

Flexible Regression

Session 2 - Introduction to Quantile Regression

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Session outline

- 1. Definitions
- 2. Motivating examples
- 3. Estimation
- 4. Asymptotics
- 5. Inference
- 6. Nonparametric quantile regression

What is quantile regression?

What is a quantile?

Y: random variable with CDF $F_Y(y) = P(Y \le y)$.

The τ th quantile of Y is

$$Q_{\tau}(Y) = \inf\{y : F_Y(y) \ge \tau\}$$

 τ : quantile level, $0 < \tau < 1$.

- au au = 0.25: first quartile
- au au = 0.5: median
- au au = 0.75: third quartile

 $Q_{\tau}(Y)$: nondecreasing function of τ .

Conditional quantile

Regression setting

Y: response variable

x: p-dimensional predictor

$$F_Y(y|\mathbf{x}) = P(Y \leq y|\mathbf{x})$$
: conditional CDF of Y given \mathbf{x}

Then the τ th conditional quantile of Y is defined as

$$Q_{\tau}(Y|\mathbf{x}) = \inf\{y : F_Y(y|\mathbf{x}) \geq \tau\}.$$

Mean vs quantile regression

Least squares linear mean regression model:

$$Y = \mathbf{x}^{\mathsf{T}} \boldsymbol{\beta} + \varepsilon, \quad E(\varepsilon) = 0.$$

Thus $\mathbb{E}(Y|\mathbf{x}) = \mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}$,

Linear quantile regression model:

$$Q_{\tau}(Y|\mathbf{x}) = \mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}(\tau), \quad 0 < \tau < 1.$$

 $Q_{\tau}(Y|\mathbf{x})$ is a non-decreasing function of τ for any given \mathbf{x} .

Example: location-scale shift model

Consider random variables Y_i , i = 1, ..., n where

$$Y_i = \alpha + \mathbf{z}_i^\mathsf{T} \boldsymbol{\beta} + (1 + \mathbf{z}_i^\mathsf{T} \boldsymbol{\gamma}) \varepsilon_i,$$

with $\varepsilon \stackrel{\text{i.i.d}}{\sim} F(\cdot)$.

Conditional quantile function:

$$Q_{\tau}(Y|\mathbf{x}_{i}) = \alpha(\tau) + \mathbf{z}_{i}^{\mathsf{T}}\boldsymbol{\beta}(\tau),$$

- $ho \ \alpha(\tau) = \alpha + F^{-1}(\tau)$ is nondecreasing in τ ;
- $\beta(\tau) = \beta + \gamma F^{-1}(\tau)$ may depend on τ .

Location shift: $\gamma = 0$, so that $\beta(\tau) = \beta$ is constant across τ .

Galton's strength of squeeze data

NATURE

[7an. 8, 1885

ANTHROPOMETRIC PER-CENTILES

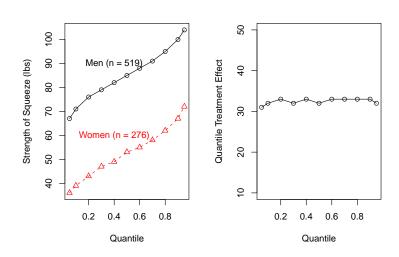
Values surpassed, and Values unreached, by various percentages of the persons measured at the Anthropometric Laboratory in the late International Health Exhibition

(The value that is unreached by n for cent, of any large group of monuterments, and surpassed by 100-n of them, is called its with

