Joint Estimation of Quantile Planes

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Linear regression through quantiles

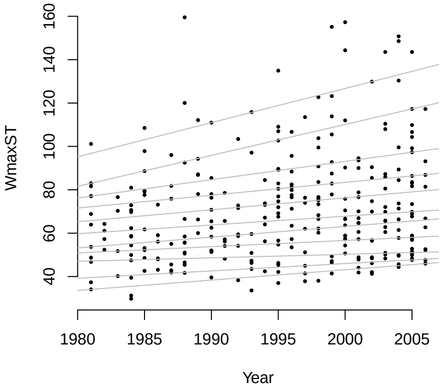
Koenker and Bassett (1978): replace $\mathbb{E}(Y|X) = \beta_0 + X^T\beta$ with

$$Q_Y(\tau \mid X) = \beta_0 + X^T\beta,$$

where

- τ is a **response proportion of interest** τ,
- $Q_Y(\tau \mid x) = \inf\{a : P(Y \leq a \mid X) \geq \tau\}$ is the corresponding (conditional) response quantile

Intensity trends of Atlantic tropical cyclones



Obvious fact: In any serious application, one looks at multiple response proportions τ

Salient features

- Analyze extreme and non-central response
  - Peer group diversity helps low achievers in elementary school!
- Capture dependence beyond changes to the mean
  - Regular vitamin intake does not improve plasma carotene level on the average, but helps the top third of the population!
- Quantify *differential* predictor effects on response distribution
  - Strongest tropical cyclones are getting stronger with time quicker than mid-range and weak cyclones!

QR as an analytic tool

- Fits are assembled from **separate single-τ analyses**
- Estimated quantiles can cross (violates probability laws)
- Little borrowing of information across response distribution

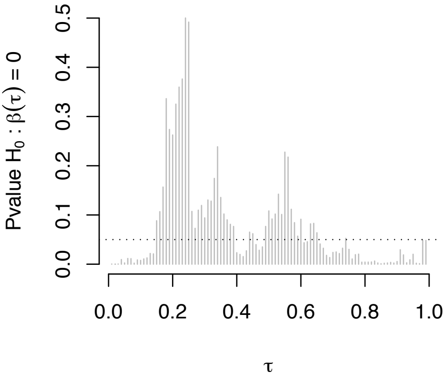
P-values from cyclone intensity analysis

Table 1 | Summary statistics

Statistic	Quantile				
	0.85	0.90	0.95	0.975	0.99
Global (2,097)					
W (m s^{-1})	51.9	55.8	62.6	68.8	75.9
Trend (m s^{-1} yr^{-1})	+0.19	+0.21	+0.18	+0.25	+0.30
s.e. (m s^{-1} yr^{-1})	0.049	0.072	0.141	0.122	0.093
P	<0.001	0.003	0.212	0.044	0.001
North Atlantic (291)					
W (m s^{-1})	48.9	54.8	60.3	72.7	77.8
Trend (m s^{-1} yr^{-1})	+0.63	+0.73	+0.81	+1.11	+1.52
s.e. (m s^{-1} yr^{-1})	0.228	0.226	0.449	0.356	NA
P	0.006	0.001	0.073	0.002	NA

From Elsner, Kossin, and Jagger (2008) published in Nature Letters

A more complete picture



In pursuit of Joint Estimation

- Model

$$Q_Y(\tau|x) = \beta_0(\tau) + x^T\beta(\tau), \quad \tau \in (0,1),$$

with function valued parameters

$$\beta_0 : (0,1) \to \mathbb{R}, \beta : (0,1) \to \mathbb{R}^p$$

- Must satisfy the monotonicity constraint

$$\beta_0(\tau_1) + x^T\beta(\tau_1) \geq \beta_0(\tau_2) + x^T\beta(\tau_2)$$

for every pair $\tau_1 > \tau_2$ and for every $x \in \mathcal{X}$ where $\mathcal{X}$ is a pre-specified domain for X

