

Intro to generalized additive models in R

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Material available at:

https://github.com/mfasiolo/workshop_BOZEN19

These slides cover:

- 1 What is an additive model?
- 2 Introducing smooth effects
- 3 Introducing random effects
- 4 Diagnostics and model selection tools
- 5 GAM modelling in mgcv

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} .

What is an additive model

Gaussian additive model:

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

where

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

and

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

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

What is an additive model

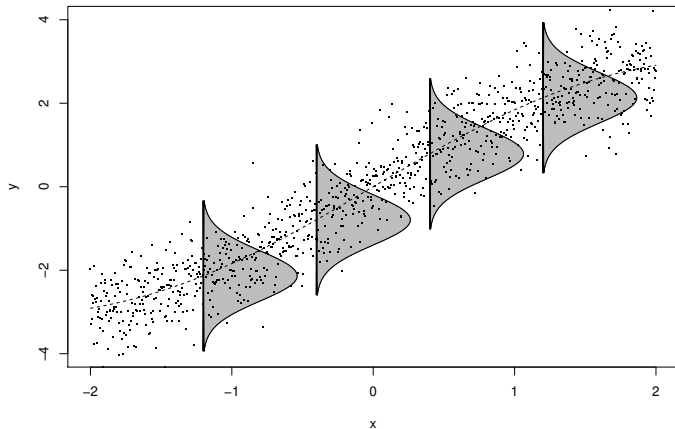


Figure: Gaussian model with variable mean.
In mgcv: `gam(y~s(x), family=gaussian)`.

What is an additive model

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

$$\mathbb{E}(y|\mathbf{x}) = \mu(\mathbf{x}) = g^{-1}\left\{\sum_{j=1}^m f_j(\mathbf{x})\right\},$$

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 $\mu(\mathbf{x}) > 0$

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

What is an additive model

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

Scaled Student's t GAM:

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

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

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

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Introducing smooth effects

Consider additive model

$$\mathbb{E}(y|\mathbf{x}) = \mu(\mathbf{x}) = g^{-1}\left\{f_1(\mathbf{x}) + f_2(\mathbf{x}) + f_3(\mathbf{x})\right\},$$

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.

Introducing smooth effects

Example: B-splines

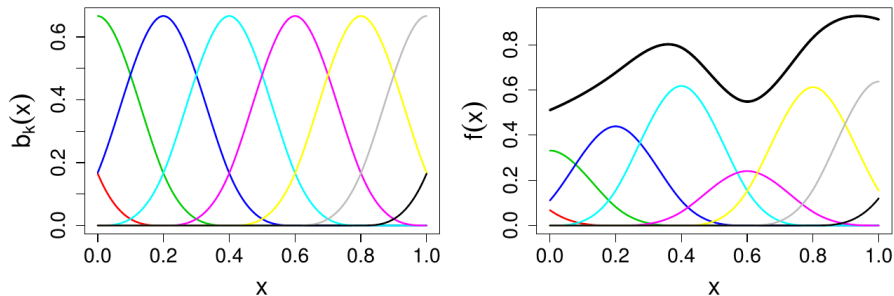
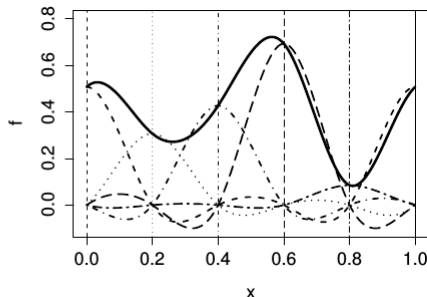
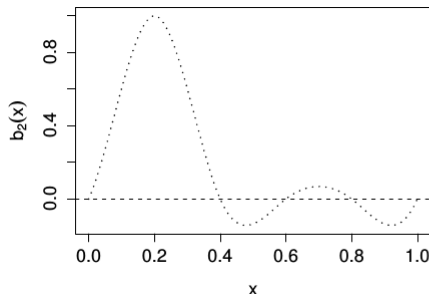


Figure: B-spline basis (left) and smooth (right).

