lqmm: Estimating Quantile Regression Models for Independent and Hierarchical Data with R

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Quantile regression

Conditional quantile regression (QR) pertains to the estimation of unknown quantiles of an outcome as a function of a set of covariates and a vector of fixed regression coefficients.

For example, consider a sample of 654 observations of FEV1 in individuals aged 3 to 19 years who were seen in the Childhood Respiratory Disease (CRD) Study in East Boston, Massachusetts [1]. We might be interested in estimating **median** FEV1 or any other **quantile** as a **function** of age, sex, smoking, etc.

[1] Data available at http://www.statsci.org/datasets.html

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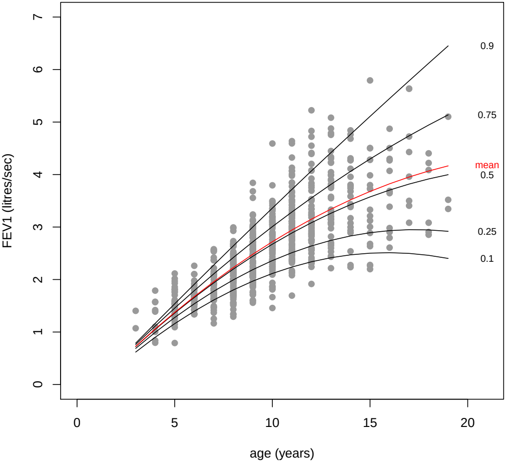

Regression quantiles (black) and mean fit (red) of FEV1 vs Age.

Quantile regression (contd)

Let's index the quantiles Q of the continuous response y_i with p, $0 < p < 1$, that is $\Pr(y_i \leqslant Q_{y_i}(p)) = p$. The conditional (linear) quantile function

$$Q_{y_i}(p|x_i) = x_i'\beta(p), \qquad i = 1, \ldots, N$$

can be estimated by solving (Koenker and Bassett, *Econometrica*, 1978)

$$\min_{\beta} \sum_i g_p(y_i - x_i'\beta(p)),$$

where $g_p(z) = z(p - I(z < 0))$ and $\beta(p)$ is the regression coefficient vector indexed by p.

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Likelihood-based quantile regression: The asymmetric Laplace

Mean regression problem
(least squares)

$$\min_{\beta} \sum (y - x'\beta)^2$$

$\updownarrow$

$$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(y - x'\beta)^2\right\}$$

Normal distribution

Quantile regression problem
(least absolute deviations)

$$\min_{\beta} \sum g_p(y - x'\beta)$$

$\updownarrow$

$$\frac{p(1-p)}{\sigma} \exp\left\{-\frac{1}{\sigma} g_p(y - x'\beta)\right\}$$

Asymmetric Laplace distribution

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Quantile regression problem
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location parameter

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Normal distribution

$$\frac{p(1-p)}{\sigma} \exp\left\{ -\frac{1}{\sigma} g_p(y - x'\beta) \right\}$$

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(least squares)

$$\min_{\beta} \sum (y - x'\beta)^2$$

Quantile regression problem
(least absolute deviations)

$$\min_{\beta} \sum g_p(y - x'\beta)$$

scale parameter

$$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(y - x'\beta)^2\right\}$$

Normal distribution

$$\frac{p(1-p)}{\sigma} \exp\left\{-\frac{1}{\sigma} g_p(y - x'\beta)\right\}$$

Asymmetric Laplace distribution

Likelihood-based quantile regression: The asymmetric Laplace

Mean regression problem
(least squares)

$$\min_{\beta} \sum (y - x'\beta)^2$$

Quantile regression problem
(least absolute deviations)

$$\min_{\beta} \sum g_p(y - x'\beta)$$

skewness parameter

$$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{ -\frac{1}{2\sigma^2}(y - x'\beta)^2 \right\}$$

Normal distribution

$$\frac{p(1-p)}{\sigma} \exp\left\{ -\frac{1}{\sigma} g_p(y - x'\beta) \right\}$$

Asymmetric Laplace distribution

Quantile regression and random effects

If $y \sim \mathrm{AL}(\mu, \sigma, p)$ then $Q_y(p) = \mu$.

