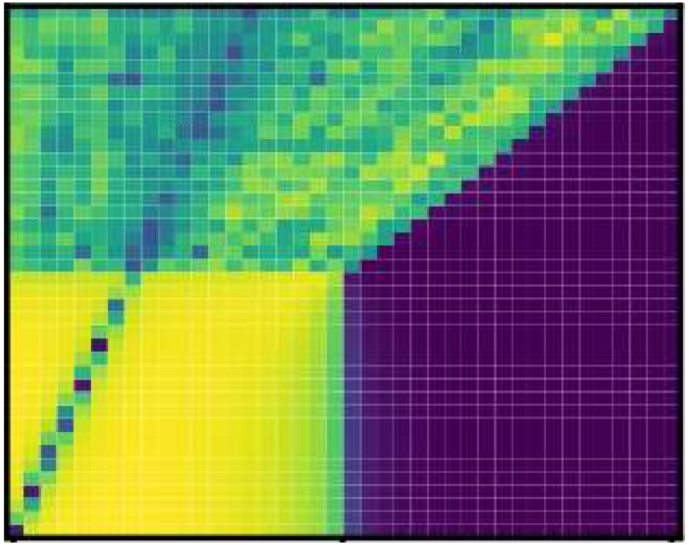
Persistent homology analysis of phase transitions



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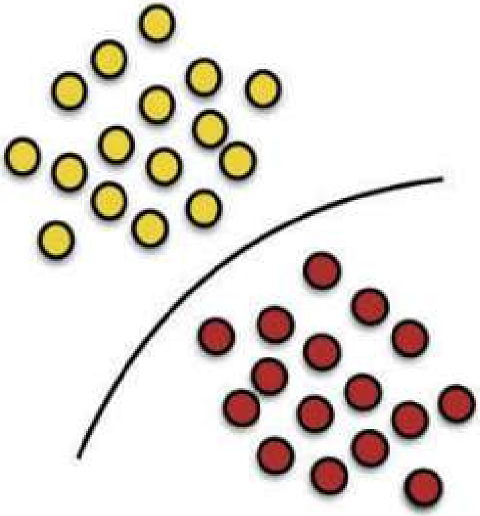
Outline

1. Introduction: machine learning for condensed matter physics
2. Topological data analysis and persistent homology
3. Persistent homology analysis of localisation transitions
4. Summary and outlook

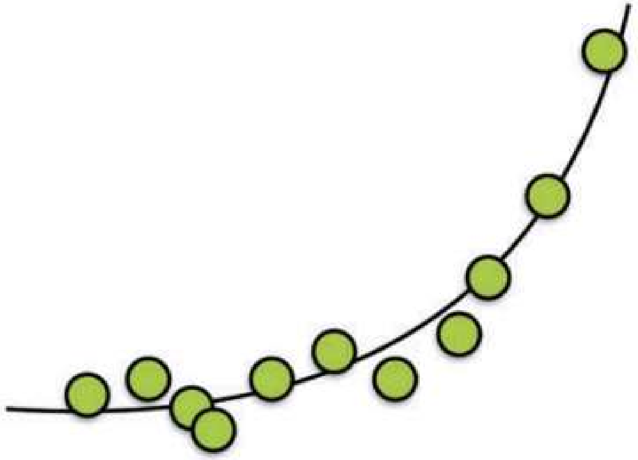
What is machine learning?

Algorithms that build models **using data** to perform tasks such as:

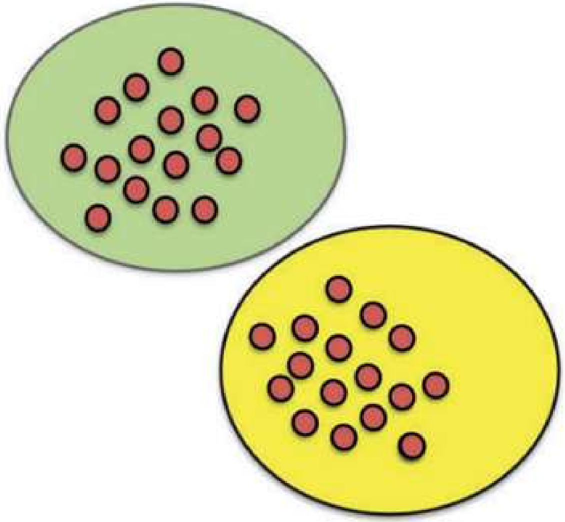
Classification



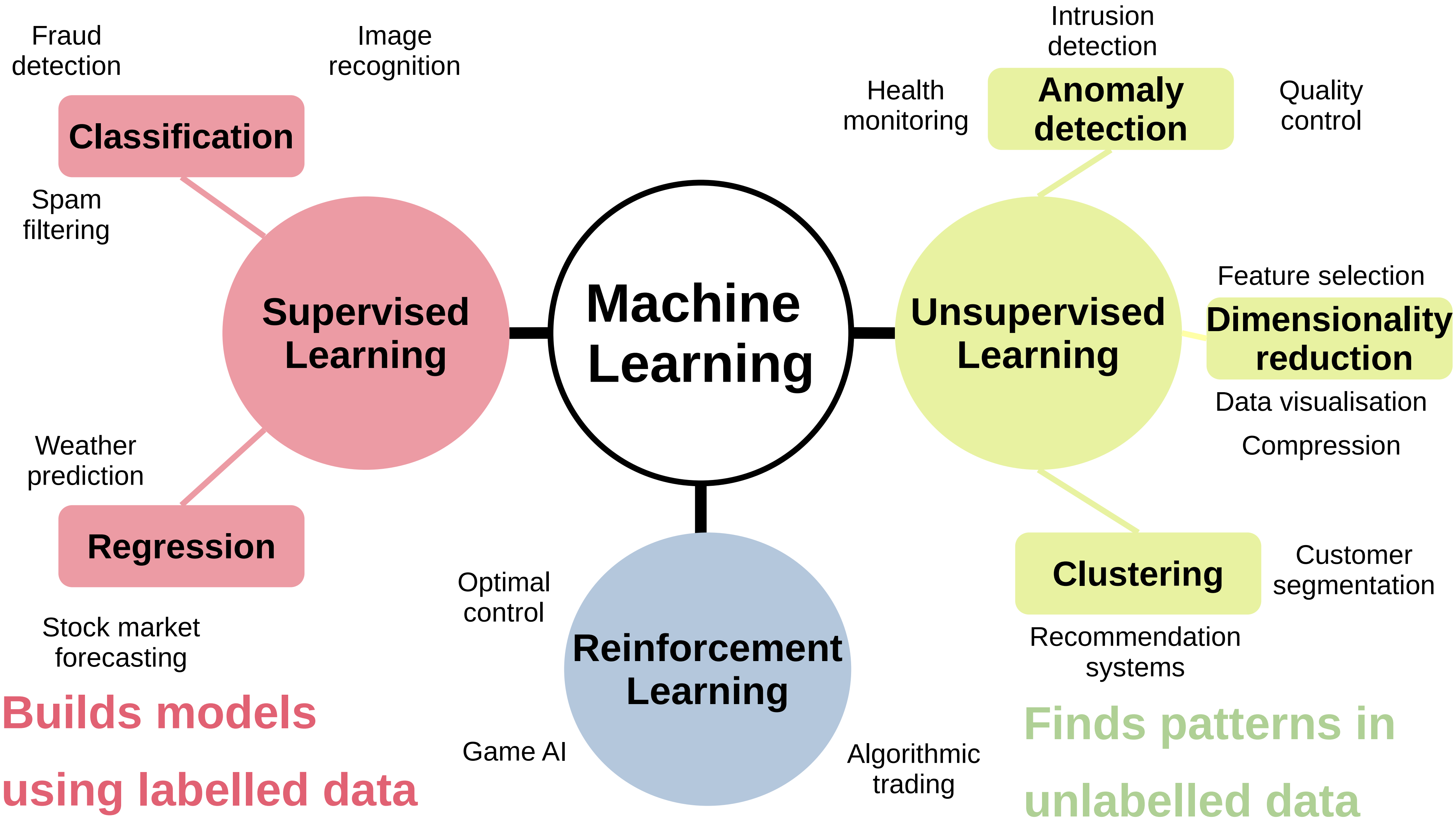
Regression



Clustering



J. Carrasquilla, Adv. Phys.: X 5, 1797528 (2020)


Machine Learning
Supervised Learning
Classification
Fraud detection
Image recognition
Spam filtering
Regression
Weather prediction
Stock market forecasting
Builds models using labelled data
Unsupervised Learning
Anomaly detection
Intrusion detection
Health monitoring
Quality control
Dimensionality reduction
Feature selection
Data visualisation
Compression
Clustering
Customer segmentation
Recommendation systems
Finds patterns in unlabelled data
Reinforcement Learning
Optimal control
Game AI
Algorithmic trading

