Generalized Additive Models

An introduction

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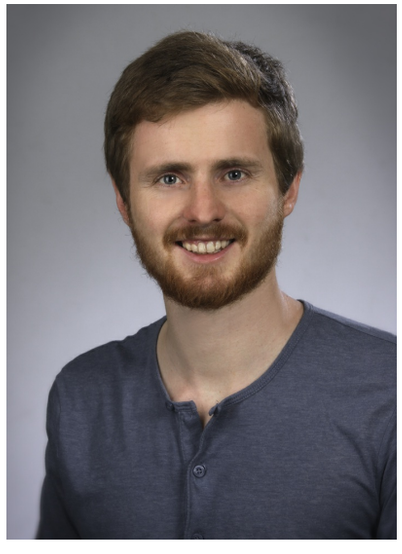
Short intro: Andreas Scharmüller



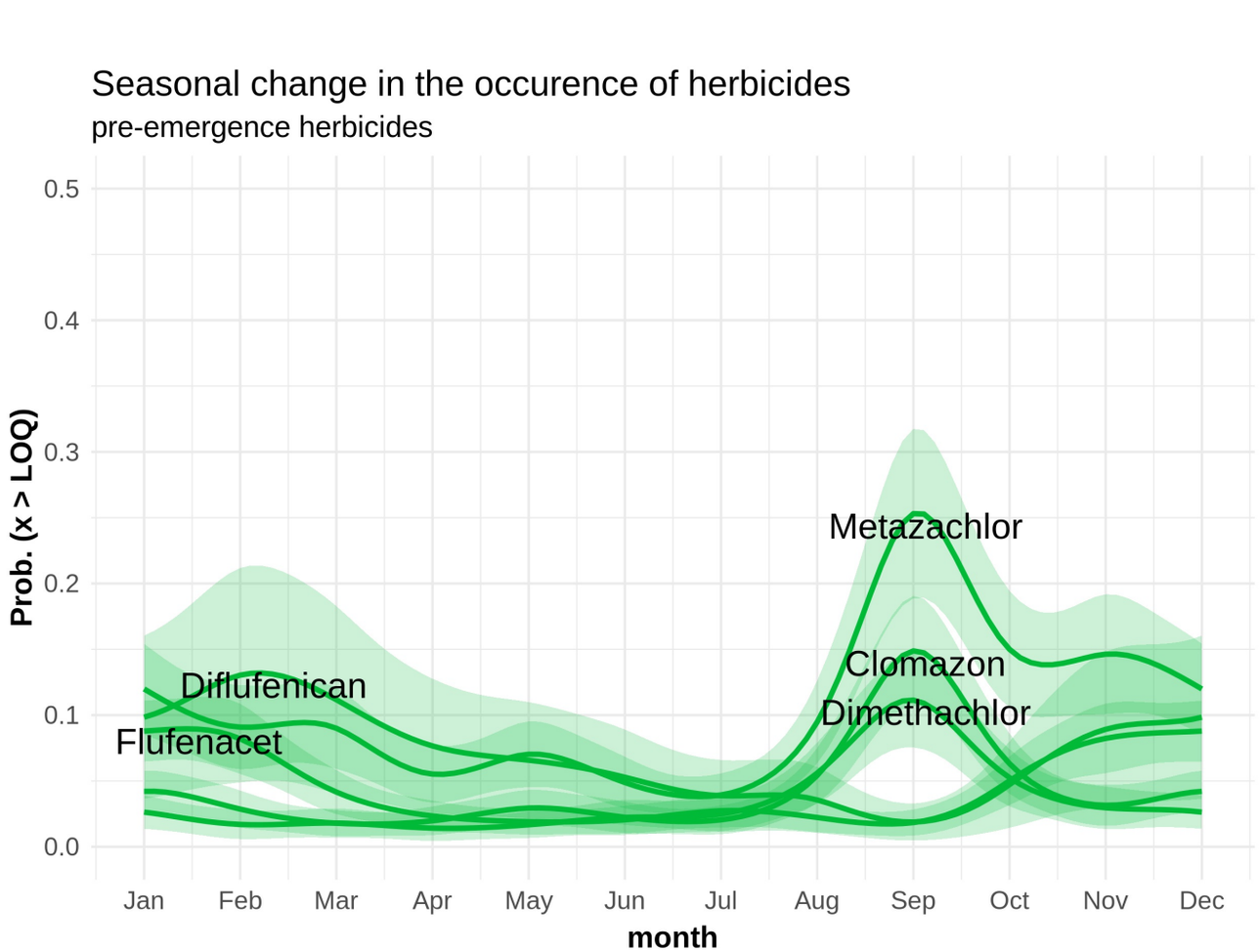
- PhD student Quantitative Landscape Ecology
- Environmental Sciences + Ecotoxicology
- Research
    - Effects and distribution of pesticides in freshwaters
    - Big(ish) ecotoxicological data processing

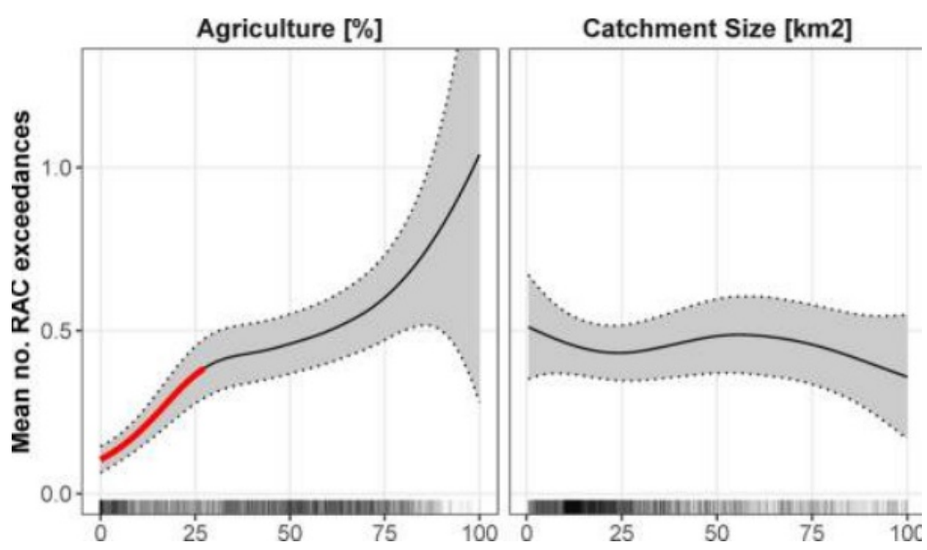
Talk: Ecotoxicology and stress responses: Monday, 14:45 (Crystall ballroom 2G)

- Teaching:
    - Statistics
    - GIS
- R programming
    - Package author: standartox (in preparation)
    - Package contributions: webchem

Research

- Seasonal occurrence patterns of **pesticides** in small waterbodies in Germany
- Modeling **benthic diatom** abundance and occurrence patterns in freshwater





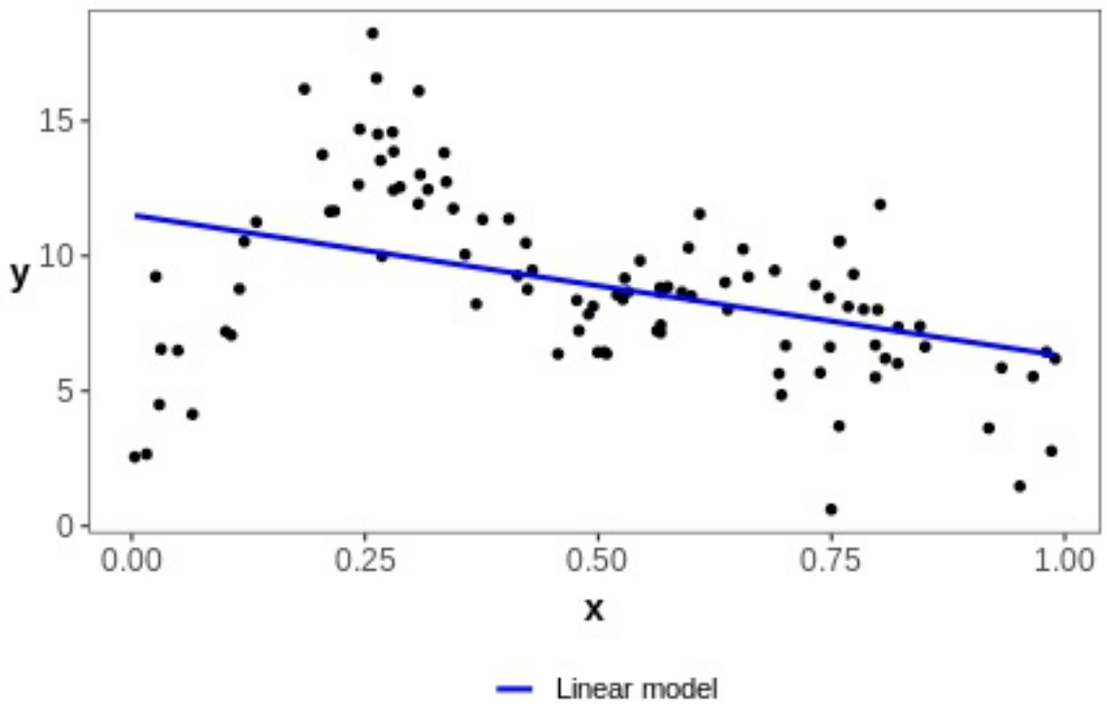
Linear Regression

Linear Models (LM)

