Time series modeling of plant protection products in aquatic systems in R

Analysis of governmental monitoring data

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Quantitative Landscape Ecology
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Quantitative Landscape Ecology

- R and other open source software
- Ecotoxicology
- Effects of Plant Protection Products (PPP) / pesticides on the environment
- Aquatic systems

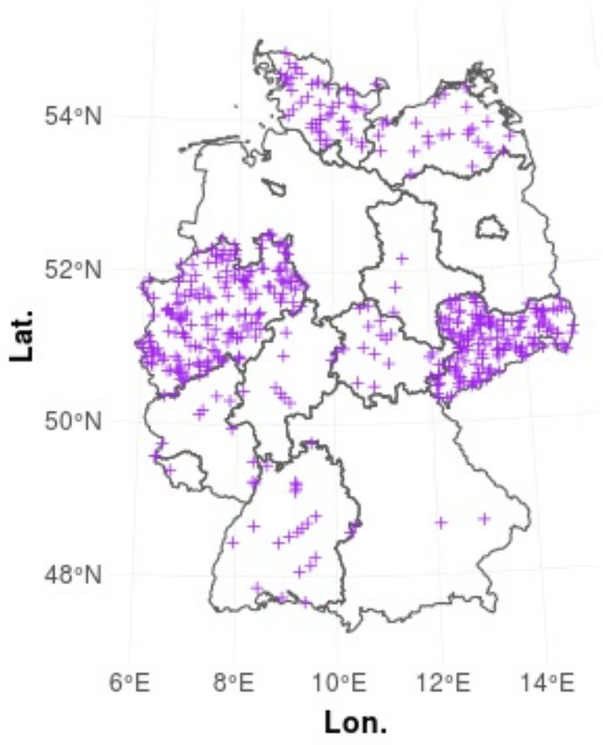
Introduction

Why study pesticides?

- Highly used in modern agriculture, gardens
- Environmental concern
- Glyphosate, Neonicotinoids, ...
- Germany (2016):
  - 753 pesticides
  - 270 substances
- Groups:
  - fungicides
  - herbicides
  - insecticides

Data

Data



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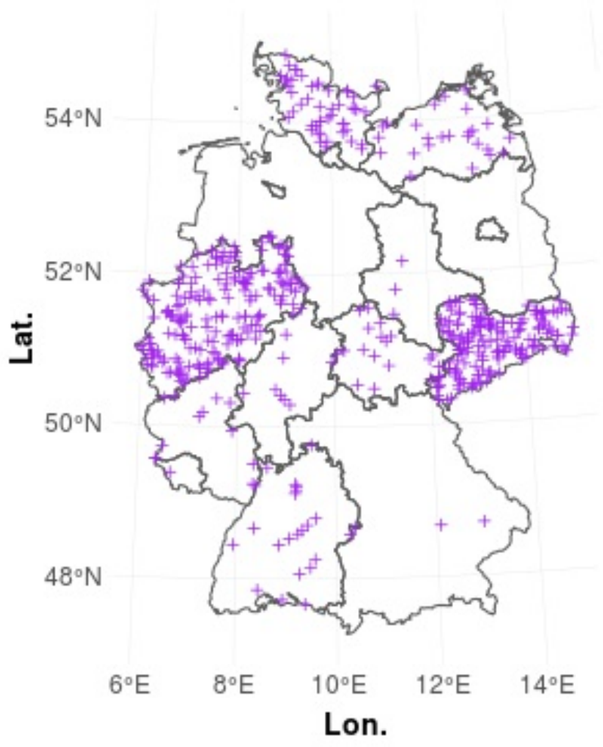
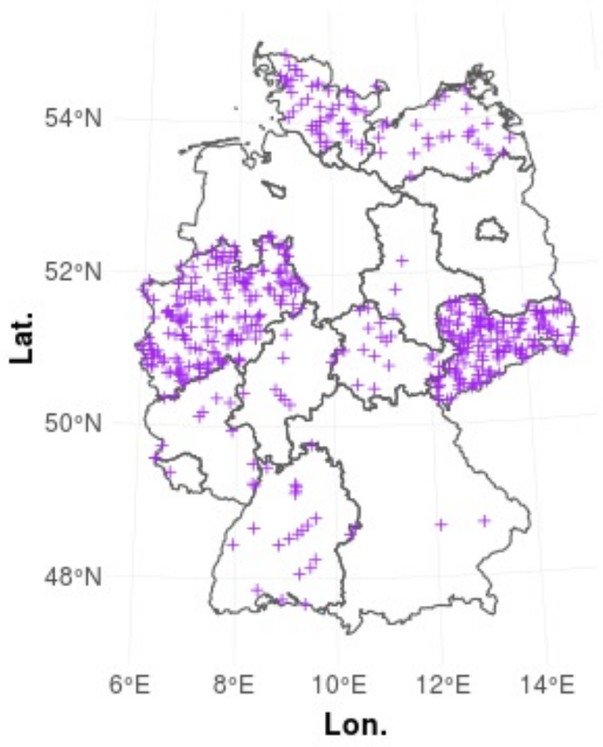


