Quantile Regression Computation: From Outside, Inside and the Proximal

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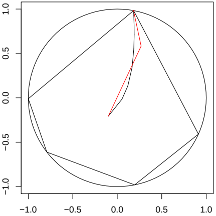
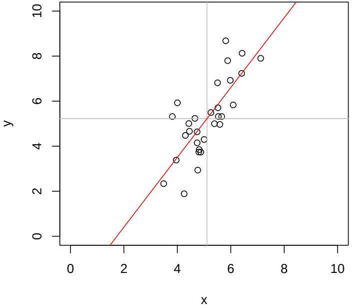


The Origin of Regression – Regression Through the Origin

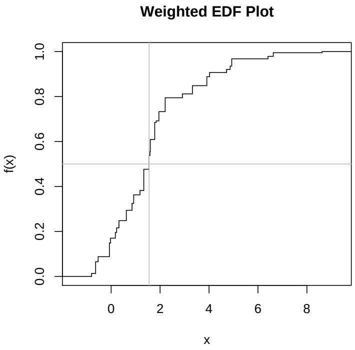
Find the line with mean residual zero that minimizes the sum of absolute residuals.



Problem: $\min_{\alpha,\beta} \sum_{i=1}^{n} |y_i - \alpha - x_i\beta| \quad \text{s.t.} \quad \bar{y} = \alpha + \bar{x}\beta.$

Boscovich/Laplace *Methode de Situation*

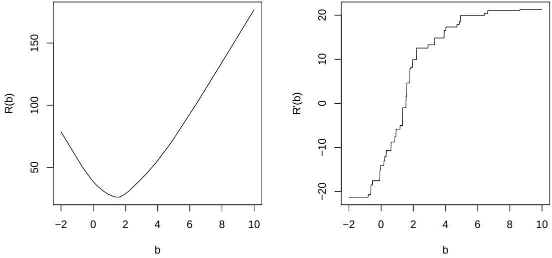
Algorithm: Order the n candidate slopes: $b_i = (y_i - \bar{y})/(x_i - \bar{x})$ denoting them by $b_{(i)}$ with associated weights $w_{(i)}$ where $w_i = |x_i - \bar{x}|$. Find the weighted median of these slopes.



Methode de Situation via Optimization

$$R(b) = \sum |\tilde{y}_i - \tilde{x}_i b| = \sum |\tilde{y}_i/\tilde{x}_i - b| \cdot |\tilde{x}_i|.$$

$$R'(b) = -\sum \mathrm{sgn}(\tilde{y}_i/\tilde{x}_i - b) \cdot |\tilde{x}_i|.$$



Quantile Regression through the Origin in R

This can be easily generalized to compute quantile regression estimates:

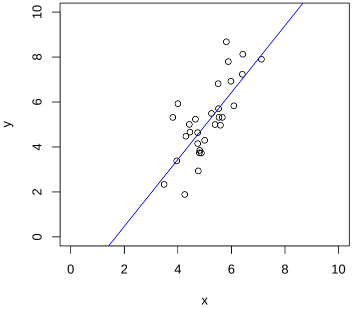
```
wquantile <- function(x, y, tau = 0.5) {
        o <- order(y/x)
        b <- (y/x)[o]
        w <- abs(x[o])
        k <- sum(cumsum(w) < ((tau - 0.5) * sum(x) + 0.5 * sum(w)))
        list(coef = b[k + 1], k = o[k+1])
}
```

Warning: When $\bar{x} = 0$ then τ is irrelevant. Why?

Edgeworth's (1888) Plural Median

What if we want to estimate both α and β by median regression?