Clustering algorithms

Group unlabelled data into different classes

Example: k-means algorithm

1. Randomly set k cluster centres $m_j^{(0)}$

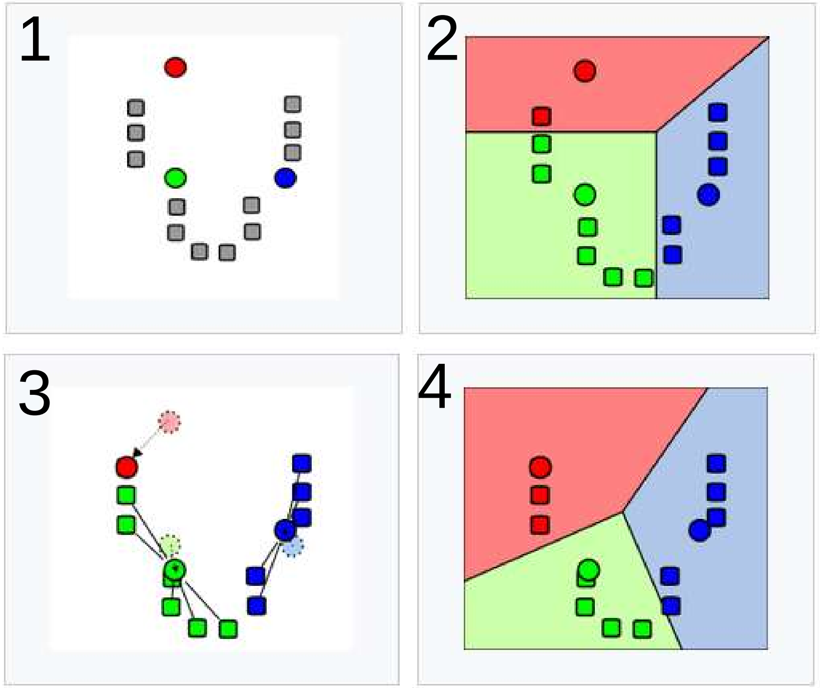
2. Assign points x_p to nearest centre

$$S_i^{(t)} = \left\{ x_p : \left\| x_p - m_i^{(t)} \right\|^2 \le \left\| x_p - m_j^{(t)} \right\|^2 \forall j, 1 \le j \le k \right\},$$

3. Cluster centroids -> new centres

$$m_i^{(t+1)} = \frac{1}{\left|S_i^{(t)}\right|} \sum_{x_j \in S_i^{(t)}} x_j$$

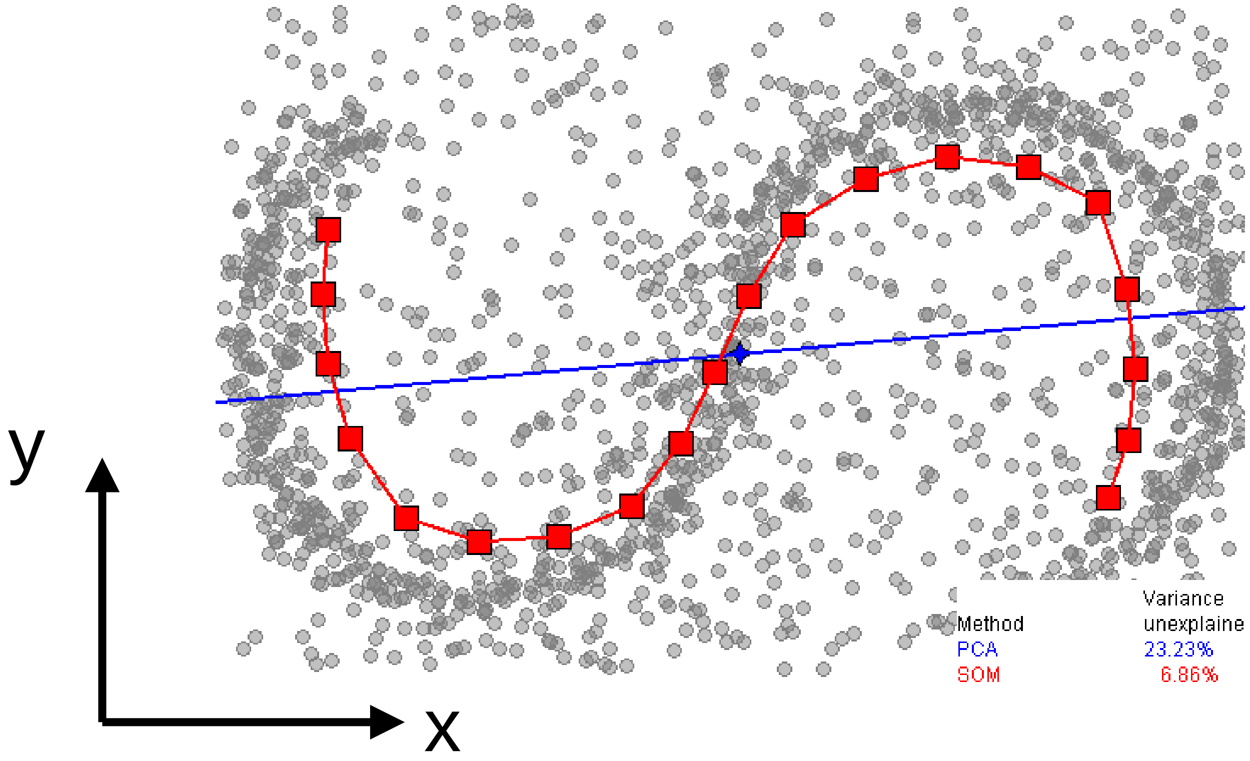
4. Repeat 2 & 3 until convergence



https://en.wikipedia.org/wiki/K-means_clustering

Dimensionality reduction

Obtain faithful lower-dimensional representations of the data



Machine learning of quantum matter

ARTICLES
https://doi.org/10.1038/s41567-019-0512-x
nature physics

Identifying topological order through unsupervised machine learning

Joaquin F. Rodriguez-Nieva* and Mathias S. Scheurer*

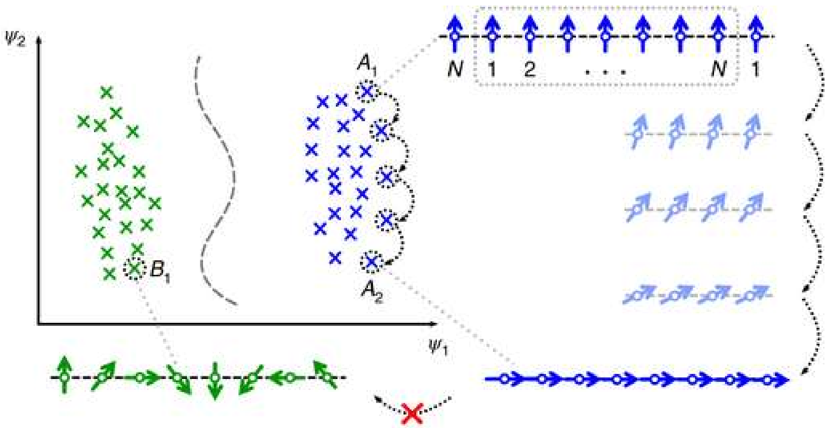


Fig. 1 | Topological classification using sample connectivity. Shown are samples of N classical XY spins, with periodic boundary conditions and winding numbers $\nu = 0,1$, projected on a two-dimensional (2D) feature space $\psi_{1,2}$. A diffusion map clusters samples that are connected via continuous deformations, such as A_1 and A_2, but not A_1 and B_1.

PHYSICAL REVIEW LETTERS **124**, 226401 (2020)

Unsupervised Machine Learning and Band Topology

Mathias S. Scheurer[1] and Robert-Jan Slager[1,2]
[1]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA
[2]TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

(Received 10 January 2020; accepted 15 May 2020; published 1 June 2020)

PHYSICAL REVIEW LETTERS **125**, 127401 (2020)

Identifying Topological Phase Transitions in Experiments Using Manifold Learning

Eran Lustig,* Or Yair,* Ronen Talmon, and Mordechai Segev
Technion–Israel Institute of Technology, Haifa 32000, Israel

(Received 17 October 2019; accepted 7 July 2020; published 14 September 2020)

PHYSICAL REVIEW B **102**, 134213 (2020)

Topological quantum phase transitions retrieved through unsupervised machine learning

Yanming Che,[1,*] Clemens Gneiting,[1] Tao Liu,[1] and Franco Nori[1,2,†]
[1]Theoretical Quantum Physics Laboratory, RIKEN Cluster for Pioneering Research, Wako-shi, Saitama 351-0198, Japan
[2]Department of Physics, The University of Michigan, Ann Arbor, Michigan 48109-1040, USA

(Received 6 February 2020; accepted 8 October 2020; published 29 October 2020)

PHYSICAL REVIEW LETTERS **125**, 225701 (2020)

