Generalized additive models in R

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Material available at:

https://github.com/mfasiolo/workshop_UseR18

Today's plan

First session

1. Intro to Generalized Additive Models (GAMs) in R
2. Hands-on session

Coffee break

Second session

1. Beyond mean modelling: GAMLSS and quantile GAMs
2. Hands-on session

Intro to Generalized Additive Models (GAMs)

Structure:

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

Structure of the talk

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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

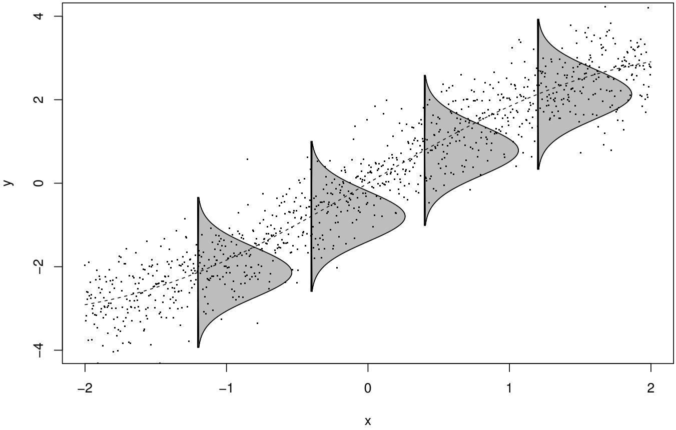

Figure: Gaussian model with variable mean.

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

What is an additive model

Generalized additive model (GAM):

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

where

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

and g is the link function.

f_j's can be fixed, random or smooth effects with coefficients $\boldsymbol{\beta}$.

Poisson GAM:

- $y|\mathbf{x} \sim \text{Pois}\{y|\mu(\mathbf{x})\}$
- $\mathbb{E}(y|\mathbf{x}) = \text{Var}(y|\mathbf{x}) = \exp\Big\{\sum_{j=1}^{m} f_j(\mathbf{x})\Big\}$
- $g = \log$ 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 see models with multiple linear predictors, eg:

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

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Introducing smooth effects

Consider additive model

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

where

- $f_1(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$
- $f_2(\mathbf{x}) = f_2(x_2)$ is a non-linear smooth function

Smooth effects built using spine bases

$$f_2(x_2) = \sum_{k=1}^{r} \beta_k b_k(x_2)$$

where β_k are unknown coeff and $b_k(x_2)$ are known spline basis functions.

NB: we call $\sum_{j=1}^{m} f_j(\mathbf{x})$ **linear predictor** because it is linear in $\boldsymbol{\beta}$.

Introducing smooth effects

B-splines:

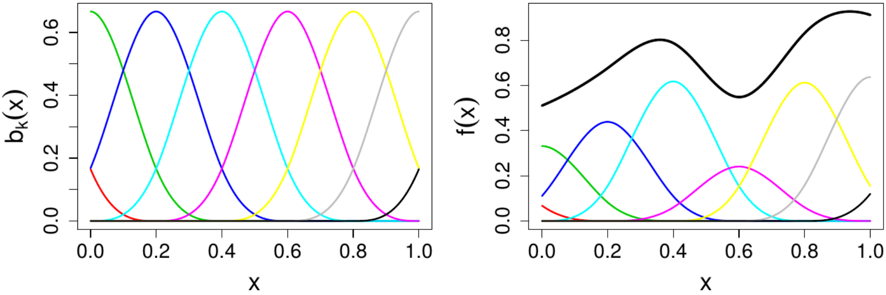
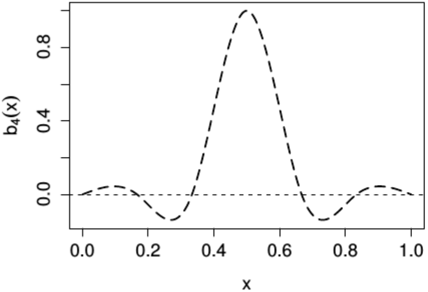
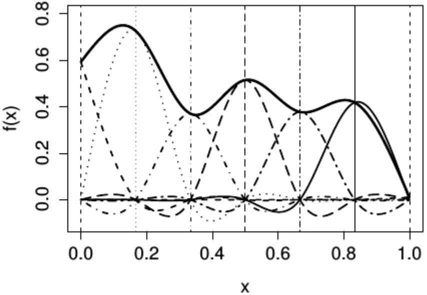


Figure: B-spline basis (left) and smooth (right).