- federal monitoring program
- period: 2005-2015
- 3116 sampling sites
- 3.246.690 susbtance detections
- 495 substances
- stored in a PostgreSQL data base:

Data



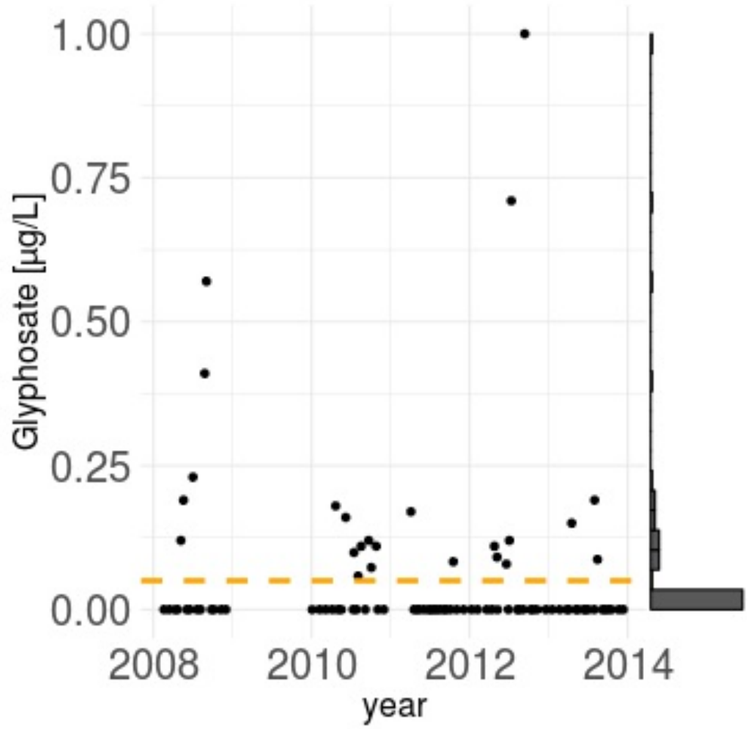

```
require(RPostgreSQL)
require(data.table)

# load data
drv = dbDriver("PostgreSQL")
con = dbConnect(...)

q = "SELECT * FROM schema.tab"
dt = dbGetQuery(con, query = q)
setDT(dt)

dbDisconnect(con)
dbUnloadDriver(drv)
```

Data



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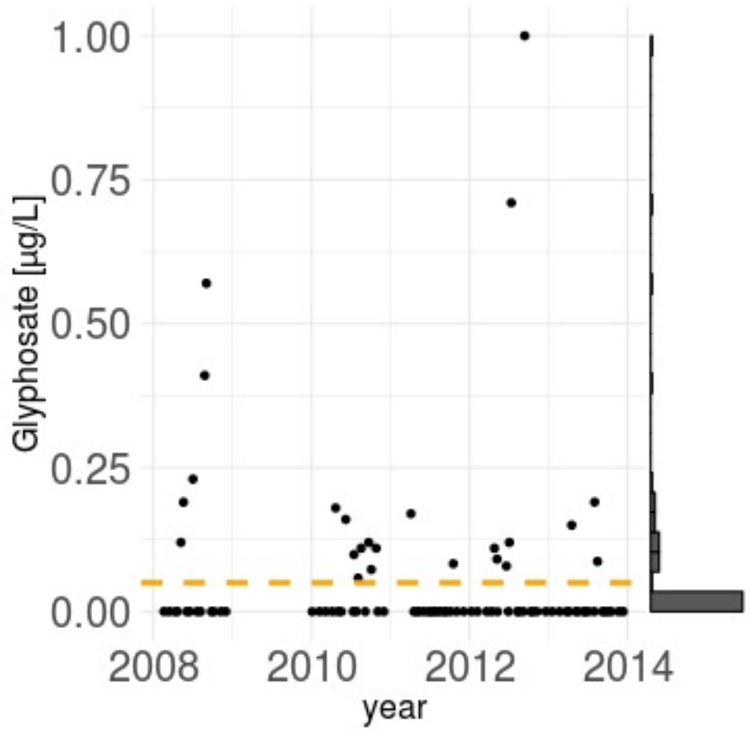

- Left skewed environmental data
  - LOQ: Limit of quantification
  - Excess of 0s
- Heterogenous data set
  - Sampling frequency
  - LOQ can change over time
  - Measured compounds
- Seasonal variability

Comparability between substances?

