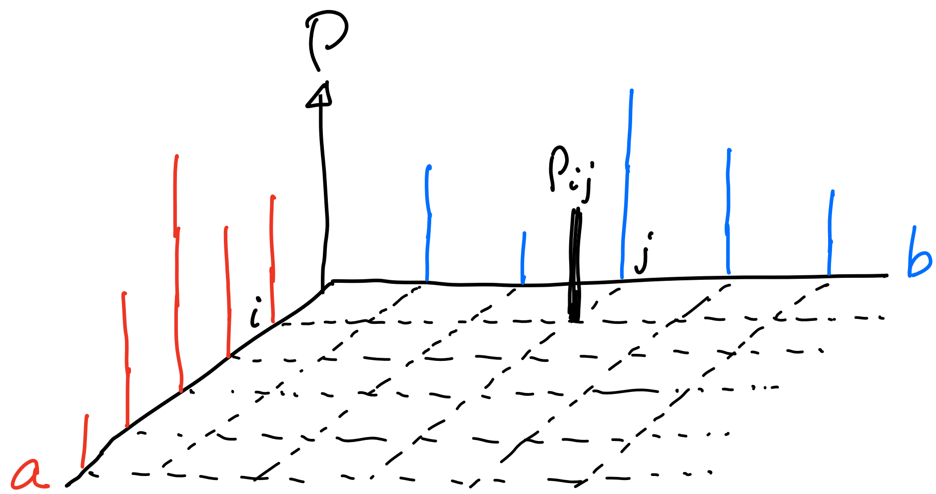
Lecture 4, Monday, April 4, 2002

Plan ⊙ More about the W-metric.

⊙ Probabilistic view of the (discrete) OT problem.

Review $\forall a \in \mathcal{P}_m \ \forall b \in \mathcal{P}_n$.

$$\mathcal{A}(a,b) \triangleq \{ P = [P_{ij}] \in \mathbb{R}^{m\times n} : P \geq 0, \ \sum_{j=1}^{n} P_{ij} = a_i \ (1 \leq i \leq m), \ \sum_{i=1}^{m} P_{ij} = b_j \ (1 \leq j \leq n) \}.$$



Given $C = [C_{ij}] \in \mathbb{R}^{m\times n}$ with $C \geq 0$.

The OT prob. (The Kantorovich discrete OT prob.)

$$W_C(a,b) \triangleq W(a,b) \triangleq \min_{P=[P_{ij}] \in \mathcal{A}(a,b)} \sum_{i=1}^{m} \sum_{j=1}^{n} P_{ij} C_{ij}.$$

Theorem If $m = n$, $C \in \mathbb{R}^{n\times n}$ is a metric matrix, then $(\mathcal{P}_n, W)$ is a metric space.

Idea of proof $W(a,c) \leq W(a,b) + W(b,c)$.

Known: $W(a,b) = \sum_{i,j} R_{ij} C_{ij}$ for some $R \in \mathcal{A}(a,b)$.

$W(b,c) = \sum_{i,j} S_{ij} \cdot C_{ij}$ for some $S \in \mathcal{A}(b,c)$.

$$W_p(a,c) \le \sum_{i,k} Q_{ik} C_{ik} \qquad [Q \in \mathcal{A}(a,c)]$$

$$= \sum_{i,k} \Big(\sum_j \widetilde{Q}_{ijk}\Big) C_{ik} \qquad [Q_{ik} \triangleq \sum_j \widetilde{Q}_{ijk}: \text{lifting}]$$

$$\le \sum_{i,k} \Big(\sum_j \widetilde{Q}_{ijk}\Big)(C_{ij}+C_{jk}) \qquad [C: \text{metric}, \widetilde{Q} \ge 0]$$

$$= \sum_{i,j} C_{ij}\Big(\sum_k \widetilde{Q}_{ijk}\Big) + \sum_{j,k} C_{j,k}\Big(\sum_i \widetilde{Q}_{ijk}\Big)$$

$$= \sum_{i,j} C_{ij} R_{ij} + \sum_{j,k} C_{j,k} S_{j,k} \qquad \begin{bmatrix} \sum_k \widetilde{Q}_{ijk} = R_{ij} & \forall i,j \\ \sum_i \widetilde{Q}_{ijk} = S_{jk} & \forall j,k \end{bmatrix} (*)$$

$$= W(a,b) + W(b,c).$$

Key: construct $\widetilde{Q}_{ijk} \ge 0$ satifing $(*)$.

$$\widetilde{Q}_{ijk} = \begin{cases} R_{ij} S_{jk} / b_j & \text{if } b_j \ne 0, \\ 0 & \text{if } b_j = 0. \end{cases}$$

<u>Theorem</u> Let $C = [C_{ij}] \in \mathbb{R}^{n\times n}$ be a metric matrix, $1 \le p < \infty$, and ~~for~~ any $a,b \in \mathcal{P}_n$

$$W_{C,p}(a,b) = W_p(a,b) = \Big[\min_{P \in \mathcal{A}(a,b)} \sum_{i,j} P_{ij} C_{ij}^p\Big]^{1/p}.$$

Then $(\mathcal{P}_n, W_p)$ is a metric space.

<u>Proof</u> Only: $W_p(a,c) \le W_p(a,b) + W_p(b,c)$ for any $a,b,c \in \mathcal{P}_n$. Choos $R \in \mathcal{A}(a,b)$, $S \in \mathcal{A}(b,c)$:

$$W_p(a,b) = \Big(\sum_{i,j} R_{ij} C_{ij}^p\Big)^{1/p}, \quad W_p(b,c) = \Big(\sum_{j,k} S_{jk} C_{jk}^p\Big)^{1/p}.$$

Using the above notation, replacing C_{ij} by C_{ij}^p, we get

$$W_p(a,c) \le \Big[\sum_{i,k} Q_{ik} C_{ik}^p\Big]^{1/p} \qquad [Q \in \mathcal{A}(a,c)]$$

$$= \Big[\sum_{i,k} \Big(\sum_j \widetilde{Q}_{ijk}\Big) C_{ik}^p\Big]^{1/p} \qquad [Q_{ik} \triangleq \sum_j \widetilde{Q}_{ijk}: \text{lifting}]$$

$$\le \Big[\sum_{i,k} \big(\sum_j \tilde{Q}_{ijk}\big)(C_{ij}+C_{jk})^p \Big]^{1/p} \quad [C\text{: metric}, \tilde{Q} \ge 0]$$

$$\le \Big(\sum_{i,j,k} \tilde{Q}_{ijk}\, C_{ij}^p\Big)^{1/p} + \Big(\sum_{ijk} \tilde{Q}_{ijk}\, C_{jk}^p\Big)^{1/p} \quad \left[\begin{array}{l} \sum_{ijk} \tilde{Q}_{ijk} = 1 \\ \text{weighted} \\ \text{Minkowski's ineq.} \end{array}\right]$$

$$\overset{(*)}{=} \Big(\sum_{i,j} R_{ij} C_{ij}^p\Big)^{1/p} + \Big(\sum_{j,k} S_{jk} C_{jk}^p\Big)^{1/p}$$

$$= W_p(a,b) + W_p(b,c). \quad \underline{\text{QED}}$$

__Example__ (Concentrated distributions) Fix $k, l \in \{1, \dots, n\}$ with $k \ne l$. Let $a = e_k$ (kth component is 1 and others 0) and $b = e_l$. Then $P = [P_{ij}] \in \mathcal{A}(a,b) = \mathcal{A}(e_k, e_l) \Longrightarrow P_{kl} = 1$ and $P_{ij} = 0$ if $i \ne k$ or $j \ne l$. So, $\mathcal{A}(e_k, e_l) = \{E_{kl}\}$, ($E_{kl}$: 1 at (k,l) and 0 at others,) a single element set. $W_C(e_k, e_l) = C_{kl} > 0$. The metric W_C = the metric C (if C is a metric matrix).

In general, it is hard to compute explicity $W_C(a,b)$. But, for a simple metric C, we can.

__Definition__ The $n \times n$ discrete metric matrix is $D = [D_{ij}] \in \mathbb{R}^{n\times n}$ with $D_{ij} = 1 - \delta_{ij}$ $(1 \le i, j \le n)$.

__Lemma__ (Wasserstein metric w.r.t. the discret metric) Let $D = [D_{ij}]$ be the $n \times n$ discrete metric matrix. Let $a = (a_i) \in \mathcal{P}_n$ and $b = (b_i) \in \mathcal{P}_n$.

(1) The cost $\sum_{i,j} P_{ij} D_{ij} = 1 - \sum_{i=1}^n P_{ii} = 1 - \mathrm{Tr}\, P \quad \forall P \in \mathcal{A}(a,b)$.

(2) $\displaystyle \max_{P\in\mathcal{A}(a,b)} \operatorname{Tr} P = \sum_{i=1}^{n} \min(a_i, b_i),$

$$W_D(a,b) = 1 - \sum_{i=1}^{n} \min(a_i, b_i).$$

<u>Proof</u> (1) This follows from the fact that $D_{ij} = 1 - \delta_{ij}$ and $\sum_{i,j} P_{ij} = 1$.

(2) Only the first equality. Note that $P \in \mathcal{A}(a,b) \Rightarrow P_{ii} \le \min(a_i, b_i)$. Hence $\operatorname{Tr} P \le \sum_{i=1}^{n} \min(a_i, b_i)$.
If $a=b$ then $\operatorname{Tr} P$ is maximized by $P = \operatorname{diag}(a_1, \dots, a_n) \in \mathcal{A}(a,b)$.

Assume $a \ne b$. Suppose for some i, $a_i = b_i$ but for some others $a_i \ne b_i$. Since $\sum_i a_i = \sum_i b_i = 1$, there are some i, $a_i > b_i$ and also some other i, $a_i < b_i$. (The case there is no i such that $a_i = b_i$ can be treated similarly.) More specifically, assume without loss of generality,

$a_i = b_i$, $i = 1, \dots, k$; $a_i > b_i$, $i = k+1, \dots, k+p$; $a_i < b_i$, $i = k+p+1, \dots, n$.

Construct $P = [P_{ij}] \in \mathcal{A}(a,b)$:

$$P = \left[\begin{array}{ccc|ccc|ccc}
a_1 & & 0 & & & & & & \\
& \ddots & & & 0 & & & 0 & \\
0 & & a_k & & & & & & \\
\hline
& & & b_{k+1} & & 0 & & & \\
& 0 & & & \ddots & & & Q & \\
& & & 0 & & b_{k+p} & & & \\
\hline
& & & & & & a_{k+p+1} & & 0 \\
& 0 & & & 0 & & & \ddots & \\
& & & & & & 0 & & a_n
\end{array}\right]
\begin{array}{l}
\Big\} \text{ row sum} = a_i \\
\text{construct } Q \in \mathbb{R}^{p\times(n-k-p)} \\
Q \ge 0, \text{ and } (*) \\
\Big\} \text{ row sum} = a_i
\end{array}$$

$$\underbrace{\qquad\qquad}_{\text{col. sum} = a_j = b_j,} \quad \underbrace{\qquad\qquad}_{\text{col. sum} = b_j}$$

row i of Q sums to $a_i - b_i$ $(i = k+1, \cdots, k+p)$, $(*)$
col. j of Q sums to $b_j - a_j$ $(j = k+p+1, \cdots, n)$.
Note: $\sum_{i=k+1}^{k+p} (a_i - b_i) = \sum_{j=k+p+1}^{n} (b_j - a_j) =: \sigma > 0$,
as this is equivalent to $\sum_{i=k+1}^{n} a_i = \sum_{j=k+1}^{n} b_j$, true since all $a_i = b_i$ $(1 \le i \le k)$ and $\sum_1^n a_i = \sum_1^n b_i = 1$.

Let $Q = [Q_{ij}]$ with $Q_{ij} = \frac{(a_i - b_i)(b_j - a_j)}{\sigma}$. Then $Q \ge 0$ and $(*)$ is satified. Hence, $P \in \mathcal{A}(a,b)$.
And $\mathrm{Tr}\, P = \mathrm{diag}(\min(a_1,b_1), \dots, \min(a_n,b_n))$ max. the trace of matrix in $\mathcal{A}(a,b)$. QED

Remarks ⊙ If $C = [C_{ij}] \in \mathbb{R}^{n \times n}$ is a metric matrix, then the cost $\sum_{i,j} P_{ij} C_{ij}$ for a feasible plan $P \in \mathcal{A}(a,b)$ is small if P_{ii}'s are large.
⊙ The example with the cost matrix being the discrete metric matrix is interesting as it has a solution formula, and any other cost metric matrix leads to equivalent distance.

Proposition If C and D are two $n \times n$ metric matrices then $\exists K_1 > 0$ and $K_2 > 0$ such that
$K_1 W_C(a,b) \le W_D(a,b) \le K_2 W_C(a,b)$ $\forall a, b \in \mathcal{A}(a,b)$.

Proof $P = [P_{ij}] \in \mathcal{A}(a,b) \Rightarrow P_{ij} \ge 0$ $\forall i,j$.
$$\sum_{i,j} P_{ij} C_{ij} = \sum_{i,j,i \ne j} P_{ij} C_{ij} \le \frac{\max_{i \ne j} C_{ij}}{\min_{i \ne j} D_{ij}} \sum_{i \ne j} P_{ij} D_{ij}$$

$$\Longrightarrow K_1 = \frac{\min_{i\neq j} D_{ij}}{\max_{i\neq j} C_{ij}} > 0, \text{ and } K_1 W_C(a,b) \leq W_D(a,b).$$

The second ineq. is similar. QED

In particular, we can compare $W_C(a,b)$ with $W_D(a,b)$ for D = discret metric matrix.

We now compare the convergence in W_C and Euclidean distance. By the above Proposition, we can fix $C = D$, the discrete metric matrix. For convenience, let us use the l_1-norm instead of the l_2 (i.e., the Euclidean) norm, as they are equivalent, and l_1 seems to be better : $\sum_{i=1}^n a_i = \sum_{i=1}^n |a_i| = |a|_1 = 1$ if $a \in \mathcal{P}_n$.

Let $a^{(k)}, a \in \mathcal{P}_n$ $(k = 1, 2, \cdots)$. $|a^{(k)} - a|_1 \to 0 \Rightarrow a_i^{(k)} \to a_i$ $(i = 1, \cdots, n) \Rightarrow W_D(a^{(k)}, a) = 1 - \sum_{i=1}^n \min(a_i^{(k)}, a_i) \to 0$, as $\min(\cdot,\cdot)$ is continuous: $\min(\alpha, \beta) = \frac{1}{2}[\alpha + \beta - |\alpha - \beta|]$.

Hence $a^{(k)} \to a$ in $(\mathcal{P}_n, |\cdot|_1) \Rightarrow a^{(k)} \to a$ in $(\mathcal{P}_n, W_D)$.

Suppose $W_D(a^{(k)}, a) \to 0$. Any subseq. of $a^{(k)}$ has a convergent subseq in $|\cdot|_1$: $a^{(k')} \to a'$ in $(\mathcal{P}_n, |\cdot|_1)$. Then $a^{(k')} \xrightarrow{W_D} a'$. But $a^{(k')} \xrightarrow{W} a$. Hence, $a' = a$. Hence, $a^{(k)} \to a$ $(\mathcal{P}_n, |\cdot|_1)$.

Now, what about equivalence of W_D-metric and Euclidean metric: $\exists K_1, K_2 > 0$ such that

$$K_1 |a - b| \leq W_D(a,b) \leq K_2 |a - b|_1 \quad \forall a, b \in \mathcal{P}_n \ ?$$

Fix $a, b \in \mathcal{P}_n$. If $a = b$ then all distances $= 0$. So, we assume $a \neq b$. We cannot have $a_i \geq b_i$ for all i as otherwise $\sum_{i=1}^n (a_i - b_i) = \Sigma a_i - \Sigma b_i = 0 \Rightarrow a_i = b_i \, \forall i$.

Let $I=\{i\in\{1,\cdots,n\}: a_i\geq b_i\}$, $J=\{j\in\{1,\cdots,n\}: a_j<b_j\}$.
$I\neq\phi$, $J\neq\phi$. $I\cup J=\{1,2,\cdots,n\}$. We have

$$|a-b|=\sum_{i\in I}(a_i-b_i)+\sum_{i\in J}(b_i-a_i)=\sum_{i\in I}a_i-\sum_{i\in I}b_i+\sum_{i\in J}(b_i-a_i)$$
$$=1-\sum_{i\in J}a_i-1+\sum_{i\in J}b_i+\sum_{i\in J}(b_i-a_i)=2\sum_{i\in J}(b_i-a_i)$$
$$W_D(a,b)=1-\sum_{i\in I}b_i-\sum_{i\in J}a_i=\sum_{i\in J}b_i-\sum_{i\in J}a_i=\sum_{i\in J}(b_i-a_i)$$

Note: $\sum_{i\in J}(b_i-a_i)=1-\sum_{i\in I}b_i-1+\sum_{i\in I}a_i=\sum_{i\in I}(a_i-b_i)$.

Denote for an $u\in\mathbb{R}^n$ $u^+=(u_1^+,\cdots,u_n^+)$, $u^-=(u_1^-,\cdots,u_n^-)$
For any $\alpha\in\mathbb{R}$, $\alpha^+=\max(\alpha,0)$, $\alpha^-=\max(-\alpha,0)$. $\alpha=\alpha^+-\alpha^-$ and $|\alpha|=\alpha^++\alpha^-$.

Summary. $$\left.\begin{array}{l}|a-b|=2|(a-b)^-|_1=2|(a-b)^+|_1\\ 2W_D(a,b)=|a-b|_1.\end{array}\right\}\ \forall a,b\in\mathcal{P}_n.$$

<u>Theorem</u> Let D be the $n\times n$ discrete metric matrix. Then
$$2W_D(a,b)=|a-b|_1\quad\forall a,b\in\mathcal{P}_n.$$
In particular, for any metric matrix C,
(1) $a^{(k)}\to a$ in $(\mathcal{P}_n,\ell_1)\iff a^{(k)}\to a$ in $(\mathcal{P}_n,W_C)$.
(2) $(\mathcal{P}_n,W_C)$ is a Polish space (i.e., it is a complete and separable metric space). <u>QED</u>