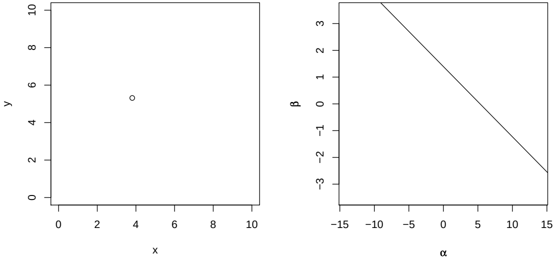
Problem: $\min_{\alpha,\beta} \sum_{i=1}^{n} |y_i - \alpha - x_i\beta|$



Edgeworth's (1888) Dual Plot: Anticipating Simplex

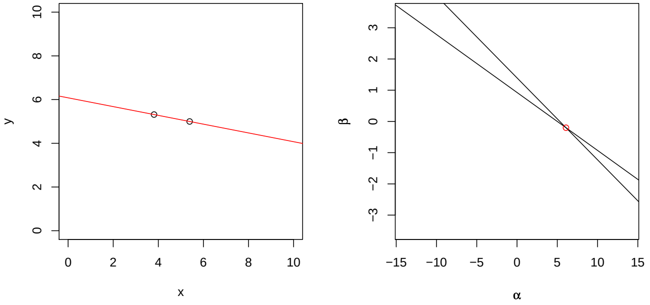
Points in sample space map to lines in parameter space.

$$(x_i, y_i) \mapsto \{(\alpha, \beta) : \alpha = y_i - x_i\beta\}$$



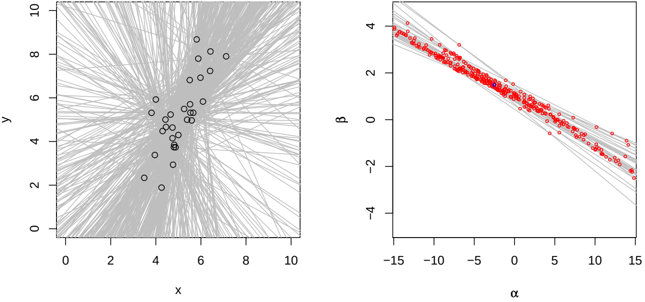
Edgeworth's (1888) Dual Plot: Anticipating Simplex

Lines through pairs of points in sample space map to points in parameter space.



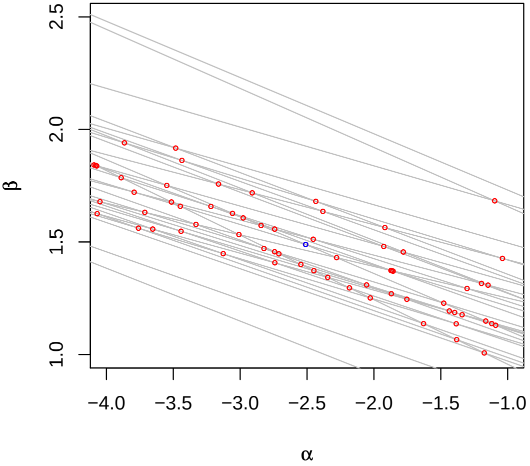
Edgeworth's (1888) Dual Plot: Anticipating Simplex

All pairs of observations produce $\binom{n}{2}$ points in dual plot.



Edgeworth's (1888) Dual Plot: Anticipating Simplex

Follow path of steepest descent through points in the dual plot.



Barrodale-Roberts Implementation of Edgeworth

```
rqx<- function(x, y, tau = 0.5, max.it = 50) { # Barrodale and Roberts -- lite
        p <- ncol(x); n <- nrow(x)
        h <- sample(1:n, size = p) #Phase I -- find a random (!) initial basis
        it <- 0
        repeat {
                it <- it + 1
                Xhinv <- solve(x[h,  ])
                bh <- Xhinv %*% y[h]
                rh <- y - x %*% bh
        #find direction of steepest descent along one of the edges
                g <-  - t(Xhinv) %*% t(x[ - h,  ]) %*% c(tau - (rh[ - h] < 0))
                g <- c(g + (1 - tau),  - g + tau)
                ming <- min(g)
                if(ming >= 0 || it > max.it) break
                h.out <- seq(along = g)[g == ming]
                sigma <- ifelse(h.out <= p, 1, -1)
                if(sigma < 0) h.out <- h.out - p
                d <- sigma * Xhinv[, h.out]
        #find step length by one-dimensional wquantile minimization
                xh <- x %*% d
                step <- wquantile(xh, rh, tau)
                h.in <- step$k
                h <- c(h[ - h.out], h.in)
        }
        if(it > max.it) warning("non-optimal solution: max.it exceeded")
        return(bh)
}
```

