Invariants for persistent homology and their stability

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Science seminars



Slide 1

Good morning everyone. My lab works in this field

Slide 40

In conclusion we have shown that under semi-hypoxic conditions non canonical XHY889-2 signaling affects the cell cycle independently of XHY33-3 withought affecting the cell cycle

Motivation

Challenges for data science:

- data arising from new technologies
- not only size of data, but also complexity

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Ideas from pure mathematics can help



Topological data analysis

TDA studies the "shape" of complex data



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- Persistent homology
 - number of components, holes, voids, and higher dimensional holes

Topological data analysis

TDA studies the "shape" of complex data



- Persistent homology
 - number of components, holes, voids, and higher dimensional holes
- Magnitude homology
 - effective number of points

A topological perspective on regimes in dynamical systems, K. Strommen, M. Chantry, J. Dorrington, N. Otter, 2021, https://arxiv.org/abs/2104.03196

(Persistent) magnitude of point-cloud data, S. Kališnik, M. O'Malley, N. Otter, in preparation

Persistent homology



Multiparameter persistent homology (MPH) Motivation

Data often depend on several parameters, e.g.:

- colored digital images
- large and noisy climate data sets

A topological perspective on regimes in dynamical systems, K. Strommen, M. Chantry, J. Dorrington, N. Otter, 2021, https://arxiv.org/abs/2104.03196

Multiparameter persistent homology (MPH) Motivation



MPH: codensity-distance bifiltration



MPH pipeline



MPH: theoretical challenges

- MPH was introduced in 2009 by Carlsson and Zomorodian¹
- ► Classification problem amounts to studying isomorphism classes of multigraded modules over K[x₁,...,x_r]
- Desiderata for invariants for applications:
 - Computability
 - Stability
 - Interpretability

 $^{^1{\}rm G.}$ Carlsson, A. Zomorodian, The theory of multidimensional persistence, Discrete & Computational Geometry, 2009

Approaches focussing on finding invariants suitable for applications

- 1) Efficient algorithms to compute homology of multifiltrations:
 - For one-critical multifiltrations²
 - For general multifiltrations³

2) Invariants of MPH modules coming from applications: Bauer and Botnan, Chachólski, Oudot

3) Restriction of 2-parameter PH to 1-parameter PH: Biasotti et al⁴, Lesnick and Wright⁵

 $^2{\rm G.}$ Carlsson, G. Singh, A. Zomorodian, Computing multidimensional persistence, ISAAC 2009, Lecture notes in computer science

³W. Chachólski, M. Scolamiero, F. Vaccarino, Combinatorial presentation of multidimensional persistent homology, Journal of Pure and Applied Algebra, 2017

⁴S. Biasotti, A. Cerri, P. Frosini, D. Giorgi, C. Landi, Multidimensional Size Functions for Shape Comparison, Journal of Mathematical Imaging and Vision, 2008

⁵M. Lesnick, M. Wright, Interactive Visualization of 2-D Persistence Modules, arxiv.org/1512.00180

Restriction of 2-parameter PH to 1-parameter PH Vertical lines





Restriction of 2-parameter PH to 1-parameter PH Lines with positive slope



Computations performed with RIVET by M. Lesnick and M. Wright. M. Lesnick, M. Wright, Interactive Visualization of 2-D Persistence Modules, arxiv.org/1512.00180

4) Stratification of MPH



In HOST⁶ proposal of invariants that distinguish between:

- transient features, support is 0-dimensional,
- partially persistent features, support is a subspace of dimension

 $1 \leq d < r$, and

 fully persistent features, support is a subspace of dimension r.

⁶H. Harrington, NO, H. Schenck, U. Tillmann, Stratifying multiparameter persistent homology, *SIAGA*, **3**(3):439–471 (2019)

Stability and distances for one-parameter PH



- Stability results for 1-parameter PH: the pipeline is Lipschitz in an appropriate sense.
- Distances on barcodes are defined using matchings between intervals in the barcode

Barcodes and persistence diagrams



from N. Otter, M. A. Porter, U. Tillmann, P. Grindrod and H. A Harrington, A roadmap for the computation of persistent homology, *EPJ Data Science*, **6**: 17 (2017)

Distances on persistence diagrams

Given two persistence diagrams:



How far apart are they?