Types of smooths

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



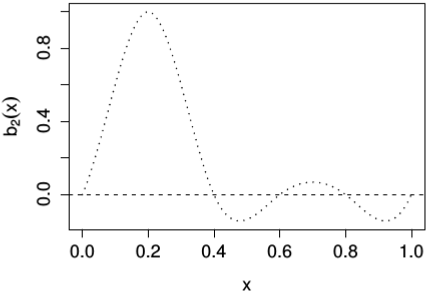


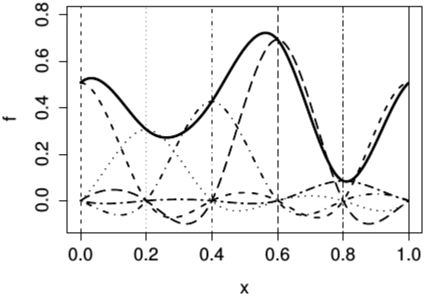
Cubic regression splines are related to the optimal solution to

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

Types of smooths

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



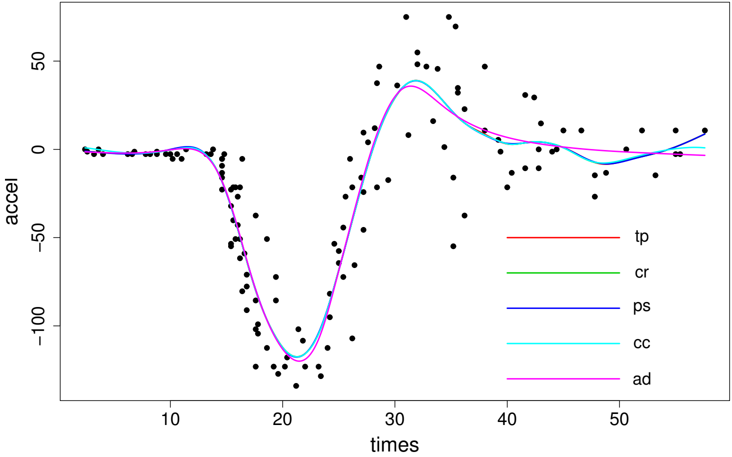


Cyclic cubic regression splines make so that

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

Types of smooths

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



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

Types of smooths

`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, ...

Types of smooths

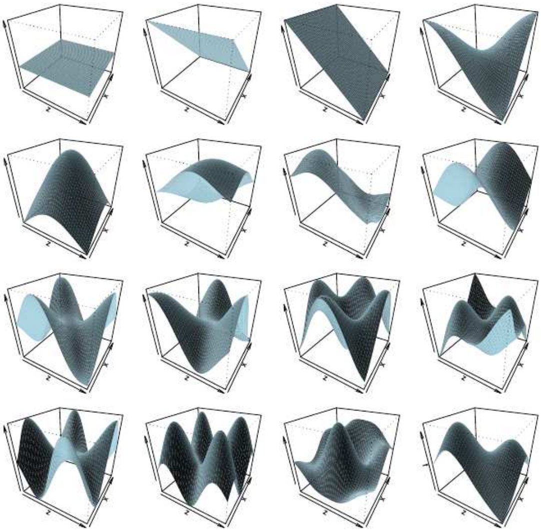


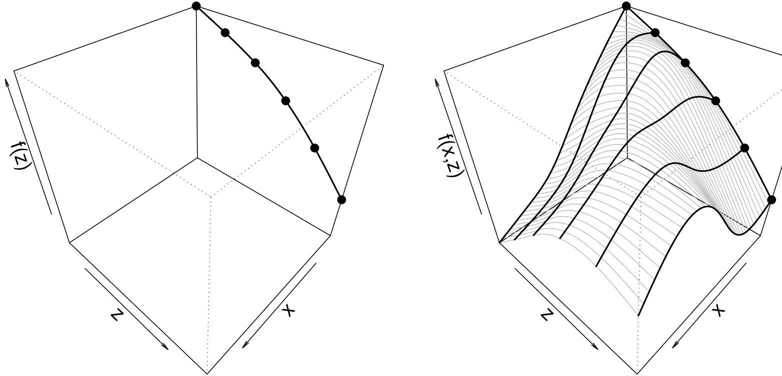
Figure: Rank 17 2D TPRS basis. Courtesy of Simon Wood.

