

Growth curves for multiple-output response variables via Bayesian quantile regression models

Joint work with Agatha Rodrigues and Thomas Kneib

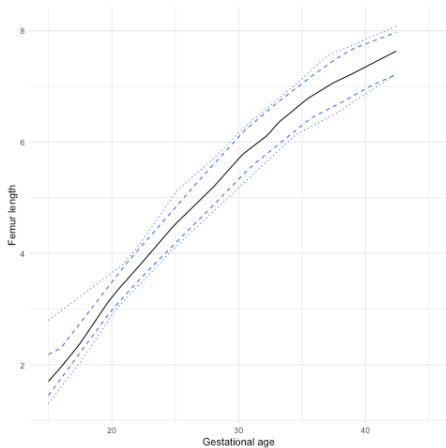
Bruno Santos

CMStatistics
University of Kent

December 20th, 2021

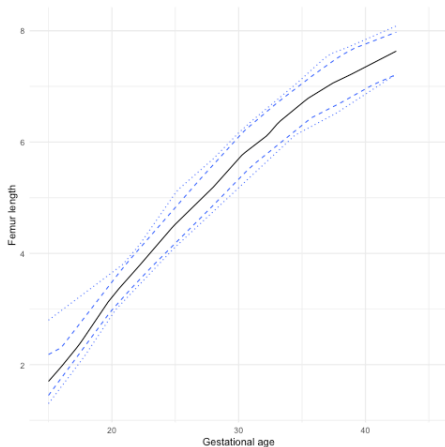
Motivation

► Growth curves - Fetus example



Motivation

► Growth curves - Fetus example

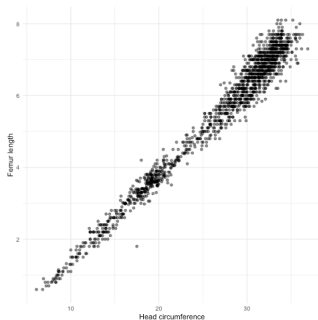
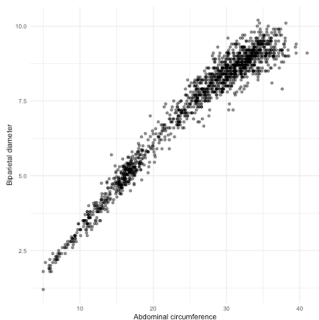


- How to build those curves when the dimension of the response variable is larger than 1?

Data set

► Data on four fetus biometric measurements:

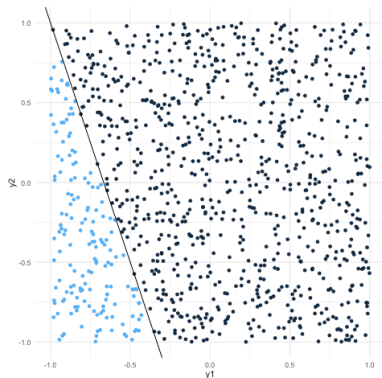
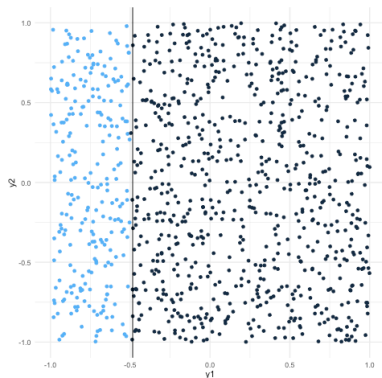
- Y_1 : femur length (F);
- Y_2 : head circumference (HC);
- Y_3 : abdominal circumference (AC);
- Y_4 : biparietal diameter (BPD).



