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Inequality Constrained Quantile Regression

Roger Koenker
University of Illinois at Urbana-Champaign, USA
Pin Ng
University of Northern Arizona, Flagstaff, USA

Abstract

An algorithm for computing parametric linear quantile regression estimates subject to linear inequality constraints is described. The algorithm is a variant of the interior point algorithm described in Koenker and Portnoy (1997) for unconstrained quantile regression and is consequently quite efficient even for large problems, particularly when the inherent sparsity of the resulting linear algebra is exploited. Applications to qualitatively constrained nonparametric regression are described in the penultimate sections. Implementations of the algorithm are available in MATLAB and R.

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1 Introduction

An early application of median regression in economics can be found in Arrow and Hoffenberg (1959). Their objective was to estimate input-output coefficients in a regression setting, but it was obviously desirable to impose the restriction that the coefficients were all positive. This was a relatively simple task given linear programming technology of the day provided that the conventional squared error fitting criterion was replaced by an absolute error criterion. Linear inequality constraints fit comfortably within the algorithmic framework of linear programming, whereas quadratic programming was still at a relatively early stage of development.

Until the mid 1980's the method of choice for solving linear programs of the sort described in the next section was the simplex method. However,

the work of Karmarker (1984) brought to fruition the idea of interior point methods, an idea that had germinated in Norway in the 1950's and been nurtured in the U.S. and U.S.S.R. during the 1960's and 1970's. Instead of traveling along the outer edges of the constraint set looking at each vertex for the direction of steepest descent, we might burrow from the center toward the boundary. This paradigm shift in thinking about linear programming has had a profound impact throughout the optimization literature. The last two decades have seen a rapid development in interior-point methods: initially for large scale linear programming applications where it produced astonishing efficiency gains, and more recently in much more general convex programming settings.

Adapting modern interior point methods to quantile regression, Koenker and Portnoy (1997) showed that dramatic improvements in computational efficiency were possible relative to earlier simplex-based methods. These improvements made quantile regression fitting comparable in speed to least squares fitting for problems throughout the full range of dimensions found in current statistical practice. Recent developments in sparse linear algebra have led to further improvements that have greatly extended the domain of applicability of these algorithms, particularly for function estimation.

The main contribution of this paper is to provide a detailed description of an interior point algorithm for solving linear quantile regression problems subject to linear inequality constraints. It may appear that this entails a relatively minor modification of existing methods designed for a relatively narrow class of new problems. However, taking Beran's (2003), definition of statistics: "the analysis of algorithms for data analysis," it seems crucial to document precisely what algorithms do. It is also crucial, we believe, for statisticians to take a more active role in the development of algorithms that widen the range of applicability of basic tools. We will argue that inequality constraints have an important role to play across a wide range of applications including constrained smoothing problems.

We will begin by introducing the basic quantile regression computational problem and briefly describe some duality theory and its relevance. We will then describe a modification of the Frisch-Newton algorithm introduced in Koenker and Portnoy (1997) that accommodates linear inequality constraints in Section 3. We will briefly describe some applications to nonparametric quantile regression in Section 4 and an empirical application to the Engel Curve in Section 5. Some details of the implementation of the algorithm and discussions of some open problems associated with inequality constrained quantile regression are provided in Sections 6 and 7.

2 Quantile Regression as a Linear Program

The quantile regression problem

$$\min_{b\in\mathbb{R}^p}\sum_{i=1}^{n}\rho_\tau(y_i - x_i^\top b) \tag{2.1}$$

where $\rho_\tau(u) = u(\tau - I(u < 0))$ is easily seen to be a linear program. This observation for median regression, i.e., $\tau = 1/2$, can be traced to Charnes, Cooper, and Ferguson (1955) and Wagner (1959). Let e denote an n-vector of ones and rewrite (2.1) as

$$\min_{(u,v,b)}\left\{\tau e^\top u + (1-\tau)e^\top v | Xb + u - v = y, \quad \left(u^\top, v^\top, b^\top\right) \in \mathbb{R}_+^{2n}\times\mathbb{R}^p\right\} \tag{2.2}$$

In this formulation we seek the minimum of a linear function of the $2n + p$ variables $(u^\top, v^\top, b^\top)$, subject to n linear equality constraints and $2n$ linear inequality constraints. It turns out to be convenient to reformulate this primal version of the problem in the following way

$$\max_d\{y^\top d | X^\top d = (1-\tau)X^\top e, \quad d\in[0,1]^n\} \tag{2.3}$$

Here, $[0,1]^n$ denotes the n-field Cartesian product of the unit interval, and d may be interpreted as a vector of Lagrange multipliers associated with the linear equality constraints of the primal problem

To understand the transition from the primal problem (2.2) to the dual problem (2.3) it is helpful to recall a somewhat more general version of the duality theory of linear programming. Using the conventional notation of linear programming [1] and following Berman (1973), consider the primal problem

$$\min_x\{c^\top x | Ax - b \in T, \quad x \in S\} \tag{2.4}$$

where the sets $T = \{y \in \mathbb{R}^n\}$ and $S = \{y \in \mathbb{R}^{2n}\times\mathbb{R}^p\}$ can be arbitrary closed convex cones. This canonical problem has dual

$$\max_y\{b^\top y | c - A^\top y \in S^*, \quad y \in T^*\} \tag{2.5}$$

[1] An inherent difficulty in describing numerical algorithms for statistical procedures is that we are faced with two well established, but mutually incompatible notational schemes; one arising in statistics, the other in numerical analysis. In Section 2 we will introduce the quantile regression problem in its familiar statistical garb and then make the connection to linear programming. For the serious business of describing the algorithm in detail in Section 3 we will revert to the well established notational conventions of numerical analysis.

where $S^* = \{y \in \mathbb{R}^{2n} \times \mathbb{R}^p | x^\top y \geq 0 \text{ if } x \in S\}$ is the dual of S and $T^* = \{y \in \mathbb{R}^n\}$. For our purposes it suffices to consider the following special case: $T = \{O_n\}$, $S = \{\mathbb{R}^{2n}_+ \times \mathbb{R}^p\}$, $S^* = \{\mathbb{R}^{2n}_+ \times O_p\}$, and $T^* = \{\mathbb{R}^n\}$ where O_n and O_p are n and p-vectors of zeros.