From exploratory to inference tool

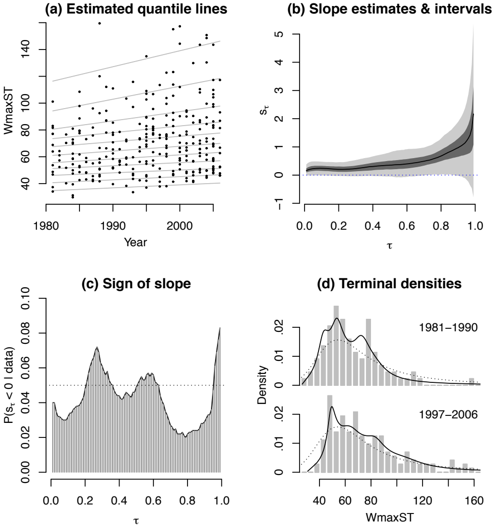
- When monotonicity holds, we have an interpretable generative model:

$$Y_i = \beta_0(U_i) + X_i^T \beta(U_i), U_i \overset{\text{IID}}{\sim} Unif(0, 1)$$

Many unsatisfactory attempts

- He (1997): imposes serious restrictions on the shape of $\beta(\tau)$
- Dunson and Taylor (2005): uses substitution likelihood, does not scale to dense τ grids
- Tokdar and Kadane (2012): complete, scalable solution when $\dim(X) = 1$; cheap shortcut when $\dim(X) > 1$

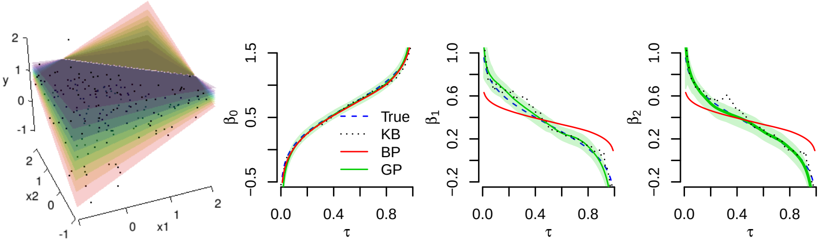
Cyclone intensity analysis from Tokdar and Kadane (2012)



Best existing approach: Reich et al. (2011)

- **Non-crossing:**
  - Bernstein basis polynomials with non-negative coefficients
  - Extending ideas from Bondell et al. (2010)
- **Prior and computing**
  - Truncated Gaussian prior distributions on coefficients
  - Gibbs sampling based Bayesian model fitting
- **BUT** require rectangular predictor domain $\mathcal{X}$
  - Getting $\mathcal{X}$ right is **important** for QR

Getting $\mathcal{X}$ right: a toy example



- X_i's simulated from the triangle $\Delta\{(-1,-1),(-1,2),(2,-1)\}$
- Crossing outside triangle but inside embedding rectangle
- GP gets it right, BP estimates are flatter

Our new approach!

- Complete characterization over **any bounded convex** $\mathcal{X}$
- **Likelihood** based estimation (penalized or Bayesian)

Characterization Theorem

- Assume non-atomic Y and 0 is an interior pt of $\mathcal{X}$
  - Non-crossing $\equiv \dot{\beta}_0(\tau) + x^T\dot{\beta}(\tau) > 0, \forall \tau \in (0,1), \forall x \in \mathcal{X}$
  - $\dot{\beta}_0(\tau) > 0 \ \forall \tau$
- Define: $a(b, \mathcal{X}) = \begin{cases} \sup_{x\in\mathcal{X}}\{-x^T b\}/\|b\| & b \neq 0, \\ \mathrm{diam}(\mathcal{X}) & b = 0. \end{cases}$
- **Theorem**. Non-crossing **if and only if**

$$\dot{\beta}_0(\tau) > 0, \quad \dot{\beta}(\tau) = \dot{\beta}_0(\tau)\frac{v(\tau)}{a(v(\tau), \mathcal{X})\sqrt{1 + \|v(\tau)\|^2}},$$

for some p-variate, real function $v(\tau) = (v_1(\tau), \cdots, v_p(\tau))^T$.

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for some p-variate, real function $v(\tau) = (v_1(\tau), \cdots, v_p(\tau))^T$.

