Multiscale 2-Mapper – Exploratory Data Analysis Guided by the First Betti Number

Halley Fritze Topological Data Visualization Workshop June 9th, 2025

The *Mapper Graph* is an unsupervised soft clustering algorithm which clusters data in the form of a graph.

G. Singh, F. Mémoli, and G. E. Carlsson, *Topological Methods for the Analysis of High Dimensional Data Sets and 3D Object Recognition*, 4th Symposium on Point Based Graphics, PBG@Eurographics 2007, Prague, Czech Republic, September 2-3, 2007, Eurographics Associa- tion, 2007, 91–100, doi: 10.2312/SPBG/SPBG07/091-100.

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Definition. Let $X \subseteq \mathbb{R}^d$ be a data set. Given a continuous lens $f: X \to \mathbb{R}^n$, cover $\mathcal{U} = \{U_i\}_{i \in I}$ of f(X), and clustering algorithm we define the *Mapper* graph as

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- Cover f(X) with overlapping squares.

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- Choose $f: X \to \mathbb{R}^2$ to be the coordinate projection to \mathbb{R}^2 .
- Cover f(X) with overlapping squares.
- Choose DBSCAN as the clustering algorithm.

























The intersection structure of a cover can yield higher dimensional nerve when $f(X) \subset \mathbb{R}^2$.

Taking this into account could yield better manifold approximations of point clouds.





Definition. Given a point cloud *X*, continuous filter $f: X \to \mathbb{R}^n$, cover \mathcal{U} and clustering algorithm, we define the *2-Mapper complex of X* as

 $M(f,\mathcal{U})\coloneqq\mathcal{N}^2\bigl(f^{-1}(\mathcal{U})\bigr)$

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<u>Definition</u>. Given a point cloud *X*, continuous filter $f: X \to \mathbb{R}^n$, cover \mathcal{U} and clustering algorithm, we define the 2-Mapper complex of *X* as $M(f, \mathcal{U}) \coloneqq \mathcal{N}^2(f^{-1}(\mathcal{U}))$

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Optimal Covers

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Cubical Cover



Four 2-Simplices



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Lattice Cover

One 2-Simplex

Defining Covers

Definition. Let $X \subset \mathbb{R}^d$ be a data set. The *bounding box* on X is the space $B = \prod_{i=1}^d [m_i, M_i]$, where $m_i = \min_{x \in X} \pi_i(x)$ and $M_i = \max_{x \in X} \pi_i(x)$ for coordinate projections π_i .

We define each cover with parameters k and g representing the scale for the number of cover sets and their overlap proportion, respectively.

Cubical Cover

Definition. Let $Z \subset \mathbb{R}^n$ be a compact topological space with bounding box *B*. The cubical cover \mathcal{U} on *Z* constructed with $k \ge 1$ -intervals and overlap fraction 0 < g < 1 is a cover of boxes $\mathcal{U} = \{U_{\alpha}\}_{\alpha \in A}$ so that each cover set is of the form

$$U_{\alpha,s} = \prod_{i=1}^{n} \left[c_{\alpha,i} - \frac{l_i}{2}, c_{\alpha,i} + \frac{l_i}{2} \right]$$

Where
$$c_{\alpha,i} = m_1 + (\alpha_i - 1)(1 - g)l_i + \frac{1}{2}l_i$$

and $l_i = \frac{M_i - m_i}{k - (k - 1)g}$.



Cubical Lattice Cover

Definition. Let $Z \subset \mathbb{R}^n$ be a compact topological space with bounding box $B = \prod_{i=1}^n [m_i, M_i]$. We define the *cubical lattice cover* \mathcal{U} over Z constructed with *k*-intervals and overlap fraction g as the cover $\mathcal{U} = \{U_{\xi}\}_{\xi \in B \cap \mathbb{Z}^n}$ whose cover sets are hypercubes defined

$$U_{\xi} = \prod_{i=1}^{n} \left[c \left(\xi_i - \frac{1}{2(1-g)} \right), c \left(\xi_i + \frac{1}{2(1-g)} \right) \right],$$

with $c = \max_{1 \le i \le n} \frac{M_i - m_i}{k - (k-1)g}$

A₂^{*}-Lattice Cover

Definition. Let $Z \subset \mathbb{R}^n$ be a compact topological space with bounding box $B = \prod_{i=1}^n [m_i, M_i]$. Let A_2^* denote the root lattice generated with matrix

$$M_{A_2^*} = \begin{pmatrix} 1 & 0\\ -1 & \sqrt{3}\\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

