

Beyond mean modelling: GAMLSS and quantile GAMs

Matteo Fasiolo (University of Bristol, UK)

Virgile Fritsch (Électricité de France R&D)

matteo.fasiolo@bristol.ac.uk

July 11, 2018

Structure:

- ① Intro to GAMs for Location Scale and Shape
- ② Intro to quantile GAMs
- ③ GAMLSS and QGAM modelling in mgcv and qgam

Beyond mean modelling: GAMLSS models

Structure:

- ① **Intro to GAMs for Location Scale and Shape**
- ② Intro to quantile GAMs
- ③ GAMLSS and QGAM modelling in mgcv and qgam

Intro to GAMLSS models

Recall GAM model structure:

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

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.

Example, Scaled Student-t distribution:

- location $\mu(\mathbf{x}) = \mathbb{E}(y|\mathbf{x})$
- scale $\theta_2 = \sigma$
- shape $\theta_3 = \nu$

Intro to GAMLSS models

In Generalized Additive Models for Location Scale and Shape (GAMLSS) (Rigby and Stasinopoulos, 2005) we let scale and shape change with the covariates \mathbf{x} .

GAMLSS model structure:

$$y|\mathbf{x} \sim \text{Distr}\{y|\theta_1 = \mu_1(\mathbf{x}), \theta_2 = \mu_2(\mathbf{x}), \dots, \theta_p = \mu_p(\mathbf{x})\},$$

where

$$\mu_1(\mathbf{x}) = g_1^{-1} \left\{ \sum_{j=1}^m f_j^1(\mathbf{x}) \right\},$$

...

$$\mu_p(\mathbf{x}) = g_p^{-1} \left\{ \sum_{j=1}^m f_j^p(\mathbf{x}) \right\},$$

and g_1, \dots, g_p are link function.

Intro to GAMLSS models

Example: **Gaussian model for location and scale**

Model is

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

where

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

$$\text{var}(y|\mathbf{x})^{1/2} = \sigma(\mathbf{x}) = \exp \left\{ \sum_{j=1}^m f_j^2(\mathbf{x}) \right\}$$

that is $g_2 = \log$ to guarantee $\sigma > 0$.

Intro to GAMLSS models

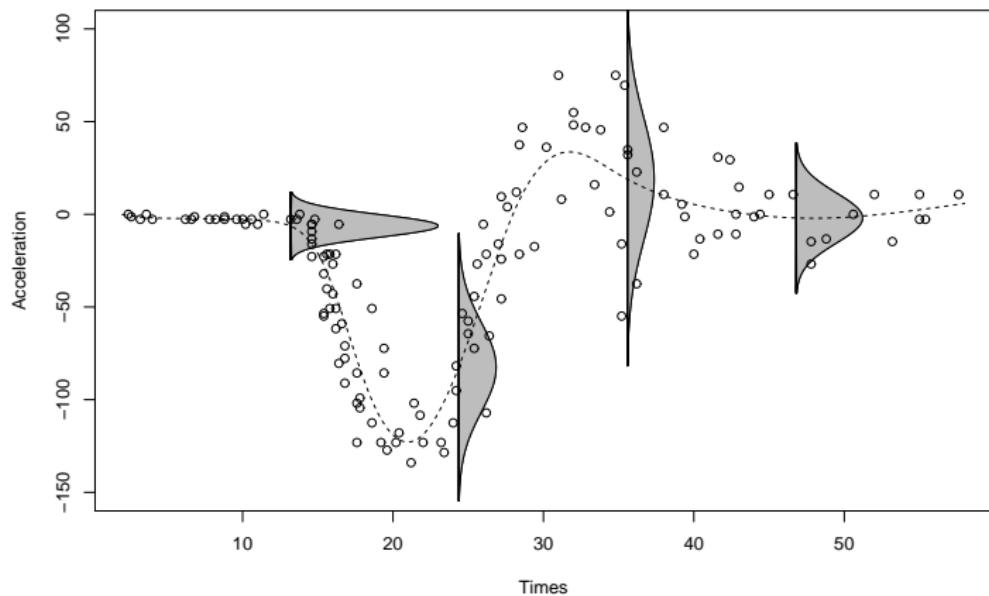
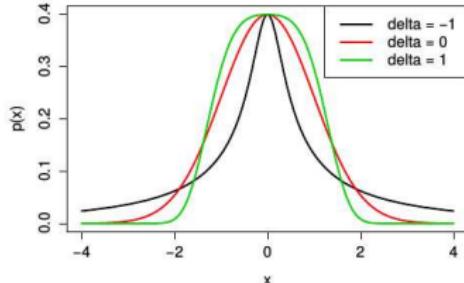
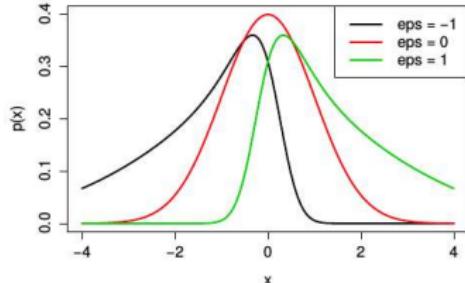
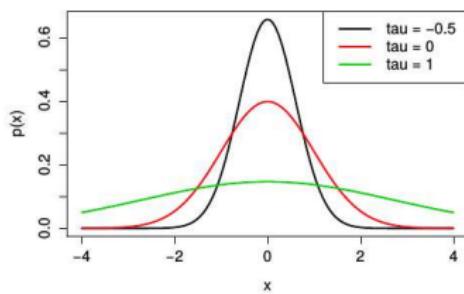
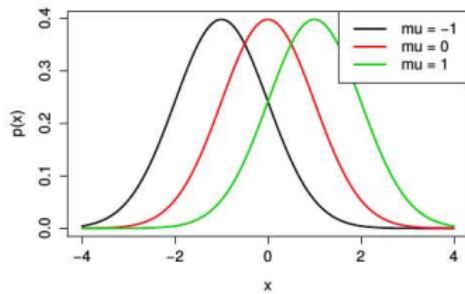


Figure : Gaussian model with variable mean and variance.
In mgcv: `gam(list(y~s(x), ~s(x)), family=gauLss)`.

