

Metric denoising: Making it more friendly for topological computation

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Introduction

- Noise in data prevalent in various applications
- Noise present in diverse forms
- Effective handling of noise depends on how they are generated and what the target uses of data are

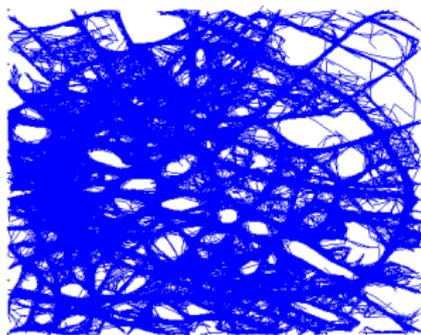


Image from brainmaps.org

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- This talk:
 - Focus on noise in metric of input data

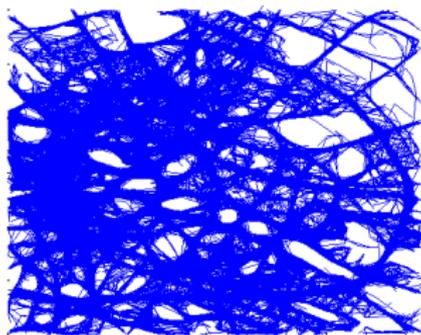


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Theorem (An example)

Given two sets of points $P, Q \subseteq \mathbb{R}^d$, let $dgm P$ and $dgm Q$ denote the persistence diagrams induced by the Čech filtration on P and Q , respectively. Then

$$d_B(dgm P, dgm Q) \leq d_H(P, Q).$$

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 - Some work handle more general noise, e.g, work on distance to measures [Chazal, Cohen-Steiner, Mériçot, 2011]

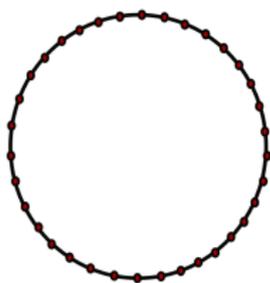
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 - Some work handle more general noise, e.g, work on distance to measures [Chazal, Cohen-Steiner, Mérigot, 2011]
- Averaging in the space of persistence diagrams may not be effective.

A graph example

Suppose our input are observed graphs

- Say, graphs G_1, G_2, \dots , are noisy observation of the same true graph G^*
- We may try to build intrinsic Čech filtration based on induced graph metric and then “average” their persistence diagrams dgm_1, dgm_2, \dots

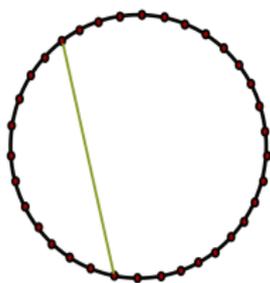


G^*

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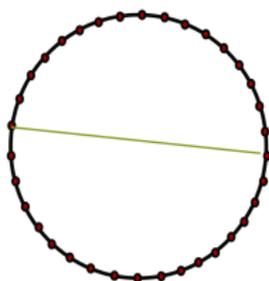


G_1

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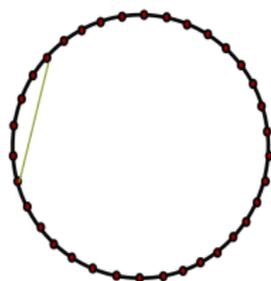


G_2

A graph example

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G_3

Our goal

To facilitate TDA tasks, our goal is to

- denoise input metric so that it is close to the “true” metric under Hausdorff-type distance

Three different settings to explore:

*What are natural ways to **model noise** in input metric, and how to process such noise efficiently **with theoretical guarantees**.*

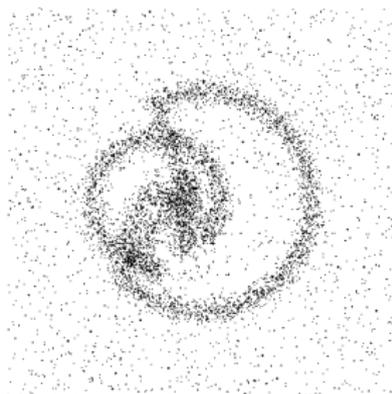
- **Setting 1:** towards parameter-free denoising for embedded point cloud data (PCD)
- **Setting 2:** metric embedding with outliers
- **Setting 3:** **recovering shortest path metrics from perturbed graphs**

Setting 1

Input: A set of points P already embedded in a metric space, which is a “noisy” sample of a hidden ground truth K

Output: A “denoised” set of points $Q \subset P$ Hausdorff-close to K

- [Buchet, Dey, J. Wang, W. SoCG 2017]