Distances on persistence diagrams

Given two persistence diagrams:



How far apart are they?

Idea: look at all possible ways to match the points in the two diagrams, and choose a way to compute distances between matched points. Then the distance is given by the optimal matching, the one minimizing these pairwise distances.

Bottleneck distance d_B

Given x, y in \mathbb{R}^2 choose



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For each matching let m be the maximum of the d_{∞} distances between matched points. The optimal matching is the one that minimizes this quantity, and the bottleneck distance is m for the optimal matching.



 $d_B(D_1, D_2) = 0.9$

The bottleneck distance Example



We have $d_B(D_1, D_2) = d_B(D_1, D_3) = \infty$

The bottleneck distance is very coarse Example



We have $d_B(D_1, D_2) = d_B(D'_1, D_2) = 1$

Wasserstein distance

Wasserstein distance

Given x, y in \mathbb{R}^2 choose



For each matching compute the the *p*-norm of all the L_p -distances between matched points. The optimal matching is the one that minimizes this *p*-norm.

For p = 2: optimal matching 6 5 . 3 2 2 3 4 5 $d_{W_2}(D_1, D_2) = \sqrt{0.82^2 + 1.2^2 + 0.8^2}$

Geometry of the spaces of persistence diagrams Means are not unique:



Two different optimal matchings, leading to two different means:





Geometry of the spaces of persistence diagrams

► In general: complicated

Geometry of the spaces of persistence diagrams

- In general: complicated
- ▶ For W₂(L₂) is a non-negatively curved Alexandroff space: Fréchet means are not necessarily unique nor continuous (Turner et al 2014)
- ► Continuous Fréchet means for probability distributions of persistence diagrams for W₂(L₂) (Munch et al 2015)
- ▶ Lots of work, e.g.: [Chazal et al 2013], [Turner 2020], ...

K. Turner, Y. Mileyko, S. Mukherjee, and J. Harer, Fréchet means for distributions of persistence diagrams, *Discrete & Computational Geometry*, **52**(2014)

E. Munch, K. Turner, P. Bendich, S. Mukherjee, J. Mattingly, and J. Harer, Probabilistic fréchet means for time varying persistence diagrams, *Electronic Journal of Statistics*, **9**(2015)

F. Chazal, B. Terese Fasy, F. Lecci, A. Rinaldo, A. Singh, and L. A. Wasserman. On the bootstrap for persistence diagrams and landscapes. *Modeling and Analysis of Information Systems*, **20**(6), 2013

K. Turner, Medians of populations of persistence diagrams, *Homology, Homotopy and Applications* **22**(1) (2020)

Alternatives



Idea: Instead of working directly with the space of persistence diagrams, map it to another space, e.g. Banach space, in which it is easier to compute means, variances, etc.

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Some approaches:

- Persistence landscapes
- Persistence images
- Tropical coordinates
- Kernels



Stability and distances for MPH



Defining distances for MPH module is a problem linked with finding suitable invariants that measure "persistence"

Interleaving distance

► Given two persistence modules N, M: (ℝ^r, ≤) → Vect, one defines a notion of "ε-approximate isomorphisms".

The interleaving distance is the smallest
e for which there is such an approximate isomorphism.

Interleaving

Let $\epsilon \in \mathbb{R}$, and use the notation $\hat{\epsilon} = (\epsilon, \dots, \epsilon) \in \mathbb{R}^r$.