Intro to GAMLSS models

Example: Sinh-arcsinh (shash) distribution

Four parameter distribution where location, scale, skewness (asymmetry) and kurtosis (tail behaviour) can depend on x (Jones and Pewsey, 2009).



Intro to GAMLSS models

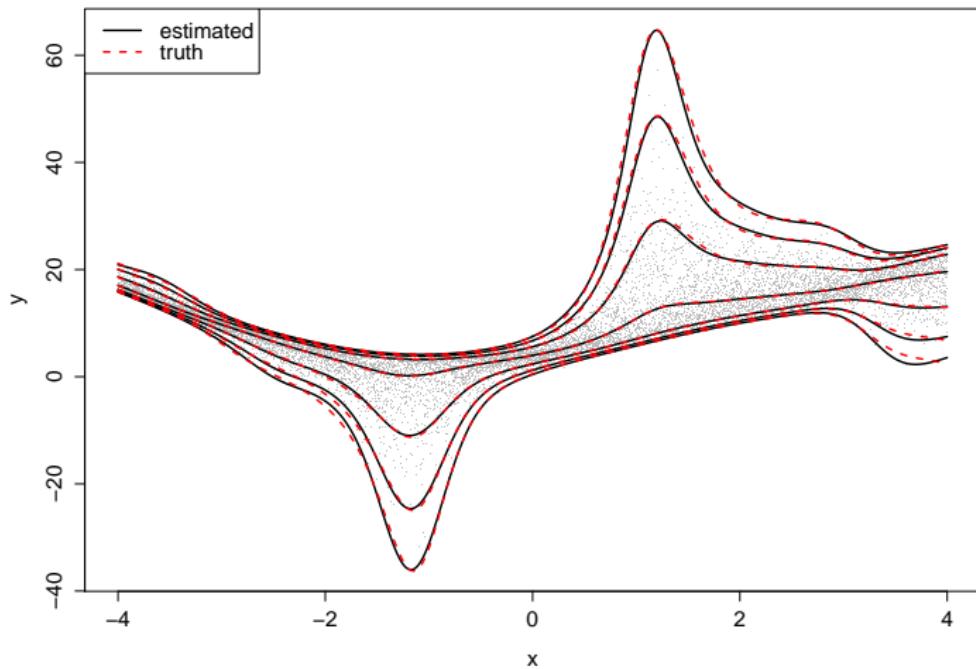
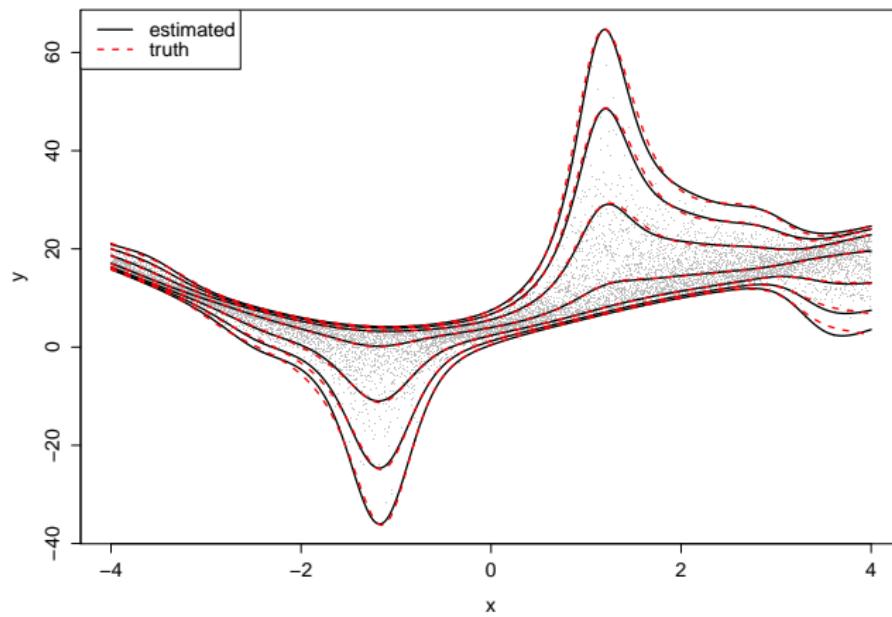


Figure : `gam(list(y~s(x), ~s(x), ~s(x), ~s(x)), family=shash).`

Intro to GAMLSS models

Why is this useful?

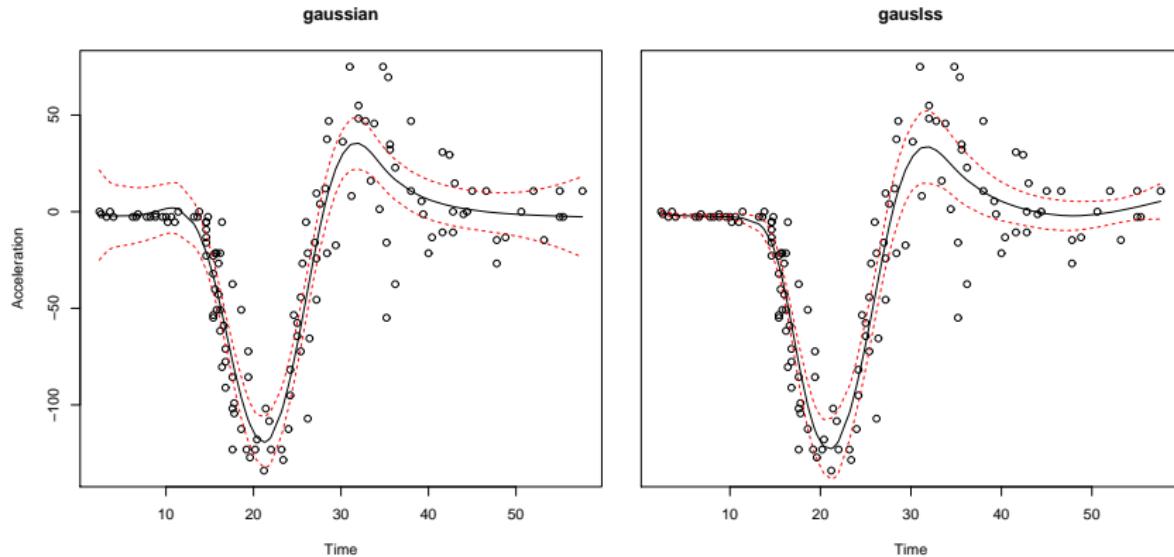
R1: you might be interested in whole distribution $y|x$ not just $\mathbb{E}(y|x)$.