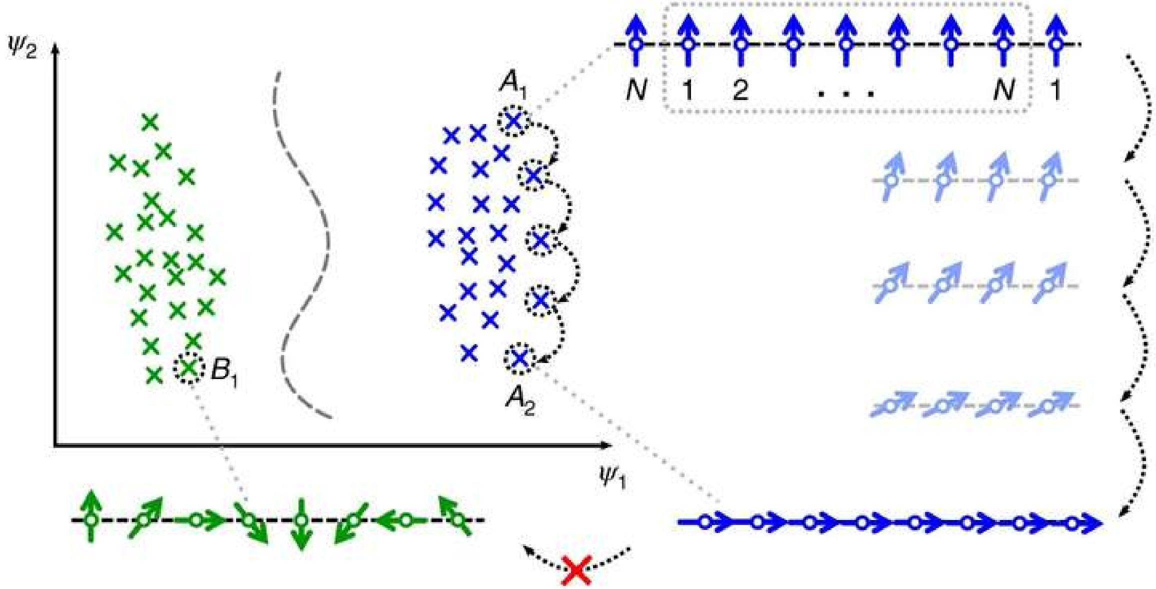
Unsupervised Machine Learning of Quantum Phase Transitions Using Diffusion Maps

Alexander Lidiak[1,*] and Zhexuan Gong[1,2,†]
[1]Department of Physics, Colorado School of Mines, Golden, Colorado 80401, USA
[2]National Institute of Standards and Technology, Boulder, Colorado 80305, USA

(Received 26 March 2020; accepted 15 October 2020; published 24 November 2020)

Unsupervised learning of (topological) phases

1. Obtain input data (e.g. eigenstates, Hamiltonians, wavefunctions)
2. Compute similarity between data points using **appropriate distance metric**
3. Apply dimensionality reduction to identify key data features
4. Perform k-means clustering on the reduced data



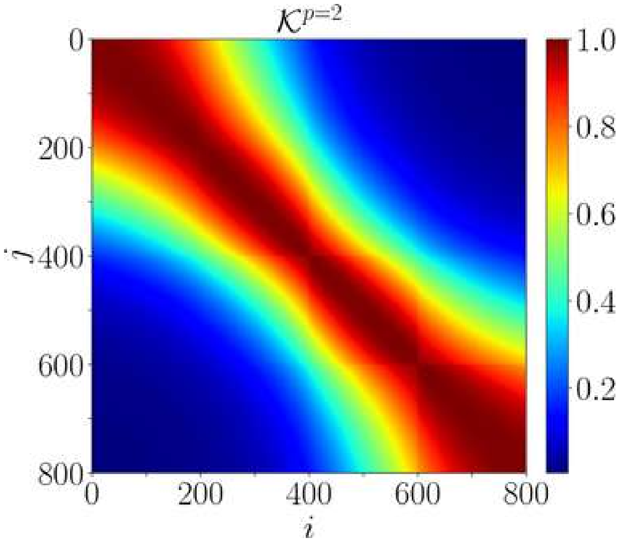
$$K_\varepsilon(x_l, x_{l'}) = \exp\left(-\frac{||x_l - x_{l'}||^2}{2N\varepsilon}\right)$$

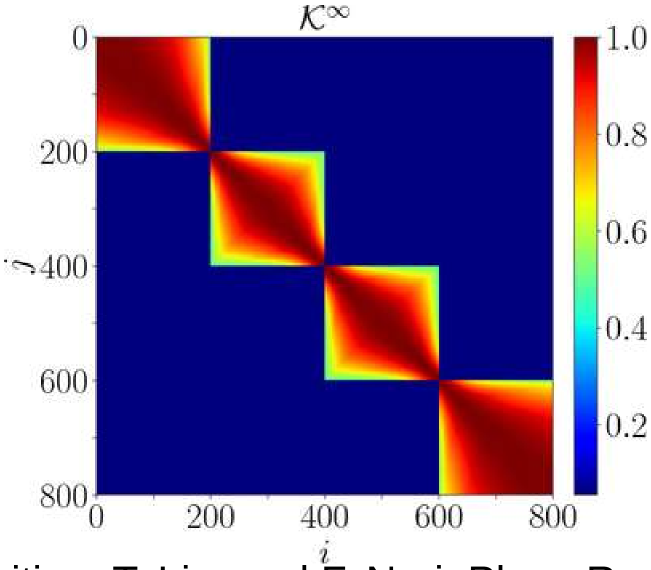
$$||x_l - x_{l'}||^2/(2N) = 1 - \frac{1}{N}\sum_{i=1}^{N} \mathbf{S}_i^{(l)} \cdot \mathbf{S}_i^{(l')}$$

J. F. Rodriguez-Nieva and M. S. Scheurer, Nat. Phys. 15, 790 (2019)

The metric matters

- 2D Chern insulator model, each data vector $\mathbf{x}_i$ constructed from band eigenstates
- Model parameters varied to sample from different topological phases
- Euclidean distance not sensitive to phase boundaries
- Chebyshev distance gives sharp separation between phases





Euclidean distance

$$\mathcal{K}_{ij}^{p=2} = \exp\left(- \frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2_{\mathbb{L}^2}}{4\epsilon (N+1)^{2D}} \right)$$

Chebyshev distance

$$\mathcal{K}_{ij}^{\infty} = \exp\left(- \frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2_{\mathbb{L}^\infty}}{4\epsilon} \right)$$

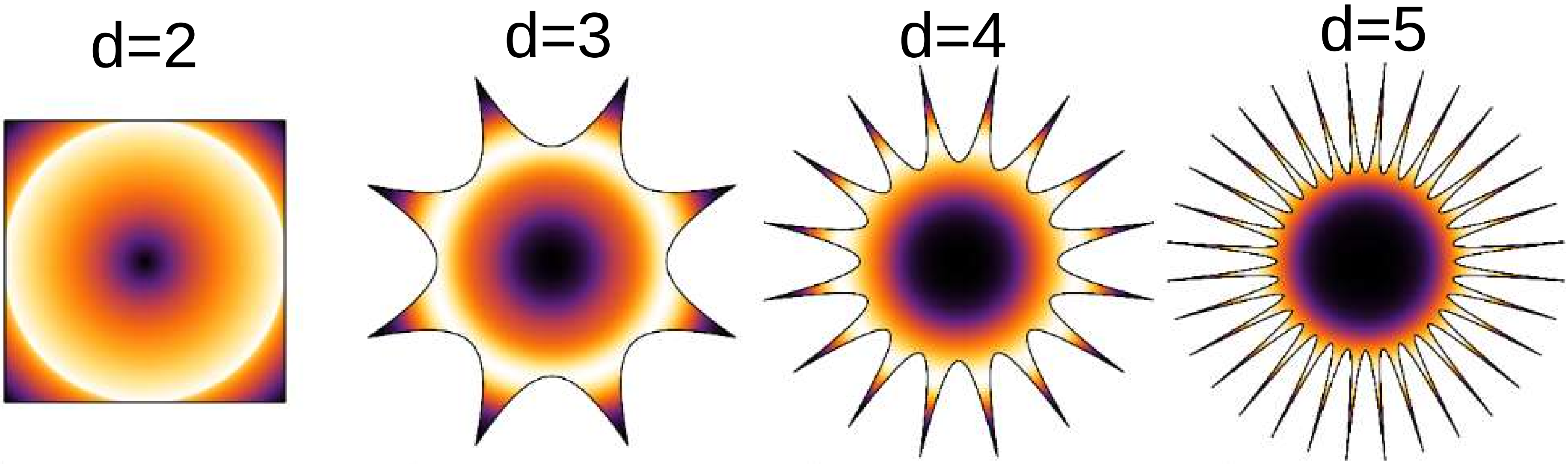
Y. Che, C. Gneiting, T. Liu, and F. Nori, Phys. Rev. B 134213 (2020)

Problem: curse of dimensionality

- **Concentration of scores and distances**: distances become numerically similar
- **Irrelevant attributes**: a significant number of attributes may be irrelevant
- **Exponential search space**: the space can no longer be systematically scanned
- **Data snooping bias**: for every desired significance a hypothesis can be found
- **Hubness**: certain states occur more frequently in neighbour lists than others

Zimek, Schubert, and Kriegel, Statistical Analy. Data Mining, 5 363 (2012);

Projections of d-dimensional hypercubes

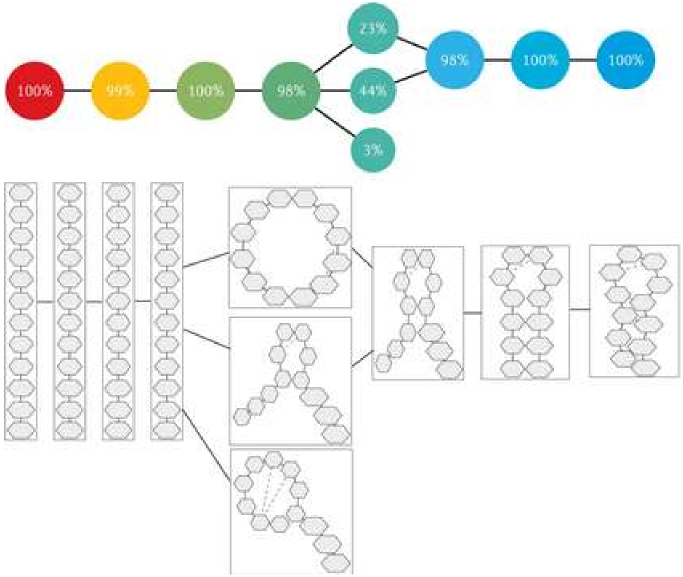


"In high dimensions, even simple compact objects present tendril-, or tentacle-like regions that extend very far but get very thin. Yet, somewhat counter-intuitively, most of the volume of high-dimensional objects is contained in these extended objects! As the dimensionality of space increases, the intersection between the hypercube and the hypersphere becomes very small."