The A_2^* -lattice cover defined with k intervals and overlap fraction g is a cover $\mathcal{L} = \{B_{\varepsilon}(c\xi M_{A_2^*})\}_{c\xi\in B\cap\mathbb{Z}^2}$ with $\varepsilon = \frac{1+g}{\sqrt{3}}\max_{i=1,2}\frac{M_i - m_i}{k}.$



Analysis of 2-Mapper through Cover Choice



Stochastic Triangle in \mathbb{R}^8

Cubical Cover

Cubical Lattice Cover A_2^* -Lattice Cover

Analysis of 2-Mapper through Cover Choice

 $_{\odot}$ 100 stochastic triangles generated in \mathbb{R}^8

 \circ 2-Mapper complexes constructed with k = 10 and g = 0.3



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Persistent Homology

Construct a filtration of simplicial complexes for $r \ge 0$,


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Construct a filtration of simplicial complexes for $r \ge 0$, $\operatorname{VR}_{r_0}(X) \subseteq \operatorname{VR}_{r_1}(X) \subseteq \cdots \subseteq \operatorname{VR}_{r_k}(X)$



Applying homology yields a *persistence vector space:* $H_*(\operatorname{VR}_{r_0}(X); \mathbb{Z}_2) \to H_*(\operatorname{VR}_{r_1}(X); \mathbb{Z}_2) \to \cdots \to H_*(\operatorname{VR}_{r_k}(X); \mathbb{Z}_2)$



Barcodes and Persistent Diagrams

We track the birth and death times for each cycle as a persistent barcode or persistence diagram.



Distances between diagrams

<u>Definition</u>. Let $D_k(V)$ and $D_k(W)$ be two degree-*k* persistence diagrams for persistence vector spaces *V* and *W*.

Let $\Pi = \{\pi : D_k(V) \to D_k(W)\}$ be the set of bijections between their points to each other or to the diagonal $\{(x, x) : x \in \mathbb{R}_+\}$.

The bottleneck distance is defined as

$$d_B(D_k(V), D_k(W)) = \inf_{\pi \in \Pi} \sup_{x \in D_k(V)} ||x - \pi(x)||_{\infty}$$

Definition. Let *X* and *Z* be topological spaces. For a well-behaved continuous map $f : X \to Z$ and finite open cover $\mathcal{U} = \{U_{\alpha}\}_{\alpha \in A}$ of *Z* the *generalized Mapper complex* is

 $\mathsf{M}(f,\mathcal{U}) \coloneqq \mathcal{N}(f^*(\mathcal{U}))$

Definition. A tower of covers with resolution $s \in \mathbb{R}_{\geq 0}$ is a collection of covers $\mathfrak{U} = {\mathcal{U}_{\varepsilon}}_{\varepsilon \geq s}$ with maps $u_{\varepsilon,\delta} \colon \mathcal{U}_{\varepsilon} \to \mathcal{U}_{\delta}$ so that $u_{\varepsilon,\varepsilon} = \text{Id}$ and $u_{\varepsilon,\gamma} = u_{\delta,\gamma} \circ u_{\varepsilon,\delta}$ for all $s \leq \varepsilon \leq \delta \leq \gamma$.

We write $res(\mathfrak{U}) = s$ for the resolution of tower \mathfrak{U} .

<u>Definition</u>. Let *X* and *Z* be topological spaces and $f: X \to Z$ be a well-behaved continuous map. Let \mathfrak{U} be a tower of covers of *Z*.

The *Multiscale Mapper* is the tower of simplicial complexes defined $MM(\mathfrak{U}, f) \coloneqq \mathcal{N}(f^*(\mathfrak{U}).$

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For a finite sequence $res(\mathfrak{U}) \leq \varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_n$,

$$H_*\left(\mathcal{N}\left(f^*(\mathcal{U}_{\varepsilon_1})\right)\right) \to H_*\left(\mathcal{N}\left(f^*(\mathcal{U}_{\varepsilon_2})\right)\right) \to \cdots \to H_*\left(\mathcal{N}\left(f^*(\mathcal{U}_{\varepsilon_n})\right)\right).$$

Tamal K. Dey, Fecundo Mèmoli, and Yusu Wang. Multiscale Mapper: Topological Summarization via Codomain Covers. *Proceedings of the 2016 Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 997-1013. 2016.













