Intro to generalized additive models in R (with mgcv)

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Material available at:

`https://github.com/mfasiolo/GAM_Workshop_Dortmund_25`

About me

BSc and MSc in Industrial Management Engineering from the University of Udine (IT) (known for Udinese F.C.).

MSc in Financial Engineering from Birkbeck College (Uni of London).

PhD in Statistic for University of Bath on Statistical Ecology.

In the School of Mathematics University of Bristol since 2015.

Research focus: methods for non-parametric regression with a focus on forecasting applications in the energy sector.

Workshop content

Today's sessions will cover:

1. Intro to standard GAMs
2. Smooth effects and penalties
3. Multi-parameter GAMs, including GAMLSS
4. Quantile GAMs and Big Data methods

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

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. Diagnostics and model selection tools
4. GAM modelling with mgcv

What is an additive model?

Regression setting:

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

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

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

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

Gaussian additive model:

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

where

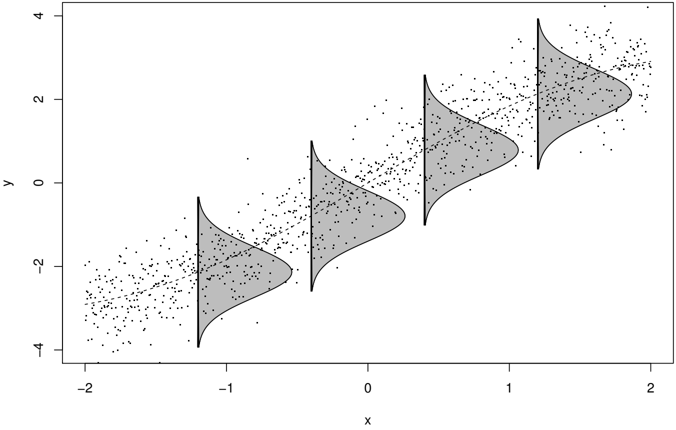
$$\mu(\boldsymbol{x}) = \mathbb{E}(y|\boldsymbol{x}) = \sum_{j=1}^{m} f_j(\boldsymbol{x}),$$

and

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

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

NB: we call $\sum_{j=1}^{m} f_j(\boldsymbol{x})$ **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):

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

where

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

and g is a one-to-one link function.

Poisson GAM:

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

Here relation between $\mathbb{E}(y|\boldsymbol{x})$ and $\text{Var}(y|\boldsymbol{x})$ is implied by model...

... or we can have extra parameters for scale and shape.

Scaled Student's t GAM:

- $y|\boldsymbol{x} \sim \text{ScaledStud}\{y|\mu(\boldsymbol{x}), \sigma, \nu\}$ (i.e. $(y-\mu)/\sigma \sim \text{Stud}(y|\nu)$)
- $\mathbb{E}(y|\boldsymbol{x}) = \mu(\boldsymbol{x}) = \sum_{j=1}^{m} f_j(\boldsymbol{x})$
- σ is scale parameter
- ν is shape parameter (degrees of freedom)
- $\text{Var}(y|\boldsymbol{x}) = \sigma^2 \frac{\nu}{\nu-2}$

Later we'll let all parameters be functions of $\boldsymbol{x}$, eg:

- $y|\boldsymbol{x} \sim N\{y|\mu(\boldsymbol{x}), \sigma(\boldsymbol{x})\}$

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Introducing smooth effects

Consider additive model

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

where

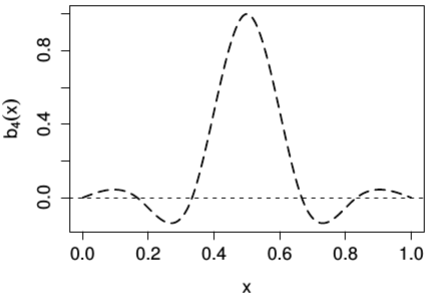
- $f_1(\boldsymbol{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$
- $f_2(\boldsymbol{x}) = \begin{cases} 0 & \text{if } x_2 = \text{FALSE} \\ \beta_4 & \text{if } x_2 = \text{TRUE} \end{cases}$
- $f_3(\boldsymbol{x}) = f_3(x_3)$ is a non-linear smooth function.