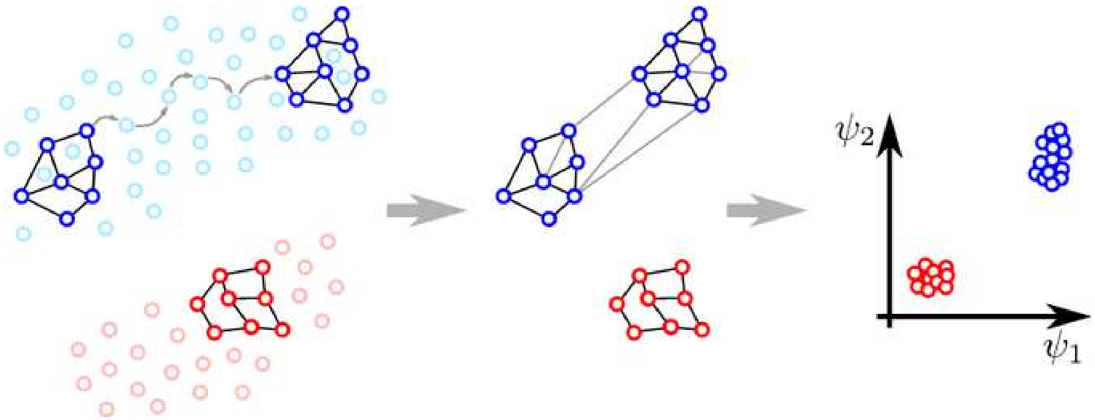
M. Casiulis and S. Martiniani, arXiv:2207.08241

Topological methods for machine learning

- Identify data features (e.g. cycles) missed by standard methods
- Intrinsic robustness to noise, deformations
- Better-suited for sparse data in high-dimensional spaces



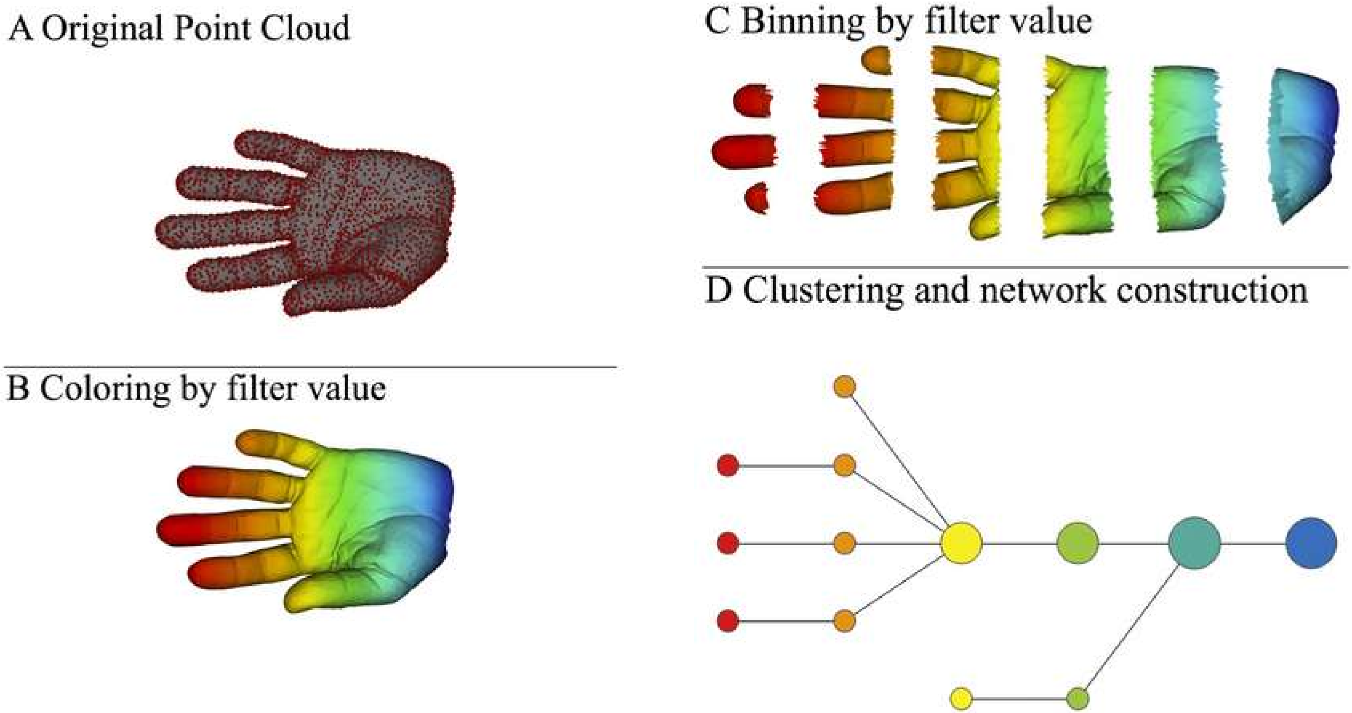
Yao, Y. et al., J. Chem. Phys. 130, 144115 (2009)



Scheurer and Slager, Phys. Rev. Lett. 124, 226401 (2020)

Topological data analysis

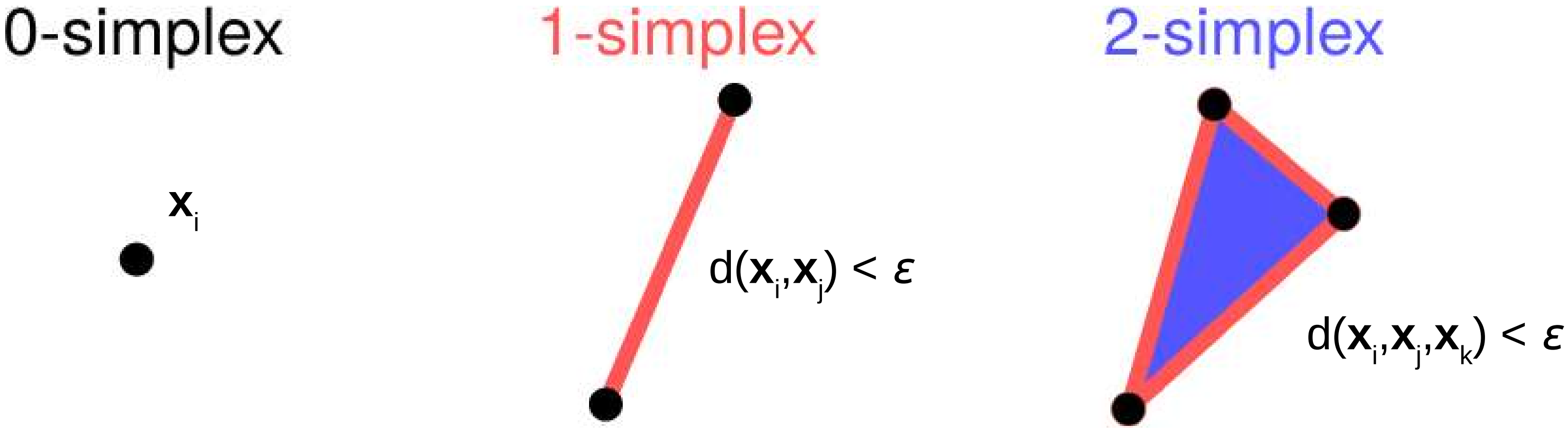
- Represents data as (families of) graphs & simplicial complexes
- Quantifies "shape" using graph topological invariants



Lum et al., Scientific Reports 3, 1236 (2013)