- easy to interpret
- confined to linear relationships
- normally distributed responses

$$y = \beta_0 + x_1\beta_1 + \epsilon, \epsilon \sim N(0, \sigma^2)$$

```
lm(y ~ x,
   data = data)
```

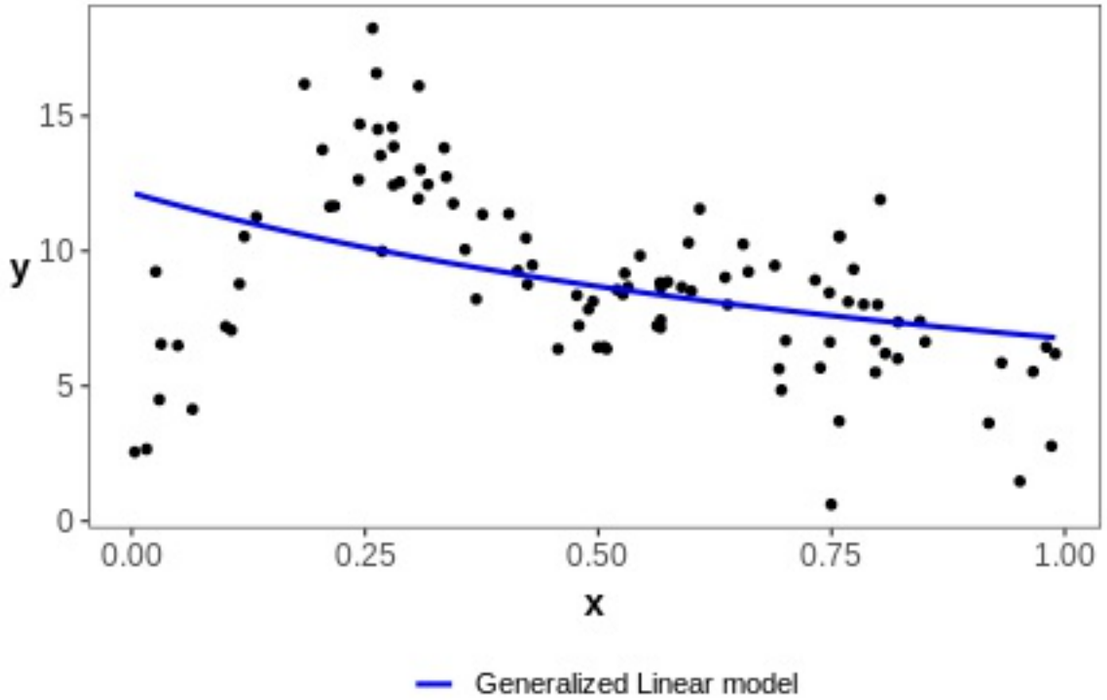


Generalized Linear Models (GLM)

- additional distributions (Poisson, Gamma, Binomial, etc.)

$$\mathrm{E}(y) = \beta_0 + x_1\beta_1 + x_2\beta_2 + \epsilon$$

```
glm(y ~ x,
    data = data,
    family = 'Gamma')
```

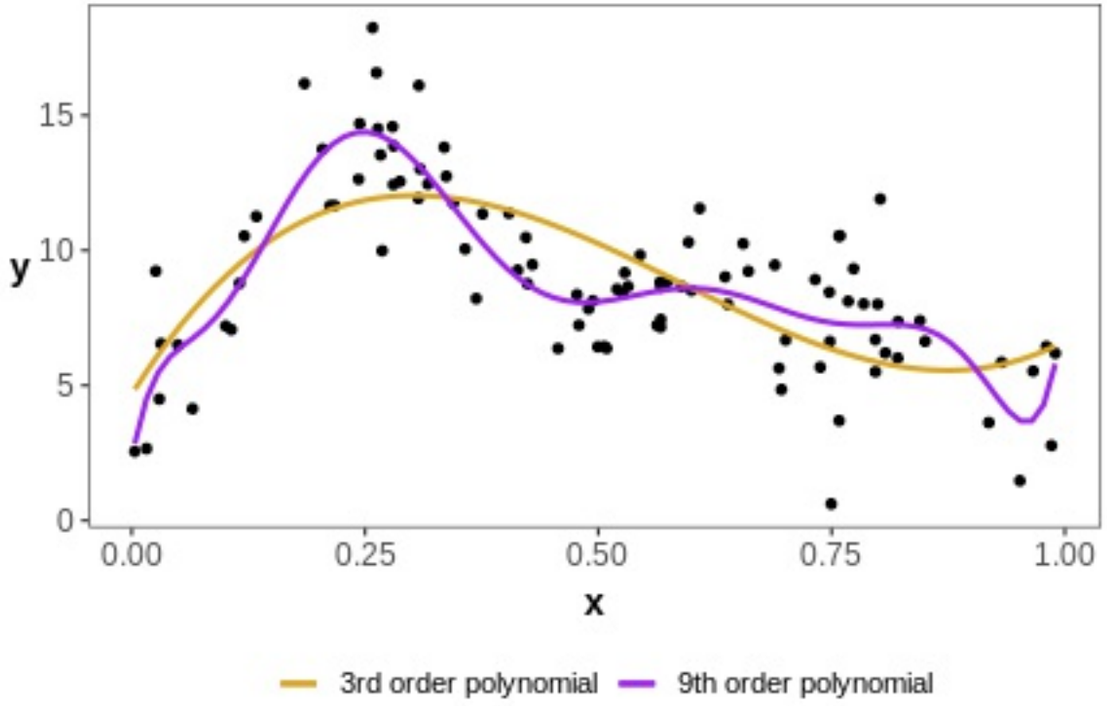


Polynomial regression

- specific patterns, not as flexible as GAMs
- might lead to poor residuals, predictions, extrapolations

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_1^3 + \epsilon, \epsilon \sim N(0, \sigma^2)$$

```
lm(y ~ poly(x, 3),
   data = data)
```



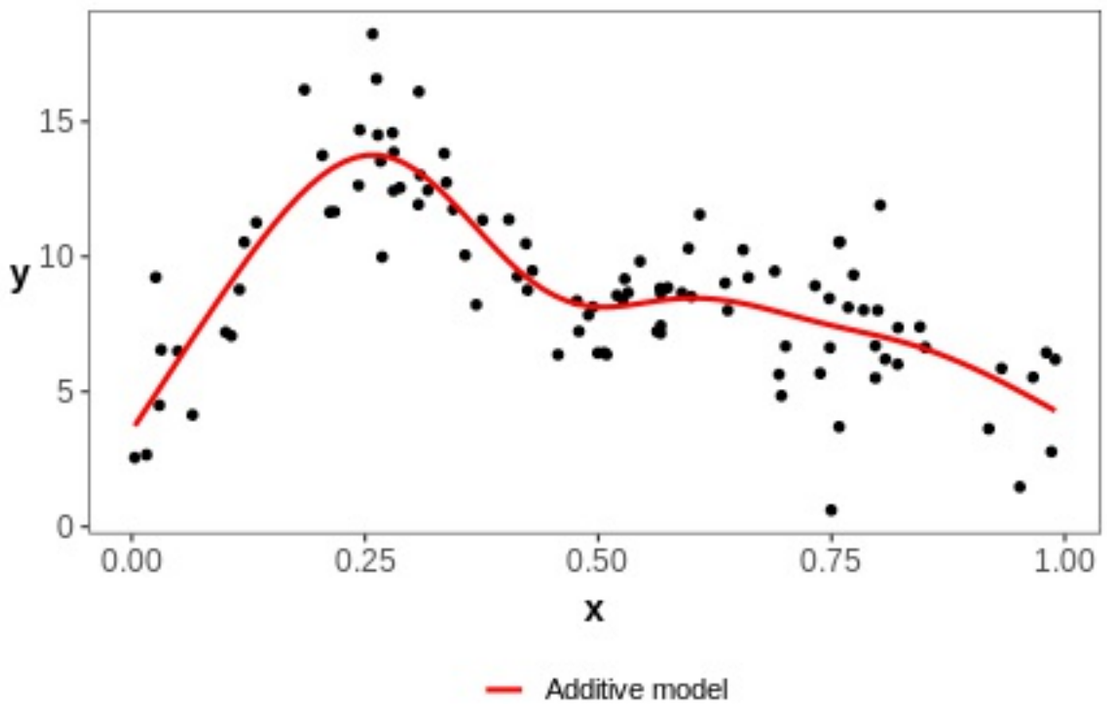
Generalized Additive models (GAM)

