Lectures on optimal transport

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1 Roadmap

L1. Discrete optimal transport
L2. Inverse optimal transport
L3. Optimal transport and quantile methods

2 Optimal transport in the discrete case

Central planner's solution
Workers characteristics $x \in X$
n_x workers of type x

Firms characteristics $y \in Y$
m_y firms of type y

$\sum_x n_x = \sum_y m_y$

A matching π_{xy} is the mass of workers of type x matched with firms of type y

Constraints:
$\sum_y \pi_{xy} = n_x$
$\sum_x \pi_{xy} = m_y$

Let Φ_{xy} be the productivity (in dollar terms) of a worker of type x matched with a firm of type y.

Central planner's problem:
$\max_{\pi \geq 0} \sum_{xy} \pi_{xy} \Phi_{xy}$
s.t.
$\sum_y \pi_{xy} = n_x$
$\sum_x \pi_{xy} = m_y$

$\max_{\pi \geq 0} \sum_{xy} \pi_{xy} \Phi_{xy} + \min_{u_x, v_y} \sum_x u_x \left(n_x - \sum_y \pi_{xy} \right) + \sum_y v_y \left(m_y - \sum_x \pi_{xy} \right)$
$\max_{\pi \geq 0} \min_{u_x, v_y} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y \right) + \sum_x u_x n_x + \sum_y v_y m_y$
$\min_{u_x, v_y} \max_{\pi \geq 0} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y \right) + \sum_x u_x n_x + \sum_y v_y m_y$

$\min_{u_x,v_y} \sum_x u_x n_x + \sum_y v_y m_y + \max_{\pi\geq 0} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y\right)$
This becomes
$\min_{u_x,v_y} \sum_x u_x n_x + \sum_y v_y m_y + \max_{\pi\geq 0} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y\right)$

hence we arrive at the **dual to the central planner's problem**
$\min_{u_x,v_y} \sum_x u_x n_x + \sum_y v_y m_y$
s.t. $u_x + v_y \geq \Phi_{xy}$

Complementary slackness
$\pi_{xy} > 0 \implies u_x + v_y = \Phi_{xy}$

The dual problem can be interpreted as the equilibrium in the wage market.
Indeed, consider the dual
$\min_{u_x,v_y} \sum_x u_x n_x + \sum_y v_y m_y$
s.t. $u_x + v_y \geq \Phi_{xy}$

Rewrite the constraint into
$v_y \geq \max_x \left\{\Phi_{xy} - u_x\right\}$

Claim: the dual can rewrite as
$\min_{u_x,v_y} \sum_x u_x n_x + \sum_y v_y m_y$
s.t. $v_y = \max_x \left\{\Phi_{xy} - u_x\right\}$

Equation
$v_y = \max_x \left\{\Phi_{xy} - u_x\right\}$
interprets as profit maximization by the firm.

2.1 Becker's theory of marriage

Becker's model of heterosexual marriage market
$x \in X$ man's characteristics in number n_x
$y \in Y$ woman's characteristics in number m_y

Assume that if x matches with y then
- x enjoys utility α_{xy}
- y enjoys utility γ_{xy}

Becker assumed **fully transferable utility**: if x gives up a quantity τ of utility to y, then after transfers
x gets $\alpha_{xy} - \tau$
y gets $\gamma_{xy} + \tau$

Note: we could get $\gamma_{xy} + f\left(\tau\right)$ but this would not be optimal transport. This is called matching with imperfectly transferable utility.

The limit without any possible transfers is called non-transferable utility model, this is Gale-Shapley's model.

Back to Becker's model

No matter the transfer, x and y if they match get joint surplus $\Phi_{xy} = \alpha_{xy} + \gamma_{xy}$.

2.2 Actual model of transportation

Koopmans-Beckmann model.

$x \in X$ the locations of plants. Production (of a commodity) by plant x is n_x per day.

$y \in Y$ the locations of cities. Consumption of the same commodity by city y is m_y per day.

Total production = total consumption

(unit) Transportation cost from plant x to city y is c_{xy} per unit of mass.

