Online lectures on optimal transport and applications to quantile regression

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Invited lectures at HU Berlin November 18-19, 2020

These lectures

- ► These two online lectures will provide a mathematical and computational introduction to optimal transport, in connection with quantile regression.
- ► Code in R is provided in the following Github directory (https://github.com/alfredgalichon/Humboldt-2020). Other language work but the LP solver used will be Gurobi, so the language of choice should have a convenient interface to these.
- Outline:
 - D1: optimal transport, quantiles, vector quantiles
 - D2: conditional quantiles, quantile regression, vector quantile regression

Texts on optimal transport

- ► Mathematical foundations:
 - ► [OTON] C. Villani, Optimal Transport: Old and New, AMS, 2008.
 - ► [OTAM] F. Santambrogio, *Optimal Transport for Applied Mathematicians*, Birkhäuser, 2015.
- ► Fluid mechanics point of view:
 - ► [TOT] C. Villani, *Topics in Optimal Transportation*, AMS, 2003.
- ► Computational focus:
 - ► [NOT] G. Peyré, M. Cuturi (2018). *Numerical optimal transport*, Arxiv.
- ► Economics focus:
 - ► [OTME] A. Galichon. *Optimal Transport Methods in Economics*, Princeton, 2016.

Today

Lecture 1. The Monge-Kantorovich duality: general overview and linear programming

Refs: [OTME], Chapters 1, 2 and 8. Complement: [TOT], Chapter 1.

Section 1

The Monge-Kantorovich theorem

Optimal Transport

- ► Consider the problem of assigning a possibly infinite number of workers and firms. Each worker should work for one firm, and each firm should hire one worker.
- ▶ Workers and firms have heterogenous characteristics; let $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ be the vector of characteristics of workers and firms respectively. For all practical purpose in this course, they will be either open or closed subsets of \mathbb{R}^d .
- ▶ Workers and firms are in equal mass, which is normalized to one. The distribution of worker's types is P, and the distribution of the firm's types is Q, where P and Q are probability measures on \mathcal{X} and \mathcal{Y} .

Couplings

- A coupling determines which workers are assigned to which firms. If we had a finite number of workers and firms, we would need to count the number of workers of a given type matched with firms of a given type. More generally, a coupling will be defined as the probability measure π of occurence of worker-firm pairs. If $(X,Y) \sim \pi$ is the joint random pair, then $X \sim P$ and $Y \sim Q$, where $X \sim P$ means "X has distribution P." In other words, the first M should be Y, while its second margin should be Y.
- ► This motivates the following definition:

Definition

The set of couplings of probability distributions P and Q is the set of probability distributions over $\mathcal{X} \times \mathcal{Y}$ with first and second margins P and Q. This set is denoted $\mathcal{M}\left(P,Q\right)$. That is, a probability measure π over $\mathcal{X} \times \mathcal{Y}$ is in $\mathcal{M}\left(P,Q\right)$ if and only if

$$\pi(A \times Y) = P(A)$$
 and $\pi(X \times B) = Q(B)$

holds for every subset A of \mathcal{X} and B of \mathcal{Y} . By extension, a random pair $(X, Y) \sim \pi$ where $\pi \in \mathcal{M}(P, Q)$ will also be called a coupling of P and Q.

Examples of couplings

- ▶ Independent coupling, a.ka. random matching: $\pi(A, B) = P(A) Q(B)$, so that, if $(X, Y) \sim \pi$, then $X \sim P$ and $Y \sim Q$ are independent.
- ▶ Pure assignment, or Monge coupling: Y is a deterministic function of X; that is, Y = T(X). In our worker-firm example, this assumes that every workers of type x will get assigned the same type of firm, $T(x) \in \mathcal{Y}$. Then if $X \sim P$, then $T(X) \sim Q$, which we denote by

$$T\#P = Q \tag{1}$$

where T#P is the distribution of T(X) when $X \sim P$ ("push-forward" of P by map T, sometimes denoted $PT^{-1} = Q$).

▶ In general, a coupling is associated to a *Markov kernels*, $\pi\left(dy|x\right)$ such that

$$\int_{\mathcal{X}} \pi(B|x) \, dP(x) = Q(B)$$

for every subset B of \mathcal{Y} .

Optimal couplings: the Monge problem

- Assume that if worker x works for firm y, this generates a quantity of output $\Phi(x,y)$, measured in some monetary unit. A social planner decides which workers to assign to which firms and seeks to maximize the total output. The theory Optimal Transport studies how to do this.
- ► The *Monge Problem* (posed at the end of the 18th century) consists of looking among all the *pure* assignments, that is,

$$\max_{T(.)} \mathbb{E}_{P} \left[\Phi \left(X, T(X) \right) \right]. \tag{2}$$
s.t. $T \# P = Q$

- ► In general, the Monge problem is difficult:
 - ▶ It is nonlinear. In the discrete case, assuming P and Q have N equally weighted sample points, this amounts to looking for T within the permutations of {1, ..., N}: N! possibilities.
 - ▶ It may not have a solution. Think e.g. of the discrete case when P has less sample points than Q.
 - ► In fact, it remained unsolved for more than a century!

Optimal couplings: the Kantorovich problem

- ▶ Kantorovich in the 1940s came up with the idea of *linear programming Relaxation*: instead of looking among Monge couplings, look among all the couplings. Hence, instead of maximizing $\mathbb{E}_P\left[\Phi\left(X,T(X)\right)\right]$ s.t. T#P=Q, simply maximize $\mathbb{E}_T\left[\Phi\left(X,Y\right)\right]$ s.t. $X\sim P$ and $Y\sim Q$.
- ► This leads to the Kantorovich problem

$$\max_{\pi \in \mathcal{M}(P,Q)} \mathbb{E}_{\pi} \left[\Phi \left(X,Y \right) \right] \tag{3}$$

- ► This formulation has many advantages:
 - ▶ it is a linear programming problem, albeit an infinite-dimensional one. The dual is very informative.
 - lt has a solution π under very weak assumptions.
 - ► In a number of relevant cases, the solution to the Monge and Kantorovich problems will coincide.

Monge-Kantorovich Duality

Theorem

Let $\mathcal X$ and $\mathcal Y$ be two finite-dimensional vector spaces, and let P and Q be two probability measures on $\mathcal X$ and $\mathcal Y$ respectively. Let $\Phi: \mathcal X \times \mathcal Y \to \mathbb R \cup \{-\infty\}$ be an upper semicontinuous surplus function bounded above by $\overline{a}(x) + \overline{b}(y)$ where \overline{a} and \overline{b} are respectively integrable with respect to P and Q. Then: (i) The value of the primal Monge-Kantorovich problem

$$\sup_{\pi \in \mathcal{M}(P,Q)} \mathbb{E}_{\pi} \left[\Phi \left(X, Y \right) \right] \tag{4}$$

coincides with the value of the dual

$$\inf_{u,v} \mathbb{E}_{P}\left[u(X)\right] + \mathbb{E}_{Q}\left[v(Y)\right] \tag{5}$$

s.t.
$$u(x) + v(y) > \Phi(x, y)$$

where the infimum is over measurable and integrable functions u and v, and the inequality constraint should be satisfied for almost every x and almost every y (all these statements are respective to measures P and Q).