The aim is to develop a QR model for hierarchical data. Inclusion of random intercepts in the conditional quantile function is straightforward (Geraci and Bottai, *Biostatistics*, 2007)

$$Q_y(p|x, u) = x'\beta(p) + u.$$

Likelihood-based estimation (MCEM – R and WinBUGS) assuming

- $y = X\beta + Zu + \epsilon$
- $u \sim \mathrm{N}\left(0, \sigma_u^2\right)$
- $\epsilon \sim \mathrm{AL}\left(0, \sigma I, p\right)$ (p is fixed a priori)
- $u \perp \epsilon$

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Linear Quantile Mixed Models

The package lqmm (S3-style) is a suite of commands for fitting linear quantile mixed models of the type

- $y = X\beta + Zu + \epsilon$
- continuous y
- two-level nested model (e.g., repeated measurements on same subject, households within same postcode, etc)
- $\epsilon \sim \mathrm{AL}(0, \sigma I, p)$
- **multiple**, symmetric random effects with covariance matrix Ψ $(q \times q)$
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LQMM estimation

Let the pair (ij), $j = 1, \ldots, n_i$, $i = 1, \ldots, M$, index the j-th observation for the i-th cluster/group/subject. The joint density of (y, u) based on M clusters for the linear quantile mixed model is given by

$$f(y, u|\beta, \sigma, \Psi) = f(y|\beta, \sigma, u)f(u|\Psi) = \prod_{i=1}^{M} f(y_i|\beta, \sigma, u_i)f(u_i|\Psi)$$

Numerical integration of likelihood (log-concave by Prékopa, 1973)

$$L_i(\beta, \sigma, \Psi|y) = \sigma_{n_i}(p) \int_{R^q} \exp\left\{-\frac{1}{\sigma} g_p\left(y_i - x_i'\beta(p) - z_i'u_i\right)\right\} f(u_i|\Psi)du_i,$$

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Numerical integration with

- normal random effects $u \sim \mathrm{N}(0, \Psi)$ $\rightarrow$ Gauss-Hermite quadrature
- robust random effects $u \sim \mathrm{Laplace}(0, \Psi)$ under the assumption $\Psi = \psi I$ $\rightarrow$ Gauss-Laguerre quadrature

Estimation of fixed effects β and covariance matrix Ψ

- gradient search for Laplace likelihood (subgradient optimization)
- derivative-free optimization (e.g., Nelder-Mead)