Generalized Additive Models (GAM)

- extension to GLMs
- more flexible
- can be harder to interpret

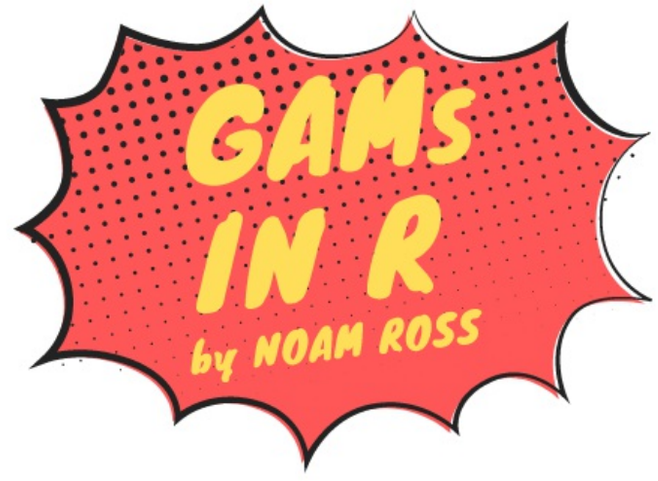
$$\mathrm{E}(y) = \beta_0 + f_1(x_1) + x_2\beta_2 + \epsilon$$

```
mgcv::gam(y ~ s(x1) + x2,
          data = data,
          family = 'gaussian')
```



Why GAMs?

https://noamross.github.io/gams-in-r-course



What are GAMs?

https://www.fromthebottomoftheheap.net

> 140 char vrsn
>
> 1 GAMs are just GLMs
> 2 GAMs fit wiggly terms
> 3 use + s(foo) not foo in frmla
> 4 use method = "REML"
> 5 gam.check()
>
> — Dr Gavin Simpson (@ucfagls) 16 march 2017

GAMs in R

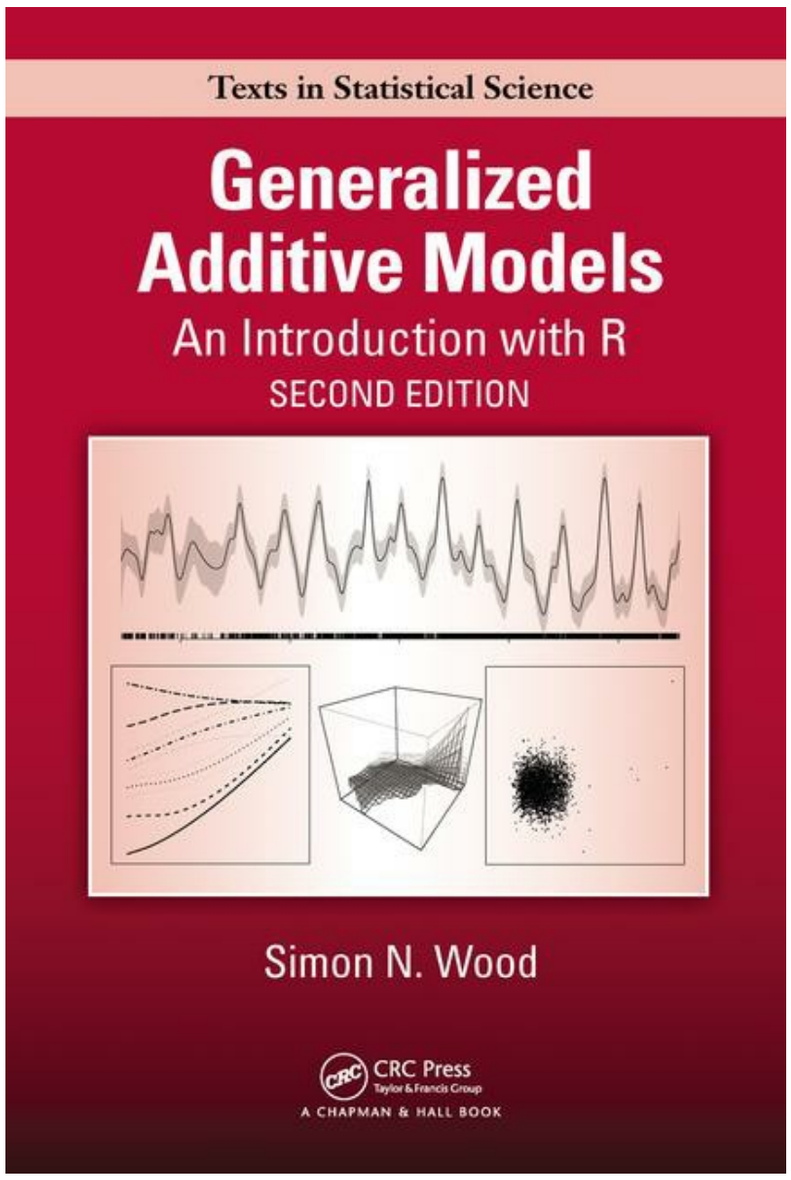
`require(mgcv)` https://cran.r-project.org/web/packages/mgcv/index.html

`require(gamlss)` https://cran.r-project.org/web/packages/gamlss/index.html

`require(brms)` https://github.com/paul-buerkner/brms

GAMs in R

`require(mgcv)` https://cran.r-project.org/web/packages/mgcv/index.html



GAMs in R

R-function:

```
require(mgcv)

gam(y ~ s(x1, bs = 'tp', k = -1) + x2, # formula
    data = data, # data
    family = 'gaussian', # family object
    method = 'REML' # default: 'GCV.Cp'
    sp = NULL) # smoothing parameter
```

GAMs in R

Formula:

```
require(mgcv)

# gam(y ~
      s(# smooth term
        x1, # predictor
        bs = 'tp', # spline basis
        k = -1, # number of basis functions
        sp = NULL  # smoothing parameter
      )
    # + x2, # linear term
    # data = data,
    # family = 'gaussian',
    # method = 'REML' # default: 'GCV.Cp'
    # sp = NULL)
```

Smoothing

Smoothing

$$Fit = Likelihood - \lambda \times Wiggliness$$

- Likelihood: How well a GAM captures patterns in the data
- Wiggliness: Complexity of a smooth
- Trade-off between Likelihood and Wiggliness
- λ is optimized in `gam()` and controls the trade-off

taken from: https://noamross.github.io/gams-in-r-course

Smoothing

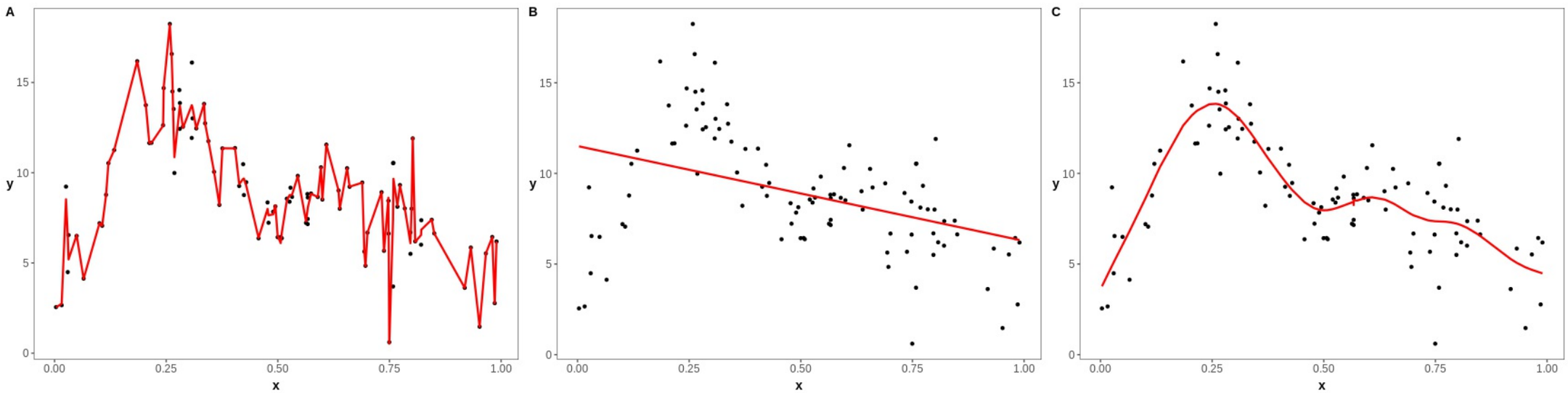
Smoothing parameter

```
gam(y ~ s(x1, sp = NULL),
    data = data,
    sp = NULL,
    method = 'REML')
```

