Towards an Optimal Bound for the Interleaving Distance on Mapper Graphs

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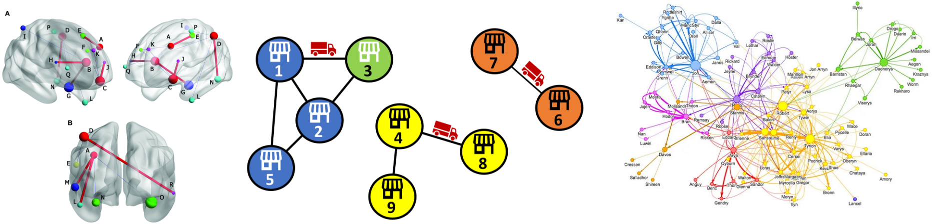
5th Workshop on Computational Topology (ComPer 2025)

October 10, 2025

Graphs in the Wild

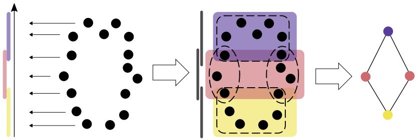
- Graphs with functions show up everywhere.
- We want to cluster and compare them.
- Need a meaningful and computable distance.
- But it's expensive to compute.

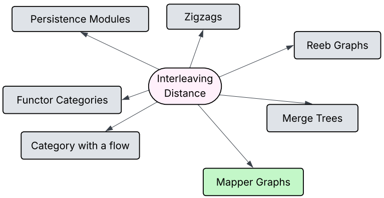


Real-world examples: brain activity, traffic flow, and social networks

Key Problem

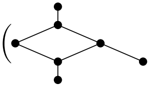
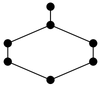
- Study graph-based topological signatures.
- Focus on Mapper graphs.
- Use interleaving distance.
- Computation is NP-hard.
- Loss function to upper bound.
- How to get the best upper bound?





TL;DR

We make Mapper graphs ML-friendly
by
optimizing a loss that bounds interleaving distance.

$d_I($  ,  $) \leq \quad n + Loss(\varphi, \psi)$

Mapper Graphs: Categorical Framework

Goal: Express mappers as cosheaves.

- Given:
  - Data $\mathbb{X}$ with function $f : \mathbb{X} \to \mathbb{R}$
  - Cover $\mathcal{U} = \{U_\alpha\}$ of $\mathbb{R}$
- Preserves connected components of $f^{-1}(U_\alpha)$
- Discretize using a grid on $\mathbb{R}$
- Represent f in cosheaf form
- Encoded as functor: $F : \mathbf{Open}(\mathcal{U}) \to \mathbf{Set}$
- Components stored in $\pi_0(f^{-1}(U))$.

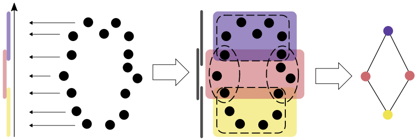


Image credit: Percival et al., 2024

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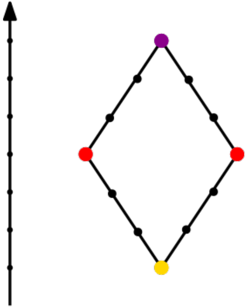
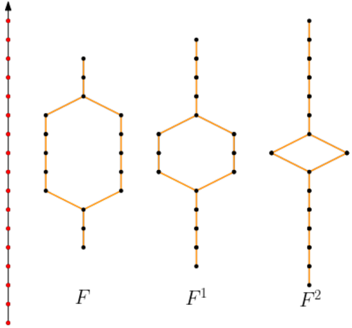


Distance Between Mappers: Interleaving Distance

Goal: to compare $F, G : \mathbf{Open}(\mathcal{U}) \to \mathbf{Set}$.

- Define n-thickening of open sets.
  - Geometrically, $(i\delta, j\delta) \to ((i-n)\delta, ((j+n)\delta)$
- Thickening of functor $F^n := F \circ (-)^n$
  - Means, $F^n(S) = F(S^n)$
- n-interleaving is $\varphi : F \Rightarrow G^n$ and $\psi : G \Rightarrow F^n$.
- Must satisfy diagram commutativity.