percentile)															
Subject of measurement	Age	Unit of measure- ment	Sex	No. of persons in the group	95	90	80	70	60 tunreache	50	40	30	20 80	10	5 95
Height, standing, without shoes	23-51	Inches {	М. F.	811	63°2 58'8	64·5 59·9	61.3 62.8	66.5 62.1	67 3 62 7	67.9 63.3	68·5 63·9	69°2 64°6	70°0 65°3	71.3 66.4	72'4 67'3
Height, sitting, from seat of chair	23-51	Inches {	M. F.	1013 775	33.6	34°2 32°3	34'9 32'9	35°3	35.4 33.6	36°0	36·3 34·2	36·7 34·6	37°1 34°9	37 ⁻⁷ 35 ⁻⁶	38.5 36.0
Span of arms	23-51	Inches {	M. F.	811	65.0 58.6	59.2 66.1	67 2 60 7	68·2 61·7	69'0 62'4	63.0 69.0	70.6 63.7	71.4 64.2	72°3 65°4	73.6 66.7	74.8 68.0
Weight in ordinary indoor clothes	23-26	Pounds {	M. F.	520 276	121 102	125 105	131	135	139 118	143 122	147 129	150 132	156 136	165 142	172 149
Breathing capacity	23-26	Cubic { inches {	M. F.	212 277	161 92	177	187 115	199 124	211 131	219 138	226 144	236 151	248 164	277 177	290 186
Strength of pull as archer with bow	23 26	Pounds {	M. F.	519 276	56 30	60 32	64 34	68 36	71 38	74 40	77 42	88 44	82 47	89 51	96 54
Strength of squeeze with strongest hand	23-26	Pounds	М. F.	519 276	67 36	71 39	76 43	79 47	82 49	85 52	88 55	91 58	95 62	100 67	104 72
Swiftness of blow.	23-26	Feet per }	M. F.	516 271	9.5 13.5	14°1 10°1	11.3	16'2 16'2	17.3	18·1 13·4	19'1 14'0	20'0 14'5	15.1 50.0	16.3 16.3	23.6 16.9
Sight, keenness of —by distance of reading diamond test-type	23-26	Inches {	M. F.	398 433	13	17 12	20 16	22 19	23 22	25 24	26 26	28 27	30 29	32 31	34 32

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Galton's strength of squeeze data



Quantile treatment effects

- \rightarrow $X_i = 0$: control; $X_i = 1$: treatment
- $Y_i|X_i=0\sim F$ (control distribution) and $Y_i|X_i=1\sim G$ (treatment distribution)
- Mean treatment effect:

$$\Delta = E(Y_i|X_i=1) - E(Y_i|X_i=0) = \int ydG(y) - \int ydF(y).$$

Quantile treatment effect:

$$\delta(au) = Q_{ au}(Y|X_i = 1) - Q_{ au}(Y|X_i = 0) = G^{-1}(au) - F^{-1}(au).$$

► Thus

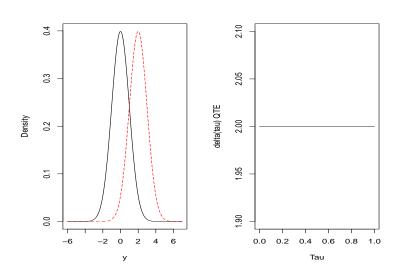
$$\Delta = \int_0^1 G^{-1}(u) du - \int_0^1 F^{-1}(u) du = \int_0^1 \delta(u) du.$$

Equivalent quantile regression model (with binary covariate):

$$Q_{\tau}(Y|X) = \alpha(\tau) + \delta(\tau)X.$$

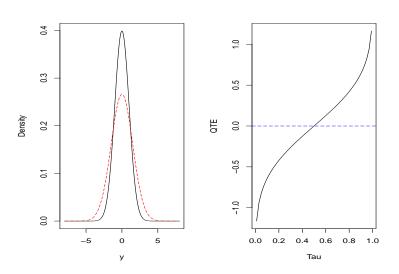
Location shift

$$F(y) = G(y + \delta) \Rightarrow \delta(\tau) = \Delta = \delta.$$

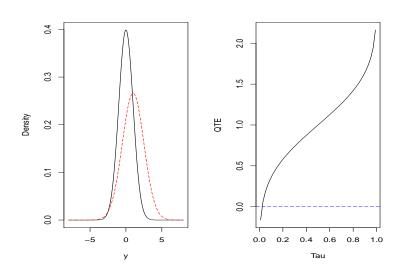


Scale shift

Scale shift: $\Delta = \delta(0.5) = 0$, but $\delta(\tau) \neq 0$ at other quantiles.