- smootghin paramter
- estimated in REML

Smoothing

Smoothing parameter

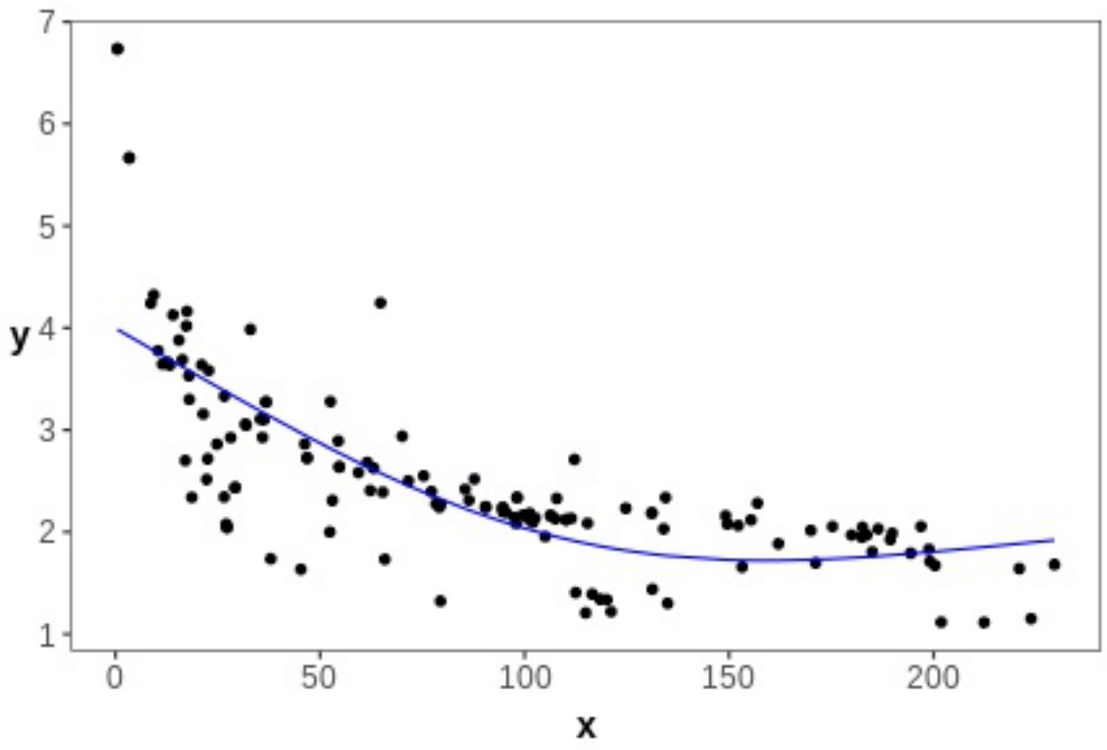


- A: `sp = 0`
- B: `sp = 1e5`
- C: `method = 'REML'`

Smoothing

Basis Functions

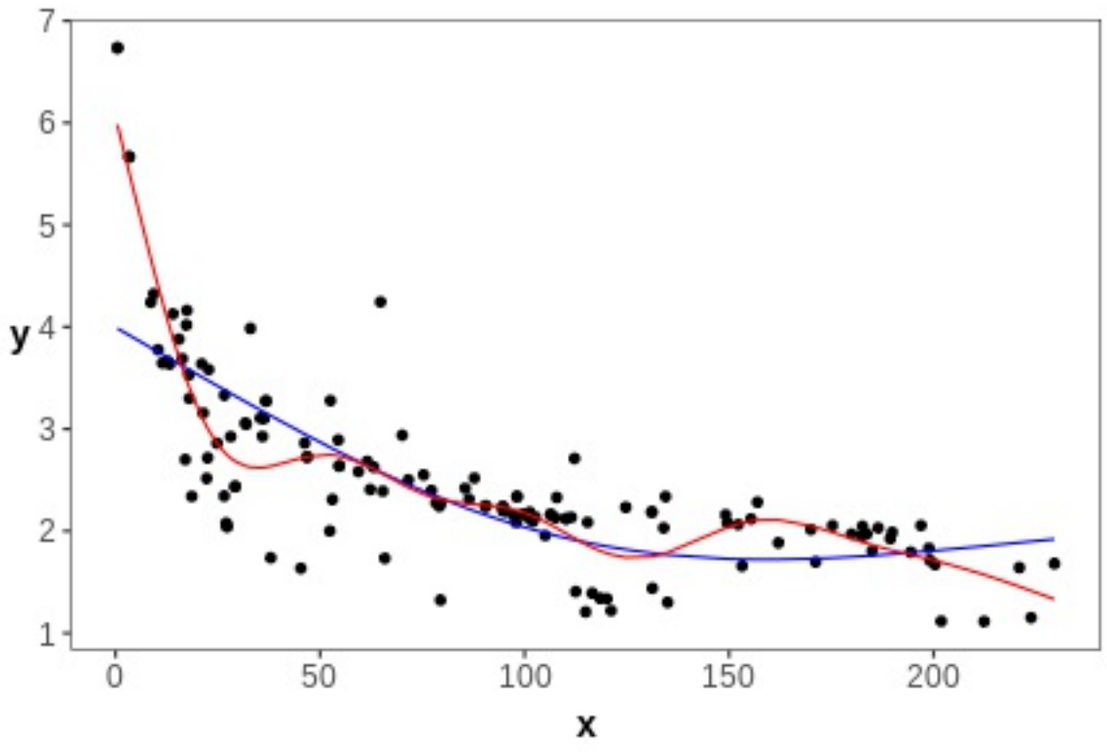
```
gam(y ~ s(x1, k = 3),
    data = data)
```



Smoothing

Basis Functions

```
gam(y ~ s(x1),
    data = data)
```



Smoothing

Basis Functions

Check for k:

```
gam.check(oc1)
```

```
k.check(oc1)
```

```
##      k'      edf  k-index p-value
## s(P)  2 1.972523 0.419655       0
```

If p-value is low, k might be too small

Smooth terms

Smooth terms

Two additive smooths

```
gam(y ~ s(x1) + s(x2))
```

Smooth-interactions

```
gam(y ~ s(x1, x2, k = 4))
gam(y ~ s(x1, by = fac))
```

Tensor product smooths

```
gam(y ~ te(x1, x2, k = c(4,8))) # interaction on different scales
```