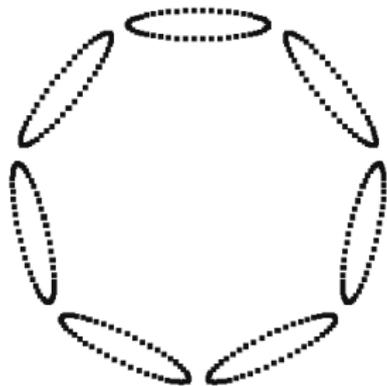


Some Existing Denoising Approaches

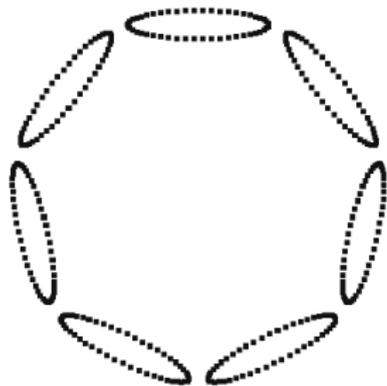
- Thresholding
 - choice of a density estimator, which involves parameter(s)
 - choice of a threshold
- Mean-shift type
 - needs additional parameters: such as step size, stopping criteria.
- Parametric methods
 - assuming knowing the noise distribution or generative model
 - often asymptotic guarantees

Require parameters and / or knowledge of noise models.
Non-uniform distribution challenging.

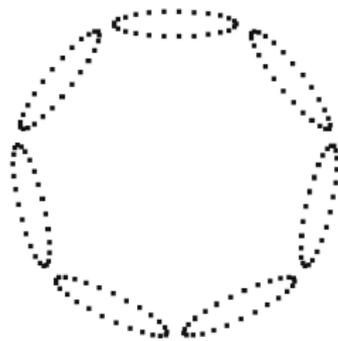
Parameter/assumptions Necessary



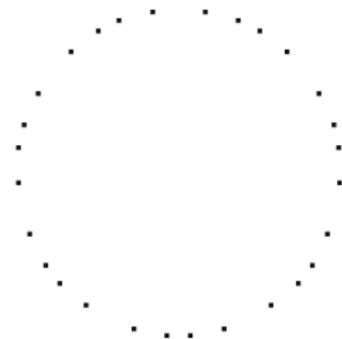
Parameter/assumptions Necessary



$k = 2$



$k = 10$



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Minimize the use of parameter in denoising embedded PCD data,
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Parameter-free? Require stronger assumptions on noise model

- Declutter+Resample algorithm

Theoretical guarantees for decluttering

Theorem

Given a point set P which is an ϵ_k *noisy sample* of a compact K , Algorithm Declutter returns a set Q such that

$$d_H(K, Q) \leq 7\epsilon_k.$$

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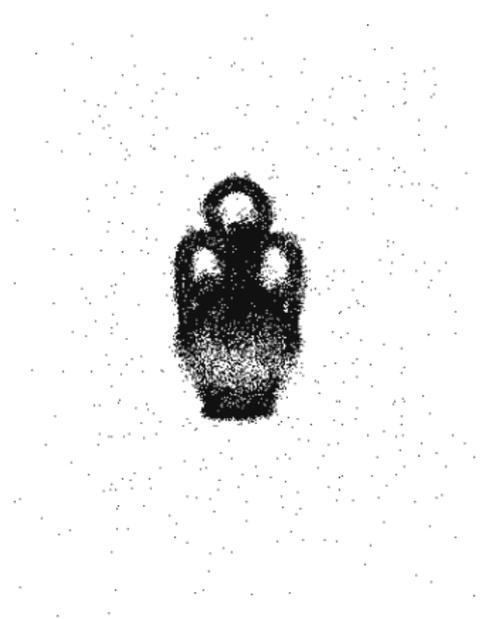
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- Can be extended to an *adaptive-noise* setting

Illustration II



Input



$k = 4$



$k = 47$

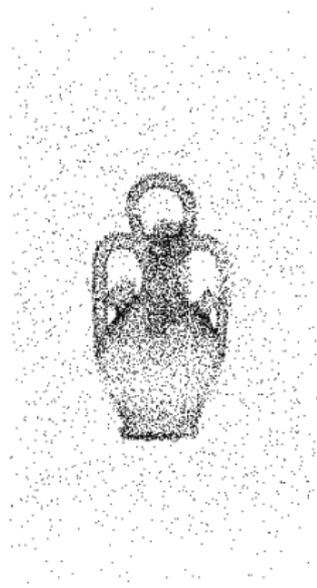
ParaFreeDecluster guarantees

Theorem

Given a point set P and i_0 such that for all $i > i_0$, P is a *weak uniform* $(\epsilon_{2^i}, 2)$ *noisy sample* of K and is also an $(\epsilon_{2^{i_0}}, 2)$ *noisy sample* of K , Algorithm ParfreeDecluster returns a point set P_0 such that $d_H(P_0, K) \leq (87 + 16\sqrt{2})\epsilon_{2^{i_0}}$.

- Require uniformity of input samples around the hidden compact set.
- Algorithm still very simple. It has $O(\log n)$ iterations of previous Decluster algorithm and another resampling procedure.