Location-scale shift

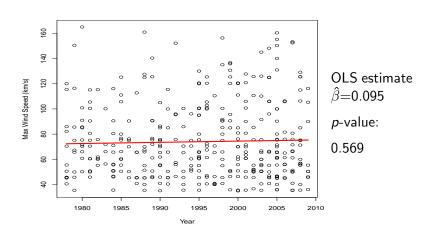


Why	quantile	regression?

1. To study the impact of predictors on different quantiles of the response distribution in order to provide a complete picture of the relationship between Y and \mathbf{x} .

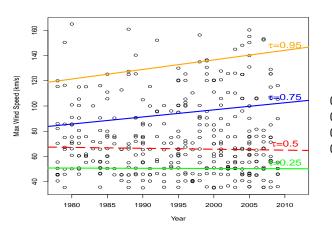
Example: Tropical cyclones

- \triangleright y_i : max wind speeds of tropical cyclones in the North Atlantic
- ► *x_i*: year 1978-2009



Example: Tropical cyclones

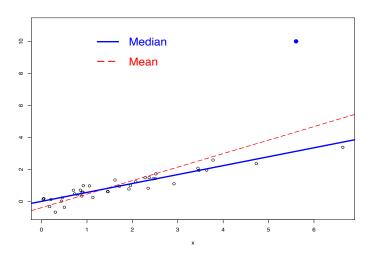
Do the quantiles of max speed change over time?



au	<i>p</i> -value
0.95	0.009
0.75	0.100
0.50	0.718
0.25	0.659

Why quantile regression?

2. It is robust to outliers in *y* observations.



Why quantile regression?

 ${\it 3. \ It \ makes \ no \ distributional \ assumptions.}$

Equivariance properties

- $\hat{eta}(\tau; ay, \mathbf{X}) = a\hat{eta}(\tau; y, \mathbf{X})$ for any constant a > 0
- $\hat{\boldsymbol{\beta}}(\tau; -ay, \mathbf{X}) = -a\hat{\boldsymbol{\beta}}(1-\tau; y, \mathbf{X})$ (scale equivariance)
- $\hat{\boldsymbol{\beta}}(\tau;y+\mathbf{X}\boldsymbol{\gamma},\mathbf{X})=\hat{\boldsymbol{\beta}}(\tau;y,\mathbf{X})+\boldsymbol{\gamma} \text{ where } \boldsymbol{\gamma}\in\mathbb{R}^p \text{ (regression shift)}$
- ▶ $\hat{\beta}(\tau; y, \mathbf{X}A) = A^{-1}\hat{\beta}(\tau; y, \mathbf{x})$ where A is any $p \times p$ nonsingular matrix (reparameterisation of design)

Equivariance to monotone transformations

Suppose $h(\cdot)$ is an increasing function on \mathbb{R} . Then for any variable Y,

$$Q_{h(Y)}(\tau) = h\{Q_{\tau}(Y)\}.$$

That is, the quantiles of the transformed random variable h(Y) are simply the transformed quantiles on the original scale.

This is not true in general for the mean, e.g.

$$\mathbb{E}(\log(Y)|X) \neq \log(\mathbb{E}(Y|X))$$

but

$$Q_{\tau}(\log(Y|X)) = \log(Q_{\tau}(Y|X).$$

Interpolation

Linear quantile regression lines exactly fit p observations (subgradient condition).

Which *p* points should be interpolated is determined by using all observations.

Estimation of quantile regression coefficients

Mean regression - ordinary least squares (OLS)

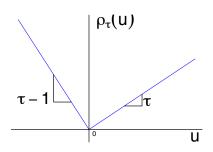
- ▶ The mean E(Y) minimises $E\{(Y a)^2\}$.
- ▶ The sample mean minimises $\sum_{i=1}^{n} (y_i a)^2$.
- ▶ The OLS estimator minimises $\sum_{i=1}^{n} (y_i \mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta})^2$.