Splines

Splines

Thin plate regression spline

- default

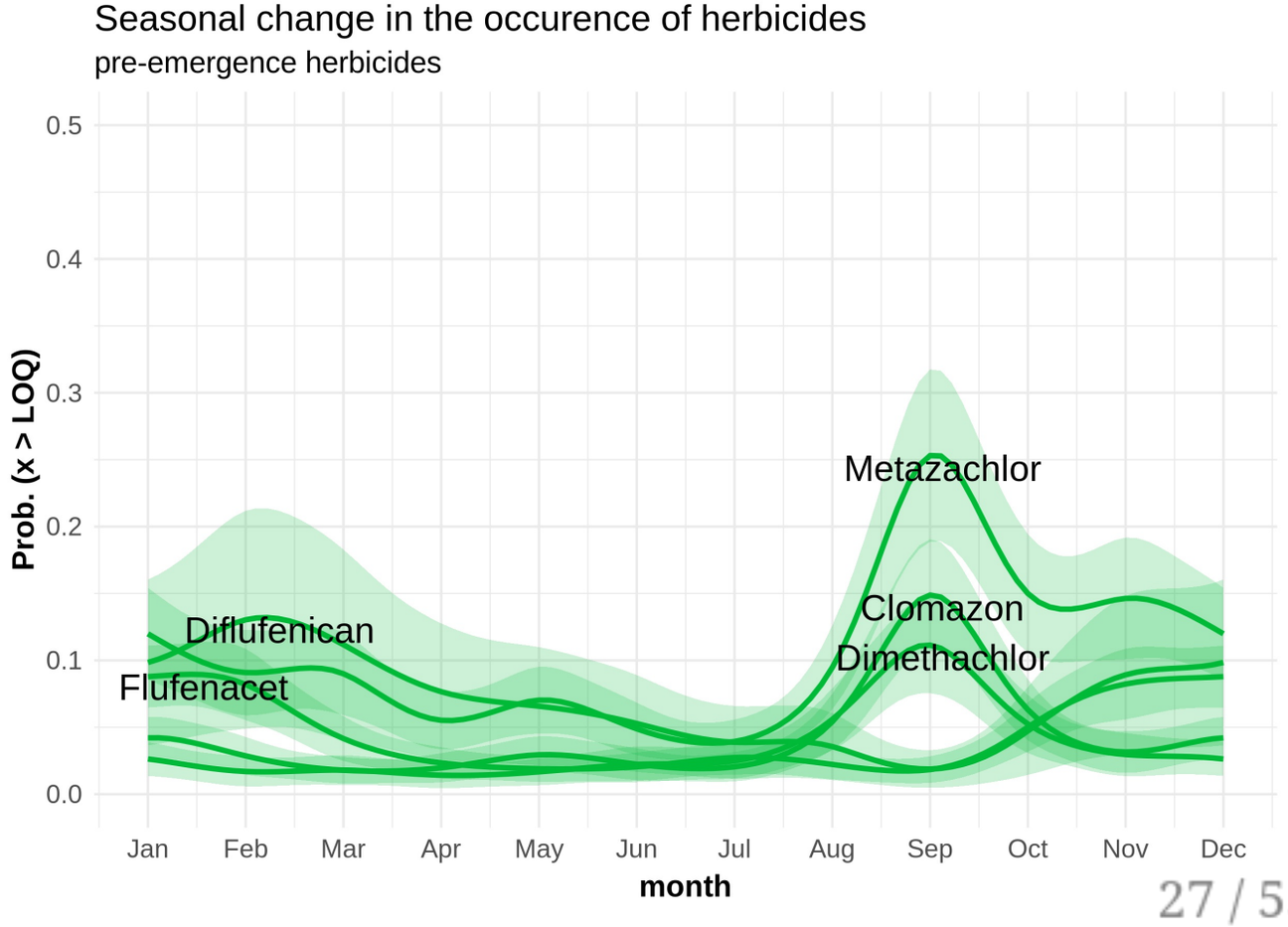
```
gam(y ~ s(x, bs = 'tp'),
    data = data)
```

Splines

Cyclic cubic regression splines

- for cyclical data (e.g. seasons)

```
gam(y ~ s(x, bs = 'cc'),
    data = data)
```



Splines

Soap Films

- boundary polygons can be introduced
- spatial models

```
gam(y ~ s(x, y, bs = 'so', xt = list(bnd = boundary_polygon)),
    data = data)
```

Splines

Discrete **random effects**

- classes (e.g. age, sex)
- sites, states, rivers, lakes
- no need to set k (equals number of levels)

```
gam(y ~ s(x, bs = 're'),
    data = data)
```

Visualisation

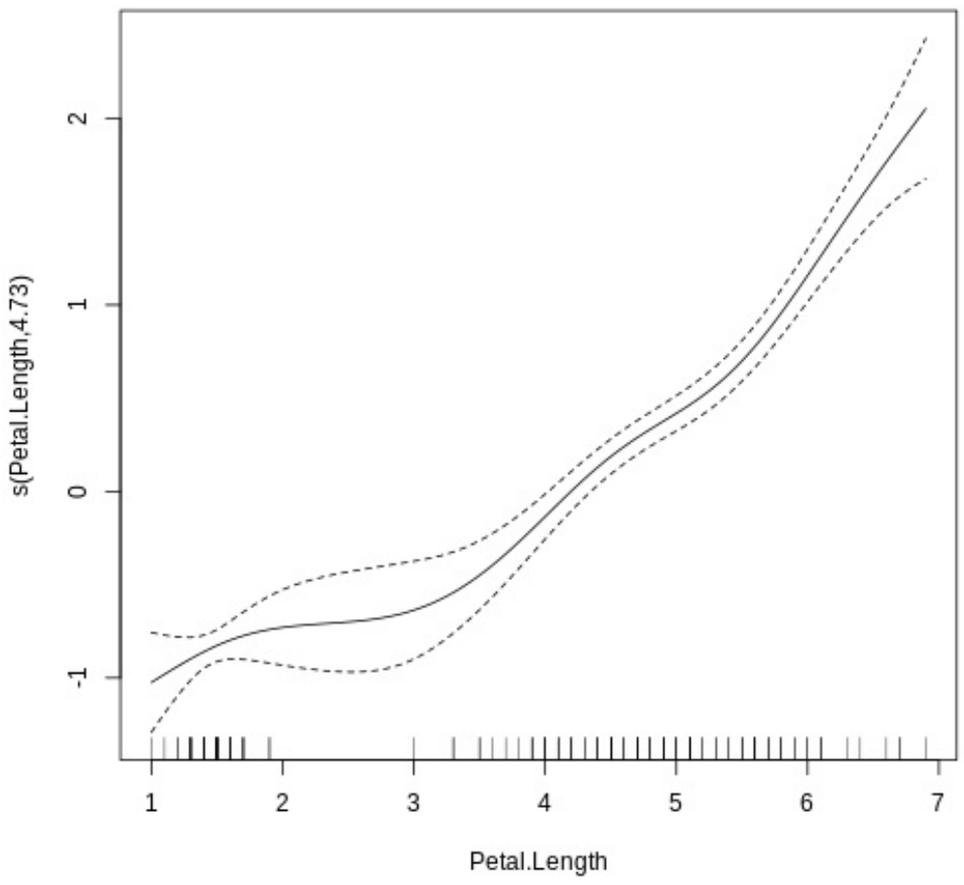
Visualisation

```
ir1 = gam(Sepal.Length ~ s(Petal.Length),
          data = iris,
          family = 'gaussian',
          method = 'REML')
```

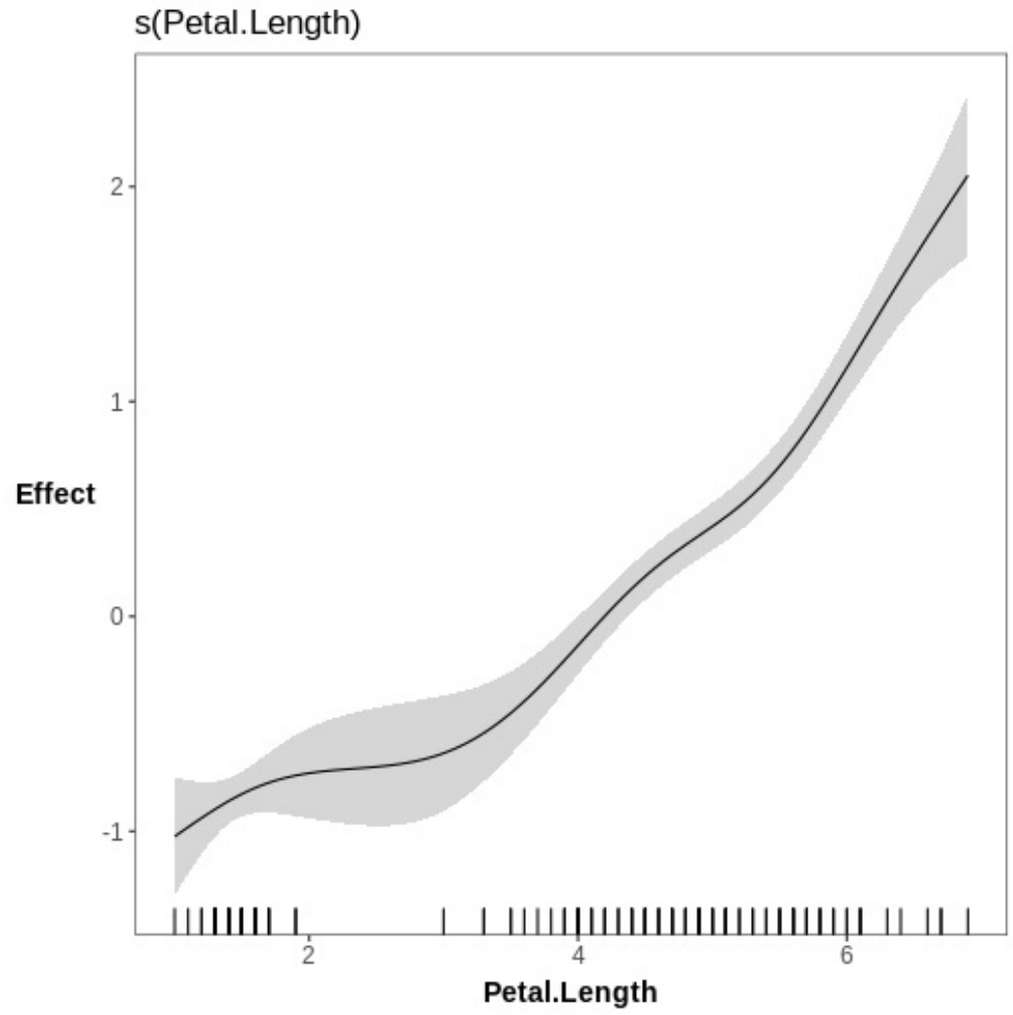
Visualisation

Partial effect plots

```
require(mgcv)
plot(ir1, pages = 1)
```




```
require(gratia)
draw(ir1)
```