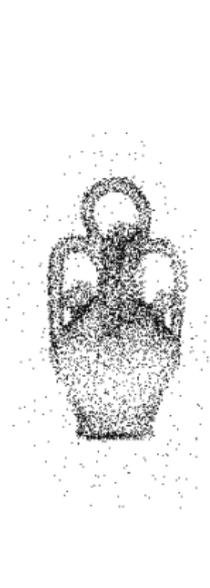
ParaFreeDeclutter results



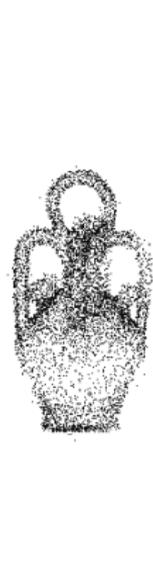
Input



$k = 1024$

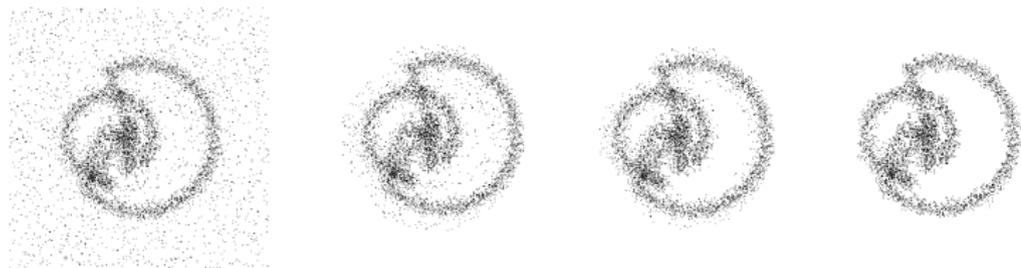


$k = 256$



$k = 1$

ParaFreeDeclutter results



Setting 2

Input: A discrete n -point metric space $(X = \{x_1, \dots, x_n\}, \rho)$

- (X, ρ) approximately comes from a “nice” *target metric space*
- some input points could have corrupted / erroneous distance to other points, they are “outliers”

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Output: A “near-optimal” set of outliers $K \subset X$ together with a “low-distortion” embedding of $(X \setminus K, \rho)$ into some target metric space

- the target space could be a tree metric, ultrametric, or constant-dimensional Euclidean space.

[Sidiropoulos, D. Wang, W. SoDA 2017]

Definition (Embedding)

Given two metric spaces $\mathcal{X} = (X, \rho_X)$ and $\mathcal{Y} = (Y, \rho_Y)$, an *embedding* of \mathcal{X} into \mathcal{Y} is simply a map $\phi : X \rightarrow Y$.

- ϕ is an *isometric embedding* if for any $x, x' \in X$,
 $\rho_X(x, x') = \rho_Y(\phi(x), \phi(x'))$.
- ϕ is an ε -*distorted embedding* if for any $x, x' \in X$,
 $|\rho_X(x, x') - \rho_Y(\phi(x), \phi(x'))| \leq \varepsilon$. Alternatively, we say that \mathcal{X} admits an embedding into \mathcal{Y} with **(additive) distortion** ε .

Optimization Problem

Minimum outlier-embedding problem: Given a discrete n -point metric space $(X = \{x_1, \dots, x_n\}, \rho)$, compute the *smallest set* $K^* \subset X$ such that $(X \setminus K^*, \rho)$ embeds into a target metric space either isometrically, or with distortion at most ε .

- Choices of target metric spaces: ultrametric, tree metric, constant-dimensional Euclidean space \mathbb{R}^d
- The set K^* is referred to as the *optimal set of outliers*

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|-------|-------|-------|-------|-------|
| x_1 | 0 | 1 | 1 | 1 |
| x_2 | 1 | 0 | 2 | 2 |
| x_3 | 1 | 2 | 0 | 2 |
| x_4 | 1 | 2 | 2 | 0 |

Input metric \mathcal{X}

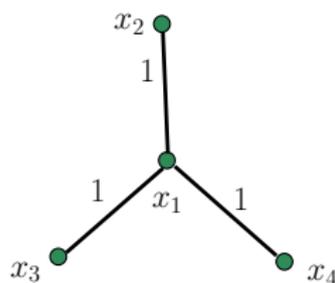
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Isometric embedding to a tree metric

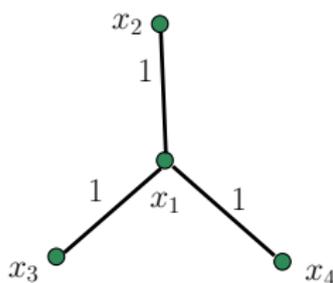
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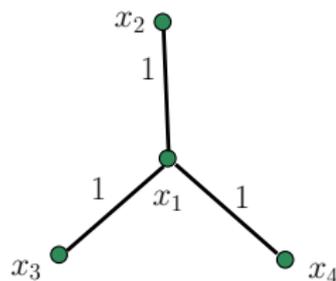
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An embedding with additive distortion 0.2

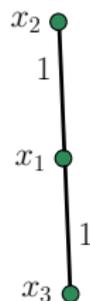
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Outlier embedding to \mathbb{R}^1 with distortion 0.13

Hardness of the Outlier Embedding

Theorem

The problem of minimum outlier embedding into a tree metric, an ultrametric, or \mathbb{R}^d , is NP-hard.