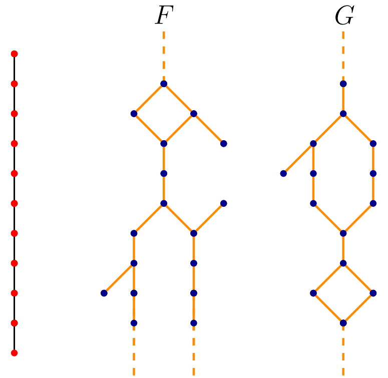


Distance Between Mappers: Interleaving Distance

- Diagrams to commute:

$$\begin{tikzcd} F(S) \arrow[rr, "{F[S\subseteq S^{2n}]}"] \arrow[dr, "\varphi_S"'] & & F(S^{2n}) \\ & G(S^n) \arrow[ur, "\psi_{S^n}"'] & \end{tikzcd} \qquad \begin{tikzcd} & F(S^n) \arrow[dr, "\varphi_{S^n}"] & \\ G(S) \arrow[ur, "\psi_S"] \arrow[rr, "{G[S\subseteq S^{2n}]}"'] & & G(S^{2n}) \end{tikzcd}$$

- Smallest n is the interleaving distance.
- NP hard.



Bounding Interleaving Distance: Assignment

- Assignment (φ, ψ): Natural transformation like maps without commutativity.
- Diagrams:
  - Triangle: Looks like interleaving
  - Parallelogram: Looks like natural transformation

$$
\begin{tikzcd}
F(S) \arrow[rr, "F[S \subseteq S^{2n}]"] \arrow[dr, "\varphi_S"'] & & F(S^{2n}) \\
& G(S^n) \arrow[ur, "\psi_{S^n}"'] &
\end{tikzcd}
\qquad
\begin{tikzcd}
& F(S^n) \arrow[dr, "\varphi_{S^n}"] & \\
G(S) \arrow[ur, "\psi_S"] \arrow[rr, "G[S \subseteq S^{2n}]"'] & & G(S^{2n})
\end{tikzcd}
$$

$$
\begin{tikzcd}
F(S) \arrow[r, "F[\subseteq]"] \arrow[dr, "\phi_S"'] & F(T) \arrow[dr, "\phi_T"] & \\
& G(S^n) \arrow[r, "G[\subseteq]"'] & G(T^n)
\end{tikzcd}
\qquad
\begin{tikzcd}
& F(S^n) \arrow[r, "F[\subseteq]"] & F(T^n) \\
G(S) \arrow[ur, "\psi_S"] \arrow[r, "G[\subseteq]"'] & G(T) \arrow[ur, "\psi_T"'] &
\end{tikzcd}
$$

Bounding Interleaving Distance: Loss Function

- Given n, how much to thicken (k), so that the diagrams commute for $n+k$?

$$\begin{tikzcd} F(S) \arrow[rr, "F[\subseteq]"] \arrow[dr, "\varphi_S"'] & & F(S^{2n}) \arrow[r] & F(S^{2(n+k)}) \\ & G(S^n) \arrow[ur, "\psi_{S^n}"'] & & \end{tikzcd}$$

$$\begin{tikzcd} F(S) \arrow[r, "F[\subseteq]"] \arrow[dr, "\varphi_S"'] & F(T) \arrow[dr, "\varphi_T"'] & \\ & G(S^n) \arrow[r, "G[\subseteq]"'] & G(T^n) \arrow[r] & G(T^{n+k}) \end{tikzcd}$$

- Diagram loss $L_{\square\!\!\!\diagdown}, L_{\square\!\!\!\diagup}, L_{\triangle}, L_{\bigtriangledown}$ is a quality measure.