1. Bayesian quantile regression models for multiple-output response variables
 - ▶ Main definitions
 - ▶ Selection of directions
2. Rearrangement of quantile hyperplanes for coverage improvement
3. Application
 - ▶ Results for our 4D data set with fetus measurements
4. Final remarks

Tukey depth (Halfspace depth)

► Halfspace example



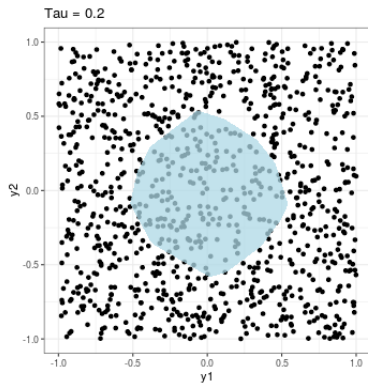
► Tukey depth:

$$HD(z, P) := \inf\{P(H) : H \text{ is a closed halfspace containing } z\}.$$

Depth region

► Definition:

$$D(\tau) := \{z \in \mathbb{R}^k : HD(z, P) \geq \tau\}$$



Directional quantile regression model

- ▶ Response variable is defined as $\mathbf{Y} \in \mathbb{R}^k$.
- ▶ Directional index can be defined by $\boldsymbol{\tau} \in \mathcal{B}^k := \{\mathbf{v} \in \mathbb{R}^k : 0 < \|\mathbf{v}\| < 1\}$.
 - ▶ $\boldsymbol{\tau} = \tau \mathbf{u}$.
 - ▶ Direction: $\mathbf{u} \in \mathcal{S}^{k-1} := \{\mathbf{z} \in \mathbb{R}^k : \|\mathbf{z}\| = 1\}$;
 - ▶ Magnitude: $\tau \in (0, 1)$.
- ▶ Define $\boldsymbol{\Gamma}_u$, an arbitrary $k \times (k-1)$ matrix of unit vectors.
 - ▶ $(\mathbf{u}; \boldsymbol{\Gamma}_u)$ is an orthonormal basis of \mathbb{R}^k .

Directional quantile regression model

- ▶ Response variable is defined as $\mathbf{Y} \in \mathbb{R}^k$.
- ▶ Directional index can be defined by $\boldsymbol{\tau} \in \mathcal{B}^k := \{\mathbf{v} \in \mathbb{R}^k : 0 < \|\mathbf{v}\| < 1\}$.
 - ▶ $\boldsymbol{\tau} = \tau \mathbf{u}$.
 - ▶ Direction: $\mathbf{u} \in \mathcal{S}^{k-1} := \{\mathbf{z} \in \mathbb{R}^k : \|\mathbf{z}\| = 1\}$;
 - ▶ Magnitude: $\tau \in (0, 1)$.
- ▶ Define $\boldsymbol{\Gamma}_u$, an arbitrary $k \times (k - 1)$ matrix of unit vectors.
 - ▶ $(\mathbf{u}; \boldsymbol{\Gamma}_u)$ is an orthonormal basis of \mathbb{R}^k .

DEFINITION:

The τ th quantile of \mathbf{Y} is the τ th quantile hyperplane obtained from the regression of $\mathbf{Y}_u := \mathbf{u}' \mathbf{Y}$ on the marginals of $\mathbf{Y}^\perp := \boldsymbol{\Gamma}_u' \mathbf{Y}$ with an intercept term.

Estimation setup

The τ th quantile of \mathbf{Y} is any element of the collection Λ_τ of hyperplanes

$$\lambda_\tau := \{\mathbf{y} \in \mathbb{R}^k : \mathbf{u}'\mathbf{y} = \hat{\mathbf{b}}_\tau \Gamma'_u \mathbf{y} + \hat{a}_\tau\},$$

such that $(\hat{a}_\tau, \hat{\mathbf{b}}_\tau)$ are the solutions of the minimization problem

$$\min_{(a_\tau, \mathbf{b}_\tau) \in \mathbb{R}^k} E[\rho_\tau(\mathbf{u}'\mathbf{y} - \mathbf{b}_\tau \Gamma'_u \mathbf{y} - a_\tau)].$$

where $\rho_\tau(u)$ is a known loss function in the quantile regression literature defined as

$$\rho_\tau(u) = u(\tau - \mathbb{I}(u < 0)), \quad 0 < \tau < 1.$$

Bayesian directional quantile regression model

- ▶ Consider the mixture representation of the asymmetric Laplace distribution

$$Y_i | w_i \sim N(\mu + \theta w_i, \psi^2 \sigma w_i)$$

$$w_i \sim \text{Exp}(\sigma)$$

$$\Rightarrow Y \sim AL(\mu, \sigma, \tau)$$

Bayesian directional quantile regression model

- ▶ Consider the mixture representation of the asymmetric Laplace distribution

$$\begin{aligned} Y_i | w_i &\sim N(\mu + \theta w_i, \psi^2 \sigma w_i) \\ w_i &\sim \text{Exp}(\sigma) \end{aligned} \quad \Rightarrow Y \sim AL(\mu, \sigma, \tau)$$