Intro to GAMLSS models

Why is this useful?

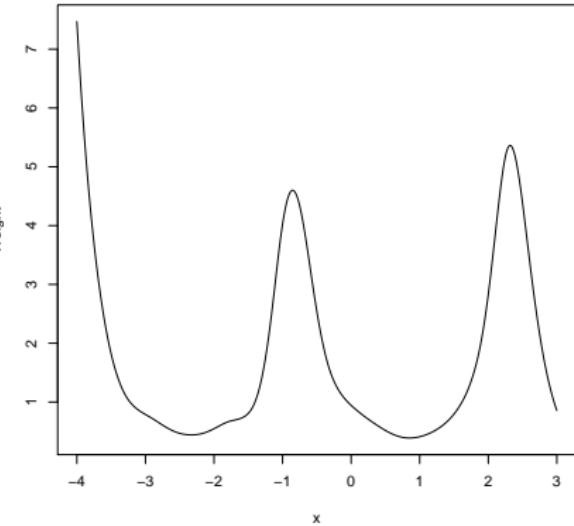
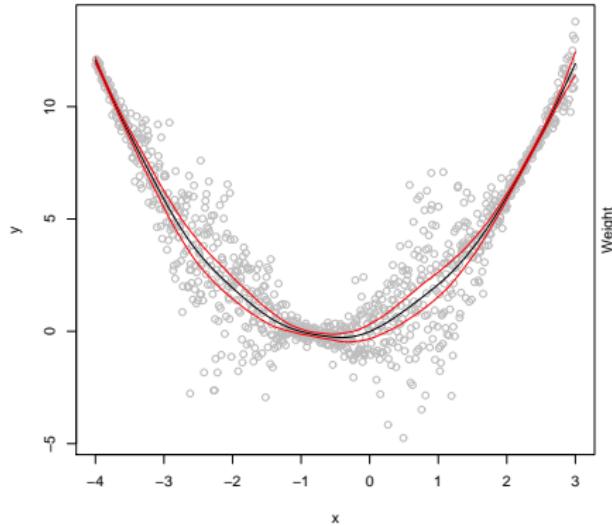
R2: standard GAM inference (e.g. p-value & confidence interval) is valid if the model for $y|x$ is correct



Intro to GAMLSS models

Why is this useful?

R3: the accuracy of the fit is improved if the weight of each observation is inversely proportional to $\text{Var}(y|x)$.



Beyond mean modelling: GAMLSS models

Structure:

- ① Intro to GAMs for Location Scale and Shape
- ② **Intro to quantile GAMs**
- ③ GAMLSS and QGAM modelling in mgcv and qgam

What is quantile regression

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 $p(y|\mathbf{x})$.

Model is $p_m\{y|\theta_1(\mathbf{x}), \dots, \theta_q(\mathbf{x})\}$, where $\theta_1(\mathbf{x}), \dots, \theta_q(\mathbf{x})$ are parameters.

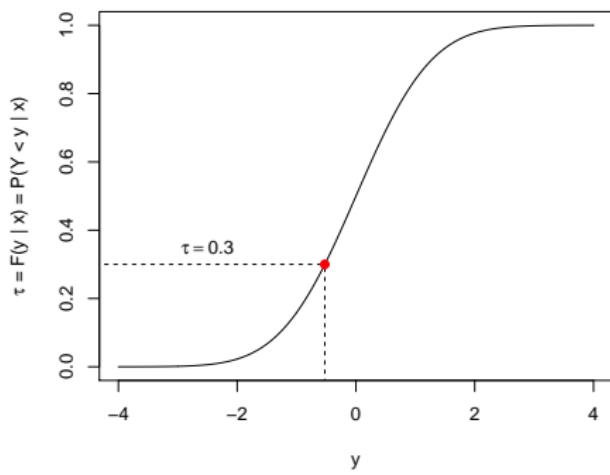
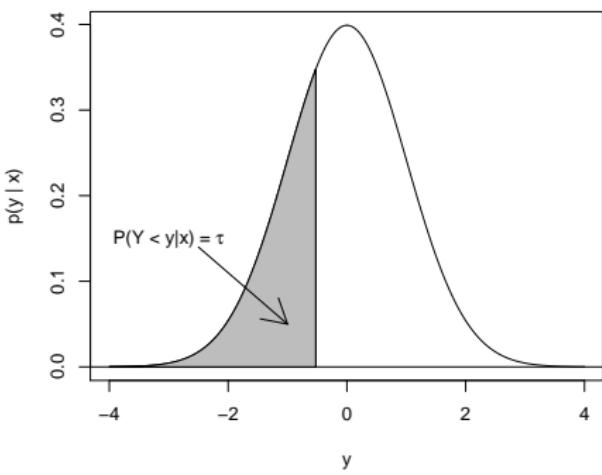
What is quantile regression

Lots of options for $p_m(y|\mathbf{x})$: binomial, gamma, Poisson, Tweedie...

We consider continuous (not discrete) y .

