Lecture 2b: optimal transport with entropic regularization

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https://www.math-econ-code.org/regularized-optimal-transport

- Entropic regularization
- The log-sum-exp trick
- The Iterated Proportional Fitting Procedure (IPFP)

References for block 9

- [OTME], Ch. 7.3
- Peyré, Cuturi, Computational Optimal Transport, Ch. 4.

- Consider the problem

$$\max_{\pi \in \mathcal{M}(p,q)} \sum_{ij} \pi_{ij} \Phi_{ij} - \sigma \sum_{ij} \pi_{ij} \ln \pi_{ij}$$

  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, $\pi_{ij} = p_i q_j$.
- Later on, we will provide microfoundations for this problem, and connect it with a number of important methods in economics (BLP, gravity model, Choo-Siow...). For now, let's just view this as an extension of the optimal transport problem.

- Let's compute the dual by the minimax approach. We have

$$\max_{\pi \geq 0} \min_{u,v} \sum_{ij} \pi_{ij} \left(\Phi_{ij} - u_i - v_j - \sigma \ln \pi_{ij} \right) + \sum_i u_i p_i + \sum_j v_j q_j$$

thus

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j + \max_{\pi \geq 0} \sum_{ij} \pi_{ij} \left(\Phi_{ij} - u_i - v_j - \sigma \ln \pi_{ij} \right)$$

- By FOC in the inner problem, one has $\Phi_{ij} - u_i - v_j - \sigma \ln \pi_{ij} - \sigma = 0$,thus

$$\pi_{ij} = \exp \left(\frac{\Phi_{ij} - u_i - v_j - \sigma}{\sigma} \right)$$

and $\pi_{ij} \left(\Phi_{ij} - u_i - v_j - \sigma \ln \pi_{ij} \right) = \sigma \pi_{ij}$, thus the dual problem is

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j + \sigma \sum_{ij} \exp \left(\frac{\Phi_{ij} - u_i - v_j - \sigma}{\sigma} \right).$$

- After replacing v_j by $v_j + \sigma$, the dual is

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j + \sigma \sum_{ij} \exp \left(\frac{\Phi_{ij} - u_i - v_j}{\sigma} \right) - \sigma. \tag{V1}$$

- Claim: the problem is equivalent to

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j + \sigma \log \sum_{i,j} \exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right) \qquad \text{(V2)}$$

- Indeed, let us go back to the minimax expression

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j + \max_{\pi \geq 0} \sum_{ij} \pi_{ij} \left(\Phi_{ij} - u_i - v_j - \sigma \ln \pi_{ij}\right)$$

we see that the solution π has automatically $\sum_{ij} \pi_{ij} = 1$; thus we can incorporate the constraint into

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j + \max_{\pi \geq 0 : \sum_{ij} \pi_{ij} = 1} \sum_{ij} \pi_{ij} \left(\Phi_{ij} - u_i - v_j - \sigma \ln \pi_{ij}\right)$$

which yields (V2).

- Expression (V2) is interesting because, taking *any* $\hat{\pi} \in M(p,q)$, (V2) reexpresses as

$$\max_{u,v} \sum_{ij} \hat{\pi}_{ij} \left(\frac{\Phi_{ij} - u_i - v_j}{\sigma} \right) - \log \sum_{ij} \exp \left(\frac{\Phi_{ij} - u_i - v_j}{\sigma} \right)$$

therefore if the parameter is $\theta = (u, v)$, observations are *ij* pairs, and the likelihood of *ij* is

$$\pi^{\theta}_{ij} = \frac{\exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right)}{\sum_{ij} \exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right)}$$

- Hence, (V2) will coincide with the maximum likelihood in this model.

- Consider

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j \tag{V3}$$
$$s.t. \sum_{i,j} \exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right) = 1$$

- It is easy to see that the solutions of this problem coincide with (V2). Indeed, the Lagrange multiplier is forced to be one. In other words,

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j \tag{V3}$$
$$s.t. \sigma \log \sum_{i,j} \exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right) = 0$$

- Recall that when $\sigma \to 0$, one has

$$\sigma \log \left(e^{a/\sigma} + e^{b/\sigma} \right) \to \max(a, b)$$

- Indeed, letting $m = \max(a, b)$,

$$\sigma \log \left(e^{a/\sigma} + e^{b/\sigma} \right) = m + \sigma \log \left(\exp\left(\frac{a-m}{\sigma} \right) + \exp\left(\frac{b-m}{\sigma} \right) \right), \tag{1}$$

  and the argument of the logarithm lies between 1 and 2.

- This simple remark is actually a useful numerical recipe called the *log-sum-exp trick*: when σ is small, using (1) to compute $\sigma \log \left(e^{a/\sigma} + e^{b/\sigma} \right)$ ensures the exponentials won't blow up.

