Statistical Ecotoxicology - Improving the utilization of data for ecological risk assessment

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Landau, 22.09.2016

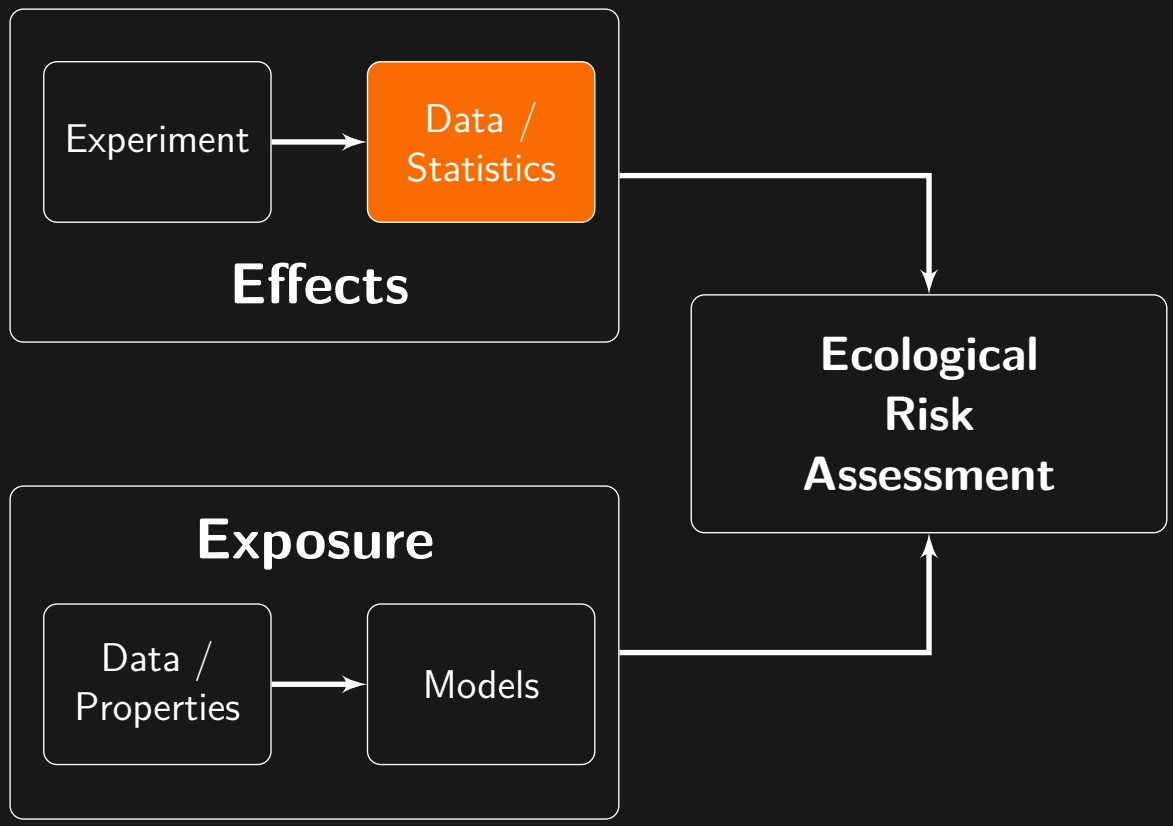
My field of research is somewhere between...

... Eco(-toxico)logy, Data Analysis & Programming

Statistical Ecotoxicology

Current use in ecotoxicology

- Ecological risk assessment (ERA) relies on statistics



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- Experiments with low replication

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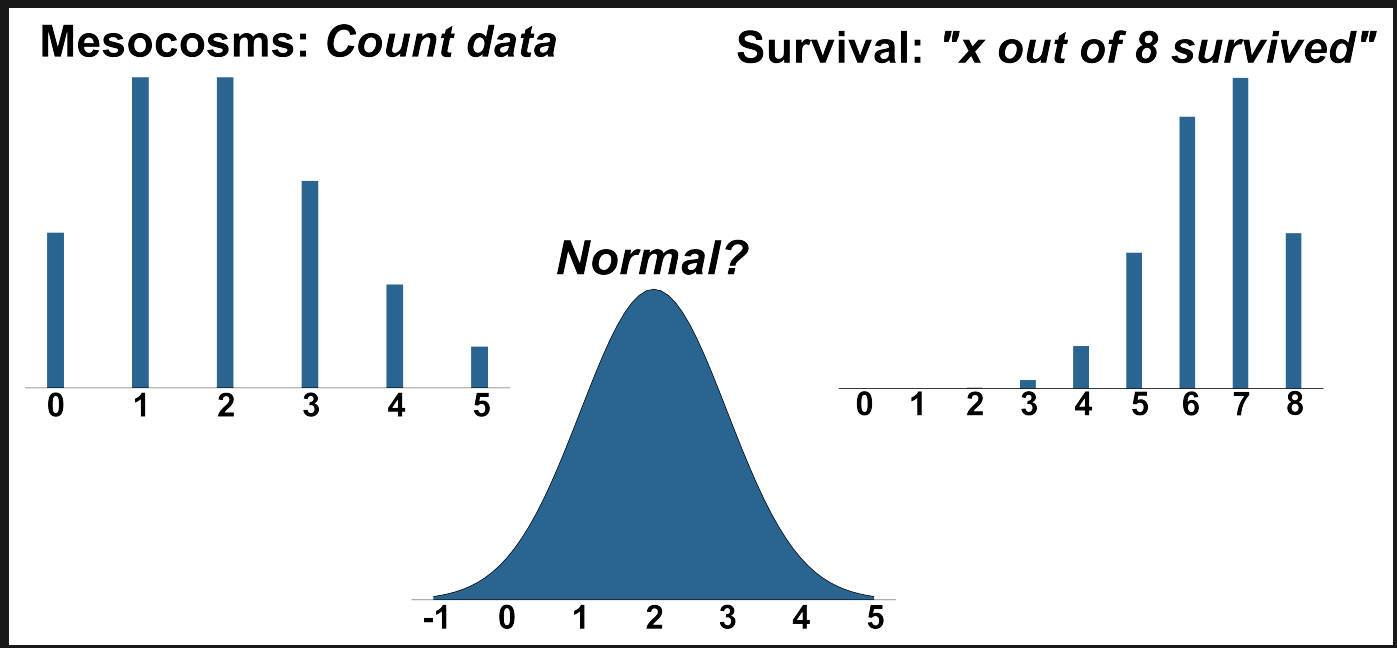
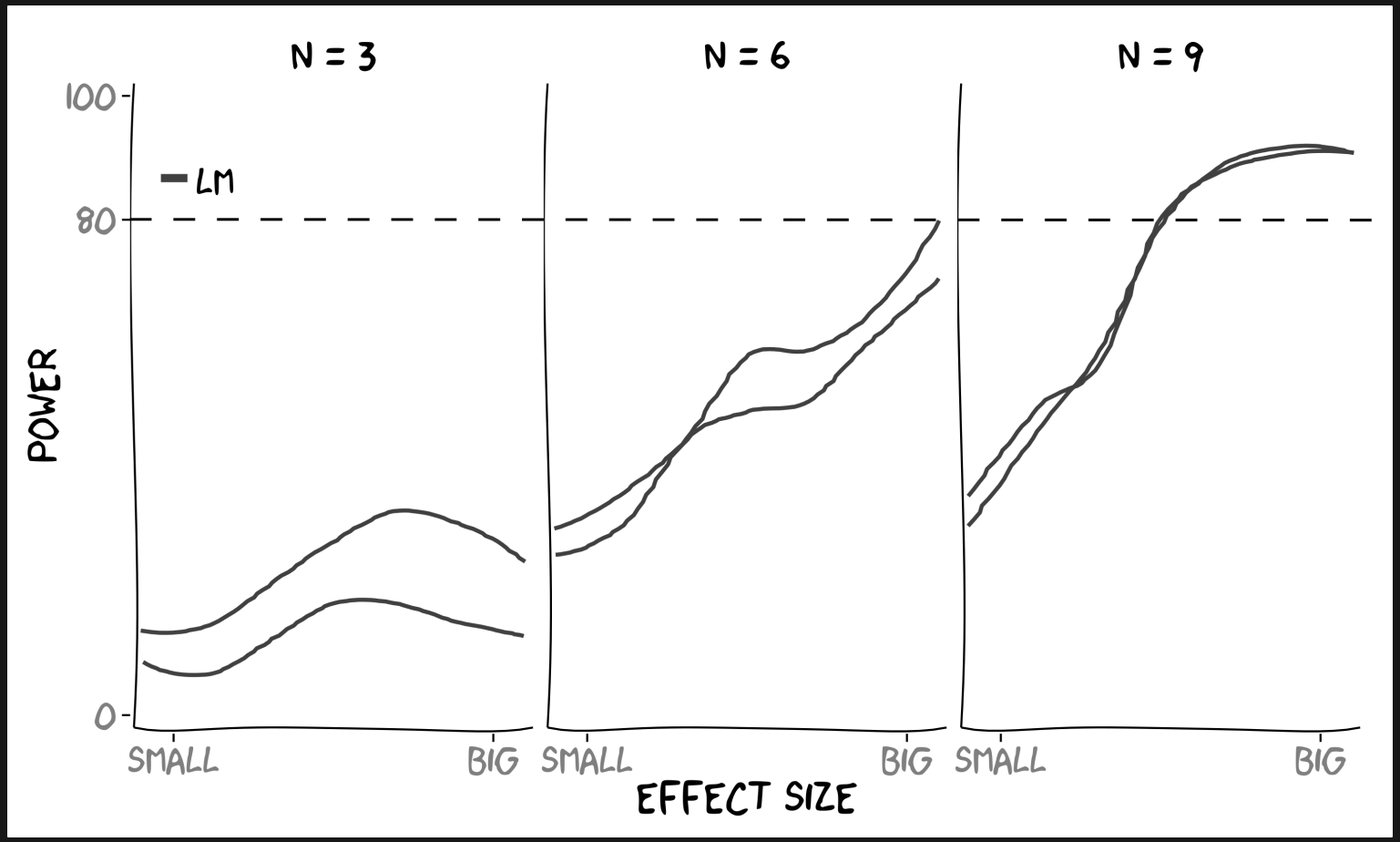
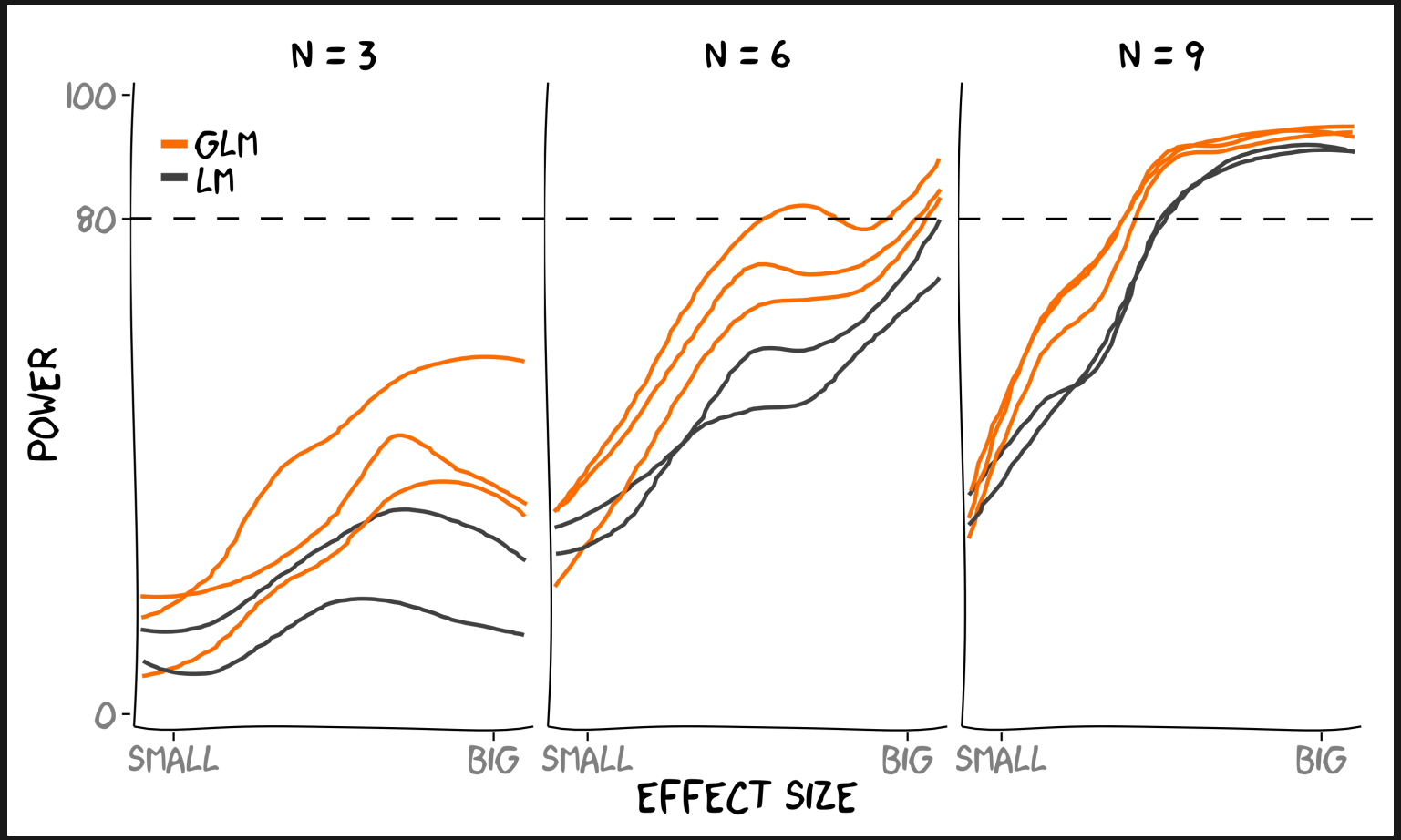
- Ecological risk assessment (ERA) relies on statistics
- Experiments with low replication
- Usually analysed using Linear Models of transformed data
- Null Hypothesis Significance Testing (=> NOEC)