- 10µg of substance A as toxic as 10µg od substance B?

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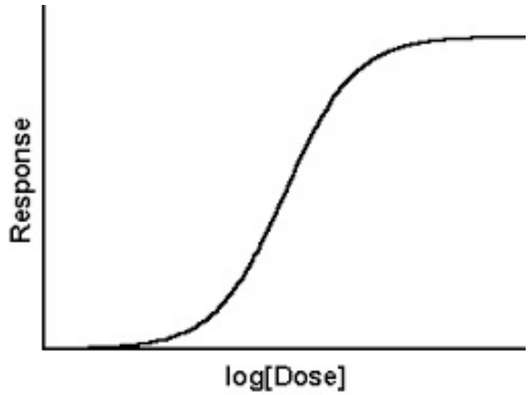
- Ecotoxicological tests
  - Effect Concentrations - EC50



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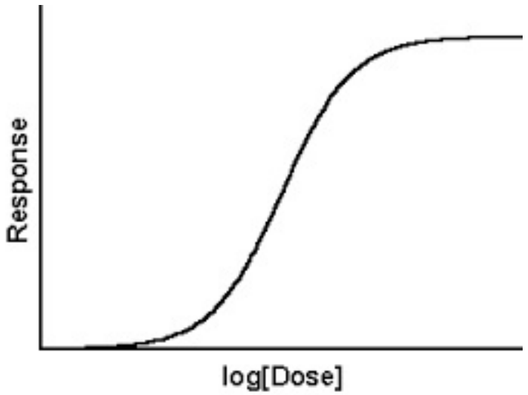


- EPA ECOTOX data base

Toxic Unit (TU)

in-stram concentrations ...

```
dt$value[1:3] # concentrations in µg/L
```

```
## [1] 0.120 0.018 0.000
```

... realte to effects

$$TU_{algae} = log_{10}(\frac{concentration}{EC50_{algae}})$$

Research questions

Research questions

Are there months of increased in-stream occurrence of pesticides?

- Occurrence model:
  - Binary data: concentration > LOQ: 1, concentration < LOQ: 0
  - pa ~ month + year + site

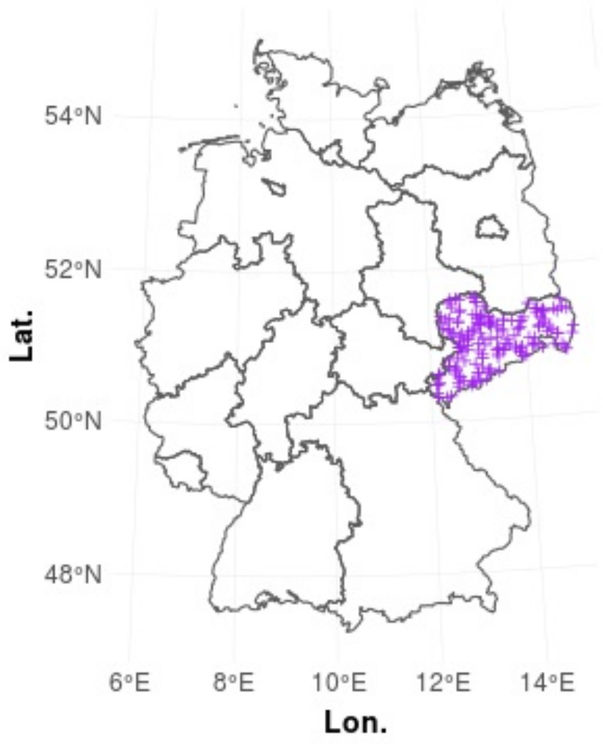
How are different organism groups (Algae, Invertebrates, Fish) effected by pesticide concentrations throughout the year?

- Effect/TU-Model:
  - Continuous data
  - TU ~ month + site

Data preparation

Filter data

```
dt = dt[state == 'SN']
dt = dt[pest_type %in% c('fungicide', 'herbicide', 'insecticide')]
```