Linear Programming Duality

Primal: $\min_x \{c^\top x | Ax - b \in T, \; x \in S\}$
Dual: $\max_y \{b^\top y | c - A^\top y \in S^*, \; y \in T^*\}$

The sets S and T are closed convex cones, with dual cones S^* and T^*. A cone K^* is dual to K if:

$$K^* = \{y \in \mathbb{R}^n | x^\top y \geqslant 0 \text{ if } x \in K\}$$

Note that for any feasible point (x, y)

$$b^\top y \leqslant y^\top Ax \leqslant c^\top x$$

while optimality implies that

$$b^\top y = c^\top x.$$

Quantile Regression Primal and Dual

Splitting the QR "residual" into positive and negative parts, yields the primal linear program,

$$\min_{(b,u,v)} \{\tau 1^\top u + (1-\tau) 1^\top v \mid Xb + u - v - y \in \{0\}, \quad (b,u,v) \in \mathbb{R}^p \times \mathbb{R}_+^{2n}\}.$$

with dual program:

$$\max_d \{y^\top d \mid X^\top d \in \{0\}, \quad \tau 1 - d \in \mathbb{R}_+^n, \quad (1-\tau)1 + d \in \mathbb{R}_+^n\},$$

$$\max_d \{y^\top d \mid X^\top d = 0, \; d \in [\tau - 1, \tau]^n\},$$

$$\max_a \{y^\top a \mid X^\top a = (1-\tau) X^\top 1, \quad a \in [0,1]^n\}$$

Quantile Regression Dual

The dual problem for quantile regression may be formulated as:

$$\max_{a}\{y^\top a | X^\top a = (1-\tau)X^\top 1,\ a \in [0,1]^n\}$$

What do these $\hat{a}_i(\tau)$'s mean statistically?
They are regression rank scores (Gutenbrunner and Jurečková (1992)):

$$\hat{a}_i(\tau) \in \begin{cases} \{1\} & \text{if} \quad y_i > x_i^\top \hat{\beta}(\tau) \\ (0,1) & \text{if} \quad y_i = x_i^\top \hat{\beta}(\tau) \\ \{0\} & \text{if} \quad y_i < x_i^\top \hat{\beta}(\tau) \end{cases}$$

The integral $\int \hat{a}_i(\tau) d\tau$ is something like the rank of the ith observation. It answers the question: On what quantile does the ith observation lie?

Linear Programming: The Inside Story

The Simplex Method (Edgeworth/Dantzig/Kantorovich) moves from vertex to vertex on the outside of the constraint set until it finds an optimum.

Interior point methods (Frisch/Karmarker/et al) take Newton type steps toward the optimal vertex from inside the constraint set.

A toy problem: Given a polygon inscribed in a circle, find the point on the polygon that maximizes the sum of its coordinates:

$$\max\{e^\top u | A^\top x = u,\ e^\top x = 1,\ x \geqslant 0\}$$

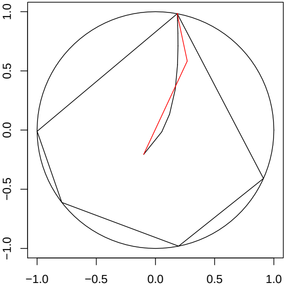
were e is vector of ones, and A has rows representing the n vertices. Eliminating u, setting $c = Ae$, we can reformulate the problem as:

$$\max\{c^\top x | e^\top x = 1, \quad x \geqslant 0\},$$

Toy Story: From the Inside

Simplex goes around the outside of the polygon; interior point methods tunnel from the inside, solving a sequence of problems of the form:

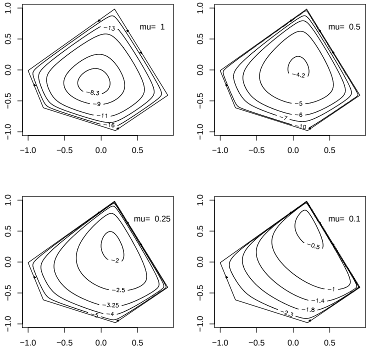
$$\max\{c^\top x + \mu \sum_{i=1}^{n} \log x_i \mid e^\top x = 1\}$$