▶ T_{ϵ} : $(\mathbb{R}^{r}, \leq) \rightarrow (\mathbb{R}^{r}, \leq)$ is the functor given by $T_{\epsilon}(a) = a + \hat{\epsilon}$

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• $\eta_{\epsilon}: id_{(\mathbb{R}^r, \leq)} \Rightarrow T_{\epsilon}$ is the natural transformation given by $\eta_{\epsilon}(a): a \leq a + \hat{\epsilon}.$
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- $\eta_{\epsilon}: id_{(\mathbb{R}^r, \leq)} \Rightarrow T_{\epsilon}$ is the natural transformation given by $\eta_{\epsilon}(a): a \leq a + \hat{\epsilon}.$
- Given two persistence modules $N, M \colon \mathbb{R}^r \to \text{Vect}$, an ϵ -interleaving of M and N consists of natural transformations $\varphi \colon M \Rightarrow NT_{\epsilon}$ and $\psi \colon N \Rightarrow MT_{\epsilon}$, i.e.



such that

 $(\psi T_{\epsilon})\varphi = M\eta_{2\epsilon}$ and $(\varphi T_{\epsilon})\psi = N\eta_{2\epsilon}$.

Interleaving distance

▶ Define the interleaving distance between modules *M* and *N* as

 $d_I(M, N) = \inf_{\epsilon} \{M \text{ and } N \text{ are } \epsilon \text{-interleaved} \}$

- ▶ We set $d_I(M, N) = \infty$ if M and N are not ϵ -interleaved for any $\epsilon \in \mathbb{R}$
- In the one-parameter case, the interleaving distance is the bottleneck distance (isometry theorem)⁷
- In the multiparameter case, the computation of the interleaving distance is NP-hard⁸

⁷Categorification of Persistent Homology, P. Bubenik, J. A. Scott *Discrete & Computational Geometry* **51**:600–627 (2014).

⁸Computing the Interleaving Distance is NP-Hard, H. B. Bjerkevik, M. B. Botnan, M. Kerber, *Foundations of Computational Mathematics* **20**:1237–1271 (2020).

Generalisation of Wasserstein distance?

In Bubenik et al.⁹:

Let d be a metric on the set of indecomposable modules, let $M \cong \bigoplus_{a \in A} M_a$ and $N \cong \bigoplus_{b \in B} N_b$ where M_a and N_b are indecomposable modules. Then define:

$$W_{p}(d)(M,N) = \min_{\varphi} \left(\left\| \left(d(M_{c}, N_{\varphi(c)}) \right)_{c \in C} \right\|_{p}^{p} + \right. \\ \left. + \left\| \left(d(M_{a}, 0) \right)_{a \in A - C} \right\|_{p}^{p} + \right. \\ \left. + \left\| \left(d(0, N_{b}) \right)_{b \in B - \varphi(C)} \right\|_{p}^{p} \right)^{1/p} \right.$$

where the minimum is over all partial matchings $\phi: A' \subset A \rightarrow B' \subset B$.

⁹P. Bubenik, J. A. Scott, and D. Stanley, An algebraic Wasserstein distance for generalized persistence modules, https://arxiv.org/abs/1809.09654, 2018.

In general, generalising distances to the multiparameter setting entails asking the question: what does "persistence" mean in the multiparameter case?

A general framework to study stability for MPH

We propose¹⁰ a shift in perspective:

- ► a choice of invariant determines a distance
- thus, rather then asking when the pipeline is Lipzschitz, we can ask for Lipschitz changes of invariants



¹⁰B. Giunti, J. Nolan, N. Otter, L. Waas, Amplitudes on abelian categories, in preparation

Amplitude

Fix an abelian category \mathcal{A} .

Definition

A class function α : ob $\mathcal{A} \to [0, \infty]$ is called an **amplitude** if $\alpha(0) = 0$, and for every short exact sequence

$$0 \rightarrow A \hookrightarrow B \twoheadrightarrow C \rightarrow 0$$

in \mathcal{A} the following inequalities hold:

$$\begin{array}{ll} \text{(Monotonicity)} & \begin{array}{l} \alpha(A) \leq \alpha(B) \\ \alpha(C) \leq \alpha(B) \end{array} & (1) \\ \text{(Subadditivity)} & \begin{array}{l} \alpha(B) \leq \alpha(A) + \alpha(C) \end{array} & (2) \end{array}$$

Moreover, α is additive if (2) is an equality and finite if $\alpha(A) < \infty$ for all A in ob A.