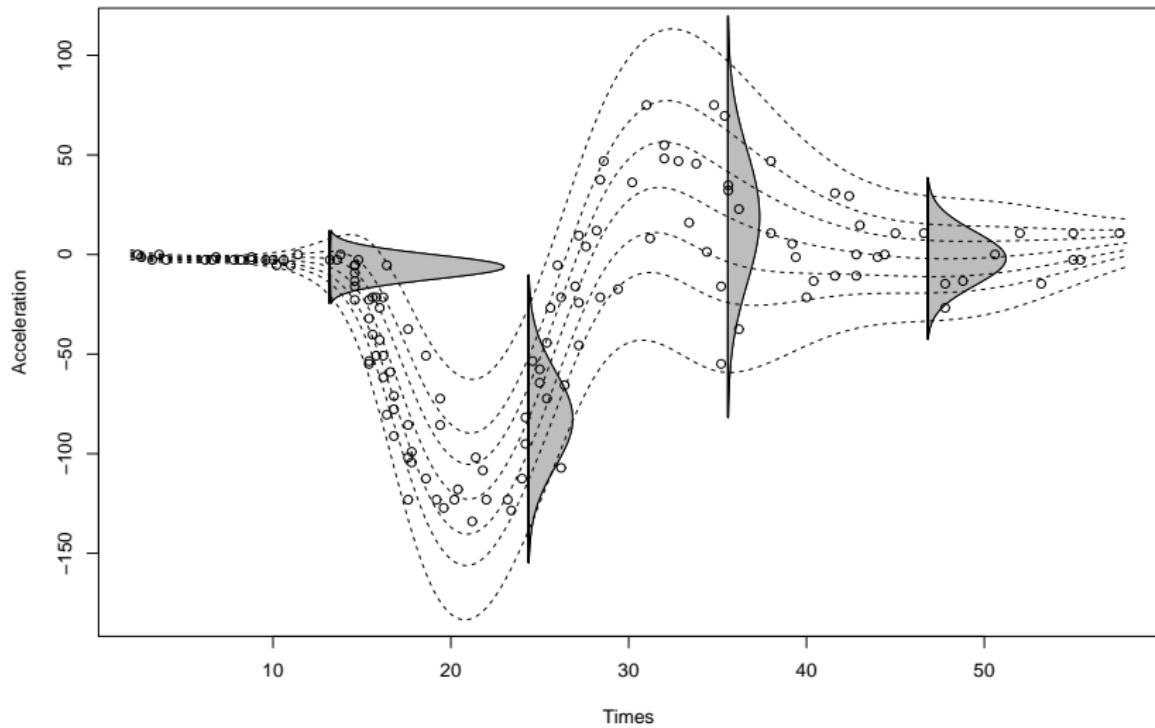
Define $F(y|\mathbf{x}) = \text{Prob}(Y \leq y|\mathbf{x})$.

The τ -th ($\tau \in (0, 1)$) quantile is $\mu_\tau(\mathbf{x}) = F^{-1}(\tau|\mathbf{x})$.



What is quantile regression

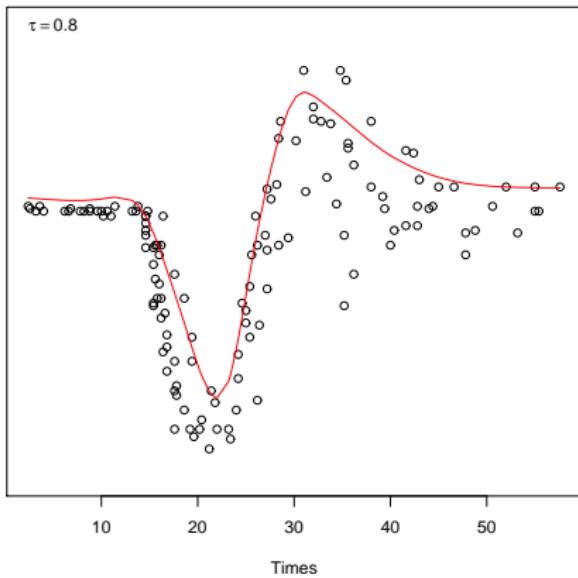
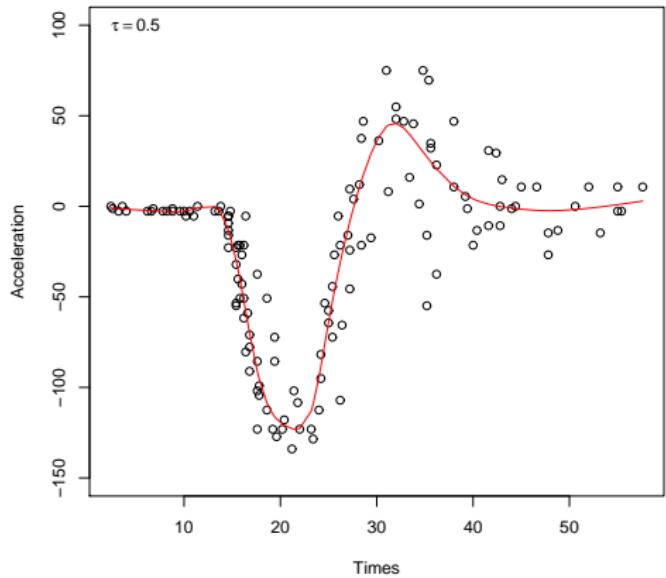
Given $p_m(y|x)$ we can get the conditional quantiles $\mu_\tau(x)$.



What is quantile regression

Quantile regression estimates conditional quantiles $\mu_\tau(\mathbf{x})$ directly.

No model for $p(y|\mathbf{x})$.



What is quantile regression

The τ -th quantile is

$$\mu = F^{-1}(\tau | \mathbf{x}),$$

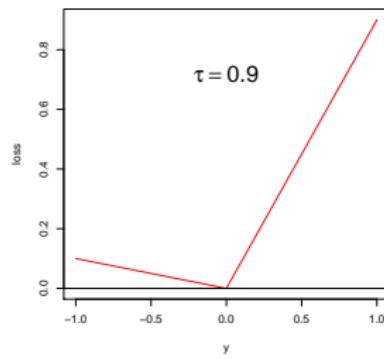
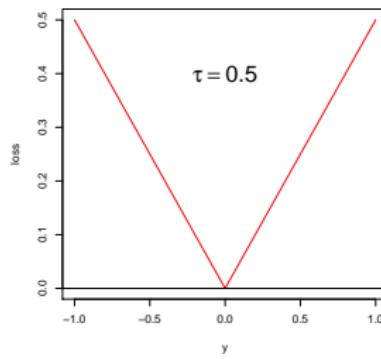
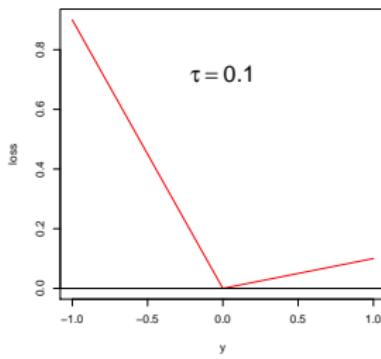
but also the minimizer of

$$L(\mu | \mathbf{x}) = \mathbb{E}\{ \rho_\tau(y - \mu) | \mathbf{x} \},$$

where

$$\rho_\tau(z) = (\tau - 1)z \mathbb{1}(z < 0) + \tau z \mathbb{1}(z \geq 0),$$

is the “pinball” loss (Koenker, 2005).



