Stable Signatures for Dynamic Graphs and Dynamic Metric Spaces via Zigzag Persistence

Facundo Mémoli
joint with Woojin Kim and Zane Smith

The Ohio State University
`https://research.math.osu.edu/networks/formigrams.`

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Woojin Kim and Facundo Memoli.
Stable signatures for dynamic graphs and dynamic metric spaces via zigzag persistence.
arXiv preprint arXiv:1712.04064, 2017.

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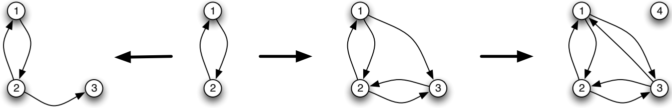
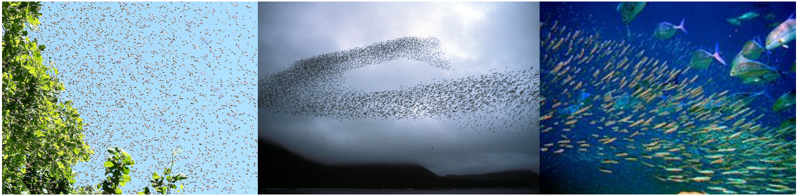
Motivations

- Study dynamic networks (social, financial, biological, ..)

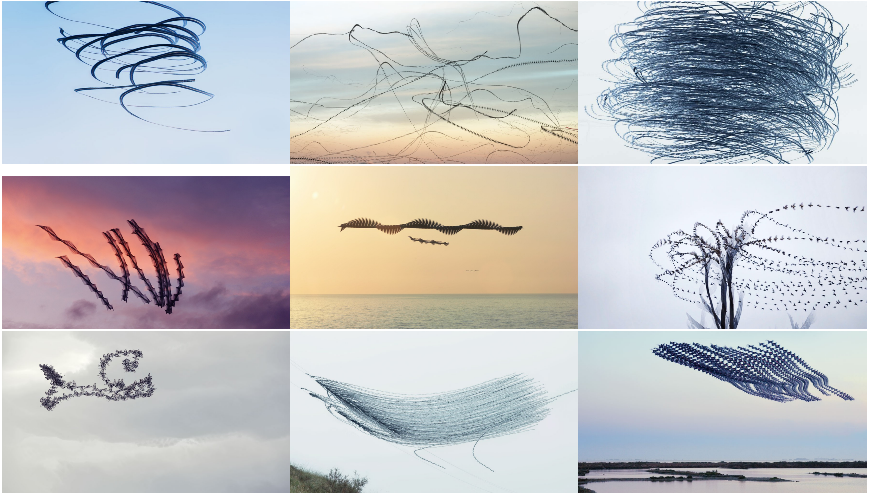


- Study/characterize flocking/swarming behavior in animals.



(wikipedia)

Ornitographies, by Xavi Bau



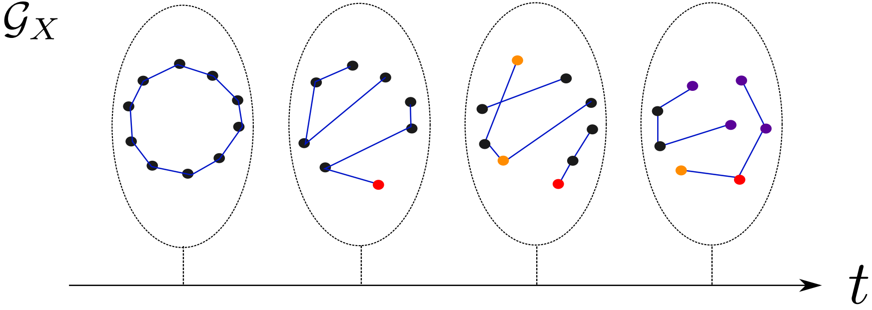
Characterization of flocking/herding behavior

Video: Murmuration of Starlings in England

`https://www.youtube.com/watch?v=NREmtGhIHew`

Dynamic graphs

Proto-definition: A *dynamic graph (DG)* $\mathcal{G}_X$ over X is a graph that is subjected to a sequence of updates such as addition/deletion of vertices/edges.



Questions

Q1. How do we **characterize** evolution of connected components of a dynamic graph (or dynamic simplicial complex)?

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Q2. How do we **quantify** the **degree** of **difference** between **two** different dynamic graphs?