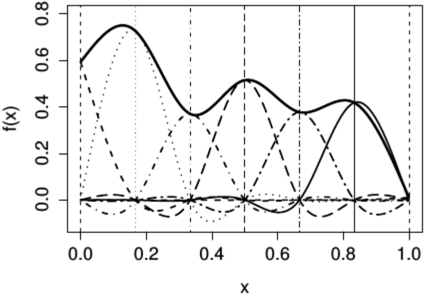
Smooth effects built using spline bases

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

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

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

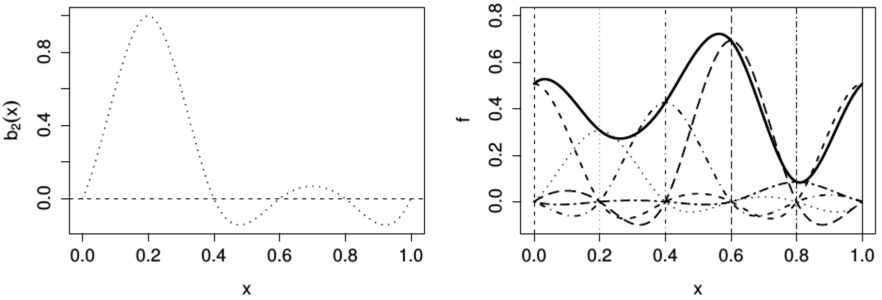




Cubic regression splines are related to the optimal solution to

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

`mgcv` offers many smooths (see `?smooth.terms`). `s(x, bs = "cc")`



Cyclic cubic regression splines make so that

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

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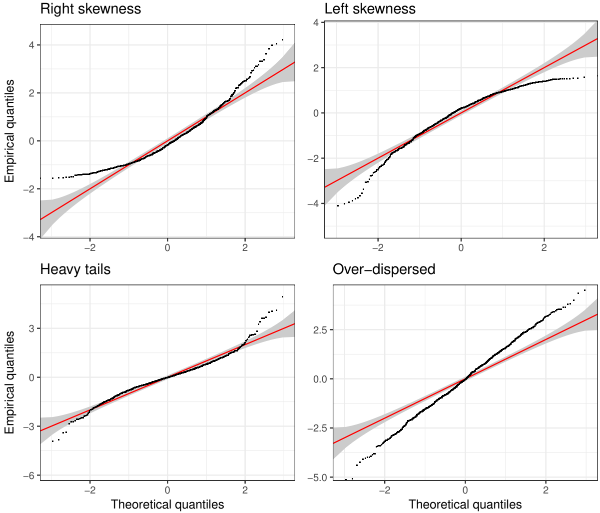
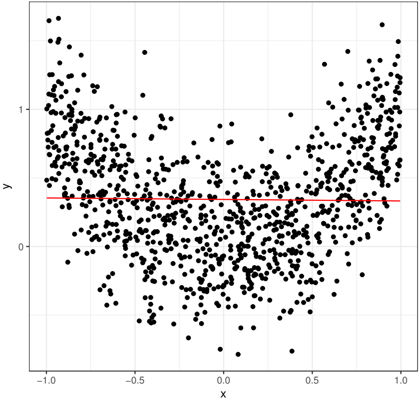
In the first hands-on session we'll use few basic diagnostics.

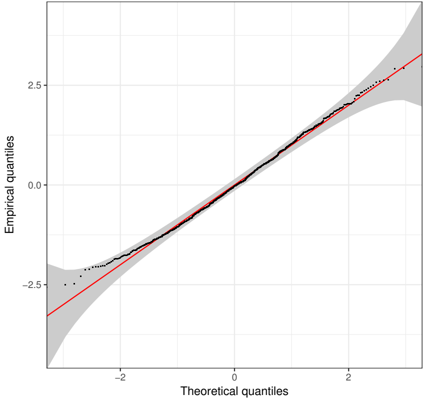
QQ-plots



Useful for choosing model $\mathrm{Dist}_m(y|\boldsymbol{x})$ (e.g. Poisson vs Neg. Binom.)

Less useful for finding omitted variables and non-linearities.





Recall structure of smooth effects:

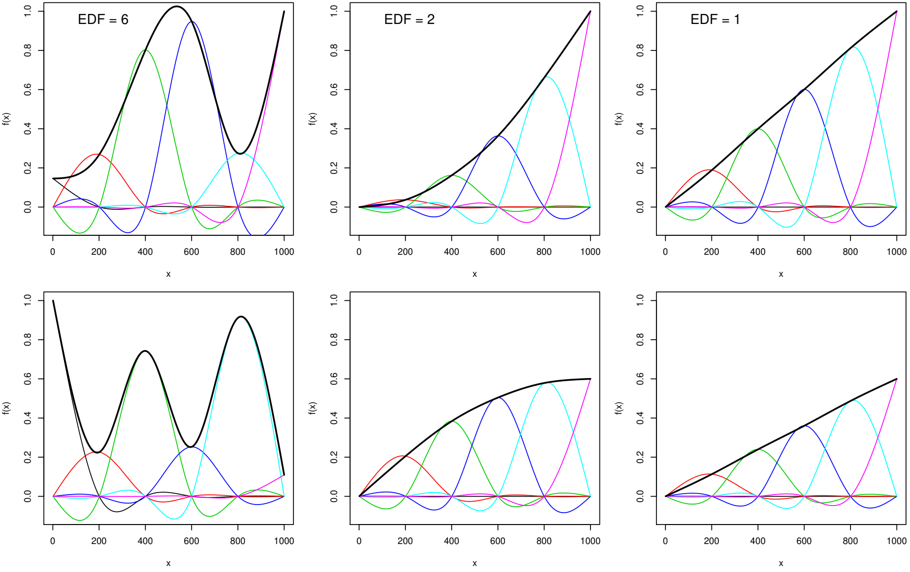
$$f(\boldsymbol{x}) = \sum_{j=1}^{k} \beta_j b_j(\boldsymbol{x}).$$

where $\boldsymbol{\beta}$ estimated by Maximum a Posterior (MAP)