Statistical Power in current experimental designs in ecotoxicology is unacceptably low



Generalized Linear Models can do better



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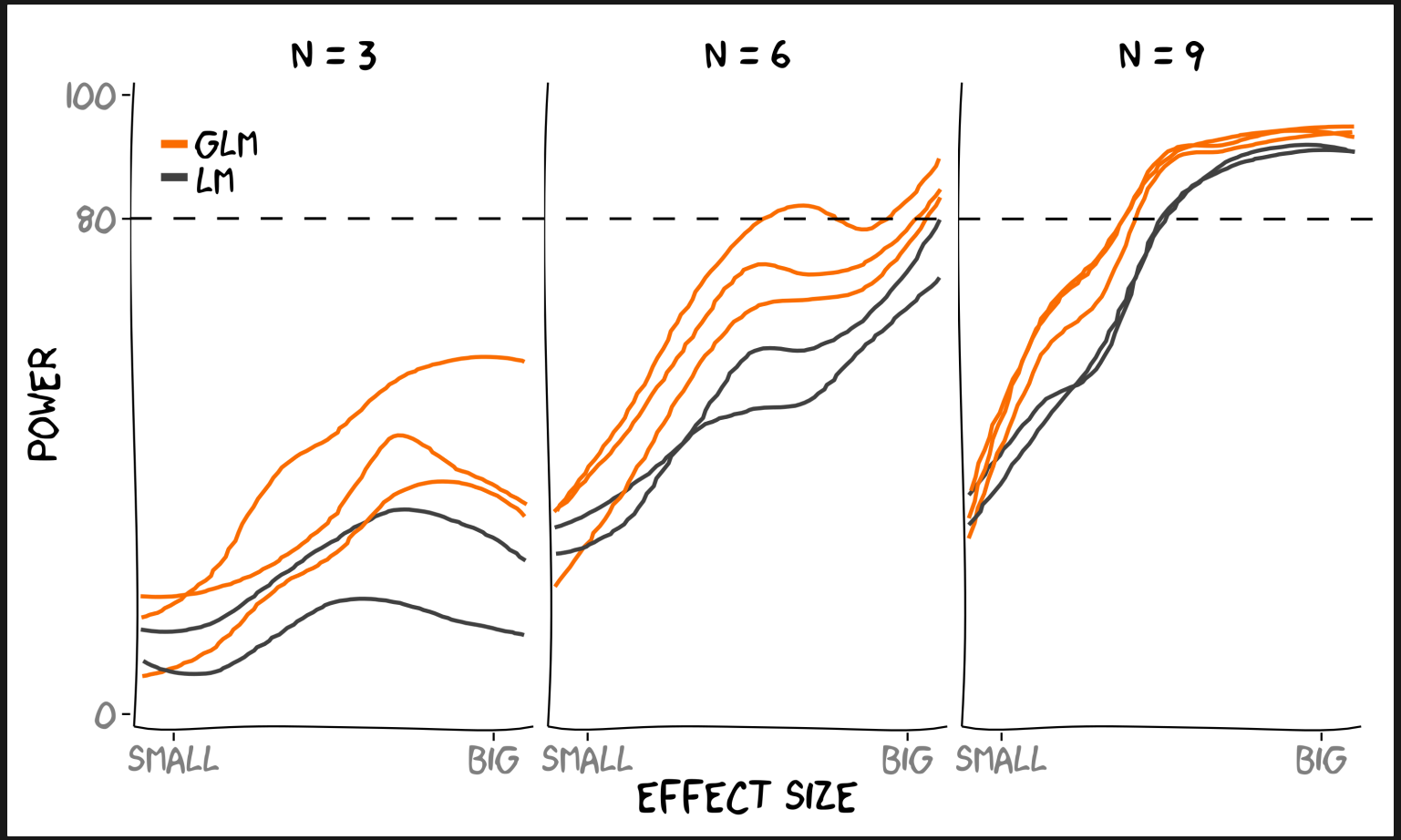

Better abandon NOEC and use a regression design [1]...

[1] debated since 30 years.