What is quantile regression

In **linear quantile regression** $\mu_\tau(\mathbf{x}) = \boldsymbol{\beta}^\top \mathbf{x} = \beta_1 x_1 + \dots + \beta_p x_p$.

$\hat{\boldsymbol{\beta}}$ is the minimizer of total pinball loss

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} L_y(\boldsymbol{\beta}) = \sum_{i=1}^n \rho_\tau(y_i - \boldsymbol{\beta}^\top \mathbf{x}_i).$$

In **additive quantile regression** $\mu_\tau(\mathbf{x}) = \sum_{j=1}^m f_j(\mathbf{x})$.

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

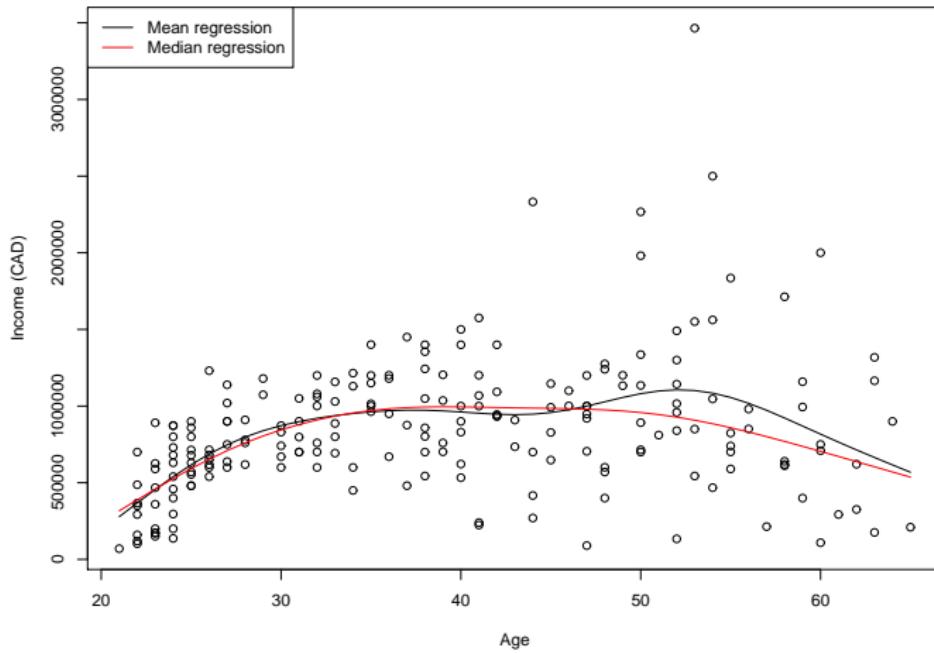
$\hat{\boldsymbol{\beta}}$ is the minimizer of total **penalized** pinball loss

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \{L_y(\boldsymbol{\beta}) + \text{Pen}(\boldsymbol{\beta})\}.$$

where $\text{Pen}(\boldsymbol{\beta})$ penalizes the complexity of the f_j 's.

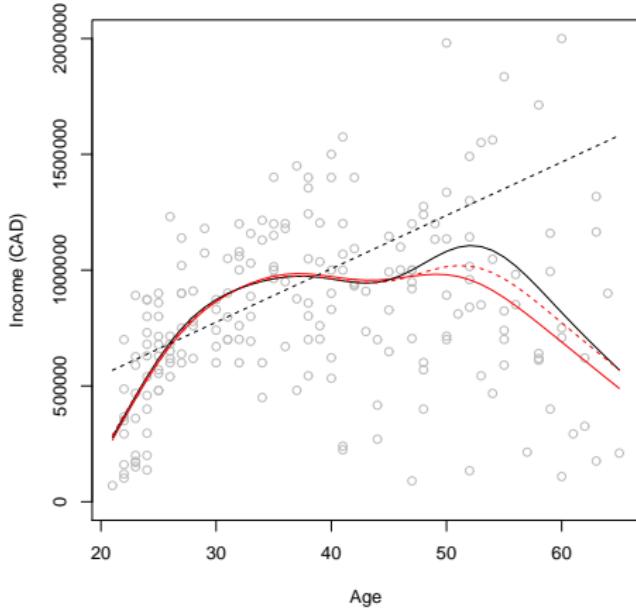
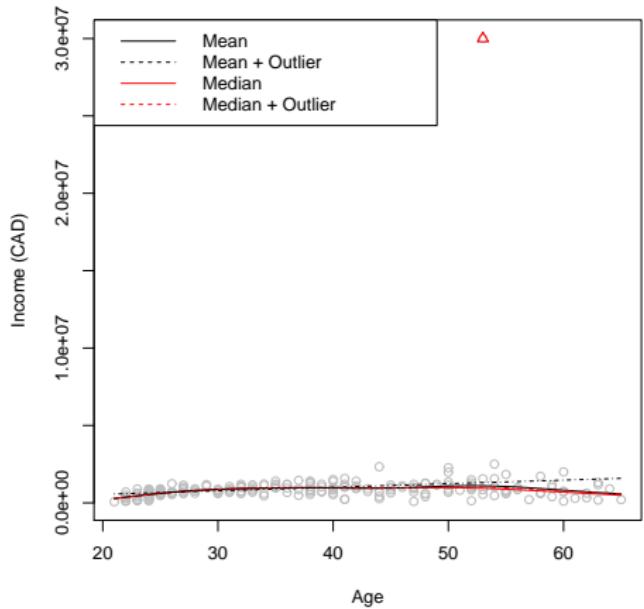
When is quantile regression useful

Median income is a better indicator of how the “average” person is doing, relative to mean income.