Types of smooths

Example: Cyclic cubic splines



Cyclic cubic regression splines make so that

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

Introducing smooth effects

Example: Thin plate regression splines (TPRS)

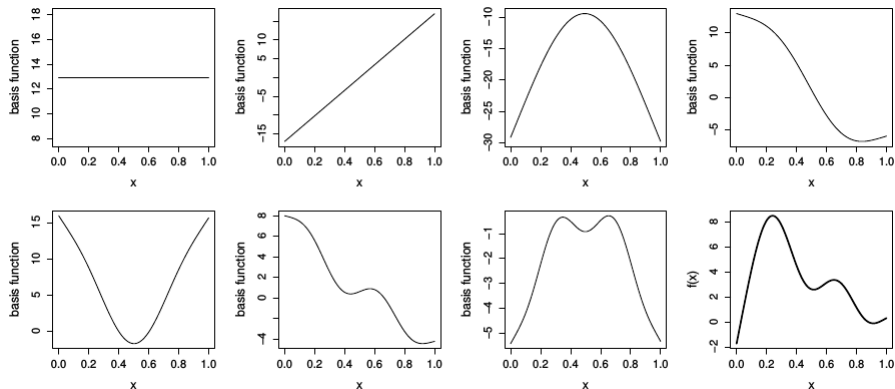


Figure: Rank 7 TPRS basis. Image from Wood (2017).

Introducing smooth effects

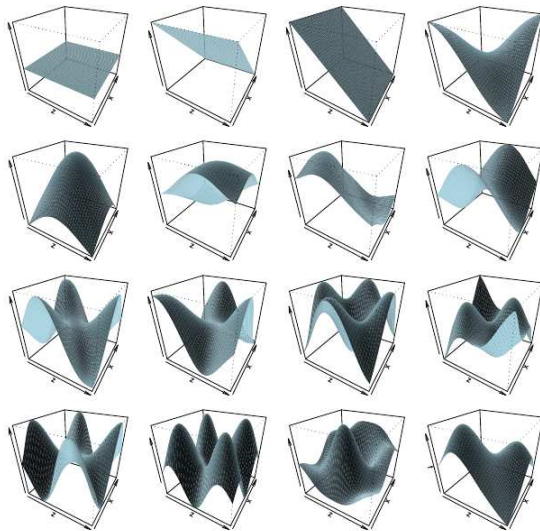


Figure: Rank 17 2D TPRS basis. Courtesy of Simon Wood.

Introducing smooth effects

In general

$$f(\mathbf{x}) = \sum_{k=1}^r \beta_k b_k(\mathbf{x}).$$

To determine complexity of $f(\mathbf{x})$:

- the basis rank r is large enough for sufficient flexibility
- a complexity penalty on β controls the wiggleness of the effects

GAM model fitting

$\hat{\beta}$ is the maximizer of **penalized** log-likelihood

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

where:

- $\log p(\mathbf{y}|\beta) = \sum_i \log p(y_i|\beta)$ is log-likelihood (i.i.d. case)
- $\operatorname{Pen}(\beta|\gamma)$ penalizes the complexity of the f_j 's
- $\gamma > 0$ smoothing parameters ($\uparrow \gamma \uparrow$ smoothness)

GAM model fitting

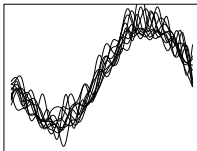
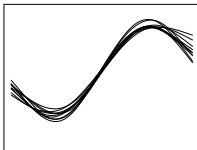
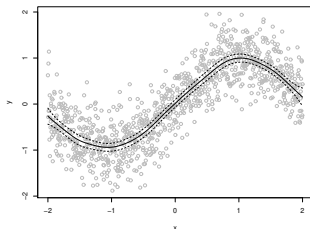
mgcv uses a hierarchical fitting framework:

- 1 Select γ to determine smoothness

$$\hat{\gamma} = \operatorname{argmax}_{\gamma} \text{LAML}(\gamma).$$

- 2 For fixed γ , estimate β to determine actual fit

$$\hat{\beta} = \operatorname{argmax}_{\beta} \text{PenLogLik}(\beta|\gamma).$$



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Introducing random effects

Suppose we have data on bone mineral density (bmd) as a function of age .

We have m subjects and n data pairs per subject

- subj 1: $\{bmd_{11}, age_{11}\}, \dots, \{bmd_{n1}, age_{n1}\}$
- subj j : $\{bmd_{1j}, age_{1j}\}, \dots, \{bmd_{nj}, age_{nj}\}$
- subj m : $\{bmd_{1m}, age_{1m}\}, \dots, \{bmd_{nm}, age_{nm}\}$