- Back to the third expression, with $\sigma \to 0$, one has

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j \tag{V3}$$
$$s.t. \max_{ij} \left(\Phi_{ij} - u_i - v_j \right) = 0$$

- This is exactly equivalent with the classical Monge-Kantorovich expression

$$\min_{u,v} \sum_i u_i p_i + \sum_j v_j q_j \tag{V3}$$
$$s.t. \Phi_{ij} - u_i - v_j \leq 0$$

- We can compute $\min F(x)$ by two methods:
  - Either by gradient descent: $x(t+1) = x_t - \epsilon_t \nabla F(x_t)$. (Steepest descent has $\epsilon_t = 1/\left|\nabla F(x_t)\right|$.)
  - Or by coordinate descent: $x_i(t+1) = \arg\min_{x_i} F(x_i, x_{-i}(t))$.
- Why do these methods converge? Let's provide some justification. We will decrease x_t by ϵd_t, were d_t is normalized by $\left|d_t\right|_p := \left(\sum_{i=1}^n d_t^i\right)^{1/p} = 1$. At first order, we have

$$F(x_t - \epsilon d_t) = F(x_t) - \epsilon d_t^\intercal \nabla F(x_t) + O\left(\epsilon^1\right).$$

- We need to maximize $d_t^\intercal \nabla F(x_t)$ over $\left|d_t\right|_p = 1$.
  - For $p = 2$, we get $d_t = \nabla F(x_t) / \left|\nabla F(x_t)\right|$
  - For $p = 1$, we get $d_t = sign\left(\partial F(x_t) / \partial x^i\right)$ if $\left|\partial F(x_t) / \partial x^i\right| = \max_j \left|\partial F(x_t) / \partial x^j\right|$, 0 otherwise.

- Here, gradient descent is

$$u_i\left(t+1\right)=u_i\left(t\right)-\epsilon\frac{\partial F}{\partial u_i}\left(u\left(t\right),v\left(t\right)\right),\text{ and}$$
$$v_j\left(t+1\right)=v_j\left(t\right)-\epsilon\frac{\partial F}{\partial v_j}\left(u\left(t\right),v\left(t\right)\right)$$

while coordinate descent is

$$\frac{\partial F}{\partial u_i}\left(u_i\left(t+1\right),u_{-i}\left(t\right),v\left(t\right)\right)=0,\text{ and }\frac{\partial F}{\partial v_j}\left(u\left(t\right),v_j\left(t+1\right),v_{-j}\left(t\right)\right)=0.$$

- Gradient of objective function in V1:

$$\left(p_i - \sum_j \exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right), q_j - \sum_i \exp\left(\frac{\Phi_{ij} - u_i - v_j}{\sigma}\right)\right)$$

- Gradient of objective function in V2:

$$\left(p_i - \frac{\sum_j \exp\left(\frac{\Phi_{ij}-u_i-v_j}{\sigma}\right)}{\sum_{ij} \exp\left(\frac{\Phi_{ij}-u_i-v_j}{\sigma}\right)}, q_j - \frac{\sum_i \exp\left(\frac{\Phi_{ij}-u_i-v_j}{\sigma}\right)}{\sum_{ij} \exp\left(\frac{\Phi_{ij}-u_i-v_j}{\sigma}\right)}\right)$$

- Coordinate descent on objective function in V1:

$$p_i = \sum_j \exp\left(\frac{\Phi_{ij} - u_i(t+1) - v_j(t)}{\sigma}\right),$$

$$q_j = \sum_i \exp\left(\frac{\Phi_{ij} - u_i(t) - v_j(t+1)}{\sigma}\right)$$

that is

$$\begin{cases} u_i(t+1) = \sigma \log\left(\frac{1}{p_i}\sum_j \exp\left(\frac{\Phi_{ij}-v_j(t)}{\sigma}\right)\right) \\ v_j(t+1) = \sigma \log\left(\frac{1}{q_j}\sum_i \exp\left(\frac{\Phi_{ij}-u_i(t)}{\sigma}\right)\right) \end{cases}$$

this is called the Iterated Fitting Proportional Procedure (IPFP), or Sinkhorn's algorithm.

- Coordinate descent on objective function in V2 does not yield a closed-form expression.

- Letting $a_i = \exp\left(-u_i/\sigma\right)$ and $b_j = \exp\left(-v_j/\sigma\right)$ and $K_{ij} = \exp\left(\Phi_{ij}/\sigma\right)$, one has $\pi_{ij} = a_i b_j K_{ij}$, and the procedure reexpresses as

$$\begin{cases} a_i\left(t+1\right) = p_i / \left(Kb\left(t\right)\right)_i \text{ and} \\ b_j\left(t+1\right) = q_j / \left(K^{\intercal} a\left(t\right)\right)_j. \end{cases}$$

- 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

$$\begin{cases} u_i^k = \mu_i + \sigma \log \sum_j \exp\left(\frac{\Phi_{ij} - v_j^{k-1}}{\sigma}\right) \\ v_j^k = \zeta_j + \sigma \log \sum_i \exp\left(\frac{\Phi_{ij} - u_i^k}{\sigma}\right) \end{cases}$$

  where $\mu_i = -\sigma \log p_i$ and $\zeta_j = -\sigma \log q_j$.

- One sees what may go wrong: if $\Phi_{ij} - v_j^{k-1}$ is positive in the exponential in the first sum, then the exponential blows up due to the small σ at the denominator. However, the "log-sum-exp trick" can be used in order to avoid this issue.

- Consider

$$\begin{cases} \tilde{v}_i^k = \max_j \left\{ \Phi_{ij} - v_j^k \right\} \\ \tilde{u}_j^k = \max_i \left\{ \Phi_{ij} - u_i^k \right\} \end{cases}$$

(the indexing is not a typo: $\tilde{v}$ is indexed by i and $\tilde{u}$ by j).

- One has

$$\begin{cases} u_i^k = \mu_i + \tilde{v}_i^{k-1} + \sigma \log \sum_j \exp\left(\frac{\Phi_{ij} - v_j^{k-1} - \tilde{v}_i^k}{\sigma} \right) \\ v_j^k = \zeta_j + \tilde{u}_j^k + \sigma \log \sum_i \exp\left(\frac{\Phi_{ij} - u_i^k - \tilde{u}_j^k}{\sigma} \right) \end{cases}$$

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