In our primal problem (2.2), $\left(\tau e^\top, (1-\tau)\, e^\top, O_p^\top\right)^\top$ and $\left(u^\top, v^\top, b^\top\right)^\top$ correspond to, respectively, c and x in (2.4), and the relation $Ax - b \in T$ in (2.4) becomes

$$[I \vdots -I \vdots X] \begin{bmatrix} u \\ v \\ b \end{bmatrix} - y \in \{O_n\} \tag{2.6}$$

while $c - A^\top y \in S^*$ becomes

$$\begin{pmatrix} \tau e \\ (1-\tau)e \\ O_p \end{pmatrix} - \begin{bmatrix} I \\ -I \\ X^\top \end{bmatrix} \lambda \in \{\mathbb{R}^{2n}_+ \times O_p\}$$

where λ denotes the n-vector of dual variables (Lagrange multipliers) associated with the equality constraints of the primal problem in (1). The requirement $y \in T^*$ in (2.5) may be translated as $\lambda \in \mathbb{R}^n$ so the dual problem in (2.5) can be expressed more concisely using the quantile regression notations as,

$$\max\{y^\top \lambda | X^\top \lambda = 0, \quad \lambda \in [\tau - 1, \tau]^n\}.$$

But this is equivalent to (2.3) after the transformation of variables, $d = 1 - \tau + \lambda$.

Now consider augmenting the constraints of the primal problem in (2.2) with the new constraints, $Rb \geq r$. This is easily accommodated into the $Ax - b \in T$ constraint, (2.6) becomes,

$$\begin{bmatrix} I & -I & X \\ 0 & 0 & R \end{bmatrix} \begin{bmatrix} u \\ v \\ b \end{bmatrix} - \begin{bmatrix} y \\ r \end{bmatrix} \in \{O_n\} \times \mathbb{R}^m_+ \tag{2.7}$$

where $m \leq p$ denotes the row dimension of R. Now we have the dual variables $\lambda = (\lambda_1^\top \ \lambda_2^\top)^\top$ where λ_1 is associated with equality constraints and λ_2 is associated with the inequality constraints. The dual constraint $c - A^\top y \in S^*$ becomes,

$$\begin{pmatrix} \tau e \\ (1-\tau)e \\ O_p \end{pmatrix} - \begin{bmatrix} I & 0 \\ -I & 0 \\ X^\top & R^\top \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} \in \{\mathbb{R}^{2n}_+ \times O_p\} \tag{2.8}$$

so the dual problem is

$$\max_{\lambda} \left\{ y^\top \lambda_1 + r^\top \lambda_2 | X^\top \lambda_1 + R^\top \lambda_2 = 0, \quad \lambda_1 \in [\tau - 1, \tau]^n, \lambda_2 \geq 0 \right\}.$$

Again, transforming variables $d_1 = 1 - \tau + \lambda_1, d_2 = \lambda_2$ we have

$$\max_{d} \left\{ y^\top d_1 + r^\top d_2 | X^\top d_1 + R^\top d_2 = (1 - \tau) X^\top e, \quad d_1 \in [0, 1]^n, d_2 \geq 0 \right\}. \tag{2.9}$$

It is this form of the inequality constrained problem for which we will describe a solution algorithm.

The advantage of the dual formulation is that it greatly reduces the effective dimensionality of the problem. This is particularly important in large problems where the primal formulation can be extremely unwieldy. The interior point algorithm described in the next section proceeds by solving at each iteration a weighted least squares problem whose parametric dimension is the column dimension of X. Fortunately, when this dimension is large, as it is in many smoothing problems, exploitation of the sparsity of the X matrix still enables the algorithm to perform efficiently.

3 A Frisch-Newton Algorithm

A pioneering early advocate of log barrier methods was Ragnar Frisch. In a series of Oslo technical reports, Frisch discovered interior point methods 30 years *avant la lettre*. Frisch (1956) described it in the following vivid terms for a talk in Paris,

> My method is altogether different than simplex. In this method we work systematically from the interior of the admissible region and employ a logarithmic potential as a guide – a sort of radar – in order to avoid crossing the boundary.

Despite considerable numerical experience with these methods, Frisch was, unfortunately, unable to establish convergence and the resolution of many practical aspects of the implementation of the methods had to wait for the intensive research effort that occurred only in the late 1980's. It is worth noting that basic Frisch idea of a logarithmic barrier, or penalty, function as a way to handle inequality constraints in convex programming was nurtured through the 1960's by Fiacco and McCormick (1968).

The algorithm that we will describe in the next section is a variant of the log-barrier algorithm described in Koenker and Portnoy (1997) for unconstrained quantile regression problems. In particular, the complications

presented by the linear algebra introduced by the inequality constraints are worked out and presented in detail.

3.1. The log-barrier formulation. An influential observation by Gill, Murray, Saunders, Tomlin, and Wright (1986) connected Karmarker's interior point methods to earlier log-barrier methods elaborated by Fiacco and McCormick (1968) and others. Following prior usage, we will refer to primal-dual interior point method as a Frisch-Newton method since the log-barrier formulation of Frisch, by replacing the sharply demarcated boundary of the inequality constraints with an objective function that smoothly tends to infinity as one approaches the boundary, enables us to take Newton steps toward a boundary solution. The strategy used to adjust the barrier parameter is based on the well-established Mehrotra (1992) predictor-corrector approach.

We adhere in this section to the notational conventions of Lustig, Marsden and Shanno (1994). We will consider the following pair of primal and dual problems:

$$\min_{(x_1,x_2)} \left\{ c_1^\top x_1 + c_2^\top x_2 | A_1 x_1 + A_2 x_2 = b,\ 0 \le x_1 \le u,\ 0 \le x_2 \right\}$$
$$\max_{(y,w)} \left\{ b^\top y - u^\top w | A_1^\top y + z_1 - w = c_1,\ A_2^\top y + z_2 = c_2,\ (z_1, z_2, w) \ge 0 \right\}.$$

Note that we have reversed the roles of primal and dual so our new primal problem corresponds to the dual problem we derived in the previous section and vice-versa. Note also that we have generalized the problem slightly to allow u to be an arbitrary vector of (positive) upper bounds.