Toy Story: From the Inside

By letting $\mu \to 0$ we get a sequence of smooth problems whose solutions approach the solution of the LP:

$$\max\{c^\top x + \mu \sum_{i=1}^{n} \log x_i | e^\top x = 1\}$$



Implementation: Meketon's Affine Scaling Algorithm

```
meketon <- function (x, y, eps = 1e-04, beta = 0.97) {
   f <- lm.fit(x,y)
   n <- length(y)
   w <- rep(0, n)
   d <- rep(1, n)
   its <- 0
   while(sum(abs(f$resid)) - crossprod(y, w) > eps) {
       its <- its + 1
       s <- f$resid * d
       alpha <- max(pmax(s/(1 - w), -s/(1 + w)))
       w <- w + (beta/alpha) * s
       d <- pmin(1 - w, 1 + w)^2
       f <- lm.wfit(x,y,d)
       }
   list(coef = f$coef, iterations = its)
   }
```

Mehrotra Primal-Dual Predictor-Corrector Algorithm

The algorithms implemented in `quantreg` for R are based on Mehrotra's Predictor-Corrector approach. Although somewhat more complicated than Meketon this has several advantages:

- Better numerical stability and efficiency due to better central path following,
- Easily generalized to incorporate linear inequality constraints.
- Easily generalized to exploit sparsity of the design matrix.

These features are all incorporated into various versions of the algorithm in `quantreg`, and coded in Fortran.

Back to Basics

Which is easier to compute: the median or the mean?

```
> x <- rnorm(100000000) # n = 10^8
> system.time(mean(x))
   user  system elapsed
 10.277   0.035  10.320
> system.time(kuantile(x,.5))
   user  system elapsed
  5.372   3.342   8.756
```

`kuantile` is a `quantreg` implementation of the Floyd-Rivest (1975) algorithm. For the median it requires $1.5n + O((n \log n)^{1/2})$ comparisons.

Portnoy and Koenker (1997) propose a similar strategy for "preprocessing" quantile regression problems to improve efficiency for large problems.

Globbing for Median Regression

Rather than solving $\min \sum |y_i - x_i b|$ consider:

1. Preliminary estimation using random $m = n^{2/3}$ subset,
2. Construct confidence band $x_i^\top \hat{\beta} \pm \kappa \|\hat{V}^{1/2} x_i\|$.
3. Find $J_L = \{i | y_i \text{ below band }\}$, and $J_H = \{i | y_i \text{ above band }\}$,
4. Glob observations together to form pseudo observations:

$$(x_L, y_L) = (\sum_{i \in J_L} x_i, -\infty), \quad (x_H, y_H) = (\sum_{i \in J_H} x_i, +\infty)$$

5. Solve the problem (with m+2 observations)

$$\min \sum |y_i - x_i b| + |y_L - x_L b| + |y_H - x_H b|$$

6. Verify that globbed observations have the correct predicted signs.

Proximal Algorithms for Large p Problems

Given a closed, proper convex function $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ the proximal operator, $P_f : \mathbb{R}^n \to \mathbb{R}^n$ of f is defined as,

$$P_f(v) = \text{argmin}_x \{f(x) + \tfrac{1}{2}\|x - v\|_2^2\}.$$

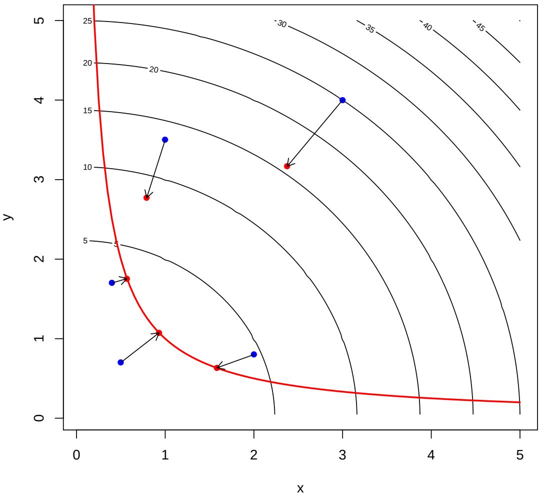
View v as an initial point and $P_f(v)$ as a half-hearted attempt to minimize f, while constrained not to venture too far away from v.
The corresponding Moreau envelope of f is

$$M_f(v) = \inf_x \{f(x) + \tfrac{1}{2}\|x - v\|_2^2\}.$$

thus evaluating M_f at $v = x$ we have,

$$M_f(x) = f(P_f(x)) + \tfrac{1}{2}\|x - P_f(x)\|_2^2\}.$$

A Toy Example:



Proximal Operators as (Regularized) Gradient Steps

Rescaling f by $\lambda \in \mathbb{R}$,

$$M_{\lambda f}(x) = f(P_{\lambda f}(x)) + \frac{1}{2\lambda}\|x - P_{\lambda f}(x)\|_2^2\}.$$

so

$$\nabla M_{\lambda f}(x) = \lambda^{-1}(x - P_{\lambda f}(x)),$$

or

$$P_{\lambda f}(x) = x - \lambda \nabla M_{\lambda f}(x).$$

So $P_{\lambda f}$ may be interpreted as a gradient step of length λ for $M_{\lambda f}$. Unlike f, which may have a nasty subgradient, M_f has a nice gradient:

$$M_f = (f^* + \tfrac{1}{2}\|\cdot\|_2^2)^*$$

where $f^*(y) = \sup_x\{y^\top x - f(x)\}$ is the convex conjugate of f.

Proximal Operators and Fixed Point Iteration

The gradient step interpretation of P_f suggests the fixed point iteration:

$$x^{k+1} = P_{\lambda f}(x^k).$$

While this may not be a contraction, it is "firmly non-expansive" and therefore convergent.

In additively separable problems of the form

$$\min_x \{f(x) + g(x)\},$$

with f and g convex, this may be extended to the ADMM algorithm:

$$\begin{aligned} x^{k+1} &= P_{\lambda f}(z^k - u^k) \\ z^{k+1} &= P_{\lambda g}(x^k - u^k) \\ u^{k+1} &= (u^k + x^k - z^k) \end{aligned}$$

Alternating Direction Method of Multipliers, Parikh and Boyd (2013).

The Proximal Operator Graph Solver

A further extension that encompasses many currently relevant statistical problems is:

$$\min_{(x,y)} \{f(y) + g(x) \mid y = Ax\},$$

where (x, y) is constrained to the graph $\mathcal{G} = \{(x, y) \in \mathbb{R}^{n+m} \mid y = Ax\}$. The modified ADMM algorithm becomes:

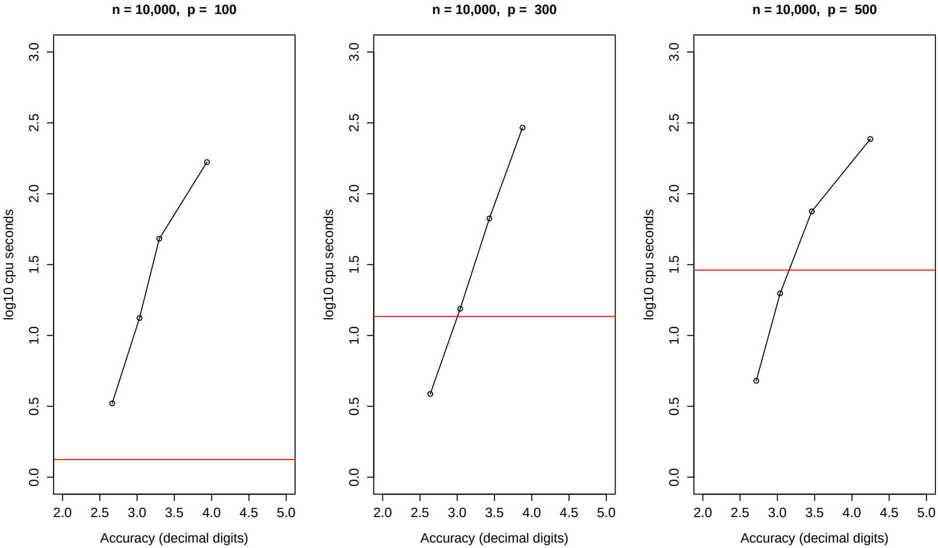
$$\begin{aligned}
(x^{k+1/2}, y^{k+1/2}) &= (P_{\lambda g}(x^k - \tilde{x}^k), P_{\lambda f}(y^k - \tilde{y}^k)) \\
(x^{k+1}, y^{k+1}) &= \Pi_A(x^{k+1/2} - \tilde{x}^k, y^{k+1/2} - \tilde{y}^k) \\
(\tilde{x}^{k+1}, \tilde{y}^{k+1}) &= (\tilde{x}^k + x^{k+1/2} - x^{k+1}, \tilde{y}^{k+1/2} + y^{k+1/2} - y^{k+1})
\end{aligned}$$