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Monge-Kantorovich Duality (continued)

Theorem

(iii) Assume further Φ is bounded below by $\underline{a}(x) + \underline{b}(y)$ where \underline{a} and \underline{b} are respectively integrable with respect to P and Q. Then the dual problem (5) also has solutions.

An informal proof of Theorem 2

The value of the primal problem $\sup_{\pi \in \mathcal{M}(P,Q)} \mathbb{E}_{\pi} [\Phi(X,Y)]$ can be rewritten

$$\sup_{\pi\in\mathcal{M}^{+}}\int\Phi\left(x,y\right)d\pi\left(x,y\right)+A_{P,Q}\left(\pi\right),$$

where \mathcal{M}^+ is the set of positive measures over $\mathcal{X} \times \mathcal{Y}$ (not necessarily of total mass one, and not necessarily with fixed marginals), and $A_{P,Q}$ should be such that

$$A_{P,Q}(\pi) = \begin{cases} 0 \text{ if } \pi \in \mathcal{M}(P,Q) \\ = -\infty \text{ else.} \end{cases}$$

One can take

$$A_{P,Q}(\pi) = \inf_{u,v} \int u(x) dP(x) + \int v(y) dQ(y) - \int (u(x) + v(y)) d\pi(x,y)$$

so that the value of the primal problem becomes

$$\sup_{\pi \in \mathcal{M}^{+}} \inf_{u,v} \left\{ \int \Phi(x,y) - (u(x) + v(y)) d\pi(x,y) + \int u(x) dP(x) + \int v(y) dQ(y) \right\}.$$

An informal proof of Theorem 2 (Ctd)

It is the case here that $\sup\inf=\inf\sup$ (this fact will be admitted without a proof), which yields

$$\inf_{u,v}\int u(x)\,dP(x)+\int v(y)\,dQ(y)+B_{\Phi}(u,v)$$

where $\mathcal{B}_{\Phi}\left(u,v
ight)=\sup_{\pi\in\mathcal{M}^{+}}\int\Phi\left(x,y
ight)-\left(u\left(x
ight)+v\left(y
ight)
ight)d\pi\left(x,y
ight)$, so that

$$B_{\Phi}\left(u,v\right) = \left\{ \begin{array}{l} 0 \text{ if } u\left(x\right) + v\left(y\right) \geq \Phi\left(x,y\right) \text{ for all } x \text{ and } y \\ = +\infty \text{ else.} \end{array} \right.$$

thus the value of the problem rewrites as (5). This argument is only a rough sketch; the minmax principle which we invoked when inverting the sup and the inf needs to be carefully established, and the spaces in which the functions u and v and the measure μ live need to be made precise. See Villani's [TOT], Ch. 1 for a rigorous argument.

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Dual problem and Walrasian equilibrium

We argue that u(x) can be interpreted as the equilibrium wage of worker x, while v(y) can be interpreted as the equilibrium profit of firm y.

Proposition

If (u, v) is a solution to the dual of the Kantorovich problem, then we can always redefine u and v so that they take value $+\infty$ outside of the supports of P and Q, respectively. In this case,

$$u(x) = \sup_{y} \left(\Phi(x, y) - v(y) \right) \tag{6}$$

$$v(y) = \sup_{x} \left(\Phi(x, y) - u(x) \right) \tag{7}$$

should hold almost surely with respect to the probabilities P and Q, respectively.

Section 2

Univariate case and quantiles

One-dimensional optimal transport

- Assume $\mathcal{X} = \mathcal{Y} = \mathbb{R}$. This implies that both workers and firms are characterized by scalar characteristics x and y. Restrictive, but most of the applied literature in Economics to this day has focused on this case, which already generates interesting economic insights.
- Assume that there is the same number of workers and firms, and this number is normalized to one. Let *P* be the probability distribution of the workers types *x*, and *Q* the probability distribution of the firms types *y*.

► E.g. the literature on CEO compensation studies the matching problem

of firms and managers: each manager has a measure of talent $x \in \mathbb{R}_+$ (extra return generated), and each firm has market capitalization $y \in \mathbb{R}_+$. Then, the economic value generated by a manager of talent x running a firm of size y is $\Phi(x,y)=xy$. Assume manager of talent x is assigned to firm of size y=T(x). The constraint on the assignment map T is that T#P=Q, which means that each firm is run by a manager and each manager runs a firm. Then the total value created is

$$\mathbb{E}_{P}\left[\Phi\left(X,T(X)\right)\right] = \mathbb{E}\left[XT(X)\right].$$

▶ Under a natural assuption on Φ , called *supermodularity*, we will see that the optimal coupling is such that Y = T(X), where T is nondecreasing. T will be given an explicit characterization

Copulas

▶ Recall that given a probability distribution P on the real line, one can define the *quantile* of that distribution, denoted F_P^{-1} , which is a map from [0,1] to R, nondecreasing and continuous from the right, and such that if $U \sim \mathcal{U} := \mathcal{U}\left([0,1]\right)$, then

$$F_{P}^{-1}\left(U\right) \sim P. \tag{8}$$

 F_P^{-1} is the generalized inverse of the c.d.f. of P, F_P , the proper inverse when P has a positive density, in which case $U=F_P(X)$. Note also that if $X\sim P$, then $F_P(X)$ has a uniform distribution if and only if P has no mass point.

▶ Representation (8) extends to the case of bivariate distributions: for $\pi \in \mathcal{M}(P,Q)$, there exists a pair (U,V) of uniform random variables such that

$$\left(F_P^{-1}(U), F_Q^{-1}(V)\right) \sim \pi,\tag{9}$$

and the c.d.f. associated with the distribution of (U, V) is called the *copula* associated with distribution π .

Comonotonicity

- ▶ A pair of random variables (X, Y) is *comonotone* if there is $U \sim \mathcal{U}$ such that $X = F_P^{-1}(U)$ and $Y = F_Q^{-1}(U)$. Equivalently, X and Y are said to exhibit *Positive Assortative Matching (PAM)*.
- ▶ The copula associated with a pair of comonotone random variables is the c.d.f. associated with (U, U), which is $F(u, v) = \min(u, v)$. This copula is called the *upper Fréchet-Hoeffding copula*.
- ▶ Note that when the cdf of *X* is continuous, there is a much simpler equivalent statement of comonotonicity:

Lemma

If the distribution of X has no mass points, then X and Y are comonotone if and only if there exists a nondecreasing map T such that Y = T(X). Moreover, one can choose $T(x) = F_Q^{-1}\left(F_P(x)\right)$.

Proof.