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\text{argmax}} \; \log p(\boldsymbol{\beta}|\boldsymbol{y}, \boldsymbol{\lambda}) = \underset{\boldsymbol{\beta}}{\text{argmax}} \Big\{ \overbrace{\log p(\boldsymbol{y}|\boldsymbol{\beta})}^{\text{goodness of fit}} + \underbrace{\log p(\boldsymbol{\beta}|\boldsymbol{\lambda})}_{\text{prior penalising complexity}} \Big\}$$

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

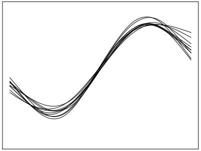
`mgcv` uses a hierarchical fitting framework:

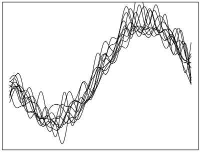
1. Select $\boldsymbol{\lambda}$ to determine smoothness

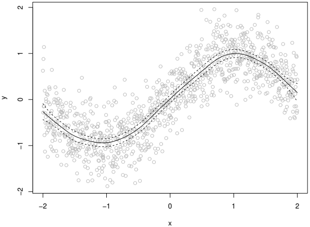
$$\hat{\boldsymbol{\lambda}} = \underset{\boldsymbol{\lambda}}{\text{argmax}} \; \text{LAML}(\boldsymbol{\lambda}).$$

2. For fixed $\boldsymbol{\lambda}$, estimate $\boldsymbol{\beta}$ to determine actual fit

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\text{argmax}} \; \log p(\boldsymbol{\beta}|\boldsymbol{y}, \boldsymbol{\lambda}).$$







Default k used by `mgcv` in $f(\boldsymbol{x}) = \sum_{j=1}^{k} \beta_j b_j(\boldsymbol{x})$ is arbitrary.

Exact choice of k not important, but it must not be too low.

Checking whether k is too low:

1. look at conditional residuals checks
2. look at output of `gam.check(fit)`:

```
##              k'  edf k-index p-value
## s(x1)      9.00 8.60    0.91  <2e-16 ***
## s(x2)      9.00 8.13    1.02    0.76
## s(x3)      8.00 2.66    1.04    0.97
```

3. increase k and see if a **model selection criterion** improves

Popular criterion is approximate Akaike Information Criterion (AIC):

$$\text{AIC} = \underbrace{-2\log p(\boldsymbol{y}|\hat{\boldsymbol{\beta}})}_{\text{goodness of fit}} \quad + \quad \underbrace{2\tau}_{\text{model complexity}}$$

where τ is EDF.

If $\text{AIC}_{m_1} < \text{AIC}_{m_2}$ choose model 1.

To select which effects to include we can also look at p-values:

```
summary(fit)
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 267.2004    75.4197   3.543 0.000405 ***
## x1            6.2854     1.0457   6.010 2.20e-09 ***
## x2           79.8459    80.4130   0.993 0.320858
## x3          -71.2728    86.1725  -0.827 0.408284
```

The exercises will be based on the `mgcv` package for GAM modelling.

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

It contains methods for:

- creating GAM models
- fitting them
- visualizing and summarizing model output

The `mgcv` ecosystem:

- `mgcViz` visualising GAMs
- `qgam` quantile GAMs
- `SCM` multivariate Gaussian GAMs
- `gamFactory` nested smooth effects in GAMs
- and many others `gamm4`, `refund`, `scam`, `vgam`, `GJRM`, `itsadug`, ...

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)
- `bamlss` (Umlauf et al., 2018)

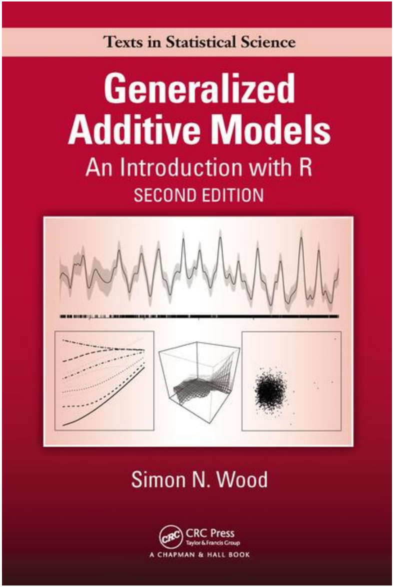
Each offers much flexibility (e.g. smooth effects types and distributions).

Strong points of `mgcv`'s methods:

1. little tuning needed (automatic smoothing parameters selection)
2. fast and stable numerical implementation

Now we'll be looking at R_demos/1_Intro_Gefcom14.html

Further reading



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Umlauf, N., N. Klein, and A. Zeileis (2018). BAMLSS: Bayesian additive models for location, scale, and shape (and beyond). *Journal of Computational and Graphical Statistics* 27(3), 612–627.