- Basic loss $L_B(\varphi, \psi)$: Measures how far from commuting.

$$L_B(\phi, \psi) = \max_{\substack{\sigma<\tau\in K \\ \rho\in K}} \left\{ L_{\square\!\!\!\diagdown}^{S_\tau, S_\sigma}, L_{\square\!\!\!\diagup}^{S_\tau, S_\sigma}, L_{\square\!\!\!\diagdown}^{S_\rho, S_\rho^n}, L_{\square\!\!\!\diagup}^{S_\rho, S_\rho^n}, L_{\triangle}^{S_\rho}, L_{\bigtriangledown}^{S_\rho} \right\}$$

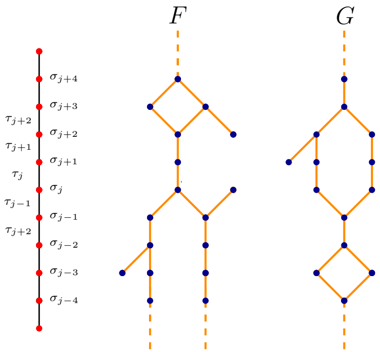
Theorem (Chambers et al. (2023))

For an n-assignment, $\varphi : F \Rightarrow G^n$ *and* $\psi : G \Rightarrow F^n$*,*

$$d_I(F, G) \leq n + L_B(\varphi, \psi).$$

Data Structure: Mapper as Graphs

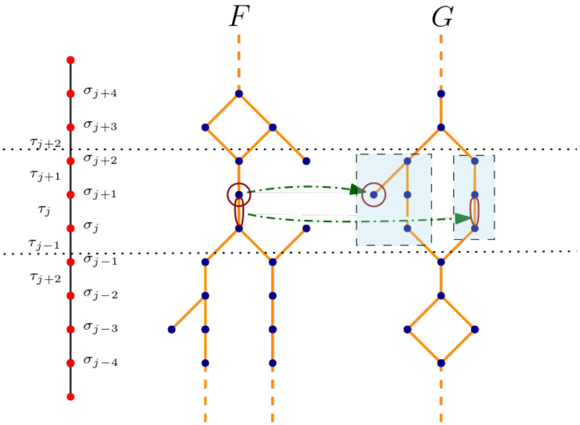
- Store $F : \textbf{Open}(\mathcal{U}) \to \textbf{Set}$ as graph $F \sim (V_F, E_F)$.
- Use grid structure on $\mathbb{R}$.
- Vertices: stored with height.
- *Assignment*: vertex and edge maps.
- Diagram commutes $\sim$ same connected component.



Commutativity and Connected Components

$$\begin{tikzcd}
F(S_\tau) \arrow[r, "F[\subseteq]"] \arrow[dr, "\varphi_{S_\tau}"'] & F(S_\sigma) \arrow[dr, "\varphi_{S_\sigma}"] & \\
& G^n(S_\tau) \arrow[r, "G[\subseteq]"'] & G^n(S_\sigma)
\end{tikzcd}$$

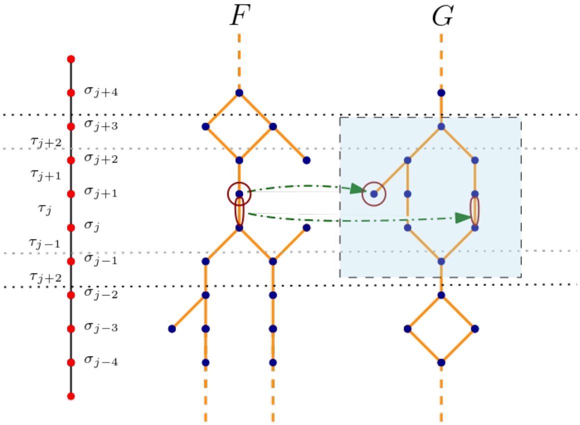
$$\begin{tikzcd}
e \arrow[r, mapsto] \arrow[dr, mapsto] & v \arrow[dr, mapsto] & \\
& {[e']} \arrow[r, mapsto] & \substack{[w] \\ {[e']}}
\end{tikzcd}$$



Commutativity and Connected Components

$$\begin{tikzcd}
F(S_\tau) \arrow[r, "F[\subseteq]"] \arrow[dr, "\varphi_{S_\tau}"'] & F(S_\sigma) \arrow[dr, "\varphi_{S_\sigma}"] & & \\
& G^n(S_\tau) \arrow[r, "G[\subseteq]"'] & G^n(S_\sigma) \arrow[r] & G(S_{\sigma_\ell}^{n+k})
\end{tikzcd}$$