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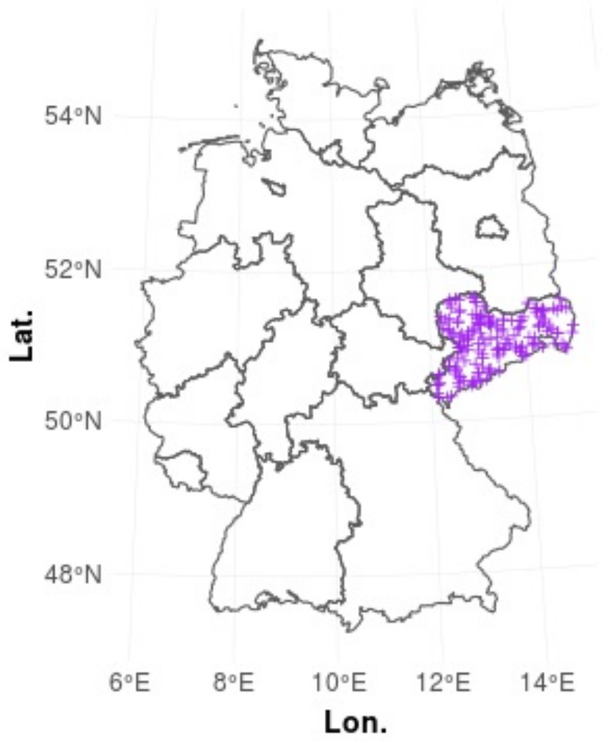



```
uniqueN(dt$site)
```

```
## [1] 413
```

```
dt[ i = value > 0,
    j = .N,
    by = pest_type]
```

```
##       pest_type     N
## 1:   fungicide  2455
## 2:   herbicide 10890
## 3: insecticide   875
```

Filter data

Substances quantification-ratio > 5%

```
subst_fin = dt[ ,
                .(perc = .SD[ value > 0, .N ] / .N),
                subst_name ][perc > 0.05][order(-perc)]
subst_fin[ , perc := round(perc,2)]
head(subst_fin)
```

```
##      subst_name perc
## 1:     Boscalid 0.39
## 2:     Bentazon 0.38
## 3:  Isoproturon 0.37
## 4:    Quinmerac 0.36
## 5:   Glyphosate 0.29
## 6: Azoxystrobin 0.27
```

```
nrow(subst_fin)
```

```
## [1] 31
```

