

Generalized additive models

Matteo Fasiolo (University of Bristol, UK)

matteo.fasiolo@bristol.ac.uk

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Today's plan

Morning session

- 1 Intro to Generalized Additive Models (GAMs)
- 2 Smooth effect types & Big Data methods

Afternoon session

- 1 Beyond mean modelling: GAMLSS models
- 2 Distribution-free modelling: Quantile GAMs

Intro to Generalized Additive Models (GAMs)

Structure:

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

Structure of the talk

Structure:

- 1 **What is an additive model?**
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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 $\text{Dist}_m\{y|\theta_1(\mathbf{x}), \dots, \theta_q(\mathbf{x})\}$, where $\theta_1(\mathbf{x}), \dots, \theta_q(\mathbf{x})$ are param.

In a Gaussian model, the mean depends on the covariates

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

where $\mu = \mathbb{E}(y|\mathbf{x})$ and $\sigma^2 = \text{Var}(y)$.

What is an additive model

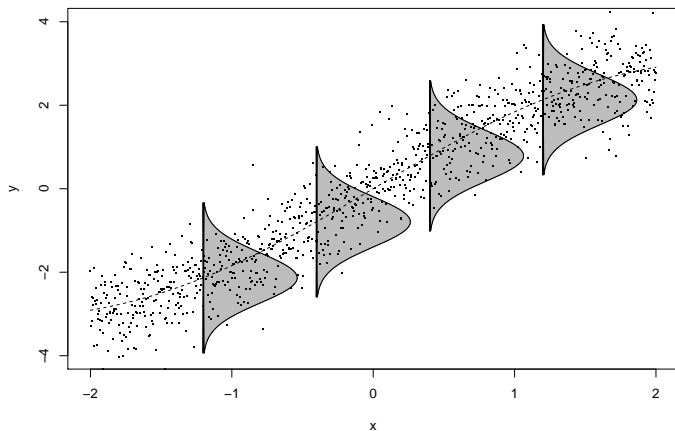


Figure : Gaussian model with variable mean.

In mgcv: `gam(y~s(x), family=gaussian)`.

What is an additive model

Gaussian additive model:

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

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

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

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

$$\hat{\beta} = \underset{\beta}{\operatorname{argmax}} \{L_y(\beta) - \operatorname{Pen}(\beta)\}.$$

where:

- $L_y(\beta) = \sum_i \log p(y_i|\beta)$ is log-likelihood
- $\operatorname{Pen}(\beta)$ penalizes the complexity of the f_j 's

What is an additive model

Generalized additive model (GAM):

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

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.

Relation between $\mathbb{E}(y|\mathbf{x})$ and $\text{Var}(y|\mathbf{x})$ might be implied by model.

Poisson GAM:

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

What is an additive model

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

Scaled Student's t GAM:

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

In the afternoon will see models with multiple linear predictors, eg:

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

What is an additive model

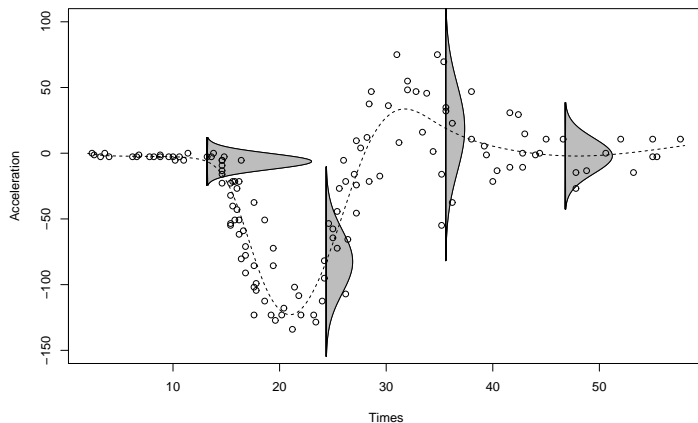


Figure : Gaussian model with variable mean and variance.
In mgcv: `gam(list(y~s(x), ~s(x)), family=gaulss).`

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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

- $f_1(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$
- $f_2(\mathbf{x}) = \begin{cases} 0 & \text{if } x_2 = \text{FALSE} \\ \alpha_4 & \text{if } x_2 = \text{TRUE} \end{cases}$
- $f_3(\mathbf{x}) = f_3(x_3)$ is a non-linear smooth function.