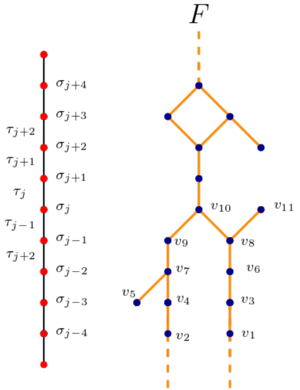
$$\begin{tikzcd}
e \arrow[r, mapsto] \arrow[dr, mapsto] & v \arrow[dr, mapsto] & & \\
& {[e']} \arrow[r, mapsto] & \begin{matrix}[w] \\ [e']\end{matrix} \arrow[r, mapsto] & \begin{matrix}[w] \\ [e']\end{matrix}
\end{tikzcd}$$



Data Structure: Maps as Matrices

Goal: Express diagram commutativity as matrix multiplication.

- Order vertices by increasing function values.
- Same for edges (lower vertex).
- Assignment: vertex and edge maps.
- Matrix whose rows and columns are these.
- Block Structure.

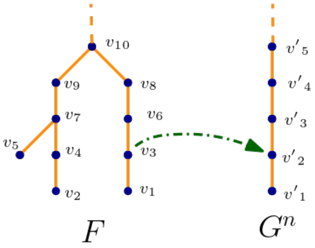


$$\{\sigma_{j-4} : (v_1, v_2), \sigma_{j-3} : (v_3, v_4), \cdots\}$$

Assignment Matrices

- Store maps like $\varphi : F \to G^n$.
- Place 1 if $\varphi(v) = v'$, 0 otherwise.
- For a valid map: only one 1 for each column.

$$
\begin{array}{cc}
 & F \\
 & \begin{array}{ccccc} v_1 & v_2 & v_3 & v_4 & \cdots \end{array} \\
G^n \begin{array}{c} v_1' \\ v_2' \\ v_3' \\ v_4' \\ \vdots \end{array} & \begin{bmatrix} & & & & \\ & & & & \\ & & 1 & & \\ & & & & \\ & & & & \end{bmatrix}
\end{array}
$$



- To have lower loss, need better assignment.

Loss Terms as Matrix Multiplication

- Diagram:

$$
\begin{tikzcd}
F(S_\tau) \arrow[r, "F[\subseteq]"] \arrow[dr, "\varphi_{S_\tau}"'] & F(S_\sigma) \arrow[dr, "\varphi_{S_\sigma}"] & \\
& G^n(S_\tau) \arrow[r, "G[\subseteq]"'] & G^n(S_\sigma)
\end{tikzcd}
\qquad
\begin{tikzcd}
e \arrow[r, mapsto] \arrow[dr, mapsto] & v \arrow[dr, mapsto] & \\
& {[e']} \arrow[r, mapsto] & \begin{smallmatrix}[w]\\ [e']\end{smallmatrix}
\end{tikzcd}
$$

- Top-right: $M_\phi^V \cdot B_F^\downarrow$
- Left-Down: $B_{G^n}^\downarrow \cdot M_\phi^E$
- In matrix terms:

$$\max_i L_{\square}^{S_{\tau_i}, S_{\sigma_i}} = \max \left\{ x \mid x \in D_{G^n}^V \left(M_\phi^V \cdot B_F^\downarrow - B_{G^n}^\downarrow \cdot M_\phi^E \right) \right\}$$

- computing loss $\rightarrow$ finding largest matrix element.

