On the Estimation of Distances Using Graph Distances

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Euclidean distance matrix completion

Undirected graph: $G = (V, E)$ where $V = \{1, \ldots, n\}$.

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Given a weighted graph, (V, E, δ), find an EDM D such that

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For example, we could (try to) solve

$$\min_{D \in \mathbb{EDM}} \sum_{(i,j) \in E} (D_{ij} - \delta_{ij})^2$$

Graph embedding

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Given a weighted graph, (V, E, δ), and embedding dimension d, find $y_1, \ldots, y_n \in \mathbb{R}^d$ such that

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For example, we could (try to) solve

$$\min_{y_1,\ldots,y_n \in \mathbb{R}^d} \sum_{(i,j)\in E} \left(\|y_i - y_j\| - \delta_{ij} \right)^2$$

(Known as non-metric scaling in the statistics literature.)

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Important connections to:

- nearest neighbor search
- embedding a finite metric space into a given Banach space

When the graph is complete and there is an exact solution, Classical Scaling finds that solution (by solving an eigenvalue problem).

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It is known to be robust to noise.
(Arias-Castro, Javanmard, and Pelletier 2018)

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Whether a graph can be uniquely embedded is a central question in rigidity theory.[1]

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A number of methods have been proposed:

[2] Kruskal and Seery 1980; Shang et al. 2003; Shang and Ruml 2004; Niculescu and Nath 2003.

[3] Eren et al. 2004; Krislock and Wolkowicz 2010.

[4] Koren, Gotsman, and Ben-Chen 2005; Cucuringu, Lipman, and Singer 2012; Singer 2008; Zhang et al. 2010; Drusvyatskiy et al. 2017.

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- Solve a semidefinite program after an appropriate relaxation.[6]

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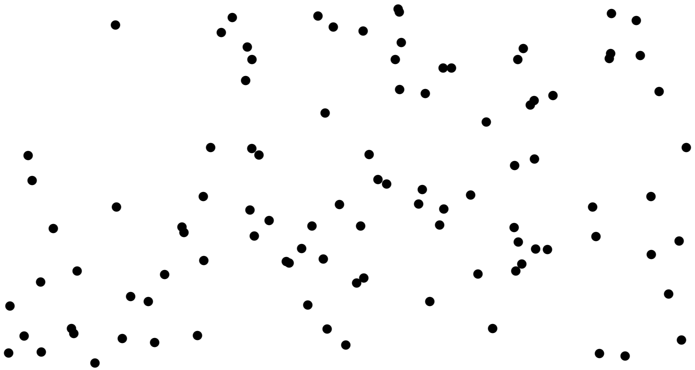

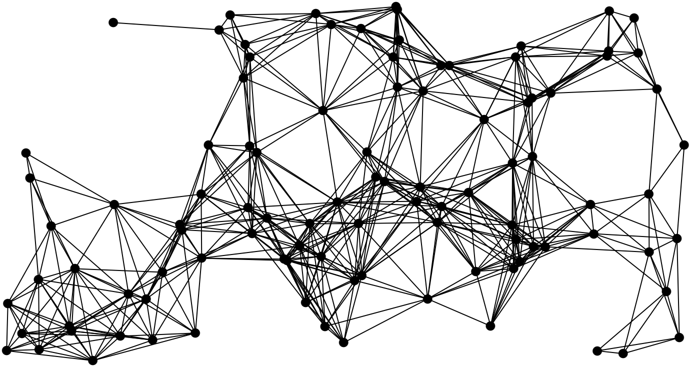

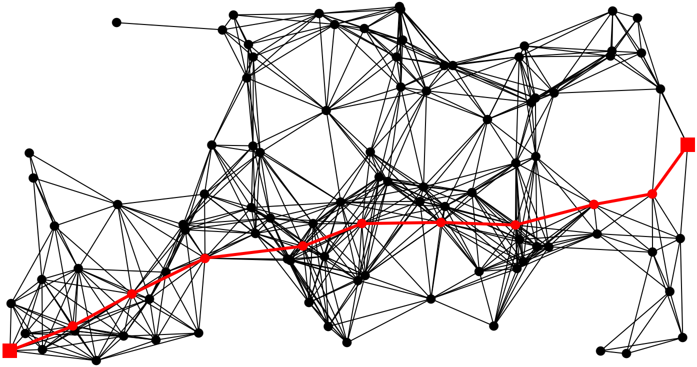

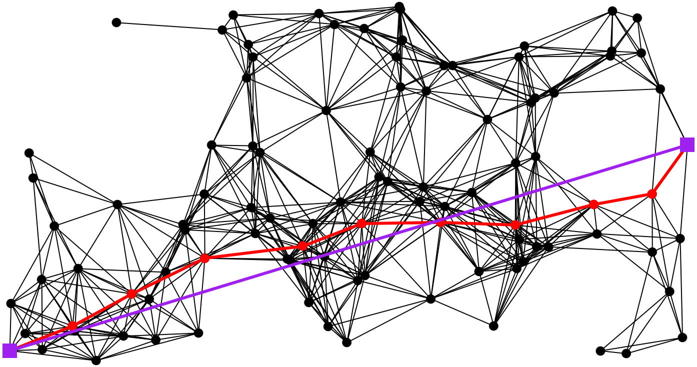

Graph distances

Based on δ, define the graph distances

$$\Delta(i,j) = \inf_{k_1,\dots,k_m} \sum_{s=0}^{m} \delta(k_s, k_{s+1}),$$

where the infimum is over paths $(k_0, \dots, k_{m+1})$ with $k_0 = i$ and $k_{m+1} = j$.

Bound for neighborhood graphs

Suppose that the graph is in fact the r-ball neighborhood graph of a set of points $x_1, \dots, x_n \in \mathbb{R}^d$, meaning

$$(i, j) \in E \iff \delta_{ij} = \|x_i - x_j\| \le r$$

[7] Arias-Castro, Javanmard, and Pelletier 2018.

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$$(i,j) \in E \;\Leftrightarrow\; \delta_{ij} = \|x_i - x_j\| \leq r$$

Proposition[7]

Take $\mathcal{X} = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$ and define

$$\varepsilon = \max_{x \in \mathrm{Conv}(\mathcal{X})} \min_{i \in [n]} \|x - x_i\|$$

When $\varepsilon / r \leq 1/c_1$,

$$\|x_i - x_j\| \leq \Delta(i,j) \leq (1 + c_2(\varepsilon/r)^2)\|x_i - x_j\|$$

where c_1, c_2 are universal constants.

[7] Arias-Castro, Javanmard, and Pelletier 2018.

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Oh, Montanari, and Karbasi 2010 prove a similar bound in the context of graph drawing for essentially the same method (MDS-MAP of Shang et al. 2003).

(The same bound above holds in that context too.)

Estimating the shortest paths distances on a surface

In manifold learning, the distances of interest are the intrinsic distances on the underlying surface.[8]

[8] Silva and Tenenbaum 2002; Tenenbaum, Silva, and Langford 2000.

[9] Karaman and Frazzoli 2011; Karaman and Frazzoli 2010; Janson et al. 2015; Schmerling, Janson, and Pavone 2015a; Schmerling, Janson, and Pavone 2015b.

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The same is true in motion planning.[9]

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Shortest paths

Consider a subset $\mathcal{S} \subset \mathbb{R}^D$.

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The intrinsic distance on $\mathcal{S}$ is defined, for $x, x' \in \mathcal{S}$, as

$$g(x, x') = \inf \Big\{ a : \exists \gamma : [0, a] \to \mathcal{S},\ 1\text{-Lipschitz}, \\ \text{with } \gamma(0) = x \text{ and } \gamma(a) = x' \Big\}$$

We have a sample of points $\mathcal{X} = \{x_1, \ldots, x_n\} \subset \mathcal{S}$, where $\mathcal{S}$ is compact and connected in $\mathbb{R}^D$. The goal is to estimate $g(x_i, x_j)$.

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$$\varepsilon = \sup_{x \in \mathcal{S}} \min_{i \in [n]} \|x - x_i\|.$$

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Define

$$\varepsilon = \sup_{x \in \mathcal{S}} \min_{i \in [n]} \|x - x_i\|.$$

Proposition (Bernstein et al. 2000)

When $\varepsilon \leq r/4$, we have

$$\Delta(x, x') \leq (1 + 4\varepsilon/r) g(x, x'), \quad \forall x, x' \in \mathcal{X}.$$

Assume that

- The intrinsic and ambient topologies coincide on $\mathcal{S}$.
- The shortest paths on $\mathcal{S}$ have curvature bounded by κ.

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Proposition (Bernstein et al. 2000; Arias-Castro and Le Gouic 2017)

There is τ depending on (the reach of) $\mathcal{S}$ and c_0 universal such that, when $r \leq \tau$ and $\kappa r \leq 1/3$,

$$g(x, x') \leq (1 + c_0 r^2)\Delta(x, x'), \quad \forall x, x' \in \mathcal{X}.$$

We also show that every shortest path on $\mathcal{S}$ between two sample points can be approximated by a shortest path in the neighborhood graph...

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Curvature-constrained shortest paths

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For $\kappa > 0$, the κ-curvature-constrained intrinsic semi-distance on $\mathcal{S}$ is defined, for $x, x' \in \mathcal{S}$, as

$$g_\kappa(x, x') = \inf \Big\{ a : \text{there is } \gamma \text{ as before} \\ \text{with curvature bounded by } \kappa \Big\}$$

We need a notion of curvature for polygonal lines (which is how paths in a neighborhood graph are embedded).

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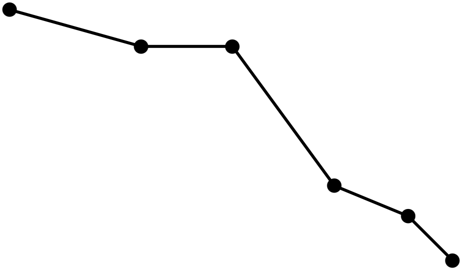
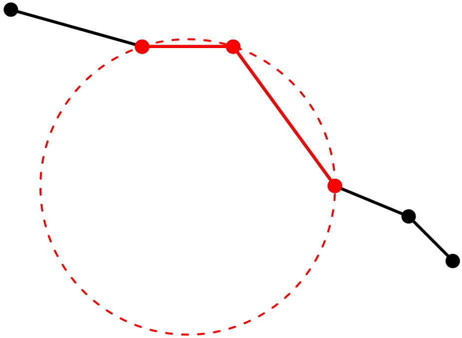
For an ordered triplet of points (x, y, z) in $\mathbb{R}^D$, define its angle as $\angle(x, y, z) = \angle(\vec{yx}, \vec{yz}) \in [0, \pi]$ and its curvature as

$$\operatorname{curv}(x, y, z) = \begin{cases} 1/R(x, y, z), & \text{if } \angle(x, y, z) \geq \frac{\pi}{2}, \\ \infty, & \text{otherwise,} \end{cases}$$

where $R(x, y, z)$ is the radius of the circle passing through x, y, z.





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Lemma

Consider a curve $\gamma : (a, b) \to \mathbb{R}^D$ which is twice continuously differentiable. Holding $s \in (a, b)$ fixed while $r \nearrow s$ and $t \searrow s$,

$$\mathrm{curv}(\gamma(r), \gamma(s), \gamma(t)) \to \text{curvature of } \gamma \text{ at } s.$$

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We also have the following key lemma.

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Lemma

Let γ be a simple curve with curvature at most κ. If $x, y, z \in \gamma$ are such that y is between x and z on γ and $\|x - z\| \leq 2/\kappa$, then

$$\mathrm{curv}(x, y, z) \leq \kappa$$

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Let $\Delta_\kappa(x, x')$ now denote the length of the shortest path in the graph with curvature bounded by κ.

Proposition

There is a numerical constant $c \geq 1$ such that, when $\varepsilon/r \leq 1/c$, $\kappa r \leq 1/c$, and $\kappa' \geq \kappa + c(\kappa^2 r + \varepsilon/r^2)$,

$$\Delta_\kappa(x, x') \leq (1 + 6\varepsilon/r) g_\kappa(x, x'), \quad x, x' \in \mathcal{X}$$

(The right-hand side may be infinite.)

We now assume in addition that all the shortest paths on $\mathcal{S}$ have curvature bounded by κ.

[11] Alexander and Alexander 1981; Alexander, Berg, and Bishop 1987; Albrecht and Berg 1991.

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Lemma

Assume that $\mathcal{S}$ is a compact and connected C^2 submanifold with boundary that is either empty or C^2. Then there is $\kappa < \infty$ such that all the shortest paths on $\mathcal{S}$ have max-curvature bounded by κ.

(Strange things near the boundary.[11])

[11] Alexander and Alexander 1981; Alexander, Berg, and Bishop 1987; Albrecht and Berg 1991.

Theorem

There is a universal constant $c > 0$ such that, if $\kappa r \leq 1/c$ and $\varepsilon/\kappa r^2 \leq 1/c$, the unconstrained shortest paths in the graph have curvature at most $\kappa' \leq \kappa + c\,\varepsilon/\kappa r^3$.

Estimating distances based on adjacency information

Latent graph models

We observe the adjacency matrix $W = (W_{ij})$ of an undirected graph. We assume the existence of points, $x_1, \ldots, x_n \in \mathbb{R}^v$, such that

$$\mathbb{P}(W_{ij} = 1 \mid x_1, \ldots, x_n) = \phi(\|x_i - x_j\|),$$

for some non-increasing link function $\phi : [0, \infty) \mapsto [0, 1]$.

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Our goal is to estimate the pairwise distances

$$d_{ij} := \|x_i - x_j\|.$$

Hoff, Raftery, and Handcock 2002 assume a parametric model.

[12] Sarkar, Chakrabarti, and Moore 2010; Liben-Nowell and Kleinberg 2007; Liben-Nowell and Kleinberg 2003.

[13] Sussman, Tang, and Priebe 2014; Tang, Sussman, and Priebe 2013.

[14] Alamgir and Luxburg 2012; Luxburg and Alamgir 2013.

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Interestingly, there is a close connection with the literature on link prediction[12], where one wants to determine which nodes are closest at a given point in time as they are the most likely to become connected in the near future.

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There is related work by Carey Priebe et al, some of it in the context of a dot product graph — where $\phi(\|x_i - x_j\|)$ is replaced by $\phi(\langle x_i, x_j \rangle)$.[13]

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Ulrike von Luxburg et al have considered the case where, instead, a K-nearest neighbor graph is available.[14]

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We estimate $d_{ij} = \|x_i - x_j\|$ by $\hat{d}_{ij} = r\Delta_{ij}$.

Define

$$\varepsilon = \max_{x \in \mathrm{Conv}(x_1, \ldots, x_n)} \min_{i \in [n]} \|x - x_i\|$$

Theorem

For all $i, j \in [n]$,

$$0 \le \hat{d}_{ij} - d_{ij} \le 4(\varepsilon / r) d_{ij} + r$$

Assume without loss of generality that $r \leq 1/2$.

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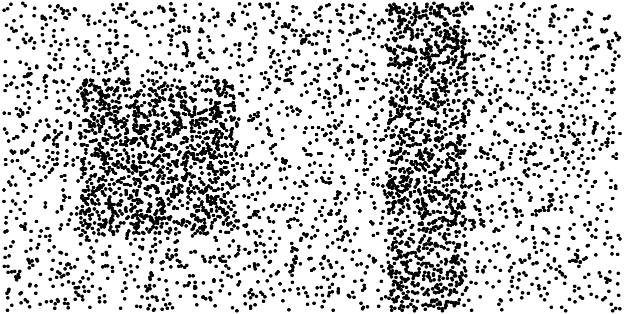
Theorem

There is a numeric constant $c > 0$ with the property that, for any $\varepsilon > 0$ and any estimator $\hat{d}$, there is $x_1, \dots, x_n \in [0,1]$ such that

$$\max_{x \in [0,1]} \min_{i \in [n]} \|x - x_i\| \leq \varepsilon$$

and, for at least half of the pairs $i \neq j$,

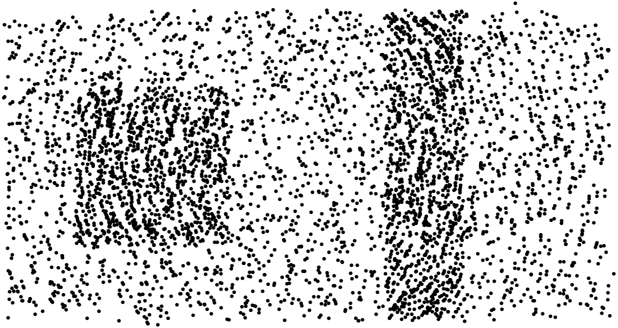
$$|\hat{d}_{ij} - d_{ij}| \geq \frac{c\,\varepsilon}{r \vee \varepsilon} d_{ij}.$$



latent positions (in $[0,2] \times [0,1]$)

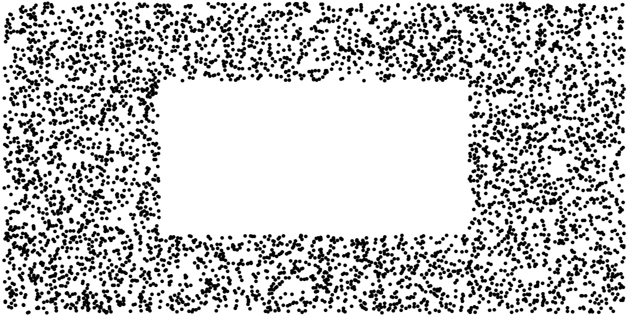
recovered positions with $r = 0.05$

recovered positions with $r = 0.1$

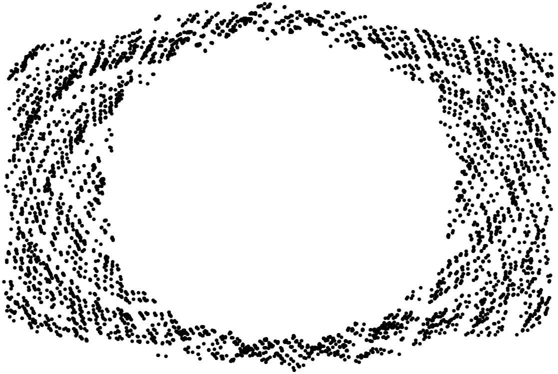


recovered positions with $r = 0.2$

The method requires convexity...



(latent positions)



(estimated positions)

More generally, assume that ϕ has support $[0, r]$, for some $r > 0$, and for some $c_0 > 0$ and $\alpha \geq 0$,

$$\phi(d) \geq c_0(1 - d/r)_+^\alpha$$

(When $\alpha = 0$, ϕ as a discontinuity at $d = r$.)

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Assume without loss of generality that $\mathrm{diam}(x_1, \ldots, x_n) \leq 1$.

Theorem

There are $C_1, C_2 > 0$ depending only on (α, c_0) such that, whenever $r/\varepsilon \geq C_1(\log n)^{1+\alpha}$, with probability at least $1-1/n$, for all $i, j \in [n]$,

$$0 \leq \hat{d}_{ij} - d_{ij} \leq C_2\Big[(\varepsilon/r)^{\frac{1}{1+\alpha}} d_{ij} + r\Big]$$

We also obtain results for the setting where the graph is the K-nearest neighbor graph of a point set $x_1, \ldots, x_n$, a setting first considered by Alamgir and Luxburg 2012.

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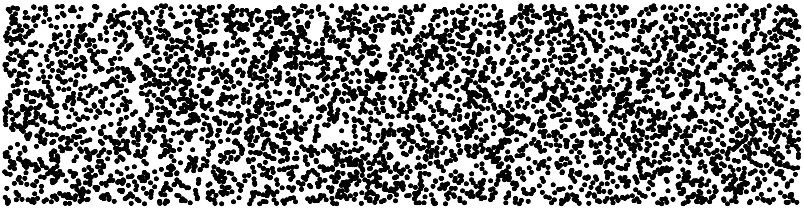
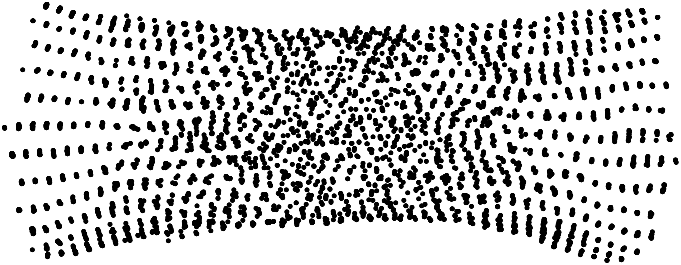
The graph distances perform similarly when $x_1, \ldots, x_n$ are generated iid from the uniform distribution on a compact and convex subset Ω... but only for pairs of points away from the boundary $\partial\Omega$.

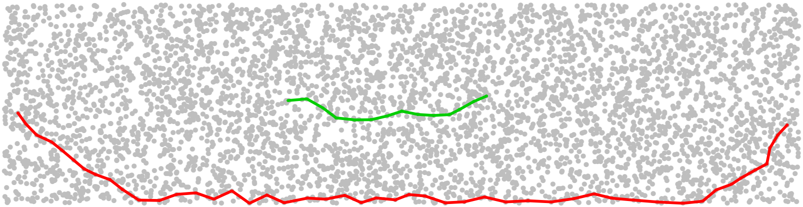


(latent positions)



(estimated positions)

The boundary acts as a high-speed freeway...



Related papers

- Ery Arias-Castro and Bruno Pelletier (2013). "On the convergence of maximum variance unfolding". In: *The Journal of Machine Learning Research* 14.1, pp. 1747–1770
- Ery Arias-Castro and Thibaut Le Gouic (2017). "Unconstrained and Curvature-Constrained Shortest-Path Distances and their Approximation". In: *arXiv preprint arXiv:1706.09441*
- Ery Arias-Castro et al. (2018). "On the Estimation of Latent Distances Using Graph Distances". In: *arXiv preprint arXiv:1804.10611*
- Ery Arias-Castro, Adel Javanmard, and Bruno Pelletier (2018). "Perturbation Bounds for Procrustes, Classical Scaling, and Trilateration, with Applications to Manifold Learning". In: *arXiv preprint arXiv:1810.09569*
- Clément Berenfeld and Ery Arias-Castro (2018). "Some Random Paths with Angle Constraints". In: *arXiv preprint arXiv:1811.01101*

Thank you

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