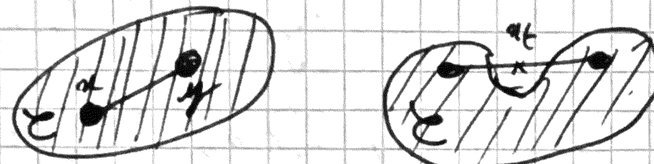
CONVEX OPIMIZATION

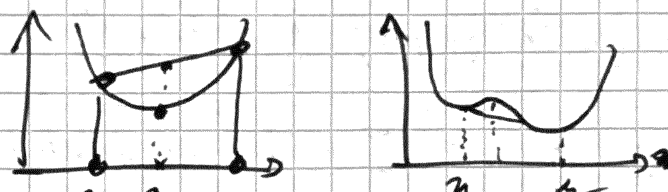
Convex set: $\mathcal{C} \subset \mathbb{R}^d$: $\forall (x,y) \in \mathcal{C}^2, \forall t \in [0,1], \underbrace{(1-t)x + ty}_{x_t} \in \mathcal{C}$



Convex NON-CONVEX

Convex functio: $f : \mathbb{R}^d \to \mathbb{R}$

$$f(x(1-t) + yt) \leq (1-t) f(x) + t f(y)$$

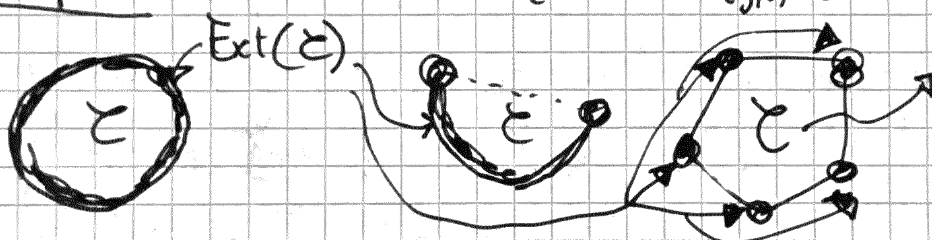


x x_t y
Convex

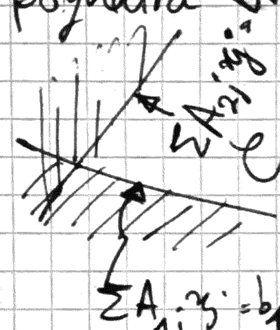
x y
Non convex

NB: $\{f \text{ convex}\} \Leftrightarrow \{ \mathrm{Epi}(f) \triangleq \{(x,y) : f(x) \geq y\} \subset \mathbb{R}^{d+1} \text{ is cvx} \}$.

Extremal points: $\mathrm{Ext}(\mathcal{C}) \triangleq \{ x \in \mathcal{C} : \text{if } x = \frac{y+z}{2}, (y,z) \in \mathcal{C}^2 \Rightarrow x = y = z \}$.



Bounded polytope
ie polyhedra

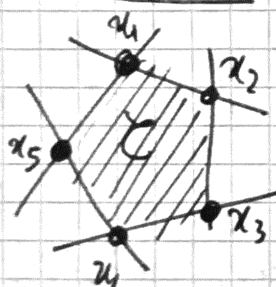


Polytope: $\mathcal{C} = \{ x : Ax \leq b, \text{ ie } \forall i, \sum_j A_{ij} x_j \leq b_i \}$.

Polyhedra: $\mathcal{C}$ needs to be bounded, and then one has

$$\mathcal{C} = \mathrm{Conv}(x_i)_{i=1}^p = \left\{ \sum_{i=1}^p \lambda_i x_i : \lambda \in \Sigma_p \right\}$$

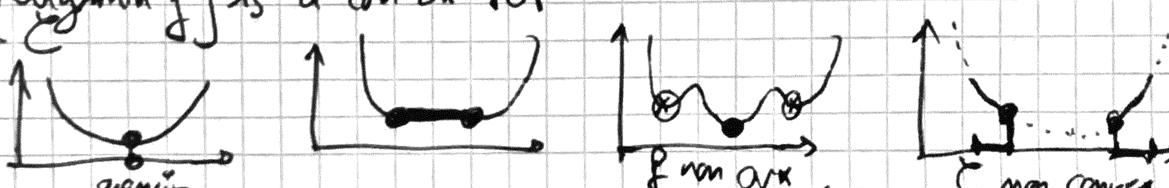
$$\Sigma_p = \{ \lambda \in \mathbb{R}_+^p : \sum_i \lambda_i = 1 \} \text{ simplex (ie discrete probabilities)}$$



CONVEX OPTIM°: solve $\min_{x \in \mathcal{C}} f(x)$ → convex

RMQ1: local minimizer $\Leftrightarrow$ global min.

Rmq2: $\{\operatorname{argmin}_{\mathcal{C}} f\}$ is a convex set



RMQ3: If $\mathcal{C}$ is closed and bounded, $\operatorname{Argmin}_{\mathcal{C}} f \neq \emptyset$

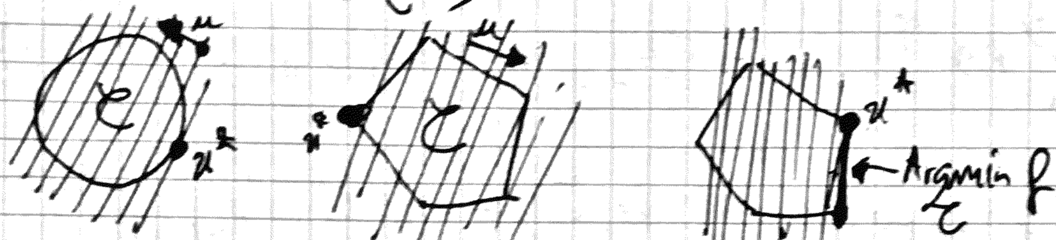
Advantages of convexity:

- local $\Rightarrow$ global
- "simple"/"fast" algorithm (eg gradient descent if $\begin{cases} f \text{ smooth} \\ \mathcal{C} = \mathbb{R}^d \end{cases}$)

Linear optimization: $\min_{x \in \mathcal{C}} f(x) = \langle x, u \rangle = \sum_i u_i x_i$

Lemma (not proved): if $\mathcal{C}$ is a closed bounded convex set, $\mathrm{Ext}(\mathcal{C}) \neq \emptyset$

Proposition: If $\mathcal{C}$ is a closed bounded convex set, $\exists x^* \in \mathrm{Argmin}_{\mathcal{C}} f$ such that $x^* \in \mathrm{Ext}(\mathcal{C})$



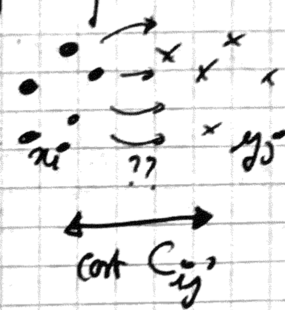
Proof: Let $\mathcal{J} \triangleq \mathrm{Argmin}_{x \in \mathcal{C}} \langle x, u \rangle$. One can show that $\mathcal{J}$ is a bounded closed convex set.

Indeed $\begin{cases} x_k \in \mathcal{J} \to x \Rightarrow x \in \mathcal{J} \text{ bc } \begin{cases} \mathcal{C} \text{ closed} \\ \langle \cdot, u \rangle \text{ continuous} \end{cases} \\ (x,y) \in \mathcal{J}^2 \Rightarrow \frac{x+y}{2} \in \mathcal{J} \text{ bc } \begin{cases} \mathcal{C} \text{ cvx} \\ \langle \cdot, u \rangle \text{ linear} \end{cases} \end{cases}$

Using previous lemma, $\mathrm{Ext}(\mathcal{J}) \neq \emptyset$. Let us show that $\mathrm{Ext}(\mathcal{J}) \subset \mathrm{Ext}(\mathcal{C})$.
Let $x \in \mathrm{Ext}(\mathcal{J})$. If we suppose $x \notin \mathrm{Ext}(\mathcal{C})$, then $x = \frac{y+z}{2}$ with $(z \neq y) \in \mathcal{C}$.
Since $x \in \mathrm{Ext}(\mathcal{J})$, it means that either $y \notin \mathcal{J}$ or $z \notin \mathcal{J}$. w.loss.g $y \notin \mathcal{J}$.
Since $(y,z) \in \mathcal{C}^2$, necessarily $\begin{cases} \langle y, u \rangle < \langle x, u \rangle \\ \langle z, u \rangle \leq \langle x, u \rangle \end{cases}$
so that $\langle x, u \rangle = \frac{1}{2}(\langle y, u \rangle + \langle z, u \rangle) < \frac{1}{2}(\langle x, u \rangle + \langle x, u \rangle)$ contradiction $\blacksquare$

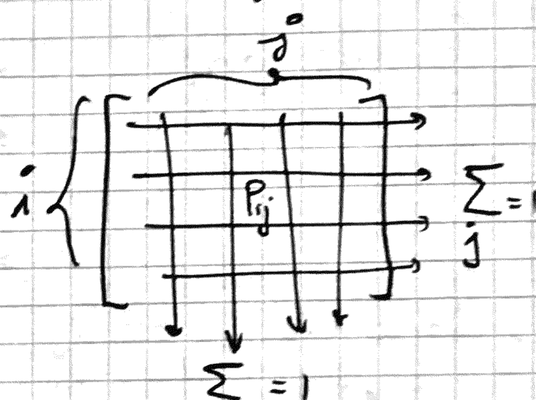
OPTIMAL TRANSPORT and ASSIGNMENTS

Special case : 2 measures (ie. distrib° of mass) uniform on two point clouds $(x_i)_{i=1}^{n}$, $(y_j)_{j=1}^{n}$



$\boxed{\text{MONGE}}$ $\min_{\substack{\sigma : \{1..n\} \to \{1..n\} \\ \text{bijection}}} \sum_{i=1}^{n} C_{i,\sigma(i)}$

$\boxed{\text{KANTOROVITCH}}$ $\min_{P \in \mathcal{B}_n} \sum_{i=1}^{n} P_{ij} C_{ij}$



$\mathcal{B}_n \triangleq \{ P \in \mathbb{R}_+^{n \times n} : \underbrace{\sum_j P_{ij} = 1, \sum_i P_{ij} = 1}_{P \mathbb{1}_n = P^T \mathbb{1}_n = \mathbb{1}_n} \}$.

Bistochastic Matrices

RMQ : $\mathcal{B}_n \subset [0,1]^n$ is a polyhedra (bounded polytope).

$\rightsquigarrow$ Kantorovitch problem is a linear program

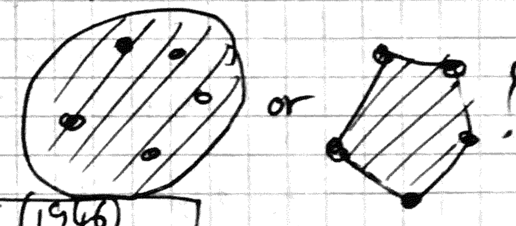
Permutation matrices : $\mathcal{P}_n \triangleq \mathcal{B}_n \cap \{0,1\}^{n \times n}$

c.a.d $P \in \mathcal{P}_n \Leftrightarrow \exists \sigma : \{1..n\} \to \{1..n\}$ permut° $P_{ij} = \begin{cases} 1 & \text{si } j = \sigma(i) \\ 0 & \text{sinon} \end{cases}$

~~[illegible]~~ : So Monge $\Leftrightarrow \min_{P \in \mathcal{P}_n} \sum_{ij} C_{ij} P_{ij}$

$\longrightarrow$ Kantorovitch is a convex relaxation of Monge (ie optimizat° on a larger cvx set)

Fundamental Q° : How larger is $\mathcal{B}_n$ from $\mathcal{P}_n$?



Answer : it is tight !

$\boxed{\begin{array}{l} \text{THM. BIRKHOFF (1946)} \\ \quad\;\;\;\; \text{VON NEUMAN (1952)} \\ \quad \text{Ext}(\mathcal{B}_n) = \mathcal{P}_n \end{array}}$

Proof : $\circlearrowleft$

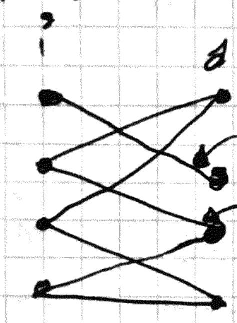
<u>Proof</u>: ① Show $\mathcal{P}_n \subset \mathrm{Ext}(\mathcal{B}_n)$: if $P \in \mathcal{P}_n$ is such that $P = \frac{U+V}{2}$

since $P_{ij} \in \{0,1\}$ and $0 \leq \begin{matrix} U_{ij} \\ V_{ij} \end{matrix} \leq 1$, nec^t $\begin{matrix} U_{ij} \\ V_{ij} \end{matrix} \in \{0,1\} \Rightarrow U = V = P$

② Show $\mathrm{Ext}(\mathcal{B}_n) \subset \mathcal{P}_n$: Take $P \in \mathcal{B}_n \setminus \mathcal{P}_n$, show that $P \notin \mathrm{Ext}(\mathcal{B}_n)$

(ie $\mathcal{P}_n^c \subset \mathrm{Ext}(\mathcal{B}_n)^c$) ie. construct $(U,V) \in \mathcal{B}_n^2$, $U \neq V$, $P = \frac{U+V}{2}$

<u>Bipartite graph</u>:



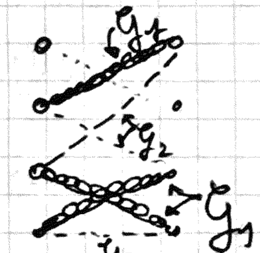
$P_{ij} = 1 \rightsquigarrow$ "isolated" edge

$P_{ij} \in (0,1)$: necessarily ≥ 2 outcoming edges at i and at j

Since $P \notin \mathcal{P}_n$, $\exists (i,j)$ with $0 < P_{ij} < 1$. One can follow a path of edge on the graph witch creates a cycle. (if not, on can always continue the process)

<u>Let</u> $(i_1, j_1, i_2, j_2, \dots, i_p, j_p)$ $i_{p+1} = i_1$, $j_{p+1} = j_1$ be the shortest of such cycles. (there is a finite #)

<u>Necessarily</u>: $0 < \underbrace{P_{i_s, j_s}, P_{i_{s+1}, j_s}}_{\text{correspond to the edges of the cycle}} < 1$



The $(i_s)_{s=1}^p$, $(j_s)_{s=1}^p$ are all differents.

Let $\varepsilon \triangleq \min_{1 \leq s \leq p} \left\{ P_{i_s j_s}, 1 - P_{i_s j_s}, P_{i_{s+1} j_s}, 1 - P_{i_{s+1} j_s} \right\}$. One has $\varepsilon > 0$, $\varepsilon < 1$

Let $\mathcal{G}_1 \triangleq \{(i_s, j_s)\}_{s=1}^p$, $\mathcal{G}_2 \triangleq \{(i_{s+1}, j_s)\}_{s=1}^p$

Let $U_{ij} = \begin{cases} P_{ij} \text{ si } (i,j) \notin \mathcal{G}_1 \cup \mathcal{G}_2 \\ P_{ij} + \frac{\varepsilon}{2} \text{ si } (i,j) \in \mathcal{G}_1 \\ P_{ij} - \frac{\varepsilon}{2} \text{ si } (i,j) \in \mathcal{G}_2 \end{cases}$ $\quad V_{ij}$ = idem mais $\left(+\frac{\varepsilon}{2}, -\frac{\varepsilon}{2}\right) \longleftrightarrow \left(-\frac{\varepsilon}{2}, +\frac{\varepsilon}{2}\right)$

One has $0 \leq U, V \leq 1$ and $\begin{cases} \sum_i U_{ij} = 1 \\ \sum_j U_{ij} = 1 \end{cases}$ Because at each vertex, there is 1 edge of $\mathcal{G}_1$ and 1 edge of $\mathcal{G}_2$

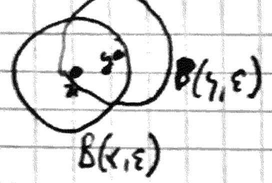
$P = \frac{U+V}{2}$, $U \neq V$ ■

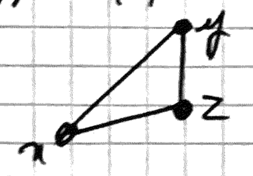
DISTANCES et TRANSPORT

Espace métrique : (X, d) : ① $d(x,y) = d(y,x)$ ② $d \geq 0$

d distance : ③ $d(x,y) = 0 \iff x = y$

Rmq : ①+③+④ ⇒ ② ④ $d(x,y) \leq d(x,z) + d(z,y)$ (inég triang)





IT important pour l'étude de la convergence de suite

$z \in B(y,\varepsilon)$, $y \in B(x,\varepsilon)$ (afin de définir une topologie, des ouverts)

$\Rightarrow z \in B(x, 2\varepsilon)$.

Exemple : • Sur $\mathbb{R}$, $d(x,y) = |x-y|$

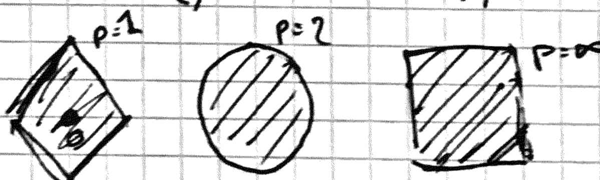
• Sur $\mathbb{R}^d$, $d(x,y) = \|x-y\|_2 \triangleq \sqrt{\sum_{i=1}^{d} |x_i - y_i|^2}$

(NB : $\|x-y\|_\infty = \max_i |x_i - y_i|$) • Plus généralement $\|x-y\|_p \triangleq \left(\sum |x_i - y_i|^p\right)^{1/p}$

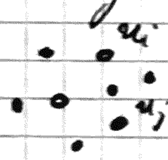
Rmq : preuve via l'inég. de Minkowski

$$\left(\sum_i \lambda_i (a_i + b_i)^p\right)^{1/p} \leq \left(\sum_i \lambda_i a_i^p\right)^{1/p} + \left(\sum_i \lambda_i b_i^p\right)^{1/p}$$

Sur $\mathbb{R}^2$, $\{x : \|x\|_p \leq 1\}$.



OT : Histogrammes $(a_i)_{i=1}^n$, $(b_i)_{i=1}^n$; $a_i, b_i \geq 0$ $\sum a_i = \sum b_i = 1$ ie. $a, b \in \Sigma_n$ simplex



Coût $C_{ij} = D_{ij}^p$ où $D_{ij} = d(x_i, y_j)$ est une distance

{Wasserstein
{Monge Kantorovitch

$$W_p(a,b) = \left(\inf_{P \geq 0} \left\{ \sum_{ij} P_{ij} D_{ij}^p : \begin{matrix} P\mathbb{1} = a \\ P^T\mathbb{1} = b \end{matrix} \right\}\right)^{1/p}$$

Thm : W_p est une distance sur Σ_n pour $1 \leq p < +\infty$

Rmq : $W_p(\delta_i, \delta_j) = d(x_i, x_j)$

Remark 2.14 (Probabilistic interpretation). Kantorovich's problem can be re-interpreted through the prism of random variables, following Remark 2.9. Indeed, problem (2.15) is equivalent to

$$\mathcal{L}_c(\alpha, \beta) = \min_{(X,Y)} \left\{ \mathbb{E}_{(X,Y)}(c(X,Y)) \ : \ X \sim \alpha, Y \sim \beta \right\} \tag{2.16}$$

where (X, Y) is a couple of random variables over $\mathcal{X} \times \mathcal{Y}$ and $X \sim \alpha$ (resp $Y \sim \beta$) means that the law of X (resp. Y), represented as a measure, must be α (resp. β). The law of the couple (X, Y) is then $\pi \in \mathcal{U}(\alpha, \beta)$ over the product space $\mathcal{X} \times \mathcal{Y}$.

2.4 Metric Properties of Optimal Transport

An important feature of OT is that it defines a distance between histograms and probability measures as soon as the cost matrix satisfies certain suitable properties. Indeed, OT can be understood as a canonical way to lift a ground distance between points to a distance between histogram or measures.

We first consider the case where, using a term first introduced by Rubner et al. [2000], the "ground metric" matrix $\mathbf{C}$ is fixed, representing substitution costs between bins, and shared across several histograms we would like to compare. The following proposition states that OT provides a valid distance between histograms supported on these bins.

Proposition 2.2. We suppose $n = m$, and that for some $p \geq 1$, $\mathbf{C} = \mathbf{D}^p = (\mathbf{D}^p_{i,j})_{i,j} \in \mathbb{R}^{n \times n}$ where $\mathbf{D} \in \mathbb{R}^{n\times n}_+$ is a distance on $[\![n]\!]$, *e.g.*

(i) $\mathbf{D} \in \mathbb{R}^{n\times n}_+$ is symmetric;

(ii) $\mathbf{D}_{i,j} = 0$ if and only if $i = j$;

(iii) $\forall (i,j,k) \in [\![n]\!]^3, \mathbf{D}_{i,k} \leq \mathbf{D}_{i,j} + \mathbf{D}_{j,k}$.

Then

$$\mathrm{W}_p(\mathbf{a}, \mathbf{b}) \stackrel{\text{def}}{=} \mathrm{L}_{\mathbf{D}^p}(\mathbf{a}, \mathbf{b})^{1/p} \tag{2.17}$$

(note that W_p depends on $\mathbf{D}$) defines the p-Wasserstein distance on Σ_n, *e.g.* W_p is symmetric, positive, $\mathrm{W}_p(\mathbf{a}, \mathbf{b}) = 0$ if and only if $\mathbf{a} = \mathbf{b}$, and it satisfies the triangle inequality

$$\forall \mathbf{a}, \mathbf{b}, \mathbf{c} \in \Sigma_n, \quad \mathrm{W}_p(\mathbf{a}, \mathbf{c}) \leq \mathrm{W}_p(\mathbf{a}, \mathbf{b}) + \mathrm{W}_p(\mathbf{b}, \mathbf{c}).$$

Proof. Symmetry and definiteness of the distance are easy to prove: since $\mathbf{C} = \mathbf{D}^p$ has a null diagonal, $\mathrm{W}_p(\mathbf{a}, \mathbf{a}) = 0$, with corresponding optimal transport matrix $\mathbf{P}^\star = \mathrm{diag}(\mathbf{a})$; by the positivity of all off-diagonal elements of $\mathbf{D}^p$, $\mathrm{W}_p(\mathbf{a}, \mathbf{b}) > 0$ whenever $\mathbf{a} \neq \mathbf{b}$ (because in this case, an admissible coupling necessarily has a non-zero element outside the diagonal); by symmetry of $\mathbf{D}^p$, $\mathrm{W}_p(\mathbf{a}, \mathbf{b})$ is itself a symmetric function.

To prove the triangle inequality of Wasserstein distances for arbitrary measures, Villani [2003, Theorem 7.3] uses the gluing lemma, which stresses the existence of couplings with a prescribed structure. In the discrete setting, the explicit constuction of this glued coupling is simple. Let $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \Sigma_n$. Let $\mathbf{P}$ and $\mathbf{Q}$ be two optimal solutions of the transport problems between $\mathbf{a}$ and $\mathbf{b}$, and $\mathbf{b}$ and $\mathbf{c}$ respectively. To avoid issues that may arise from null coordinates in $\mathbf{b}$, we define a vector $\tilde{\mathbf{b}}$ such that $\tilde{\mathbf{b}}_j \stackrel{\text{def}}{=} \mathbf{b}_j$ if $\mathbf{b}_j > 0$, and $\tilde{\mathbf{b}}_j \stackrel{\text{def}}{=} 1$ otherwise, to write

$$\mathbf{S} \stackrel{\text{def}}{=} \mathbf{P}\,\mathrm{diag}(1/\tilde{\mathbf{b}})\mathbf{Q} \in \mathbb{R}^{n\times n}_+,$$

and notice that $\mathbf{S} \in U(\mathbf{a}, \mathbf{c})$ because

$$\mathbf{S}\mathbb{1}_n = \mathbf{P}\,\mathrm{diag}(1/\tilde{\mathbf{b}})\mathbf{Q}\mathbb{1}_n = \mathbf{P}(\mathbf{b}/\tilde{\mathbf{b}}) = \mathbf{P}\mathbb{1}_{\mathrm{Supp}(\mathbf{b})} = \mathbf{a}$$

where we denoted $\mathbb{1}_{\mathrm{Supp}(\mathbf{b})}$ the vector of size n with ones located at those indices j where $\mathbf{b}_j > 0$ and zero otherwise, and we use the fact that $\mathbf{P}\mathbb{1}_{\mathrm{Supp}(\mathbf{b})} = \mathbf{P}\mathbb{1} = \mathbf{a}$ because necessarily $\mathbf{P}_{i,j} = 0$ for those j where $\mathbf{b}_j = 0$. Similarly one verifies that $\mathbf{S}^\top \mathbb{1}_n = \mathbf{c}$. The triangle inequality follows then from

$$\begin{aligned}
\mathrm{W}_p(\mathbf{a}, \mathbf{c}) &= \left(\min_{\mathbf{P} \in U(\mathbf{a},\mathbf{c})} \langle \mathbf{P}, \mathbf{D}^p \rangle \right)^{1/p} \leq \langle \mathbf{S}, \mathbf{D}^p \rangle^{1/p} \\
&= \left(\sum_{ik} \mathbf{D}^p_{ik} \sum_j \frac{\mathbf{P}_{ij}\mathbf{Q}_{jk}}{\tilde{\mathbf{b}}_j} \right)^{1/p} \leq \left(\sum_{ijk} (\mathbf{D}_{ij} + \mathbf{D}_{jk})^p \frac{\mathbf{P}_{ij}\mathbf{Q}_{jk}}{\tilde{\mathbf{b}}_j} \right)^{1/p} \\
&\leq \left(\sum_{ijk} \mathbf{D}^p_{ij} \frac{\mathbf{P}_{ij}\mathbf{Q}_{jk}}{\tilde{\mathbf{b}}_j} \right)^{1/p} + \left(\sum_{ijk} \mathbf{D}^p_{jk} \frac{\mathbf{P}_{ij}\mathbf{Q}_{jk}}{\tilde{\mathbf{b}}_j} \right)^{1/p}.
\end{aligned}$$

The first inequality is due to the suboptimality of $\mathbf{S}$, the second is the triangle inequality for elements in $\mathbf{D}$, and the third comes from Minkowski's inequality. One thus has

$$\begin{aligned}
\mathrm{W}_p(\mathbf{a}, \mathbf{c}) &\leq \left(\sum_{ij} \mathbf{D}^p_{ij} \mathbf{P}_{ij} \sum_k \frac{\mathbf{Q}_{jk}}{\tilde{\mathbf{b}}_j} \right)^{1/p} + \left(\sum_{jk} \mathbf{D}^p_{jk} \mathbf{Q}_{jk} \sum_i \frac{\mathbf{P}_{ij}}{\tilde{\mathbf{b}}_j} \right)^{1/p} \\
&= \left(\sum_{ij} \mathbf{D}^p_{ij} \mathbf{P}_{ij} \right)^{1/p} + \left(\sum_{jk} \mathbf{D}^p_{jk} \mathbf{Q}_{jk} \right)^{1/p} \\
&= \mathrm{W}_p(\mathbf{a}, \mathbf{b}) + \mathrm{W}_p(\mathbf{b}, \mathbf{b}).
\end{aligned}$$

□

Remark 2.15 (The cases $0 < p \leq 1$). Note that if $0 < p \leq 1$, then $\mathbf{D}^p$ is itself distance. This implies that while for $p \geq 1$, $\mathrm{W}_p(\mathbf{a}, \mathbf{b})$ is a distance, in the case $p \leq 1$, it is actually $\mathrm{W}_p(\mathbf{a}, \mathbf{b})^p$ which defines a distance on the simplex.