Loss in Matrix Terms

	Loss Term	Diagram	Matrix Multiplication	Eval.
Edge-vertex Parallelogram	$L^{S_\tau,S_\sigma}_{\text{▱}}$	$\begin{tikzcd} F(S_\tau) \arrow[r, "F[\subseteq]"] \arrow[dr, "\varphi_{S_\tau}"'] & F(S_\sigma) \arrow[dr, "\varphi_{S_\sigma}"] & \\ & G^n(S_\tau) \arrow[r, "G[\subseteq]"'] & G^n(S_\sigma) \end{tikzcd}$	$D^V_{G^n}\left(M^V_\varphi \cdot B^\uparrow_F - B^\uparrow_{G^n} \cdot M^E_\varphi\right)$ $D^V_{G^n}\left(M^V_\varphi \cdot B^\downarrow_F - B^\downarrow_{G^n} \cdot M^E_\varphi\right)$	$\max\limits_{x_{ij}\in A} x_{ij}$
	$L^{S_\tau,S_\sigma}_{\text{▱}}$	$\begin{tikzcd} & F^n(S_\tau) \arrow[r, "F[\subseteq]"] & F^n(S_\sigma) \\ G(S_\tau) \arrow[ur, "\psi_{S_\tau}"] \arrow[r, "G[\subseteq]"'] & G(S_\sigma) \arrow[ur, "\psi_{S_\sigma}"'] & \end{tikzcd}$	$D^V_{F^n}\left(M^V_\psi \cdot B^\uparrow_G - B^\uparrow_{F^n} \cdot M^E_\psi\right)$ $D^V_{F^n}\left(M^V_\psi \cdot B^\downarrow_G - B^\downarrow_{F^n} \cdot M^E_\psi\right)$	
Thickening Parallelogram	$L^{S_\rho,S_\rho^n}_{\text{▱}}$	$\begin{tikzcd} F(S_\rho) \arrow[r, "F[\subseteq]"] \arrow[dr, "\varphi_{S_\rho}"'] & F^n(S_\rho) \arrow[dr, "\varphi_{S_\rho^n}"] & \\ & G^n(S_\rho) \arrow[r, "G[\subseteq]"'] & G^{2n}(S_\rho) \end{tikzcd}$	$D^V_{G^n}\left(M^V_{\varphi^n} \cdot I^V_F - I^V_{G^n} \cdot M^V_\varphi\right)$ $D^E_{G^n}\left(M^E_{\varphi^n} \cdot I^E_F - I^E_{G^n} \cdot M^E_\varphi\right)$	
	$L^{S_\rho,S_\rho^n}_{\text{▱}}$	$\begin{tikzcd} & F^n(S_\rho) \arrow[r, "F[\subseteq]"] & F^{2n}(S_\rho) \\ G(S_\rho) \arrow[ur, "\psi_{S_\rho}"] \arrow[r, "G[\subseteq]"'] & G(S_\rho^n) \arrow[ur, "\psi_{S_\rho^n}"'] & \end{tikzcd}$	$D^V_{F^n}\left(M^V_{\psi^n} \cdot I^V_G - I^V_{F^n} \cdot M^V_\psi\right)$ $D^E_{F^n}\left(M^E_{\psi^n} \cdot I^E_G - I^E_{F^n} \cdot M^E_\psi\right)$	
Triangle	$L^{S_\rho}_{\triangledown}$	$\begin{tikzcd} F(S_\rho) \arrow[rr, "F[\subseteq]"] \arrow[dr, "\varphi_{S_\rho}"'] & & F^{2n}(S_\rho) \\ & G^n(S_\rho) \arrow[ur, "\psi_{S_\rho^n}"'] & \end{tikzcd}$	$D^V_{F^{2n}}\left(I^V_{F^n} \cdot I^V_F - M^V_{\psi^n} \cdot M^V_\varphi\right)$ $D^E_{F^{2n}}\left(I^E_{F^n} \cdot I^E_F - M^E_{\psi^n} \cdot M^E_\varphi\right)$	$\max\limits_{x_{ij}\in A} \left\lceil \frac{x_{ij}}{2} \right\rceil$
	$L^{S_\rho}_{\triangle}$	$\begin{tikzcd} & F^n(S_\rho) \arrow[dr, "\varphi_{S_\rho^n}"] & \\ G(S_\rho) \arrow[ur, "\psi_{S_\rho}"] \arrow[rr, "G[\subseteq]"'] & & G^{2n}(S_\rho) \end{tikzcd}$	$D^V_{G^{2n}}\left(I^V_{E^n} \cdot I^V_G - M^V_{\varphi^n} \cdot M^V_\psi\right)$ $D^E_{G^{2n}}\left(I^E_{G^n} \cdot I^E_G - M^E_{\varphi^n} \cdot M^E_\psi\right)$	