Occurrence model

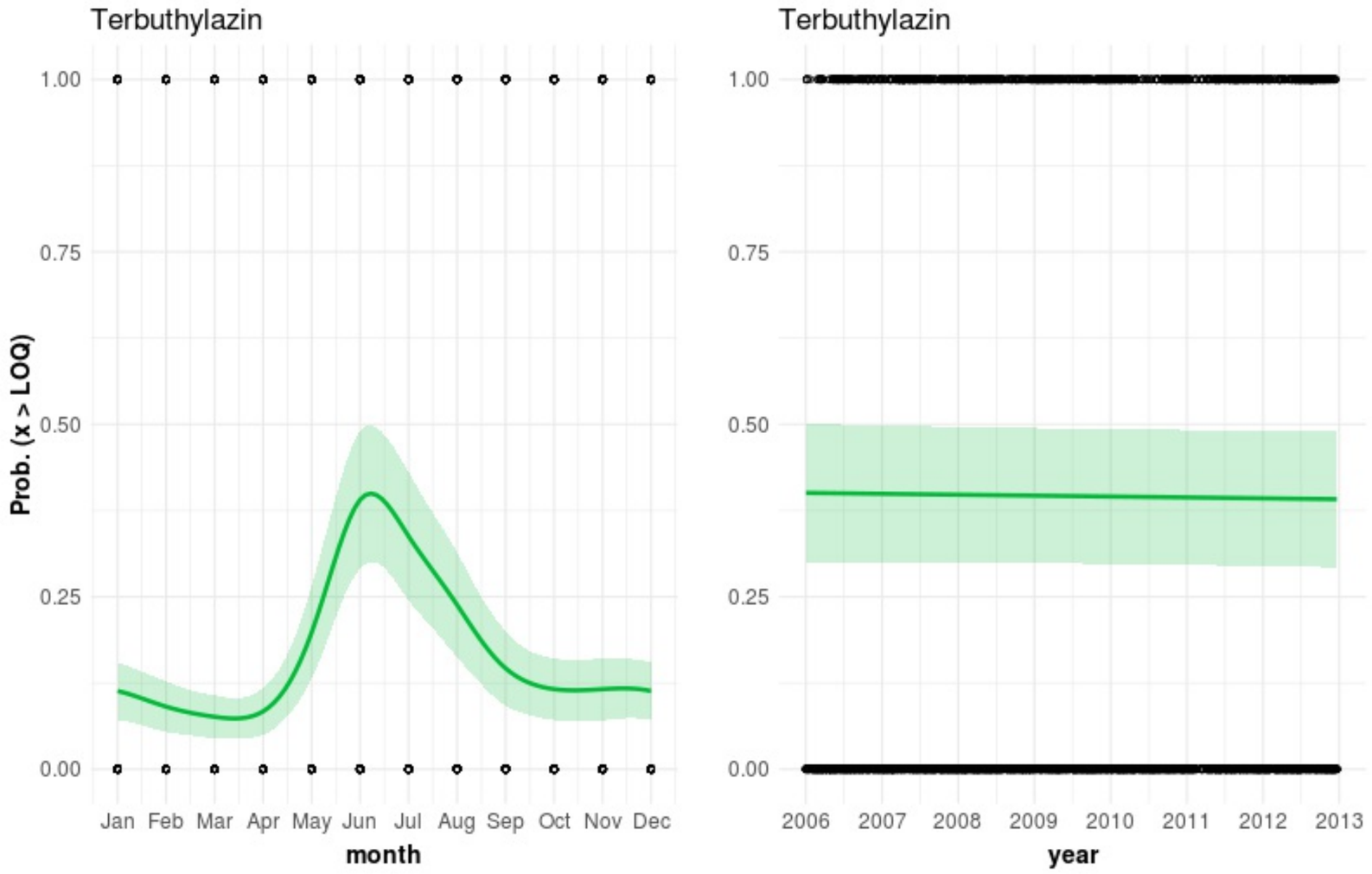
Occurrence model

fit the model for each substancre individually

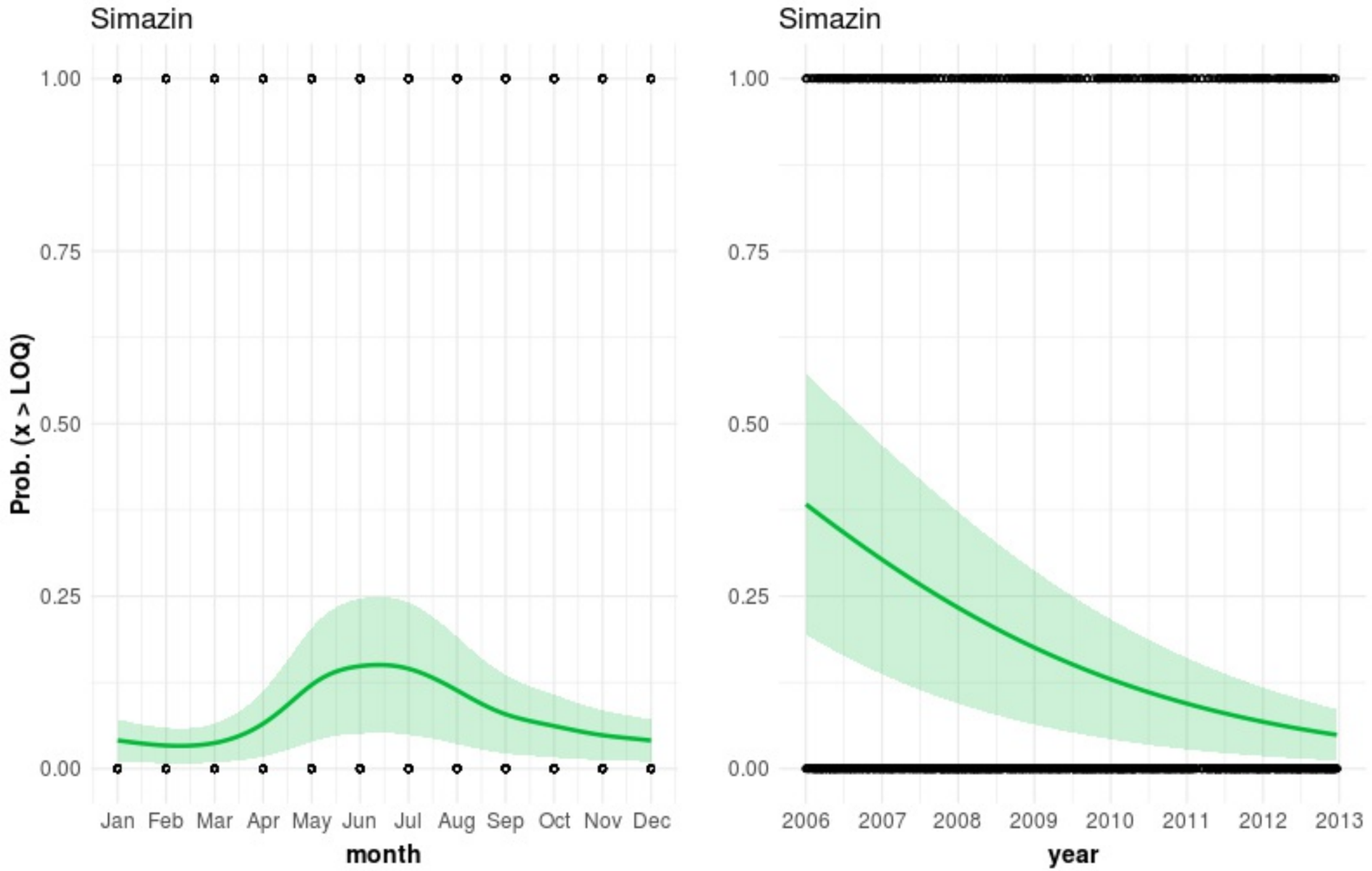
```
mdt[ , pa := as.numeric(as.logical(value)) ]
mdt[ , time := as.numeric(date) / 1000 ]
```

```
require(mgcv)
for (i in seq_along(substances)) { # for 31 pesticides
  # ...
  mdt = dt[ subst == substances[i] ]
  mod_pa = gam(pa ~
                 s(month, bs = 'cc', k = 12) +
                 s(time, k = 20) +
                 s(year, bs = 're') +
                 s(site, bs = 're'),
               data = mdt,
               family = binomial(link = 'logit'),
               method = 'REML')
  # ...
}
```