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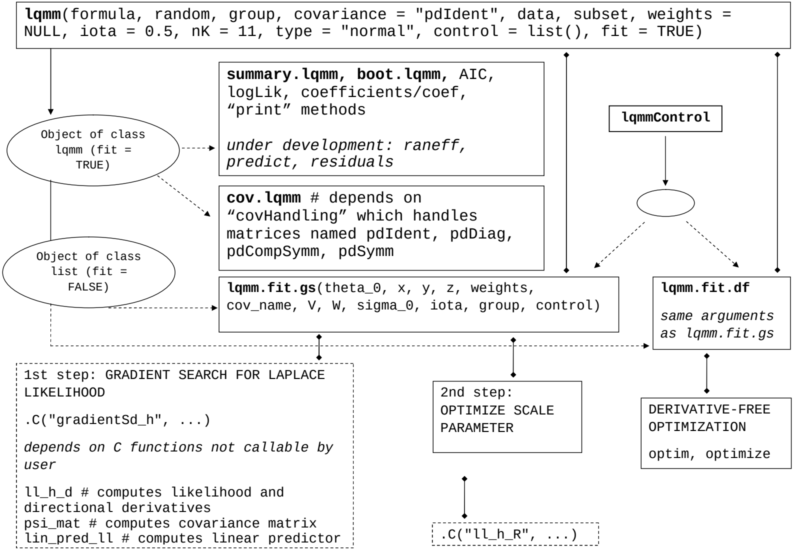
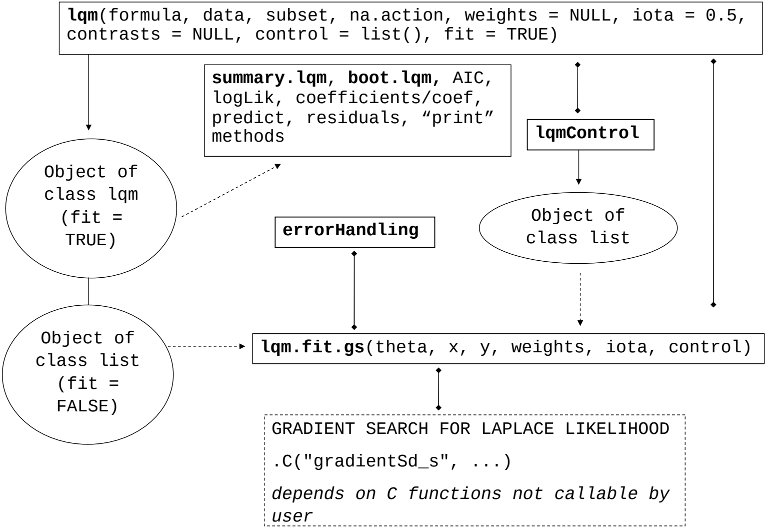
lqmm package




lqm(formula, data, subset, na.action, weights = NULL, iota = 0.5, contrasts = NULL, control = list(), fit = TRUE)
summary.lqm, boot.lqm, AIC, logLik, coefficients/coef, predict, residuals, “print” methods
lqmControl
Object of class lqm (fit = TRUE)
errorHandling
Object of class list
Object of class list (fit = FALSE)
lqm.fit.gs(theta, x, y, weights, iota, control)
GRADIENT SEARCH FOR LAPLACE LIKELIHOOD
.C("gradientSd_s", ...)
depends on C functions not callable by user

Labor pain data

- repeated measurements of self-reported amount of pain (response) on 83 women in labor
- 43 randomly assigned to a pain medication group and 40 to a placebo group
- response measured every 30 min on a 100-mm line (0 no pain - 100 extreme pain)

Aim

- to assess the effectiveness of the medication

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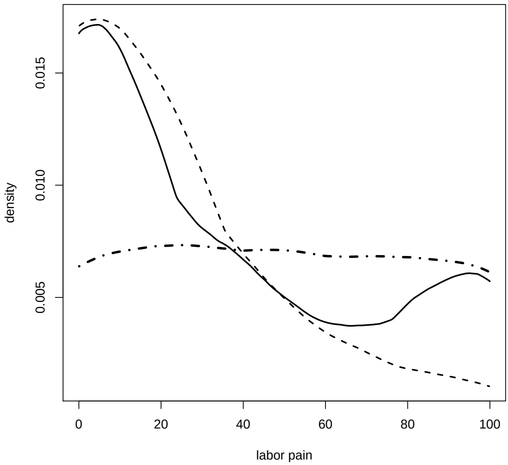
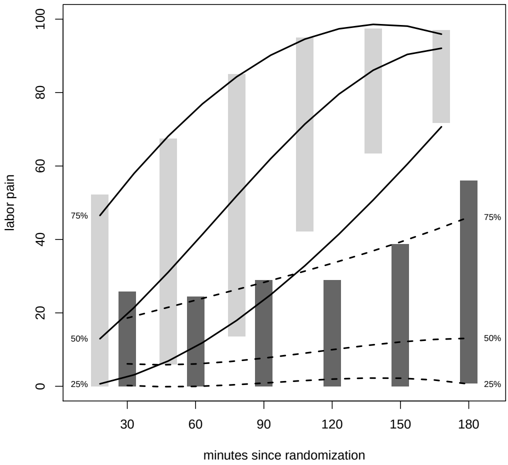


Density of the labor pain score plotted for the entire sample (solid line), for the pain medication group only (dashed line) and for the placebo group only (dot-dashed line). Source: Geraci and Bottai (2007).