Related work: TDA of dynamic data

- H. Edelsbrunner, J. Harer, A. Mascarenhas, V. Pascucci; (2004). *Time-varying Reeb graphs for continuous space–time data.*

- D. Cohen-Steiner, H. Edelsbrunner, D. Morozov; (2006). *Vines and vineyards by updating persistence in linear time.*

- E. Munch; (2013). *Applications of Persistent Homology to Time Varying Systems.*

- M. Hajij, B. Wang, C. Scheidegger, P. Rosen; (2017) *Visual Detection of Structural Changes in Time-Varying Graphs Using Persistent Homology.*

Dynamic Graphs

Definition: A **dynamic graph** $\mathcal{G}_X$ over the finite set X consists of a pair of maps as below satisfying four conditions:

$$V_X(\cdot) : \mathbb{R} \to \mathrm{pow}(X) \quad \text{and} \quad E_X(\cdot) : \mathbb{R} \to \mathrm{pow}\left(\mathrm{pow}_2\left(V_X(\cdot)\right)\right),$$

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[1] $\mathrm{crit}(\mathcal{G}_X)$ is the union of the sets of discontinuity points of $V_X(\cdot)$ and $E_X(\cdot)$.

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1. (Self-loops) For all $t \in \mathbb{R}$, $E_X(t) \supseteq \mathrm{diag}(V_X(t) \times V_X(t))$.

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4. (Comparability) for every $t \in \mathbb{R}$, it holds that

   $$\mathcal{G}_X(t - \varepsilon) \subseteq \mathcal{G}_X(t) \supseteq \mathcal{G}_X(t + \varepsilon)$$

   for all sufficiently small $\varepsilon > 0$.

---

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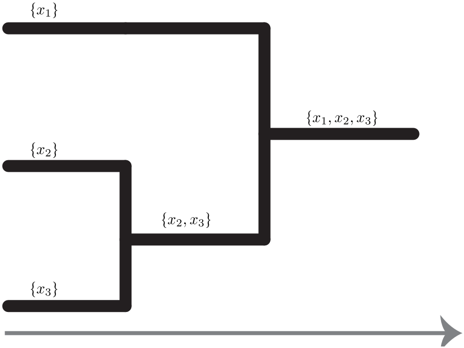
Encoding evolution of connected components of a dynamic graph.

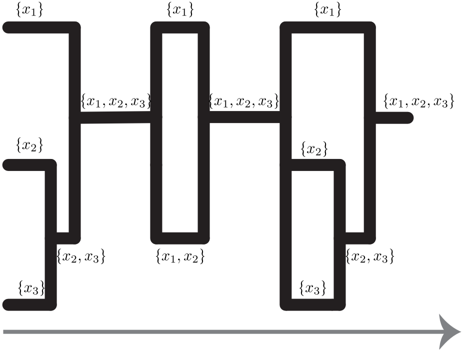
Want to be able to encode both **merging** and **splitting** of connected components of dynamic graphs.

Dendrograms

Merging only



Formigrams (Formicarium + Diagram)



Merging and splitting

(↑ Wikipedia)

(Formica = ant in latin.)

Formigrams

A *formigram* over a finite set X is any function

$$\theta_X : \mathbb{R} \to \mathcal{P}^{\mathrm{sub}}(X)$$

such that:

1. (Tameness) the set $\mathrm{crit}(\theta_X)$ of points of discontinuity of θ_X is locally finite. We call the elements of $\mathrm{crit}(\theta_X)$ *the critical points of* θ_X.
2. (Interval lifespan) for every $x \in X$, the set $I_x := \{t \in \mathbb{R} : x \in B \in \theta_X(t)\}$, said to be the *lifespan of* x, is a non-empty closed interval,
3. (Comparability) for every point $c \in \mathbb{R}$ it holds that $\theta_X(c-\varepsilon) \leq \theta_X(c) \geq \theta_X(c+\varepsilon)$ for all sufficiently small $\varepsilon > 0$.[2]

---

[2] If θ_X is discontinuous at c, then at least one of the relations of $\theta_X(c-\varepsilon) \leq \theta_X(c) \geq \theta_X(c+\varepsilon)$ will be strict for small $\varepsilon > 0$. Otherwise, $\theta_X(c-\varepsilon) = \theta_X(c) = \theta_X(c+\varepsilon)$ for small $\varepsilon > 0$.

Dynamic Graph $\to$ Formigram

Recall the π_0 functor: If $G_X = (X, E_X)$ is a graph on the vertex set X, then $\pi_0(G_X) :=$ Partition of X into connected components.