The classical (Karush-Kuhn-Tucker) KKT conditions for an optimum are:

$$\begin{aligned} A_1^\top y + z_1 - w &= c_1 \\ A_2^\top y + z_2 &= c_2 \\ Ax &= b \\ x_1 + s &= u \\ XZe &= 0 \\ SWe &= 0 \end{aligned}$$

Here we employ the convention that upper case letters corresponding to vectors in lower case are diagonal matrices with the elements of the vector along the diagonal, so for example $X = \mathrm{diag}(x)$. An easy way to see the

KKT conditions is to write the primal problem above as the Lagrangian expression,

$$L = c^\top x - y^\top (Ax - b) - w^\top (u - x_1 - s) - \mu(\sum \log x_{1i} + \sum \log x_{2i} + \sum \log s_i).$$

This log-barrier formulation replaces the inequality constraints with a barrier function that penalizes feasible solutions as they approach the boundary of the constraint set. The parameter μ controls the severity of this penalization, and the strategy will be to gradually reduce μ. As μ tends to zero we approach the solution on the boundary of the constraint set. Differentiating with respect to x_1 and x_2 yields

$$\begin{aligned} A_1^\top y - w + \mu X_1^{-1} e &= c_1 \\ A_2^\top y + \mu X_2^{-1} e &= c_2. \end{aligned}$$

Writing $z = \mu X^{-1} e$, we have the first two equations of the KKT system. Differentiating with respect to y and w yields the next two. For fixed μ we have, from the definitions of z,

$$XZe = \mu e$$

and, from differentiating with respect to s, we obtain,

$$w = \mu S^{-1} e.$$

Substituting $\mu = 0$ yields the last two KKT conditions. The motivation for setting $\mu = 0$ stems from the question: 'What is the best value for μ at each iteration toward the optimal solution on the boundary of the constraint set?' The affine-scaling step described in Section 3.2 suggests computing the primal-dual step with $\mu = 0$. When the step thus obtained is feasible, we take it and continue the iteration. If it takes us outside the feasible region determined by the inequality constraints, i.e., the barrier function dominates the Lagrangian, we compute a Mehrotra predictor-corrector step described in Section 3.3 to modify the affine-scaling step to bring us back into the interior of the feasible region. The iterations stop when the duality gap is smaller than a specified tolerance, which is the requirement for optimality implied by the complementary slackness.

3.2. The affine scaling step. We are looking for a solution to the KKT equations, say $g(\xi) = 0$. Suppose we have an initial point $\xi_0 = (y_0, z_0, x_0, s_0, w_0)$, for which x_0 is feasible for our primal problem. Denote $g(\xi_0) = g_0$. We differentiate to get

$$g(\xi) \approx \nabla_\xi g(\xi_0) d\xi + g_0$$

and we choose a direction by setting this equal zero, i.e.,

$$d\xi = -[\nabla_\xi g(\xi_0)]^{-1} g_0.$$

This is just Newton's Method. The linear system we obtain looks like

$$\begin{bmatrix} A_1^\top & I & 0 & 0 & 0 & 0 & -I \\ A_2^\top & 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A_1 & A_2 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & I & 0 \\ 0 & X_1 & 0 & Z_1 & 0 & 0 & 0 \\ 0 & 0 & X_2 & 0 & Z_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W & S \end{bmatrix} \begin{bmatrix} dy \\ dz_1 \\ dz_2 \\ dx_1 \\ dx_2 \\ ds \\ dw \end{bmatrix}$$

$$= - \begin{bmatrix} A_1^\top y + z_1 - w - c_1 \\ A_2^\top y + z_2 - c_2 \\ Ax - b \\ x_1 + s - u \\ X_1 Z_1 e \\ X_2 Z_2 e \\ SWe \end{bmatrix} \equiv \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \\ r_7 \end{bmatrix}$$

To solve, substitute out dw and dz to get

$$\begin{aligned} Wds + Sdw &= -SWe \\ dw &= -S^{-1}(SWe + Wds) = -We - S^{-1}Wds \\ Xdz + Zdx &= -XZe \\ dz &= -X^{-1}(XZe + Zdx) = -Ze - X^{-1}Zdx. \end{aligned}$$

This reduces the system to,

$$\begin{aligned} A_1^\top dy - X_1^{-1}Z_1 dx_1 + S^{-1}Wds &= r_1 - We + Z_1 e \\ A_2^\top dy - X_2^{-1}Z_2 dx_2 &= r_2 + Z_2 e \\ Adx &= r_3 \\ dx_1 + ds &= r_4, \end{aligned}$$

which we can assemble as,

$$\begin{bmatrix} A_1^\top & -X_1^{-1}Z_1 & 0 & S^{-1}W \\ A_2^\top & 0 & -X_2^{-1}Z_2 & 0 \\ 0 & A_1 & A_2 & 0 \\ 0 & I & 0 & I \end{bmatrix} \begin{bmatrix} dy \\ dx_1 \\ dx_2 \\ ds \end{bmatrix}$$

$$= \begin{bmatrix} c_1 + w - z_1 - A_1^\top y - w + z_1 \\ c_2 - z_2 - A_2^\top y + z_2 \\ b - Ax \\ 0 \end{bmatrix}.$$

Note that we have assumed that we start with $u = x_1 + s$. Now, substitute out $ds = -dx_1$ to reduce further the system, and set $Q_1 = X_1^{-1}Z_1 + S^{-1}W$, and $Q_2 = X_2^{-1}Z_2$. We now have,

$$\begin{bmatrix} A_1^\top & -Q_1 & 0 \\ A_2^\top & 0 & -Q_2 \\ 0 & A_1 & A_2 \end{bmatrix} \begin{bmatrix} dy \\ dx_1 \\ dx_2 \end{bmatrix} = \begin{bmatrix} c_1 - A_1^\top y \\ c_2 - A_2^\top y \\ b - Ax \end{bmatrix} \equiv \begin{bmatrix} \tilde{r}_1 \\ \tilde{r}_2 \\ \tilde{r}_3 \end{bmatrix}.$$