When is quantile regression useful

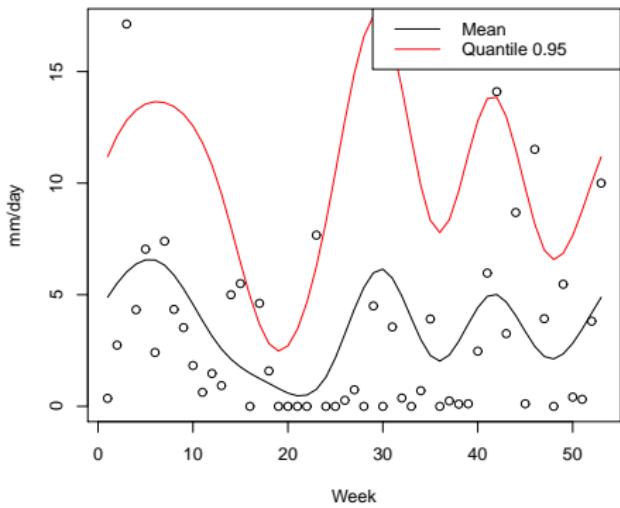
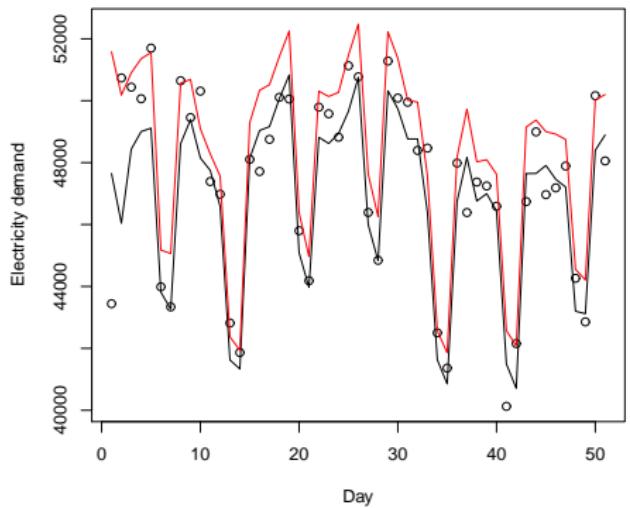
The median is also more **resistant to outliers**.



When is quantile regression useful

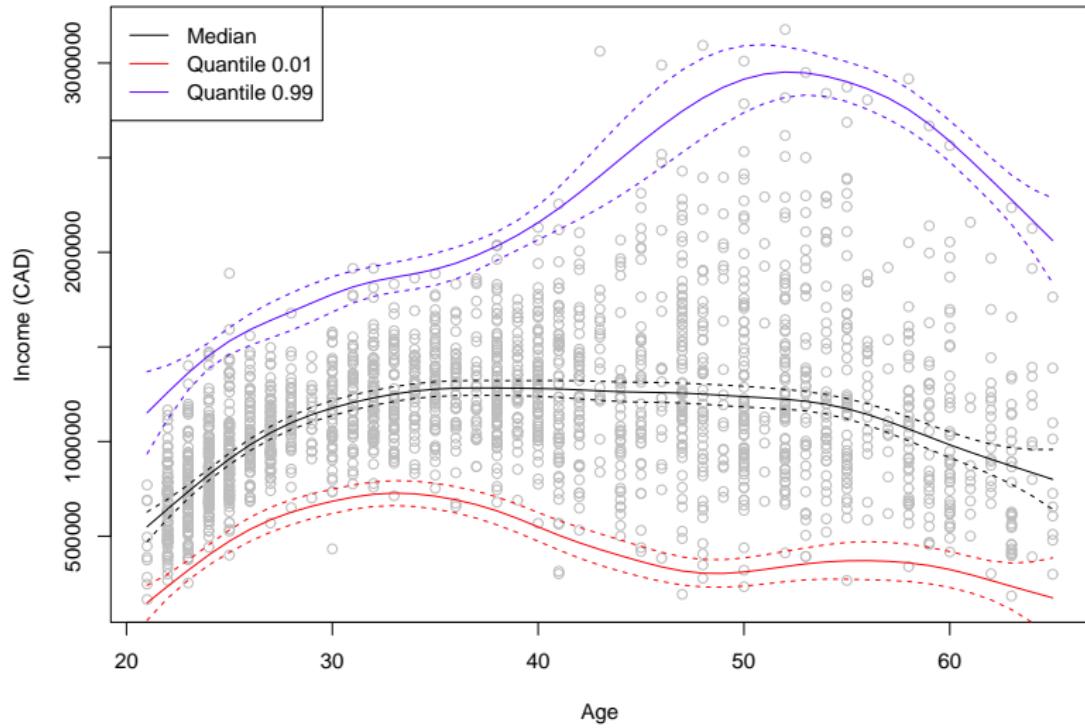
Some quantiles are more important than others:

- electricity producers need to satisfy top electricity demand
- urban planners need estimates of extreme rainfall



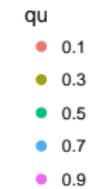
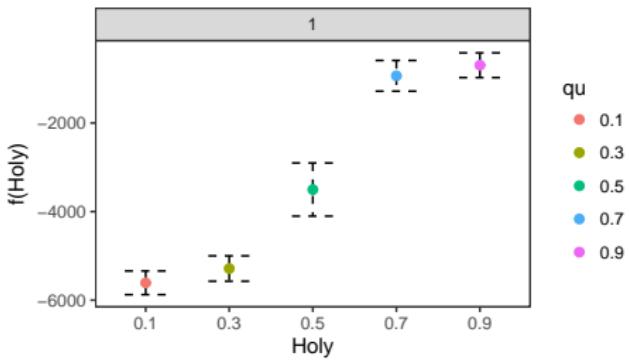
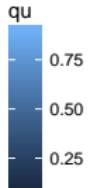
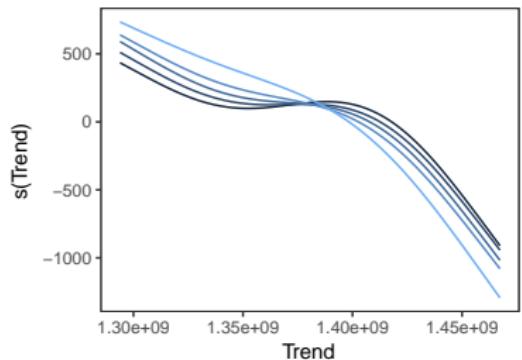
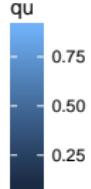
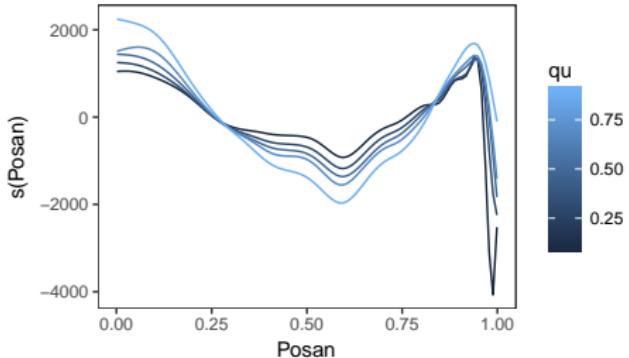
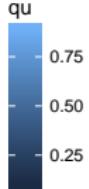
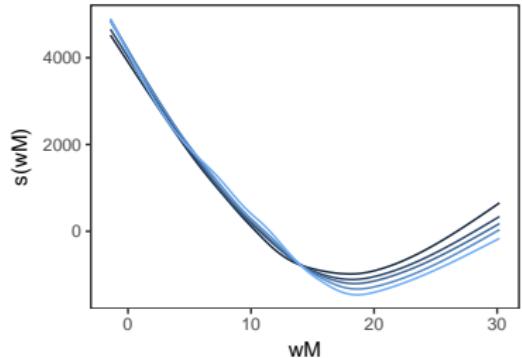
When is quantile regression useful