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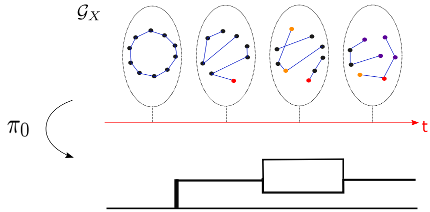

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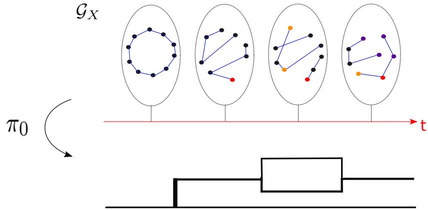


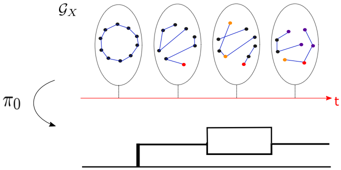
Proposition. For any $\mathcal{G}_X$,

$$\pi_0(\mathcal{G}_X) : \mathbb{R} \to \mathcal{P}^{sub}(X)$$

is a formigram.

Here $\mathcal{P}^{sub}(X)$ is the set of all sub-partitions of X.

Remarks about formigrams.



Remarks.

- Formigrams generalize dendrograms:

Standard simplicial filtration → Dendrogram

Zigzag simplicial filtration → Formigram[3]

- Any formigram has an underlying (Reeb) graph.
- Underlying graph is **not** always planar.

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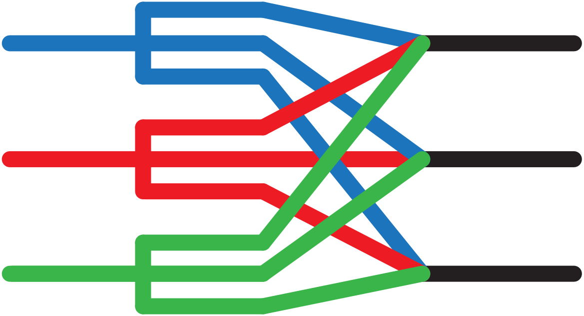
[3] A dynamic graph is an 1-dim zigzag simplicial filtration.

Non-planar formigram:[4]



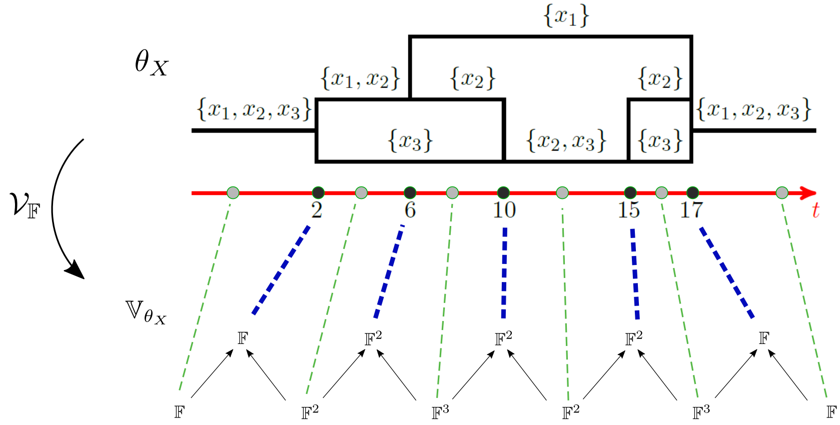
⇒ We want further simplification step to facilitate:

1. **simpler visualization**, and
2. **reduced computational cost of comparison**.

---

[4] By Z. Smith.

Simplification: Formigrams ⇒ Zigzag modules



$\mathcal{V}_{\mathbb{F}}$ is the free functor.

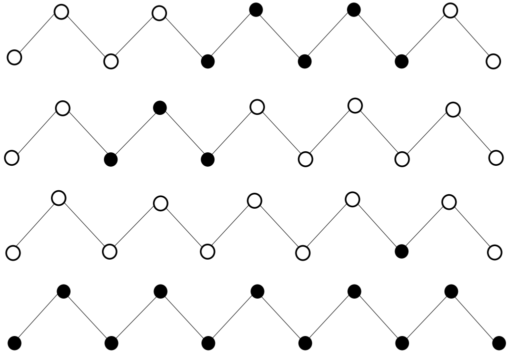
Simplification: Zigzag modules ⇒ Barcodes