Now solve for dx_1 and dx_2 in terms of dy in the first two equations:

$$\begin{aligned} A_1^\top dy - Q_1 dx_1 = \tilde{r}_1 \quad &\Rightarrow \quad dx_1 = Q_1^{-1}(A_1^\top dy - \tilde{r}_1) \\ A_2^\top dy - Q_2 dx_2 = \tilde{r}_2 \quad &\Rightarrow \quad dx_2 = Q_2^{-1}(A_2^\top dy - \tilde{r}_2) \end{aligned}$$

Substitution gives us one equation[2] in dy

$$(A_1 Q_1^{-1} A_1^\top + A_2 Q_2^{-1} A_2^\top) dy = \tilde{r}_3 + A_1 Q_1^{-1} \tilde{r}_1 + A_2 Q_2^{-1} \tilde{r}_2$$

We can now write the solution to the linear system for the "affine step" as:

$$\begin{aligned} dy &= (AQ^{-1}A^\top)^{-1}[\tilde{r}_3 + A_1 Q_1^{-1}\tilde{r}_1 + A_2 Q_2^{-1}\tilde{r}_2] \\ dx_1 &= Q_1^{-1}(A_1^\top dy - \tilde{r}_1) \\ dx_2 &= Q_2^{-1}(A_2^\top dy - \tilde{r}_2) \\ ds &= -dx_1 \\ dz &= -z - X^{-1}Z dx = -Z\left(e + X^{-1}dx\right) \\ dw &= -w - S^{-1}W ds = -W\left(e + S^{-1}ds\right). \end{aligned}$$

The real effort at each iteration involves the Cholesky decomposition of the matrix $AQ^{-1}A^\top$ where Q is the diagonal matrix with Q_1 and Q_2 on the diagonal. And in this respect the algorithm is essentially the same as the case without the inequality constraints.

[2]Note that in prior implementations, Koenker and Portnoy (1997), we assumed that we had initial primal-dual feasibility, i.e., that the equality constraints were all satisfied and the starting value satisfied $0 \leq x \leq u$. This was easy since $x_0 = (1 - \tau)e$ was a natural initial point. Here we have not assumed initial primal feasibility so the right hand side becomes a bit more complicated. But *crucially* we do not need to have $Ax = b$ at the start; this simplifies life in the inequality constrained case considerably.

3.3. The Mehrotra predictor – corrector step. The tentative affine scaling step length is given by,

$$\phi_p = \min\left\{1, \sigma \min_{i:\, dx_i<0}\{x_i/dx_i\}, \sigma \min_{i:\, ds_i<0}\{s_i/ds_i\}\right\} \tag{3.10}$$

$$\phi_d = \min\left\{1, \sigma \min_{i:\, dz_i<0}\{z_i/dz_i\}, \sigma \min_{i:\, dw_i<0}\{w_i/dw_i\}\right\} \tag{3.11}$$

where the scaling factor σ determines how close the step is allowed to come to the boundary of the constraint set. In accordance with Lustig, Marsden and Shanno (1992, 1994) we take $\sigma = .99995$.

When the full affine scaling step is infeasible, that is when $\min\{\phi_p, \phi_d\} < 1$, we attempt to modify the length and direction of the step. For fixed $\mu > 0$, the first order conditions corresponding to our Lagrangian expression are,

$$\begin{aligned} A_1^\top y + z_1 - w &= c_1 \\ A_2^\top y + z_2 &= c_2 \\ Ax &= b \\ x_1 + s &= u \\ XZe &= \mu e \\ SWe &= \mu e \end{aligned} \tag{3.12}$$

Substituting $x \to x + dx, y \to y + dy$ etc., we obtain, assuming $x_1 + s = u$

$$\begin{aligned} A_1^\top dy + dz - dw &= c_1 - A_1^\top y - z_1 + w \\ A_2^\top dy + dz_2 &= c_2 - A_2^\top y - z_2 \\ Adx &= b - Ax \\ dx_1 + ds &= 0 \\ Xdz + Zdx &= \mu e - XZe - dXdZe \\ Sdw + Wds &= \mu e - SWe - dSdWe. \end{aligned}$$

Note that our provisional affine scaling step has been computed by solving almost the same system except that the bilinear terms $dXdZe$ and $dSdWe$ were ignored and μ was set to zero. The Mehrotra predictor-corrector step

brings both of these aspects of the problem back into play by solving:

$$\begin{aligned} A_1^\top \delta y + \delta z_1 - \delta w &= 0 \\ A_2^\top \delta y + \delta z_2 &= 0 \\ A\delta x &= 0 \\ \delta x_1 + \delta s &= 0 \\ X\delta z + Z\delta x &= \mu e - dXdZe \\ S\delta w + W\delta s &= \mu e - dSdWe \end{aligned}$$

Solving, we proceed as before,

$$\begin{aligned} W\delta s + S\delta w &= \mu e - dSdWe \\ \delta w &= -S^{-1}W\delta s + S^{-1}(\mu e - dSdWe) \\ X\delta z + Z\delta x &= \mu e - dXdZe \\ \delta z &= -X^{-1}Z\delta x + X^{-1}(\mu e - dXdZe) \end{aligned}$$

substituting, and eliminating δs as before, we have

$$\begin{aligned} A_1^\top \delta y - Q_1\delta x_1 &= S^{-1}(\mu e - dSdWe) - X_1^{-1}(\mu e - dX_1dZ_1e) \\ A_2^\top \delta y - Q_2\delta x_2 &= -X_2^{-1}(\mu e - dX_2dZ_2e) \\ A\delta x &= 0, \end{aligned}$$

rewritten in matrix form,

$$\begin{bmatrix} A_1^\top & -Q_1 & 0 \\ A_2^\top & 0 & -Q_2 \\ 0 & A_1 & A_2 \end{bmatrix} \begin{bmatrix} \delta y \\ \delta x_1 \\ \delta x_2 \end{bmatrix} = \begin{bmatrix} \hat{r}_1 \\ \hat{r}_2 \\ 0 \end{bmatrix}$$

where

$$\begin{aligned} \hat{r}_1 &= S^{-1}(\mu e - dSdWe) - X_1^{-1}(\mu e - dX_1dZ_1e) \\ &= \mu(S^{-1} - X_1^{-1})e + X_1^{-1}dX_1dZ_1e - S^{-1}dSdWe \\ \hat{r}_2 &= -X_2^{-1}(\mu e - dX_2dZ_2e) \end{aligned}$$