Smooth effects built using spine 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 1: B-splines

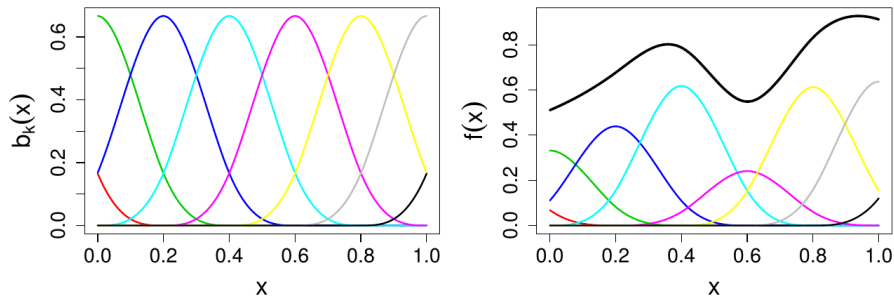


Figure : B-spline basis (left) and smooth (right).

Introducing smooth effects

Example 2: Thin plate regression splines (TPRS)

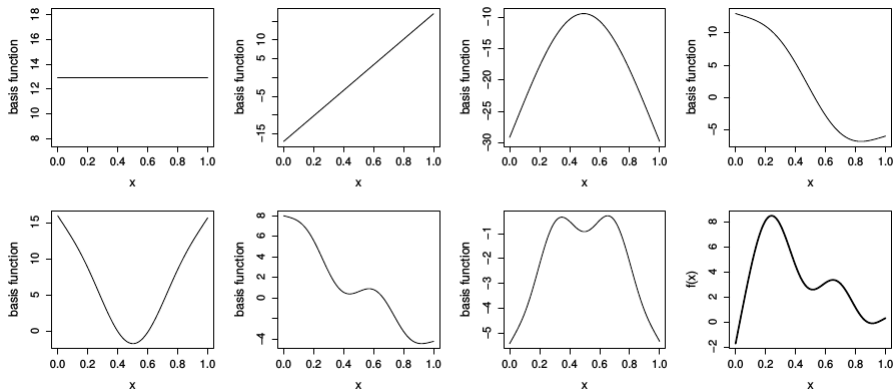


Figure : Rank 7 TPRS basis. Image from Wood (2006).

Introducing smooth effects

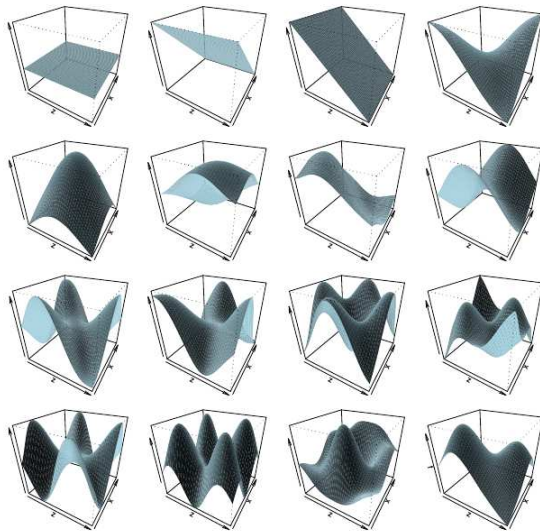


Figure : Rank 17 2D TPRS basis. Courtesy of Simon Wood.

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

In first morning practical we'll see only 1D effects.

In mgcv:

```
gam(y ~ 1 + x0 + s(x1, bs = "tp", k = 15), ...)
```


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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

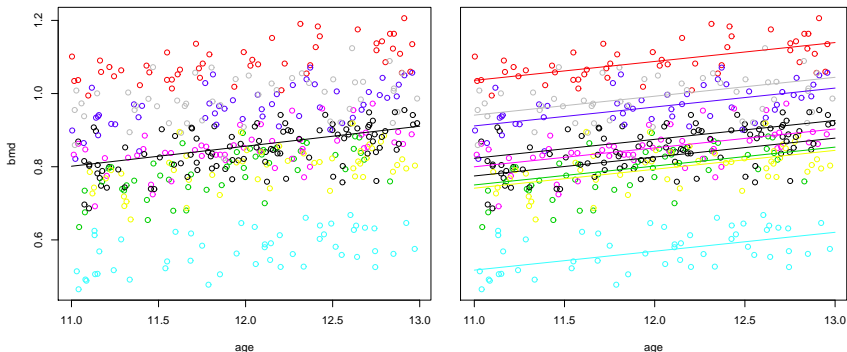
$$\mathbb{E}(bmd|age_{ij}) = \mu(age_{ij}) = \alpha + \beta age_{ij}.$$

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).