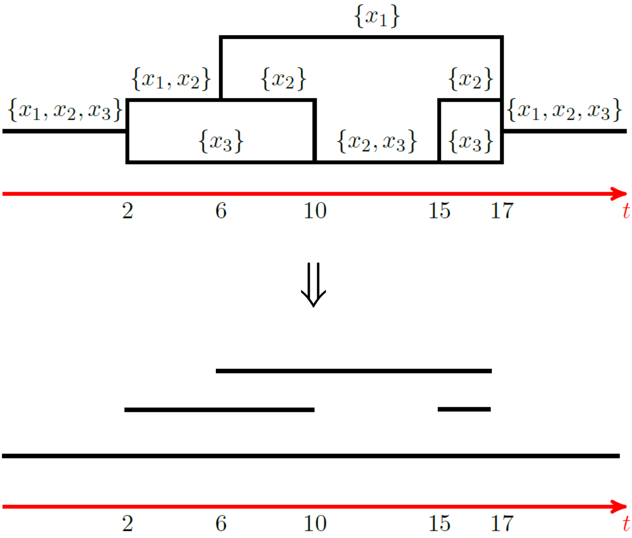
Gabriel 1972, de Silva-Carlsson 2010

$$\begin{tikzcd}[column sep=small]
\mathbb{V}_{\theta_X} & & \mathbb{F} & & \mathbb{F}^2 & & \mathbb{F}^2 & & \mathbb{F}^2 & & \mathbb{F} & \\
& \mathbb{F} \arrow[ur] & & \mathbb{F}^2 \arrow[ul] \arrow[ur] & & \mathbb{F}^3 \arrow[ul] \arrow[ur] & & \mathbb{F}^2 \arrow[ul] \arrow[ur] & & \mathbb{F}^3 \arrow[ul] \arrow[ur] & & \mathbb{F} \arrow[ul]
\end{tikzcd}$$

$$\cong$$

$$\bigoplus \Bigg\{$$




$\{x_1\}$
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$\{x_1, x_2, x_3\}$
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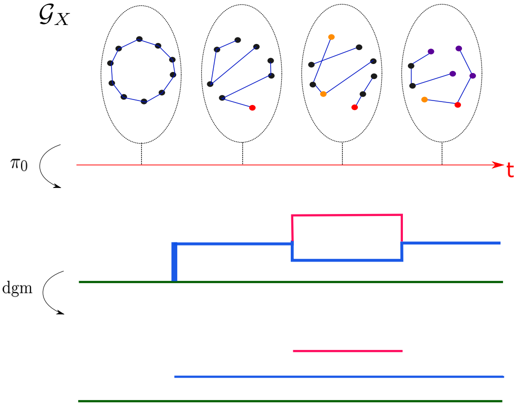
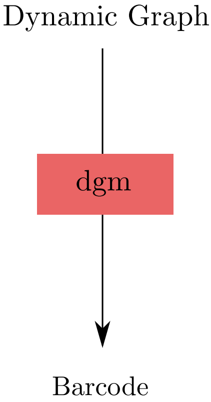
Summary




Dynamic Graph

dgm

Barcode

Questions (again)

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Q1+. Is the process $\text{Dynamic Graph} \longrightarrow \boxed{\text{dgm}} \longrightarrow \text{Barcode}$ **stable**?

Q2. How do we **quantify** the **degree** of **difference** between **two** different dynamic graphs?

Stability Theorem (Kim-M 2018) [KM17]

We construct $d_{\mathrm{I}}^{\mathrm{dynG}}$, a metric on DGs and prove:

Theorem. For any two dynamic graphs $\mathcal{G}_X$ and $\mathcal{G}_Y$,

$$2\ d_{\mathrm{I}}^{\mathrm{dynG}}(\mathcal{G}_X, \mathcal{G}_Y) \geq d_{\mathrm{B}}\left(\mathrm{dgm}(\mathcal{G}_X), \mathrm{dgm}(\mathcal{G}_Y)\right).$$

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Structure of $d_{\mathrm{I}}^{\mathrm{dynG}}$ is some sort of hybrid of:

- the interleaving distance between Reeb graphs (de Silva, Munch, Patel 2015), and
- the Gromov-Hausdorff distance.

Interconnecting dynamic graphs via correspondences

Let $\mathcal{G}_X = (V_X(\cdot), E_X(\cdot))$ and $\mathcal{G}_Y = (V_Y(\cdot), E_Y(\cdot))$ be two dynamic graphs, and let R be a correspondence between X and Y.

By $\mathcal{G}_X \xrightarrow{R} \mathcal{G}_Y$, we mean:

For any $(x, y), (x', y') \in R$ and any $t \in \mathbb{R}$,

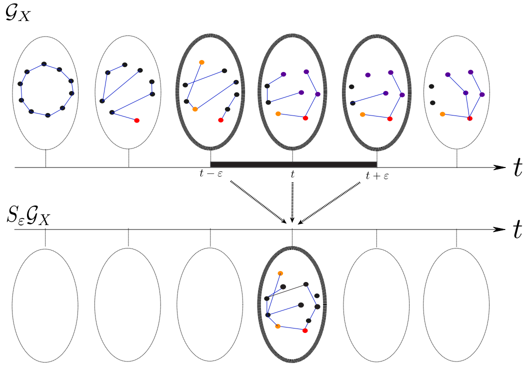
$$(x, x') \in E_X(t) \Rightarrow (y, y') \in E_Y(t).$$

(This implies that if $x \in V_X(t)$, then $y \in V_Y(t)$.)

