APPENDIX – SUPPLEMENTARY MATERIAL
On a Connection between Maximum Variance Unfolding, Shortest Path Problems and IsoMap

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Proof of Proposition 1

For $\mathbb{EDM}^N$, this is well-known (see [Dat05]).

It remains to show that $\mathbb{DM}^N$ is a proper closed convex cone. By definition, $\mathbb{DM}^N$ is the intersection of pre-images of closed sets under continuous functions. Hence, $\mathbb{DM}^N$ is closed.

It is trivially clear that $\lambda\mathbb{DM}^N \subseteq \mathbb{DM}^N$ for all $\lambda \geq 0$. Hence, it suffices to show that $\mathbb{DM}^N + \mathbb{DM}^N \subseteq \mathbb{DM}^N$ to obtain that $\mathbb{DM}^N$ is a convex cone. To this end, let $D, \tilde{D} \in \mathbb{DM}$. The fact that $\mathbb{DM}^N + \mathbb{DM}^N \subseteq (\mathbb{S}^N_{\geq O})^*$ is obvious. Thus, we may complete the proof by showing that

$$\sqrt{d_{ij} + \tilde{d}_{ij}} \leq \sqrt{d_{ik} + \tilde{d}_{ik}} + \sqrt{d_{kj} + \tilde{d}_{kj}},\ i, j, k \in \underline{N},$$

for all $D, \tilde{D} \in \mathbb{DM}$.

We have

$$\begin{aligned}
&d_{ij} + \tilde{d}_{ij} \\
&\leq (\sqrt{d_{ik}} + \sqrt{d_{kj}})^2 + (\sqrt{\tilde{d}_{ik}} + \sqrt{\tilde{d}_{kj}})^2 \\
&= d_{ik} + d_{kj} + \tilde{d}_{ik} + \tilde{d}_{kj} + 2(\sqrt{d_{ik}d_{kj}} + \sqrt{\tilde{d}_{ik}\tilde{d}_{kj}}) \\
&= d_{ik} + d_{kj} + \tilde{d}_{ik} + \tilde{d}_{kj} + 2\sqrt{\left(\sqrt{d_{ik}d_{kj}} + \sqrt{\tilde{d}_{ik}\tilde{d}_{kj}}\right)^2} \\
&= d_{ik} + d_{kj} + \tilde{d}_{ik} + \tilde{d}_{kj} + \\
&\quad + 2\sqrt{d_{ik}d_{kj} + \tilde{d}_{ik}\tilde{d}_{kj} + 2\sqrt{d_{ik}d_{kj}\tilde{d}_{ik}\tilde{d}_{kj}}} \\
&\leq d_{ik} + d_{kj} + \tilde{d}_{ik} + \tilde{d}_{kj} + \\
&\quad + 2\sqrt{d_{ik}d_{kj} + \tilde{d}_{ik}\tilde{d}_{kj} + d_{ik}\tilde{d}_{kj} + d_{kj}\tilde{d}_{ik}} \\
&= d_{ik} + d_{kj} + \tilde{d}_{ik} + \tilde{d}_{kj} + 2\sqrt{(d_{ik} + \tilde{d}_{ik})(d_{kj} + \tilde{d}_{kj})} \\
&= \left(\sqrt{d_{ik} + \tilde{d}_{ik}} + \sqrt{d_{kj} + \tilde{d}_{kj}}\right)^2,
\end{aligned}$$

where we used the geometric-arithmetic mean inequality $\sqrt{ab} \leq \frac{1}{2}(a + b)\ \forall\ a, b \geq 0$.

Sketch of a Proof of Theorem 4

Lifting the constraint into the objective of (5.3) by means of a suitably chosen Lagrange multiplier $z \geq 0$, we obtain that any optimizer of the above also optimizes

$$\min_{K \in \mathbb{S}^N_{\succeq O}} \langle L, K \rangle + z(d - \langle I, K \rangle). \tag{0.1}$$

Rescaling the objective yields the equivalent program

$$\max_{K \in \mathbb{S}^N_{\succeq O}} \langle I, K \rangle - \tilde{z} \langle L, K \rangle\,, \tag{0.2}$$

where $\tilde{z} := 1/z$. To complete our discussion, we make use of the subsequent trivial lemma.

Lemma 1 *Let $\mathcal{S}$ be a set and $f, g : \int \to \mathbb{R}$. Then, for any $z > 0$, any optimizer x^* of*

$$\max f(x) - zg(x)$$

is also an optimizer of

$$\max f(x)\ s.t.\ g(x) \leq g(x^*).$$

Let K be feasible for (0.2) and let $D := \mathcal{D}(K)$. We have

$$\langle L, K \rangle = \sum_{\{i,j\} \in E} w_{ij} \langle E_{ij}, K \rangle$$

Hence, we may consider $-\tilde{z}w_{ij}$ as Lagrange multipliers. Invoking Lemma 1 iteratively eventually gives rise to Theorem 4.

Proof of Proposition 3

From the proof of Theorem 2, any $D \in \mathbb{DM}$ is feasible for (5.5) if and only if $D \le D^G$, where D^G. This immediately implies that D^G is an optimizer of (5.5). Hence, any feasible D is an optimizer if and only if

$$\sum_{\{i,j\}\in\tilde{E}} w_{ij}(d_{ij}^G - d_{ij}) = 0.$$

Since, by virtue of $D \le D^G$, all terms in the summation are nonnegative, this identity is equivalent to $d_{ij} = d_{ij}^G,\ w_{ij} > 0$.