Monitoring Data

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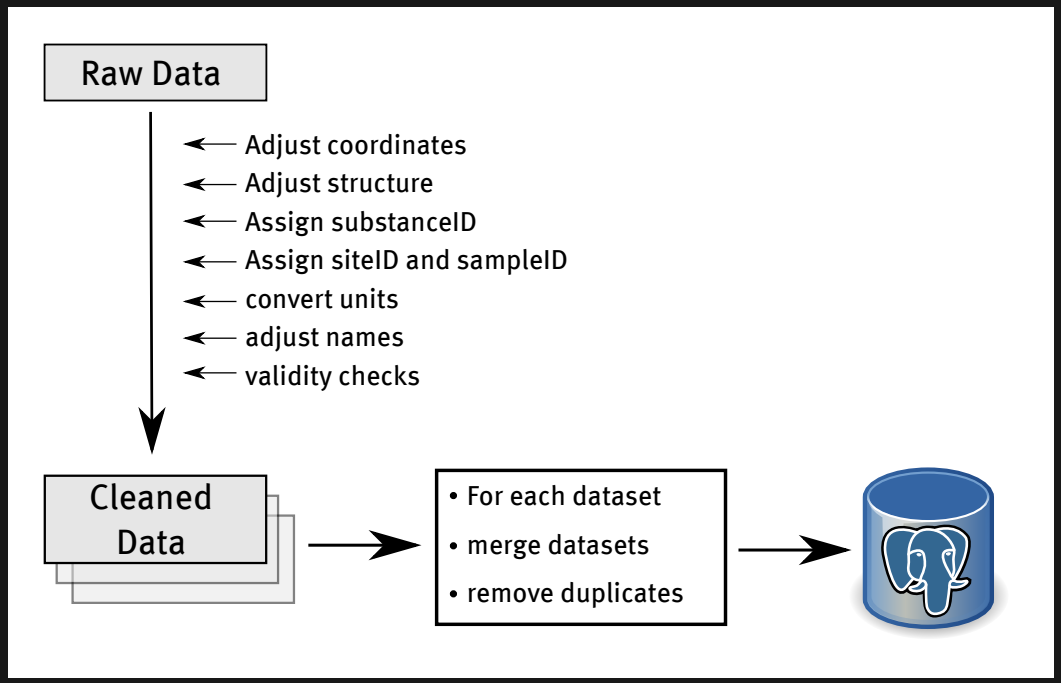
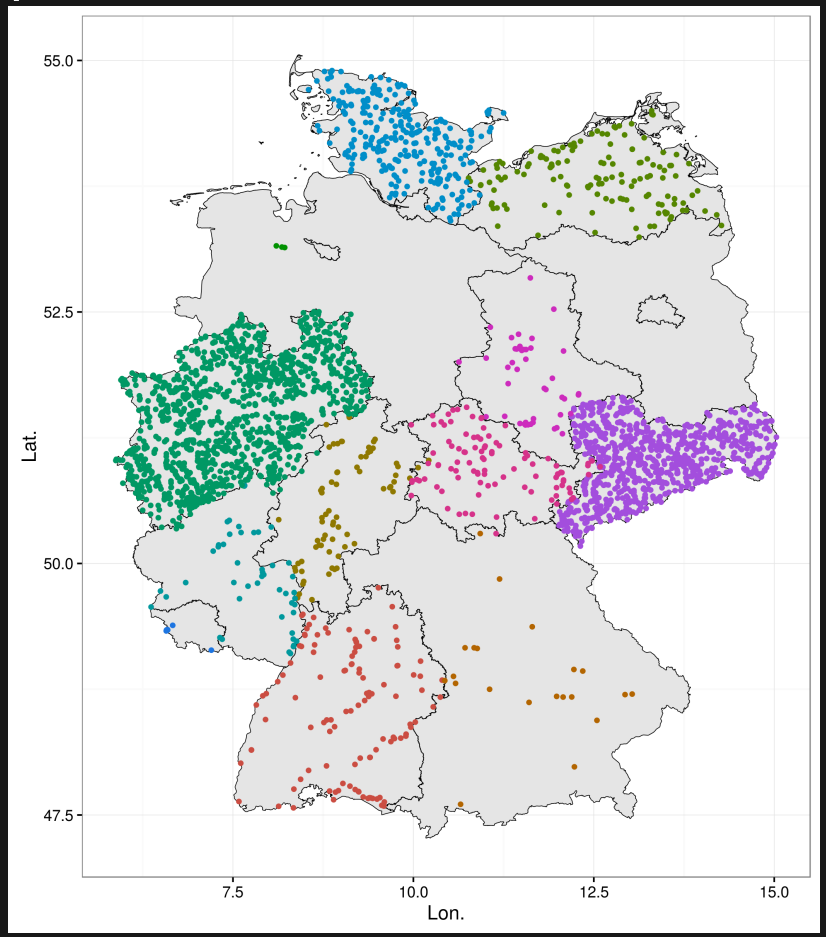
- ... provides the biggest amount of data available
- ... is really messy



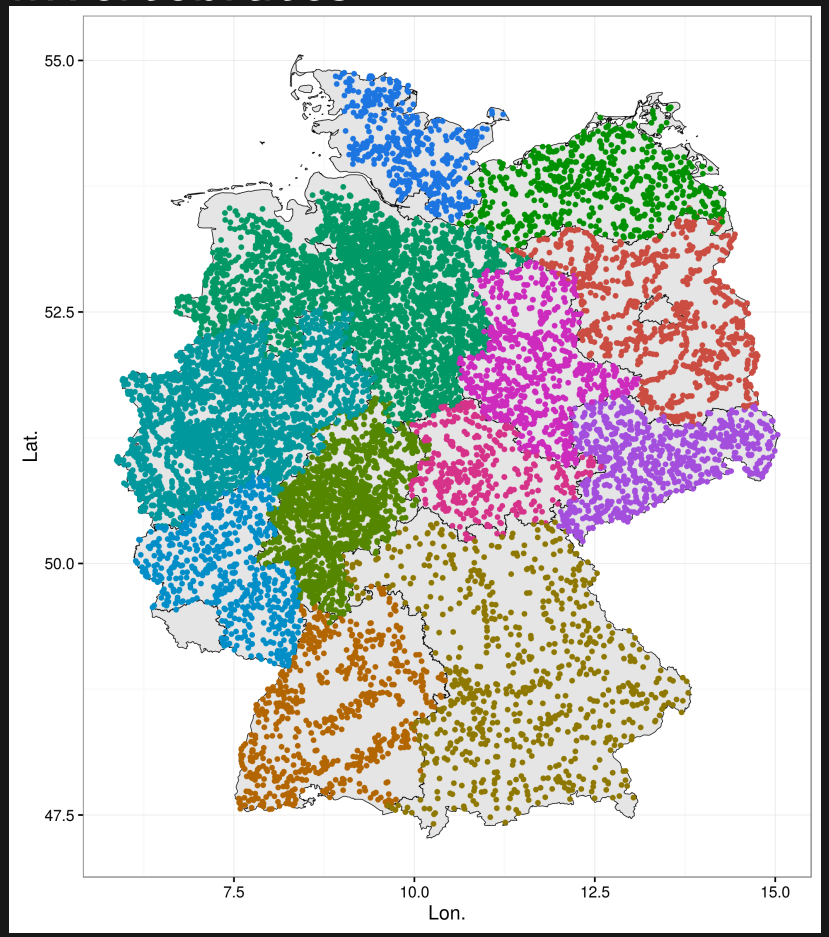
The biggest currently available dataset on

pesticides



3,000 sites, 45,000 samples, 500 pesticides

invertebrates



14,000 sites, 27,000 samples, 3000 taxa

Additional data on

Sites

- catchment size
- agriculture within catchment

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Compounds

- RAC, LC50, EQS
- chemical group
- identifiers
- properties

Results - Thresholds

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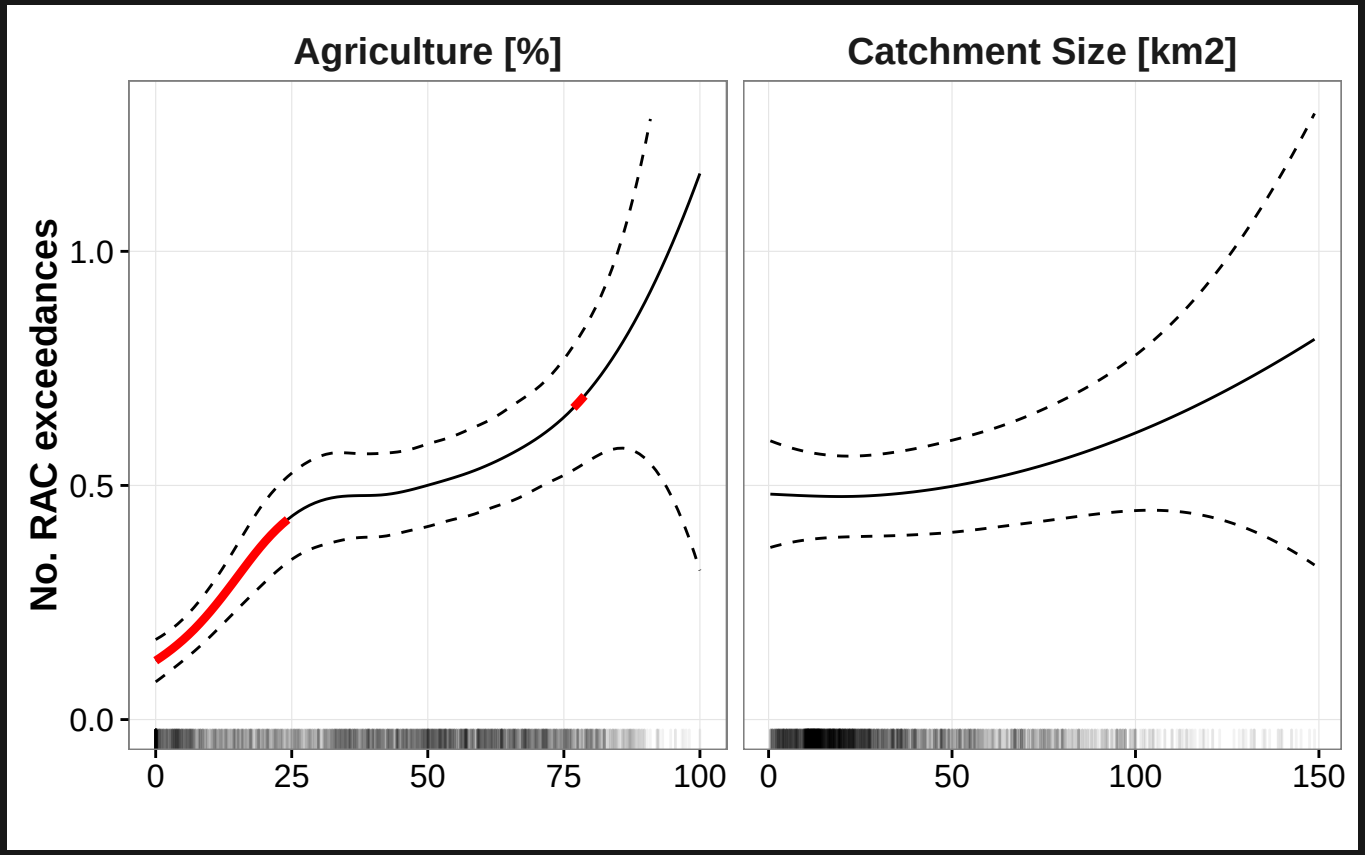