Consider $U \sim \mathcal{U}$ such that $X = F_P^{-1}(U)$ and $Y = F_Q^{-1}(U)$. If the distribution of X has no mass point, then $U = F_P(X)$. Hence, $Y = F_Q^{-1}(F_P(X))$.

Supermodular surplus

▶ Assume Φ is *supermodular*, that is, for every scalars x, x', y and y',

$$\Phi\left(x \vee x', y \vee y'\right) + \Phi\left(x \wedge x', y \wedge y'\right) \ge \Phi\left(x, y\right) + \Phi\left(x', y'\right), \quad (10)$$

where $x \lor x'$ and $x \land x'$ denote respectively the maximum and the minimum between scalars x and x'. When Φ is twice continuously differentiable (which we will assume from now on), this is equivalent to

$$\frac{\partial^2 \Phi\left(x,y\right)}{\partial x \partial y} \ge 0. \tag{11}$$

Assume that there are two types of workers $\mathcal{X} = \{\underline{x}, \bar{x}\}$ and firms $\mathcal{Y} = \{\underline{y}, \bar{y}\}$. An equivalent restatement of Condition (10) is then

$$\bar{x} \ge \underline{x} \text{ and } \bar{y} \ge \underline{y} \text{ implies } \Phi(\bar{x}, \bar{y}) + \Phi(\underline{x}, \underline{y}) \ge \Phi(\bar{x}, \underline{y}) + \Phi(\underline{x}, \bar{y})$$
 (12)

which asserts that the total output created is higher if the high types match together and the low types match together (assortative matching) rather than if mixed high/low pairs are formed.

Supermodular surplus: examples

Example

The following examples of surplus functions are supermodular:

- (i) Cobb-Douglas function: $\Phi(x, y) = x^a y^b$ $(x, y \ge 0)$, with $a, b \ge 0$,
- (ii) General multiplicative form: $\Phi(x, y) = \zeta(x) \xi(y)$ with ζ and ξ nondecreasing,
- (iii) Leontieff: $\Phi(x, y) = \min(x, y)$,
- (iv) C.E.S. function: $\Phi(x, y) = (x^{-\rho} + y^{-\rho})^{-1/\rho}, \rho \ge 0$,
- (v) $\Phi(x, y) = \phi(x y)$ where ϕ is concave; in particular,
- $\Phi(x, y) = -|x y|^p$, $p \ge 1$ or $\Phi(x, y) = -(x y k)^+$,
- (vi) $\Phi(x, y) = \phi(x + y)$, where ϕ convex.

The rearrangement theorem

Theorem

(i) Assume that $\boldsymbol{\Phi}$ is supermodular. Then the primal of the Monge-Kantorovich problem

$$\sup_{\pi \in \mathcal{M}(P,Q)} \mathbb{E}_{\pi} \left[\Phi \left(X, Y \right) \right] \tag{13}$$

has a comonotone solution.

(ii) Conversely, if Problem (13) has a comonotone solution for any choice of probability distributions P and Q on the real line, then Φ is supermodular.

(iii) If, in addition, P has no mass points, then there is an optimal assignment which is is pure and satisfies Y = T(X) where

$$T(x) = F_Q^{-1} \circ F_P(x). \tag{14}$$

The rearrangement theorem, proof (1)

The proof of part (i) is based on the following lemma.

Lemma

Let Z_1 and Z_2 be two Bernoulli random variables of respective success probability p_1 and p_2 . Then $\mathbb{E}\left[Z_1Z_2\right] \leq \min\left(p_1,p_2\right)$.

Proof.

As
$$Z_2 \leq 1$$
, $\mathbb{E}\left[Z_1Z_2\right] \leq \mathbb{E}\left[Z_1\right] = p_1$. Similarly $\mathbb{E}\left[Z_1Z_2\right] \leq \mathbb{E}\left[Z_2\right] = p_2$. Thus, $\mathbb{E}\left[Z_1Z_2\right] \leq \min\left(p_1,p_2\right)$.

We are now ready to sketch the proof of Theorem 7.

The rearrangement theorem, proof (2)

Sketch of proof of Theorem 7.

(i) Take $U \sim \mathcal{U}$, and $X = F_P^{-1}(U)$ and $Y = F_Q^{-1}(U)$. By (8), $X \sim P$ and $Y \sim Q$ and (X, Y) is comonotone by definition. The proof is in three steps.

Step 1. For $a, b \in \mathbb{R}$, consider surplus function

$$\phi_{ab}(x, y) := 1 \{x \ge a\} 1 \{y \ge b\}$$
, and let $Z_1 = 1 \{X \ge a\}$ and $Z_2 = 1 \{Y \ge b\}$. Z_1 and Z_2 are two Bernoulli random variables of respective

 $Z_2 = 1 \{ r \ge b \}$. Z_1 and Z_2 are two Bernoulli random variables of respective

success probability $p_1 = 1 - F_P(a)$ and $p_2 = 1 - F_Q(b)$, thus

 $\mathbb{E}[Z_1Z_2] \le \min(p_1, p_2)$, but a straightforward calculation shows that the inequality actually holds as an equality. Hence (X, Y), which is comonotone, is entired for each curplus function A

is optimal for each surplus function ϕ_{ab} .

Step 2. Assume $\mathcal{X}=[\underline{x},\bar{x}]$ and $\mathcal{Y}=[\underline{y},\bar{y}]$ are compact intervals. Then

$$F(x,y) = \frac{\Phi(x,y) - \Phi(\underline{x},y) - \Phi(x,\underline{y}) + \Phi(\underline{x},\underline{y})}{\Phi(\bar{x},\bar{y}) - \Phi(\underline{x},\bar{y}) - \Phi(\bar{x},\underline{y}) + \Phi(\underline{x},\underline{y})}$$

is a c.d.f. associated to a probability measure ζ , and hence

$$F(x,y) = \iint \phi_{ab}(x,y) \, d\zeta(a,b).$$

The rearrangement theorem, proof (3)

Proof.

As a result, if $\pi \in \mathcal{M}(p,q)$ is the distribution of (X,Y) where X and Y are comonotone, then

$$\int F(x,y) d\pi(x,y) \ge \int F(x,y) d\tilde{\pi}(x,y)$$

for every $\tilde{\pi} \in \mathcal{M}(p,q)$. But as F is of the form $F(x,y) = K\Phi(x,y) + f(x) + g(y) + c$ with K>0, and because $\int \left\{f(x) + g(y) + c\right\} d\pi(x,y) = \int \left\{f(x) + g(y) + c\right\} d\tilde{\pi}(x,y)$ for every $\tilde{\pi} \in \mathcal{M}(p,q)$, it results that

$$\int \Phi\left(x,y\right) d\pi\left(x,y\right) \geq \int \Phi\left(x,y\right) d\tilde{\pi}\left(x,y\right) \ \forall \tilde{\pi} \in \mathcal{M}\left(p,q\right)$$

which completes step 2.

The rearrangement theorem, proof (4)

Proof.