Now solve again for δx in terms of δy, and substituting we have

$$\begin{aligned}
\delta y &= (AQ^{-1}A^\top)^{-1}[A_1Q_1^{-1}\hat{r}_1 + A_2Q_2^{-1}\hat{r}_2] \\
\delta x_1 &= Q_1^{-1}(A_1^\top \delta y - \hat{r}_1) \\
\delta x_2 &= Q_2^{-1}(A_2^\top \delta y - \hat{r}_2) \\
\delta s &= -\delta x_1 \\
\delta z &= -X^{-1}Z\delta x + X^{-1}(\mu e - dXdZe) \\
\delta w &= -S^{-1}W\delta s + S^{-1}(\mu e - dSdWe)
\end{aligned} \tag{3.13}$$

We can interpret the solution of this system for the vector $(\delta y, \delta z, \delta x, \delta s, \delta w)$ as simply taking another Newton step, this time starting from the proposed affine scaling point. Since the left hand sides of the two linear systems are exactly the same, only the right hand side has been altered, a solution to the new system can be found by backsolving the triangular system using the Cholesky factorization of the affine step.

Comparing the corrector step in (3.13) with equation (4.18) in Koenker and Portnoy (1997), we can see the complications that are introduced by the inequality constraints. The effect of the A_2 inequality constrained matrix propagates through all the corrector steps and there is an additional corrector step for the Lagrange multiplier x_2 that is not present in the Koenker and Portnoy (1997). Similar intricacy occur in the affine step as well.

The crucial remaining question is: how does μ get updated? The duality gap is given by the expression,

$$\gamma = x^\top z + s^\top w.$$

Complementary slackness requires that the duality gap vanish at an optimum, so γ provides a direct measure of progress toward the solution. Iterations stop when γ is reduced below a prespecified tolerance. Solving the last two equations of the system (3.12) for μ we obtain,

$$\mu = \gamma/(2n_1 + n_2)$$

where n_1 is the dimension of the vectors: x_1, z_1, s, w, and n_2 is the dimension of the vectors: x_2, z_2. Were we to take the affine scaling step the duality gap would be

$$\hat{\gamma} = (x + \phi_p dx)^\top (z + \phi_d dz) + (s + \phi_p ds)^\top (w + \phi_d dw)$$

If $\hat{\gamma} \ll \gamma$ the step has made considerable progress toward the solution and it is reasonable to reduce μ considerably. On the other hand, if the duality gap

is only slightly reduced, we should consider the affine step to be poor and conclude that μ should not be substantially reduced. Note that repeated Newton steps with a fixed value of μ bring the iterations toward a point on the "central path", that is a point that minimizes the Lagrangian for a fixed μ.

Good performance of any interior point algorithm must balance the objectives of trying to stay close to the central path while trying to rapidly reduce the barrier parameter μ and thus moving toward the boundary. See Gonzago (1992) for a detailed analysis. The heuristics described above are embodied in the updating rule,

$$\mu_{(k+1)} \to (\hat{\gamma}/\gamma)^3 \gamma/(2n_1 + n_2)$$

Substituting this new value of μ into the system and solving we obtain the modified step. The step length is again determined by the rules (3.10) and (3.11). The step is taken, and the iterations continue until the duality gap is reduced to satisfy the specified tolerance.

4 Quantile Smoothing Splines

In Koenker, Ng, and Portnoy (1994) we proposed a variant of the classical cubic smoothing spline solving

$$\min_{g \in \mathcal{G}_2} \sum (y_i - g(x_i))^2 + \lambda \int (g''(x))^2 dx.$$

This quantile smoothing spline was constructed by solving,

$$\min_{g \in \mathcal{G}_1} \sum \rho_\tau (y_i - g(x_i)) + \lambda \bigvee (g'). \tag{4.14}$$

Here $\bigvee(f)$ denotes the total variation of the function f. Recall, e.g., Natanson (1955) for absolutely continuous $f : \mathbb{R} \to \mathbb{R}$,

$$\bigvee (f) = \int |f'(x)| dx.$$

Thus, for sufficiently smooth g, we can interpret the roughness penalty in (4.14) as $\mathcal{L}_1$ norm of the *second* derivative,

$$\bigvee (g') = \int |g''(x)| dx.$$

However, solutions of the variational problem (4.14) turn out to take the form of piecewise linear functions, so the total variation interpretation of the penalty is preferable.[3]

The problem (4.14) has a simple linear programming formulation. Writing

$$g(x) = \alpha_i + \beta_i(x - x_i) \quad \text{for } x \in [x_i, x_{i+1})$$

for the ordered, distinct values $x_1, \ldots, x_n$, we have by the continuity of g, that

$$\beta_i = (\alpha_{i+1} - \alpha_i)/h_i \quad i = 1, 2, \ldots, n-1$$

where $h_i = x_{i+1} - x_i$. So the penalty becomes

$$\bigvee(g') = \sum_{i=1}^{n-2} |\beta_{i+1} - \beta_i| = \sum_{i=1}^{n-2} |(\alpha_{i+2} - \alpha_{i+1})/h_{i+1} \quad - (\alpha_{i+1} - \alpha_i)/h_i|,$$

and the original problem may be written as,

$$\min_{\alpha \in \Re\mathbb{R}^n} \sum_{i=1}^{n} \rho_\tau(y_i - \alpha_i) + \lambda \sum_{j=1}^{n-2} |d_j^\top \alpha|$$

where $d_j^\top = (0, \ldots, 0, h_j^{-1}, (h_{j+1}^{-1} - h_j^{-1}), h_{j+1}^{-1}, 0, \ldots, 0)$. In the important median special case, $\tau = 1/2$, we can view this as simply a data-augmented ℓ_1 regression. We have the pseudo-design matrix,

$$X = \begin{bmatrix} I_n \\ D \end{bmatrix}$$

where $d_j^\top$ is the j^{th} row of D, and the pseudo response is $y^\top = (y_1, \ldots, y_n, 0, \ldots, 0) \in \mathbb{R}^{2n-2}$. In the case that $\tau \neq 1/2$ the situation is almost the same, except that in the dual formulation of the problem we have equality constraints whose right hand side is $(1 - \tau)e_n + 1/2D^\top e_{n-2}$ rather than $1/2e_n + 1/2D^\top e_{n-2}$.

