

# Intro to generalized additive models in R

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Material available at:

[https://github.com/mfasiolo/workshop\\_WARSAW19](https://github.com/mfasiolo/workshop_WARSAW19)

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

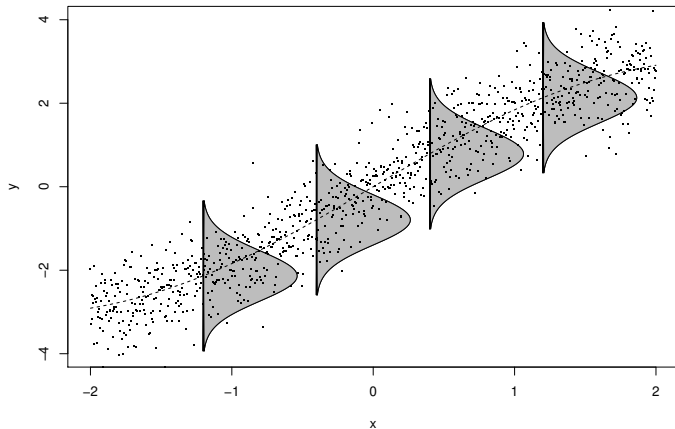
$$\mu(\mathbf{x}) = \mathbb{E}(y|\mathbf{x}) = \sum_{j=1}^m f_j(\mathbf{x}),$$

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:

- $y|\mathbf{x} \sim \text{ScaledStud}\{y|\mu(\mathbf{x}), \sigma, \nu\}$
- $\mathbb{E}(y|\mathbf{x}) = \mu(\mathbf{x}) = \sum_{j=1}^m f_j(\mathbf{x})$
- $\sigma$  is scale parameter
- $\nu$  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  $\beta_k$  are unknown coeff and  $b_k(x_3)$  are known spline basis functions.

# Introducing smooth effects

## Example: B-splines

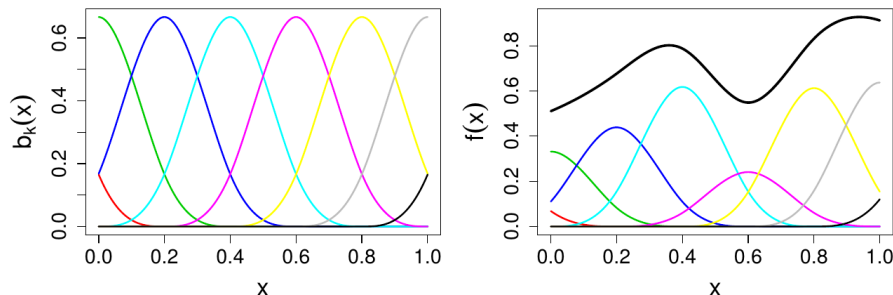


Figure: B-spline basis (left) and smooth (right).

# Introducing smooth effects

## Example: Thin plate regression splines (TPRS)

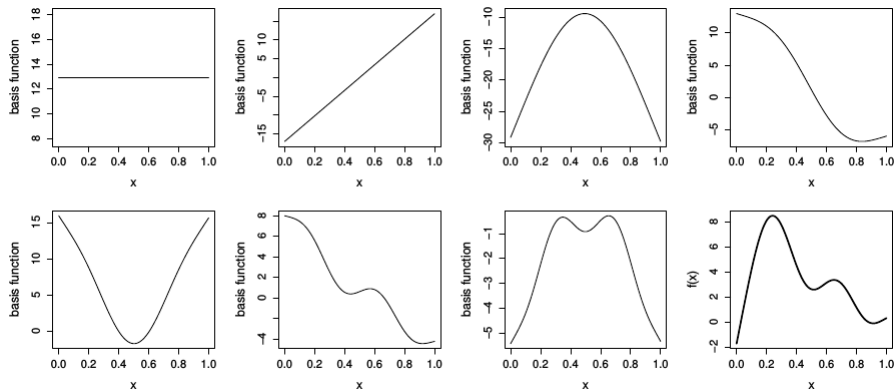


Figure: Rank 7 TPRS basis. Image from Wood (2017).