Results - Precipitation & Seasonality

- Used a mixture model

$$RQ_i \sim ZAGA(\mu_i, \sigma, \pi_i) = \begin{cases} (1 - \pi_i) & \text{if } y < LOQ \\ \pi_i \times f_{Gamma}(\mu_i, \sigma) & \text{if } y \geq LOQ \end{cases}$$

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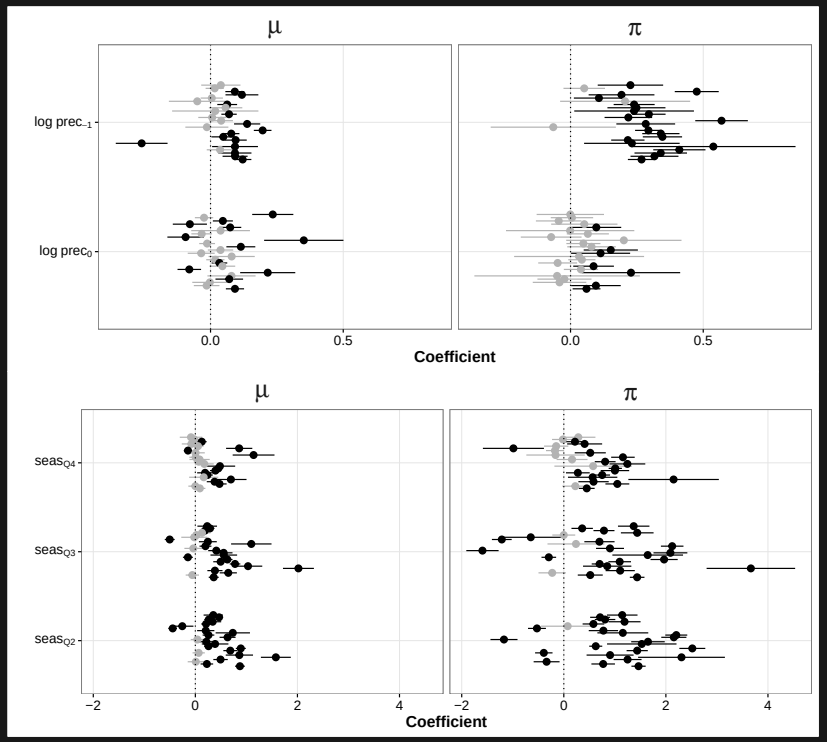

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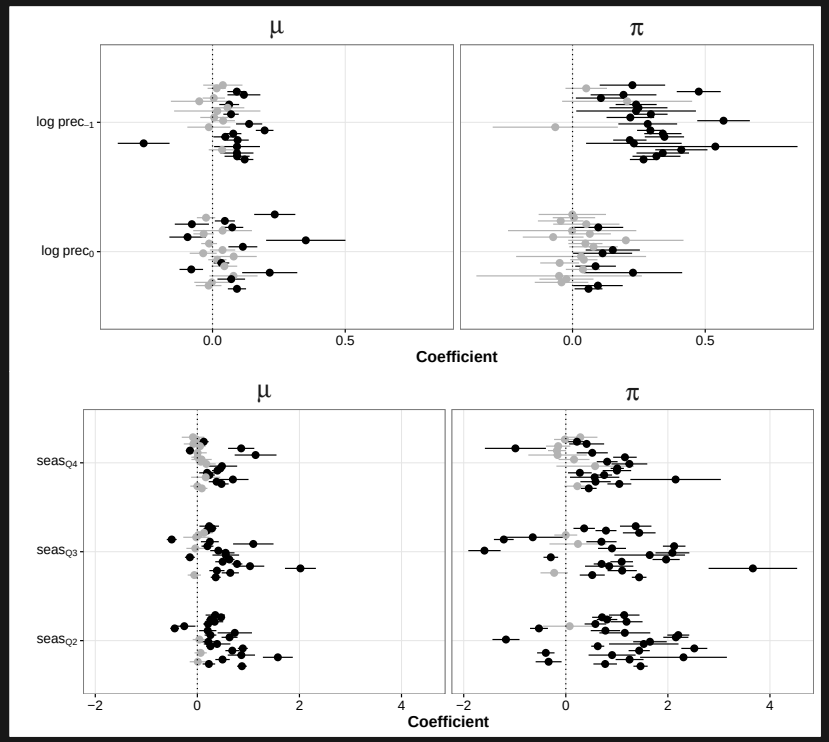
- Precipitation and Quarter as predictors
- Site within state as random intercept
- Precipitation before sampling increases RQ
- Summer higher RQ, but compound specific



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- most streams are *small*
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- High risk of pollution
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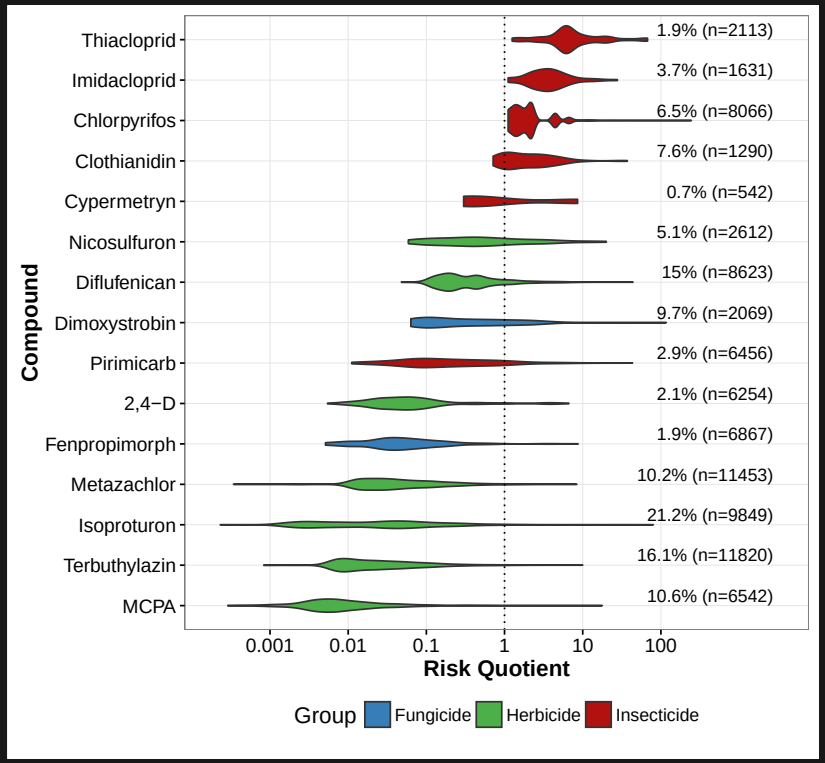
- Neonicotinoids
- up to 244x RAC
- ecological effects likely



Software

Biologists and Chemists face similar problems...

Names

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

Chlorpyrifos, Chlorpyriphos,
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Hymenoptera/ Apoidea/ Megachilidae/ Osmia/ rufa

organophospate, ester, insecticide

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

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Amount of data

2993 taxa

489 pesticides
(+ 590 other organics)

Instead of wasting time...

