# Intro to generalized additive models in R (with mgcv)

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Material available at:

`https://github.com/mfasiolo/GAM_Workshop_Enbis_EDF_23`

We will firstly cover:

1. What is an additive model?
2. Introducing smooth effects
3. GAM modelling with mgcv and mgcViz

# What is an additive model

Regression setting:

- $y$ is our response or dependent variable
- $\mathbf{x}$ is a vector of covariates or independent variables

In **distributional regression** we want a good model for $\text{Dist}(y|\mathbf{x})$.

Model is $\text{Dist}_m\{y|\theta_1(\mathbf{x}), \theta_2, \dots, \theta_q\}$, where $\theta_1, \dots, \theta_q$ are param.

We assume that $\theta_2, \dots, \theta_q$ do not depend on $\mathbf{x}$.

**Gaussian additive** model:

$$y|\mathbf{x} \sim N\{y|\mu(\mathbf{x}), \sigma^2\},$$

where

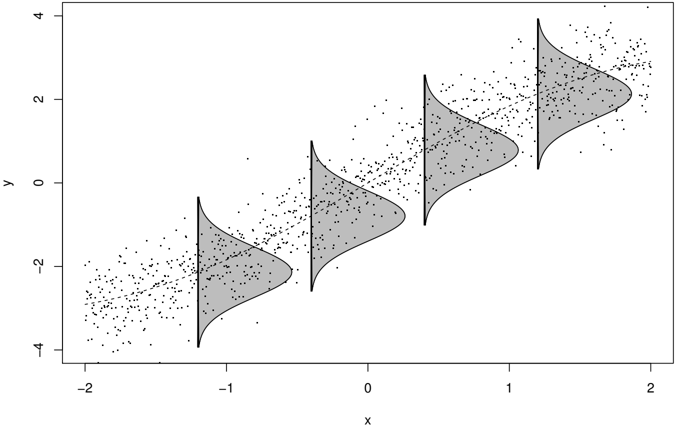
$$\mu(\mathbf{x}) = \sum_{j=1}^{m} f_j(\mathbf{x}),$$

and

$$\sigma^2 = \text{Var}(y).$$

$f_j$'s can be fixed, random or smooth effects.

NB: we call $\sum_{j=1}^{m} f_j(\mathbf{x})$ **linear predictor** because it is linear in $\boldsymbol{\beta}$.




Gaussian model with variable mean.
In mgcv: `gam(y~s(x), family=gaussian)`.

**Generalized** additive model (GAM) (Hastie and Tibshirani, 1990):

$$y|\mathbf{x} \sim \text{Distr}\{y|\theta_1 = \mu(\mathbf{x}), \theta_2, \dots, \theta_p\},$$

where

$$g\{\mu(\mathbf{x})\} = \sum_{j=1}^{m} f_j(\mathbf{x}),$$

and $g$ is the link function.

Poisson GAM:

- $y|\mathbf{x} \sim \text{Pois}\{y|\mu(\mathbf{x})\}$
- $\mathbb{E}(y|\mathbf{x}) = \text{Var}(y|\mathbf{x}) = \exp\left\{\sum_{j=1}^{m} f_j(\mathbf{x})\right\}$
- $g = \log$ assures $\mu(\mathbf{x}) > 0$

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# Introducing smooth effects

Consider additive model

$$g\{\mu(\mathbf{x})\} = f_1(\mathbf{x}) + f_2(\mathbf{x}) + f_3(\mathbf{x}),$$

where

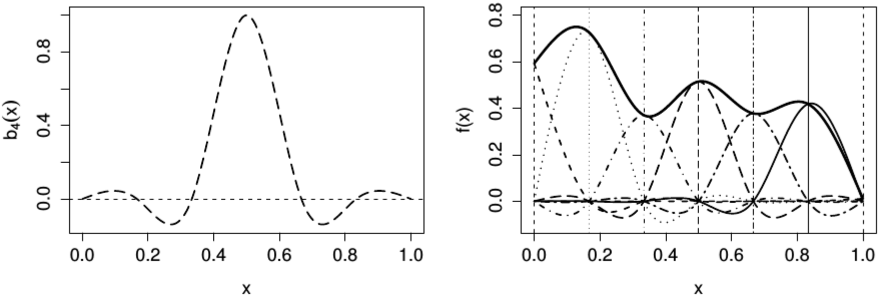
- $f_1(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$
- $f_2(\mathbf{x}) = \begin{cases} 0 & \text{if } x_2 = \text{FALSE} \\ \beta_4 & \text{if } x_2 = \text{TRUE} \end{cases}$
- $f_3(\mathbf{x}) = f_3(x_3)$ is a non-linear smooth function.