S_ε: ε-smoothing of dynamic graphs

Let $\varepsilon \geq 0$. For $t \in \mathbb{R}$,

$$S_\varepsilon \mathcal{G}_X(t) := \left(\bigcup_{s \in [t]^\varepsilon} V_X(s), \bigcup_{s \in [t]^\varepsilon} E_X(s) \right).$$

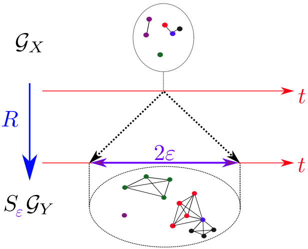


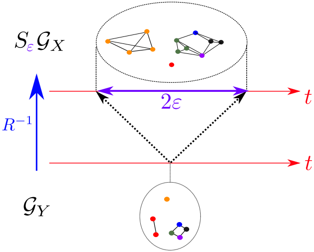
Proposition. S_ε maps DGs to DGs.

$d_{\mathrm{I}}^{\mathrm{dynG}}$ for dynamic graphs

Definition. Given $\mathcal{G}_X$ and $\mathcal{G}_Y$ be dynamic graphs, define:

$$d_{\mathrm{I}}^{\mathrm{dynG}}(\mathcal{G}_X, \mathcal{G}_Y) := \inf \left\{ \varepsilon \geq 0 : \exists R,\ \mathcal{G}_X \xrightarrow{R} S_\varepsilon \mathcal{G}_Y \text{ and } \mathcal{G}_Y \xrightarrow{R^{-1}} S_\varepsilon \mathcal{G}_X \right\}.$$





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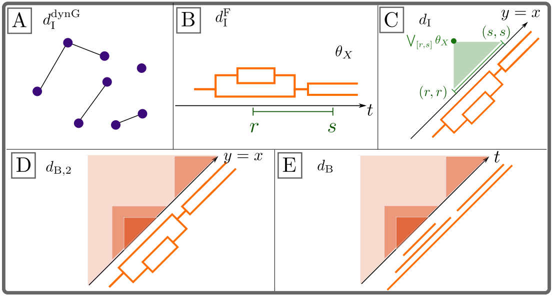
The proof uses ideas and results from the recent papers by Botnan-Lesnick, and by Bjerkevik.



Flocking

(Xavi Bau)

Flocking: Questions

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- Very large literature in biology.
- C.Topaz, L. Ziegelmeier, T. Halverson; (2015). *Topological Data Analysis of Biological Aggregation Models.*
- P. Corcoran and C. B. Jones; (2017). *Modeling Topological Features of Swarm Behavior in Space and Time With Persistence Landscapes.*

Dynamic Metric Spaces

A **dynamic metric space** is a pair $(X, d_X(\cdot))$ where X is finite set and $d_X(\cdot) : \mathbb{R} \times X \times X \to \mathbb{R}_{\geq 0}$ is such that

- $\forall t \in \mathbb{R}$, $d_X(t) : X \times X \to \mathbb{R}_{\geq 0}$ is a pseudo-metric on X.
- $\forall x, x' \in X$, $t \mapsto d_X(t)(x, x')$ is continuous and *tame*.

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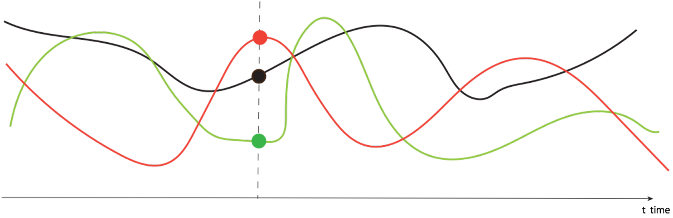
Example: Trajectory data in $\mathbb{R}^d$. Case $d = 1$ shown here:

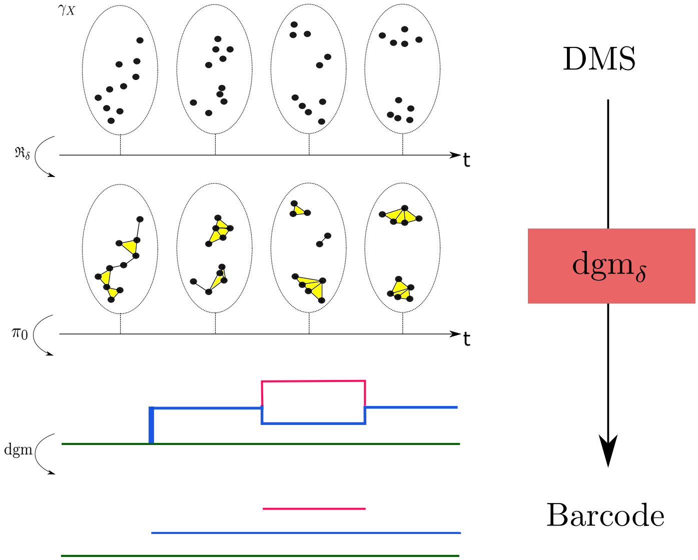


Encoding clustering behavior of DMSs.

Fix $\delta \geq 0$. Given a metric space (X, d_X), let $\mathcal{R}^1_\delta(X, d_X)$ be the 1-skeleton of the Rips complex $\mathcal{R}_\delta(X, d_X)$.

Proposition. Let $\gamma_X = (X, d_X(\cdot))$ be a DMS. Then, $\mathcal{R}^1_\delta(\gamma_X)$ is a dynamic graph.

The map $\mathrm{dgm}_\delta : \mathcal{M}^{\mathrm{dyn}} \to \mathrm{Barcodes}$.



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We introduce a family $\{d_{\mathrm{I},\lambda}^{\mathrm{dynM}}\}_{\lambda\geq 0}$ of metrics on DMSs. Here λ is a slack parameter.
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Theorem. For DMSs γ_X and γ_Y,

$$2\ d_{\mathrm{I}}^{\mathrm{dynM}}(\gamma_X,\gamma_Y) \geq \sup_{\delta\geq 0}\ d_{\mathrm{I}}^{\mathrm{dynG}}(\mathcal{R}_{\delta}^{1}(\gamma_X),\mathcal{R}_{\delta}^{1}(\gamma_Y)).$$

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Corollary (Formigram barcodes are stable). For DMSs γ_X and γ_Y,

$$2\ d_{\mathrm{I}}^{\mathrm{dynM}}(\gamma_X,\gamma_Y) \geq \sup_{\delta\geq 0} d_{\mathrm{B}}\left(\mathrm{dgm}_\delta(\gamma_X),\mathrm{dgm}_\delta(\gamma_Y)\right),$$

where $\mathrm{dgm}_\delta(\gamma_X) = \mathrm{dgm}\circ\mathcal{R}_\delta^1(\gamma_X)$.

What about (δ, t)-persistence? SLHC of DMSs

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Let $\mathcal{H}$ denote the single linkage functor.

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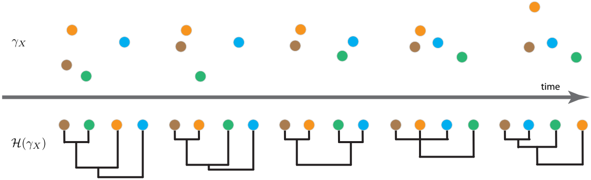
Given a DMS γ_X, one obtains an ultrametric DMS $\mathcal{H}(\gamma_X)$.



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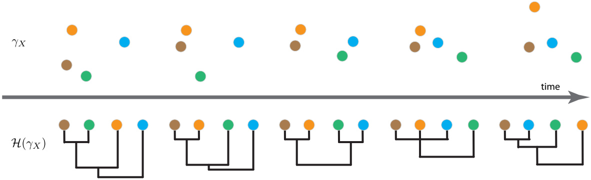

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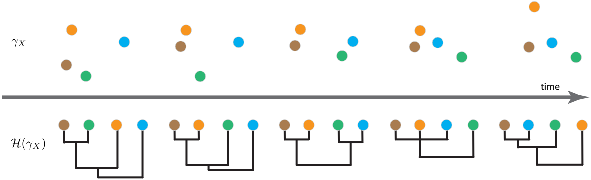

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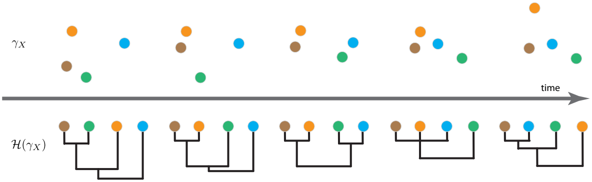

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Theorem (Kim-M, 2018). For $\ell > 0$, let γ_X and γ_Y be any ℓ-Lipschitz DMSs. Then for any $\lambda > 0$,

$$\lambda + \ell \qquad d^{\mathrm{dyn}}(\gamma_X, \gamma_Y) \geq d^{\mathrm{dyn}}(\mathcal{H}(\gamma_X), \mathcal{H}(\gamma_Y))$$