- ▶ Then one can consider that, for each direction u ,

$$Y_u | \mathbf{b}_\tau, \beta_\tau, \sigma, w \sim N(Y^\perp b_\tau + \mathbf{x}' \beta_\tau + \theta w_i, \psi^2 \sigma w_i),$$

Bayesian directional quantile regression model

- ▶ Consider the mixture representation of the asymmetric Laplace distribution

$$\begin{aligned} Y_i | w_i &\sim N(\mu + \theta w_i, \psi^2 \sigma w_i) \\ w_i &\sim \text{Exp}(\sigma) \end{aligned} \quad \Rightarrow Y \sim AL(\mu, \sigma, \tau)$$

- ▶ Then one can consider that, for each direction u ,

$$Y_u | \mathbf{b}_\tau, \beta_\tau, \sigma, w \sim N(Y^\perp b_\tau + \mathbf{x}' \beta_\tau + \theta w_i, \psi^2 \sigma w_i),$$

- ▶ That result makes it possible:
 - ▶ to use interesting developments of the univariate in the multivariate case.

Upper and lower halfspaces

With predictor variables, we have

$$\lambda_\tau(\mathbf{X}) = \{\mathbf{u}'\mathbf{y} = \hat{\mathbf{b}}_\tau\Gamma'_u\mathbf{y} + \mathbf{x}'\hat{\boldsymbol{\beta}}_\tau + \hat{a}_\tau\},$$

Upper and lower halfspaces

With predictor variables, we have

$$\lambda_{\tau}(\mathbf{X}) = \{\mathbf{u}'\mathbf{y} = \hat{\mathbf{b}}_{\tau}\Gamma'_{\mathbf{u}}\mathbf{y} + \mathbf{x}'\hat{\beta}_{\tau} + \hat{a}_{\tau}\},$$

We can say that each element $(\hat{a}_{\tau}, \hat{\mathbf{b}}_{\tau}, \hat{\beta}_{\tau})$ define an upper closed quantile halfspace

$$H_{\tau\mathbf{u}}^{+} = H_{\tau\mathbf{u}}^{+}(\hat{a}_{\tau}, \hat{\mathbf{b}}_{\tau}, \hat{\beta}_{\tau}) = \{\mathbf{y} \in \mathbb{R}^k : \mathbf{u}'\mathbf{y} \geq \hat{\mathbf{b}}_{\tau}\Gamma'_{\mathbf{u}}\mathbf{y} + \mathbf{x}'\hat{\beta}_{\tau} + \hat{a}_{\tau}\}$$

and an analogous lower open quantile halfspace switching \geq for $<$.

Upper and lower halfspaces

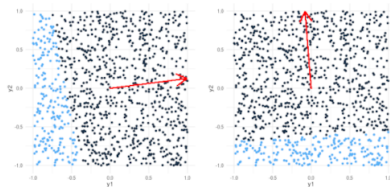
With predictor variables, we have

$$\lambda_{\tau}(\mathbf{X}) = \{\mathbf{u}'\mathbf{y} = \hat{\mathbf{b}}_{\tau}'\Gamma'_{\mathbf{u}}\mathbf{y} + \mathbf{x}'\hat{\beta}_{\tau} + \hat{a}_{\tau}\},$$

We can say that each element $(\hat{a}_{\tau}, \hat{\mathbf{b}}_{\tau}, \hat{\beta}_{\tau})$ define an upper closed quantile halfspace

$$H_{\tau\mathbf{u}}^{+} = H_{\tau\mathbf{u}}^{+}(\hat{a}_{\tau}, \hat{\mathbf{b}}_{\tau}, \hat{\beta}_{\tau}) = \{\mathbf{y} \in \mathbb{R}^k : \mathbf{u}'\mathbf{y} \geq \hat{\mathbf{b}}_{\tau}'\Gamma'_{\mathbf{u}}\mathbf{y} + \mathbf{x}'\hat{\beta}_{\tau} + \hat{a}_{\tau}\}$$