Graphs and simplicial complices

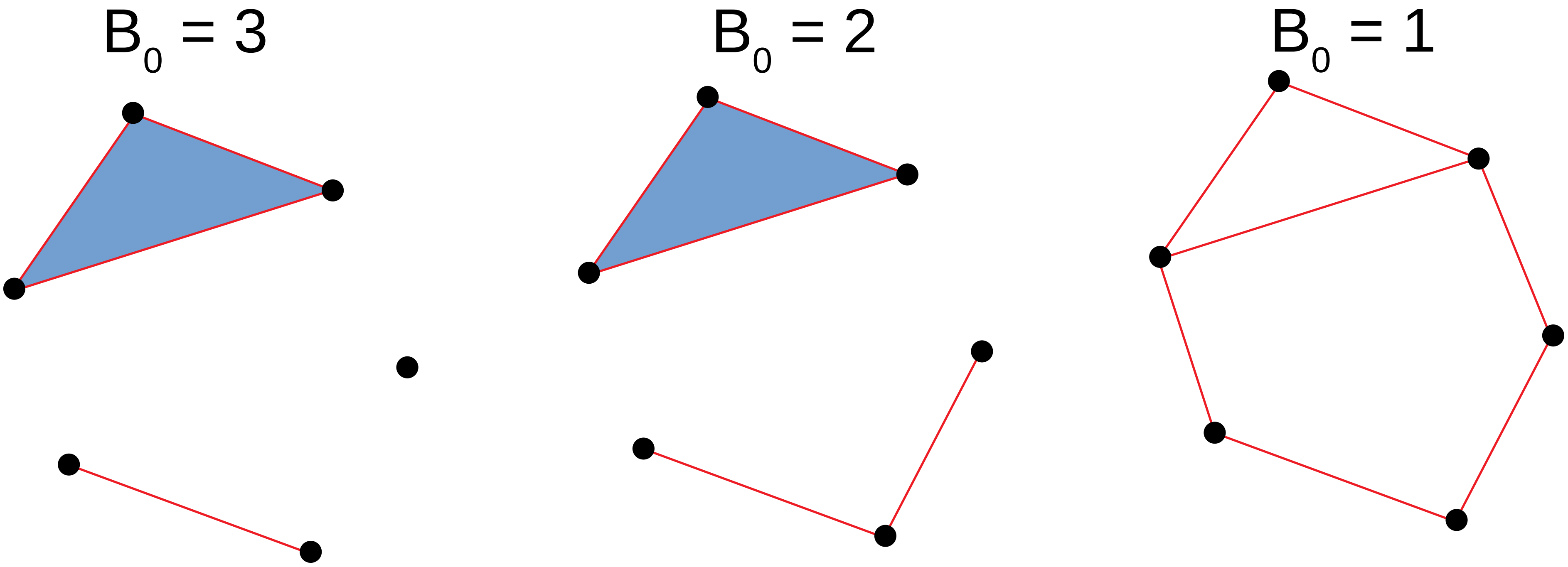
- Graph: vertices connected by edges
- Simplicial complex: higher dimensional generalization
- Simplicial complex constructed from points using distance measure d



J. Murugan, D. Robertson, arXiv:1904.11044; G. Carlsson, Nature Rev. Phys. 2, 697 (2020)

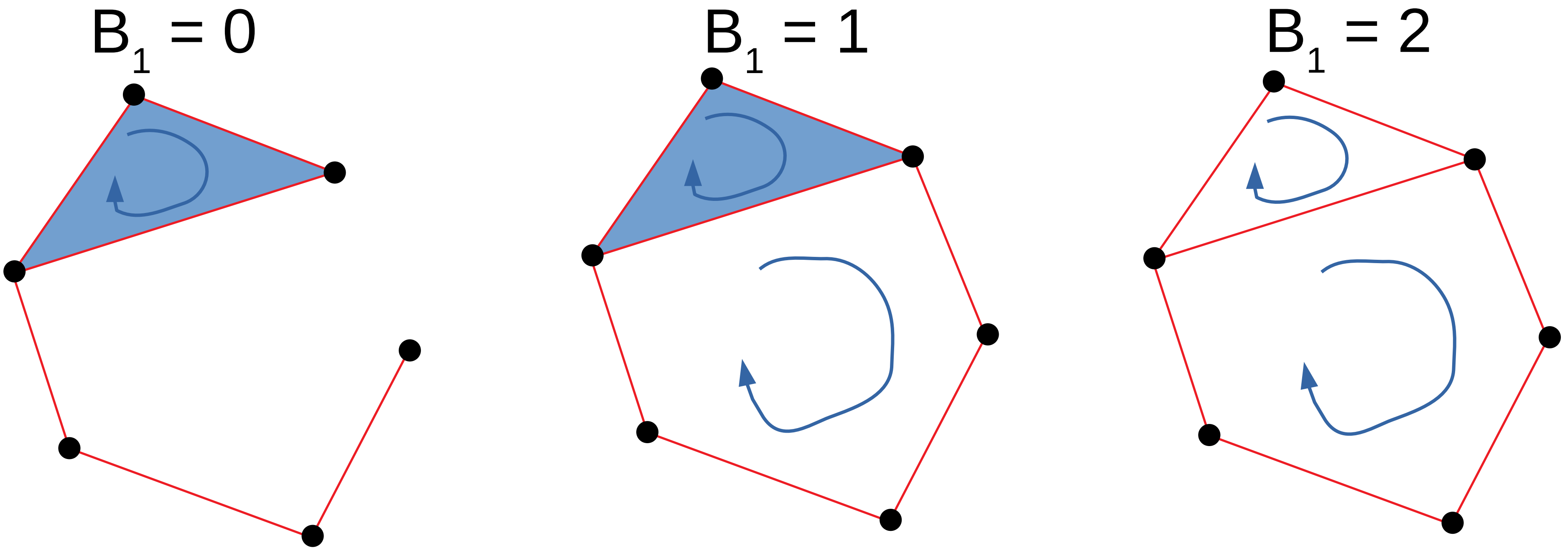
Topological invariants: Betti numbers

- kth Betti number B_k = number of k-dimensional cycles
- B_0 = number of disconnected components



Topological invariants: Betti numbers

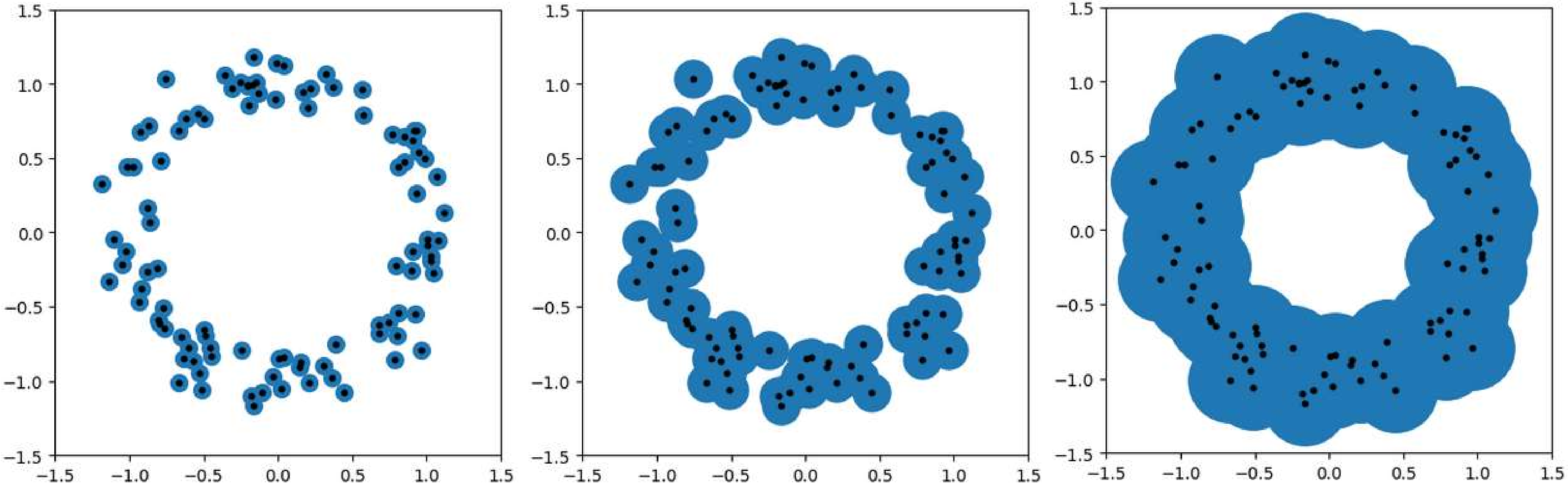
- kth Betti number B_k = number of k-dimensional cycles
- B_1 = number of non-contractible loops