Boxplot of labor pain score. The lines represent the estimate of the quartiles for the placebo group (solid) and the pain medication group (dashed). Source: Geraci and Bottai (2007).

```
# LQMM FIT

> tmp <- labor$y/100; tmp[tmp == 0] <- 0.025; tmp[tmp == 1] <- 0.975
> labor$pain_logit <- log(tmp/(1-tmp)) # outcome
> system.time(
+ fit.int <- lqmm(pain_logit ~ time_center*treatment, random = ~ 1, group =
labor$id, data = labor, iota = c(0.1,0.5,0.9))
+ )
   user  system elapsed
   0.22    0.00    0.22

# PRINT LQMM OBJECTS

> fit.int
Call: lqmm(formula = pain_logit ~ time_center * treatment, random = ~1,
    group = labor$id, data = labor, iota = c(0.1, 0.5, 0.9))

Fixed effects:
                       iota = 0.1  iota = 0.5  iota = 0.9
Intercept              -0.9828      0.3702      1.8547
time_center             0.7739      0.7569      0.8009
treatment              -2.6808     -2.5201     -1.8623
time_center:treatment  -0.7740     -0.7523     -0.5908

Number of observations: 357
Number of groups: 83
```

```
# EXTRACTING STATISTICS

> logLik(fit.int)
'log Lik.' -640.5730, -628.0026, -695.6520 (df=6)

> coef(fit.int)
                            0.1        0.5        0.9
Intercept             -0.9827571  0.3702043  1.8546808
time_center            0.7738773  0.7569301  0.8009082
treatment             -2.6808118 -2.5200997 -1.8623206
time_center:treatment -0.7739989 -0.7522610 -0.5907584

> cov.lqmm(fit.int)
$`0.1`
Intercept
 2.093377

$`0.5`
Intercept
 2.630906

$`0.9`
Intercept
  2.78936
```

```
# RANDOM SLOPE

> system.time(
+ fit.slope <- lqmm(pain_logit ~ time_center*treatment, random = ~ time_center,
group = labor$id, covariance = "pdSymm", data = labor, iota = c(0.1,0.5,0.9))
+ )
   user  system elapsed
   8.24    0.00    8.24
> cov.lqmm(fit.slope)
$`0.1`
            Intercept time_center
Intercept   1.4655346  0.31884671
time_center 0.3188467  0.07266096

$`0.5`
             Intercept time_center
Intercept   2.52996615 0.091073866
time_center 0.09107387 0.004447338

$`0.9`
             Intercept time_center
Intercept    1.7134076 -0.17001109
time_center -0.1700111  0.02155449
> AIC(fit.int)
[1] 1293.146 1268.005 1403.304
> AIC(fit.slope)
[1] 1375.718 1268.372 1401.859
```