The parameter λ in (4.14) controls the smoothness of the fitted function $\hat{g}$. The parametric dimension of $\hat{g}$ can be associated with the number of points interpolated exactly by $\hat{g}$, i.e., $\#\{i : y_i = \hat{g}(x_i)\}$. Koenker, Ng, and Portnoy (1994) discuss using this quantity in a Schwartz-type model selection criterion. They also suggest that further qualitative constraints on the fitted

[3]The $\mathcal{L}_1$ interpretation can be extended to the piecewise linear case, but we then need to interpret the integral as a limiting form in the sense of (Schwartz) distributions. See Koenker and Mizera (2002) for details.

function such as monotonicity or convexity could be imposed by adding linear inequality constraints. This approach was implemented in He and Ng (1999b) using the Bartels and Conn (1980) projected gradient/Simplex algorithm.

4.1. Monotonicity. There is a vast literature on estimating non-parametric regression relationships subject to monotonicity constraints. The classical reference is Barlow, Bartholomew, Bremner, and Brunk (1972), recent developments are treated in Robertson, Wright and Dykstra (1988). Much of the early work focused on minimizing a squared error objective subject to a monotonicity constraint, but more recently there has been interest in adding a smoothing objective as well. Mammen (1991), for example, considers kernel smoothing followed by a pooled-adjacent-violators (PAV) step as well as a procedure that reverses the order of these operations. More in line with the approach suggested here is the work of Utreras (1985), Villalobos and Wahba (1987), Ramsay (1988), Mammen Marron, Turlach, and Wand (2001), and most closely He and Ng (1999a) who all explore smoothing spline methods subject to linear inequality constraints as a way to impose monotonicity

Adding a monotonicity constraint to the quantile smoothing spline problem is quite straightforward given the algorithm described in the earlier sections. The function g is monotone increasing if

$$\beta_i = (\alpha_{i+1} - \alpha_i)/h_i \geq 0 \quad i = 1, 2, \ldots, n-1$$

so our constraint $Rb \geq r$ becomes,

$$\begin{bmatrix} -1 & 1 & 0 & \ldots & \ldots & 0 \\ 0 & -1 & 1 & \ldots & \ldots & 0 \\ \vdots & & & & & \\ 0 & \ldots & \ldots & \ldots & -1 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \vdots \\ \alpha_n \end{bmatrix} \geq 0.$$

To illustrate the method, in Figure 4.1 we plot observations from the model

$$y_i = x_i + u_i$$

where the x_i are equally spaced on $[0, 5]$, and the u_i are Student t on 2 degrees of freedom. There are 100 observations. The pooled-adjacent-violators curve appears in gray, and the monotone median smoothing spline with $\lambda = 0.1$ appears in black. Note that the outliers in the response tend to produce extended flat segments in the pooled-adjacent-violators fit. There are several

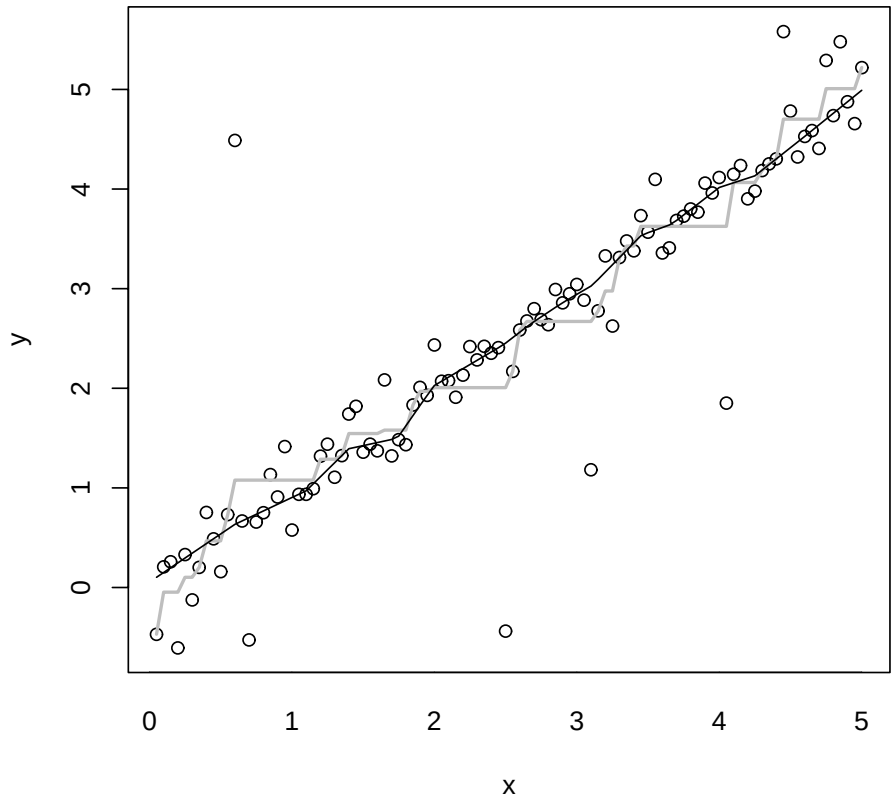

Figure 4.1. A comparison of the pooled-adjacent-violators estimate (in gray) and a monotone median smoothing spline fit (in black). Note the sensitivity of the PAV solution to outliers in the response y, and the need for further smoothing.

advantages of the spline: it has a "knob" to control the smoothness of the fitted function, it has an inherent robustness that PAV fitting based on Gaussian fidelity does not, and there is also a knob to control the desired conditional quantile of the fit.

