Graphs in Machine Learning

Similarity Graphs Construction

Building Graphs from Data

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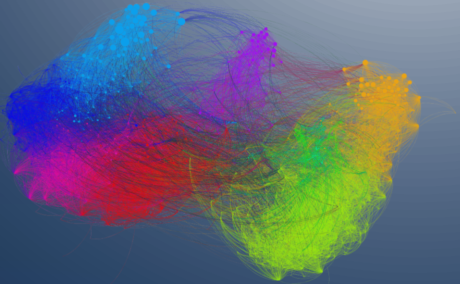
Partially based on material by: Ulrike von Luxburg, Gary Miller, Doyle & Schnell, Daniel Spielman



Similarity Graphs

Input: $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_N$

- raw data
- flat data
- vectorial data

Similarity Graphs

Similarity graph: $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ — **(un)weighted**

Task 1: For each pair i, j: define a **similarity function** s_{ij}

Task 2: Decide which edges to include

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ε-neighborhood graphs – connect the points with the distances smaller than ε

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This is art (not much theory exists).

http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/Luxburg07_tutorial.pdf

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- choose a “meaningful” similarity function s
- default choice:

$$s_{ij} = \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

- why the exponential decay with the distance?

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- why the exponential decay with the distance?
- σ controls the width of the neighborhoods
  - **a** practical rule of thumb: 10% of the average empirical std
  - possibility: learn σ_i for each feature independently
- metric learning (a whole field of ML)

Similarity Graphs: ε-neighborhood graphs

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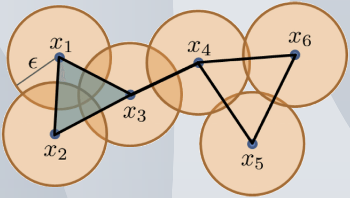

Figure: An ε-graph. Source: Illustration of a Rips complex

Similarity Graphs: ε-neighborhood graphs

Edges connect the points with the distances smaller than ε.

- distances are roughly on the same scale (ε)
- weights may not bring additional info $\rightarrow$ unweighted
- equivalent to: similarity function is at least ε
- theory [Penrose, 1999]: $\varepsilon = ((\log N)/N)^d$ to guarantee connectivity N nodes, d dimension
- practice: choose ε as the length of the longest edge in the MST - minimum spanning tree

What could be the problem with this MST approach?

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Anomalies can make ε too large.

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- asymmetric (or directed graph)
  - option OR: ignore the direction
  - option AND: include if we have both direction (mutual k-NN)
- how to choose k?
- $k \approx \log N$ - suggested by asymptotics (practice: up to $\sqrt{N}$)
- for mutual k-NN we need to take larger k
- mutual k-NN does not connect regions with different density
- why don't we take $k = N - 1$?
  - space and time
  - manifold considerations (preserving local properties)

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- these rules have little theoretical underpinning
- similarity is very data-dependent

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https://misovalko.github.io/mva-ml-graphs.html