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Graph Approximations to Geodesics on Metric Graphs

MOTIVATION

Proximity graphs are often used to approximate geodesics

Used for various dimensionality reduction methods



- Laplacian Eigenmaps
- Locally Linear Embedding
- ISOMAP
- Maximum Variance Unfolding
- Local Tangent Space Alignment
- ...

Used as intermediate representations for topological inference [1, 2, 3]

THE PROBLEM

Existing results for approximating geodesic distances [4]

- Only apply to smooth submanifolds of \mathbb{R}^n
 - No singularities (such as bifurcations) allowed
- Conditions under which approximated and true

OUR APPROACH

New geometric characteristics for metric graphs

Definition 3. Given a connected metric graph M. For any $\epsilon > 0$ we define the branch separation $s_{\epsilon}(M) \in \mathbb{R}^+ \cup \{\infty\}$ of M at resolution $1/\epsilon$ as

 $s_{\epsilon}(M) \coloneqq \sup \{s \in \mathbb{R} : ||x - y|| < s \implies d_M(x, y) \le \epsilon\}.$

Definition 4. Given a connected metric graph M. For any

geodesic distances are close are stringent

- Must approximate all local patterns well
- However, global patterns may be approximated well without local patterns



REFERENCES

 $0 \leq \epsilon' < \epsilon \text{ we define the linearity of } M \text{ between resolutions}$ $1/\epsilon \text{ and } 1/\epsilon' \in \mathbb{R}^+ \cup \{\infty\} \text{ as}$ $\lambda_{\epsilon',\epsilon}(M) \coloneqq \sup \{\lambda \in \mathbb{R} : \epsilon' \leq d_M(x,y) \leq \epsilon \implies$ $\lambda d_M(x,y) \leq ||x-y||\}.$

- More flexibility (account for data at hand)
- Is also necessary to extend to singularities (proof in paper)

Theorem 3. Let M be a connected metric graph in \mathbb{R}^d and let X be a finite set of data points in M. Suppose a graph G = (X, E) is given, defining the following three thresholds: 1) $||x - y|| \ge \epsilon'$ for all $\{x, y\} \in E$, 2) $||x - y|| < s_{\epsilon}(M)$ for all $\{x, y\} \in E$, with $\epsilon > 0$, 3) for all $x, y \in X$ with $||x - y|| \le \tau$, we have $\{x, y\} \in E$. If for $0 < 4\delta < \tau$, X satisfies the δ -sampling condition, *i.e.*, for every $m \in M$ there is $x \in X$ with $d_M(m, x) \le \delta$, then for all $x, y \in M$

 $\lambda_{\epsilon,\epsilon'}(M)d_M(x,y) \le d_G(x,y) \le (1+4\delta/\tau)d_M(x,y).$ (1)



[1] R. Vandaele et al, "Mining Topological Structure in Graphs through Forest Representations," Journal of Machine Learning Research, 21(215):1–68, 2020.

[2] R. Vandaele. "Topological Data Analysis of Metric Graphs for Evaluating Cell Trajectory Data Representations," Master's thesis, Ghent University, 2020.

[3] R. Vandaele. "Topological Inference in Graphs and Images," Doctoral thesis, Ghent University, 2020.

[4] M. Bernstein et al, "Graph approximations to geodesics on embedded manifolds," 2000.

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