<u>Definition</u>. Let $c \ge 1$ and s > 0. A finite tower of covers $\mathfrak{W} = {\mathcal{W}_{\varepsilon}}$ over a compact metric space (Z, d_Z) is (c, s)-good if

- 1. $res(\mathfrak{B}) = s$, and $s \leq diam(Z)$
- 2. diam $(W_{\varepsilon,\alpha}) \leq \varepsilon$ for all $W_{\varepsilon,\alpha} \in \mathcal{W}_{\varepsilon}, \varepsilon \geq s$
- *3.* $\forall 0 \subset Z$ with diam $(0) \geq s$, there exists $W \in \mathcal{W}_{c \cdot \text{diam}(0)}$ such that $0 \subset W$.

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Example. A tower of covers $\mathfrak{U} = {\mathcal{U}_{\varepsilon}}_{\varepsilon \ge s}$ with $\mathcal{U}_{\varepsilon} = {B_{\varepsilon/2}(z) | z \in Z}$ is a (2, s)-good tower of covers of compact metric space *Z*.

<u>**Theorem (Dey, M., W.).</u>** For two (c, s)-good tower of covers $\mathfrak{U}, \mathfrak{V}$, the bottleneck distance between two diagrams produced from their multiscale mappers is bounded,</u>

$$d_B\left(D_k(MM(f,\mathfrak{U})), D_k(MM(f,\mathfrak{V}))\right) \leq c.$$

Definition. Let $Z \subset \mathbb{R}^n$ be a compact topological space. Then for lens function $f: Z \to \mathbb{R}^m$ and tower of covers $\mathfrak{U} = {\mathcal{U}_{\varepsilon}}_{\varepsilon \ge s}$ over f(Z), the *Multiscale 2-Mapper*, denoted $MM_2(f, \mathfrak{U})$, for a finite sequence $s \le \varepsilon_1 \le \cdots \le \varepsilon_k$ is of filtration of 2-Mapper complexes

$$\mathcal{N}^{2}(f^{*}(\mathcal{U}_{s})) \to \mathcal{N}^{2}(f^{*}(\mathcal{U}_{\varepsilon_{1}})) \to \cdots \to \mathcal{N}^{2}(f^{*}(\mathcal{U}_{\varepsilon_{k}})).$$

Tower of Cubical Covers

<u>Definition</u>. Let $X \subset \mathbb{R}^n$ be a compact topological space with bounding box *B* and cubical cover \mathcal{U}_s constructed with *k*-intervals and overlap fraction *g* so that each cover set is of the form

$$U_{\alpha,s} = \prod_{i=1}^{n} \left[c_{\alpha,i} - \frac{l_i}{2}, c_{\alpha,i} + \frac{l_i}{2} \right]$$

Where $c_{\alpha,i} = m_1 + (\alpha_i - 1)(1 - g)l_i + \frac{1}{2}l_i$ and $l_i = \frac{M_i - m_i}{k - (k - 1)g}$.

Tower of Cubical Covers

<u>Definition</u>. The *tower of cubical covers* \mathfrak{U} on X is a tower $\mathfrak{U} = {\mathcal{U}_{\varepsilon}}_{\varepsilon \ge s}$ with resolution $\operatorname{res}(\mathfrak{U}) = s = ||(l_1, \dots, l_n)||_2$. For $\varepsilon \ge s$, each cover $\mathcal{U}_{\varepsilon} = {U_{\alpha,\varepsilon}}_{\alpha \in A}$ such that for each $\alpha \in A$,

$$U_{\alpha,\varepsilon} = \prod_{i=1}^{n} \left[c_{\alpha,i} - \frac{1}{2} (l_i - \varepsilon'), c_{\alpha,i} + \frac{1}{2} (l_i + \varepsilon') \right],$$

For some $\varepsilon' \ge 0$ so that $\operatorname{diam}(U_{\alpha,\varepsilon}) = \varepsilon$.

This is a filtration over the parameter g.

Tower of Cubical Covers constructed with $0.1 \le g \le 0.5$ and k = 6.



$$g = 0.1$$

g = 0.3

g = 0.5

Tower of Lattice Covers

Definition. For $X \subset \mathbb{R}^n$ with bounding box *B*, let \mathcal{U}_s be a cubical lattice cover constructed with *k*-intervals and overlap fraction *g*.