Types of smooths

Isotropic effect of x_1, x_2 are in same unit (e.g. Km).

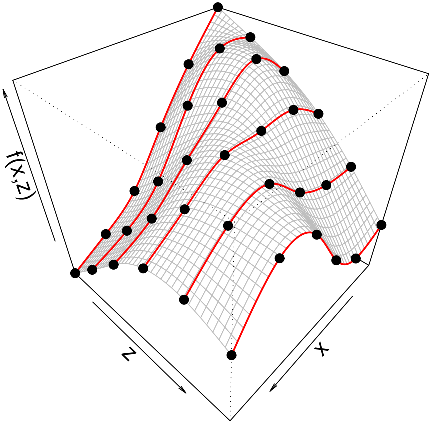
If different units better use tensor product smooths `te(x1, x2)`.

Construction: make a spline $f_z(z)$ a function of x by letting its coefficients vary smoothly with x



Types of smooths

- x-penalty: average wiggliness of red curves
- z-penalty: average wiggliness of green curves



Types of smooths

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), k=c(20,10), 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)
```

Types of smooths

By-factor smooths

Approach (1) is `s(x, by = subject)`, which means

- $\mu(x) = f_1(x) + \ldots \qquad$ if subject $= 1$
- $\mu(x) = f_2(x) + \ldots \qquad$ if subject $= 2$
- ...

Approach (2) is `s(x, subject, bs = "fs")`, which means

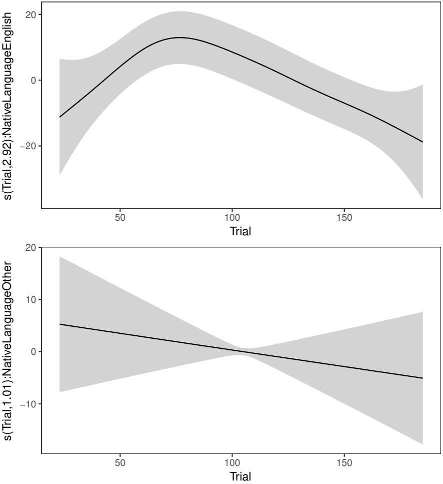
- $\mu(x) = b_1 + f_1(x) + \ldots \qquad$ if subject $= 1$
- $\mu(x) = b_2 + f_2(x) + \ldots \qquad$ if subject $= 2$
- ...

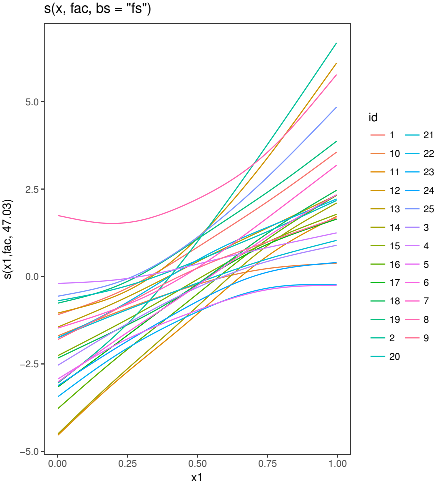
where $b_1, b_2, \cdots \sim N(0, \gamma_{\mathbf{b}} \mathbf{I})$ are random effects.

In (1) each f_j has its own smoothing parameter.

In (2) all f_j's have the same smoothing parameter.

Types of smooths





GAM model fitting

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 $\boldsymbol{\beta}$ controls the wiggliness of the effects

GAM model fitting

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

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

where:

- $L_y(\boldsymbol{\beta}) = \sum_i \log p(y_i|\boldsymbol{\beta})$ is log-likelihood
- $\text{Pen}(\boldsymbol{\beta}|\boldsymbol{\gamma})$ penalizes the complexity of the f_j's
- $\boldsymbol{\gamma} > 0$ smoothing parameters ($\uparrow \boldsymbol{\gamma}$ $\uparrow$smoothness)

Concrete example $\mu(\mathbf{x}) = f(x_1) + g(x_2, x_3)$:

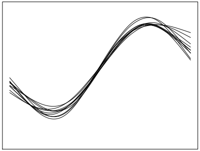
$$\text{Pen}(\boldsymbol{\beta}|\boldsymbol{\gamma}) \approx \gamma_1 \int f_{x_1 x_1}^2 dx_1 + \gamma_2 \int g_{x_2 x_2}^2 + 2 g_{x_2 x_3}^2 + g_{x_3 x_3}^2 dx_2 dx_3$$