An almost constraint-free parametrization

- Fixed quantities:
  - A $\tau_0 \in (0,1)$, an anchoring quantile, e.g., $\tau_0 = 0.5$
  - A base pdf f_0 [e.g., $t(\nu)$], with cdf F_0, $Q_0 = F_0^{-1}$, $q_0 = \dot{Q}_0$
  - A bounded convex $\mathcal{X}$ [e.g., convex hull of observed X_i's]
- Specification

$$\beta_0(\tau_0) = \gamma_0, \beta(\tau_0) = \gamma, \qquad \beta_0(\tau) = \gamma_0 + \sigma \int_{\zeta(\tau_0)}^{\zeta(\tau)} q_0(u) du$$

$$\beta(\tau) = \gamma + \sigma \int_{\zeta(\tau_0)}^{\zeta(\tau)} \frac{w(u)}{a(w(u), \mathcal{X})\sqrt{1 + \|w(u)\|^2}} q_0(u) du$$

- Model parameters:
  - $\gamma_0 \in \mathbb{R}$, $\gamma \in \mathbb{R}^p$, $\sigma > 0$
  - $w : [0,1] \to \mathbb{R}^p$ (unconstrained)
  - $\zeta : [0,1] \to [0,1]$ a diffeomorphism

Relating back to the Characterization Theorem

$$\dot{\beta}_0(\tau) = \sigma q_0(\zeta(\tau))\dot{\zeta}(\tau) > 0 \text{ for all } \tau \in (0,1)$$

$$\begin{aligned}\dot{\beta}(\tau) &= \sigma \frac{w(\zeta(\tau))}{a(w(\zeta(\tau)),\mathcal{X})\sqrt{1+\|w(\zeta(\tau))\|^2}} q_0(\zeta(\tau))\dot{\zeta}(\tau) \\ &= \dot{\beta}_0(\tau)\frac{v(\tau)}{a(v(\tau),\mathcal{X})\sqrt{1+\|v(\tau)\|^2}}\end{aligned}$$

with $v := w \circ \zeta$

Role of f_0: centrally embedded linear model

- When $\zeta = \mathrm{Identity}$, $w \equiv 0$ (and $Q_0(\tau_0) = 0$)

$$Q_Y(\tau|X) = \gamma_0 + X^T\gamma + \sigma Q_0(\tau)$$

  i.e.,

$$Y = \gamma_0 + X^T\gamma + \sigma\epsilon, \quad \epsilon \sim f_0.$$

- The prior can be made to center around this linear model

Role of f_0: tail and support control

- Prior supports $f(y|x)$ with tails decaying at least as quickly as those of f_0
- To gain more control we allow a family $\{f_0(\cdot|\nu) : \nu \in S\}$ of varying tails. Our R package **qrjoint** uses the Student-t family as default.
- Can take f_0 to be supported on $[0, \infty)$ to analyze positive valued response variables

Likelihood score evaluation

- Basic math
  - $f(y|x) = \left.\frac{1}{\frac{\partial}{\partial\tau}Q_Y(\tau|x)}\right|_{\tau=\tau_x(y)}$; $\tau_x(y)$ solves $Q_Y(\tau|x) = y$
  - Log-likelihood score equals

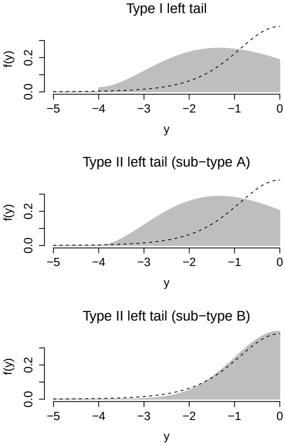
$$\sum_i \log f(y_i|x_i) = -\sum_i \log\left\{\dot{\beta}_0\left(\tau_{x_i}(y_i)\right) + x_i^T\dot{\beta}\left(\tau_{x_i}(y_i)\right)\right\}$$

- Calculations based on dense grid: $\{\tau_k = \frac{k}{N} : k = 0, \ldots, N\}$
  - Mostly quick vector-matrix multiplications
  - $a(w(\zeta(\tau)), \mathcal{X})$ is calculated as an automatic byproduct

