'MATH+ECON+CODE' MASTERCLASS ON MATCHING MODELS, OPTIMAL TRANSPORT AND APPLICATIONS

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Day 3, January 17 2018: "Optimal transport II"
Block 7. Continuous multivariate matching

- Existence of potentials in the quadratic case
- Knott-Smith criterion and Brenier's and McCann's theorems
- Entropic regularization
- The iterated proportional fitting procedure

- [OTME], Ch. 6
- [TOT] Villani (2003). *Topics in Optimal Transportation*. AMS. Ch. 1 and 2.

Section 1

THEORY

- As a consequence of the previous lecture, we have seen that if P is a continuous distribution over $\mathbb{R}^d$ (distribution of the inhabitants' locations), and if $Q = \sum_{k=1}^{M} q_k \delta_{y_k}$ is a discrete distribution over $\mathbb{R}^d$ (distribution of the fountains' locations), then there exists a mapping T such that $T\#P = Q$, that is

$$Y = T(X)$$

  where:
  - $X \sim P$ and $Y \sim Q$, and $T(x)$ is the location of the fountain assigned to the inhabitant at x.
  - $T(x) = \nabla u(x)$, where u is a convex function which is given by $u(x) = \max_k \{x^\intercal y_k - v_k\}$.
- Note the connection with Becker's model: when the dimension $d = 1$, T is piecewise constant and nondecreasing (positive assortative matching).
- In this lecture, we shall generalize these results to the case when Q is a general distribution (not necessarily discrete). P will have a density, and the support of P and Q will be assumed to be convex.

- Assume that $\mathcal{X}$ and $\mathcal{Y}$ are convex subsets of $\mathbb{R}^d$, and that

$$\Phi\left(x, y\right) = x^{\intercal} y.$$

and P and Q are two probability distributions on $\mathcal{X}$ and $\mathcal{Y}$.

- The Monge-Kantorovich theorem provides assumptions under which the value of the primal problem

$$\mathcal{W} = \sup_{\pi \in \mathcal{M}(P,Q)} \mathbb{E}_{\pi}\left[X^{\intercal} Y\right] \tag{1}$$

coincides with the value of the dual

$$\mathcal{W} = \inf_{u(x)+v(y) \geq x^{\intercal} y} \mathbb{E}_P\left[u\left(X\right)\right] + \mathbb{E}_Q\left[v\left(Y\right)\right]. \tag{2}$$

- Note, however, that the M-K theorem requires Φ to be bounded by above, which is not the case of $\Phi\left(x, y\right) = x^{\intercal} y$ unless we assume P and Q have bounded support. We could alternatively work with $\Phi\left(x, y\right) = -\left|x - y\right|^2/2$, in which case we should assume that P and Q have finite second moment and replace $u\left(x\right)$ by $u\left(x\right) + \left|x\right|^2/2$, and v by a similar quantity. We shall assume away these concerns for now.

The following result ensures that u and v exist as soon as P and Q have finite second moments.

THEOREM

If P and Q have finite second moments, then there exists a pair (u, v) solution to the dual Monge-Kantorovich problem

$$\inf_{u(x)+v(y)\geq x^{\intercal}y} \mathbb{E}_P\left[u\left(X\right)\right] + \mathbb{E}_Q\left[v\left(Y\right)\right].$$

See theorem 2.9 in [TOT].

- Assume that a dual minimizer (u, v) exists; if needed, redefine u and v so that they take value $+\infty$ outside of the support of P and Q, assumed to be convex. As argued, u and v are then related by

$$v(y) = \max_{x \in \mathbb{R}^d} \left\{ x^\intercal y - u(x) \right\} \tag{3}$$

$$u(x) = \max_{y \in \mathbb{R}^d} \left\{ x^\intercal y - v(y) \right\} \tag{4}$$

hence we see immediately that if (u, v) is a solution to the dual problem, then u and v are convex functions. Further, the expression of v as a function of u is the same as the expression of u as a function of v.

We want to relate the solutions to the primal and dual problems. Recall that in the finite-dimensional case, where the primal and the dual problems are related by a complementary slackness condition. In the present case, let $(X, Y) \sim \pi$ be a solution to the primal problem, and (u, u^*) be a solution to the dual problem. Then almost surely X and Y are willing to match, which, by the previous discussion, implies that

$$u(X) + u^*(Y) = X^\intercal Y, \tag{5}$$

that is, the support of π is included in the set $\{(x, y) : u(x) + u^*(y) = x^\intercal y\}$. This condition appears as the correct generalization of the complementary slackness condition in the finite-dimensional case. Without surprise, taking the expectation with respect to π of equality (5) yields the equality between the value of the dual problem on the left-hand side, and the value of the primal problem on the right-hand side.

The following statement provides a generalization of the complementary slackness condition in finite dimension.