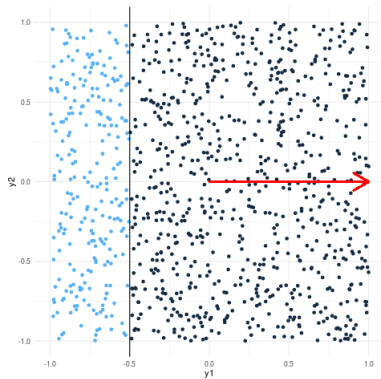
and an analogous lower open quantile halfspace switching \geq for $<$.



Properties

- Probabilistic nature of quantiles:

$$P(\mathbf{Y} \in H_{\tau u}^-) = \tau,$$



Quantile region

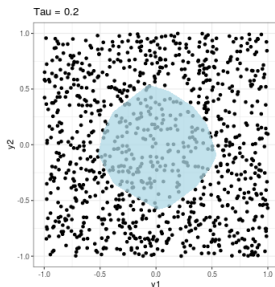
Moreover, fixing τ we are able to define the τ quantile region $R(\tau)$ as

$$R(\tau) = \bigcap_{\boldsymbol{u} \in \mathcal{S}^{k-1}} H_{\tau \boldsymbol{u}}^+.$$

Quantile region

Moreover, fixing τ we are able to define the τ quantile region $R(\tau)$ as

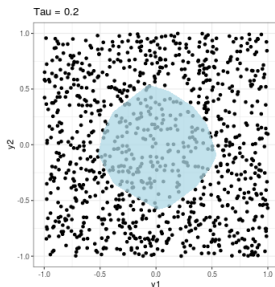
$$R(\tau) = \bigcap_{\mathbf{u} \in \mathcal{S}^{k-1}} H_{\tau \mathbf{u}}^+.$$



Quantile region

Moreover, fixing τ we are able to define the τ quantile region $R(\tau)$ as

$$R(\tau) = \bigcap_{\mathbf{u} \in \mathcal{S}^{k-1}} H_{\tau \mathbf{u}}^+.$$



Depth and quantile regions

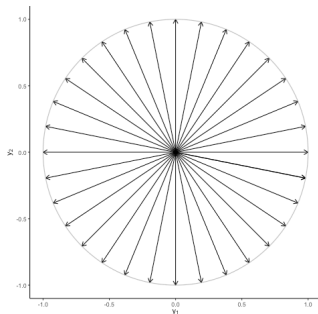
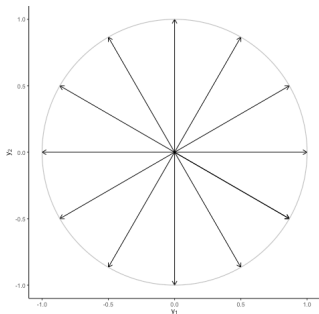
$$R(\tau) = D(\tau)$$

Selection of directions

- ▶ For 2 dimensions, one can easily split the unit ball with considering same angles in the interval $[0, 2\pi]$.

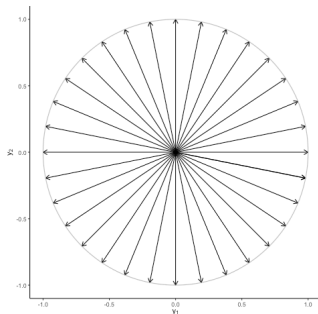
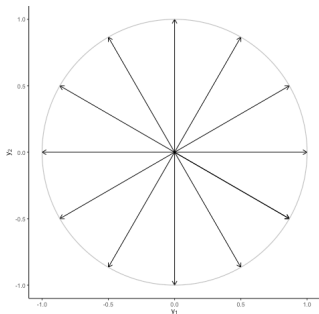
Selection of directions

- For 2 dimensions, one can easily split the unit ball with considering same angles in the interval $[0, 2\pi]$.