ε-smoothing of DMSs

For $\varepsilon \geq 0$, consider ε-smoothing $S_\varepsilon : \mathcal{M}^{\mathrm{dyn}} \to \mathcal{M}^{\mathrm{dyn}}$ s.t.

$$S_\varepsilon : \quad \gamma_X = (X, d_X(\cdot)) \longmapsto \gamma_X^\varepsilon = (X, d_X^\varepsilon(\cdot))$$

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$$d_X^\varepsilon(t)(x, x') = \min_{s \in [t]^\varepsilon} d_X(s)(x, x')$$

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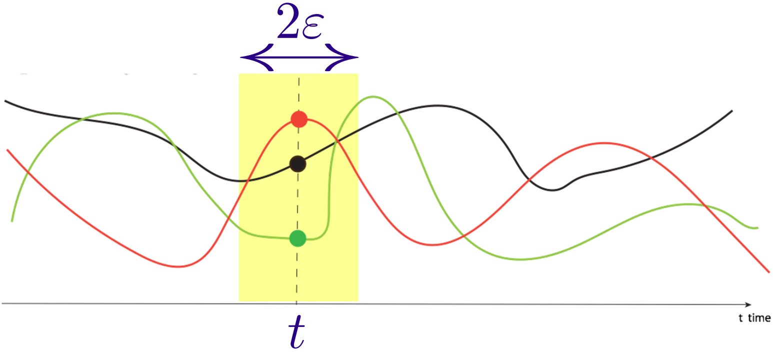

$d_{\mathrm{I},\lambda}^{\mathrm{dyn}}$: λ-slack interleaving distance

Construction inspired on the GH distance and the interleaving distance between Reeb graphs (de Silva, Munch, Patel 2015)

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Definition

Two DMSs γ_X, γ_Y are (λ,ε)-interleaved when there is a correspondence $R \subseteq X \times Y$ s.t. $\forall t \in \mathbb{R}, \forall (x,y),(x',y') \in R$

- $d_X^{\varepsilon}(t)(x,x') \leq d_Y(t)(y,y') + \lambda \cdot \varepsilon$
- $d_Y^{\varepsilon}(t)(y,y') \leq d_X(t)(x,x') + \lambda \cdot \varepsilon$

Whenever this happens we write $\gamma_X \approx_{(\lambda,\varepsilon)} \gamma_Y$. Define:

$$d_{\mathrm{I},\lambda}^{\mathrm{dyn}}(\gamma_X,\gamma_Y) := \inf\{\varepsilon \geq 0 : \gamma_X \approx_{(\lambda,\varepsilon)} \gamma_Y\}.$$

Remark. For $\lambda \in [0, +\infty)$, $d^{\mathrm{dyn}}_{\mathrm{I},\lambda}$ can be $+\infty$.

Remark. $\lambda \leq \lambda' \quad \Rightarrow \quad d^{\mathrm{dyn}}_{\mathrm{I},\lambda} \geq d^{\mathrm{dyn}}_{\mathrm{I},\lambda'}$.

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Theorem. For $\lambda \geq 0$, $d_{\mathrm{I},\lambda}^{\mathrm{dyn}}$ is an **extended metric** on $\mathcal{M}^{\mathrm{dyn}}$.

Theorems. For $\lambda > 0$,

- $d_{\mathrm{I},\lambda}^{\mathrm{dyn}}$ is a **metric** on **bounded** DMSs.
- $d_{\mathrm{I},\lambda}^{\mathrm{dyn}}$ recovers the Gromov-Hausdorff distance between constant DMSs (up to a constant factor).[5]
- The metrics $d_{\mathrm{I},\lambda}^{\mathrm{dyn}}$ for different $\lambda > 0$ are bilipschitz equivalent.

---

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Theorem. There is an **isometric embedding** $\Delta : \mathcal{M} \hookrightarrow \mathcal{M}^{\mathrm{dyn}}$, i.e.

$$d_{\mathrm{GH}}(X, Y) = d_{\mathrm{I}}^{\mathrm{dyn}}(\Delta(X), \Delta(Y)).$$

Recall
Corollary. For any DMSs γ_X and γ_Y,

$$2\ d_{\mathrm{I}}^{\mathrm{dyn}}(\gamma_X, \gamma_Y) \geq \sup_{\delta \geq 0} d_{\mathrm{B}}\left(\mathrm{dgm}_\delta(\gamma_X), \mathrm{dgm}_\delta(\gamma_Y)\right)$$

LHS is **NP-hard** whereas the RHS is **poly time**.