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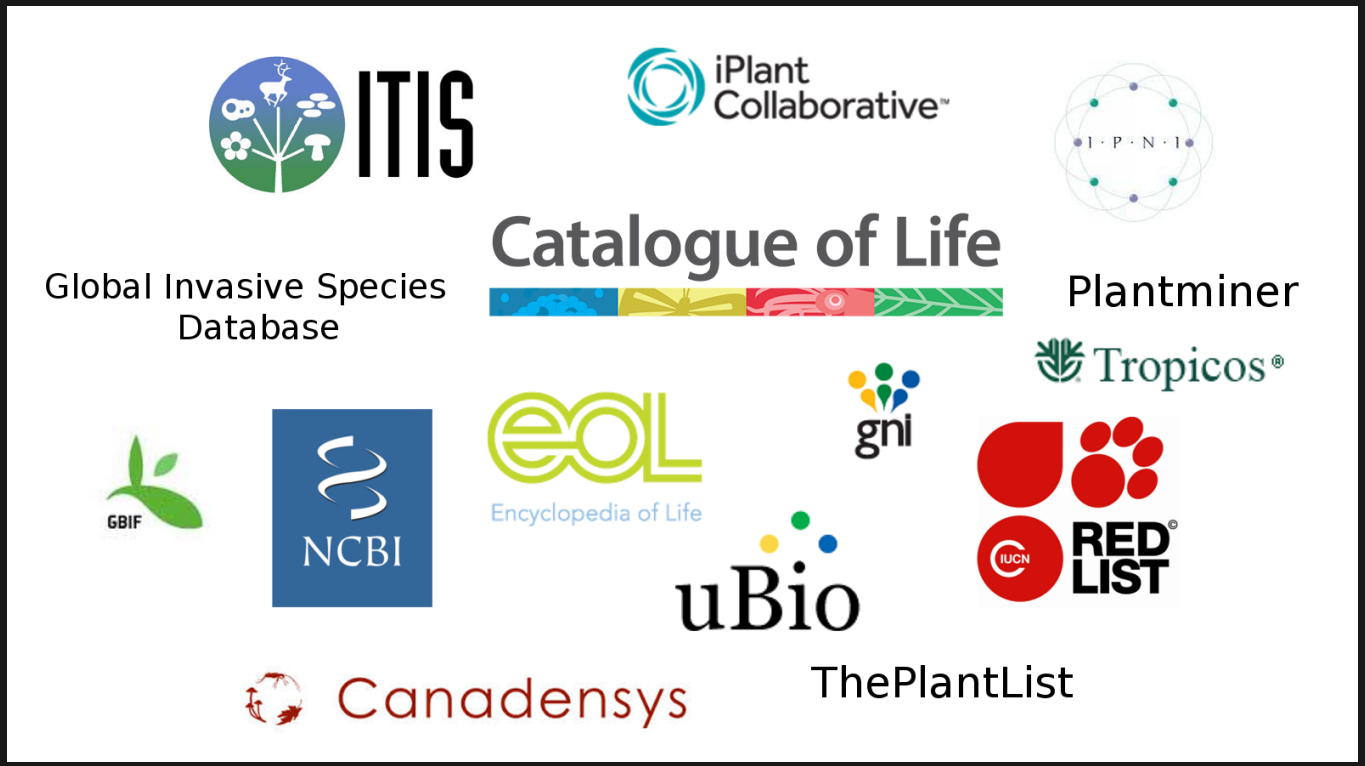
taxize - taxonomic search and retrieval in R



RopenSci

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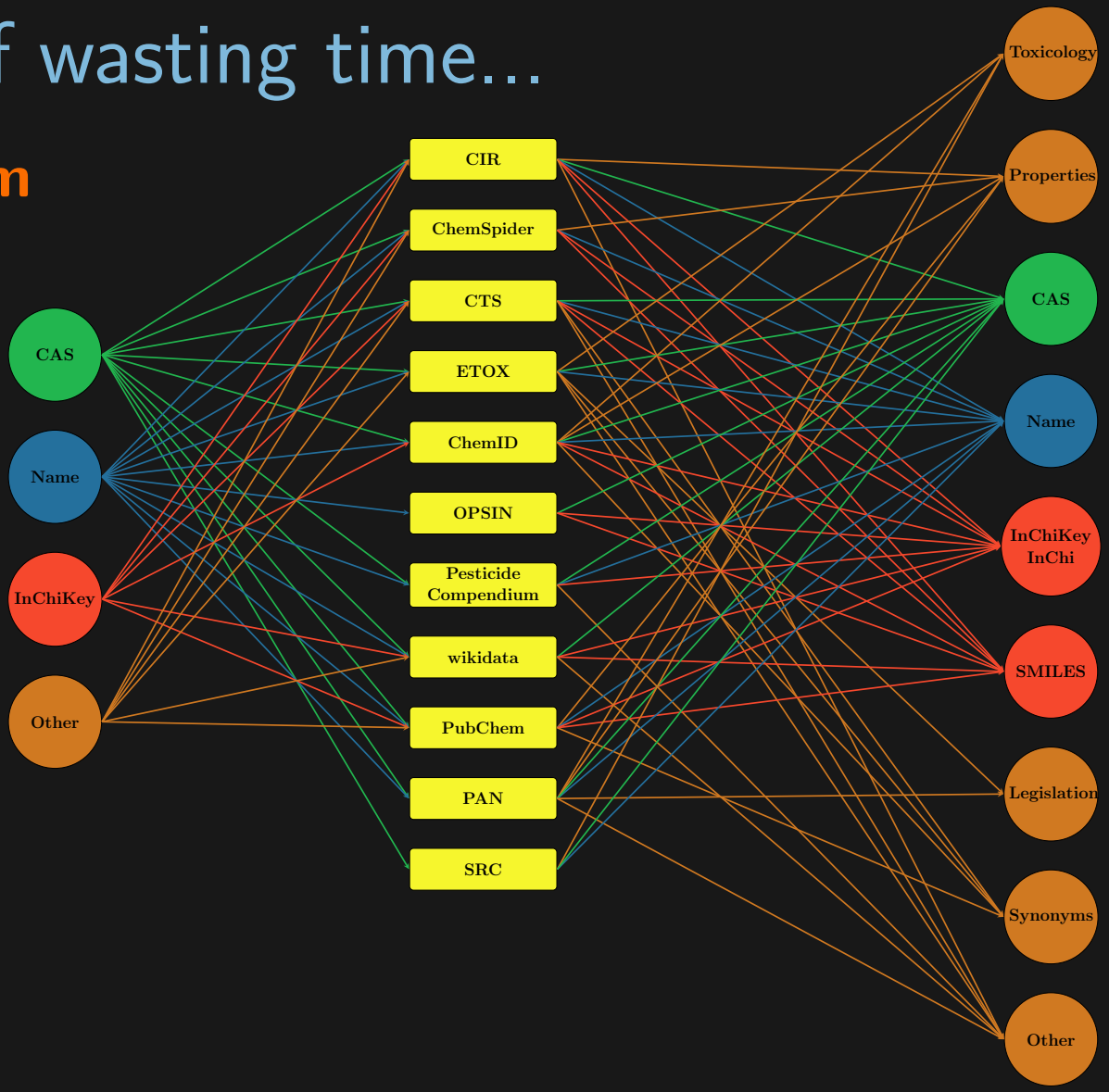
webchem



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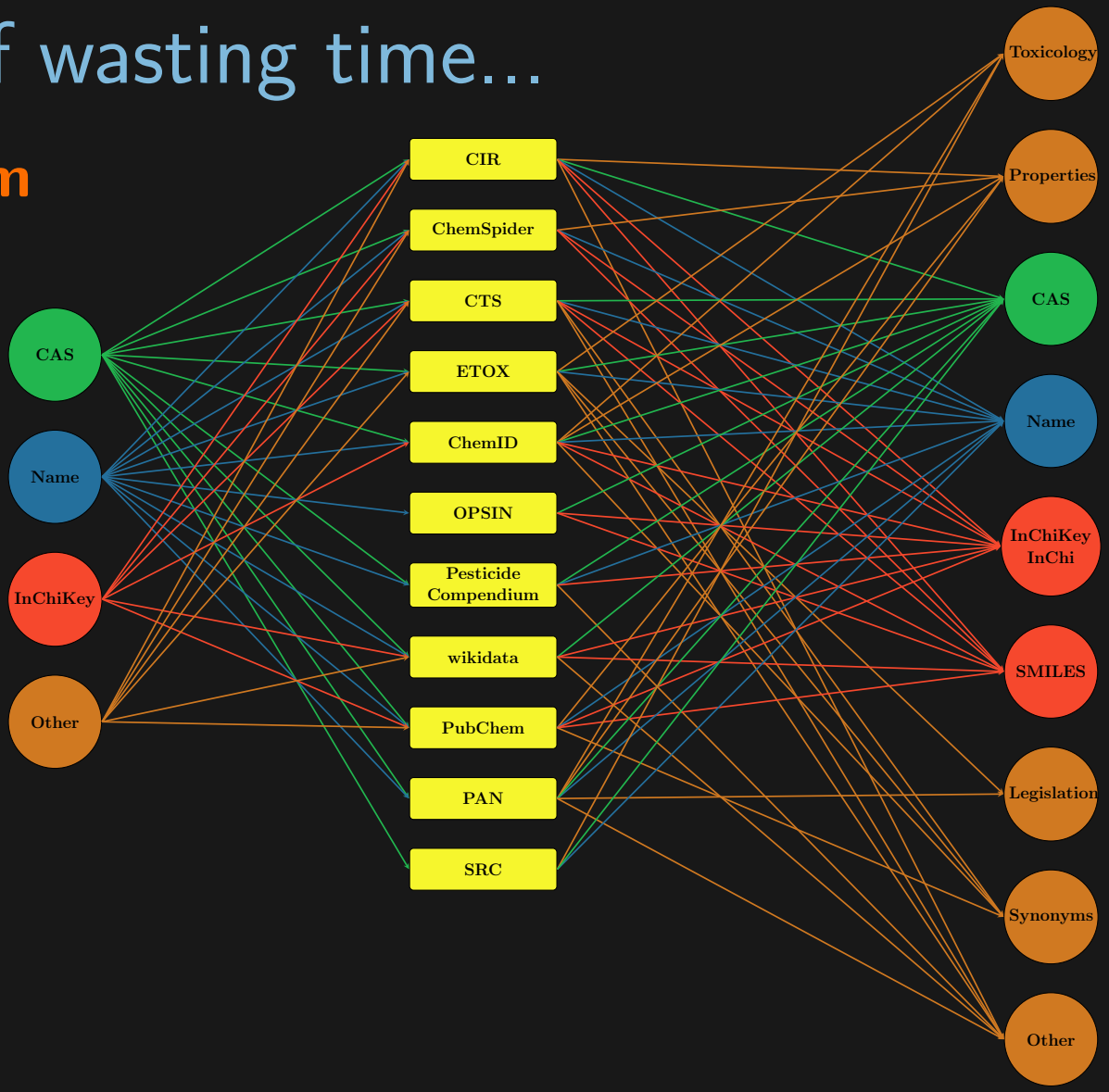