THEOREM (KNOTT-SMITH)

Let $\pi \in \mathcal{M}(P, Q)$ and u be a convex function. Then π and (u, u^*) are respective solutions to the primal and the dual Monge-Kantorovich problems if and only if

$$u(x) + u^*(y) = x^\intercal y \text{ holds for } \pi\text{-almost all } (x, y). \quad (6)$$

PROOF.

Assume that (6) holds. Then, note that (u, u^*) satisfies the constraints of the dual; further, taking expectation with respect to π yields $\mathbb{E}_P[u(X)] + \mathbb{E}_Q[v(Y)] = \mathbb{E}_\pi[X^\intercal Y]$, which implies that π is an optimal primal solution and (u, u^*) is an optimal dual solution. Conversely, assume that π is an optimal primal solution and (u, u^*) is an optimal dual solution. Then $\mathbb{E}_\pi[u(X) + u^*(Y) - X^\intercal Y] = 0$; but $(x, y) \to u(x) + u^*(y) - x^\intercal y$ is nonnegative, thus (6) holds. □

THEOREM (BRENIER)

Assume that P and Q have finite second moments, and P has a density. Then the solution $(X, Y) \sim \pi \in \mathcal{M}(P, Q)$ to the primal problem is represented by

$$Y = \nabla u(X)$$

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

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

While we evoked the case when the Kantorovich potentials u and v are differentiable, there is no a-priori guarantee that they are so. However, an important result in Analysis called Rademacher's theorem implies that the set of non-differentiable points of a convex function is of zero Lebesgue measure, and hence can be ignored for practical purposes as soon as P is continuous. Thus the Monge map solution, $T(x)$, can be defined as $T(x) = \nabla u(x)$ wherever the latter quantity exists, and $T(x)$ can be defined arbitrarily elsewhere, without affecting the distributional properties of $T(X)$.

The previous result allows to provide a representation of a large class of probability distributions Q over $\mathbb{R}^d$ as the probability distribution of $\nabla u(X)$, for X with a fixed distribution P. There is however a limitation, in the sense that it requires that Q has finite second moments, which is needed to interpret u as entering the solution to the dual problem. Fortunately, McCann's theorem addresses this issue:

Theorem (Brenier)

Assume that P and Q are probability distributions such that P has a density. Then the solution $(X, Y) \sim \pi \in \mathcal{M}(P, Q)$ to the primal problem is represented by

$$Y = \nabla u(X)$$

for some convex function u which is unique up to a constant.

- When $P = \mathcal{N}(0, \Sigma_X)$ and $Q = \mathcal{N}(0, \Sigma_Y)$, one can get a solution in closed form.
  - Consider first the case when $\Sigma_X = I$. Then the optimal transport map $T(x) = \Sigma_Y^{1/2} x$ is a linear map.
  - General case is done by wrting $X = \Sigma_X^{1/2} U$, where $U \sim \mathcal{N}(0, I)$. Then $\max \mathbb{E}\left[U \Sigma_X^{1/2} Y\right]$ is obtained when $\Sigma_X^{1/2} Y = \left(\Sigma_X^{1/2} \Sigma_Y \Sigma_X^{1/2}\right)^{1/2} U$, so the solution is

$$Y = \Sigma_X^{-1/2} \left(\Sigma_X^{1/2} \Sigma_Y \Sigma_X^{1/2}\right)^{1/2} \Sigma_X^{-1/2} X.$$

- Actually, one has even a closed-form solution in the case when $\Phi(x, y) = x^{\intercal} A y$. (This is left as an exercise).

- Consider the problem

$$\max_{\pi \in \mathcal{M}(P,Q)} \iint_{\mathcal{X}\times\mathcal{Y}} x^{\intercal} y \pi(x,y)\, dxdy - \sigma \iint_{\mathcal{X}\times\mathcal{Y}} \pi(x,y) \ln \pi(x,y)\, dxdy$$

where $\sigma > 0$. The problem coincides with the optimal assignment problem when $\sigma = 0$. When $\sigma \to +\infty$, the solution to this problem approaches the independent coupling, $\pi(x,y) = f_P(x) f_Q(y)$.

- The dual problem yields

$$\min_{u,v} \left\{ \begin{array}{c} \int_{\mathcal{X}} u(x)\, dP(x) + \int_{\mathcal{Y}} v(y)\, dQ(y) + \\ \sigma \left(\iint_{\mathcal{X}\times\mathcal{Y}} \exp\left(\frac{x^{\intercal} y - u(x) - v(y)}{\sigma} \right) dxdy - 1 \right) \end{array} \right\},$$

and the classical optimal transport duality is recovered when $\sigma \to 0$.

