Intro to generalized additive models in R (with mgcv)

Matteo Fasiolo (University of Bristol, UK)

matteo.fasiolo@bristol.ac.uk

Material available at:

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

Workshop content

Today we will cover:

1. Intro to standard GAMs
2. Multi-parameter GAMs, including GAMLSS
3. Quantile GAMs

Focus on **GAM modelling**, not fitting/inferential/computational aspects.

We will mention but not explain Big Data methods for GAMs.

On Github you can find:

1. slides
2. html files for R demos
3. exercises and solutions

We 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

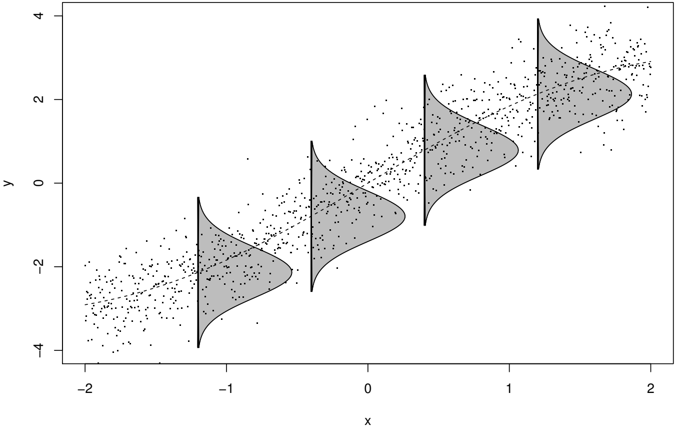
$$\mu(\mathbf{x}) = \sum_{j=1}^{m} f_j(\mathbf{x}),$$

and

$$\sigma^2 = \mathrm{Var}(y|\mathbf{x}).$$

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):

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

where

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

and g is a one-to-one function.

Poisson GAM:

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

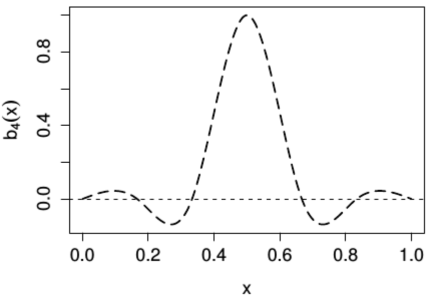
- $f_1(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$
- $f_2(\mathbf{x}) = \begin{cases} 0 & \text{if } x_2 = \text{FALSE} \\ \beta_4 & \text{if } x_2 = \text{TRUE} \end{cases}$
- $f_3(\mathbf{x}) = f_3(x_3)$ is a non-linear smooth function.

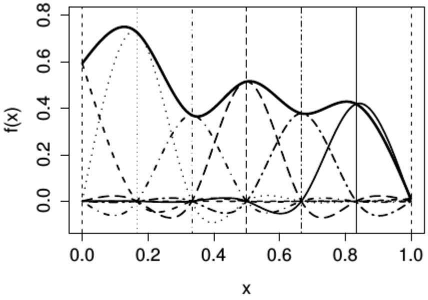
Smooth effects built using spline bases

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

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

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





Knot-based 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

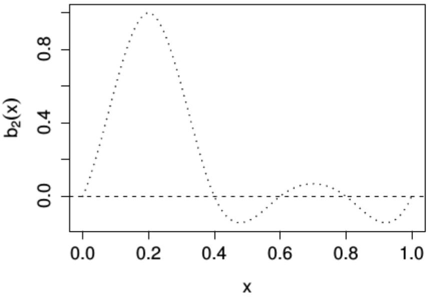
Multivariate type:

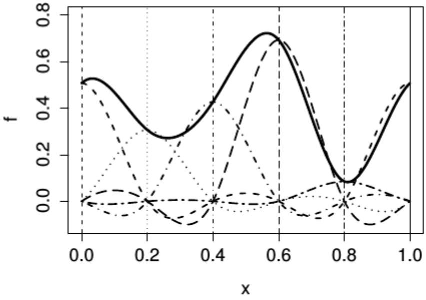
- `s(x1, x2) = s(x1, x2, bs = "tp")` thin-plate-splines (isotropic)
- `te(x1, x2)` tensor-product-smooth (anisotropic)
- `s(x, y, bs = "sos")` smooth on sphere

They can depends on factors:

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

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

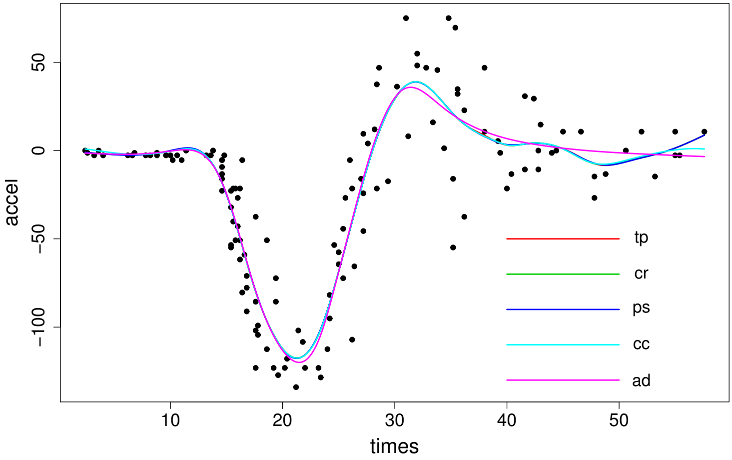




Cyclic cubic regression splines make so that

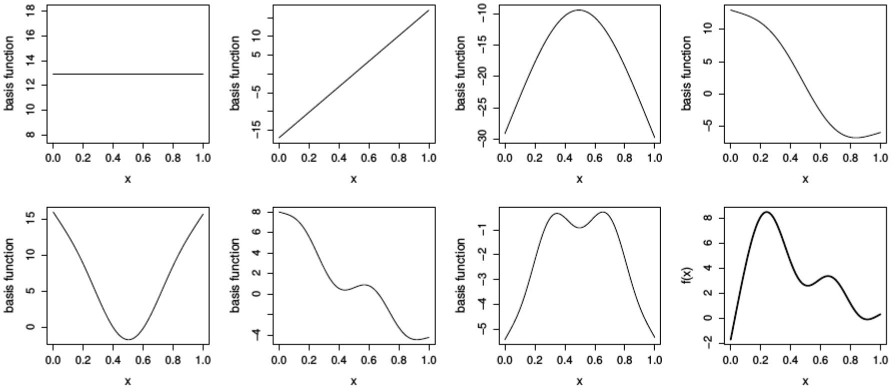
- $f(x_{min}) = f(x_{max})$
- $f'(x_{min}) = f'(x_{max})$
- $f''(x_{min}) = f''(x_{max})$

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

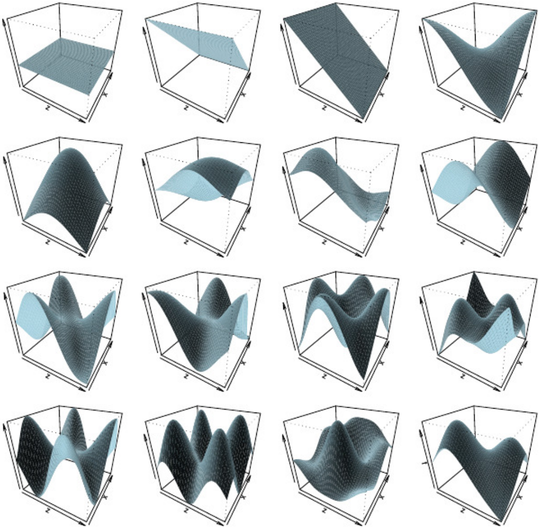


The wiggliness or smoothness of $f(x)$ depends on x.

`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:

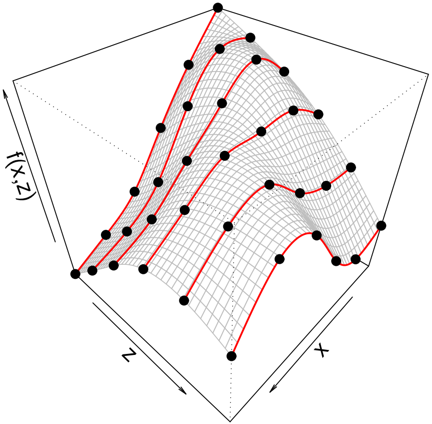
$$\sum_i \{y_i - f(x_i, z_i)\}^2 + \gamma \int f_{xx}^2 + 2f_{xz}^2 + f_{zz}^2 dxdz$$

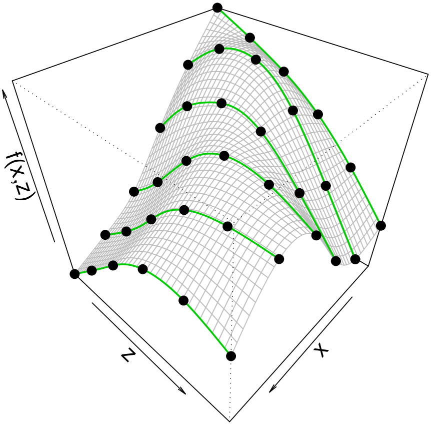
A single smoothing parameter γ.