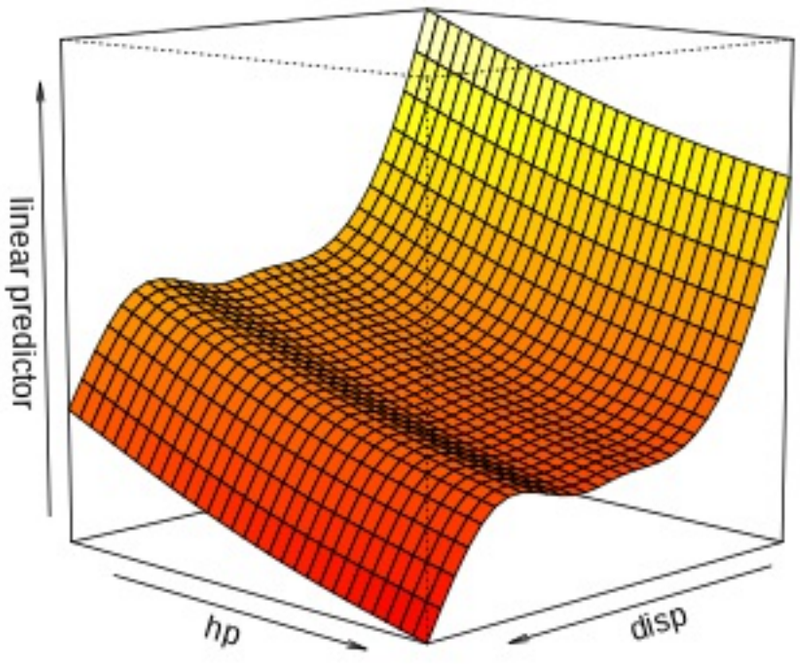
Visualisation

Multiple covariates

```
mt1 = gam(mpg ~ s(disp) + s(hp),
          data = mtcars,
          family = 'gaussian',
          method = 'REML')
```

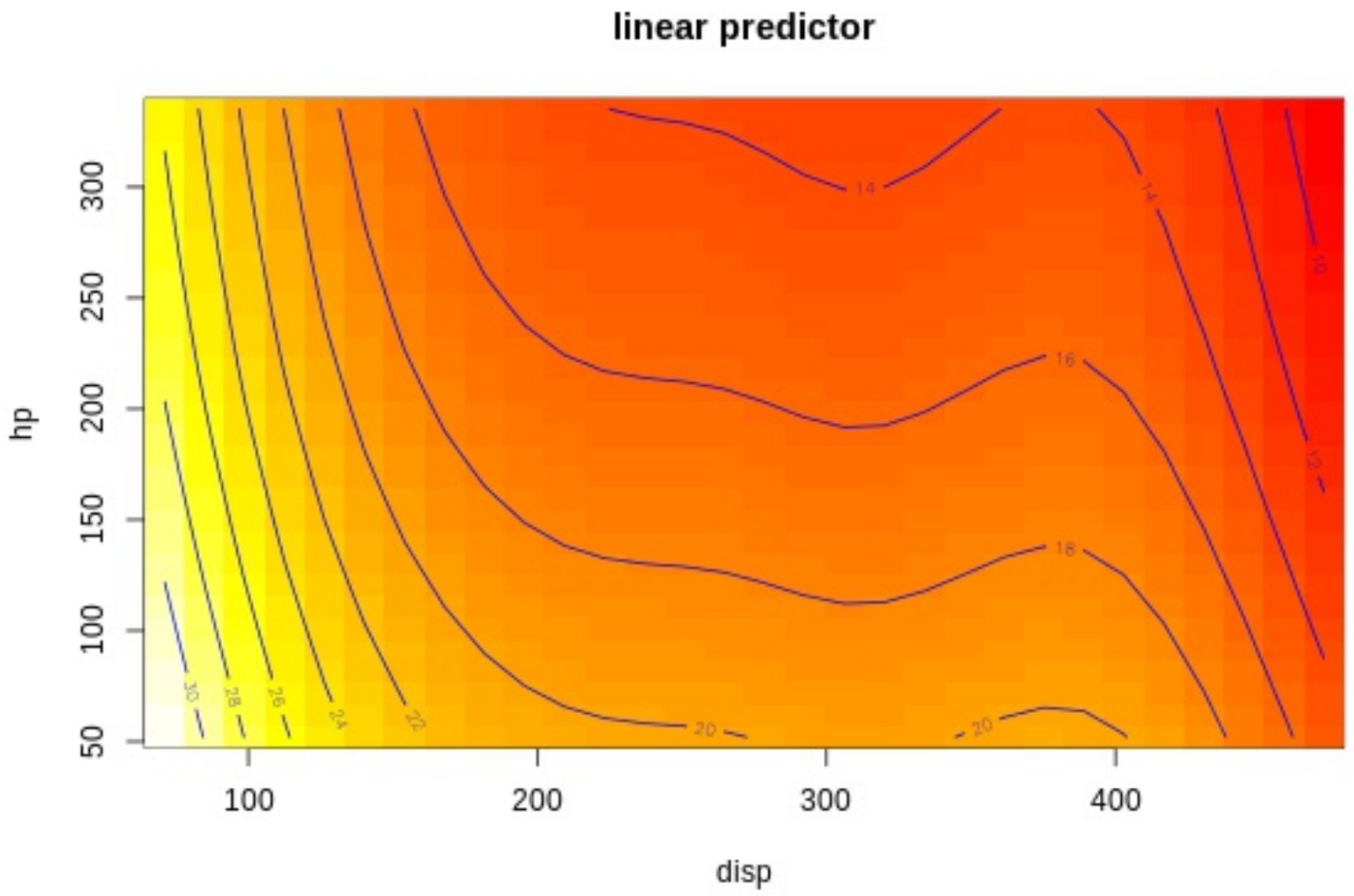
Visualisation

```
vis.gam(mt1, # GAM object
        view = c("disp", "hp"), # variables
        plot.type = "persp", # 3D plot
        theta = 135, # horizontal rotation
        phi = 10, # phi vertical rotation
        r = 10) # zoom
```



Visualisation

```
vis.gam(mt1, # GAM object
        view = c("disp", "hp"), # variables
        plot.type = "contour") # contour plot or heatmap
```



Exercise 1

Hierachical GAMs

Hierachical GAMs

- Hierachical data: grouped data (factor!)
- non-linear relationships
- shape of function can vary between grouping/factor levels

Hierarchical generalized additive models in ecology: an introduction with mgcv

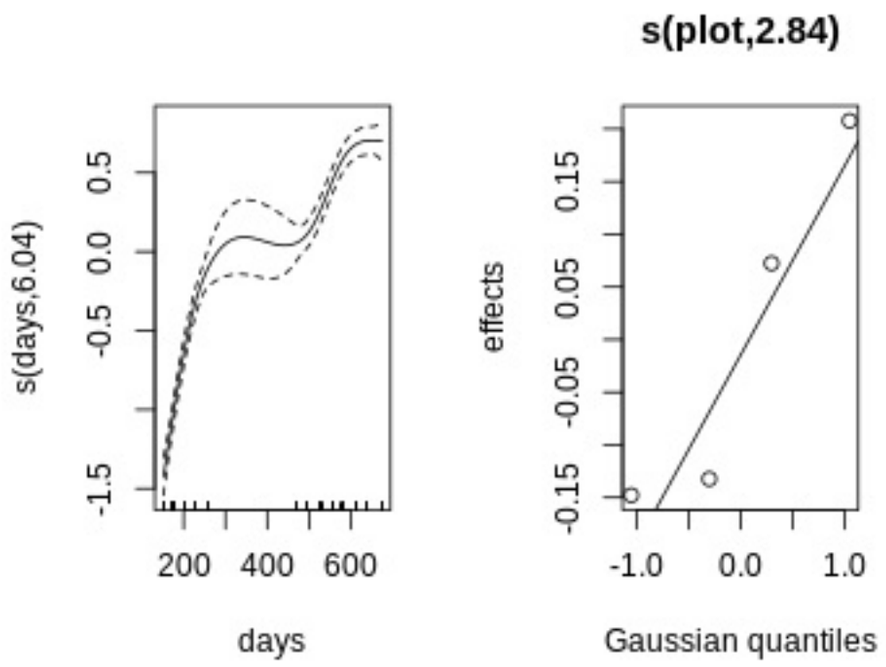
Eric J. Pedersen[1,2], David L. Miller[3,4], Gavin L. Simpson[5,6] and Noam Ross[7]