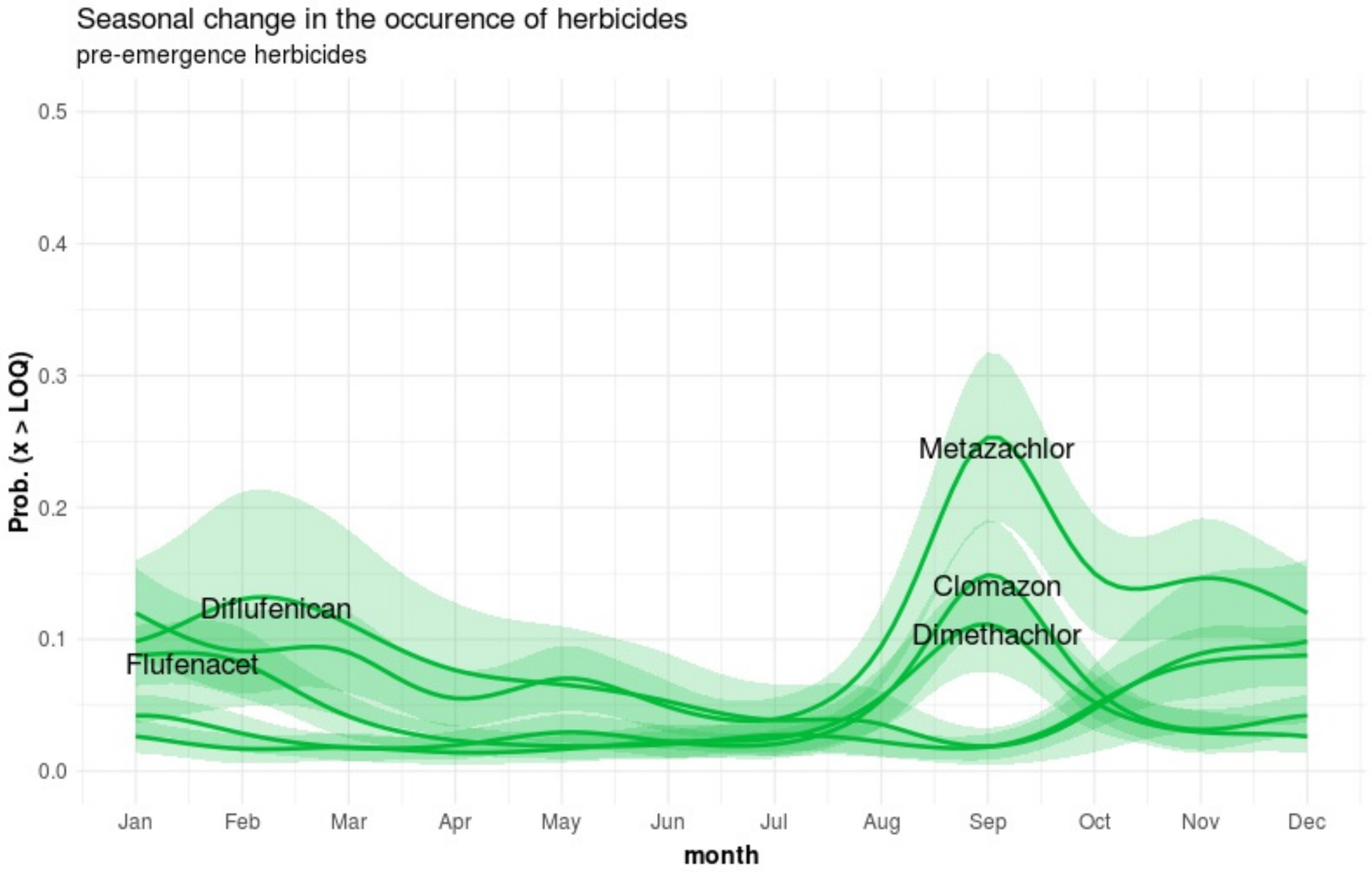
Occurrence model - Herbicides



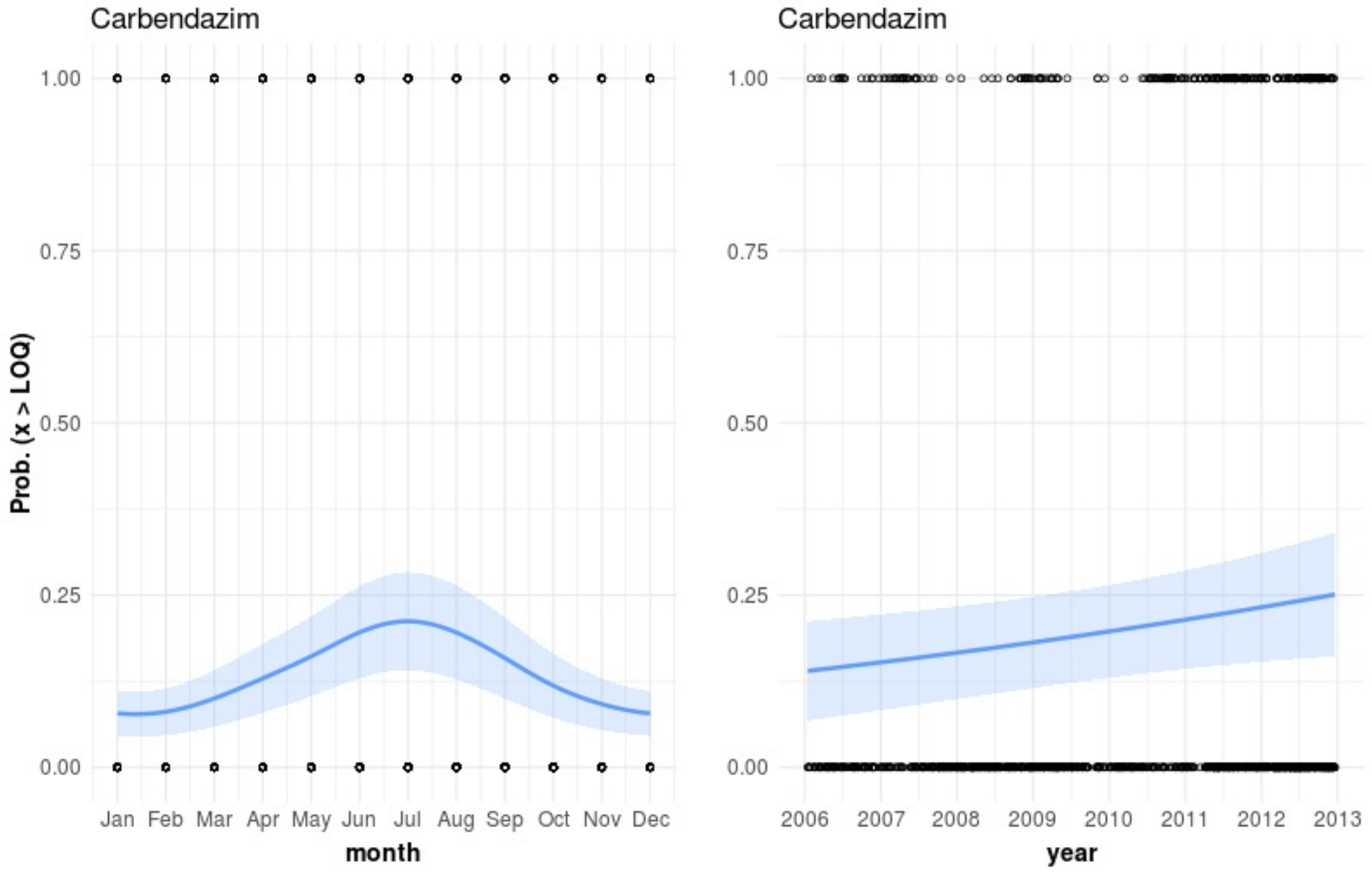
Occurrence model - Herbicides



Occurrence model - Herbicides



Occurrence model - Fungicides



Effect model

Effect model

Effect model

```
dt[ , TU_algae := log10(value / EC50_algae) ]
dt[ , TU_inv := log10(value / EC50_inv) ]
dt[ , TU_fish := log10(value / EC50_fish) ]
```

Maximum per site & month

```
dt_agg = dt[ ,
             .(maxTU_al = max(TU_algae),
               maxTU_iv = max(TU_inv),
               maxTU_fi = max(TU_fish)),
             .(site, month) ]
```