Smooth effects built using spline bases

$$f_3(x_3) = \sum_{k=1}^{r} \beta_k b_k(x_3)$$

where $\beta_k$ are unknown coeff and $b_k(x_3)$ are known spline basis functions.

```
s(x, bs = "cr", k = 20)
```




Cubic regression splines are related to the optimal solution to

$$\sum_{i=1}^{n} \{y_i - f(x_i)\}^2 + \gamma \int f''(x)^2 \, dx.$$

`mgcv` offers a wide variety of smooths (see `?smooth.terms`).

Univariate types:

- `s(x) = s(x, bs = "tp")` thin-plate-splines
- `s(x, bs = "cr")` cubic regression spline
- `s(x, bs = "ad")` adaptive smooth

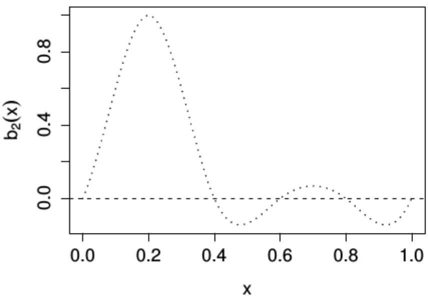
Multivariate type:

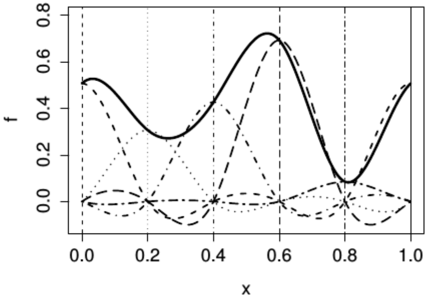
- `s(x1, x2) = s(x1, x2, bs = "tp")` thin-plate-splines (isotropic)
- `te(x1, x2)` tensor-product-smooth (anisotropic)
- `s(x, y, bs = "sos")` smooth on sphere

They can depends on factors:

- `s(x, by = Subject)`
- `s(x, Subject, bs = "fs")`

```
s(x, bs = "cc")
```

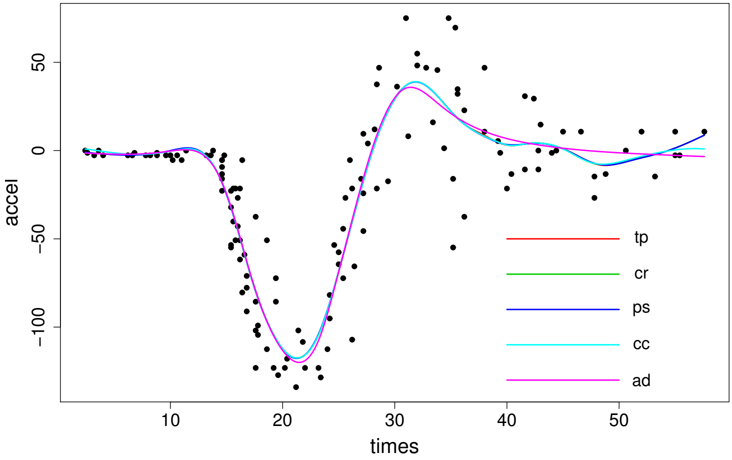



Cyclic cubic regression splines make so that

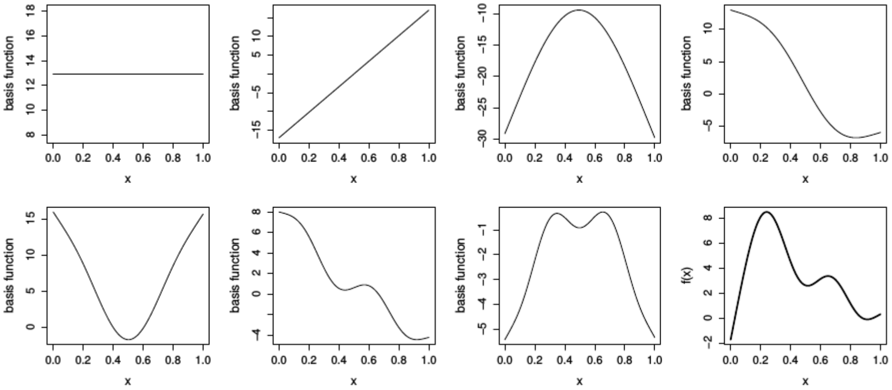
- $f(x_{min}) = f(x_{max})$
- $f'(x_{min}) = f'(x_{max})$
- $f''(x_{min}) = f''(x_{max})$

```
s(x, bs = "ad")
```

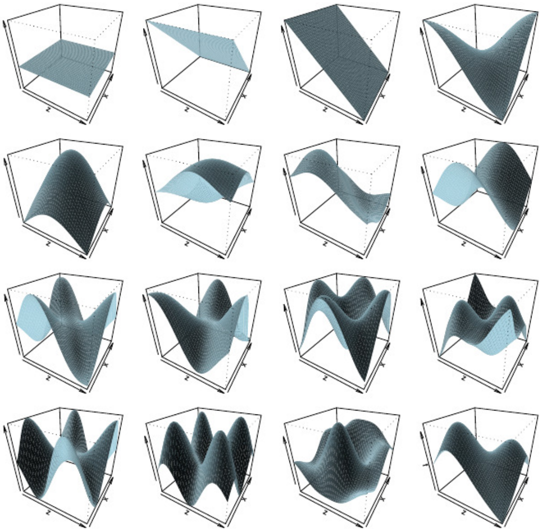



The wiggliness or smoothness of $f(x)$ depends on $x$.

## `s(x, bs = "tp")` or `s(x)`: Thin plate regression splines (TPRS)




Rank 7 TPRS basis. Image from Wood (2017).



Rank 17 2D TPRS basis. Courtesy of Simon Wood.

`s(x1, x2)`, `s(x1, x2, x3)`, ...

Based on thin plate regression splines basis.

Related to optimal solution to:

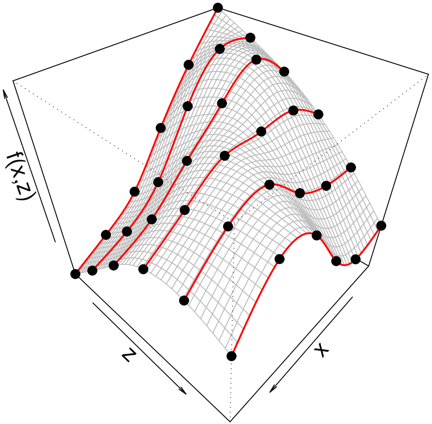
$$\sum_i \{y_i - f(x_i, z_i)\}^2 + \gamma \int f_{xx}^2 + 2f_{xz}^2 + f_{zz}^2 dxdz$$

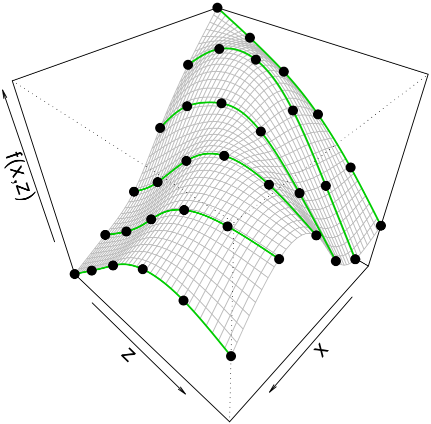
A single smoothing parameter $\gamma$.

Isotropic: same smoothness along $x_1$, $x_2$, ...

Isotropic effect of $x_1$, $x_2$ are in same unit (e.g. Km).
If different units better use tensor product smooths `te(x1, x2)`.

- $x$-penalty: average wiggliness of red curves
- $z$-penalty: average wiggliness of green curves



Can use (almost) any kind of marginal:

- `te(x1, x2, x3)` product of 3 cubic regression splines bases
- `te(x1, x2, bs = c("cc", "cr"), k = c(10, 6))`
- `te(LO, LA, t, d=c(2,1), bs=c("tp","cc"))`

Basis of `te` contains functions of the form $f(x_1)$ and $f(x_2)$.

