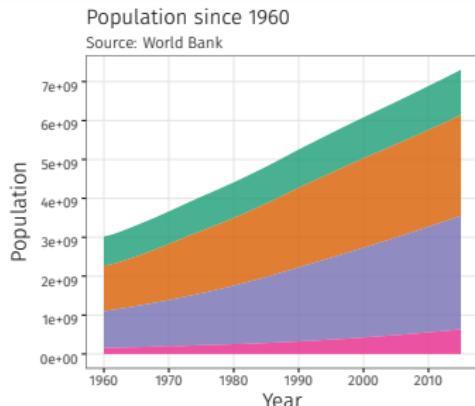
Bereswill, Streloke, Schulz (2014). Risk mitigation measures for diffuse pesticide entry into aquatic ecosystems: Proposal of a guide to identify appropriate measures on a catchment scale: Guide to Identify Pesticide Risk Mitigation Measures. IEAM 10, 286–298.

Biotic field effects



- biological data with good spatial coverage
- 60% of spatial congruence
- Large scale effects largely unknown.
- Some work left...
- Future....

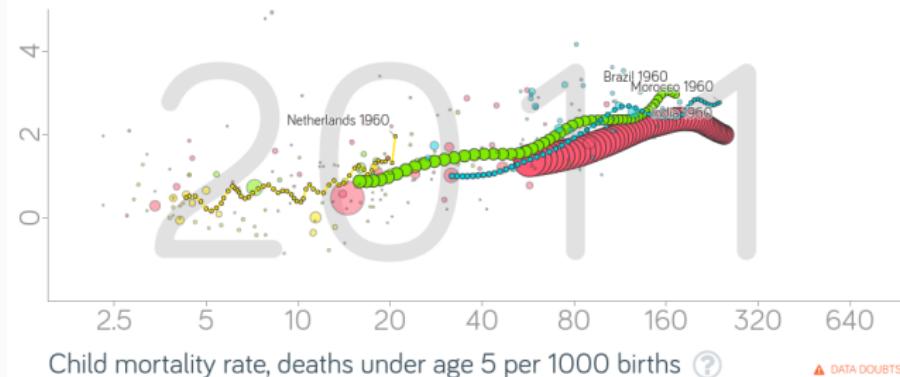
A global perspective (I)



Source code to retrieve data and reproduce results: <http://uni-ko-l.de/g7>

A global perspective (II)

Population growth, annual % ⓘ



Software availability

Stable versions on CRAN, dev versions on github.

`webchem` github.com/ropensci/webchem

`taxize` github.com/ropensci/taxize

Best practices for Software:

- open source (permissive MIT License)
- version control (git)
- automated tests (Travis-CI)
- in source documentation (roxygen)