Furthermore, assuming the Unique Games Conjecture, it is NP-hard to approximate the isometric version with a factor of $2 - \nu$ for any $\nu > 0$.

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- We developed various approximation algorithms
- Present results for special case: *(near-)isometric outlier-embedding into \mathbb{R}^d*

Isometric outlier-embedding case

Theorem (First 2-approximation)

Given an n -point metric space (X, ρ) , there is an algorithm that can compute at most $2|K^|$ number of points $K \subset X$, such that $(X \setminus K, \rho)$ admits an isometric embeddign into \mathbb{R}^d . The algorithm runs in $O(n^{d+1})$ time.*

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Theorem (Improved Approximation)

Given an n -point metric space (X, ρ) , there is a $O(n^2)$ time *randomized algorithm* that can compute $3|K^*|$ number of points $K \subset X$, such that with constant probability, $(X \setminus K, \rho)$ admits an isometric embeddign into \mathbb{R}^d .

- The big O notation hides constants depending exponentially on the dimension d .

Theorem (Bicriteria-Approximation)

Given an n -point metric space (X, ρ) , suppose it admits an $X \setminus K^$ admits a δ^* -distortion embedding into \mathbb{R}^d . Then there is a $O(n^2)$ time randomized algorithm that can compute $O(|K^*|d)$ number of points $K \subset X$, such that with constant probability, $(X \setminus K, \rho)$ admits an embeddign into \mathbb{R}^d with distortion $O(\sqrt{\delta^*})$ -distortion.*

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- The big O notation hides constants depending exponentially on the dimension d .
- Algorithm still reasonably simple, but analysis is much more involved.
 - We have implemented it!

Talk Outline

In this talk, we consider three different settings to explore:

What are natural ways to model noise in input metric, and how to process such noise efficiently with theoretical guarantees.

- **Setting 1:** towards parameter-free denoising for embedded point cloud data (PCD)
- **Setting 2:** metric embedding with outliers
- **Setting 3:** recovering shortest path metric from perturbed graphs

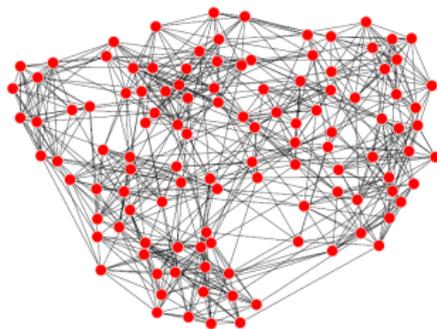
Problem Setup

Input: An observed **unweighted** graph $G = (V, E)$

- G is a “noisy” observation of a true graph G^*
- the metric of interest is the shortest path metric d_{G^*}

Output: Recover (approximately) the “true” shortest path metric d_{G^*} from G

- [Parthasarathy, Sivakoff, Tian, W. 2017]



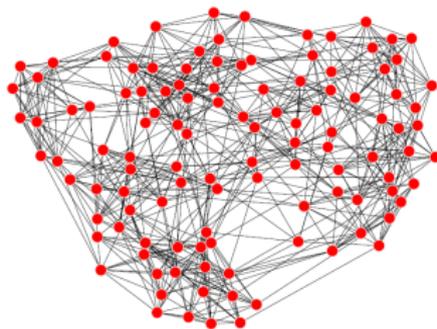
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The model

The true graph $G^* = (V, E^*)$: given n ,

- $V = V_n$ sampled i.i.d from a L -doubling measure $\mu : M \rightarrow \mathbb{R}^+$ on a compact geodesic metric space (M, d_M)
- $E^* = E_{r,n}^* = \{(u, v) \mid d_M(u, v) \leq r, u, v \in V\}$ is the r -neighborhood graph for some parameter $r > 0$

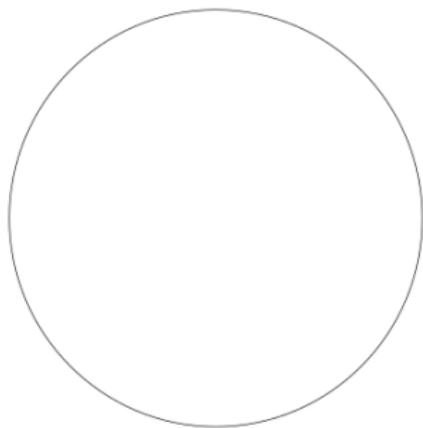
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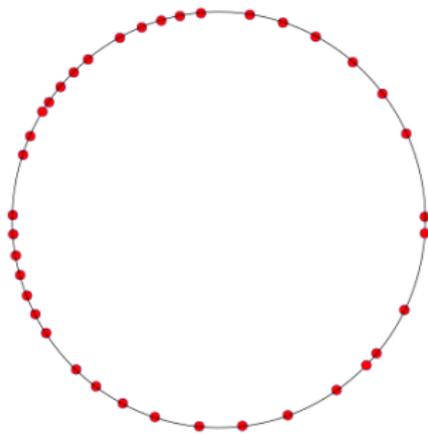
The observed graph $G = (V, E)$: A (p, q) -perturbation of G^* where