# Introducing smooth effects

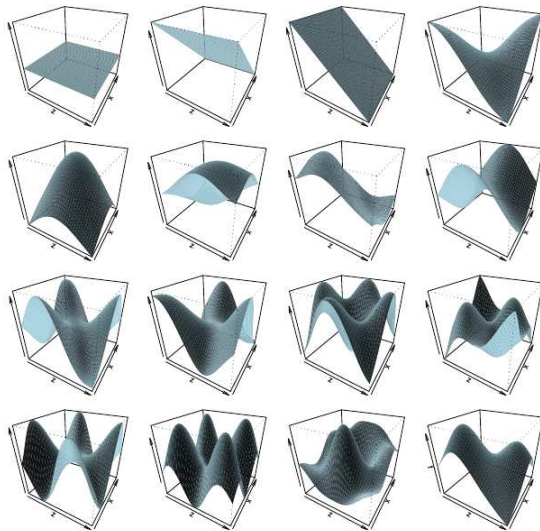


Figure: Rank 17 2D TPRS basis. Courtesy of Simon Wood.

# 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  $\beta$  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

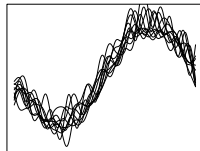
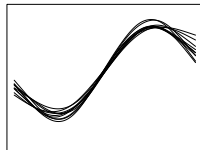
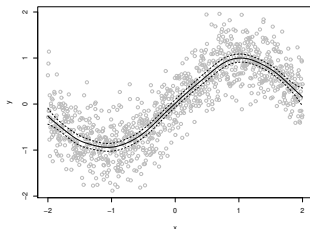
mgcv uses a hierarchical fitting framework:

- 1 Select  $\gamma$  to determine smoothness

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

- 2 For fixed  $\gamma$ , estimate  $\beta$  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

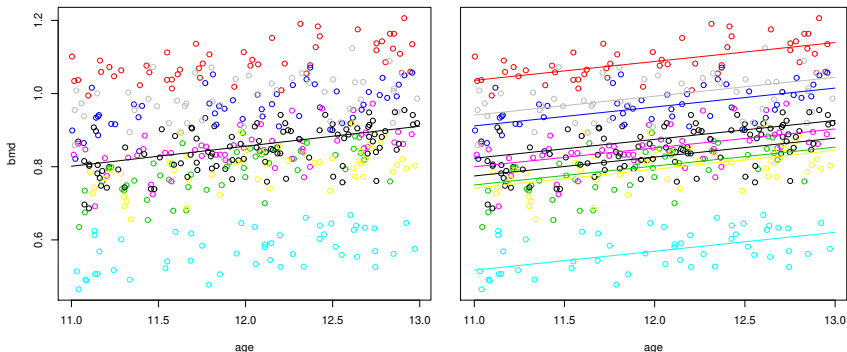
$$\mathbb{E}(bmd|age_{ij}) = \mu(age_{ij}) = \alpha + \beta age_{ij}.$$

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.

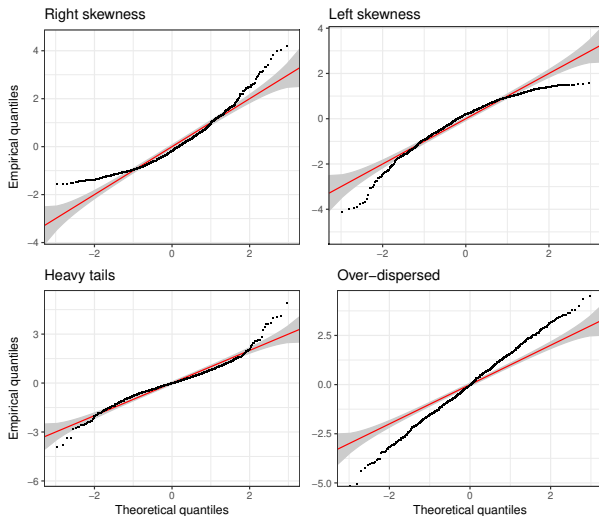
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# Diagnostics and model selection tools