Summary: Stability theorems for DGs and DMSs

$\Rightarrow$ **Clustering (formigram) barcodes are $d_{\mathrm{I}}^{\mathrm{dyn}}$- stable.**

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$\Rightarrow$ **Clustering (formigram) barcodes are $d_{\mathrm{I}}^{\mathrm{dyn}}$- stable.**

$\Rightarrow$ **HC is $d_{\mathrm{I},\lambda}^{\mathrm{dyn}}$ stable.**

Q. What about higher-dimensional homological features?

$\mathrm{PH}_{k\geq 1}$?

Q. Extension to high-dimensional PH?

Any DG $\mathcal{G}_X$ induces a ZZ simplicial filtration (and its barcode) for **each** dimension $k \in \mathbb{Z}_+$.

For every t, just consider the associated *clique complex* $\mathcal{C}(\mathcal{G}_X(t))$.

Bad news..

Theorem (Kim-M). For each integer $k \geq 1$, there exists a finite set X_k and a pair of DGs $\mathcal{G}_{X_k}$ and $\mathcal{G}'_{X_k}$ over X_k such that

$$d_{\mathrm{I}}^{\mathrm{dynG}}\left(\mathcal{G}_{X_k}, \mathcal{G}'_{X_k}\right) < \infty,$$

but

$$d_{\mathrm{B}}\left(\mathrm{dgm}\left(H_k(\mathcal{C}(\mathcal{G}_{X_k}))\right), \mathrm{dgm}\left(H_k(\mathcal{C}(\mathcal{G}'_{X_k}))\right)\right) = \infty.$$

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These two DGs are finitely interleaved but the bottleneck distance between their associated H_1 barcodes is ∞.

Application: classifying flocking behaviors [KMS]

- a variation of Boids simulation (parameters: Cohesion, Alignment, Separation, etc.)
- Consider 4 behaviors by tuning parameters.
- Repeat simulation 20 times for each behavior with random initial configurations.
- Compute clustering barcodes (Morozov's Dionysus).
- Construct 80×80-matrix of bottleneck distances. Carry out hierarchical clustering and MDS plot of it.

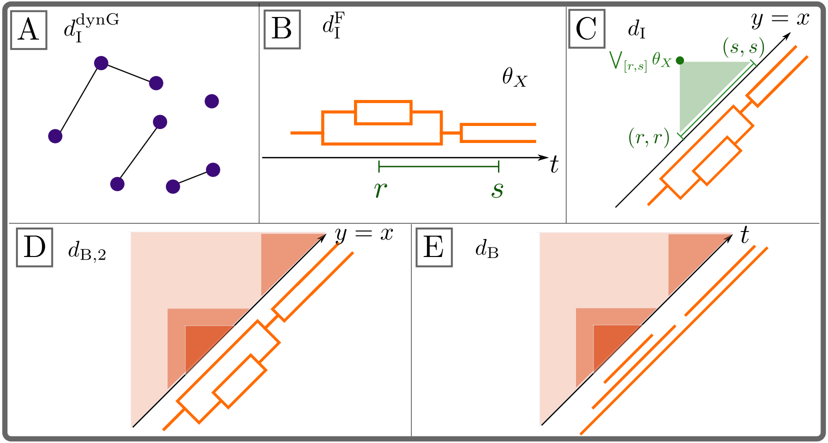
`https://research.math.osu.edu/networks/formigrams`

Discussion

- Extensions: dynamic networks.
- Extensions: dynamical systems?
- $\gamma_X \mapsto \mathrm{PH}_{k\geq 1}(\gamma_X)$ stably?

Proof of Stability Theorem

Inspired by M. Botnan and M.Lesnick (2016)



Tameness

A continuous map $f : \mathbb{R} \to \mathbb{R}$ is **tame** if for all $r \in \mathbb{R}$, the closed set $f^{-1}(r)$ has only finitely many connected components.

A DMS $\gamma_X = (X, d_X(\cdot))$ is **tame** if for every $x, x' \in X$,

$$d_X(\cdot)(x, x') : \mathbb{R} \to \mathbb{R}$$

is tame.

Example of $d_{\mathrm{I}}^{\mathrm{dyn}} < \infty$.

- $X := \{x, x'\}$. $\gamma_X := (X, d_X(\cdot))$. $\overline{\gamma_X} := (X, \overline{d_X}(\cdot))$.

  $d_X(t) = 1 + \cos(t)$

  $\overline{d_X}(t) = 1 + \cos(t + \tau)$ for some $\tau \in (0, 2\pi)$.

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$$d_{\mathrm{I}}^{\mathrm{dyn}}(\gamma_X, \overline{\gamma_X}) = \min(\tau, 2\pi - \tau) \leq \tau$$