The tower of cubical lattice covers $\mathfrak{U} = \{\mathcal{U}_{\varepsilon}\}_{\varepsilon \ge s}$ is a tower of covers with resolution $\operatorname{res}(\mathfrak{U}) = s = \frac{c\sqrt{n}}{1-g}$. For each $\varepsilon \ge s$ we define each cover $\mathcal{U}_{\varepsilon} = \{\mathcal{U}_{\alpha,\varepsilon}\}_{\alpha \in A}$ so that $\mathcal{U}_{\alpha,\varepsilon} = \prod_{\alpha,\varepsilon} \left[c\xi_{\alpha,i} - \frac{1}{2} \left(\frac{c}{2} - \varepsilon' \right), c\xi_{\alpha,i} + \frac{1}{2} \left(\frac{c}{2} + \varepsilon' \right) \right].$

$$U_{\alpha,\varepsilon} = \prod_{i=1}^{l} \left[c\xi_{\alpha,i} - \frac{1}{2} \left(\frac{c}{1-g} - \varepsilon' \right), c\xi_{\alpha,i} + \frac{1}{2} \left(\frac{c}{1-g} + \varepsilon' \right) \right],$$

For some $\varepsilon' \ge 0$ so that $\operatorname{diam}(U_{\alpha,\varepsilon}) = \varepsilon$.

Tower of A_2^* **-Lattice Covers**

Definition. For $X \subset \mathbb{R}^n$ with bounding box *B*, let \mathcal{L}_s be an A_2^* -lattice cover constructed with *k*-intervals and overlap fraction *g*.

The tower of A_2^* -lattice covers $\mathfrak{L} = \{\mathcal{L}_{\varepsilon}\}_{\varepsilon \ge s}$ is a tower of covers with resolution $\operatorname{res}(\mathfrak{L}) = s = \frac{2c(1+g)}{\sqrt{3}}$. For each $\varepsilon \ge s$ we define each cover $\mathcal{L}_{\varepsilon} = \left\{B\left(c\xi_{\alpha}M_{A_2^*}, \frac{1}{2}\varepsilon\right)\right\}_{\alpha \in A}$ with $\varepsilon = s + \varepsilon'$ for some $\varepsilon' \ge 0$.

Tower of A_2^* -Lattice Covers constructed with $0.1 \le g \le 0.5$ and k = 6.



g = 0.1

g = 0.3

g = 0.5

Stability for Covers

<u>Theorems (F.).</u> A tower of cubical (lattice) covers with resolution *s* constructed with *k*-intervals and overlap fraction *g* is (3, s)-good for $k \ge \sqrt{n}$.

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 Two Multiscale 2-Mapper objects with these towers are close with respect to the bottleneck distance!

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$$U_{\alpha} = C_{1,\alpha} \sqcup C_{2,\alpha} \sqcup N_{\alpha}$$

Theorem (Bungula, Darcy). Let *X* be a data set with tower of covers \mathcal{U} and use DBSCAN to cluster *X* with fixed parameters ϵ and Minpts ≤ 2 . Define $C_{\varepsilon} = \{C_{p,\varepsilon} : p \in U_{\varepsilon} \text{ is a core point}\}$. Then $\mathfrak{C} = \{C_{\varepsilon}\}_{\varepsilon \geq s}$ is a tower of covers with maps $c_{\varepsilon,\delta} : C_{\varepsilon} \to C_{\delta}$ for all $\mathcal{U}_{\varepsilon} \subseteq \mathcal{U}_{\delta}$ which are closed under composition.

<u>**Theorem (Bungula, Darcy).</u>** Let *X* be a data set and assume DBSCAN is used to cluster *X* with fixed hyperparameters ϵ and Minpts ≤ 2 . Then for all $\mathcal{U}_{\varepsilon} \subseteq \mathcal{U}_{\delta}$,</u>

 \circ There is a filtration of simplicial complexes $\phi_{ε,δ}$: $\mathcal{N}(\mathcal{C}_ε) \rightarrow \mathcal{N}(\mathcal{C}_\delta)$.

○ There is a filtration of homology groups $f_{\varepsilon,\delta} : H_k(\mathcal{N}(\mathcal{C}_{\varepsilon})) \to H_k(\mathcal{N}(\mathcal{C}_{\delta}))$ for each degree *k*.