Tolstoi's problem (1920).

Define π_{xy} the mass of commodity which will route from x to y. The optimal shipping plan is given by

$\min_{\pi \geq 0} \sum_{xy} \pi_{xy} c_{xy}$

s.t.

$\sum_y \pi_{xy} = n_x$

$\sum_x \pi_{xy} = m_y$

The dual of this problem is

$\max_{p_x, p_y} \sum_y m_y p_y - \sum_x n_x p_x$

$p_y - p_x \leq c_{xy}$

$\sum_y m_y p_y = \sum_x n_x p_x + \sum_{xy} \pi_{xy} c_{xy}$: total price at destination=total price at origin+total shipping cost

The constraint in the dual

$p_y \leq c_{xy} + p_x$

says that there is no pair xy such that

$p_y > c_{xy} + p_x$

this is a no-arbitrage conditions.

$\Phi(x, y) = x^\top A y = \sum_{kl} A_{kl} x^k y^l$

Most LP solvers compute

$\max_{z \geq 0} c^\top z$

s.t. $Mz = d$

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

s.t.
$\sum_y \pi_{xy} = n_x$
$\sum_x \pi_{xy} = m_y$

$vec\left(\pi\right)$

$I_X \pi 1_Y = n$
$1_X^\top \pi I_Y = m^\top$

Get $vec\left(\pi 1_Y\right) = (...)vec\left(\pi\right)$ and $vec\left(1_X^\top \pi\right) = (...)\, vec\left(\pi\right)$
We have
$vec\left(AXB^\top\right) = \left(A \otimes B\right) vec\left(X\right)$

THis gives
$vec\left(I_X \pi 1_Y\right) = n$
$vec\left(1_X^\top \pi I_Y\right) = m$
therefore
$\left(I_X \otimes 1_Y^\top\right) vec\left(\pi\right) = n$
$\left(1_X^\top \otimes I_Y\right) vec\left(\pi\right) = m$

The OT problem can be computed as
$\max_{\pi \geq 0} vec\left(\pi\right)^\top vec\left(\Phi\right)$
s.t.
$\left(I_X \otimes 1_Y^\top\right) vec\left(\pi\right) = n$
$\left(1_X^\top \otimes I_Y\right) vec\left(\pi\right) = m$

3 Entropic regularization

$\max_{\pi \geq 0} \sum_{xy} \pi_{xy} \Phi_{xy} - \sigma \sum_{xy} \pi_{xy} \ln \pi_{xy}$
s.t.
$\sum_y \pi_{xy} = n_x \;\; [u_x]$
$\sum_x \pi_{xy} = m_y \;\; [v_y]$

$\max_{\pi \geq 0} \sum_{xy} \pi_{xy} \Phi_{xy} - \sigma \sum_{xy} \pi_{xy} \ln \pi_{xy} + \min_{u_x, v_y} \sum_x u_x \left(n_x - \sum_y \pi_{xy}\right) + \sum_y v_y \left(m_y - \sum_x \pi_{xy}\right)$
$\max_{\pi \geq 0} \min_{u_x, v_y} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y - \sigma \log \pi_{xy}\right) + \sum_x u_x n_x + \sum_y v_y m_y$
$\min_{u_x, v_y} \max_{\pi \geq 0} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y - \sigma \log \pi_{xy}\right) + \sum_x u_x n_x + \sum_y v_y m_y$
$\min_{u_x, v_y} \sum_x u_x n_x + \sum_y v_y m_y + \max_{\pi \geq 0} \sum_{xy} \pi_{xy} \left(\Phi_{xy} - u_x - v_y - \sigma \log \pi_{xy}\right)$

FOC in the inner problem
$\left(\Phi_{xy} - u_x - v_y - \sigma \log \pi_{xy}\right) - \sigma = 0$
thus
$\pi_{xy} = \exp\left(\frac{\Phi_{xy} - u_x - v_y - \sigma}{\sigma}\right)$
and the value of the inner problem is $\sigma \sum_{xy} \pi_{xy} = \sigma \sum_{xy} \exp\left(\frac{\Phi_{xy} - u_x - v_y - \sigma}{\sigma}\right)$.