Structure of the talk

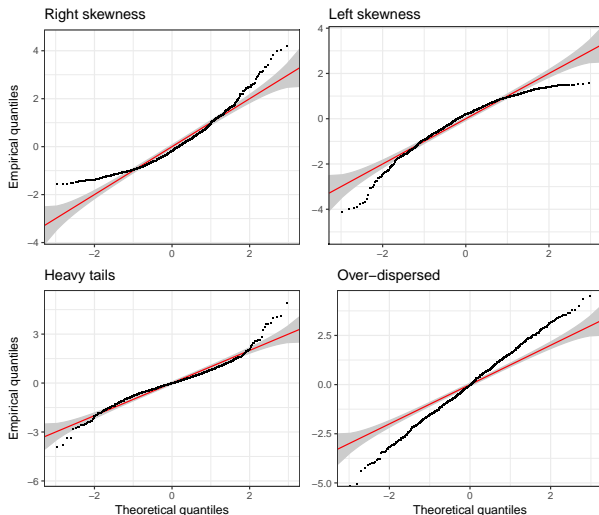
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Diagnostics and model selection tools

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

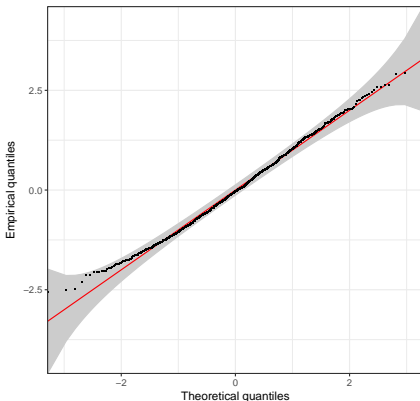
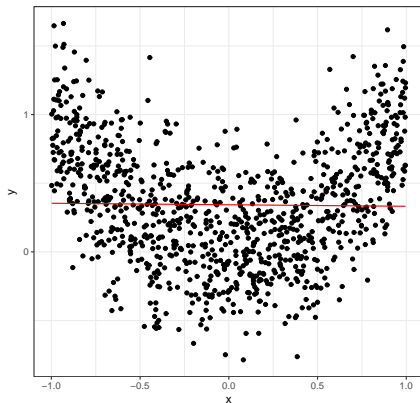
QQ-plots



Diagnostics and model selection tools

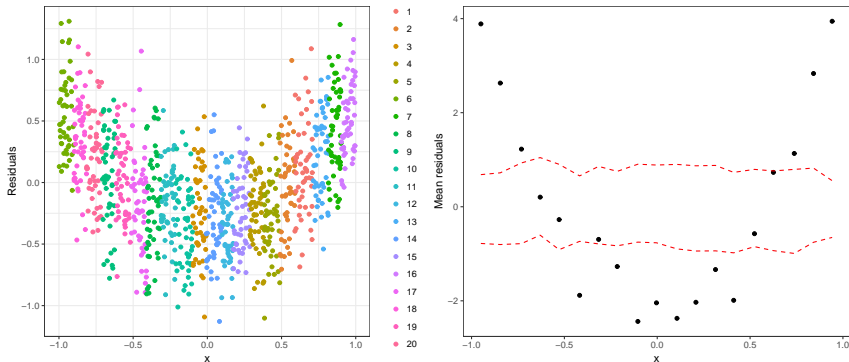
Useful for choosing model $\text{Dist}_m(y|\mathbf{x})$ (e.g. Poisson vs Neg. Binom.)

Less useful for finding omitted variables and non-linearities.



Diagnostics and model selection tools

Conditional residuals checks are more helpful here.



```
fit <- gamV(... some model ...)  
qq(fit) # QQ-plot  
check1D(fit, "x") + l_gridCheck1D() # Check along x
```


Diagnostics and model selection tools

Recall structure of smooth effects:

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

where β shrunk toward zero by smoothness penalty.

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

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

By default $k = 10$ but this is arbitrary.

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

Diagnostics and model selection tools

Checking whether k is too low:

- 1 look at conditional residuals checks
- 2 look at output of `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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GAMs in mgcv and mgcViz

`mgcv` is the recommended R package for fitting GAMs.

It contains methods for:

- creating GAM models
- fitting them
- summarizing model output

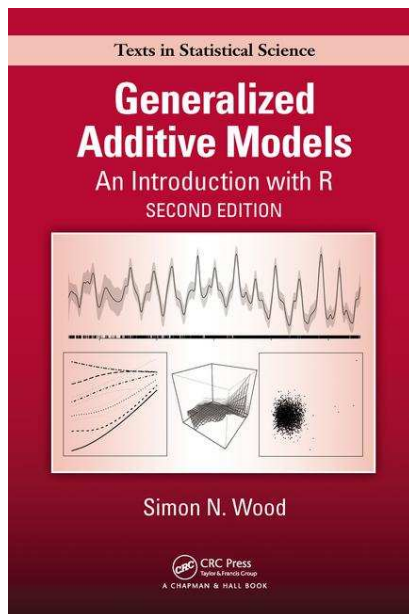
`mgcViz` extends `mgcv`'s tools for:

- plotting the estimated effects
- doing visual model checking

Today we'll work with `mgcViz`'s interface.

But most of the computation is done by `mgcv` under the hood.

Further reading



References I

Fasiolo, M., Y. Goude, R. Nedellec, and S. N. Wood (2017). Fast calibrated additive quantile regression. *arXiv preprint arXiv:1707.03307*.