Step 3. When ${\mathcal X}$ and ${\mathcal Y}$ are the real line, the result still holds by approximation.

- (ii) The converse follows by taking for P the discrete probability with two mass points \underline{x} and \bar{x} with probability 1/2 each, and Q the discrete probability with two mass points \underline{y} and \bar{y} also each with probability 1/2. Then if (13) has a solution such that $F_P^{-1}(U)$ and $Y=F_Q^{-1}(U)$, for $U\sim \mathcal{U}\left([0,1]\right)$, it follows that condition (12) holds.
- (iii) follows from (i) and Lemma 5.

The rearrangement theorem, strict version

Note that the assumptions made in Theorem 7 do not guarantee that all the optimal assignments are comonotone. Indeed, the trivial example where $\Phi\left(x,y\right)=0$ for every x and y provides an example of supermodular surplus function, for which any assignment is optimal. For this reason, we provide a strengthening of the previous result, which ensures uniqueness. We will assume Φ is strictly supermodular, that is if both $\bar{x}>_{\underline{X}}$ and $\bar{y}>_{\underline{Y}}$ hold, then $\Phi\left(\bar{x},\bar{y}\right)+\Phi\left(\underline{x},\underline{y}\right)>\Phi\left(\bar{x},\underline{y}\right)+\Phi\left(\underline{x},\bar{y}\right).$

Theorem

Assume that Φ is strictly supermodular, and P has no mass point. Then the primal Monge-Kantorovich problem (13) has a unique optimal assignment, and this assignment is characterized by Y = T(X) where T is given by (14).

The wage equation

Assume (u, v) is a solution to the dual of the Monge-Kantorovich problem

$$\inf \mathbb{E}_{P}[u(X)] + \mathbb{E}_{Q}[v(Y)]$$
s.t. $u(x) + v(y) \ge \Phi(x, y)$ (15)

▶ Then v(y) is interreted as the value of the problem of a firm of type y, choosing the optimal worker x. Then the firm's program is

$$v(y) = \max_{x} \left\{ \Phi\left(x, y\right) - u\left(x\right) \right\}$$

thus by first order conditions, one is led to the wage equation

$$u'(x) = \frac{\partial \Phi}{\partial x}(x, T(x)), \tag{16}$$

where T is given by (14).

Dual Solution

Theorem

(i) Assume Φ is supermodular and continuously differentiable with respect to its first variable. Assume P has no mass point. Then the dual Monge-Kantorovich problem (15) has a solution (u,v). Further, u solves the wage equation (16). Hence, u is determined up to a constant c by

$$u(x) = c + \int_{x_0}^{x} \frac{\partial \Phi}{\partial x} (t, T(t)) dt.$$
 (17)

(ii) Assume further that Q has no mass point, and that Φ is also continuously differentiable with respect to its second variable. Then v is given by

$$v(y) = c' + \int_{T(x_0)}^{y} \frac{\partial \Phi}{\partial y} \left(T^{-1}(z), z \right) dz, \tag{18}$$

where c and c' are related by $c + c' = \Phi(x_0, T(x_0))$.

Application: quantiles as a solution to the optimal transport problem

As a consequence of the previous considerations, we have the following result:

Theorem

Assume $\mu=\mathcal{U}\left([0,1]\right)$ is the uniform distribution on the [0,1] interval, and Q is a probability distribution on the real line. Consider the optimal transport problem

$$\sup_{\pi \in \mathcal{M}(\mu, Q)} \mathbb{E}_{\pi}\left[\mathit{UY}\right] = \inf_{\varphi(u) \; \mathit{convex lsc}} \int_{0}^{1} \varphi\left(u\right) du + \int \varphi^{*}\left(y\right) dQ\left(y\right)$$

then a solution of the prial problem is given by $\left(U,F_{Q}^{-1}\left(U\right)\right)$, while a solution of the dual problem is given by

$$\varphi\left(u\right) = \int_{0}^{u} F_{Q}^{-1}\left(t\right) dt.$$

Section 3

Vector quantiles

Brenier's theorem

Theorem (Brenier)

Assume that μ and ν have finite second moments, and μ has a density. Then the solution $(\textit{U},\textit{Y}) \sim \pi \in \mathcal{M}\left(\mu,\nu\right)$ to the primal problem is represented by

$$Y = \nabla \varphi(U)$$

where (φ, φ^*) is a solution to the dual problem. Such φ is unique up to a constant.

Intuition of the proof: if φ is differentiable, then y is matched with u that maximizes $\{u^{\mathsf{T}}y - \varphi(u)\}$ over $u \in \mathbb{R}^d$. By first order conditions, such u satisfy $\nabla \varphi(u) = y$. It turns out, however, that differentiability is not a serious concern (at least, almost never).

McCann's theorem

The previous result allows to provide a representation of a large class of probability distributions ν over \mathbb{R}^d as the probability distribution of $\nabla \varphi \left(U \right)$, for U with a fixed distribution $\mu.$ There is however a limitation, in the sense that it requires that ν has finite second moments, which is needed for the optimal transport problem to have a finite value. Fortunately, McCann's theorem addresses this issue:

Theorem (McCann)

Assume that μ and ν are probability distributions such that μ has a density. Then there is a unique (up to a constant) function u such that

$$Y = \nabla \varphi (U)$$

holds almost surely with $U \sim \mu$ and $Y \sim \nu$.

The latter is denoted $\nabla \varphi \# \mu = \nu$.

Vector quantile: definition

▶ Definition. Let μ be a distribution on \mathbb{R}^d . For every distribution ν on \mathbb{R}^d , the μ -vector quantile associated with distribution ν is the map

$$Q_{\nu}(u) = \nabla \varphi(u)$$

where φ is a convex function such that $\nabla \varphi \# \mu = \nu$.

- ► The existence and uniqueness of this object are provided by McCann's theorem.
- ▶ We will take $\mu = \mathcal{U}([0,1]^d)$. In that case, when $\nu = \nu_1 \otimes \nu_2 \otimes ... \otimes \nu_d$, we have

$$\varphi\left(u\right)=\sum_{i=1}^{d}\varphi_{i}\left(u_{i}\right),$$

$$\begin{array}{l} \text{so } Q_{\mathcal{V}}\left(u\right) = \left(\varphi_{1}'\left(u_{1}\right), \varphi_{2}'\left(u_{2}\right), ..., \varphi_{d}'\left(u_{d}\right)\right) = \\ \left(F_{\nu_{1}}^{-1}\left(u_{1}\right), F_{\nu_{2}}^{-1}\left(u_{2}\right), ..., F_{\nu_{d}}^{-1}\left(u_{d}\right)\right). \end{array}$$

Section 4

Discrete case and linear programming

- Assume that the type spaces \mathcal{X} and \mathcal{Y} are finite, so $\mathcal{X} = \{1, ..., N\}$, and $\mathcal{Y} = \{1, ..., M\}$.
- ► The total mass of workers and jobs is normalized to one. The mass of workers of type x is p_x ; the mass of jobs of type y is q_y , with $\sum_x p_x = \sum_y q_y = 1$.
- Let π_{xy} be the mass of workers of type x assigned to jobs of type y. Every worker is occupied and every job is filled, thus

$$\sum_{y=1}^{M} \pi_{xy} = p_x \text{ and } \sum_{x=1}^{N} \pi_{xy} = q_y.$$
 (19)

(Note that this formulation does not restrict to Monge couplings, i.e. it allows for $\pi_{xy} > 0$ and $\pi_{xy'} > 0$ to hold simultaneously with $y \neq y'$.)