"webchem ...likely saved hundreds of working hours"

Münch (2016)

Conclusions from my PhD

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- Monitoring data can be used to
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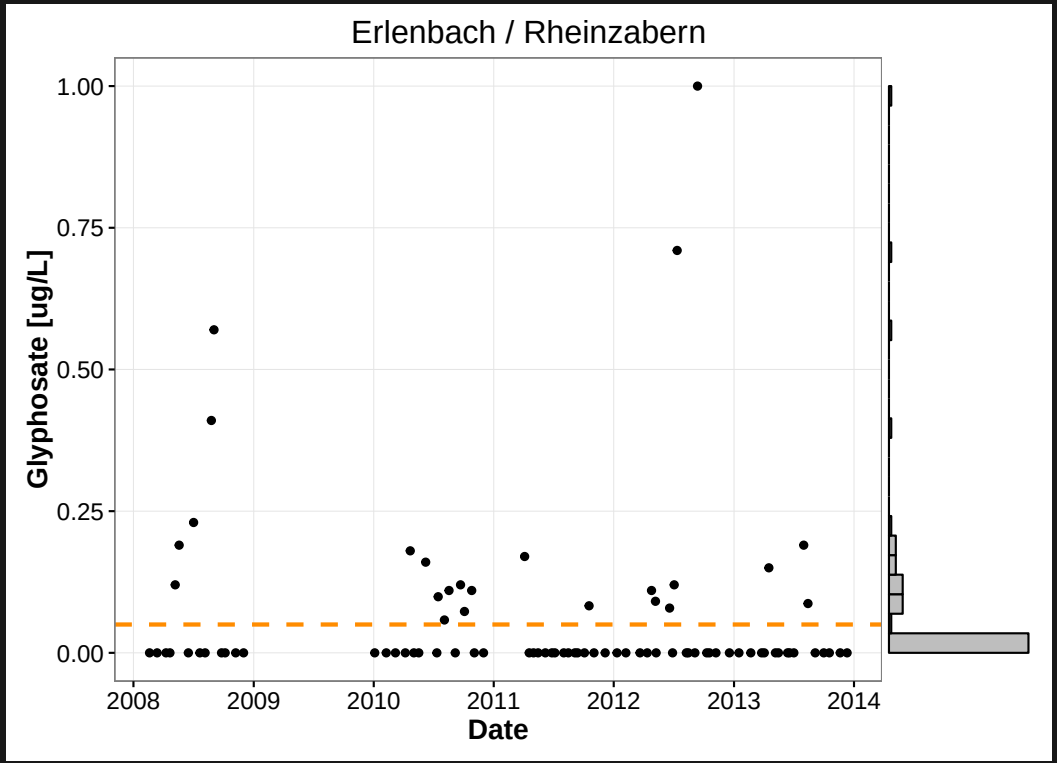
- SWB at risk
- Handling big eco(toxico-)logical data not easy
  - now easier

Outlook

Analysing chemical concentrations is not easy, because of

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



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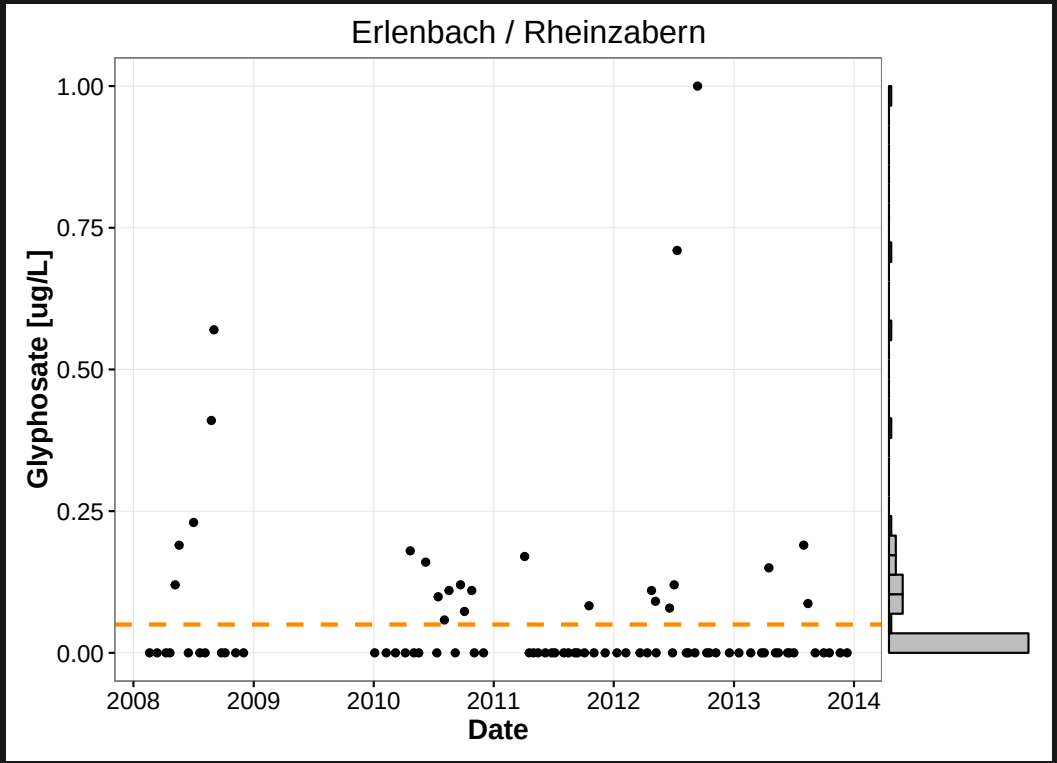
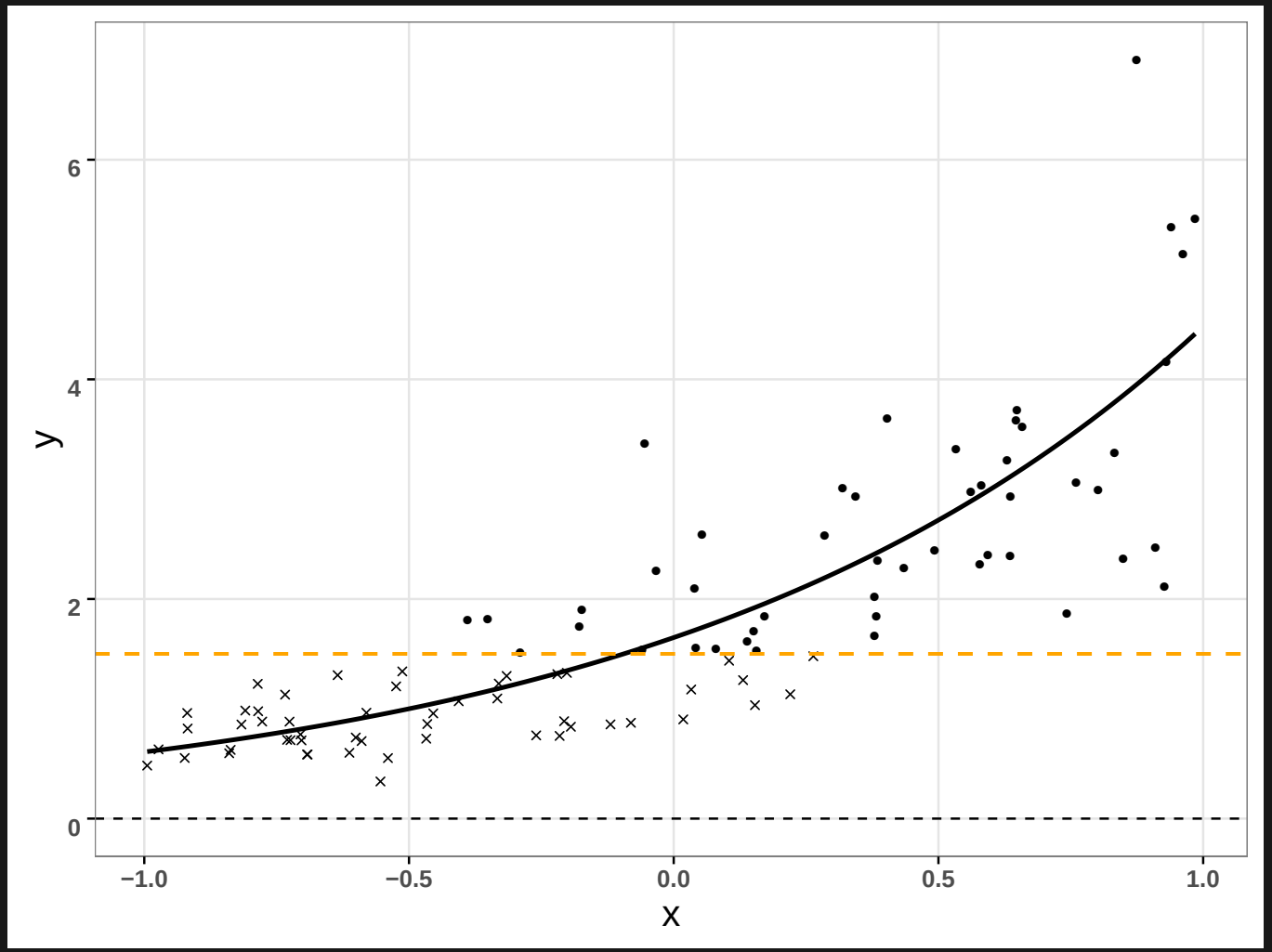
- continuous distribution in $\mathbb{R}_0^+$
- censoring (x $<$LOQ)
- non-linearity (season, trends)
- dependency (spatial, temporal)