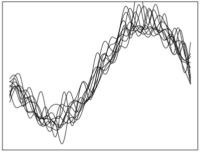
We use a hierarchical fitting framework:

1. Select γ determine smoothness

$$\hat{\gamma} = \underset{\gamma}{\text{argmax}}\ \text{LAML}(\gamma)$$

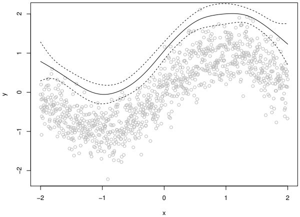
   where $\text{LAML}(\gamma) \approx p(y|\gamma) = \int p(y, \boldsymbol{\beta}|\gamma) d\boldsymbol{\beta}$.





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

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\text{argmax}}\ \text{PenLogLik}(\boldsymbol{\beta}|\gamma).$$



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Big Data methods

Recall the GAM model structure

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

Here $\mu(\mathbf{x}_i)$ can be written as $g^{-1}(\mathbf{X}_i\beta)$, where $\mathbf{X}_i$ row of

$$\mathbf{X} = \begin{bmatrix} A_{11} & A_{12} & \cdots & b_{11}(x_{11}) & b_{12}(x_{11}) & \cdots & b_{21}(x_{21}) & \cdots \\ A_{21} & A_{22} & \cdots & b_{11}(x_{12}) & b_{12}(x_{12}) & \cdots & b_{21}(x_{22}) & \cdots \\ . & . & \cdots & . & . & \cdots & . & \cdots \\ . & . & \cdots & . & . & \cdots & . & \cdots \end{bmatrix}$$

with n rows and

$$d = p + k_1 + \cdots + k_j + \cdots + k_m$$

columns.

Big Data methods

Bottom line: $\mathbf{X}$ can get very big, which causes problems:

- storing $\mathbf{X}$ takes too much memory
- computing things involving $\mathbf{X}$ (e.g. $\mathbf{X}^\mathsf{T}\mathbf{X}$) takes time

Solution implemented in `mgcv::bam` function:

- do not create $\mathbf{X}$ but only sub-blocks:

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{11} & \mathbf{X}_{12} \\ \mathbf{X}_{21} & \mathbf{X}_{22} \end{bmatrix}$$

  do not store them either, but create them when needed;
- any computation involving $\mathbf{X}$ is based on the blocks;
- use parallelization when possible;

Big Data methods

Further acceleration and memory savings by discretization.

Instead of having n unique rows of $\mathbf{X}$ discretize to $b << n$ rows.

In `mgcv`:

```
fit <- bam(y ~ s(x),
           discrete = TRUE,
           nthreads = 2,
           ...)
```

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3. Introducing random effects
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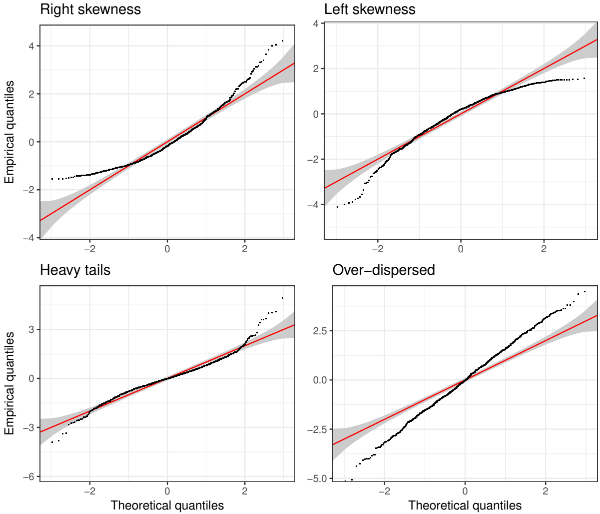
Diagnostics and model selection tools

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

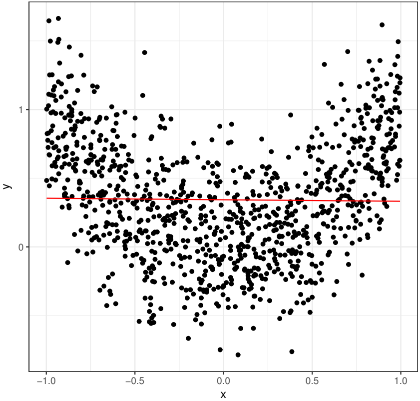
QQ-plots

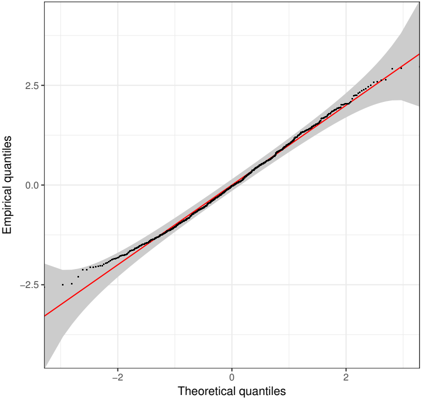


Diagnostics and model selection tools

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

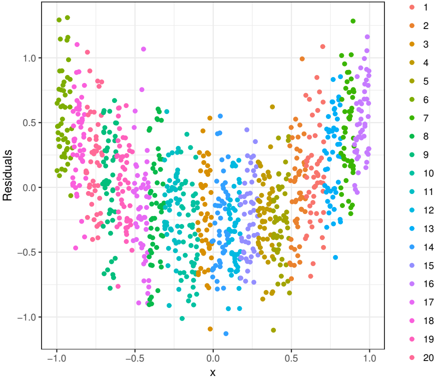
Less useful for finding omitted variables and non-linearities.

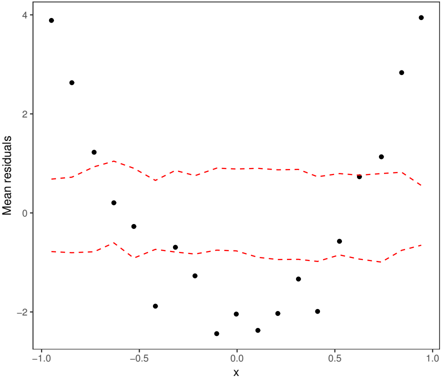




Diagnostics and model selection tools

Conditional residuals checks are more helpful here.





Diagnostics and model selection tools

Recall structure of smooth effects:

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

where $\boldsymbol{\beta}$ 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):

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

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.

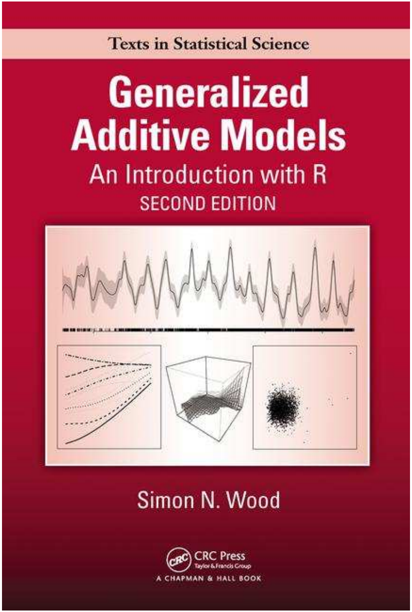
Today we'll work with `mgcViz`'s interface.

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

- plotting the estimated effects
- doing visual model checking

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

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*.