Implement Loss Optimization

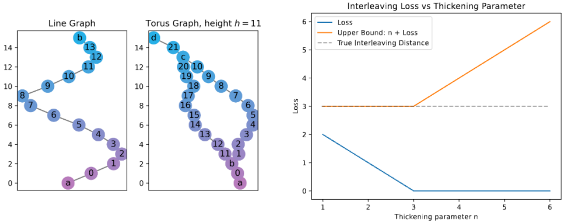
- Question: Can we formulate loss optimization as a linear program?
  - Yes! Both the objective function and constraints can be linearized.
- Discretized setup calls for integer linear programming.
- ILP is formulated as follows:

$$
\begin{aligned}
\text{Minimize} \quad & \ell \\
\text{Subject to} \quad & \ell \geq x_{ij}^{F,\uparrow} \quad \forall\, x_{ij}^{F,\uparrow} \in D_{G^n}^{V} \left(M_{\varphi}^{V} \cdot B_{F}^{\uparrow} - B_{G^n}^{\uparrow} \cdot M_{\varphi}^{E} \right) \\
& \sum_i x_{ij}^{\eta,A} = 1 \quad \forall x_{ij}^{\eta,A} \in M_{\eta}^{A},\ \eta \in \{\phi, \phi^n, \psi, \psi^n\},\ A \in \{V, E\} \\
& x_{ij} \geq 0 \\
& \vdots \quad \text{(more constraints)}
\end{aligned}
$$

- Nonlinearity in triangles (e.g., $M_{\psi^n}^{V} \cdot M_{\varphi}^{V}$) is linearized with additional variables.

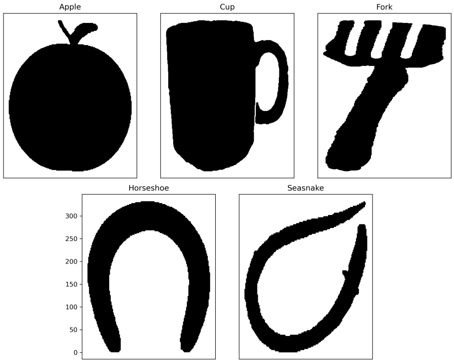
Experiments with Small Mappers

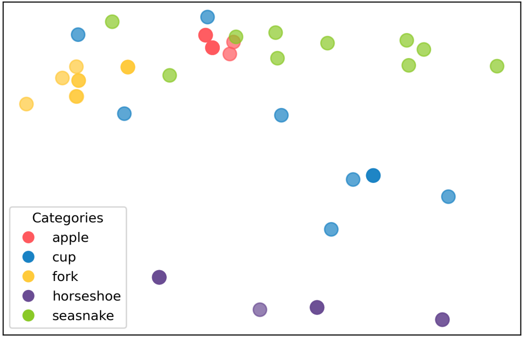
- Small mappers where interleaving distance can be computed.
- Line mapper: One vertex at every height.
- Torus mapper: A loop in the middle.
- Interleaving distance is $\lceil \frac{h}{4} \rceil$.



Experiments with Images

- Mappers of images from the MPEG7 image dataset.
- Pairwise distance with the optimized mapper loss.
- MDS to preserve pairwise dissimilarities.

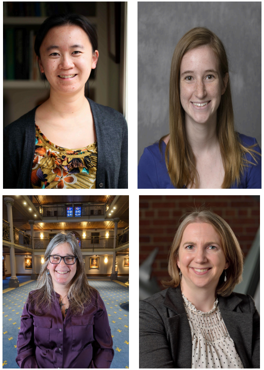




Summary and Future Work

- First available method to compute a bound for the interleaving distance.
- Mapper as graphs, maps as matrices.
- Loss optimization using ILP.
- Initial experiments support the approach.
- Future: test on more datasets, improve efficiency.
- Explore mapper construction and parameter selection.
- Integrate into ML pipelines.

Thank You!



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