Median regression – least absolute deviation (LAD)

- ▶ The median $Q_{0.5}(Y)$ minimises E|Y-a|.
- ▶ The sample median minimises $\sum_{i=1}^{n} |y_i a|$.
- Assuming $Q_{0.5}(y|x) = \mathbf{x}_i^\mathsf{T} \boldsymbol{\beta}(0.5)$, $\hat{\boldsymbol{\beta}}(0.5)$ can be obtained by minimising $\sum_{i=1}^n |y_i \mathbf{x}_i^\mathsf{T} \boldsymbol{\beta}|$.

Quantile coefficient estimation

► The τ th quantile $Q_{\tau}(Y)$ minimises $E\{\rho_{\tau}(Y-a)\}$, where $\rho_{\tau}(u) = u\{\tau - I(u < 0)\}$ is the quantile loss function.



- ▶ The τ th sample quantile of Y minimises $\sum_{i=1}^{n} \rho_{\tau}(y_i a)$.
- Assuming $Q_{\tau}(Y|\mathbf{x}) = \mathbf{x}^{\mathsf{T}}\boldsymbol{\beta}(\tau)$, then $\hat{\boldsymbol{\beta}}(\tau)$ minimises $\sum_{i=1}^{n} \rho_{\tau}(y_{i} \mathbf{x}_{i}^{\mathsf{T}}\boldsymbol{\beta})$.

How to minimise the objective function?

Linear programming problem

 $\min_{\mathbf{y} \in \mathbb{R}^m} \mathbf{y}^\mathsf{T} \mathbf{b},$

subject to the constraints

$$y^T A \ge c^T$$
,

and

$$y_1 \geq 0, \cdots, y_m \geq 0,$$

where **A** is an $m \times n$ matrix, $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{c} \in \mathbb{R}^n$.

How to minimise the objective function?

Dual problem

 $\max_{\mathbf{x} \in \mathbb{R}^n} \mathbf{c}^\mathsf{T} \mathbf{x},$

subject to constraints

 $\mathbf{A}\mathbf{x} \leq \mathbf{b}$

and

 $\mathbf{x} \geq 0$.

Quantile regression as a linear programming problem

$$y_i = \mathbf{x}_i^\mathsf{T} \boldsymbol{\beta}(\tau) + e_i$$

= $\mathbf{x}_i^\mathsf{T} \boldsymbol{\beta}(\tau) + (u_i - v_i),$

where

$$u_i = e_i I(e_i > 0),$$

 $v_i = |e_i| I(e_i < 0).$

So

$$\begin{aligned} \min_{\mathbf{b}} \sum_{i=1}^{n} \rho_{\tau} (y_{i} - \mathbf{x}_{i}^{\mathsf{T}} \mathbf{b}) \\ \Leftrightarrow & \min_{\{\mathbf{b}, \mathbf{u}, \mathbf{v}\}} \tau \mathbf{1}_{n}^{\mathsf{T}} \mathbf{u} + (1 - \tau) \mathbf{1}_{n}^{\mathsf{T}} \mathbf{v} \\ s.t. & \mathbf{y} - \mathbf{X}^{\mathsf{T}} \mathbf{b} = \mathbf{u} - \mathbf{v} \\ & \mathbf{b} \in \mathbb{R}^{p}, & \mathbf{u} \geq 0, & \mathbf{v} \geq 0. \end{aligned}$$

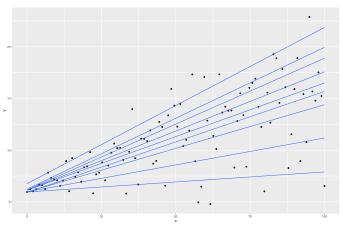
Implementation in R

- ► Function rq() from library(quantreg) fits quantile regression models.
- Syntax:

```
rq(y ~ x, tau=.5, data,method=...)
```

- method="br" (default) implements the simplex method of Barrodale and Roberts (1974) for optimising the objective function.
- method="fn" implements the Frisch-Newton interior point algorithm (Portnoy and Koenker, 1997).
- method="sfn" implements a version of the interior point algorithm suitable for sparse design matrices (Koenker and Ng, 2003).