Shape depends on scale

Solution: study topology over a range of spatial scales

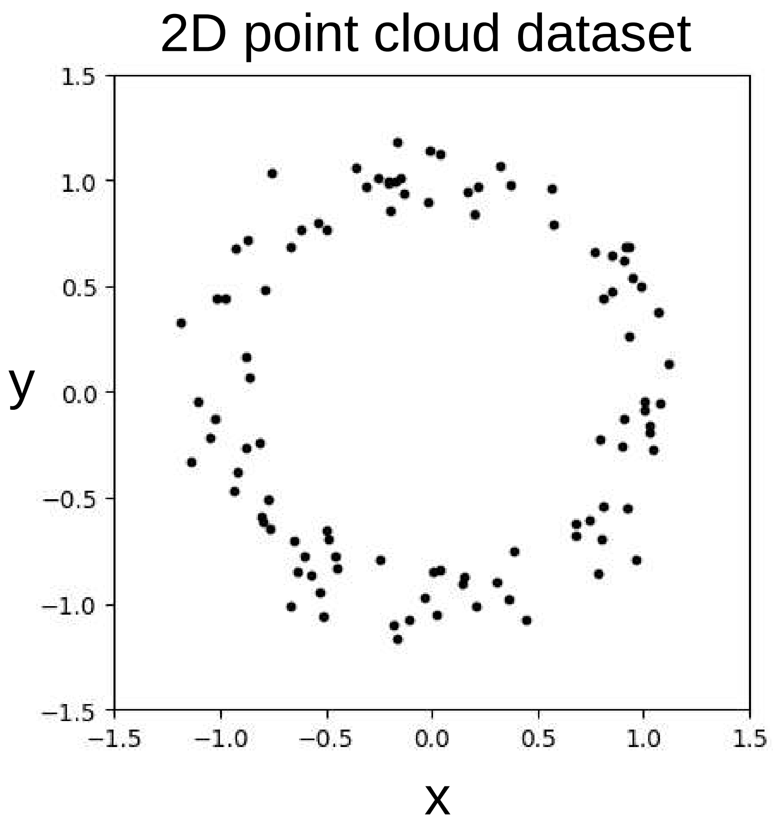
Isolated clusters | Clusters merging | Annulus

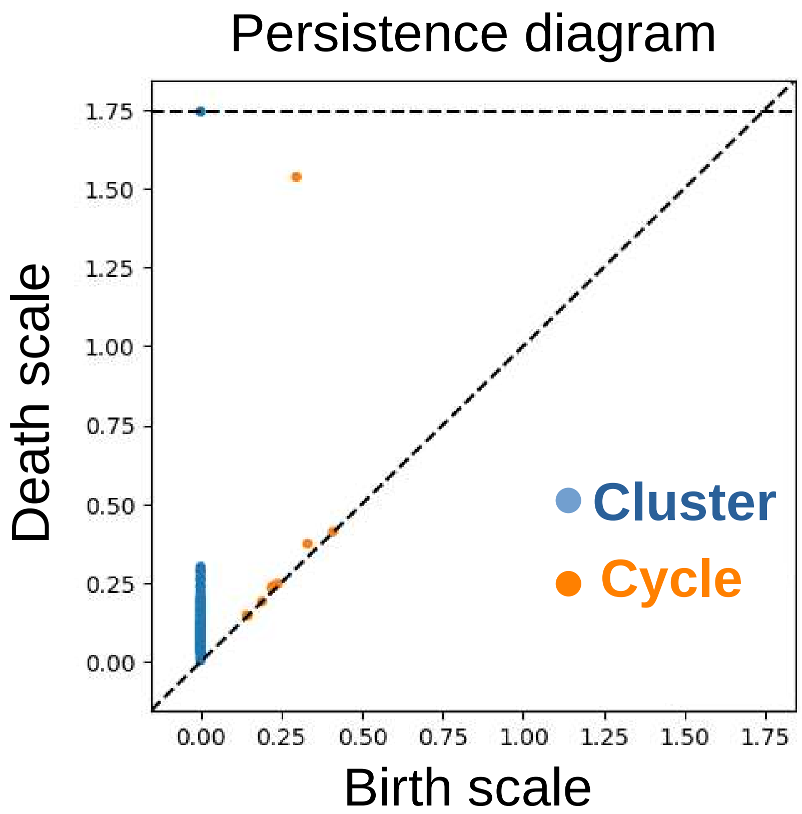


Increasing characteristic distance scale ε

Persistence diagrams

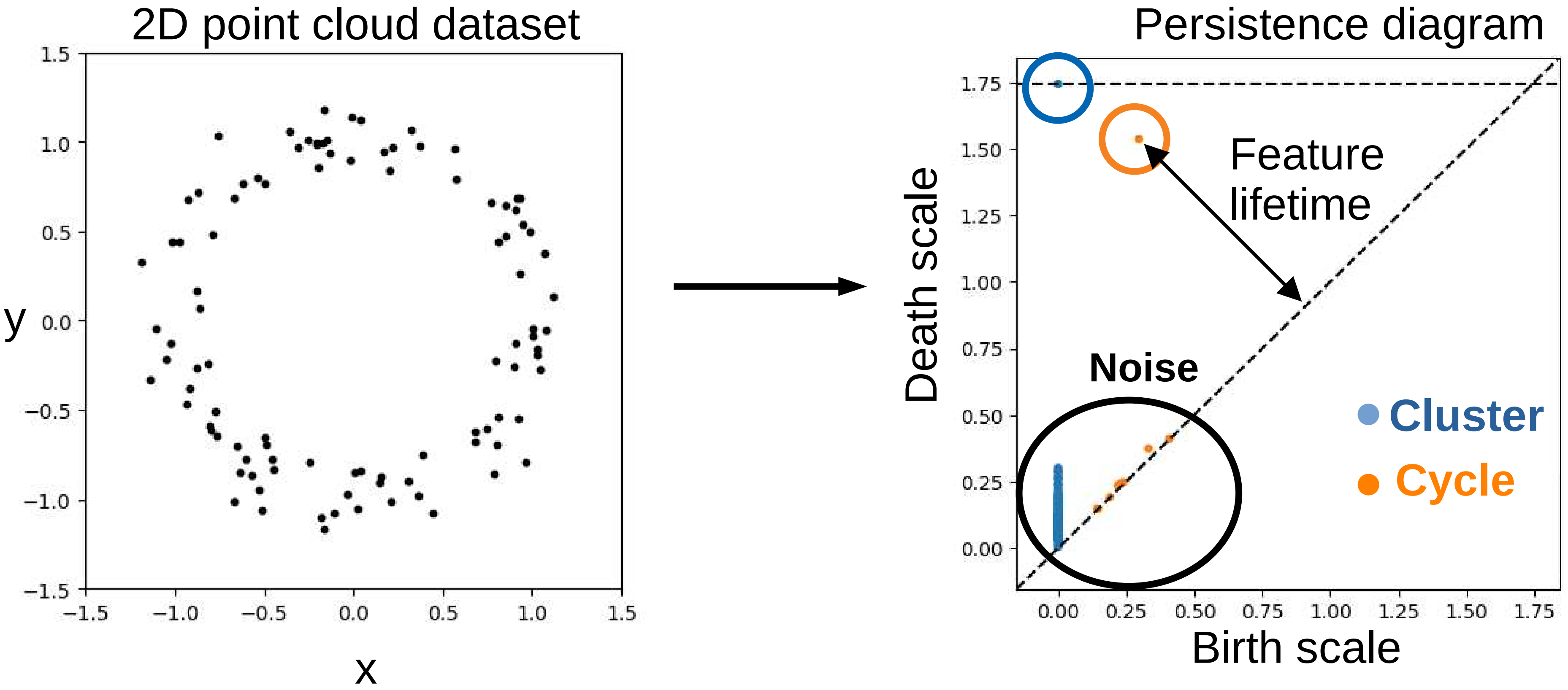
Show scales at which features are created and destroyed