Dealing with censored, non-normal data



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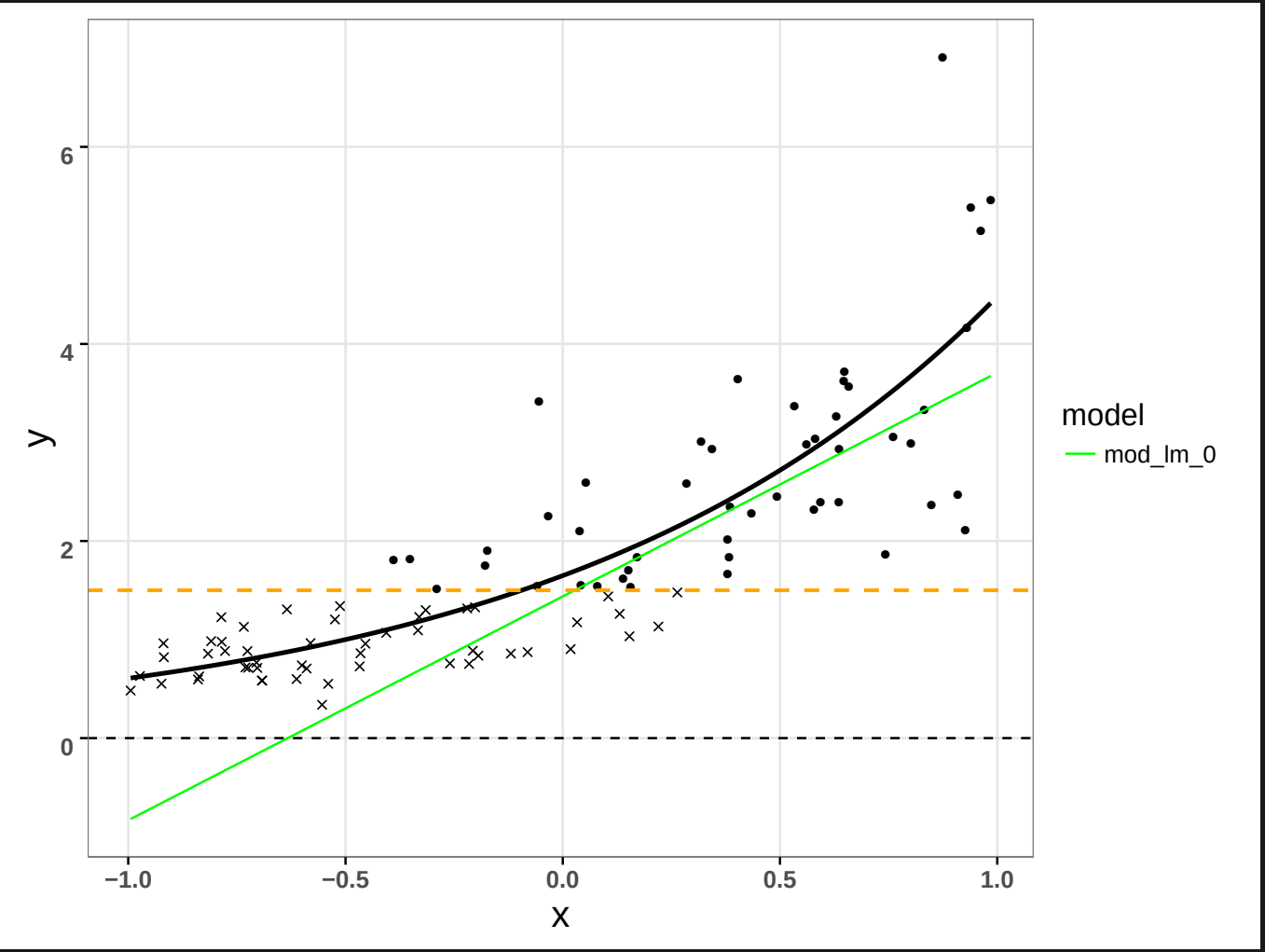

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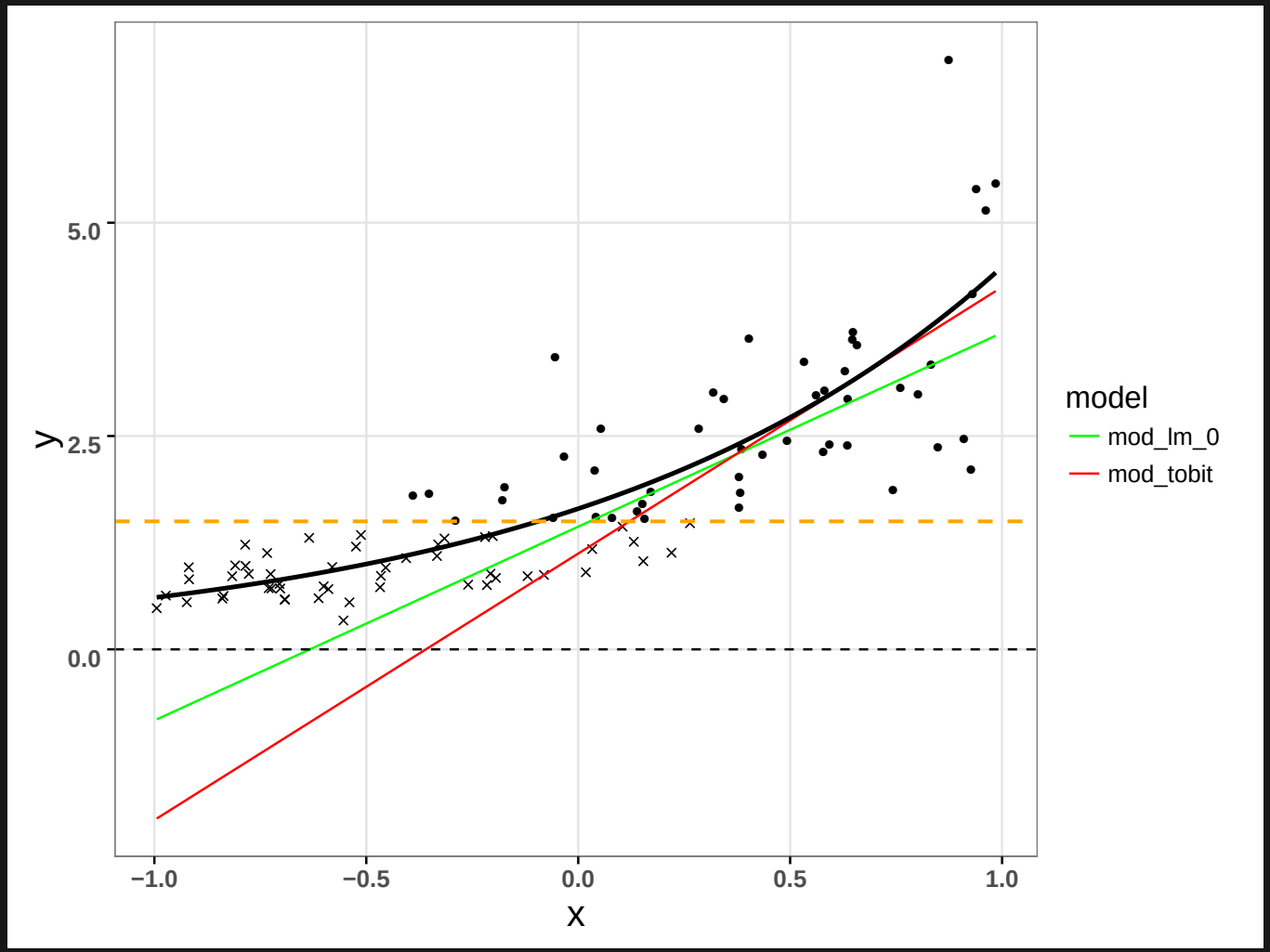