Optimal assignment

- Assume the economic output created when assigning worker x to job y is Φ_{xy} . Hence, under assignment π , the total output is $\sum_{xy} \pi_{xy} \Phi_{xy}$.
- ► Thus, the optimal assignment is

$$\max_{\pi \geq 0} \sum_{xy} \pi_{xy} \Phi_{xy}$$

$$s.t. \sum_{y=1}^{M} \pi_{xy} = p_{x} [u_{x}]$$

$$\sum_{x=1}^{N} \pi_{xy} = q_{y} [v_{y}]$$

$$(20)$$

and it is now a finite-dimensional linear programming problem.

Note that it is nothing else than the Monge-Kantorovich problem when P and Q are discrete probability measures on $\mathcal{X} = \{1, ..., N\}$, and $\mathcal{Y} = \{1, ..., M\}$.

Theorem (M-K, finite-dimensional case)

(i) The value of the primal problem (20) coincides with the value of the dual problem

$$\min_{u,v} \sum_{x=1}^{N} p_{x} u_{x} + \sum_{y=1}^{M} q_{y} v_{y}.$$

$$s.t. u_{x} + v_{y} \ge \Phi_{xy} \left[\pi_{xy} \ge 0 \right]$$
(21)

(ii) Both the primal and the dual problems have optimal solutions. If π is a solution to the primal problem and (u, v) a solution to the dual problem, then by complementary slackness,

$$\pi_{xy} > 0 \text{ implies } u_x + v_y = \Phi_{xy}. \tag{22}$$

(iii) If (u, v) is a solution to the dual problem, then

$$u_{x} = \max_{y \in \{1, \dots, M\}} \left\{ \Phi_{xy} - v_{y} \right\} \text{ and } v_{y} = \max_{x \in \{1, \dots, N\}} \left\{ \Phi_{xy} - u_{x} \right\}. \tag{23}$$

Computation (1)

- ▶ This problem of computation of the Optimal Assignment Problem, more specifically of (π, u, v) , is arguably the most studied problem in Computer Science, and dozens, if not hundreds of algorithms exist, whose running time is polynomial in $\max(n, m)$, typically a power less than three of the latter.
- ► Famous algorithms include: the Hungarian algorithm (Kuhn-Munkres); Bertsekas' auction algorithm; Goldberg and Kennedy's pseudoflow algorithm. See an introduction to these algorithms in http://www.assignmentproblems.com/doc/LSAPIntroduction.pdf.
- ▶ Here, we will show how to solve the problem with the help of a linear programming solver used as a black box; our challenge here will be to carefully set up the constraint matrix as a sparse matrix in order to let a large scale linear programming solvers such as Gurobi recognize and exploit the sparsity of the problem.

Computation (2)

▶ Let Π and Φ be the matrices with typical elements (π_{xy}) and (Φ_{xy}) . We let p, q, u, v, and 1 the column vectors with entries (p_x) , (q_y) , (u_x) , (v_y) , and 1, respectively. Problem (20) rewrites using matrix algebra as

$$\max_{\Pi \ge 0} Tr(\Pi'\Phi)$$

$$\Pi 1_{M} = p$$

$$1'_{N}\Pi = q'.$$
(24)

• We need to convert matrices into vectors; this can be done for instance by stacking the columns of Π into a single column vector (typical in R or Matlab). This operation is called *vectorization*, which we will denote

$$vec(A)$$
,

which reshapes a $N \times M$ matrix into a $nm \times 1$ vector. In R, this is implemented by c(A); in Matlab, by reshape(A, [n*m, 1]).

► The objective function rewrites as

$$vec(\Phi)'vec(\Pi)$$
.

Computation (3)

▶ Recall that if A is a $M \times p$ matrix and B a $N \times q$ matrix, then the Kronecker product $A \otimes B$ of A and B is a $mn \times pq$ matrix such that

$$vec(BXA') = (A \otimes B) vec(X)$$
. (25)

In R, $A \otimes B$ is implemented by kronecker(A,B); in Matlab, by kron(A,B).

► The first constraint $I_N\Pi 1_M = p$, vectorizes therefore as

$$(1_{M}' \otimes I_{N}) \operatorname{vec}(\Pi) = \operatorname{vec}(p)$$
,

and similarly, the second constraint $1'_{N}\Pi I_{M} = q'$, vectorizes as

$$(I_{\mathcal{M}} \otimes 1'_{\mathcal{N}}) \operatorname{vec}(\Pi) = \operatorname{vec}(q)$$
.

Note that the matrix $1_M' \otimes I_N$ is of size $N \times NM$, and the matrix $I_M \otimes 1_N'$ is of size $M \times NM$; hence the full matrix involved in the left-hand side of the constraints is of size $(N+M) \times NM$. In spite of its large size, this matrix is *sparse*. In R, the identity matrix I_N is coded as sparseMatrix(1:N,1:N), in Matlab as Speye(N).

Computation (4)

▶ Setting $z = vec(\Pi)$, the linear programming problem then becomes

$$\max_{z \ge 0} \operatorname{vec}(\Phi)' z$$

$$s.t. \ (1'_{M} \otimes I_{N}) z = \operatorname{vec}(p)$$

$$(I_{M} \otimes 1'_{N}) z = \operatorname{vec}(q')$$

$$(26)$$

which is ready to be passed on to a linear programming solver such as Gurobi.

► A LP solver typically computes programs of the form

$$\max_{z \ge 0} c'z$$

$$s.t. Az = d.$$
(27)

In R, Gurobi is called to compute program (27) by gurobi(list(A=A,obj=c,modelsense="max",rhs=d,sense="=")).

► See https://github.com/math-econ-code/mec_optim/tree/master/04-appli-optassign

Section 5

Quantile regression

References

- ► [OTME], Ch. 6.3 and 9.5
- ► Hedonic models: Ekeland, Heckman and Nesheim, Heckman, Nesheim and Matzkin
- ▶ Quantile regression: Koenker and Bassett (1978), Koenker (2005)
- ▶ Vector quantiles: Ekeland, G and Henry (2012), Carlier, G and Santambrogio (2010), Carlier, G. and Chernozhukov (2016, 2017) Chernozhukov, G, Hallin and Henry (2016), Carlier, Chernozhukov, De Bie, and G (2020).