Standard linear model ignores individual differences

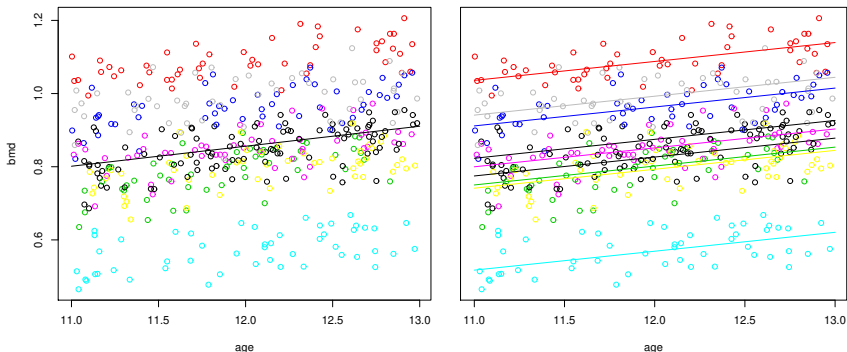
$$\mathbb{E}(bmd|age_{ij}) = \mu(age_{ij}) = \alpha + \beta age_{ij}.$$

We can include random intercept per subject

$$\mu(age_{ij}) = \alpha + \beta age_{ij} + a_j,$$

where $\mathbf{a} = \{a_1, \dots, a_m\} \sim N(\mathbf{0}, \Sigma)$.

Introducing random effects



We can also include random slopes

$$\mu(\text{age}_{ij}) = \alpha + (\beta + b_j)\text{age}_{ij} + a_j,$$

where $\mathbf{a} \sim N(\mathbf{0}, \Sigma_{\mathbf{a}})$ and $\mathbf{b} \sim N(\mathbf{0}, \Sigma_{\mathbf{b}})$.

Introducing random effects

In `mgcv` random effect are specified as:

```
gam(bmd ~ 1 + s(subject, bs = "re") +  
      age + s(age, subject, bs = "re"), ...)
```

In simplest case $\Sigma_{\mathbf{a}} = \gamma_{\mathbf{a}}\mathbf{I}$ and $\Sigma_{\mathbf{b}} = \gamma_{\mathbf{b}}\mathbf{I}$, that is

$$\Sigma_{\mathbf{a}} = \begin{bmatrix} \gamma_{\mathbf{a}} & 0 & 0 & \dots & 0 \\ 0 & \gamma_{\mathbf{a}} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \gamma_{\mathbf{a}} \end{bmatrix}$$

Variances $\gamma_{\mathbf{a}}$ and $\gamma_{\mathbf{b}}$ must be estimated (later I'll explain how).

Introducing random effects

Using the `gam` function in `mgcv` we can create and estimate simple random effects:

```
gam(bmd ~ 1 + s(subject, bs = "re") +  
      age + s(age, subject, bs = "re"), ...)
```

For more complex random effects (e.g. introducing correlation between random slopes and intercepts) we can use:

- `gamm` function estimates generalized additive mixed models using `nlme`
- `gamm4` package based on `lme4` package

Here we will use only simple effects.

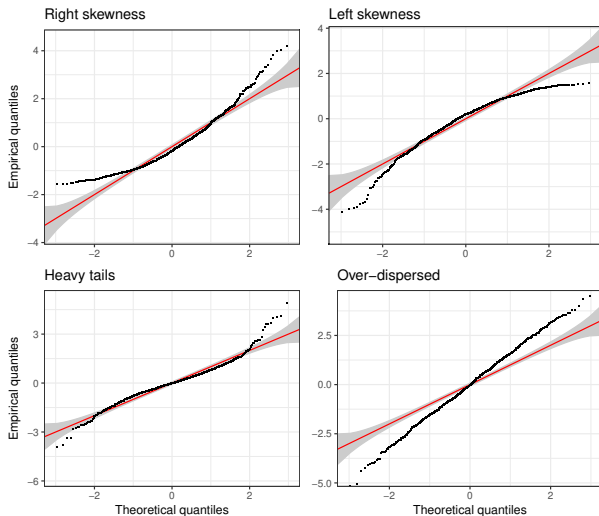
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Diagnostics and model selection tools

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

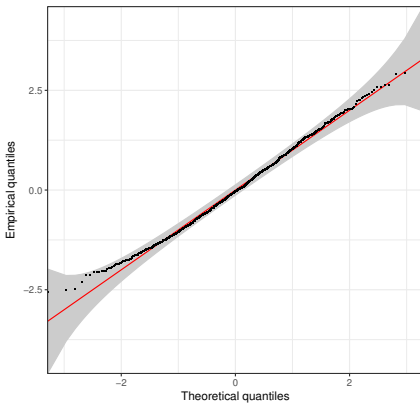
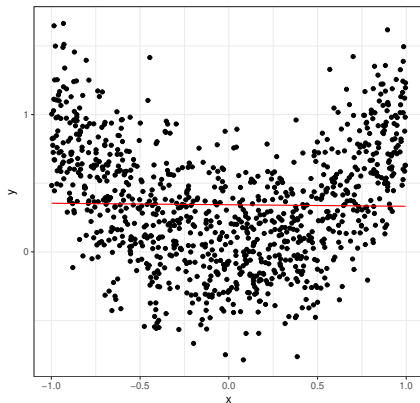
QQ-plots



Diagnostics and model selection tools

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

Less useful for finding omitted variables and non-linearities.