4.2. Convexity. There is also an extensive literature on estimating functions constrained to be convex, or concave. Such conditions are also easy to impose. Convexity is equivalent in our setting of linear splines to the monotonicity of the slope parameters, β_i, i.e. to the conditions,

$$\beta_{i+1} - \beta_i \geq 0 \quad i = 1, 2, ..., n-1.$$

So to impose convexity we need simply to add the constraint,

$$D\alpha \geq 0,$$

where D is the matrix defining the total variation roughness penalty introduced above. For concavity, D is replaced by $-D$. In Figure 4.2 we illustrate a simple application to fitting the quadratic model,

$$y_i = x_i + x_i^2 + u_i$$

where the u_i are iid $\mathcal{N}(0, 4)$. The plot illustrates two median smoothing spline fits, both with λ chosen to be 0.08, one with the convexity constraint, the other without the constraint. Clearly the convexity constraint acts as a powerful additional smoothing effect.

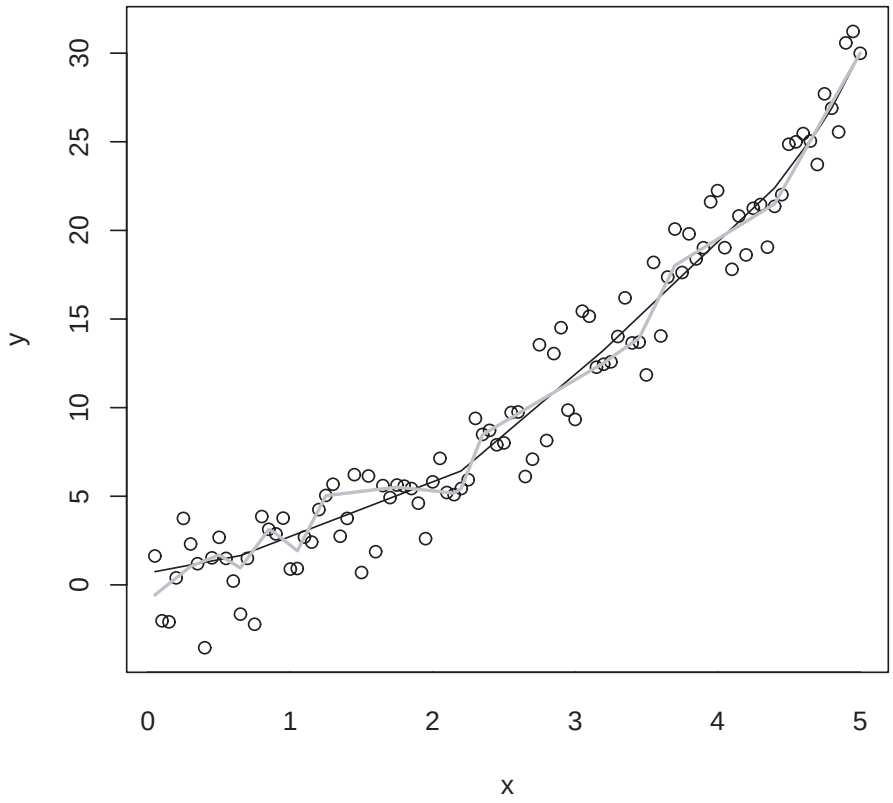

Figure 4.2. A comparison of the convex constrained median smoothing spline (in black) and the unconstrained median smoothing spline (in gray). Both of the fitted curves use the same smoothing parameter $\lambda = 0.08$.

4.3. $\mathcal{L}_\infty$ Roughness penalty. In earlier work, Koenker and Ng (1992), we have suggested that $\mathcal{L}_\infty$ penalties on the roughness of the fitted function,

$$\sup_x |g''(x)|$$

might serve as a useful alternative to the total variation penalty for some applications. For linear splines we may interpret this as,

$$\sup_i |\beta_{i+1} - \beta_i| \leq \nu.$$

Rather than assigning a Lagrange multiplier to determine the relative weight received by the roughness penalty we may choose a value for ν and vary the smoothness of the fitted function by adjusting the ν knob. It is well known that there is a one to one correspondence between the solutions determined by the Lagrange multiplier formulation and those indexed by the constraint parameter ν. Again the matrix D plays a crucial role, and we may express the constraints as restricting both $D\alpha$ and $-D\alpha$ to exceed $-\nu$ times a vector of ones.

4.4. Boundary constraints. In many smoothing problems there are natural constraints on the function being estimated near the boundary of the region of support. These might entail inequality constraints on the function itself, or on its derivatives, or even equality constraints. Note that equality constraints, say $R\beta = r$ can easily be imposed by requiring both $R\beta \geq r$ and $R\beta \leq r$.

5 An Engel Curve Example

To illustrate the approach of the preceding section we consider an application to the estimation of Engel curves. The data is taken from the U.K. Family Expenditure Survey for 1995. There are 3296 observations. The observations on household income were rounded to 4 significant digits; this yielded 1537 distinct values representing the parametric dimension of the model prior to smoothing. Expenditure on alcohol and tobacco is modeled solely as a function of household total expenditure with both variables taken in natural logarithms, so the slope of the estimated curves can be taken as an estimate of the Engel elasticity. We estimate six distinct conditional quantile functions for $\tau \in \{.15, .25, .50, .75, .95, .99\}$. Quantiles below .15 can not be estimated since the proportion of reported zeros exceeds this level at lower household expenditure levels. Note that the treatment of the zero expenditure households when taking logarithms is not an issue for the estimation

of these lower quantiles. Such observations can be notionally coded at $-\infty$. Only the sign of their residuals influences the estimate of the model, so the actual coding only has to insure that they lie below the fitted function. In Figure 4.3 we depict six families of estimated conditional quantile Engel curves. All of the estimates are based on the total variation penalty method (4.14). We illustrate results for two different values of the smoothing parameter λ: the upper panels use $\lambda = 1.0$, while the lower panels use $\lambda = 0.5$. The left panels of the figure depict the unconstrained estimates, the middle panels illustrates the estimates constrained to be monotone increasing, and the right panels were constrained to be increasing and concave. It is apparent that the qualitative constraints are effective in imposing some additional discipline on the fitting and this is even more clear as one explores fitting with smaller values of the smoothing parameter, λ.

Here the fitting was carried out using the sparse versions of the algorithms in R described in the next section, as a consequence it would be straightforward to add further complexity to the model in the form of parametric or nonparametric components. See the documentation for the function `rqss` in the `quantreg` package for R, Koenker (1991-), and the `SparseM` package for sparse linear algebra, Koenker and Ng (2003). The use of sparse algebra is quite essential since without it the size of underlying regression problems with column dimension 1537 and up to about 10,000 rows would be prohibitive on many machines; with it, required cpu time for fitting is about half a second on a Sun Ultra 2 for each quantile.