- By optimality conditions,

$$\pi(x,y) = \exp\left(\frac{x^\intercal y - u(x) - v(y)}{\sigma}\right)$$

where $u(x)$ and $v(y)$ satisfy the Bernstein-Schrödinger equation

$$\left\{\begin{array}{l} \int_{\mathcal{Y}} \exp\left(\frac{x^\intercal y - u(x) - v(y)}{\sigma}\right) dy = f_P(x) \\ \int_{\mathcal{X}} \exp\left(\frac{x^\intercal y - u(x) - v(y)}{\sigma}\right) dx = f_Q(y) \end{array}\right. .$$

- Hence, letting $A(x) = \exp(-u(x)/\sigma)$ and $B(y) = \exp(-v(y)/\sigma)$ and $K(x,y) = \exp(x^\intercal y/\sigma)$, one has $\pi(x,y) = A(x)B(y)K(x,y)$, and

$$\left\{\begin{array}{l} A(x) = f_P(x) / \int_{\mathcal{Y}} K(x,y)B(y)\,dy \text{ and} \\ B(y) = f_Q(y) / \int_{\mathcal{X}} K(x,y)A(x)\,dx. \end{array}\right.$$

Section 2

CODING

- The iterated proportional fitting procedure (ipfp) consists of taking an initial guess $B^0(x)$, and do

$$\begin{cases} A^1(x) = f_P(x) \,/\, \int_{\mathcal{Y}} K(x,y) \, B^0(y) \, dy \\ B^1(y) = f_Q(y) \,/\, \int_{\mathcal{X}} K(x,y) \, A^1(x) \, dx \end{cases}$$

  and iterate.

- This is implemented by IPFP1:

```
K=exp(Phi/sigma)
B=rep(1,nbY)
while (cont) {
A = p / (K %*% B)
KA = c(A %*% K)
if (max(abs(KA*B - q))<tol ) {cont=FALSE}
B = q / KA }
```

- The previous program is extremely fast, partly due to the fact that it involves linear algebra operations. However, it breaks down when σ is small; this is best seen taking a log transform and returning to $u^k = -\sigma \log A^k$ and $v^k = -\sigma \log B^k$, that is

$$\left\{ \begin{array}{l} u^k(x) = \mu(x) + \sigma \log \int_{\mathcal{Y}} \exp\left(\frac{x^\intercal y - v^{k-1}(y)}{\sigma}\right) dy \\ v^k(y) = \nu(y) + \sigma \log \int_{\mathcal{X}} \exp\left(\frac{x^\intercal y - u^k(x)}{\sigma}\right) dx \end{array} \right.$$

  where $\mu(x) = -\sigma \log f_P(x)$ and $\nu(y) = -\sigma \log f_Q(y)$.
- One sees what may go wrong: if $x^\intercal y - v^{k-1}(y)$ is positive in the exponential in the first sum, then the exponential blows up due to the small σ at the denominator. However, a very simple trick, called the "log-sum-exp trick" in order to avoid this issue.

- Consider

$$\left\{ \begin{array}{l} \left(v^{k-1}\right)^{*}(x) = \max_{y} \left\{x^{\intercal}y - v^{k-1}(y)\right\} \\ \left(u^{k}\right)^{*}(y) = \max_{x} \left\{x^{\intercal}y - u^{k}(x)\right\} \end{array} \right.$$

(as we shall see next block, these will be interpreted as the Legendre-Fenchel transforms of v^{k-1} and u^{k}, respectively).

- One has

$$\left\{ \begin{array}{l} u^{k}(x) = \mu(x) + \left(v^{k-1}\right)^{*}(x) + \sigma \log \int_{\mathcal{Y}} \exp\left(\frac{x^{\intercal}y - v^{k-1}(y) - \left(v^{k-1}\right)^{*}(x)}{\sigma}\right) dy \\ v^{k}(y) = \nu(y) + \left(u^{k}\right)^{*}(y) + \sigma \log \int_{\mathcal{X}} \exp\left(\frac{x^{\intercal}y - u^{k}(x) - \left(u^{k}\right)^{*}(y)}{\sigma}\right) dx \end{array} \right.$$

and now the arguments of the exponentials are always nonpositive, ensuring the exponentials don't blow up.

- This is implemented as IPFP2:

```
vstar = apply(t(t(Phi) - v), 1, max)
u=mu + vstar + sigma * log(apply(exp( (Phi -
matrix(v,nbX,nbY,byrow=T)- vstar)/sigma) ,1,sum))
ustar = apply( Phi - u , 2, max)
v=nu + ustar + sigma * log(apply(exp( (Phi -
matrix(ustar,nbX,nbY,byrow=T)- u)/sigma) ,2,sum))
```

- When we run it on the example in '07-appli-ipfp', we see that IPFP1 is faster, but more fragile; indeed:
  - for $\sigma = 10^{-2}$, both algorithms converge, the IPFP1 in 0.05s, and IPFP2 in 0.11s.
  - for $\sigma = 10^{-3}$, IPFP1 fails, and IPFP2 converges in 109s.