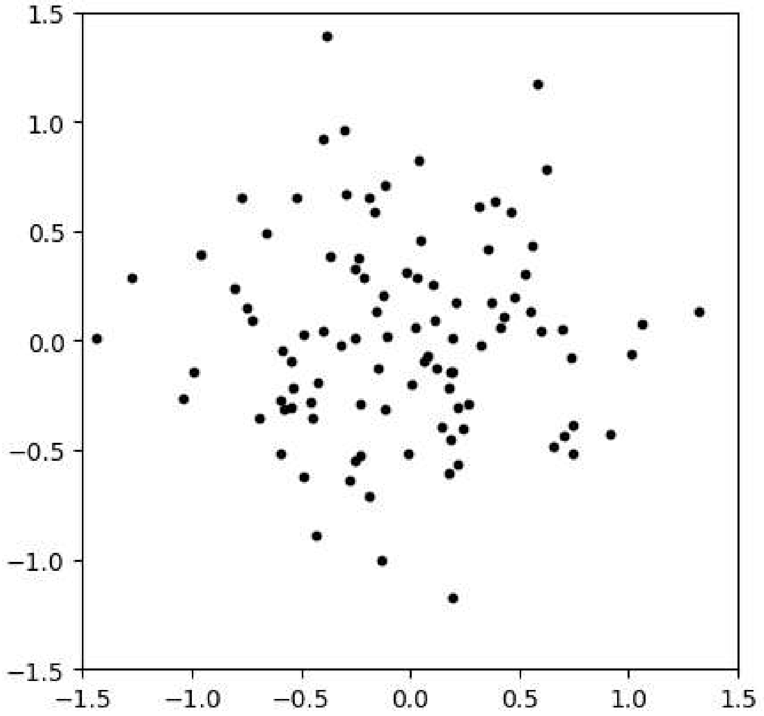
Persistence diagrams

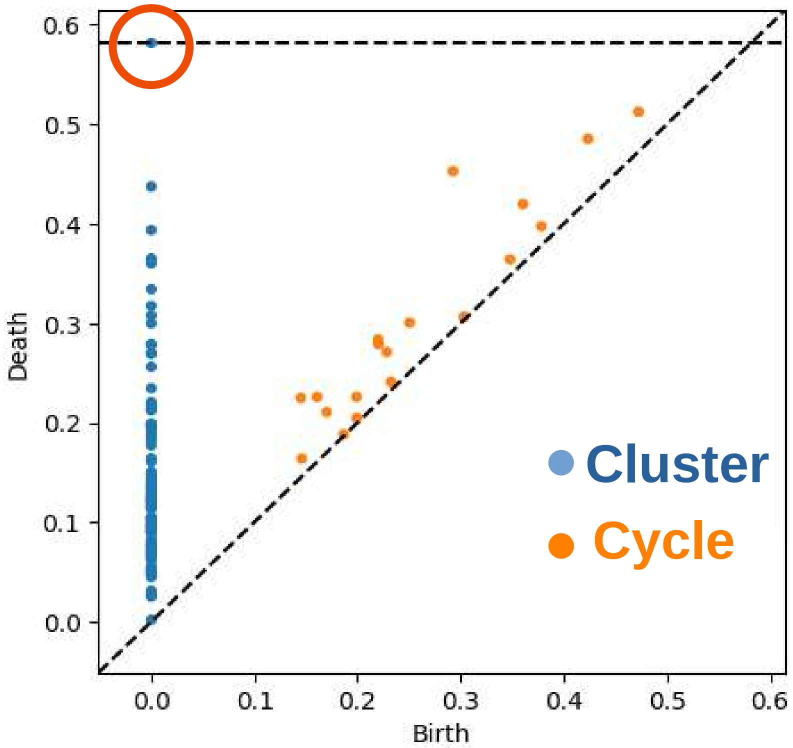
- Low persistence features (near diagonal) sensitive to noise
- High persistence features are robust, reveal shape of data



Persistence diagrams: examples

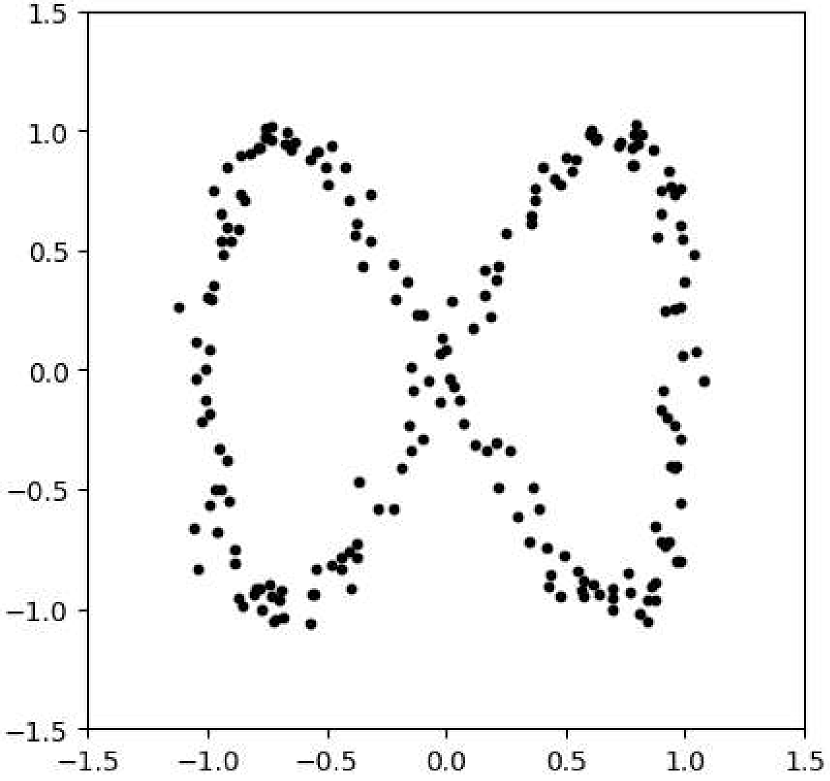
- Loops have low persistence, sensitive to noise
- Single high persistence connected component

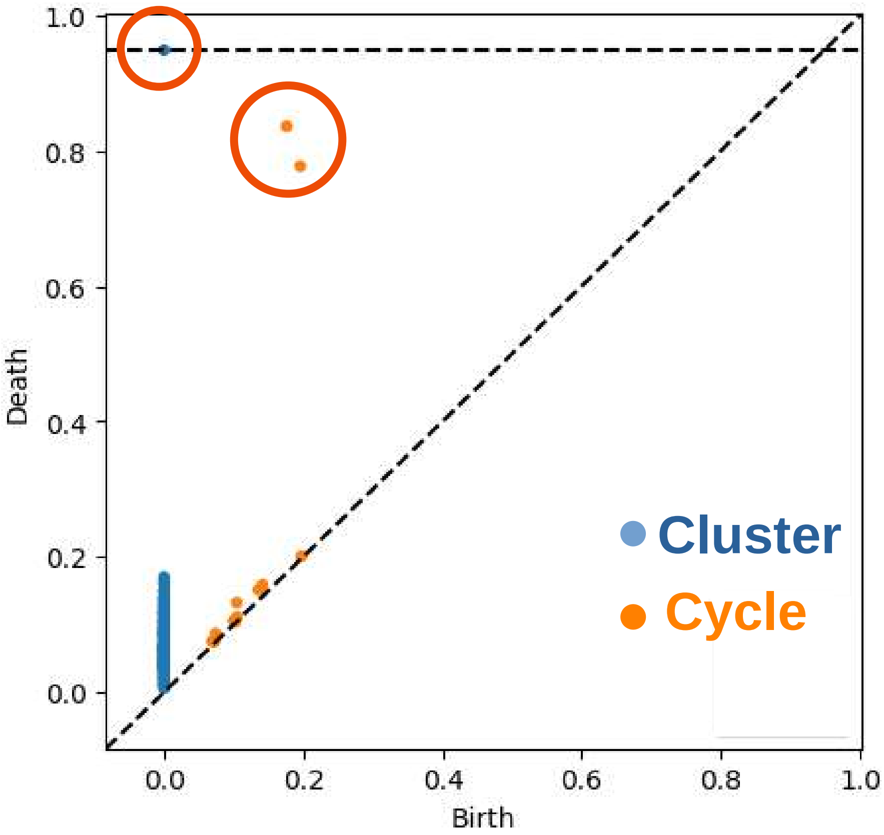




Persistence diagrams: examples

High persistence features: single cluster forming two loops





Applications of persistent homology to physics

- Detecting phase transitions
- Classifying quantum entanglement
- Characterising nonlinear dynamics

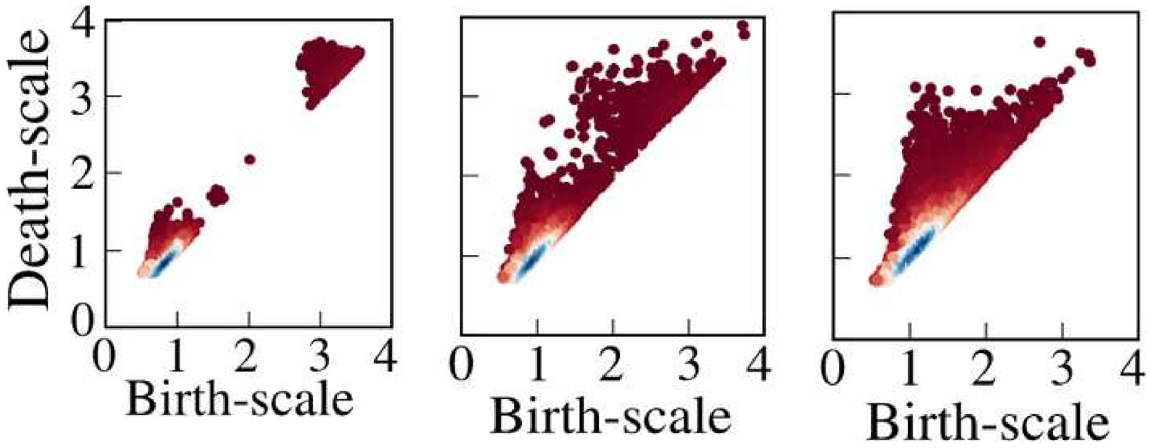
Phys. Rev. Research 2, 043308 (2020)
Phys. Rev. B 104, 104426 (2021)

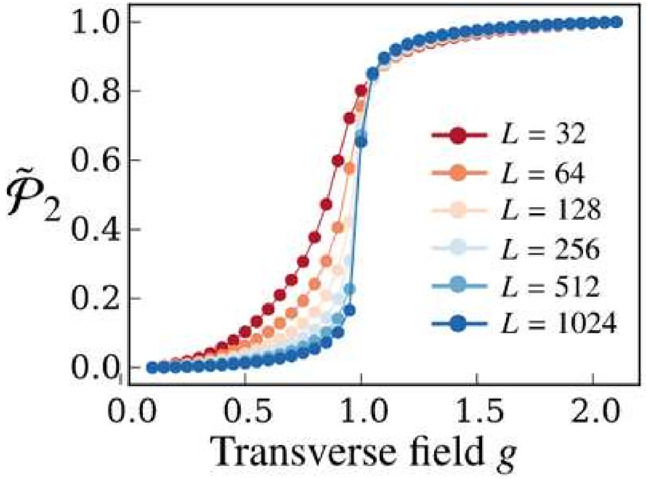
Quantum Inf. Comput. 20, 0375 (2020)