Selection of directions

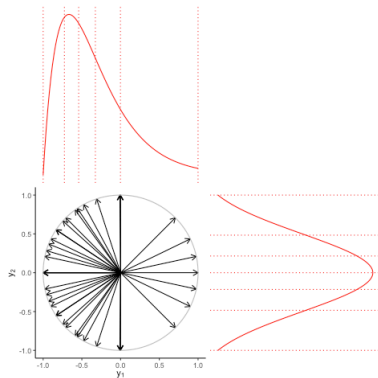
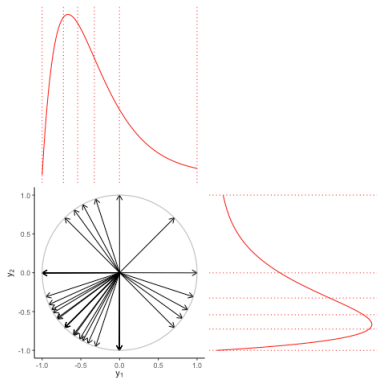
- ▶ For 2 dimensions, one can easily split the unit ball with considering same angles in the interval $[0, 2\pi]$.



- ▶ The same idea becomes more difficult with 3 or more dimensions.
 - ▶ And possibly it is not efficient.

Selection of directions based on marginal quantiles

- ▶ We propose selecting the directions based on marginal quantiles.
 - ▶ Example in 2 dimensions:



Adjustment of quantile hyperplanes

- ▶ Quantile regions do not show good properties regarding their coverage.
- ▶ In fact,

$$P(Y \in R(\tau)) \leq 1 - \tau$$

Adjustment of quantile hyperplanes

- ▶ Quantile regions do not show good properties regarding their coverage.
- ▶ In fact,

$$P(Y \in R(\tau)) \leq 1 - \tau$$

- ▶ This issue gets worse as the dimensions grow.

Adjustment of quantile hyperplanes

- ▶ Quantile regions do not show good properties regarding their coverage.
- ▶ In fact,

$$P(Y \in R(\tau)) \leq 1 - \tau$$

- ▶ This issue gets worse as the dimensions grow.

Readjustment of intercept for all directions

$$H_{\tau \mathbf{u}_a}^+ = \{\mathbf{y} \in \mathbb{R}^k : \mathbf{u}' \mathbf{y} \geq \hat{\mathbf{b}}_\tau \Gamma'_u \mathbf{y} + \mathbf{x}' \hat{\boldsymbol{\beta}}_\tau + \alpha_\tau^\lambda\},$$

where

$$\alpha_\tau^\lambda = \hat{a}_\tau - \lambda, \quad \lambda > 0,$$

such that

$$P(Y \in \bigcap_{\mathbf{u} \in \mathcal{S}^{k-1}} H_{\tau \mathbf{u}_a}^+) = 1 - \tau$$

Adjustment of quantile hyperplanes

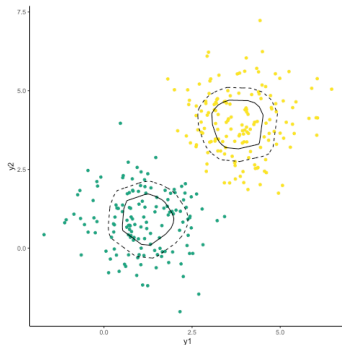
- ▶ Advantages:
 - ▶ it maintains all the conclusions regarding the covariates and their effects;
 - ▶ the same value of adjustment is used for all directions.

Adjustment of quantile hyperplanes

- ▶ Advantages:
 - ▶ it maintains all the conclusions regarding the covariates and their effects;
 - ▶ the same value of adjustment is used for all directions.
- ▶ Disadvantage:
 - ▶ It violates the subgradient conditions of the estimation process.