Proof of Theorem 5

Assume that $\tilde{E}$ be a geodesic covering and let D be an optimizer of (5.5). We show that $D = D^G$. Let $\{i,j\} \in \underline{N}^2$. If $\{i,j\} \in \tilde{E}$, then, by Proposition 3, we have $d_{ij} = d_{ij}^G$. If $\{i,j\} \notin \tilde{E}$, then, again by Proposition 3, we have $d_{ij} \le d_{ij}^G$. Now assume that $d_{ij} < d_{ij}^G$. Since $\tilde{E}$ is a geodesic covering, there is $\{k,l\} \in \tilde{E}$ and a shortest path $\gamma \in \Pi_{kl}^G$ such that $i = \gamma_{s_1}, j = \gamma_{s_2}$ for some $1 \le s_1, s_2 \le |\gamma|$. Since γ is a shortest path in G, so is the restricted path $\gamma|_{s_1 \le s \le s_2} \in \Pi_{ij}^G$.

The triangle inequality and $D \le D^G$ from Proposition 3 yield

$$\begin{aligned}\sqrt{d_{kl}} &\le \underbrace{\tilde{l}(\gamma|_{s\le s_1})}_{\le l(\gamma|_{s\le s_1})} + \underbrace{\sqrt{d_{ij}}}_{<\sqrt{d_{ij}^G}} + \underbrace{\tilde{l}(\gamma|_{s\ge s_2})}_{\le l(\gamma|_{s\ge s_2})} \\ &< l(\gamma|_{s\le s_1}) + \sqrt{d_{ij}^G} + l(\gamma|_{s\ge s_2}) \\ &= \sqrt{d_{kl}^G},\end{aligned}$$

where $\tilde{l}(\tilde{\gamma})$ denotes the length of $\tilde{\gamma}$ with respect to the weighting $\tilde{d}_{ij}^w = d_{ij},\ \{i,j\} \in E$. The strict inequality contradicts the fact that $d_{ij} = d_{ij}^G$ by Proposition 3. This proves sufficiency.

To show necessity, assume that $\tilde{E}$ is not a geodesic covering and let $i,j \in V$ such that for all $\{k,l\} \in \tilde{E}$, no shortest path in Π_{kl}^G passes through i and j. We shall construct an optimal solution other than D^G. To this end, define

$$\begin{aligned}S := \{\{s,t\}\ \mid\ & s,t \in V, \\ & \text{there is a shortest path from } s \text{ to } t \\ & \text{passing through } i,j\}.\end{aligned} \tag{0.3}$$

Since S contains at least $\{i,j\}$, S is nonempty. Let

$$\epsilon := \min_{\{q,r\}\notin S,\ \{q,k\}\in S \vee \{k,r\}\in S} \frac{\sqrt{d_{qr}^G}}{\sqrt{d_{qk}^G} + \sqrt{d_{kr}^G}}.$$

It holds that $\epsilon < 1$, since, otherwise, we would obtain that $\sqrt{d_{qr}^G} = \sqrt{d_{qk}^G} + \sqrt{d_{kr}^G}$ for some $\{q,k\} \notin S$, $\{q,k\} \in S$, which, in turn, gives rise to the contradiction that there is a shortest path from q to r traversing i,j. Now define $\tilde{D}$ by

$$\tilde{d}_{qr} = \begin{cases} \epsilon^2 d_{qr}^G, & \{q,r\} \in S, \\ d_{qr}^G, & \{q,r\} \notin S. \end{cases}$$

Since $\epsilon < 1$ and S is nonempty, we obtain $\tilde{D} \ne D^G$. Clearly, $S \cap \tilde{E} = \emptyset$. Therefore, $\tilde{D}$ and D^G have the same objective value. To complete the proof, it remains to show that $\tilde{D}$ is feasible. Obviously, $\tilde{D}$ is symmetric, $\tilde{d}_{ii} = 0$, and $O \le \tilde{D} \le D^G$, which, in particular, yields $\tilde{d}_{ij} \le d_{ij}^w,\ \{i,j\} \in E$. Hence, $\tilde{D} \in \mathbb{DM}^N$ if

$$\sqrt{\tilde{d}_{qr}} \le \sqrt{\tilde{d}_{qk}} + \sqrt{\tilde{d}_{kr}}\ \forall\ q,k,r \in V,$$

which is verified as follows: If $\{q,k\}, \{k,r\} \notin S$, then

$$\sqrt{d_{qr}^G} \le \sqrt{d_{qk}^G} + \sqrt{d_{kr}^G} = \sqrt{\tilde{d}_{qk}^G} + \sqrt{\tilde{d}_{kr}^G}.$$

Otherwise, we have

$$\sqrt{d_{qr}^G} \le \epsilon(\sqrt{d_{qk}^G} + \sqrt{d_{kr}^G}) \le \sqrt{\tilde{d}_{qk}} + \sqrt{\tilde{d}_{kr}}.$$

As $\tilde{d}_{qr} \le d_{qr}^G$, the desired inequality follows.

References

[Dat05] Jon Dattorro. *Convex optimization & Euclidean distance geometry.* Meboo, 2005.