[1] Northwest Atlantic Fisheries Center, Fisheries and Oceans Canada, St. John's, NL, Canada
[2] Department of Biology, Memorial University of Newfoundland, St. John's, NL, Canada
[3] Centre for Research into Ecological and Environmental Modelling, University of St Andrews, St Andrews, UK
[4] School of Mathematics and Statistics, University of St Andrews, St Andrews, Scotland, UK
[5] Institute of Environmental Change and Society, University of Regina, Regina, SK, Canada
[6] Department of Biology, University of Regina, Regina, SK, Canada
[7] EcoHealth Alliance, New York, NY, USA

Global Smoother

- single global smooth term for each variable
- level-individual **random effect intercepts** (`bs = 're'`)

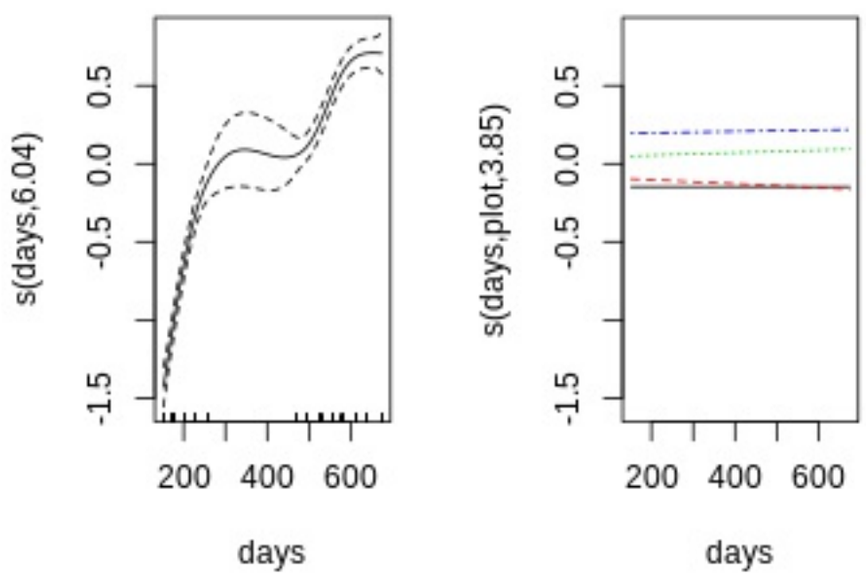
```
spr_G = gam(logSize ~ s(days) +
                      s(plot, bs = 're'),
            data = Spruce,
            method = 'REML')
plot(spr_G, pages = 1)
```



Global Smoother + Group Level Smoother

- factor-smooth interaction (`bs = 'fs'`)
- single global smooth term for each variable
- **varying slopes**
- same wiggliness (i.e. complexity) of smooths

```
spr_GS = gam(logSize ~ s(days) +
                       s(days, plot, bs = 'fs'),
             data = Spruce,
             method = 'REML')
plot(spr_GS, pages = 1)
```



Global Smoother + Group Level Smoother

- `s(x, by = fac)` and `s(fac, bs = 're')`
- similar to GS
- varying slopes
- **different wiggliness** (i.e. complexity) of smooths

```
spr_GI = gam(logSize ~ s(days) +
                       s(days, by = plot) +
                       s(plot, bs = 're'),
             data = Spruce,
             method = 'REML')
```

Model output

Model output

Summary

```
summary(mod)
```

Checking

```
gam.check(mod)
```

AIC

```
AIC(mod)
```

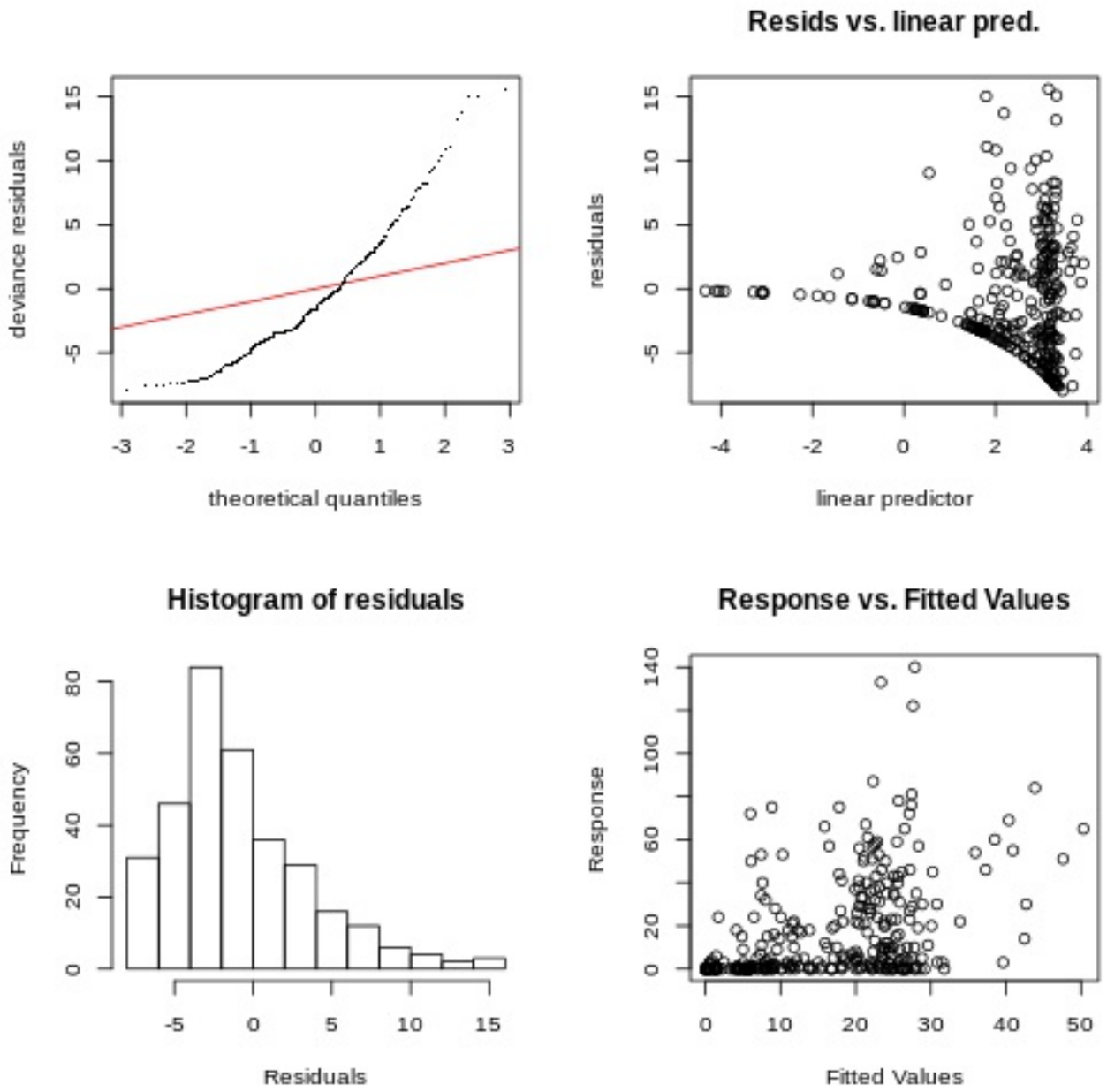
Predict

```
predict(mod)
```

Model summary

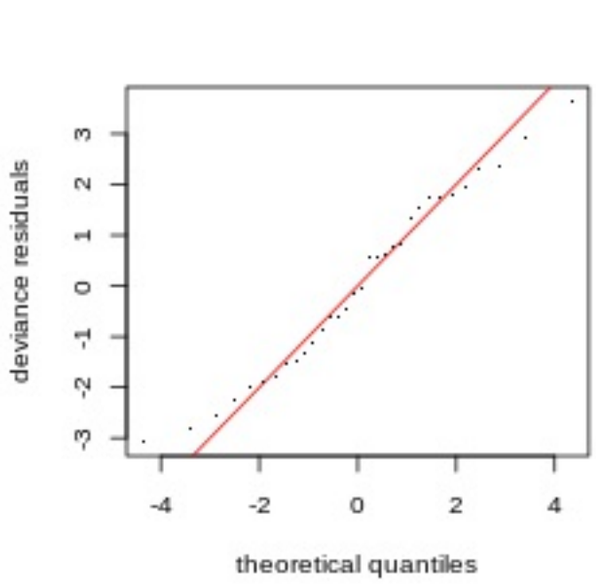
```
##
## Family: poisson
## Link function: log
##
## Formula:
## egg.count ~ s(c.dist) + s(salinity)
##
## Parametric coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  2.22458    0.04077   54.57   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##                edf Ref.df Chi.sq p-value
## s(c.dist)    8.559  8.938  255.8  <2e-16 ***
## s(salinity) 8.886  8.992 1204.7  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.165   Deviance explained = 28.9%
## UBRE = 19.928  Scale est. = 1         n = 330
```