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- The map δ(C) = max{n ∈ N | C_n ≠ 0} gives an amplitude on ch;

Examples

- The map M → rank_RM gives an additive amplitude on the category of (left) R-modules;
 - The map $V \rightarrow \dim V$ gives an additive amplitude on Vect;
- The map δ(C) = max{n ∈ N | C_n ≠ 0} gives an amplitude on ch;
- Given two amplitudes α and β on A, the assignments max{α, β} and α + β are two amplitudes on A.

Relationship to other work

- Noise systems (Scolamiero, Chachólski, Lundman, Ramanujam, and Öberg)¹¹: to each ε ≥ 0 they assign a collection of objects.
- p-norms (Skraba and Turner)¹²
- Weight functions (Bubenik, Scott, and Stanley) ¹³

¹¹M. Scolamiero, W. Chachólski, A. Lundman, R. Ramanujam, and S. Öberg, Multidimensional persistence and noise, *Foundations of Computational Mathematics*, **17**:1367–1406, 2017

 $^{^{12}\}text{P.}$ Skraba and K. Turner, Wasserstein stability for persistence diagrams,https://arxiv.org/2006.16824, 2020

¹³P. Bubenik, J. A. Scott, and D. Stanley, An algebraic Wasserstein distance for generalized persistence modules, https://arxiv.org/abs/1809.09654, 2020.

Examples in TDA: *p*-norms

Definition

Let $X \cong \bigoplus_{i=1}^{n} \mathbb{I}[b_i, d_i) \in \operatorname{PerM}(\mathbb{R})$ and $p \in [1, \infty]$. The *p*-norm of X is defined by

$$\rho_p(X) = \begin{cases} \left(\sum_{i=1}^n |d_i - b_i|^p\right)^{1/p} & \text{if } p < \infty \\ \max_{i=1,\dots,n} |d_i - b_i| & \text{if } p = \infty \end{cases}$$

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Proposition

For all $p \in [1, \infty]$, ρ_p is an amplitude on $\operatorname{PerM}(\mathbb{R})$, additive if p = 1.

Proof. Skraba and Turner, arXiv, (2020).

Examples in TDA: Tropical coordinates

Definition (Kališnik¹⁴)

Let $X = \bigoplus_{i=1}^{n} \mathbb{I}[b_i, b_i + \ell_i)$. Then ℓ -trop^k(X) is defined to be the sum of the length of the k-longest intervals in X, while ∂ -trop^p_m(X) is defined to the sum of the p largest expressions of the form $\min\{b_i + \ell_i, (m+1)\ell_i\}$, for $m \in \mathbb{N}$.

Proposition (Giunti, Nolan, NO, Waas)

- The tropical coordinate ℓ-trop^k is an amplitude, for all k ∈ N on PerM(R);
- The tropical coordinate ∂-trop^p_m is an amplitude on PerM(ℝ), for all m, p ∈ N;
- The tropical coordinate given by the sum of I largest expressions of the form min{b_i, mℓ_i} is not an amplitude on PerM(ℝ) for any m, I ∈ ℕ.

¹⁴S. Kališnik, Tropical coordinates on the space of persistence barcodes. *Foundations of Computational Mathematics*, **19**(1):101–129, 2019.

Examples in TDA: Persistent magnitude

Definition

Let $X \cong \bigoplus_{i=1}^{n} \mathbb{I}[b_i, d_i) \in \operatorname{PerM}(\mathbb{R})$. The **persistent magnitude** of X is

$$\operatorname{PMagn}(X) = \sum_{i=1}^n e^{-b_i} - e^{-d_i}$$

¹⁵D. Govc and R. Hepworth, Persistent magnitude, *Journal of Pure and Applied Algebra*, **225**, 2021.