The outer problem becomes
$\min_{u_x,v_y} F(u,v) := \sum_x u_x n_x + \sum_y v_y m_y + \sigma \sum_{xy} \exp\left(\frac{\Phi_{xy}-u_x-v_y-\sigma}{\sigma}\right)$

Foc yield
wrt u_x: $n_x = \sum_y \exp\left(\frac{\Phi_{xy}-u_x-v_y-\sigma}{\sigma}\right)$
wrt v_y: $m_y = \sum_x \exp\left(\frac{\Phi_{xy}-u_x-v_y-\sigma}{\sigma}\right)$

(Blockwise) Coordinate descent.
Given v_y's compute u_x by $\min_{u_x} F(u,v)$
$n_x = \sum_y \exp\left(\frac{\Phi_{xy}-u_x-v_y-\sigma}{\sigma}\right)$
yields
$\exp(u_x/\sigma) = \sum_y \exp\left(\frac{\Phi_{xy}-v_y-\sigma}{\sigma}\right)/n_x$
similarly Given u_x's compute v_y by $\min_{v_y} F(u,v)$
yields
$\exp(v_y/\sigma) = \sum_x \exp\left(\frac{\Phi_{xy}-u_x-\sigma}{\sigma}\right)/m_y$

Sinkhorn's algorithm / Itererated Proportional Fitting Procedure
https://arxiv.org/abs/1609.06349

Write $A_x = \exp(-u_x/\sigma)$ and $B_y = \exp(-v_y/\sigma)$
and $K_{xy} = \exp\left(\frac{\Phi_{xy}-\sigma}{\sigma}\right)$, we have
$A_x = n_x / \sum_y K_{xy} B_y$
similarly Given u_x's compute v_y by $\min_{v_y} F(u,v)$
yields
$B_y = m_y / \sum_x K_{xy} A_y$

When σ is small
$u_x = \sigma \log\left(\sum_y \exp\left(\frac{\Phi_{xy}-v_y-\sigma}{\sigma}\right)\right) - \sigma \log n_x$
log-sum-exp trick
When computing numerically
$\sigma \log \sum_y \exp\left(\frac{z_y}{\sigma}\right)$
you should
$m = \max_y \{z_y\}$
and use the fact that for any c
$\sigma \log \sum_y \exp\left(\frac{z_y-c}{\sigma}\right) + c = \sigma \log \sum_y \exp\left(\frac{z_y}{\sigma}\right)$
use this with $c = m$ and get
$\sigma \log \sum_y \exp\left(\frac{z_y}{\sigma}\right) = \sigma \log \sum_y \exp\left(\frac{z_y-m}{\sigma}\right) + m$

4 Inverse optimal transport

Go back to the labor market, but this time introducing unmatched agents

Consider primal problem

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

s.t.

$\sum_y \pi_{xy} \leq n_x$

$\sum_x \pi_{xy} \leq m_y$

which has dual

$\min_{u_x \geq 0, v_y \geq 0} \sum_x n_x u_x + \sum_y m_y v_y$

s.t.

$u_x + v_y \geq \Phi_{xy}$

Introduce unobserved heterogeneity.

Now we assume that n_x and m_y are very large.

Individual worker $i \in I$ has type $x_i \in X$

Individual firm $j \in J$ has type $y_j \in Y$

Assume that the joint output generated by i and j together is

$\Phi_{ij} = \Phi_{x_i y_j} + \varepsilon_{i y_j} + \eta_{x_i j}$. (Separability assumption).

The dual is

$\min \sum_{i \in I} u_i + \sum_{j \in J} v_j$

s.t.