Example: illustration with simulated data



Example: illustration with simulated data

Statistical properties

Coefficient estimator

$$\hat{\boldsymbol{\beta}}(\tau) = \arg\min_{\mathbf{b} \in \mathbb{R}^p} \sum_{i=1}^n \rho_{\tau}(y_i - \mathbf{x}_i^{\mathsf{T}} \mathbf{b}).$$

Consistency

Under regularity conditions A1 and A2(i) (see next slide)

$$\hat{\boldsymbol{\beta}}(\tau) \stackrel{p}{\to} \boldsymbol{\beta}(\tau).$$

Statistical properties

Regularity conditions

- A1. The distribution functions of Y given \mathbf{x}_i , $F_i(\cdot)$, are absolutely continuous with continuous densities $f_i(\cdot)$ that are uniformly bounded away from 0 and ∞ at $\xi_i(\tau) = Q_{\tau}(Y|\mathbf{x}_i)$.
- A2. There exist positive definite matrices D_0 and D_1 such that
 - (i) $\lim_{n\to\infty} n^{-1} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\mathsf{T} = D_0$;
 - (ii) $\lim_{n\to\infty} n^{-1} \sum_{i=1}^n f_i(\xi_i(\tau)) \mathbf{x}_i \mathbf{x}_i^{\mathsf{T}} = D_1(\tau);$
 - (iii) $\max_{i=1,...,n} ||\mathbf{x}_i|| = o(n^{\frac{1}{2}}).$

Statistical properties

Asymptotic normality

Under Conditions A1 and A2

$$\sqrt{n}\left(\hat{\boldsymbol{\beta}}(\tau) - \boldsymbol{\beta}(\tau)\right) \overset{d}{\to} N\left(0, \tau(1-\tau)D_1^{-1}D_0D_1^{-1}\right).$$

Simplification in the case of i.i.d. errors

$$\sqrt{n}\left(\hat{\boldsymbol{\beta}}(\tau)-\boldsymbol{\beta}(\tau)\right)\stackrel{d}{\to} N\left(0,\frac{\tau(1-\tau)}{f_{\varepsilon}^2(0)}D_0^{-1}\right),$$

where $f_i(\xi_i(\tau)) = f_{\varepsilon}(0)$.

Inference

- ▶ Idea: use asymptotic normality results to perform Wald-type hypothesis tests and construct confidence intervals.
- ▶ **Problem:** Asymptotic covariance matrix involves the unknown densities $f_i(\mathbf{x}_i^\mathsf{T}\boldsymbol{\beta}(\tau))$ in non-i.i.d. settings, and $f_\varepsilon(0)$ in i.i.d. settings.

How do we estimate these?

Estimation in i.i.d. setting

Sparsity parameter

$$s(\tau) = \frac{1}{f(F^{-1}(\tau))}$$
 (derivative of the quantile function $F^{-1}(t)$ with respect to t)

Difference quotient estimator (Siddiqui, 1960)

$$\hat{s}_n(t) = \frac{\hat{F}_n^{-1}(t + h_n|\bar{\mathbf{x}}) - \hat{F}_n^{-1}(t - h_n|\bar{\mathbf{x}})}{2h_n},$$

where

$$ightharpoonup h_n o 0$$
 as $n o \infty$,

•
$$\hat{F}_n^{-1}(t|\bar{\mathbf{x}})$$
 is the estimated t th conditional quantile of Y given $\bar{\mathbf{x}} = n^{-1} \sum_{i=1}^n \mathbf{x}_i$.