What is the right definition of a quantile?

In dimension one, the following statements equivalently define quantiles of a distribution $Y \sim \nu$:

- ▶ The quantile map is the (generalized) inverse of the cdf of ν : F_{ν}^{-1} .
- ▶ The quantile map is the nondecreasing map T such that if $U \sim \mathcal{U}([0,1])$, then $T(U) \sim \nu$.
- The quantile at $t F_{\nu}^{-1}(t)$ is the solution of $\min_{q} \mathbb{E}\left[\rho_{t}(Y-q)\right]$, where $\rho_{t}(z) = tz^{+} + (1-t)z^{-}$.
- ▶ The quantile map is the solution to the Monge problem between distribution $\mathcal{U}\left([0,1]\right)$ and ν relative to cost $\Phi\left(u,y\right)=uy$.

Quantile: properties

Quantiles have a number of enjoyable properties that make them easy to work with.

- ▶ They fully characterize the distribution ν .
- They allow to construct a representation of ν : $F_{\nu}^{-1}(U)$, $U \sim \mu := \mathcal{U}([0,1])$ has distribution ν .
- ► They embed the median $(F_{\nu}^{-1}(1/2))$ and the extreme values $(F_{\nu}^{-1}(0))$ and $F_{\nu}^{-1}(1)$.
- ▶ They allow to provide a construction of distance between distributions: for $p \ge 1$,

$$\left(\int\left|F_{\nu}^{-1}\left(t\right)-F_{\nu}^{-1}\left(t\right)\right|^{p}dt\right)^{1/p}$$

is the *p*-Wasserstein distance between μ and ν .

- ► They allow for a natural construction of robust statistics by trimming the interval [0, 1].
- ► They lend themselves to a natural notion of regression: quantile regression (Koenker and Bassett, 1978; Koenker 2005).

Quantile/quantile regression: applications

Quantiles are widely used in economics, finance and statistics.

- ▶ Comonotonicity: $(F_{\nu_1}^{-1}(U), F_{\nu_2}^{-1}(U))$ for $U \sim \mu := \mathcal{U}([0,1])$ is a comonotone representation of ν_1 and ν_2 .
- ► Mesures of risk: Value-at-risk $F_{\nu}^{-1}(1-\alpha)$; CVaR $\int_{1-\alpha}^{1} F_{\nu}^{-1}(t) dt$.
- Non-expected utility: Yaari's rank-dependent EU (Choquet integral) $\int_0^1 F_{\nu}^{-1}(t) \, w(t) \, dt.$
- ▶ Demand theory: Matzkin's identication of hedonic models. (See later)
- ► Income and inequality: Chamberlain (1994)'s study of the effect of unionization on wages.
- ► Biometrics: growth charts.

Quantile regression

▶ Quantile regression therefore adopts a parameterization of the conditional quantile which is linear in *Z*. That is

$$Q_{Y|X}(\tau|x) = x^{\mathsf{T}}\beta_{\tau}$$

(note that one can always augment x with nonlinear functions of x, so this parameterization is quite general).

▶ In order to estimate β_{τ} , first note that

$$Q_{Y|X}(\tau|x) = \arg\min_{q} \mathbb{E}\left[\rho_{\tau}\left(Y - q\right) | X = x\right]$$

where $\rho_{\tau}\left(w\right)=\tau w^{+}+\left(1-\tau\right)w^{-}$.

▶ Therefore, if the conditional quantile has the specified form, β_u is the solution to

$$\min_{\beta \in \mathbb{R}^k} \mathbb{E}\left[\rho_{\tau}\left(Y - X^{\mathsf{T}}\beta\right) \middle| X = x\right]$$

for each x, and therefore it is the solution to the quantile regression problem introduced by Koenker and Bassett (1978)

$$\min_{\beta \in \mathbb{R}^{k}} \mathbb{E}\left[\rho_{\tau}\left(Y - X^{\mathsf{T}}\beta\right)\right].$$

Quantile regression as linear programming

Koenker and Bassett showed that this problem has a linear programming formulation. Indeed, consider its sample version

$$\min_{\beta \in \mathbb{R}^k} \sum_{i=1}^n \rho_{\tau} \left(Y_i - X_i^{\mathsf{T}} \beta \right)$$

▶ Introducing $Y_i - X_i^{\mathsf{T}} \beta = P_i - N_i$ with P_i , $N_i \geq 0$, we have

$$\min_{ \substack{\beta \in \mathbb{R}^k \\ P_i \geq 0, N_i \geq 0}} \sum_{i=1}^n \tau P_i + (1 - \tau) N_i$$
 s.t. $P_i - N_i = Y_i - X_i^\mathsf{T} \beta$

therefore β can be obtained by simple linear programming.

Computing classical quantile regression (1)

- ► The package 'quantreg' performs classical quantile regression.
- Do:

```
thedata = data.frame(X0,Y)

QRres = rq(Y ~X0, data=thedata, tau = t )
print(summary(QRres))
```

Computing classical quantile regression (2)

Alternatively, we can code it ourselves using Gurobi

$$\min_{\substack{\beta \in \mathbb{R}^k \\ P_i \ge 0, N_i \ge 0}} \sum_{i=1}^n \tau P_i + (1 - \tau) N_i$$
s.t. $(I_n P)_i + (-I_n N)_i + (X\beta)_i = Y_i$

Do:

```
X=cbind(1,X0)
k=dim(X)[2]
obj=c(rep(t,n),rep(1-t,n),rep(0,k))
A=cbind(sparseMatrix(1:n,1:n),-sparseMatrix(1:n,1:n),X)
result = gurobi
(list(A=A,obj=obj,modelsense="min",rhs=c(Y),
lb=c(rep(0,2*n),rep(-Inf,k)),sense="="))
thebeta = result$x[(2*n+1):(2*n+k)]
```

Section 6

Vector quantile regression

Quantile regression a linear programming problem (recalled)

Recall

$$\begin{aligned} \min_{P \geq 0, N \geq 0, \beta} \mathbb{E} \left[\tau P + (1 - \tau) \ N \right] \\ s.t. \ P - N = Y - X^\top \beta \ \left[V \right] \end{aligned}$$
 where $P = \left(Y - X^\top \beta \right)^+$ and $N = \left(Y - X^\top \beta \right)^-$, or equivalently,
$$\min_{P \geq 0, N \geq 0, \beta} \mathbb{E} \left[P + (1 - \tau) \ X^\top \beta \right]$$
 s.t. $P - N = Y - X^\top \beta \ \left[V \right]$

which we call the "dual" problem.