- (**p-deletion**): For each edge $e = (u, v) \in E^*$, we have $e \in E$ with probability $1 - p$
- (**q-insertion**): For any pair of nodes $u, v \in V$ s.t. $(u, v) \notin E^*$, we have $(u, v) \in E$ with probability q



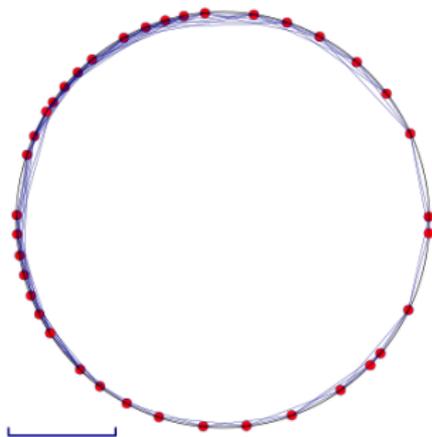
Hidden domain M

Illustration



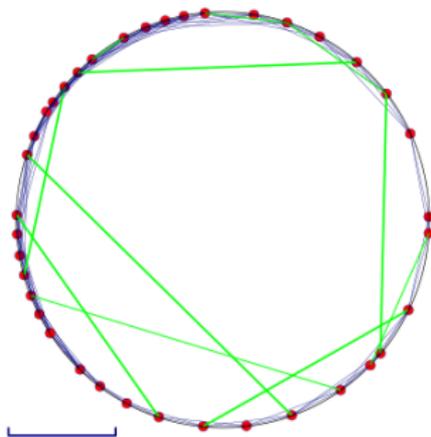
Graph Nodes V

Illustration



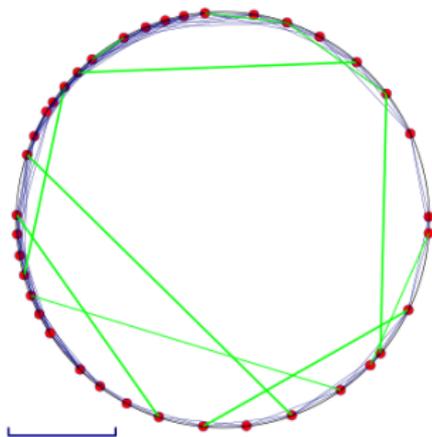
True graph G^*

Illustration



Random perturbation G

Illustration



Random perturbation G

The goal

Recover the shortest path metric d_{G^*} from G with approximation guarantee.

Remarks

- In many graphs, e.g social networks, nodes sampled from a hidden feature space, and edges encode proximity between graph nodes in certain feature space.

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- Shortest path metric natural choice in many situations (especially for sparse graphs), reflects the metric of the feature space
 - Other graph-induced metrics, e.g, diffusion distance?

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- Sampling from a measure allows varying degree distribution
- Random Erdős-Rényi type perturbation allows exceptions / noise
- Shortest path metric natural choice in many situations (especially for sparse graphs), reflects the metric of the **feature space**
 - Other graph-induced metrics, e.g, diffusion distance?
- However, shortest path metric sensitive to random perturbations (especially “short-cuts”)

Further remarks

- The model related to superposing a “structured subgraph” and a “random subgraph”
 - e.g, [Bollobás and Chung, 1988], [Watts and Strogatz, 1998], [Kleinberg 2000] (the small-world phenomenon), ...

Further remarks

- The model related to superposing a “structured subgraph” and a “random subgraph”
 - e.g, [Bollobás and Chung, 1988], [Watts and Strogatz, 1998], [Kleinberg 2000] (the small-world phenomenon), ...
- However, the metric recovery problem is somewhat orthogonal to goals in typical network analysis

Definition (Doubling measure)

A measure $\mu : X \rightarrow \mathbb{R}^+$ on a metric space (X, d) is said to be *L-doubling* if all metric balls have finite and positive measure and that there is a constant L such that for all $x \in X$ and $R > 0$,

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Assumption-R: The parameter r (neighborhood size) is large enough such that $\mu(B(x, \frac{r}{2})) \geq s \geq \frac{12 \ln n}{n}$ for any $x \in M$.

Effect of Deletion

Theorem (Deletion only)

Let G^* be the true graph generated as described, and G a graph obtained by deleting each edge in G^* with probability p . Assuming Assumption-R, then for $p < \frac{1}{2} e^{-\frac{2 \ln n}{sn}}$ with probability at least $1 - \frac{1}{n^{\Omega(1)}}$, the shortest path metric d_G in the observed graph is a 2-approximation of the shortest path metric d_{G^*} in the true graph; that is,

$$\frac{1}{2} d_G(u, v) \leq d_{G^*}(u, v) \leq 2 d_G(u, v).$$

Since $s \geq 12 \ln n/n$ by Assumption-R, $p < \frac{1}{2e^{3/4}}$. As s increases, the upper bound on p gets closer to $1/2$.