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Proposition

The persistent magnitude is an additive amplitude on $\operatorname{PerM}(\mathbb{R})$.

Proof.

Govc and Hepworth¹⁵.

¹⁵D. Govc and R. Hepworth, Persistent magnitude, *Journal of Pure and Applied Algebra*, **225**, 2021.

Additive amplitudes

Theorem (Giunti, Nolan, NO, Waas) Let Q be a finite poset. The following map is a bijection: $\psi = \text{Meas}(Q) \longrightarrow \text{AdAmp}(\text{PerM}(Q))$ $\mu \mapsto \int_{Q} \text{dim}(\cdot) d\mu.$

Additive amplitudes

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Theorem (Giunti, Nolan, NO, Waas)

Each additive amplitude on $\operatorname{PerM}(\mathbb{R}^d)$ is uniquely given by integrating the Hilbert function with respect to a content.

Amplitudes in multi-parameter persistence

- L^p-amplitudes;
- Shift amplitudes;
- Support amplitude;
- Maximal dimension amplitude;
- Rank and multirank amplitude;

▶ ...

Distances from amplitudes Absolute-value distance

Definition

The **absolute-value distance**, for every $X, Y \in ob \mathcal{A}$, is defined as

$$d_{|\alpha|}(X,Y) = |\alpha(X) - \alpha(Y)|.$$

- ► d_{|ρ1|} is used in one of the first stability results in persistent homology¹⁶.
- ▶ d_{|ℓ-trop^k|} and d_{|∂-trop^p|} are used in the stability results for tropical coordinates¹⁷.

¹⁶David Cohen-Steiner, Herbert Edelsbrunner, John Harer, and Yuriy Mileyko. Lipschitz functions have I_p -stable persistence, Foundations of Computational Mathematics, **10**(2):127–139, 2010.

¹⁷S. Kališnik, Tropical coordinates on the space of persistence barcodes. *Foundations of Computational Mathematics*, **19**(1):101–129, 2019.

Distances from amplitudes Path metric

$$c_{lpha}(arphi) = lpha(\ker arphi) + lpha(\operatorname{coker} arphi)$$
 .

Distances from amplitudes Path metric

Definition

Given a morphism φ in \mathcal{A} , its **cost** is

$$c_{\alpha}(\varphi) = \alpha(\ker \varphi) + \alpha(\operatorname{coker} \varphi).$$

For any $X, Y \in ob \mathcal{A}$, the **path metric** associated to α is

$$\mathrm{d}_{\alpha}\left(X,Y\right) = \inf\left\{\varepsilon \in [0,\infty) \mid c_{\alpha}(\varphi) + c_{\alpha}(\psi) \leq \varepsilon \text{ with } X \xleftarrow{\varphi} Z \xrightarrow{\psi} Y\right\}.$$

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Lemma

For each $X \in A$, $\alpha(X) = d_{\alpha}(X, 0)$.

Interleaving distance as a distance from an amplitude

Let C be a cone in \mathbb{R}^r . A shift amplitude σ on $\operatorname{PerM}(\mathbb{R}^r)$ is defined for any $X \in \operatorname{ob}\operatorname{PerM}(\mathbb{R}^r)$ as

 $\sigma(X) = \inf \left\{ \ ||c|| \ | \ c \in C \text{ and } X(t \leq t + c) = 0 \text{ for all } t \in \mathbb{R}^r \right\}.$

¹⁸Oliver Gäfvert and Wojciech Chachólski. Stable invariants for multidimensional persistence, arXiv:1703.03632, 2017

Interleaving distance as a distance from an amplitude

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 $\sigma(X) = \inf \left\{ \ ||c|| \ | \ c \in C \text{ and } X(t \leq t + c) = 0 \text{ for all } t \in \mathbb{R}^r \right\}.$

Theorem For any $X, Y \in PerM(\mathbb{R}^r)$, we have:

$$d_I(X, Y) \leq d_\sigma(X, Y) \leq 6 d_I(X, Y).$$

Proof. Prop. 12.2 in [GC17]¹⁸.