► The corresponding primal problem is

$$\begin{aligned} \max_{V} \mathbb{E} \left[YV \right] \\ s.t. \ V &\geq 0 \ \left[N \geq 0 \right] \\ V &\leq 1 \ \left[P \geq 0 \right] \\ \mathbb{E} \left[VX \right] &= (1-\tau) \, \mathbb{E} \left[X \right] \ \left[\beta \right] \end{aligned}$$

Complementary slackness

▶ Let $V(\tau)$ and $\beta(\tau)$ be solutions to the above program. Complementary slackness yields

$$Y - X^{T} \beta(\tau) < 0 \implies V(\tau) = 0$$

 $Y - X^{T} \beta(\tau) > 0 \implies V(\tau) = 1$

therefore

$$\mathbf{1}\left\{Y > X^{\top}\beta\left(\tau\right)\right\} \leq V(\tau) \leq \mathbf{1}\left\{Y \geq X^{\top}\beta\left(\tau\right)\right\}.$$

Assume (X, Y) has a continuous distribution,. Then for any β , $\Pr\left(Y - X^{\top}\beta = 0\right) = 0$, and therefore one has almost surely

$$V(\tau) = 1 \left\{ Y \ge X^{\top} \beta(\tau) \right\}.$$

Quantile curve regression

Consider

$$\begin{aligned} \max_{V(.)} \int_0^1 \mathbb{E} \left[YV(\tau) \right] d\tau \\ s.t. \ V(\tau) &\geq 0 \ \left[N(\tau) \geq 0 \right] \\ V(\tau) &\leq 1 \ \left[P(\tau) \geq 0 \right] \\ \mathbb{E} \left[V(\tau) X \right] &= (1 - \tau) \, \mathbb{E} \left[X \right] \ \left[\beta \left(\tau \right) \right] \end{aligned}$$

The problem has dual

$$\min_{P \geq 0, N \geq 0, \beta} \int_{0}^{1} \mathbb{E}\left[P(\tau) + (1 - \tau) X^{T} \beta(\tau)\right] d\tau$$
s.t. $P(\tau) - N(\tau) = Y - X^{T} \beta(\tau) \left[V(\tau)\right]$

► The solution to these problems are the same as the solutions to each of the previous problem — the contraints don't interfere.

Quantile curve regression under dual monotonicity constraint

► Koenker and Ng (2005) consider imposing the monotonicity constraint of the estimated quantile curves. Thus, they impose a constraint on the dual, that is $X^{\top}\beta(\tau) \geq X^{\top}\beta(\tau')$ for $\tau \geq \tau'$, that is

$$\begin{aligned} \min_{P \geq 0, N \geq 0, \beta} \int_{0}^{1} \mathbb{E} \left[P(\tau) + (1 - \tau) X^{T} \beta(\tau) \right] d\tau \\ s.t. \ P(\tau) - N(\tau) &= Y - X^{T} \beta(\tau) \quad [V(\tau)] \\ X^{T} \beta(\tau) &\geq X^{T} \beta(\tau'), \ \tau \geq \tau' \end{aligned}$$

► This is the most natural approach to solve the non-monotonicity problem.

Quantile curve regression under primal monotonicity constraint

- ▶ By contrast, we impose the constraint that the primal variable $\tau \to V(\tau)$ should be nonincreasing. This is justified by the fact that $V(\tau) = 1 \left\{ Y \ge X^\top \beta(\tau) \right\}$, so $\tau \to X^\top \beta(\tau)$ nondecreasing implies $V(\tau)$ nonincreasing.
- ► Therefore, we let

$$\max_{V(\tau)} \int_{0}^{1} \mathbb{E} \left[YV(\tau) \right] d\tau$$
s.t. $V(\tau) \ge 0 \quad [N(\tau) \ge 0]$

$$V(\tau) \le 1 \quad [P(\tau) \ge 0]$$

$$\mathbb{E} \left[V(\tau) X \right] = (1 - \tau) \mathbb{E} \left[X \right] \quad [\beta(\tau)]$$

$$V(\tau) \le V(\tau'), \quad \tau \ge \tau'$$

Primal monotonicity constraint, sample

► Consider $\tau_1 = 0 < ... < \tau_T \le 1$ and let \bar{x} be the $1 \times K$ row vector whose k-th entry is $\mathbb{E}[X_k]$. One has

$$\max_{V_{ti} \geq 0} \sum_{\substack{1 \leq i \leq N \\ 1 \leq t \leq T}} V_{ti} Y_i$$

$$V_{ti} \leq 1$$

$$\frac{1}{N} \sum_{1 \leq i \leq n} V_{ti} X_{ik} = (1 - \tau_t) \bar{x}_k$$

$$V_{(t+1)i} \leq V_{ti}$$

 \blacktriangleright As $\tau_1 = 0$, one has necessarly $V_{1i} = 1$ and the program becomes

$$\begin{aligned} \max_{V_{ti}} \sum_{\substack{1 \leq i \leq N \\ 1 \leq t \leq T}} V_{ti} Y_i \\ V_{1i} &= 1 \\ \frac{1}{N} \sum_{1 \leq i \leq n} V_{ti} X_{ik} = (1 - \tau_t) \, \bar{x}_k \\ V_{t1} \geq V_{t2} \geq ... \geq V_{t(m-1)} \geq V_{T,i} \geq 0. \end{aligned}$$

Matrix notations

- ▶ Let τ be the $T \times 1$ row matrix with entries τ_k .
- \blacktriangleright Let D be a $T \times T$ matrix with

$$D = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 1 & 0 & \ddots & \vdots & \vdots \\ 0 & -1 & 1 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 & 0 \\ \vdots & & 0 & -1 & 1 & 0 \\ 0 & & 0 & 0 & -1 & 1 \end{pmatrix}$$

we have $V^{\top}D \geq 0$ if and only if $V_{1i} \geq V_{2i} \geq ... \geq V_{(T-1)i} \geq V_{Ti} \geq 0$.

Matrix formulation

► One can write

$$\max_{V} 1_{N}^{\top} V Y$$

$$\frac{1}{N} V X = (1_{T} - \tau) \bar{x}$$

$$V^{\top} D 1_{T} = 1_{N}$$

$$V^{\top} D \ge 0$$

thus, setting $\pi = D^{\top} V/N$, and $U = D^{-1} 1_N$, $\mu = D^{\top} (1_T - \tau)$, and $p = 1_N/N$, one has

$$\max_{\pi} U^{\top} \pi Y$$

$$\pi X = \mu \bar{x}$$

$$\pi^{\top} 1_{T} = p$$

$$\pi \ge 0$$

▶ It is easy to compute U = (1/T, 2/T, ..., 1) and $\mu = (1/T, ..., 1/T)$.

Matrix formulation (ctd)

Assume that the first entry of X is one. One has that if π satisfies the constraints, then

$$\sum\limits_{i=1}^{N}\pi_{ti}=\mu_{t}$$
 and $\sum\limits_{t=1}^{T}\pi_{ti}=\mathit{p_{i}}$

thus π can be thought of as a joint probability on τ and X.