A Bayesian implementation

- Prior specification
  - Flat/Horseshoe type shrinkage prior on γ
  - A GP prior on every w_j, $j = 1, \ldots, p$
    - Square exponential covariance function
    - Hyperpriors on range and scale
  - A logistic-GP prior on ζ:
$$\zeta(\tau) = \frac{\int_0^\tau e^{w_0(u)} du}{\int_0^1 e^{w_0(u)} du}$$
    where w_0 is a GP
- Computation:
  - Adaptive MCMC and blocking over preidctor index
  - 'Standard' GP approximations (low-rank, discretized range)
- Posterior consistency holds (well-/ill-specified wrt f_0)

Consistency holds under mild tail conditions



Defn: Type I left tail.

- $Q(0) > -\infty$
- $c(\sigma) := \lim_{t \downarrow 0} \frac{\frac{1}{\sigma} f_0(m + \frac{Q(t)-m}{\sigma})}{f(Q(t))} \in (0, \infty)$,
- $c(\sigma) \to 0$ as $\sigma \downarrow 0$.

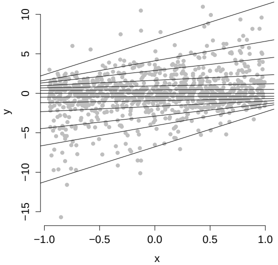
Defn: Type II left tail.

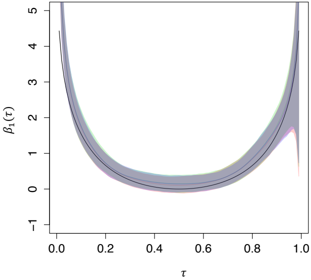
- $\lim_{t \downarrow 0} \frac{\frac{1}{\sigma} f_0(m + \frac{Q(t)-m}{\sigma})}{f(Q(t))} \to \infty$
- $u(\sigma) :=$ $\inf \left\{ t > 0 : \frac{\frac{1}{\sigma} f_0(m + \frac{Q(t)-m}{\sigma})}{f(Q(t))} \leq 1 \right\} > 0$
- $u(\sigma) \to 0$ as $\sigma \downarrow 0$.

Theorem

- **Assumptions:**
  - $\dot{\beta}^*/\dot{\beta}_0^*$ has cont. extension to $[0,1]$
  - $\exists c_0 > 0$ s.t. $\dot{\beta}_0^*(t) + x^T\dot{\beta}^*(t) \geq c_0\dot{\beta}_0^*(t)\ \forall x \in \mathcal{X}, t \in (0,1)$.
- **Result.** $f^* \in KL(\Pi)$ whenever $f_Y^*(\cdot|0)$ has type I or II tails with respect to t_ν for all small enough $\nu > 0$.

Efficient and reproducible computation

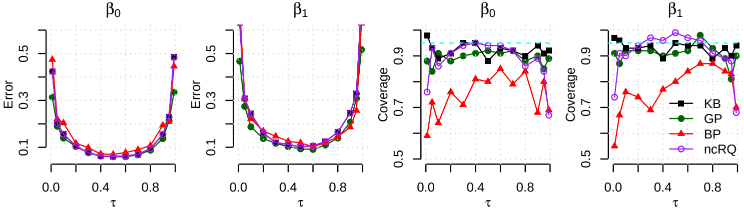




- Left: True quantile lines and synthetic data ($n = 1000$)
- Right: Posterior summaries of $\beta_1(\tau)$ from **four** runs of MCMC

Estimation accuracy

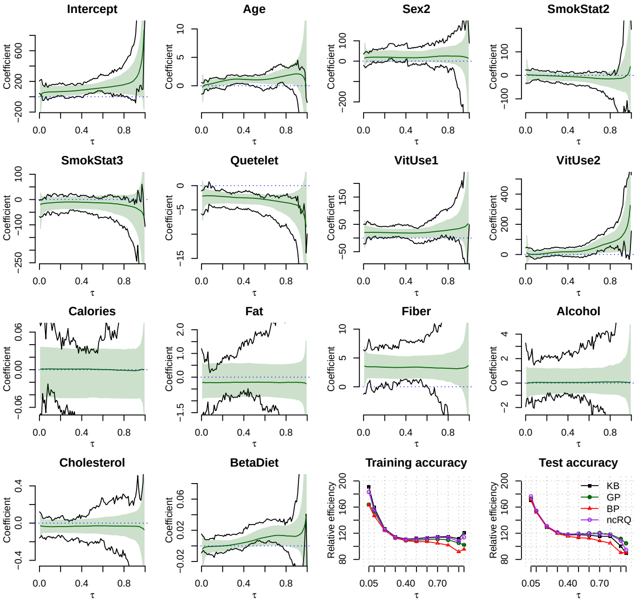
- 100 datasets from the above setting
- Pointwise mean absolute estimation error and coverage:



Application to plasma concentration of beta-carotene

- Low plasma concentration of beta-carotene may lead to higher risk of cancer
- What are the determinants of low concentration?
- $Y =$ log transform of beta-carotene concentration
- $X =$ age; smoking status; Quetelet (BMI); vitamin use, dietary intake (fat, fiber, alcohol, cholesterol, beta-carotene)

Parameter estimation



Results

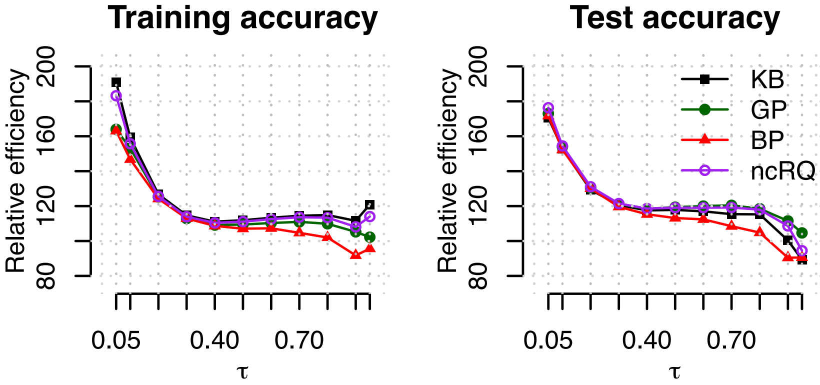
- Being female, use of vitamin and consumption of fiber have reasonably strong positive effect on plasma concentration of beta-carotene.
- Smoking and BMI have reasonably strong negative effect.
- Calories, fat, alcohol or cholesterol consumption appears to have little effect.
- Dietary intake of beta-carotene appears to have a positive effect, but the inference is not conclusive.
- More enhanced positive and negative effects, respectively for heavy vitamin use and BMI, on the upper quantiles

More dramatic effects on upper tail

j	Predictor	$\beta_j(0.9) - \beta_j(0.1)$	$\beta_j(0.9) - \beta_j(0.5)$
1	Age	$1.6_{(-0.33,4.07)}$	$0.97_{(-0.81,3.34)}$
2	Sex2	$4.6_{(-50.75,57.83)}$	$6.5_{(-42.93,57.27)}$
3	SmokStat2	$-13.43_{(-69.5,38)}$	$-5.94_{(-55.69,43.85)}$
4	SmokStat3	$-19.11_{(-94.84,31.17)}$	$-20.9_{(-90,26.57)}$
5	Quetelet	$-1.93_{(-5.61,0.91)}$	$-1.51_{(-4.79,1.02)}$
6	VitUse1	$14.37_{(-26.87,81.3)}$	$16.65_{(-22.72,81.83)}$
7	**VitUse2**	$\mathbf{113.05}_{(19.86,209.36)}$	$\mathbf{93.53}_{(12.62,185.14)}$
8	Calories	$0_{(-0.02,0.02)}$	$0_{(-0.02,0.02)}$
9	Fat	$-0.02_{(-0.37,0.36)}$	$-0.02_{(-0.37,0.32)}$
10	Fiber	$-0.16_{(-3.31,3.19)}$	$-0.22_{(-3.27,2.85)}$
11	Alcohol	$0.04_{(-0.74,1.28)}$	$0.05_{(-0.62,1.11)}$
12	Cholesterol	$0_{(-0.12,0.13)}$	$0_{(-0.12,0.12)}$
13	BetaDiet	$0.01_{(0,0.04)}$	$0.01_{(-0.01,0.03)}$