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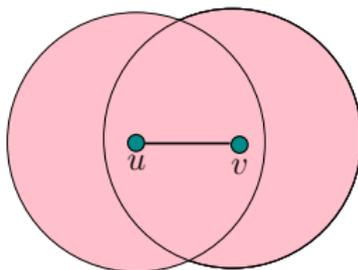
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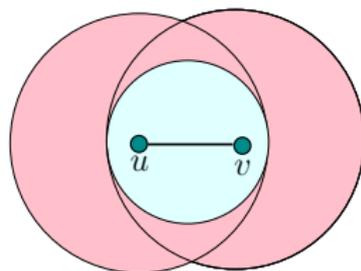
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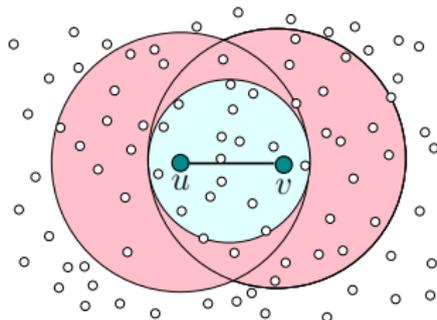
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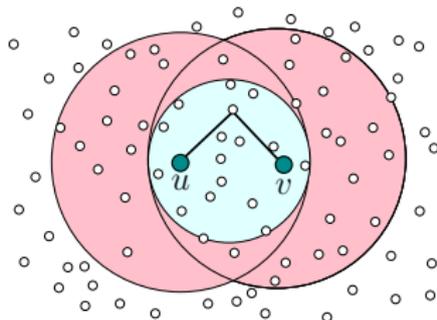
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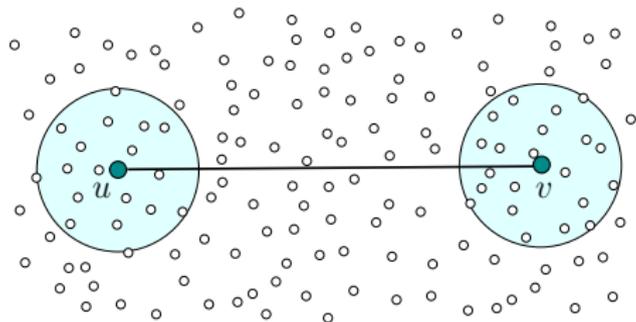
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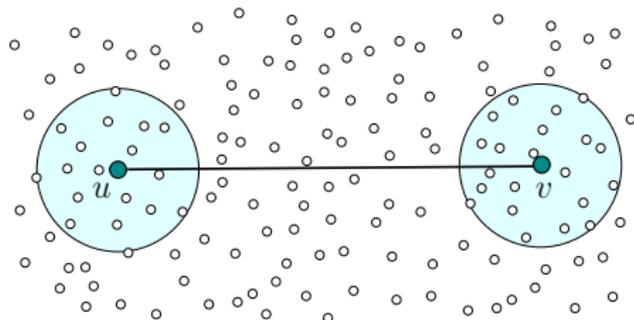
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τ -Jaccard-Cleanup: Given graph G , for each edge $(u, v) \in G$, we keep the edge in a filtered graph \widehat{G} iff

$$\rho_{u,v}(G) = \frac{|N_u^G \cap N_v^G|}{|N_u^G \cup N_v^G|} \geq \tau.$$

Insertion only – Good edges

Good edges have “large” Jaccard index.

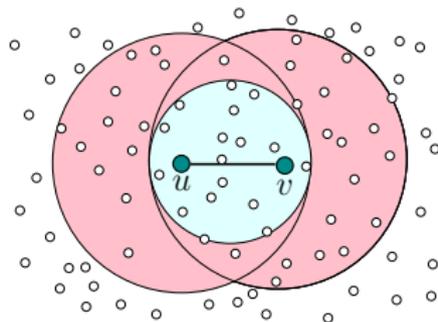
Lemma

Let V be n points sampled i.i.d. from L -doubling measure $\mu : M \rightarrow \mathbb{R}$. Let G^* be the r -neighborhood graph for V and \widehat{G} obtained by inserting each edge not in G^* independently with probability q . Suppose Assumption-R holds and the insertion probability satisfies $q \leq cs$. Then w.h.p., for any $\tau \leq \frac{1}{(6+12c)L^2}$, $\rho_{u,v}(\widehat{G}) \geq \tau$ for all pairs of nodes $u, v \in V$ with $(u, v) \in E(G^*)$.