Recall structure of smooth effects:

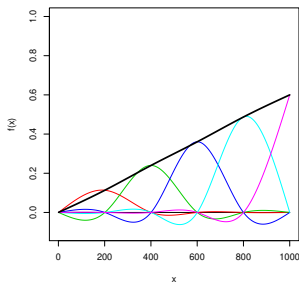
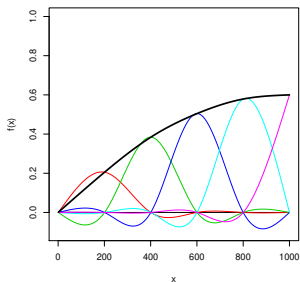
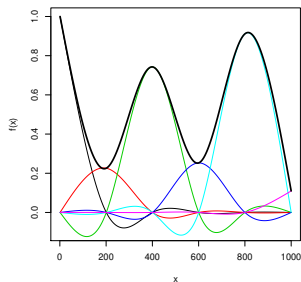
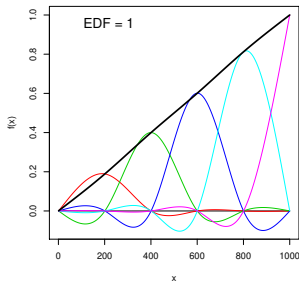
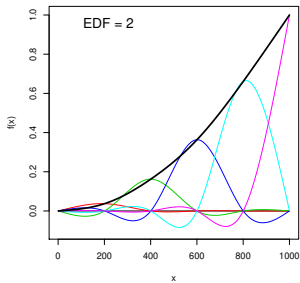
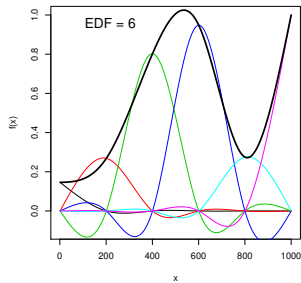
$$f(\mathbf{x}) = \sum_{j=1}^k \beta_j b_j(\mathbf{x}).$$

where β shrunk toward smoothness by penalty.

Effective number of parameters we are using is $< k$.

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

Diagnostics and model selection tools



Diagnostics and model selection tools

By default $k = 10$ but this 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(wM)	9.00	8.60	0.91	<2e-16 ***
## s(wM_s95)	9.00	8.13	1.02	0.76
## s(Posan)	8.00	2.66	1.04	0.97

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

Diagnostics and model selection tools

Model selection

General criterion is approximate Akaike Information Criterion (AIC):

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

where τ is EDF.

If $\text{AIC}_{m1} < \text{AIC}_{m2}$ 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	***
## Fl	6.2854	1.0457	6.010	2.20e-09	***
## loc2	79.8459	80.4130	0.993	0.320858	
## loc3	-71.2728	86.1725	-0.827	0.408284	

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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

There are alternatives to `mgcv`, such as:

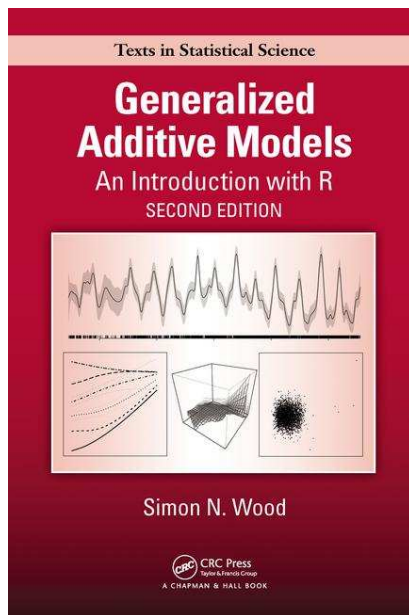
- `mboost` (Hothorn et al., 2010)
- `gamlss` (Rigby and Stasinopoulos, 2005)
- `brms` (Bürkner et al., 2017)
- BayesX (Brezger et al., 2003)
- INLA (Rue et al., 2009)

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

Further reading



References I

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