Adjustment of quantile hyperplanes

- ▶ Advantages:
 - ▶ it maintains all the conclusions regarding the covariates and their effects;
 - ▶ the same value of adjustment is used for all directions.
- ▶ Disadvantage:
 - ▶ It violates the subgradient conditions of the estimation process.
- ▶ Example:

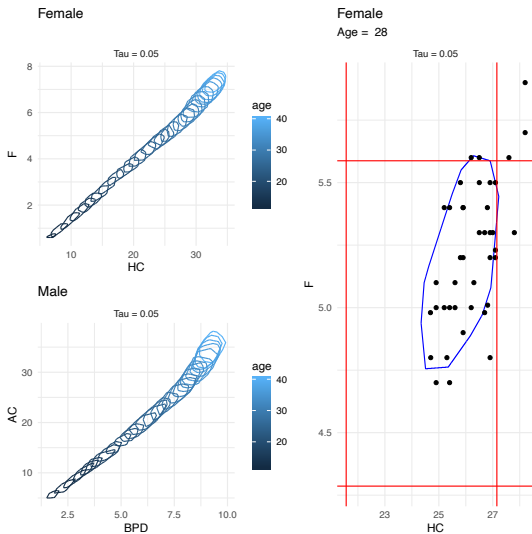


- ▶ 1445 ultrasonographic examinations of 434 pregnancies at 12-42 gestational weeks.
 - ▶ babies were born between July 1, 2014 and December 31, 2017
 - ▶ University Hospital of University of São Paulo, Brazil

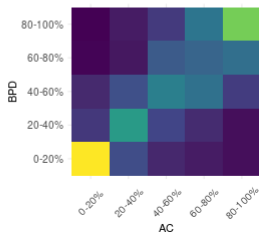
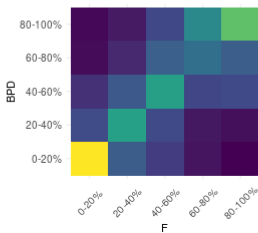
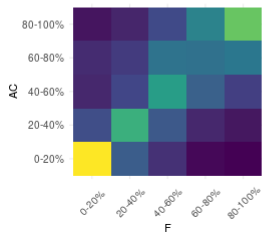
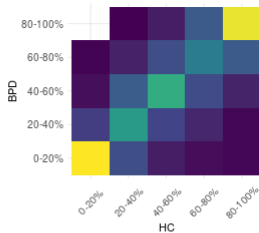
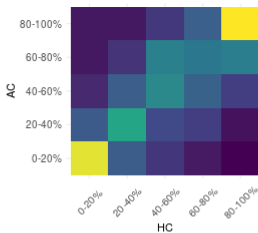
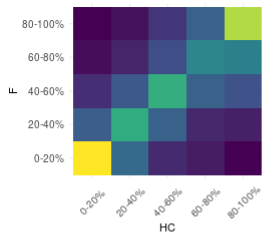
- ▶ 1445 ultrasonographic examinations of 434 pregnancies at 12-42 gestational weeks.
 - ▶ babies were born between July 1, 2014 and December 31, 2017
 - ▶ University Hospital of University of São Paulo, Brazil
- ▶ Measurements:
 - ▶ Y_1 : femur length (F);
 - ▶ Y_2 : head circumference (HC);
 - ▶ Y_3 : abdominal circumference (AC);
 - ▶ Y_4 : biparietal diameter (BPD).

- ▶ 1445 ultrasonographic examinations of 434 pregnancies at 12-42 gestational weeks.
 - ▶ babies were born between July 1, 2014 and December 31, 2017
 - ▶ University Hospital of University of São Paulo, Brazil
- ▶ Measurements:
 - ▶ Y_1 : femur length (F);
 - ▶ Y_2 : head circumference (HC);
 - ▶ Y_3 : abdominal circumference (AC);
 - ▶ Y_4 : biparietal diameter (BPD).
- ▶ Covariates:
 - ▶ gestational age (nonlinear effect);
 - ▶ sex;
 - ▶ mother BMI;

Examples of results



Distributions of observations outside quantile region



Final remarks

- ▶ We consider Bayesian quantile regression models for multiple-outputs to build growth curves for fetus measurements.
- ▶ We propose a method to select directions for higher dimensions based on marginal quantiles.
- ▶ We consider an adjustment in the quantile hyperplanes in order to improve the coverage of the conditional quantile regions.
- ▶ Next steps:
 - ▶ Add random effects to this framework.
 - ▶ Study the effects of the intercept adjustment for higher dimensions.

Thank you for your attention!

e-mail: b.santos@kent.ac.uk