Additive quantile regression with qgam

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Joint work with:

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Structure:

- Distributional vs quantile regression
- Additive quantile regression
- The qgam R package

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In distributional regression we want a good model for $p(y|\mathbf{x})$.

We indicate it with $p_m\{y|\theta_1(\mathbf{x}),\ldots,\theta_q(\mathbf{x})\}$, where $\theta_1(\mathbf{x}),\ldots,\theta_q(\mathbf{x})$ are model parameters.

For instance, if we use a Gaussian model, we can make its mean and/or variance depend on the covariates, that is

$$y|\mathbf{x} \sim N\{y|\mu = \theta_1(\mathbf{x}), \sigma^2 = \theta_2(\mathbf{x})\},$$

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



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

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Figure: We are using of Gaussian model with variable mean and variance. In mgcv: $gam(list(y^s(x), s(x)), family=gaulss)$.

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There are lots of models for $p(y|\mathbf{x})$ that can be used for distributional regression: binomial, gamma, Poisson, Tweedie, etc...

But sometimes it is difficult to find a good model.



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In QR we do not have a model for $p(y|\mathbf{x})$, but we model quantiles directly. Let $F(y|\mathbf{x})$ be $\operatorname{Prob}(Y \leq y|\mathbf{x})$. The τ -th $(\tau \in (0,1))$ quantile is

$$\mu_{\tau}(\mathbf{x}) = F^{-1}(\tau | \mathbf{x}).$$



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Obviously, given a set of fitted quantiles, we can approximate $p(y|\mathbf{x})$.



So we can use QR when we can't model $p(y|\mathbf{x})$ directly.

But we could be genuinely interested in estimating a quantile $\mu_{\tau}(\mathbf{x})$.

We might want to model median, rather than mean, income because:

- a) it is more robust to outliers then mean income;
- b) it is a better indicator of how the "average" person is doing.



Age

For electricity producers and/or distributors the top electricity demand on a given day might be more important that mean demand.



Structure:

Distributional vs quantile regression

Additive quantile regression

- The qgam R package
- Limitations and future developments

We are in an additive framework

$$\mu_{ au}(\mathbf{x}) = \sum_{j=1}^m f_j(\mathbf{x}),$$

where the effects $f_j(\mathbf{x})$ can be parametric, smooth or random effects. Given τ , how is $\mu_{\tau}(\mathbf{x})$ estimated?

Key fact is that $\mu_{\tau}(\mathbf{x})$ is minimizer of

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

where

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

is the so-call "check" function or "pinball" loss.



Given *n* observations, $\{y_1, \mathbf{x}_1\}, \ldots, \{y_n, \mathbf{x}_n\}$, the total loss is

$$\hat{\mu}_{\tau}(\mathbf{x}) = \operatorname*{argmin}_{\mu} \sum_{i=1}^{n} \rho_{\tau}[y_i - \mu(\mathbf{x}_i)],$$

hence we could estimate $\mu_{ au}(\mathbf{x})$ by minimizing

$$PL\{\mu(\mathbf{x})\} = L\{\mu(\mathbf{x})\} + \sum_{j=1}^{m} \gamma_j \int f_j''(x_j)^2 dx_j.$$

but $L{\mu(\mathbf{x})}$ is not differentiable!

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We use a modified loss based on the Extended log-F (ELF) density:

$$ilde{
ho}(y|\mu,\sigma, au,\lambda) \propto -(1- au)rac{y-\mu}{\sigma} + \lambda \log{\left[1+e^{rac{y-\mu}{\lambda\sigma}}
ight]},$$

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 $\downarrow \lambda$).

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For fixed $\gamma = \{\gamma_1, \dots, \gamma_m\}$ we can estimate $\mu_{\tau}(\mathbf{x}) = \underset{\mu}{\operatorname{argmin}} PL\{\mu(\mathbf{x})\}.$

But how to select γ in the first place?

We minimize the marginal loss

$$G(\boldsymbol{\gamma}, \sigma) = -\int \underbrace{\exp\left[-\frac{1}{\sigma}L\{\mu(\mathbf{x})\}\right]}_{\text{fit the data well}} \underbrace{\exp\left[\frac{1}{\sigma}L\{\mu(\mathbf{x})\}\right]}_{\boldsymbol{\beta}} \underbrace{\exp\left[\frac{1}{\sigma}H(\boldsymbol{\beta}|\boldsymbol{\gamma})\right]}_{\boldsymbol{\beta}} d\boldsymbol{\beta}.$$

where $p(\beta|\gamma)$ is related to the penalties $\sum_{j=1}^{m} \gamma_j \int f_j''(x_j)^2 dx_j$.

Here σ is the reciprocal of the "learning rate" and it needs to be selected as well...

If $\uparrow \sigma$ then $\uparrow \hat{\gamma}$ (smoother fit) and wider conf. int. for $\mu_{\tau}(\mathbf{x})$. If $\downarrow \sigma$ then $\downarrow \hat{\gamma}$ (more wiggly fit) and narrower conf. int. for $\mu_{\tau}(\mathbf{x})$.



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We choose σ so that confidence intervals for $\mu_{\tau}(\mathbf{x})$ are well calibrated.



In practice we use bootstrapping to calibrate σ .

In qgam this is implemented by tuneLearn() and tuneLearnFast().

To recap, we have three nested iterations:

- **Q** Calibration to estimate reciprocal of learning rate, σ .
- **2** Minimize ML to select smoothing parameters γ (fixed σ):

$$G(\boldsymbol{\gamma}, \sigma) = -\int \exp\left[-\sigma^{-1}L\{\mu(\mathbf{x})\}\right] \rho(\boldsymbol{\beta}|\boldsymbol{\gamma}) d\boldsymbol{\beta}.$$

Solution Minimize PL to estimate regression coefficients β (fixed σ and γ):

$$PL\{\mu(\mathbf{x})\} = L\{\mu(\mathbf{x})\} + \sum_{j=1}^{m} \gamma_j \int f_j''(x_j)^2 dx_j.$$

For more methodology, see Fasiolo et al. (2017) on arXiv.

Structure of the seminar

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- **3** The qgam R package