To fit $f(x_1) + f(x_2) + f(x_1, x_2)$ separately use:

```
y ~ ti(x1) + ti(x2) + ti(x1, x2)
```

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`mgcv` is a recommended R package, included in R by default.

There are alternatives to `mgcv`, such as:

- `mboost` (Hothorn et al., 2010)
- `gamlss` (Rigby and Stasinopoulos, 2005)
- `brms` (Bürkner et al., 2017)
- `BayesX` (Brezger et al., 2003)
- `INLA` (Rue et al., 2009)

The `mgcv` ecosystem:

- `mgcViz` visualising GAMs
- `qgam` quantile GAMs
- `SCM` multivariate Gaussian GAMs
- `gamFactory` aggregation of experts with GAMs
- and many others `gamm4`, `refund`, `scam`, `vagam`, `GJRM`, `itsadug`, ...

# GAM modelling with mgcv and mgcViz

Recall structure of smooth effects:

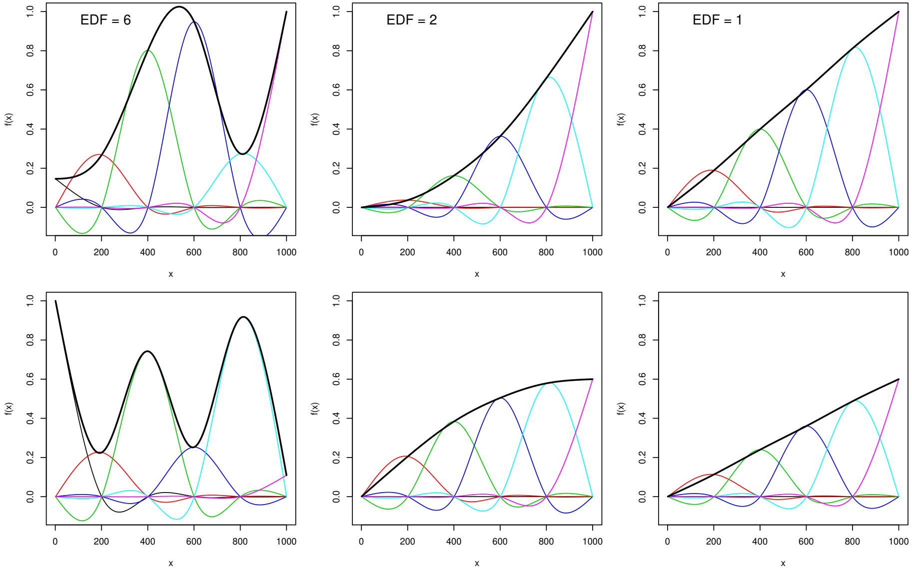
$$f(\mathbf{x}) = \sum_{j=1}^{k} \beta_j b_j(\mathbf{x}).$$

where $\boldsymbol{\beta}$ shrunk toward smoothness by penalty.

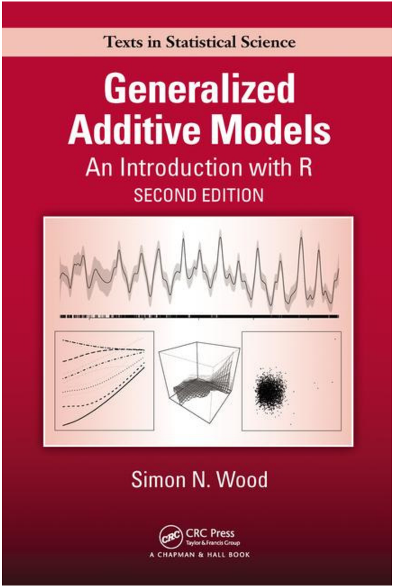
Exact $k$ is unimportant, we choose it large enough and let penalty work.

Effective number of parameters we are using is $\leq k$.

Approximation is **Effective Degrees of Freedom** (EDF) $\leq k$.


EDF = 6
EDF = 2
EDF = 1
f(x)
x
0 200 400 600 800 1000
0.0 0.2 0.4 0.6 0.8 1.0

# Further reading



# References I

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