Effect model

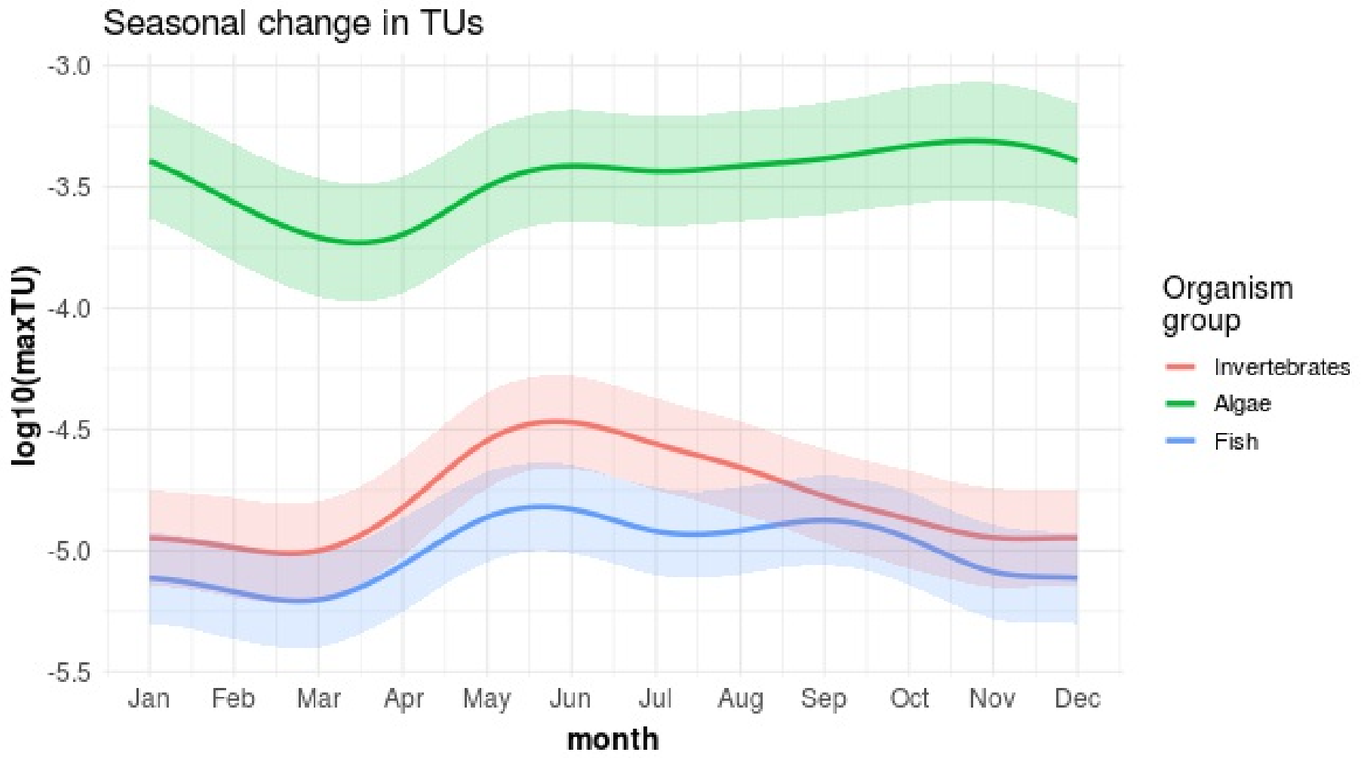
maximum: TU-Algae, TU-Invertebrates, TU-Fish

```
require(mgcv)

for (i in seq_along(todo)) { # for 3 TUs
  # ...
  mod_al = gam(maxTU_al ~
                 s(month, bs = 'cc', k = 12) +
                 s(site, bs = 're'),
               family = gaussian(),
               data = mdt_agg,
               method = 'REML')
  # ...
}
```

Effect model

All organism groups (Algae, Fish, Invertebrates)



Conclusions

- Occurrence model
  - identify peaks in occurence (for well measured substances)
- Effect model
  - underestimation of effects
  - sampling effort
  - different physical chemical properties of susbstances
- Improve model
  - include interactions
  - refine selection of EC50 vlaues for TU calculations
  - other covariates:
  - percentage of agriculture in catchments
  - precipitation on/before sampling date

R packages + tools

- data storage + preparation

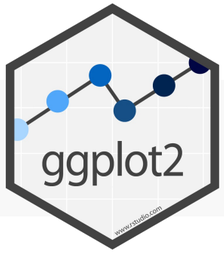
PostgreSQL

```
require(RPostgreSQL)
require(data.table)
```

- modeling

```
require(mgcv)
```

- visualization




```
require(ggplot2)
require(sf)
```

- slides


```
require(rmarkdown)
require(knitr)
require(xaringan)
```

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Thank you for your attention!

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LANDSCAPE ECOLOGY

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