Estimation in non-i.i.d. settings

Estimation of $D_1(\tau)$

- ▶ Suppose the conditional quantiles of Y given \mathbf{x} are linear at quantile levels around τ .
- ► Then fit quantile regression at $(\tau \pm h_n)$ th quantiles, resulting in $\hat{\beta}(\tau h_n)$ and $\hat{\beta}(\tau + h_n)$.
- ▶ Estimate $f_i(\xi_i(\tau))$ by

$$\tilde{f}_i(\xi_i(\tau)) = \frac{2h_n}{\mathbf{x}_i^{\mathsf{T}} \hat{\boldsymbol{\beta}}(\tau + h_n) - \mathbf{x}_i^{\mathsf{T}} \hat{\boldsymbol{\beta}}(\tau - h_n)},$$

where $\xi_i(\tau) = Q_{\tau}(Y|\mathbf{x}_i)$.

"Hendricks-Koenker sandwich"

Implementation in R

```
> # Assuming iid errors:
> summary.rq(fit, se="iid")
> # Hendricks-Koenker sandwich:
> summary.rq(fit, se="nid") # assuming non-iid errors
tau: [1] 0.5
Coefficients:
           Value Std. Error t value Pr(>|t|)
(Intercept) 6.13147 0.17754 34.53611 0.00000
            0.10376 0.00888 11.67973 0.00000
X
> # Based on Powell kernel estimator
> summary.rq(fit, se="ker")
```

Rank score test

- ► Model: $Q_{\tau}(Y|\mathbf{x}_i, \mathbf{z}_i) = \mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta}(\tau) + \mathbf{z}_i^{\mathsf{T}} \boldsymbol{\gamma}(\tau)$
- ▶ Hypotheses: $H_0: \gamma(\tau) = 0$ vs $H_1: \gamma(\tau) \neq 0$ where $\beta(\tau) \in \mathbb{R}^p$ and $\gamma(\tau) \in \mathbb{R}^q$.
- Score function:

$$S_n = \sqrt{n} \sum_{i=1}^n z_i^* \psi_\tau(y_i - \mathbf{x}_i^\mathsf{T} \hat{\boldsymbol{\beta}}(\tau)),$$

where

- $\psi_{\tau}(u) = \tau I(u < 0);$
- $\mathbf{z}^* = (\mathbf{z}_i^*) = \mathbf{z} \mathbf{x} (\mathbf{x}^\mathsf{T} \mathbf{\Psi} \mathbf{x})^{-1} \mathbf{x}^\mathsf{T} \mathbf{\Psi} \mathbf{z}, \ \mathbf{\Psi} = \mathrm{diag}(f_i(Q_\tau(Y|\mathbf{x}_i,\mathbf{z}_i));$
- $\hat{eta}(au)$ is the quantile coefficient estimator under H_0 .

Rank score test

▶ Under H_0 , as $n \to \infty$,

$$S_n = AN(0, M_n^{\frac{1}{2}}),$$

where
$$M_n = n^{-1} \sum_{i=1}^n \mathbf{z}_i^* \mathbf{z}_i^{*T} \tau (1 - \tau)$$
.

▶ Then the rank-score test statistic

$$T_n = S_n^{\mathsf{T}} M_n^{-1} S_n \stackrel{d}{\to} \chi_q^2$$
, under H_0 .

- ▶ In *i.i.d.* settings $\mathbf{z}^* = (\mathbf{z}_i^*) = \{\mathbf{I} \mathbf{x}(\mathbf{x}^\mathsf{T}\mathbf{x})^{-1}\mathbf{x}^\mathsf{T}\}\mathbf{z}$ and $M_n = \tau(1-\tau)n^{-1}\sum_{i=1}^n \mathbf{z}_i^*\mathbf{z}_i^{*\mathsf{T}}$ no need to estimate the nuisance parameters $f_i\{Q_\tau(Y|\mathbf{x}_i,z_i)\}$.
- The rank score test can be inverted to give confidence intervals.