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

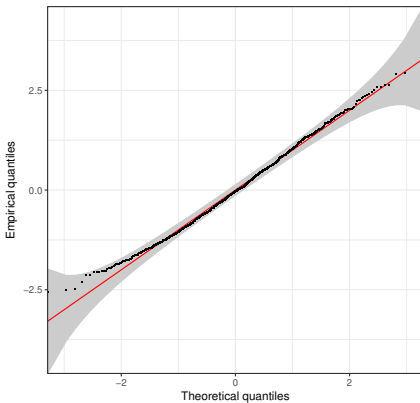
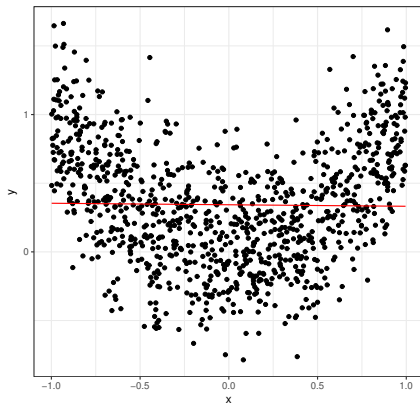
## QQ-plots



# 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:

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

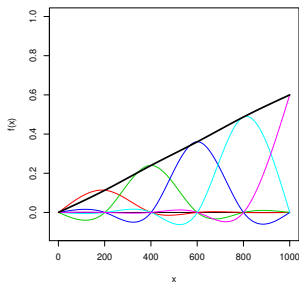
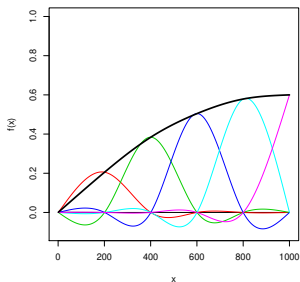
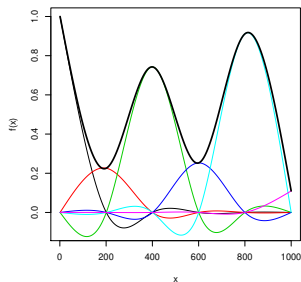
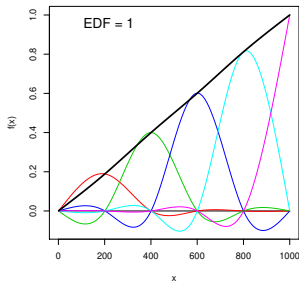
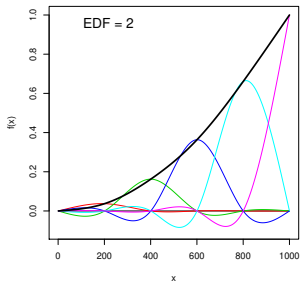
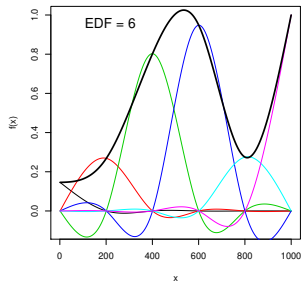
where  $\beta$  shrunk toward smoothness by penalty.

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  $\tau$  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:

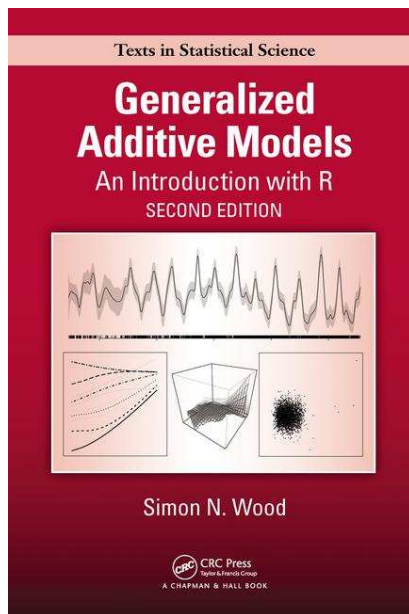
- `mboost` (Hothorn et al., 2010)
- `gamlss` (Rigby and Stasinopoulos, 2005)
- `brms` (Bürkner et al., 2017)
- BayesX (Brezger et al., 2003)
- INLA (Rue et al., 2009)

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

- 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.