$u_i + v_j \geq \Phi_{ij} := \Phi_{x_i y_j} + \varepsilon_{i y_j} + \eta_{x_i j}$

$u_i \geq \varepsilon_{i0}$

$v_j \geq \eta_{0j}$

Take a look at the constraint

$u_i + v_j \geq \Phi_{x_i y_j} + \varepsilon_{i y_j} + \eta_{x_i j}$

rewrtie this as

$u_i - \varepsilon_{iy} + v_j - \eta_{xj} \geq \Phi_{xy}$ for all $i : x_i = x$ and for all $j : y_j = y$

$\min_{i:x_i=x} \{u_i - \varepsilon_{iy}\} + \min_{j:y_j=y} \left\{v_j - \eta_{xj}\right\} \geq \Phi_{xy}$

define $U_{xy} = \min_{i:x_i=x} \{u_i - \varepsilon_{iy}\}$ and $V_{xy} = \min_{j:y_j=y} \left\{v_j - \eta_{xj}\right\}$, in which case the constraints become

$U_{xy} + V_{xy} \geq \Phi_{xy}$

We have $U_{xy} = \min_{i:x_i=x} \{u_i - \varepsilon_{iy}\}$, therefore $u_i \geq \max_y \{U_{xy} + \varepsilon_{iy}, \varepsilon_{i0}\}$ and similarly $v_j \geq \max_x \left\{V_{xy} + \eta_{xj}, \eta_{0j}\right\}$

The micro problem rewrites

$\min \sum_{i \in I} u_i + \sum_{j \in J} v_j$

s.t.

$U_{xy} + V_{xy} \geq \Phi_{xy}$

$u_i \geq \max_y \{U_{xy} + \varepsilon_{iy}, \varepsilon_{i0}\}$

$v_j \geq \max_x \left\{V_{xy} + \eta_{xj}, \eta_{0j}\right\}$

and in fact
$\min \sum_{i\in I} u_i + \sum_{j\in J} v_j$
s.t.
$U_{xy} + V_{xy} \geq \Phi_{xy}$
$u_i = \max_y \{U_{xy} + \varepsilon_{iy}, \varepsilon_{i0}\}$
$v_j = \max_x \left\{V_{xy} + \eta_{xj}, \eta_{0j}\right\}$

which can rewrite
$\min \sum_{i\in I} \max_y \{U_{xy} + \varepsilon_{iy}, \varepsilon_{i0}\} + \sum_{j\in J} \max_x \left\{V_{xy} + \eta_{xj}, \eta_{0j}\right\}$
s.t.
$U_{xy} + V_{xy} \geq \Phi_{xy}$

that is
$\min \sum_x n_x \sum_{i:x_i=x} \frac{1}{n_x} \max_y \{U_{xy} + \varepsilon_{iy}, \varepsilon_{i0}\} + \sum_y m_y \sum_{j:y_j=y} \frac{1}{m_y} \max_x \left\{V_{xy} + \eta_{xj}, \eta_{0j}\right\}$
s.t.
$U_{xy} + V_{xy} \geq \Phi_{xy}$

We shall assume a statistical behaviour of ε_{iy} and η_{xj}'s. Assume that $(\varepsilon_{iy})_y$ is distributed according to P
and that $\left(\eta_{xj}\right)_x$ is distributed according to Q.
By the law of large numbers the above expression converges to
$\min_{U,V} \sum_x n_x E_P \left[\max_y \{U_{xy} + \varepsilon_y, \varepsilon_0\}\right] + \sum_y m_y E_Q \left[\max_x \{V_{xy} + \eta_x, \eta_0\}\right]$
s.t.
$U_{xy} + V_{xy} \geq \Phi_{xy}$

Define $G_x(U) = E_P \left[\max_y \{U_{xy} + \varepsilon_y, \varepsilon_0\}\right]$ and $H_y(V) = E_Q \left[\max_x \{V_{xy} + \eta_x, \eta_0\}\right]$
and $G(U) = \sum_x n_x G_x(U)$ and $H(V) = \sum_y m_y H_y(V)$
the problem becomes

$\min_{U,V} G(U) + H(V)$
s.t.
$U_{xy} + V_{xy} = \Phi_{xy}$

$\min_U G(U) + H(\Phi - U)$
FOC
$\frac{\partial G(U)}{\partial U_{xy}} = \frac{\partial H}{\partial V_{xy}} (\Phi - U)$