Implementation in R

The rank score method is the default method for standard error and confidence interval estimation in library(quantreg):

Bootstrap methods

- An alternative approach is to use bootstrap for standard error estimation
- Options include:
 - residual bootstrap
 - paired bootstrap
 - Markov chain marginal bootstrap (MCMB)
 - **▶** ...
- See boot.rq() in library(quantreg)
- > summary.rq(fit, se="boot", alpha=0.05) # default: paired
 tau: [1] 0.5

Coefficients:

```
Value Std. Error t value Pr(>|t|)
(Intercept) 6.13147 0.20251 30.27766 0.00000
x 0.10376 0.00772 13.43691 0.00000
```

Nonparametric quantile regression

- ► The ideas of
 - local polynomial models,
 - ► regression splines,
 - penalised splines,

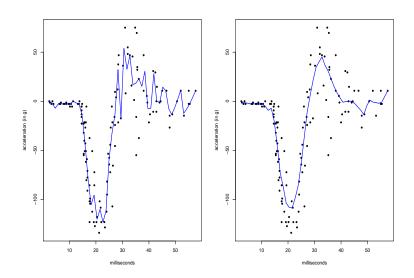
introduced earlier, can be applied to quantile regression.

▶ Decisions about the order of the spline, number of knots or penalty parameter need to be made.

Example: motorcycle data

- ► Locally linear approach using the lprq function from library(quantreg).
- ► This function computes a quantile regression fit at each of *m* equally spaced *x*-values over the support of the observed *x* points.
- ► The value of the smoothing parameter (bandwidth h) must be provided.
- ► In R:
 - > library(MASS) # to get the mcycle data
 - > fit1 <- lprq(mcycle\$times,mcycle\$accel,h=.5,tau=0.5)</pre>
 - > fit2 <- lprq(mcycle\$times,mcycle\$accel,h=2,tau=0.5)</pre>

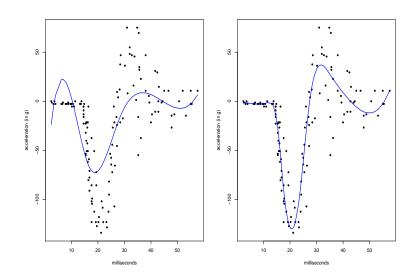
Local linear median regression fit for the motorcycle data with h=0.5 and h=2



Example: motorcycle data

- ▶ B-splines can be implemented using the function bs() in the package splines in R.
- Here we control the level of smoothing via the degrees of freedom.
 - > fit3 <- rg(accel~bs(times,df=5),tau=0.5, data=mcycle)</pre>
 - > fit4 <- rq(accel~bs(times,df=10),tau=0.5, data=mcycle)</pre>

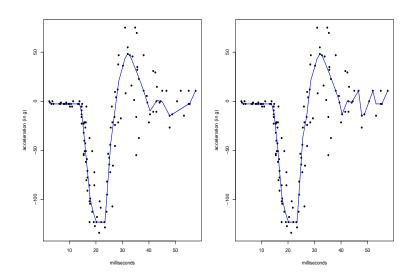
Median regression fit using cubic B-splines with df=5 and df=10 for the motorcycle data



Example: motorcycle data

- Quantile smoothing splines using a roughness penalty can be implemented via the rqss() function in library(quantreg) in R.
- This function is quite flexible and allows specification of monotonicity and convexity constraints.
- ▶ Penalty parameter λ has to be specified by the user (default value is lambda=1).
- ▶ In R:

Median regression fit for the motorcycle data using quantile smoothing splines with penalty $\lambda=1$ and $\lambda=0.5$.



Remarks

- ▶ Spline methods are better than local linear methods in general.
- All methods require decisions to be made about the degree of smoothing to be applied.
- ▶ Quantile crossing is an issue in general, and even more so with nonparametric quantile regression, especially for τ near 0 or 1.

Summary

Quantile regression

- Quantiles and quantile regression
- ▶ Why use quantile regression?
- ▶ How to fit quantile regression models in R
- ► Splines for nonparametric quantile regression

Aknowledgements



Prof. Judy H. Wang, GWU



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