- For example, if $c = \frac{1}{2}$ (i.e, $q \leq \frac{s}{2}$), then $\rho_{u,v}(\widehat{G}) \geq \frac{1}{13L^2}$ w.h.p.
- c can be super-constant, and tradeoff the requirement on q and Jaccard index on good edges.
 - As c increases, q is larger, but the upper bound on τ decreases.

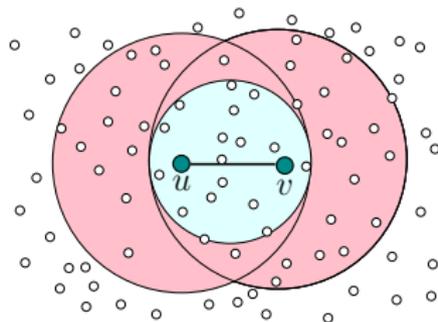
Requirement of $q \leq cs$

Recall the Jaccard index for an edge (u, v) is $\rho_{u,v}(G) = \frac{|N_u^G \cap N_v^G|}{|N_u^G \cup N_v^G|}$.



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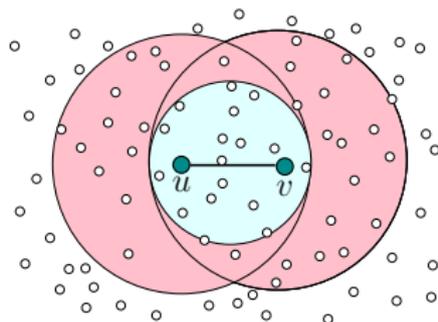


For an good edge $(u, v) \in E(G^*)$,

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For an good edge $(u, v) \in E(G^*)$,

- When $q = 0$, $\rho_{u,v}(G)$ is a constant depending on L
- As q increases, randomly inserted edges dominates, and $\rho_{u,v}(G)$ tends to q
 - $|N_u^G \cap N_v^G| \rightarrow nq^2$ while $|N_u^G \cup N_v^G| \rightarrow nq$

Insertion only – Bad edges

Very-bad edges have “small” Jaccard index.

Lemma

Let V be n points sampled i.i.d. from L -doubling measure μ . Let G^* be the r -neighborhood graph for V and \hat{G} obtained by inserting each edge not in G^* independently with probability q . Suppose Assumption-R holds and the insertion probability satisfies $q \leq cs$.

Then for any $\tau \geq (c + 2)q + 2(c + 2)\sqrt{\frac{\ln n}{sn}}$, w.h.p., $\rho_{u,v}(\hat{G}) < \tau$ for all pairs of nodes $u, v \in V$ such that (u, v) is very-bad.

- For example, if $c = 1$ and $sn = \omega(\ln n)$, then w.h.p. $\rho_{u,v}(\hat{G}) \leq 3q + o(1)$ for all very-bad edges (u, v) .

Main Result

Theorem

Given an observed graph G as a perturbed version of G^* as described before. Suppose Assumption-R holds, $sn = \omega(\ln n)$, the deletion probability $p < \min\{1 - \frac{\sqrt{3}}{2}, \frac{1}{2}e^{-\frac{9 \ln n}{sn}}\}$, and that the insertion probability $q \leq cs$. Let \widehat{G}_τ denote the graph after τ -Jaccard-cleanup of G with $\tau \in (\frac{c}{1-p}q + o(1), \frac{2(1-p)^2}{15L^2(1+2c)})$. Then the shortest path distance metric $d_{\widehat{G}_\tau}$ from \widehat{G}_τ is a 2-approximation of the shortest path metric d_{G^*} of the true graph G^* with high probability.

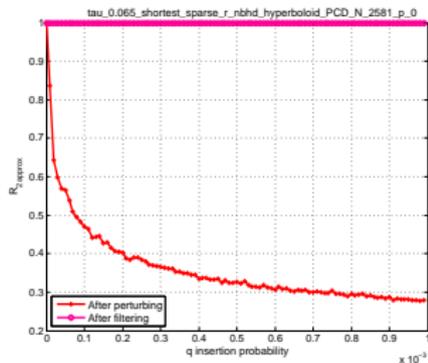
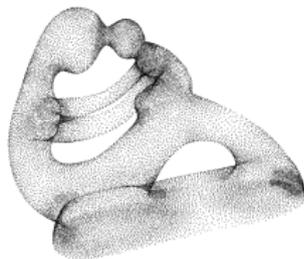
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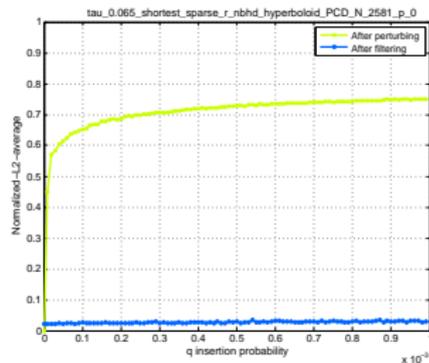
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- L -doubling measure can be extended to a **local version**