► One has

$$\max_{\substack{\pi \geq 0}} \sum_{\substack{1 \leq t \leq T \\ 1 \leq i \leq N}} \pi_{ti} U_t Y_i$$

$$\sum_{1 \leq i \leq N} \pi_{ti} X_{ik} = \mu_t \bar{x}_k$$

$$\sum_{1 \leq t \leq T} \pi_{ti} = p_i$$

Section 7

Vector quantile regression

Link with optimal transport

► This rewrites as a "Vector quantile regression" (yet for now in the scalar case) of CCG (2016)

$$\begin{aligned} \max_{\pi} & \mathbb{E}_{\pi} \left[UY \right] \\ s.t.U \sim \mu \\ & (X, Y) \sim P \\ & \mathbb{E} \left[X | U \right] = \mathbb{E} \left[X \right] \end{aligned}$$

► This is an extension of the optimal transport problem of Monge and Kantorovich. As a matter of fact, when X is restricted to the constant, this is *exactly* an optimal transport problem.

Vector quantile regression, primal problem

Recall our previous problem

$$\max_{\pi} \mathbb{E}_{\pi} [UY]$$

$$s.t.U \sim \mu$$

$$(X, Y) \sim P$$

$$\mathbb{E} [X|U] \sim \mathbb{E} [X]$$

and replace mean-independence by independence; one has

$$\max_{\pi} \mathbb{E}_{\pi} [UY]$$
s.t. $U \sim \mu$

$$(X, Y) \sim P$$

$$X \perp U$$

► The solution to the latter problem is simply

$$U = F_{Y|X}(Y|X)$$

which yields the nonparametric conditional quantile representation

$$Y = F_{V|X}^{-1}(U|X)$$
.

Vector quantile regression, dual problem

► The dual problem yields

$$\begin{aligned} & \min_{\psi,b} & \mathbb{E}_{P} \left[\psi \left(X, Y \right) \right] + \bar{\mathbf{x}}^{\top} \mathbb{E}_{\mu} \left[b \left(U \right) \right] \\ & \text{s.t.} \ \psi \left(\mathbf{x}, \mathbf{y} \right) + \mathbf{x}^{\top} b \left(\tau \right) \geq \tau \mathbf{y}, \ \forall \mathbf{x}, \mathbf{y}, \tau \end{aligned}$$

▶ Optimality of (ψ, b) yields

$$\psi\left(x,y\right) = \sup_{\tau \in \left[0,1\right]} \left\{ \tau y - x^{\top} b\left(\tau\right) \right\}$$

which yields, if b is differentiable,

$$Y = X^{T} \beta(U)$$

where (U, X, Y) are the solutions to the primal problem and $\beta(\tau) = b'(\tau)$.

Multivariate quantile regression

- ▶ Vector quantile regression yields a natural way to extend classical quantile regression to the case when the dependent variable is multivariate. If Y is valued in \mathbb{R}^d , one may take τ in \mathbb{R}^d , $\mu = \mathcal{U}\left(\left[0,1\right]^d\right)$. We replace the product τ by the scalar product $\tau^\top \beta\left(\mathcal{U}\right)$, and the analysis goes unmodified.
- ▶ We get a nice tensorization of vector quantile regression that way: when the components of *Y* are independent, the previous propal amounts to running the scalar version component by component.

Why mean-independence?

Quantile regression is specified when

$$Q_{Y|X}(\tau|x) = x^{\top}\beta(\tau)$$

Letting

$$U:=F_{Y|X}(Y|X),$$

it follows that $U \sim \mathcal{U}([0,1])$ and independent from X.

► Therefore the model is specified if and only if $\tau \to x^{\top} \beta(\tau)$ is increasing for all $x \in Supp(F_X)$, and

$$Y = X^{\top} \beta (U)$$
 , $U \sim \mathcal{U} ([0,1])$, $X \perp \!\!\! \perp U$

Note that when QR is specified, then $\tau \to V(\tau) = 1 \left\{ 1 \left\{ Y \geq X^\top \beta \left(\tau \right) \right\} \right\} \text{ is a.s. nonincreasing. Is the converse true?}$

Why mean-independence? (ctd)

- ▶ Quantile regression is quasi-specified when for all $x \in Supp(F_X)$, $\tau \to x^\top \beta(\tau)$ is continuous and increasing from [0,1] to $Supp(F_{Y|X=x})$.
- ▶ In this case, let $U = \tau(X, Y)$, where $\tau(x, y)$ is the solution τ to $y = x^{\top}\beta(\tau)$. We have

$$V(\tau) = 1\left\{Y \ge X^{\top}\beta\left(\tau\right)\right\} = 1\left\{X^{\top}\beta\left(U\right) \ge X^{\top}\beta\left(\tau\right)\right\} = 1\left\{U \ge \tau\right\}$$

and $\mathbb{E}[VX] = (1 - \tau) \mathbb{E}[X]$ rewrites as

$$\mathbb{E}\left[1\left\{U \geq \tau\right\} X\right] = (1 - \tau) \,\mathbb{E}\left[X\right]$$

which, assuming that the first dimension of X is the constant 1, yields mean independence

$$\mathbb{E}\left[X|U\right] = \mathbb{E}\left[X\right].$$

► Therefore, when the model is quasi-specified, one has the representation

$$Y = X^{\top} \beta(U)$$
 , $U \sim \mathcal{U}([0,1])$, $\mathbb{E}[X|U] = \mathbb{E}[X]$

Computation of problem using Gurobi

► Recall the problem to compute

$$\max_{\pi \ge 0} U^{\top} \pi Y$$
$$\pi X = \mu \bar{x}$$
$$\pi^{\top} 1_T = p$$

which we sill vectorize using $vec(A\pi B) = (B^{\top} \otimes A) vec(\pi)$ so that the constraint becomes

$$\begin{pmatrix} \mathbf{X}^{\top} \otimes \mathbf{I}_{T} \\ \mathbf{I}_{N} \otimes \mathbf{1}_{T}^{\top} \end{pmatrix} \operatorname{vec}\left(\boldsymbol{\pi}\right) = \begin{pmatrix} \operatorname{vec}\left(\boldsymbol{\mu}\bar{\mathbf{x}}\right) \\ \mathbf{p} \end{pmatrix}$$

- ▶ There are NT primal variables and KT + N constraints.
- ▶ One-line computation in a linear programming solver like Gurobi. Large-scale linear programming solvers make use of sparsity of constraint matrix. However, if dimension of *Y* is larger, *T* will need to be large.

Vector quantile regression

► For vector quantile regression, we solve the problem using
A1 = kronecker(sparseMatrix(1:n,1:n),matrix(1,1,m))
A2 = kronecker(t(X),sparseMatrix(1:m,1:m))
f1 = matrix(t(nu),nrow=n)
f2 = matrix(mu %*% xbar,nrow=m*r)
e = matrix(1,m*n,1)
A = rbind2(A1,A2)
f = rbind2(f1,f2)
result = gurobi
(list(A=A,obj=c,modelsense="min",rhs=f,ub=e,sense="="),
params=NULL)

► See https://github.com/alfredgalichon/VQR/