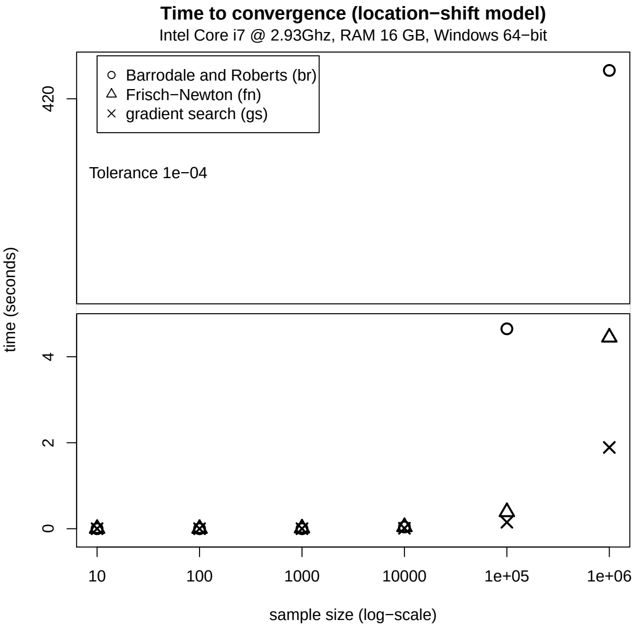
```
# SUMMARY LQMM OBJECT

> fit.int <- lqmm(pain_logit ~ time_center*treatment, random = ~ 1, group =
labor$id, data = labor, iota = 0.5, type = "robust")
> summary(fit.int)
Call: lqmm(formula = pain_logit ~ time_center * treatment, random = ~1,
    group = labor$id, data = labor, iota = 0.5, type = "robust")

Quantile 0.5
                          Value Std. Error lower bound upper bound  Pr(>|t|)
Intercept              0.011624   0.161867   -0.313661      0.3369     0.943
time_center            0.708198   0.074178    0.559132      0.8573 9.158e-13 ***
treatment             -2.989943   0.134250   -3.259729     -2.7202 < 2.2e-16 ***
time_center:treatment -0.627419   0.092040   -0.812381     -0.4425 1.275e-08 ***
scale                  0.428443   0.031258    0.365628      0.4913 < 2.2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
Null model (likelihood ratio):
[1] 183 (p = 0)
AIC:
[1] 1304 (df = 6)
Warning message:
In errorHandling(OPTIMIZATION$low_loop, "low", control$low_loop_max_iter,  :
  Lower loop did not converge in: lqmm. Try increasing max number of iterations
(500) or tolerance (0.001)
```

Performance assessment

- pilot simulation: confirmed previous bias and efficiency results but much faster than MCEM
- main simulation: extensive range of models and scenarios
- algorithm speed (preview):
    - lqmm method "gs" ranged from 0.03 (random intercept models) to 14 seconds (random intercept + slope) on average, for sample size between 250 ($M = 50 \times n = 5$) and 1000 ($M = 100 \times n = 10$)
    - linear programming (quantreg::rq) vs gradient search (lqmm::lqm)


Time to convergence (location−shift model)
Intel Core i7 @ 2.93Ghz, RAM 16 GB, Windows 64−bit
Barrodale and Roberts (br)
Frisch−Newton (fn)
gradient search (gs)
Tolerance 1e−04
time (seconds)
420
4
2
0
10
100
1000
10000
1e+05
1e+06
sample size (log−scale)

Concluding remarks

Work in progress

- estimation algorithms: "A Gradient Search Algorithm for Estimation of Laplace Regression" (with Prof. Matteo Bottai and Dr Nicola Orsini – Karolinska Institutet) and "Geometric Programming for Quantile Mixed Models"
- methodological: "Linear Quantile Mixed Models" (with M. Bottai) (available upon request `m.geraci@ich.ucl.ac.uk`)
- software: lqmm for Stata (with M. Bottai and N. Orsini)

Concluding remarks

To-do list (as usual, very long)

- submit to CRAN!
- plot functions
- adaptive quadrature
- integration on sparse grids (Smolyak, *Soviet Mathematics Doklady*, 1963, Heiss and Winschel, *J Econometrics*, 2008)
- missing data
- smoothing
- interface with other packages
- S4-style
- ...

Acknowledgements

Function	Package	Version	Author(s)
is./make.positive.definite	corpcor	1.5.7	J. Schaefer, R. Opgen-Rhein, K. Strimmer
permutations	gtools	2.6.2	G.R. Warnes
gauss.quad, gauss.quad.prob	statmod	1.4.8	G. Smyth

References

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