Preliminary Results – Proof of principle examples



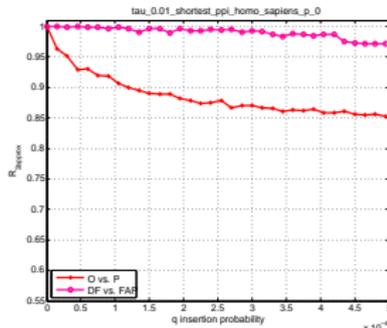
2-approximation rate



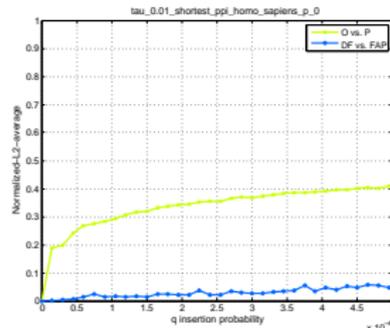
normalized L_2 error

Preliminary Results – Real networks w/o ground truth

- Given observed graph G , let G_q denote G with random $(p = 0, q)$ -perturbation
- Let G^τ and G_q^τ be the graphs after τ -Jaccard filtering of G and G_q , respectively.
 - "O vs P": comparison between d_G and d_{G_q} as q increases
 - "DP vs FAP": comparison between d_{G^τ} and $d_{G_q^\tau}$



2-approximation rate



normalized L_2 error

In this talk:

- **Setting 1:** towards parameter-free denoising for embedded point cloud data (PCD)
- **Setting 2:** metric embedding with outliers
- **Setting 3:** shortest path metric recovery from perturbed graphs

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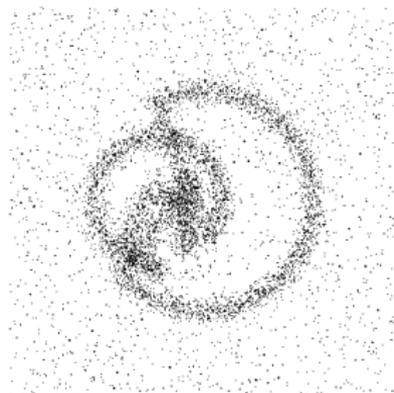
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 - E.g., for graph metrics, better tolerance in insertion probability, or better model to include more general graphs
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- Other natural noise models?
 - E.g., for graph metrics, better tolerance in insertion probability, or better model to include more general graphs
 - for weighted graphs?
- What are other ways to handle noise in metric?
 - Do we have to perform explicit denoising?

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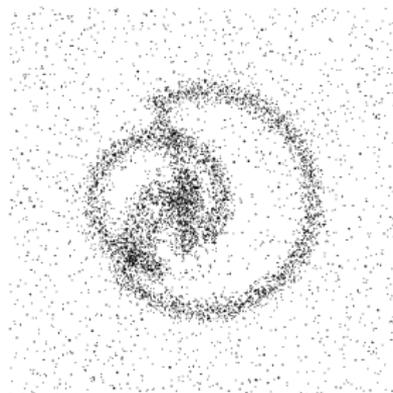
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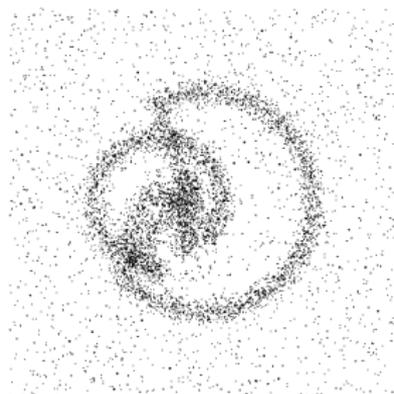
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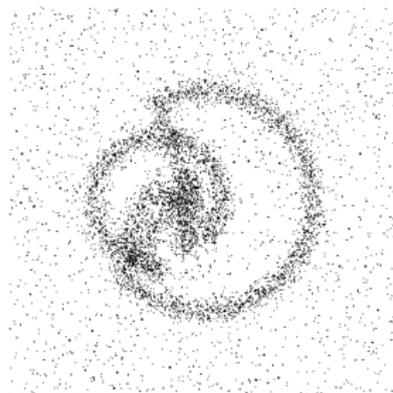
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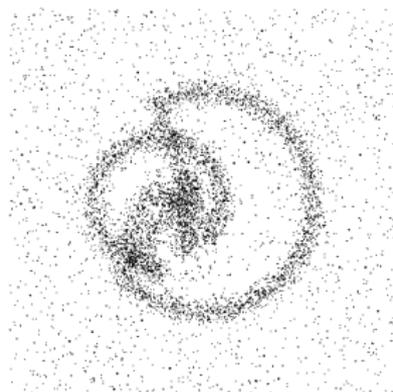
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Goal: depending on input noise model, develop theoretical guarantee for the output.

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The geometry of the underlying space where graph nodes are sampled from may help.

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What can we obtain if we are given multiple sets of samples of input data

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- graph case?
 - Averaging resulting persistence diagrams may not “cancel” noise.
 - Maybe “decorated” persistence diagrams?