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

Isotropic effect are ok if 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`, ...

Recall structure of smooth effects:

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

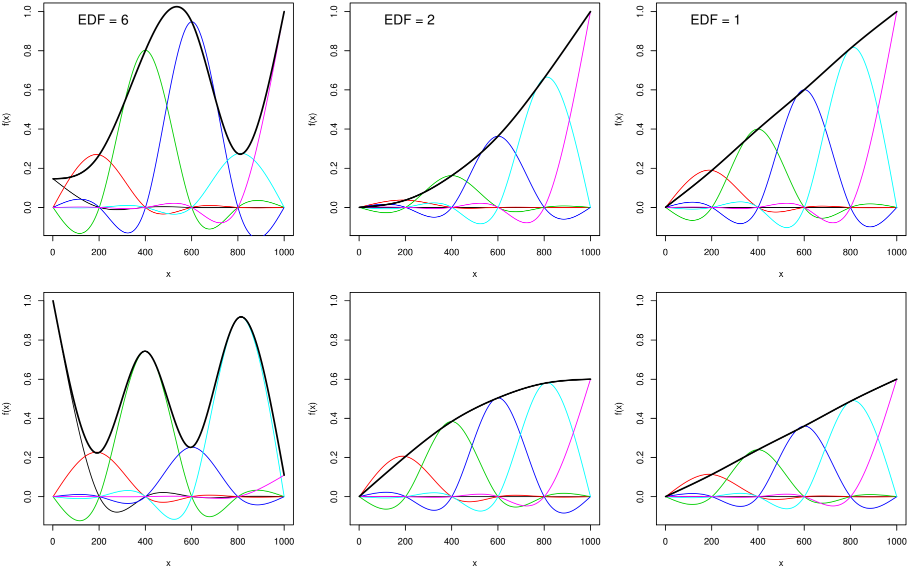
where $\boldsymbol{\beta}$ shrunk toward smoothness by penalty

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\text{argmax}}\ \text{PenLogLik}(\boldsymbol{\beta}|\gamma) = \underset{\boldsymbol{\beta}}{\text{argmax}} \Big\{ \overbrace{\log p(\mathbf{y}|\boldsymbol{\beta})}^{\text{goodness of fit}} - \underbrace{\text{Pen}(\boldsymbol{\beta}|\gamma)}_{\text{penalize complexity}} \Big\}$$

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

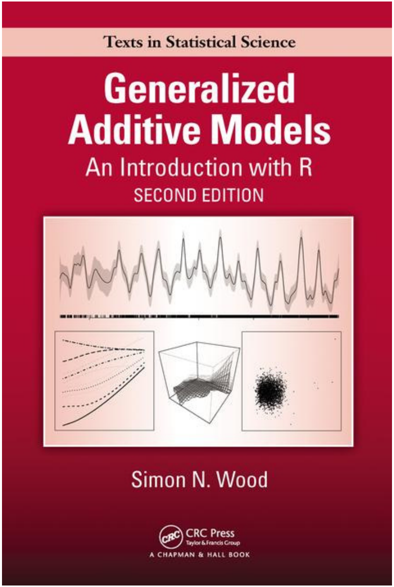
Effective number of parameters we are using is $\leq k$.

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

Brezger, A., T. Kneib, and S. Lang (2003). Bayesx: Analysing bayesian structured additive regression models. Technical report, Discussion paper//Sonderforschungsbereich 386 der Ludwig-Maximilians .

Bürkner, P. C. et al. (2017). brms: An r package for bayesian multilevel models using stan. *Journal of Statistical Software 80*(1), 1–28.

Hastie, T. and R. Tibshirani (1990). *Generalized Additive Models*, Volume 43. CRC Press.

Hothorn, T., P. Bühlmann, T. Kneib, M. Schmid, and B. Hofner (2010). Model-based boosting 2.0. *The Journal of Machine Learning Research 11*, 2109–2113.

Rigby, R. A. and D. M. Stasinopoulos (2005). Generalized additive models for location, scale and shape. *Journal of the Royal Statistical Society: Series C (Applied Statistics) 54*(3), 507–554.

Rue, H., S. Martino, and N. Chopin (2009). Approximate bayesian inference for latent gaussian models by using integrated nested laplace approximations. *Journal of the royal statistical society: Series b (statistical methodology) 71*(2), 319–392.

Wood, S. (2017). *Generalized additive models: an introduction with R*. CRC press.