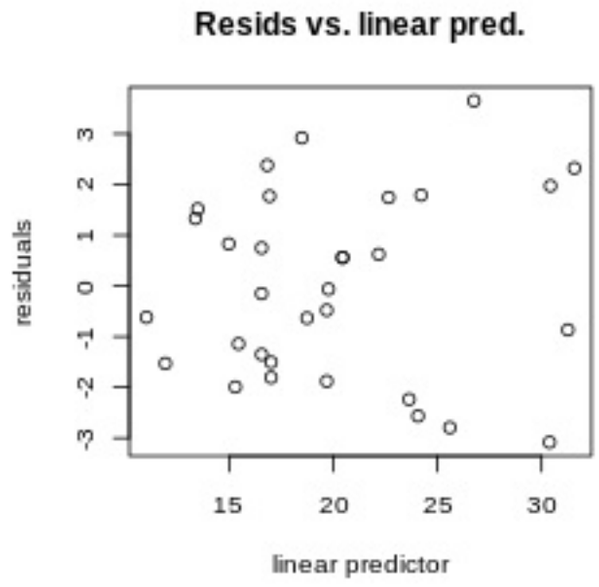
Model checking

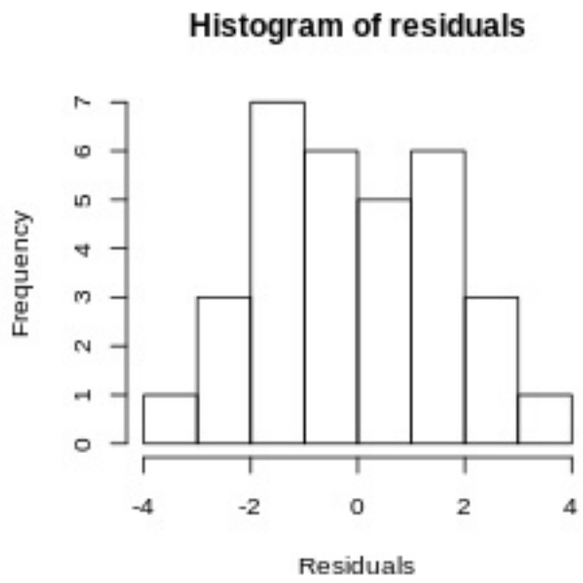


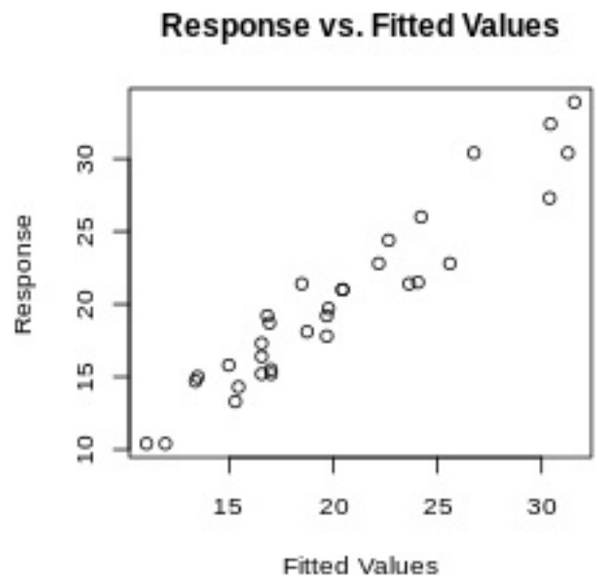

```
##
## Method: UBRE   Optimizer: outer newton
```

Model checking










```
##
## Method: REML   Optimizer: outer newton
```

Exercise 2

Thank you for participating in the course!

Structural Equation Modelling (Moritz Link) 15.00 - 16.30

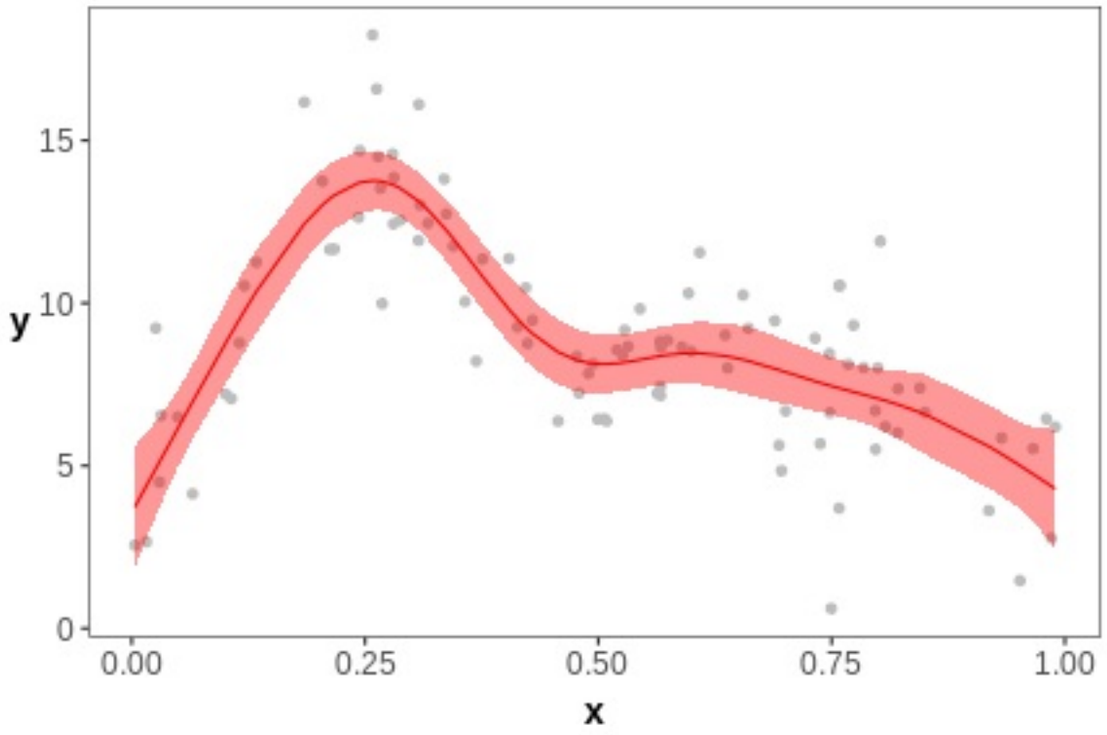
Tutorials, Blogs

- Generalized Additive Models in R (Noam Ross)
  - https://noamross.github.io/gams-in-r-course
- Doing magic and analyzing seasonal time series with GAM (Generalized Additive Model) in R
  - https://petolau.github.io/Analyzing-double-seasonal-time-series-with-GAM-in-R/
- From the Bottom of the Heap - Blog by Gavin Simpson
  - https://www.fromthebottomoftheheap.net/
- Introducing gratia
  - https://www.fromthebottomoftheheap.net/2018/10/23/introducing-gratia/
- Noam Ross Github
  - https://github.com/noamross/gam-resources
- Environmental computing
  - http://environmentalcomputing.net/intro-to-gams

Prediction

```
gam_sim = gam(y ~ s(x),
              data = sim,
              family = 'gaussian')
pred = predict(gam_sim, type = 'response', se.fit = TRUE)

sim$fit = pred$fit
sim$lwr = pred$fit - (2 * pred$se.fit)
sim$upr = pred$fit + (2 * pred$se.fit)
```



Model selection

Model selection

If you are not interested in prediction, but the most parsimonious model

- penalty on overall slope (in addition to wiggliness penalty)
- similar to ridge regression, lasso

```
select = TRUE
```

```
gam(y ~ s(x1) + s(x2) + s(x3),
    select = TRUE,
    data = data,
    method = 'REML')
```

Model selection

- AIC
- expert subject
- computational time
- inferential goals of the study