¹⁸Oliver Gäfvert and Wojciech Chachólski. Stable invariants for multidimensional persistence, arXiv:1703.03632, 2017

Categories of amplitudes

Definition

The category of amplitudes, Amp , is the category where:

- 1. Objects are pairs (A, α) consisting of an abelian category A together with an amplitude α on it;
- 2. Morphisms $(\mathcal{A}, \alpha) \to (\mathcal{A}', \alpha')$ are **amplitude-bounding** functors, i.e. additive functors $F : \mathcal{A} \to \mathcal{A}'$ such that there exists $K \ge 0$ so that $\alpha'(FX) \le K\alpha(X)$ for all $X \in \text{ob } \mathcal{A}$.

Amplitude-bounding functors

Lemma (Giunti, Nolan, NO, Waas)

Let id: $(\operatorname{PerM}(\mathbb{R}), \rho_p) \to (\operatorname{PerM}(\mathbb{R}), \rho_q)$, where ρ_p is the p-norm amplitude. Then id is amplitude-bounding, with K = 1, if and only if $p \leq q \in [1, \infty]$.

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Lemma (Giunti, Nolan, NO, Waas)

Let id: $(\operatorname{PerM}(\mathbb{R}), \rho_1) \to (\operatorname{PerM}(\mathbb{R}), \operatorname{PMagn})$, where PMagn is the persistent magnitude. Then id is amplitude-bounding with K = 1.

Continuous changes of invariants



Continuous changes of invariants



Inferred stability results

Proposition (Giunti, Nolan, NO, Waas)

Let $F: (\mathcal{A}, \alpha) \to (\mathcal{A}', \alpha')$ be an exact, amplitude-bounding functor with constant K. Then, for all $X, Y \in ob \mathcal{A}$,

 $d_{\alpha'}(FX,FY) \leq K d_{\alpha}(X,Y).$

Inferred stability results

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Corollary (Giunti, Nolan, NO, Waas) Given any persistence modules $X, Y \in PerM(\mathbb{R})$, we have that $d_{PMagn}(X, Y) \leq W_1(Dgm(X), Dgm(Y))$.

Future work

- Extend stability results.
- Study the computability of the distances.
- Explore the discriminating power of distances from amplitudes on a data set of tropical diseases.

Non-example: Number of indecomposables

In general, the number of indecomposables of an object in an abelian, Krull-Schmidt category is not an amplitude. Example¹⁹:

¹⁹M. Buchet and E. G. Escolar, Realizations of Indecomposable Persistence Modules of Arbitrarily Large Dimension, *In 34th International Symposium on Computational Geometry(SoCG 2018)*, **99** 15:1–15:13, Dagstuhl, Germany, 2018

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Non-example: *c*_p-rank

Let *M* be an \mathbb{N} -graded module over $\mathbb{K}[x_1, \ldots, x_r]$. Let *p* be an associated prime of *M*. Its 0th local cohomology with respect to *p* is

$$H^0_p(M)=\{m\in M\mid p^n\cdot m=0 ext{ for all }n>>0\}\,.$$

W.l.o.g. assume that $p = \langle x_1, \ldots, x_k \rangle$. The c_p -rank of M^{20} is the rank of H_p^0 as a module over $\mathbb{K}[x_{k+1}, \ldots, x_r]$.

²⁰H. Harrington, NO, H. Schenck, U. Tillmann, Stratifying multiparameter persistent homology, *SIAGA*, **3**(3):439–471 (2019)
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The c_p -rank gives a count of the ways that the module goes to infinity in the directions orthogonal to the coordinate subspace spanned by x_1, \ldots, x_k [Proposition 4.20, HOST].

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In general, the c_p -rank is not an amplitude.

²⁰H. Harrington, NO, H. Schenck, U. Tillmann, Stratifying multiparameter persistent homology, *SIAGA*, **3**(3):439–471 (2019)