Effect of explanatory variables may depend on quantile



When is quantile regression useful

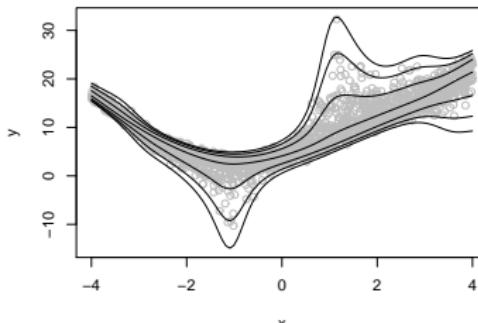
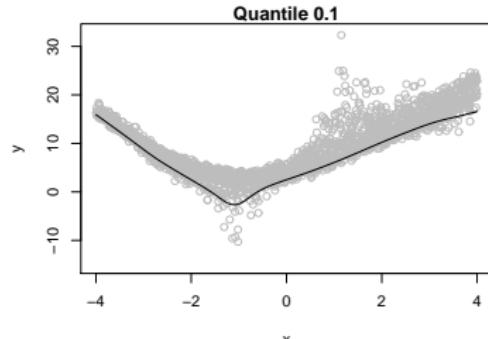
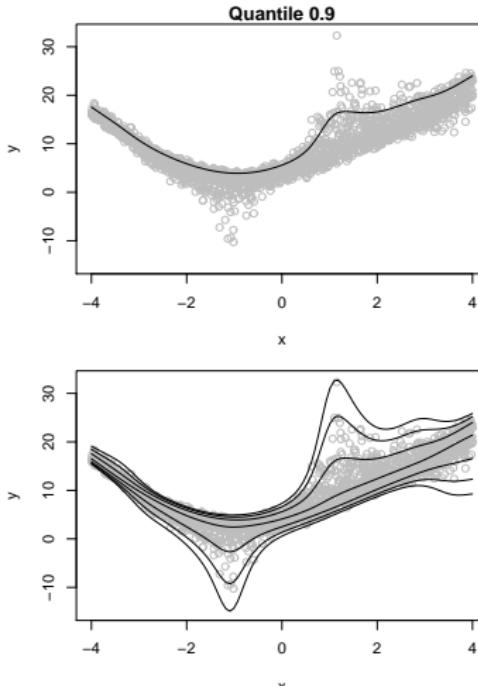
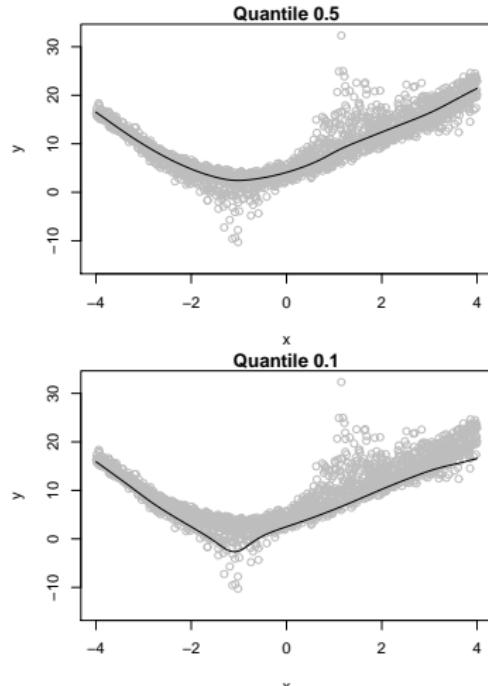
$$q_\tau(\text{Demand}) = f_1(\text{Temp}) + f_2(\text{TimeOfYear}) + f_3(\text{Trend}) + f_4(\text{Holiday}) + \dots$$



When is quantile regression useful

No assumptions on $p(y|x)$:

- no need to find good model for $p(y|x)$;
- no need to find normalizing transformations (e.g. Box-Cox);



Beyond mean modelling: GAMLSS models

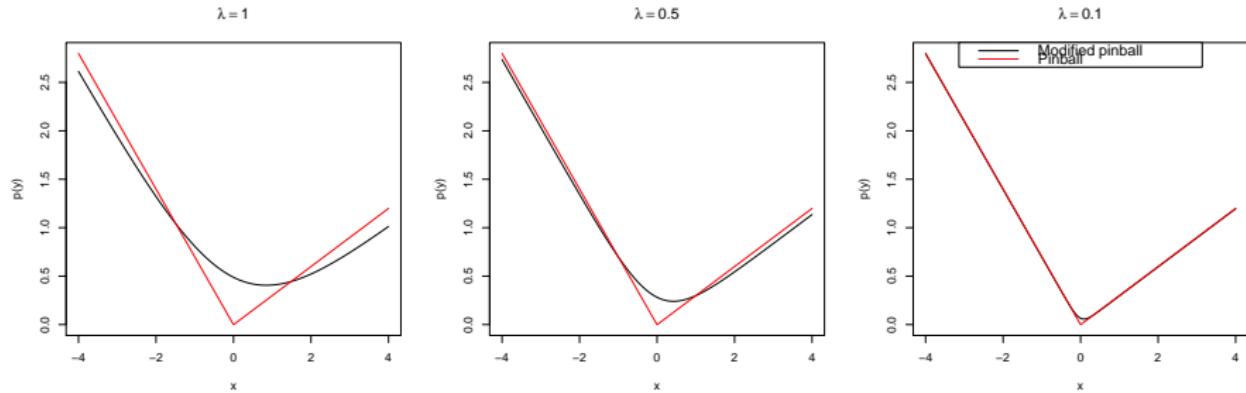
Structure:

- ① Intro to GAMs for Location Scale and Shape
- ② Intro to quantile GAMs
- ③ **GAMLSS and QGAM modelling in mgcv and qgam**

Smoothing the pinball loss

`qgam` uses a modified loss which we call Extended log-F (ELF) loss.