Assessment of fit

- 10 sets of random 2:1 train/test split of data
- Risk = Ave 'check' loss[1] $\rho_\tau(Y_i - \hat{\beta}_0(\tau) - X_i^T \hat{\beta}(\tau))$ at each τ
- Accuracy is inverse relative risk with LM as benchmark



[1] $\rho_\tau(r) = r\{\tau - I(r < 0)\}$

Survival analysis

- Censored observations
- Log-likelihood score calculation now changes to

$$\sum_i [(1 - c_i) \log f_Y(y_i|x_i) + c_i \log\{1 - F_Y(y_i|x_i)\}]$$
$$= \sum_i \Big[c_i \log\{1 - \tau_{x_i}(y_i)\}$$
$$- (1 - c_i) \log \left\{ \dot{\beta}_0(\tau_{x_i}(y_i)) + x_i^T \dot{\beta}(\tau_{x_i}(y_i)) \right\} \Big],$$

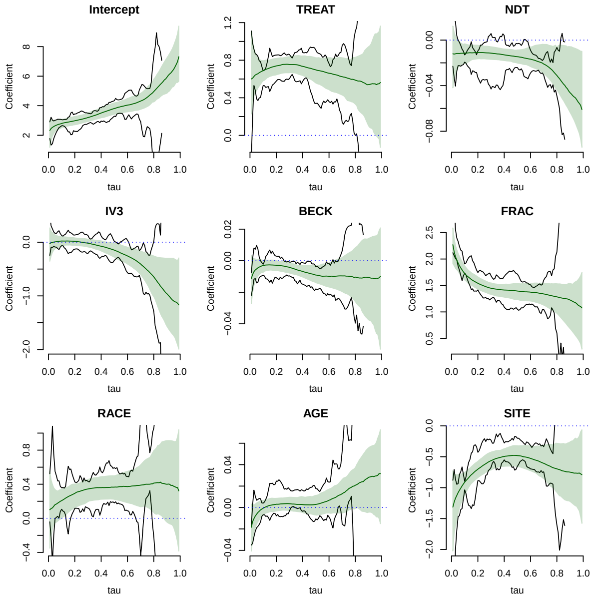
c_i = censoring status (1= right censored, 0 = observed).

- That's all that needs changing!

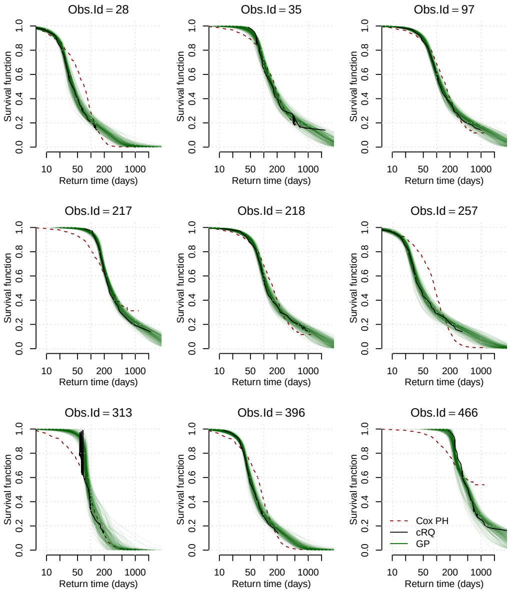
Return to drug study

- Data from University of Massachusetts Aids Research Unit IMPACT Study data (UIS, Hosmer and Lemeshow, 1998, Table 1.3)
- Response = (log) time to return to drug
- Predictors include current treatment assignment , drug use history, compliance factor, depression score, race, age, treatment site
- Total 575 subjects. Return times were right censored for 111

Parameter estimation



Survival curves – crossing!



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Package 'qrjoint'

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Title Joint Estimation in Linear Quantile Regression

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Depends R (>= 2.6), stats, graphics, grDevices, quantreg

Imports splines, coda, Matrix, kernlab

Description
Joint estimation of quantile specific intercept and slope parameters in a linear regression setting.

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NeedsCompilation yes

R topics documented: