

# GRAPH APPROXIMATIONS TO GEODESIC DISTANCES IN NONLINEAR DIMENSIONALITY REDUCTION

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ABSTRACT. Nonlinear dimensionality reduction (NLD) methods attempt to recover a low-dimensional, geometrically faithful representation of data drawn from an unknown low-dimensional submanifold of a high-dimensional Euclidean space. Estimating geodesic distances between data points is an essential part of many of these methods, e.g., [TdSL00, LZ08, BN03].

Maximum Variance Unfolding (MVU) [WS06b, WS06a, WS04] is a heuristic approach to NLD, which is based on a semidefinite optimization problem which, intuitively, aims at maximizing the variance of the data while preserving local proximity relations stipulated in terms of a neighborhood graph. We present an equivalent formulation of this problem in terms of Euclidean distance matrices [Dat05, BB07] and consider a relaxation thereof to the cone of general distance matrices [PG12]. We show that the unique solution of the latter is precisely the distance matrix of the underlying neighborhood graph. Invoking results on graph approximations to geodesic distances, we may consider MVU as a regularized geodesic distance approximation problem. This insight enables us to establish a convergence result for MVU, provided that the underlying manifold be intrinsically flat and convex. This is surprising, since the authors of [WS04] explicitly intended to design the algorithm in such a way that graph approximations to global geodesic distances be avoided. (This part of the talk is based on [PG12]).

The above mentioned hitherto known convergence results on graph approximations to geodesic distances are restricted to manifolds without boundary and convex manifolds-with-boundary. In the second part of the talk, we shall present generalizations of these convergence results to (not necessarily convex) manifolds-with-boundary. These extensions are based on differential properties of geodesics in manifolds-with-boundary established in [AA81, ABB87, ABB93, PG12].

## REFERENCES

- [AA81] Ralph Alexander and S. Alexander. Geodesics in Riemannian manifolds-with-boundary. *Indiana Univ. Math. J.*, 30(4):481–488, 1981.
- [ABB87] Stephanie B. Alexander, I. David Berg, and Richard L. Bishop. The Riemannian obstacle problem. *Ill. J. Math.*, 31:167–184, 1987.
- [ABB93] Stephanie B. Alexander, I. David Berg, and Richard L. Bishop. The distance-geometry of Riemannian manifolds with boundary. In *Differential geometry: Riemannian geometry (Los Angeles, CA, 1990)*, volume 54 of *Proc. Sympos. Pure Math.*, pages 31–36. Amer. Math. Soc., Providence, RI, 1993.
- [BB07] R. Balaji and R. B. Bapat. On Euclidean distance matrices. *Linear Algebra Appl.*, 424(1):108–117, 2007.
- [BN03] Mikhail Belkin and Partha Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Computation*, 15:1373–1396, 2003.
- [Dat05] Jon Dattorro. *Convex optimization & Euclidean distance geometry*. Meboo, 2005.
- [LZ08] Tong Lin and Hongbin Zha. Riemannian manifold learning. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 30(5):796–809, May 2008.
- [PG12] Alexander Paprotny and Jochen Garcke. On a connection between maximum variance unfolding, shortest path problems and isomap. In *15th International Conference on Artificial Intelligence and Statistics (AISTATS 2012)*, La Palma, Canary Islands, Spain, April 21-23 2012.

- [TdSL00] J. B. Tenenbaum, V. de Silva, and J.C Langford. A global geometric framework for nonlinear dimensionality reduction. *Science*, 290(5500):2319–2323, 22 December 2000.
- [WS04] Kilian Q. Weinberger and Lawrence K. Saul. Unsupervised learning of image manifolds by semidefinite programming. In *CVPR (2)*, pages 988–995, 2004.
- [WS06a] Kilian Q. Weinberger and Lawrence K. Saul. An introduction to nonlinear dimensionality reduction by maximum variance unfolding. In *Unfolding, Proceedings of the 21st National Conference on Artificial Intelligence*. AAAI, 2006.
- [WS06b] Kilian Q. Weinberger and Lawrence K. Saul. Unsupervised learning of image manifolds by semidefinite programming. *International Journal of Computer Vision*, 70(1):77–90, 2006.