This is smooth and convex and, as $\lambda \rightarrow 0$, we have recover pinball loss.



NB in `qgam`, λ reparametrized as `err` $\in (0, 1)$ (\downarrow `err` implies $\downarrow \lambda$).

Smoothing the pinball loss

Increasing `err` leads to:

- faster and more stable computation
- more bias

By default:

```
qgam(..., err = 0.05, ...)
```

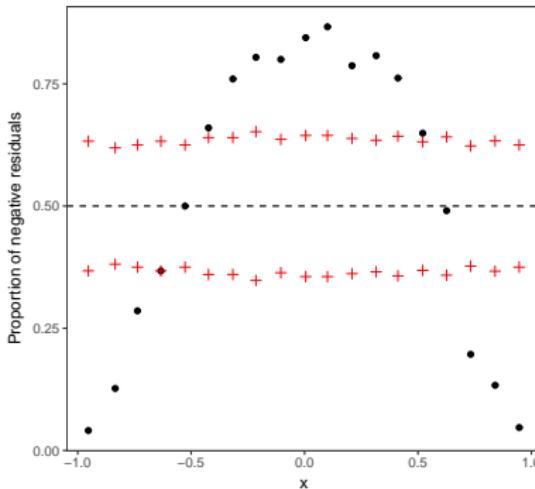
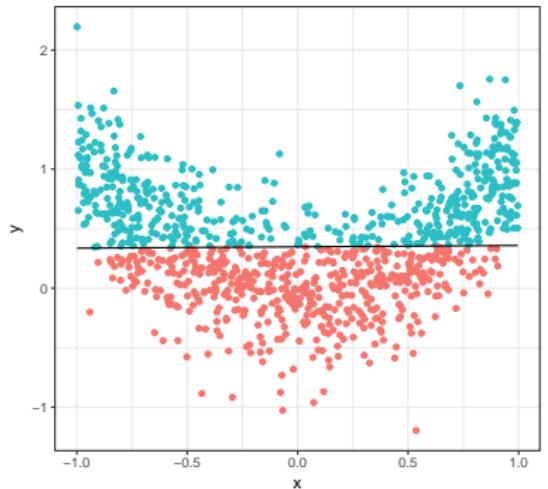
which is a compromise between bias and speed.

Residual checking

We have no model for $p(y|x) \rightarrow$ QQ-plots are useless.

We can check the proportion of residuals < 0 , which should be $\approx \tau$.

```
check1D(b, "x") + l_gridQCCheck1D(qu = 0.5)
```



Conclusions

THANK YOU!

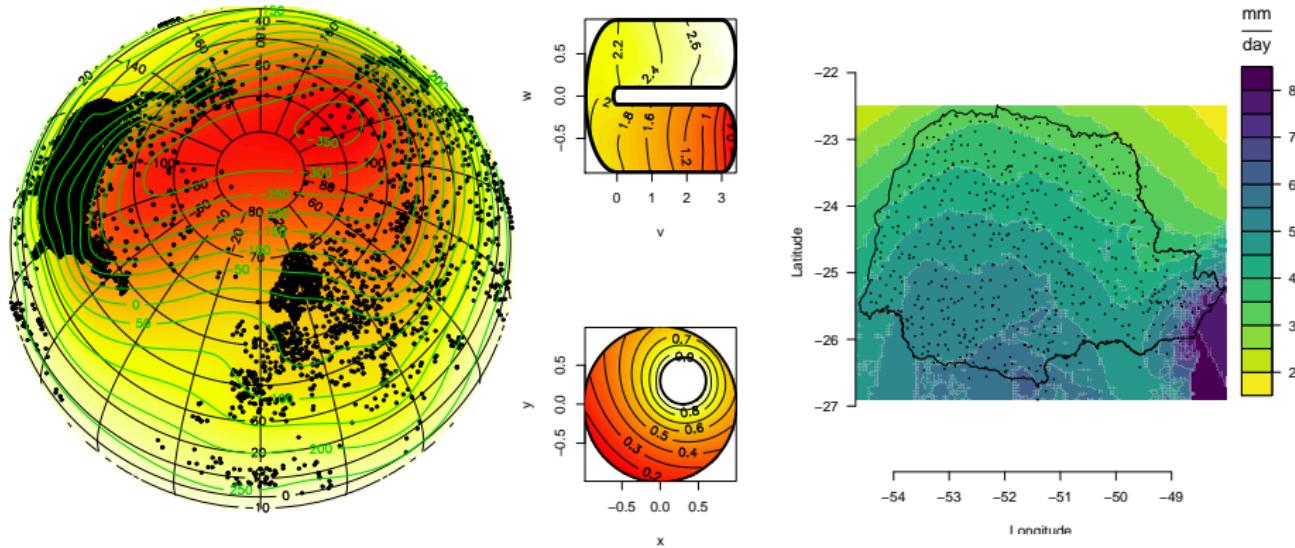


Figure : Examples of quantile GAMs from Fasiolo et al. (2017).

References I

- Fasiolo, M., Y. Goude, R. Nedellec, and S. N. Wood (2017). Fast calibrated additive quantile regression. *arXiv preprint arXiv:1707.03307*.
- Jones, M. and A. Pewsey (2009). Sinh-arcsinh distributions. *Biometrika* 96(4), 761–780.
- Koenker, R. (2005). *Quantile regression*. Number 38. Cambridge university press.
- 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.