6 Implementation

The algorithm described above has been implemented in four distinct versions.[4] Versions written in "R" and "Matlab" provide accessible and convenient tools for studying qualitative features of performance since they are written in higher-level, matrix-oriented languages. R, Ihaka and Gentleman (1996), is a open source dialect of the statistical language S developed by Chambers (1998). We have used the pure "R" version primarily as a debugging tool, but the Matlab version is reasonably efficient for problems of moderate size.[5]

[4]Code is available at: `http://www.econ.uiuc.edu~/roger/rq/rq.html` for all four versions.

[5]Careful examination of the Matlab code reveals that some additional efficiency gain would be possible by reusing the Cholesky factorization in the computation of the modified step, as described in the preceding section.

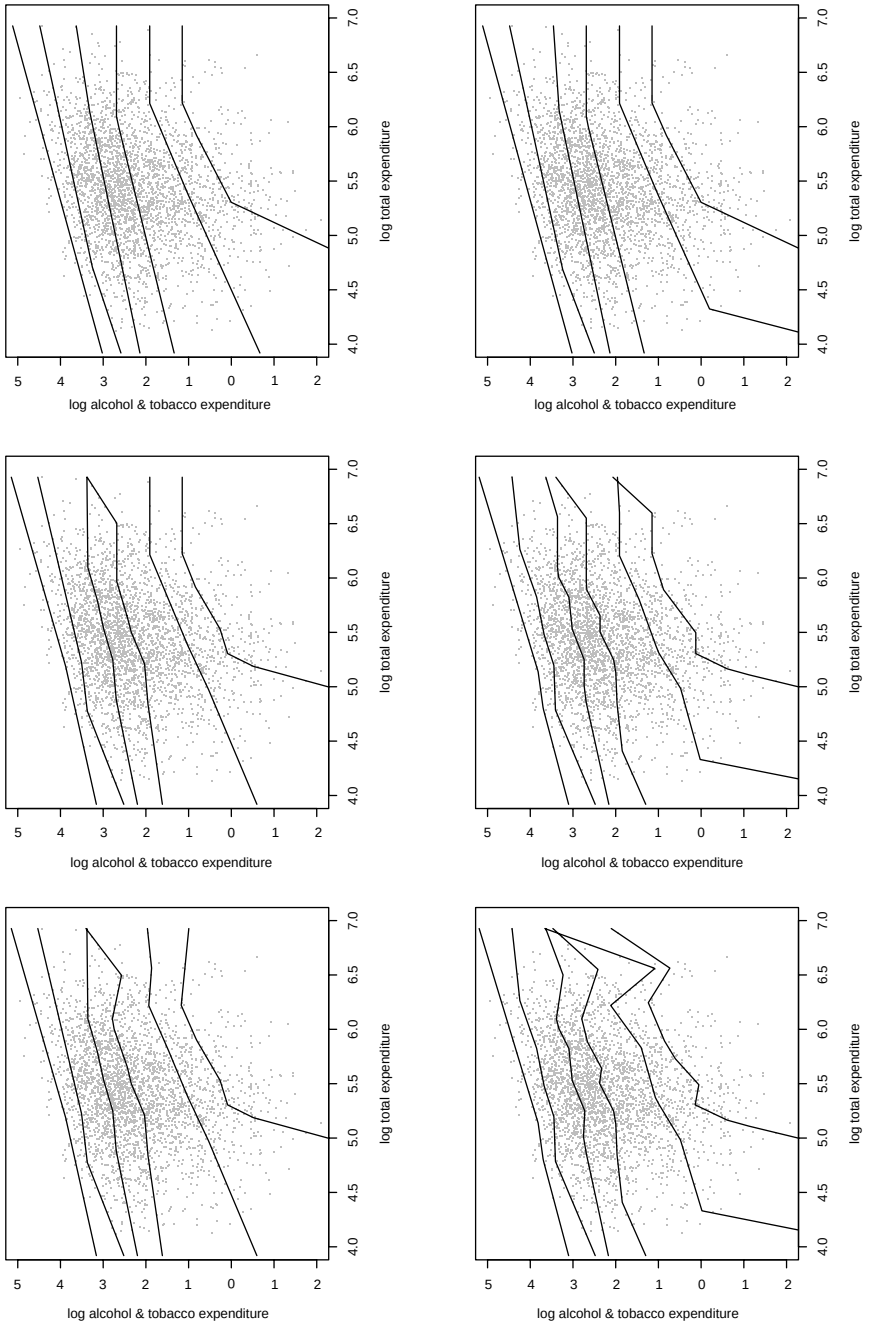

Figure 4.3. Families of Estimated Quantile Engel Curves.

Two distinct versions of the algorithm have also been written in Fortran and linked to "R". One employs standard (dense) linear algebra routines from LAPACK, the other uses more specialized sparse linear algebra to improve performance for problems having a high proportion of zeros in the matrix A. The latter formulation is particularly well-suited to the nonparametric regression problems we describe in the previous two sections. We discuss in more detail the sparse matrix implementation aspects in Koenker and Ng (2004).

7 Prospects and Conclusions

Inequality constraints are relatively easy to impose in the context of quantile regression estimation and provide a flexible means of imposing qualitative restrictions in non-parametric quantile regression problems. Interior point methods based on Frisch's log-barrier approach offer an extremely efficient approach to the computation of such estimators. And sparse linear algebra leads to significant further gains in efficiency of computation.

There are several important open problems associated with inequality constrained quantile regression. There is an extensive literature on inference in the classical Gaussian regression setting subject to inequality restrictions, and there is also an extensive literature on tests of qualitative features in nonparametric mean regression. It would be very useful to extend this inference apparatus to the present context.

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Roger Koenker
Department of Economics
University of Illinois at Urbana-Champaign
Champaign, IL 61820, USA
E-mail: rkoenker@uiuc.edu

Pin Ng
College of Business Administration
University of Northern Arizona
P.O. Box 15066
Flagstaff, AZ 86011, USA
E-mail: pin.ng@nau.edu

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