$\frac{\partial G(U)}{\partial U_{xy}} = n_x \frac{\partial G_x(U)}{\partial U_{xy}} = n_x \Pr\left(y \in \arg\max \{U_{xy} + \varepsilon_y, \varepsilon_0\}\right)$
$\frac{\partial H(V)}{\partial V_{xy}} = m_y \Pr\left(x \in \arg\max \{V_{xy} + \eta_x, \eta_0\}\right)$

Dual problem:
Start from the penalized problem
$\min_{U,V} G(U) + H(V) + \max_{\pi\geq 0} \sum \pi_{xy} (\Phi_{xy} - U_{xy} - V_{xy})$
$\max_{\pi\geq 0} \sum \pi_{xy}\Phi_{xy} + \min_{U,V} \left\{G(U) + H(V) - \sum \pi_{xy} (U_{xy} + V_{xy})\right\}$
$\max_{\pi\geq 0} \sum \pi_{xy}\Phi_{xy} - \max_U \left\{\sum \pi_{xy}U_{xy} - G(U)\right\} - \max_V \left\{\sum \pi_{xy}V_{xy} - H(V)\right\}$

Define the convex conjugates / Legendre-Fenchel transforms of G and H as
$G^*(\pi) = \max_U \left\{\sum \pi_{xy} U_{xy} - G(U)\right\}$
$H^*(\pi) = \max_V \left\{\sum \pi_{xy} V_{xy} - H(V)\right\}$
and the problem becomes
$\max_{\pi_{xy} \geq 0} \left\{\sum \pi_{xy} \Phi_{xy} - G^*(\pi) - H^*(\pi)\right\}$

FOC yield
$\Phi_{xy} = \frac{\partial G^*(\pi)}{\partial \pi_{xy}} + \frac{\partial H^*(\pi)}{\partial \pi_{xy}}$

When P (the distribution of $(\varepsilon_{iy})_y$) is the Gumbel distribution (extreme-value type 1 – distribution with cdf $\exp(-\exp(-z))$)
https://en.wikipedia.org/wiki/Gumbel_distribution

then $G_x(U) = \log\left(1 + \sum_y \exp U_{xy}\right)$, and therefore $G(U) = \sum_x n_x \log\left(1 + \sum_y \exp U_{xy}\right)$.
We have
$G_x^*(\pi) = \sum_{y \in Y} \frac{\pi_{xy}}{n_x} \log \frac{\pi_{xy}}{n_x} + \frac{\pi_{x0}}{n_x} \log \frac{\pi_{x0}}{n_x}$ where $\pi_{x0} = n_x - \sum_y \pi_{xy}$

Therefore the primal problem in this case rewrites
$\max_{\pi_{xy} \geq 0} \left\{\sum \pi_{xy} \Phi_{xy} - \sum_x n_x \sum_{y \in Y} \frac{\pi_{xy}}{n_x} \log \frac{\pi_{xy}}{n_x} - \pi_{x0} \log \frac{\pi_{x0}}{n_x} - \sum_y m_y \sum_{x \in X} \frac{\pi_{xy}}{m_y} \log \frac{\pi_{xy}}{m_y} - \pi_{0y} \log \frac{\pi_{0y}}{m_y}\right\}$
which yields
$\max_{\pi_{xy} \geq 0} \left\{\sum \pi_{xy} \Phi_{xy} - \sum_{xy} \pi_{xy} \log \frac{\pi_{xy}^2}{n_x m_y} - \pi_{x0} \log \frac{\pi_{x0}}{n_x} - \pi_{0y} \log \frac{\pi_{0y}}{m_y}\right\}$

First order conditions wrt π_{xy}:
$\Phi_{xy} = 2 + 2\log \pi_{xy} - \log(n_x m_y) - (1 + \log \pi_{x0} - \log n_x) - (1 + \log \pi_{0y} - \log m_y)$.
This is Choo and Siow's formula (Journal of Political Economy, 2006)

$$\Phi_{xy} = \log \frac{\pi_{xy}^2}{\pi_{x0} \pi_{0y}}.$$