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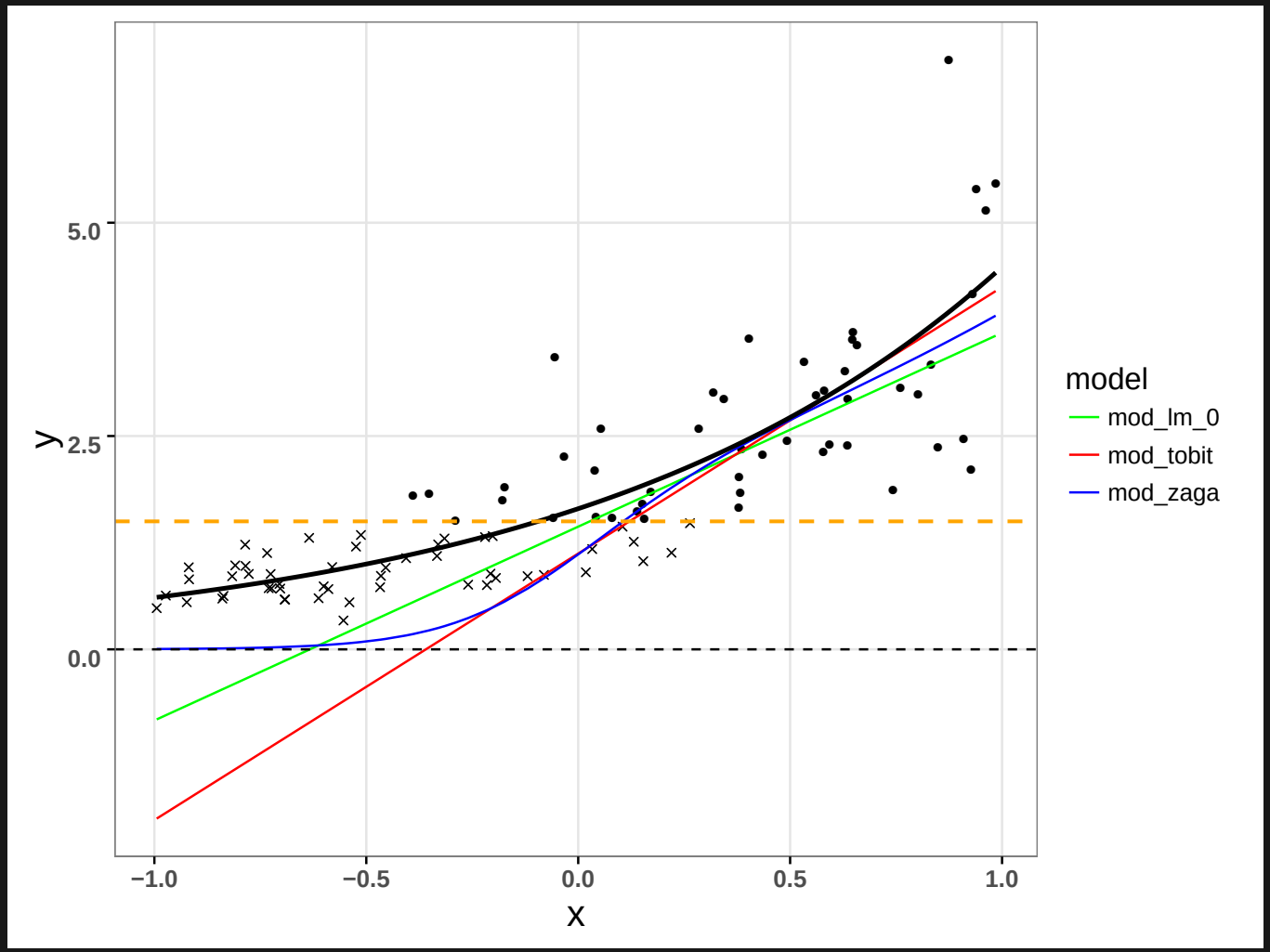

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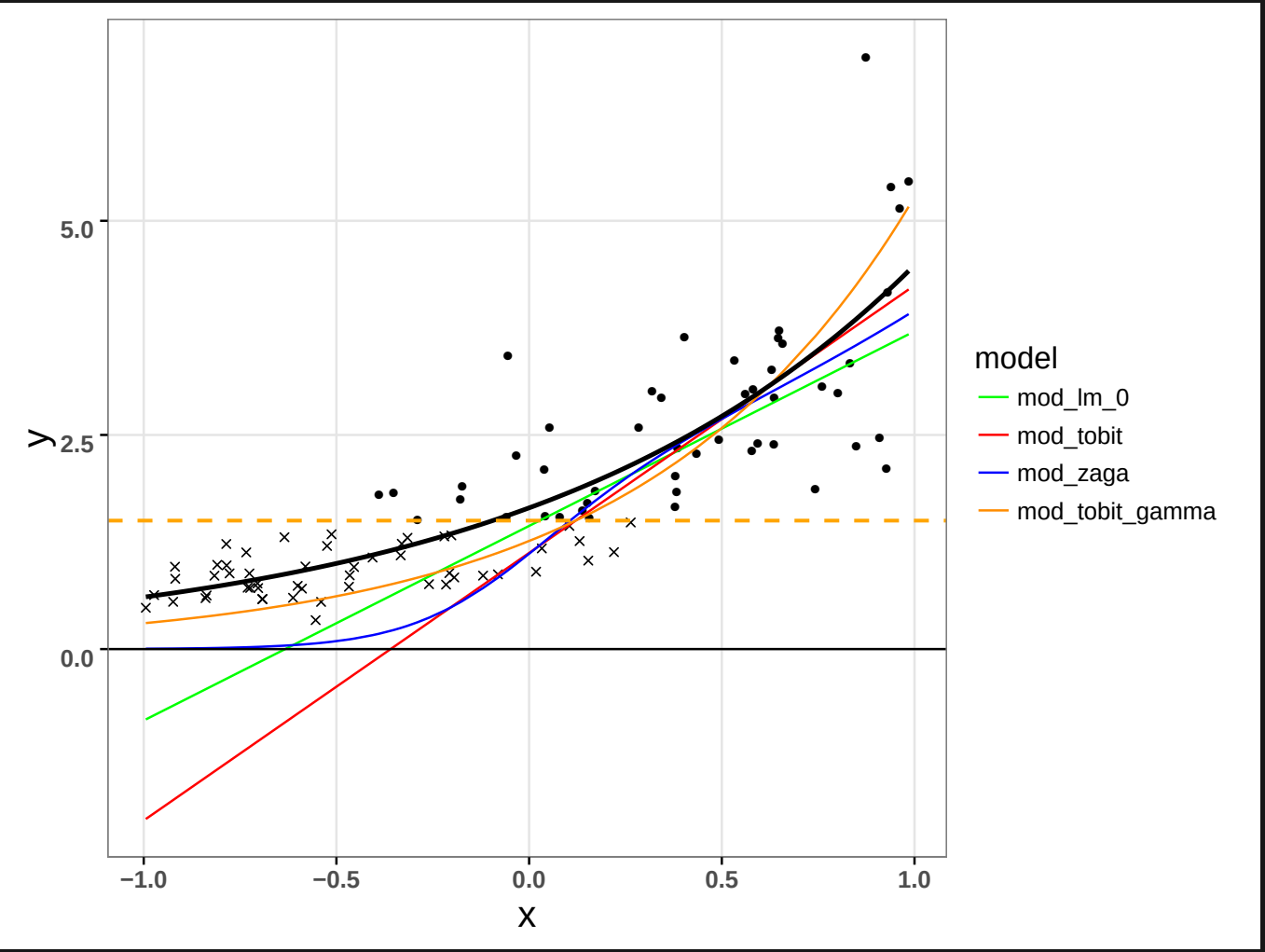

Guidance how to model environmental concentrations is missing

Temporal dynamics of pesticide occurrence

- Pesticides show compound specific dynamics
- Mixture dynamics? - Multivariate response.

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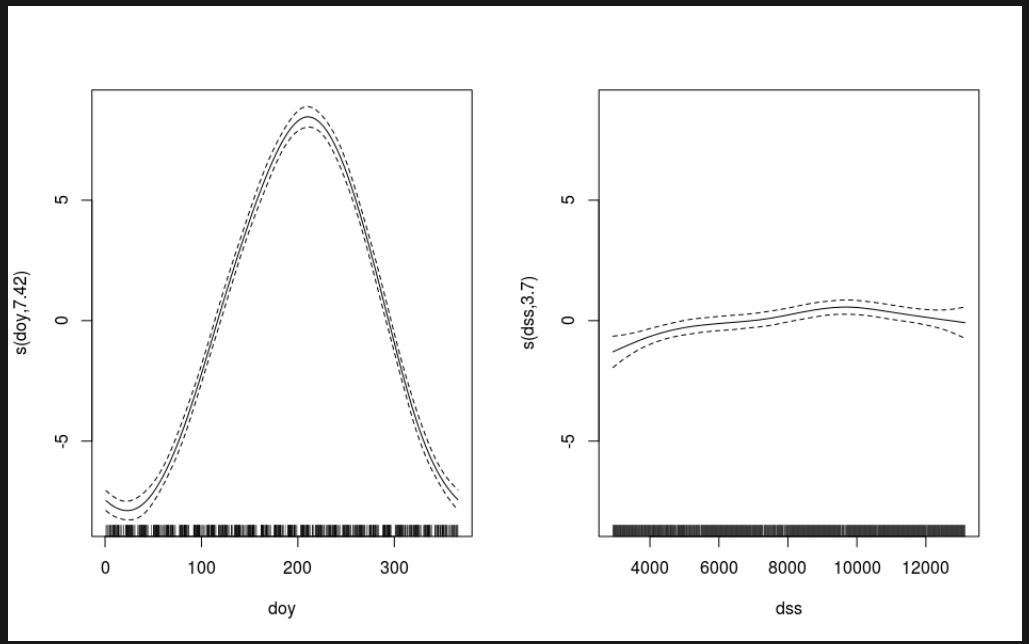
- Pesticides show compound specific dynamics
- Mixture dynamics? - Multivariate response.
- Seasonality, Trends (Fade out...)?
  $y = \beta_0 + f_{seasonal}(x_1) + f_{trend}(x_2) + \epsilon; \epsilon \sim ???$



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https://github.com/edild/talk_work2