Stability for Covers with DBSCAN

Theorem (F.). Let \mathfrak{U} be a tower of cubical, cubical lattice, or A_2^* -lattice covers with resolution *s* over a data set *X*. Define $\mathfrak{C} = \{\mathcal{C}_{\varepsilon}\}_{\varepsilon \ge s'}$ to be the cluster cover subordinate to \mathfrak{U} using DBSCAN with fixed parameters ϵ and $Minpts \le 2$. Then \mathfrak{C} is a (4, s')-good cover where $s' \le s$.

Stability for Covers with DBSCAN

Theorem (F.). Let $X \subset \mathbb{R}^m$ be a data set, $f : X \to \mathbb{R}^n$ be a continuous lens, and $\mathfrak{U}, \mathfrak{W}$ be two towers of covers (cubical, cubical lattice, or A_2^* -lattice). Cluster X using DBSCAN with fixed parameters ϵ and Minpts ≤ 2 . Then for each $k \geq 0$,

 $d_B(D_k(\mathsf{MM}_2(f,\mathfrak{C}_{\mathfrak{U}})), D_k(\mathsf{MM}_2(f,\mathfrak{C}_{\mathfrak{W}}))) \le 4$


The bottleneck distances for these two barcodes is 0.0894 in degree zero and 0.1789 in degree one.

Let $MM_2(f, \mathfrak{C})$ be the Multiscale 2-Mapper computed over data set *X* with finite tower of covers \mathfrak{U} and clustered with DBSCAN using parameters ϵ and Minpts.

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$$\mathsf{M}_{2}(\mathsf{f}, \mathcal{C}_{\varepsilon_{0}}) \xrightarrow{c_{0,1}^{*}} \mathsf{M}_{2}(\mathsf{f}, \mathcal{C}_{\varepsilon_{1}}) \xrightarrow{c_{1,2}^{*}} \cdots \xrightarrow{c_{t-1,t}^{*}} \mathsf{M}_{2}(f, \mathcal{C}_{\varepsilon_{t}})$$

Write $M_i := M_2(f, C_{\varepsilon_i})$ where M_i has vertex set V_i .

For each node $n \in V_i$ we write $n = (X_n, U_{\alpha, \varepsilon_i}, C_{p_{\alpha}, \varepsilon_i})$ $\uparrow \qquad \uparrow \qquad \uparrow$ Data Cover set Cluster

Simplex trees are used for computing with simplicial complexes and filtrations of simplicial complexes.



Each simplex σ is stored with filtration time t_{σ} .

J.-D. Boissonnat and C. Maria, The Simplex Tree: An Efficient Data Structure for General Simplicial Complexes, Algorithmica 70 (2014), no. 3, 406–427, doi: 10.1007/s00453-014-9887-3.

<u>Dream Construction</u>. For data set *X*, lens $f : X \to \mathbb{R}^n$, tower of covers \mathfrak{U} , and DBSCAN parameters ϵ and Minpts.

 \circ Create 2-Mapper complexes M_i for each cover in cluster cover \mathfrak{C} .

 $_{\odot}$ Start with an empty simplex tree.

 \circ Insert each M_i sequentially.

o Done!

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Clustering complicates our algorithm.



W. Bungula and I. Darcy, Bi-Filtration and Stability of TDA Mapper for Point Cloud Data, arXiv: 2409.17360 [math.AT], 2024.

Building an Algorithm

Single Cluster Collapse









Double Cluster Collapse









Sketch: For data set *X*, lens $f : X \to \mathbb{R}^n$, tower of covers \mathfrak{U} , and DBSCAN parameters ϵ and Minpts.

 \circ Create 2-Mapper complexes M_i for each cover in cluster cover \mathfrak{C} .

◦ For pairs (M_i , M_{i+1}) create maps $\varphi_i : M_i \rightarrow M'_{i+1}$ which deal with single and double collapses of clusters.

 \circ Create Simplex Tree with 2-Mapper complexes M_0, M'_1, \dots, M'_t











g = 0.1











Persistence barcode







Persistence barcode





$$g = 0.2$$



Persistence barcode





g = 0.2







Future Directions

- Estimation for likely trajectories in dynamical systems: *Trajectory Mapper.*
- *Engineering Mapper Complexes:* Computing probabilities for 2-Mapper given certain parameters.
- Visualization of clustering in genetic ancestry for human populations