where Π_A denotes the (Euclidean) projection into graph $\mathcal{G}$. This has been elegantly implemented by Fougner and Boyd (2015) and made available by Fougner in the R package `POGS`.

When Is POGS Most Attractive?

- f and g must:
  - Be closed, proper convex
  - Be additively (block) separable
  - Have easily computable proximal operators
- A should be:
  - Not too thin
  - Not too sparse
- Other Problem Aspects
  - Available parallelizable hardware, cluster, GPUs, etc.
  - Not too stringent accuracy requirement

POGS Performance – Large p Quantile Regression



Global Quantile Regression?

Usually quantile regression is local, so solutions,

$$\hat{\beta}(\tau) = \text{argmin}_{b \in \mathbb{R}^p} \sum_{i=1}^{n} \rho_\tau(y_i - x_i^\top b)$$

are sensitive only to $\{y_i\}$ near $Q(\tau | x_i)$, the τth conditional quantile function of $Y_i | X = x_i$.
But recently there has been more interest in jointly estimating several $\beta(\tau_i)$:

$$\{\hat{\beta}(\tau) \mid \tau \in \mathcal{T}\} = \text{argmin} \sum_{\tau \in \mathcal{T}} \sum_{i=1}^{n} w_\tau \rho_\tau(y_i - x_i^\top b_\tau)$$

This is sometimes called "composite quantile regression" as in Zou and Yuan (2008). Constraints need to be imposed on the $\beta(\tau)$ otherwise the problem separates.

Example 1: Choquet Portfolios

Bassett, Koenker and Kordas (2004) proposed estimating portfolio weights $\pi \in \mathbb{R}^p$ by solving:

$$\min_{\pi \in \mathbb{R}^p,\, \xi \in \mathbb{R}^m} \{\sum_{k=1}^{m} \sum_{i=1}^{n} w_{\tau_k} \rho_{\tau_k}(x_i^\top \pi - \xi_{\tau_k}) \mid \bar{x}^\top \pi = \mu_0\}$$

where $x_i \in \mathbb{R}^p : i = 1, \cdots, n$ denote historical returns, and μ_0 is a required mean rate of return. This approach replaces the traditional Markowitz use of variance as a measure of risk with a lower-tail expectation measure.

- The number of assets, p, is potentially quite large in these problems.
- Linear inequality constraints can easily be added to the problem to prohibit short sales, etc.
- Interior point methods are fine, but POGS may have advantages in larger problems.

Example 2: Smoothing the Quantile Regression Process

Let $\tau_1, \cdots, \tau_m \subset (0,1)$ denote an equally spaced grid and consider

$$\min_{\beta(\tau) \in \mathbb{R}^{mp}} \{ \sum_{k=1}^{m} \sum_{i=1}^{n} w_{\tau_k} \rho_{\tau_k}(y_i - x_i^\top \beta(\tau_k)) \mid \sum_k (\Delta^2 \beta(\tau_k))^2 \leqslant M \}.$$

Imposes a conventional L_2 roughness penalty on the quantile regression coefficients.

- Implemented recently in POGS by Shenoy, Gorinevsky and Boyd (2015) for forecasting load in a large power grid setting,
- Smoothing, or borrowing strength from adjacent quantiles, can be expected to improve performance,
- Many gory details of implementation remain to be studied.

Conclusions and Lingering Doubts

- Optimization can replace sorting
- Simplex is just steepest descent at successive vertices
- Log barriers revive Newton method for linear inequality constraints
- Proximal algorithms revive gradient methods
- Statistical vs computational accuracy?
- Quantile models as global likelihoods?
- Multivariate, IV, extensions?