SciPost Phys. 11, 060 (2021)

$$\mathcal{P}_p(D) = \left[\sum_{(b,d) \in D} |d - b|^p \right]^{1/p}$$

Root mean square feature lifetime

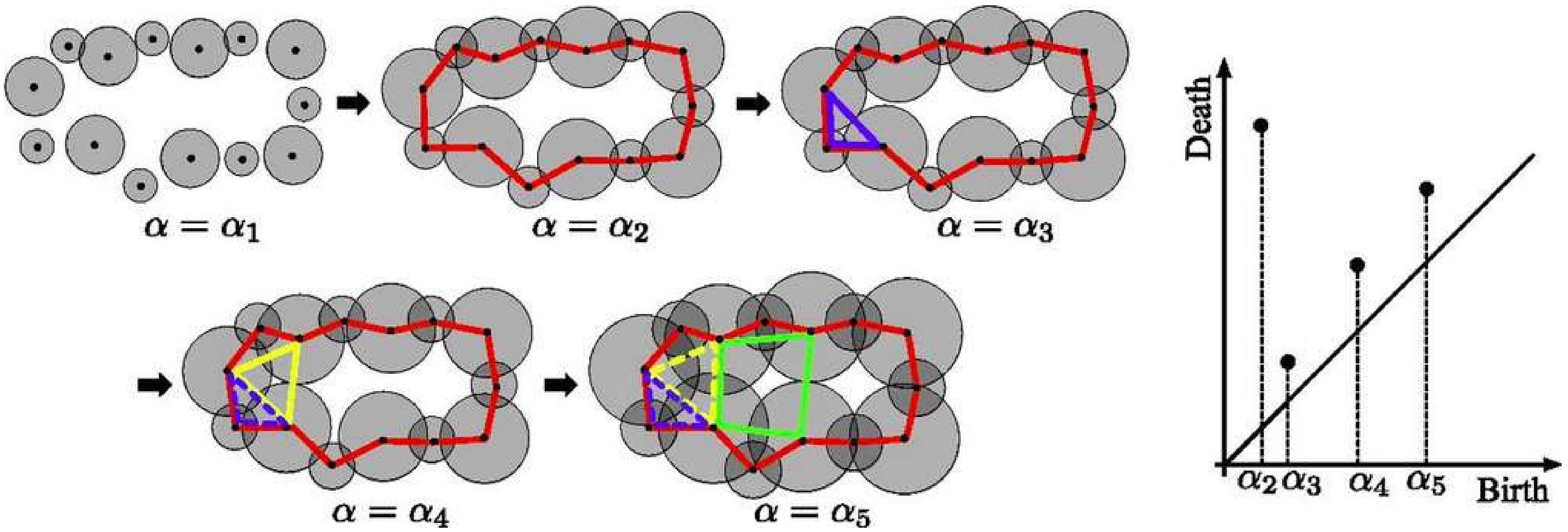




Tran, Chen, and Hasegawa, Phys. Rev. E 103, 052127 (2021)

Characterising amorphous materials

- Data obtained from molecular dynamics simulations
- TDA Inputs: atomic positions in 3D space, Euclidean metric
- Persistence diagrams reveal hidden glassy short range order

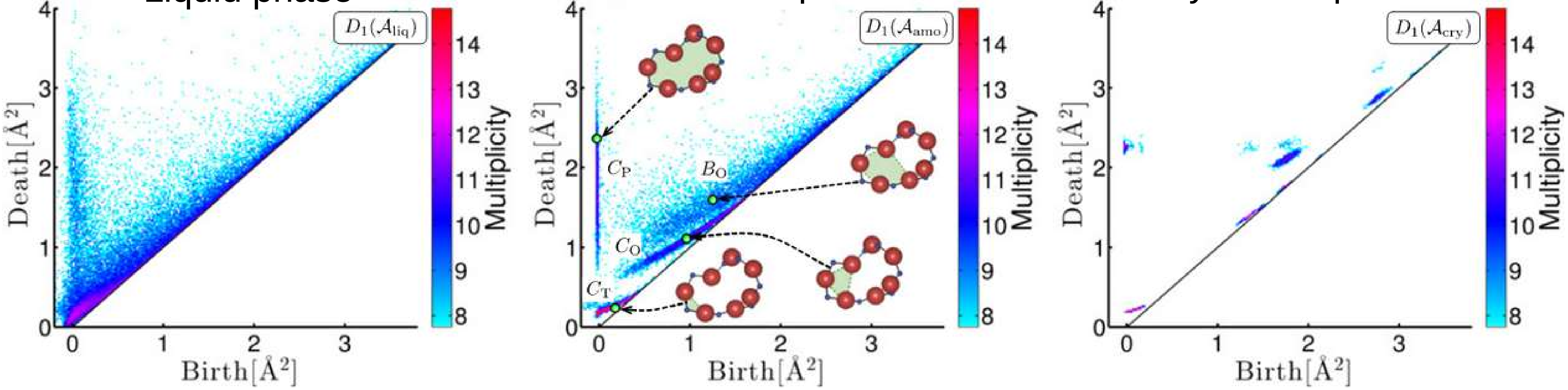


T. Nakamura et al., Nanotechnology 26, 3040001 (2015); Y. Hiraoka et al., PNAS 113, 7035 (2016)

Characterising amorphous materials

- Data obtained from molecular dynamics simulations
- TDA Inputs: atomic positions in 3D space, Euclidean metric
- Persistence diagrams reveal hidden glassy short range order

Liquid phase | Glass phase | Crystalline phase



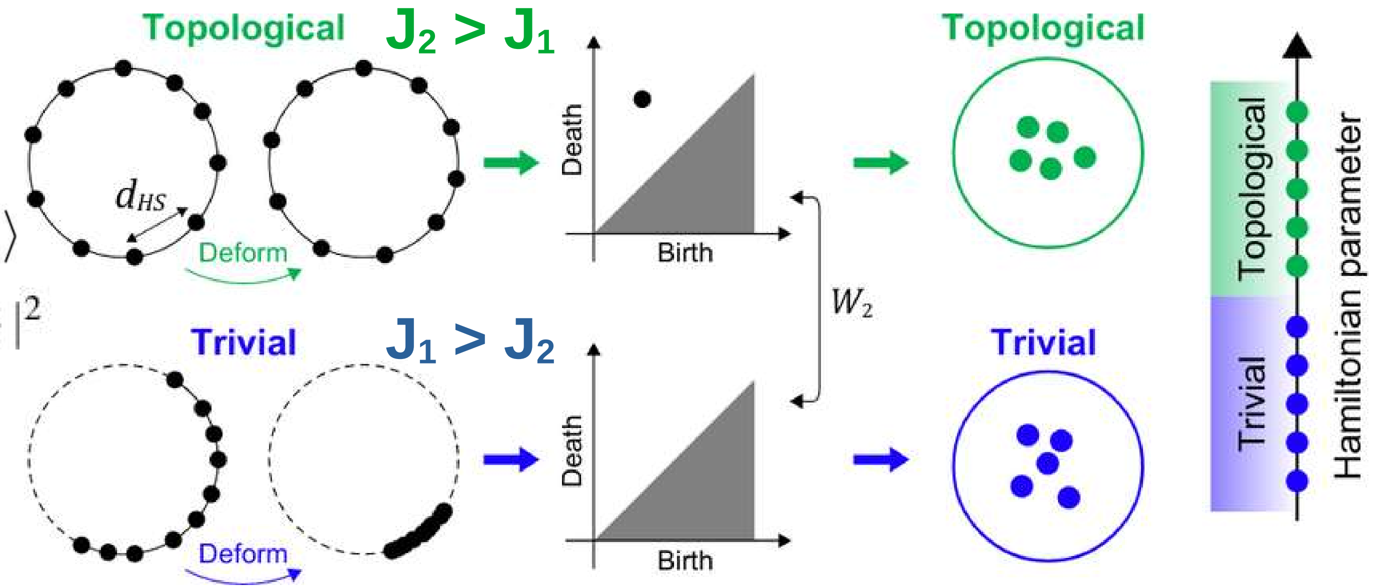
T. Nakamura et al., Nanotechnology 26, 3040001 (2015); Y. Hiraoka et al., PNAS 113, 7035 (2016)

Shape of Fermi levels and Bloch functions

- Quantum distance: distance measure for Bloch functions
- Persistent homology identifies Bloch function clusters and loops
- Applied to unsupervised learning of topological phase diagrams

$$\hat{H}(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = \omega_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$$

$$d^2(\boldsymbol{k},\boldsymbol{k}') = 1 - |\langle u_n(\boldsymbol{k})|u_n(\boldsymbol{k}')\rangle|^2$$

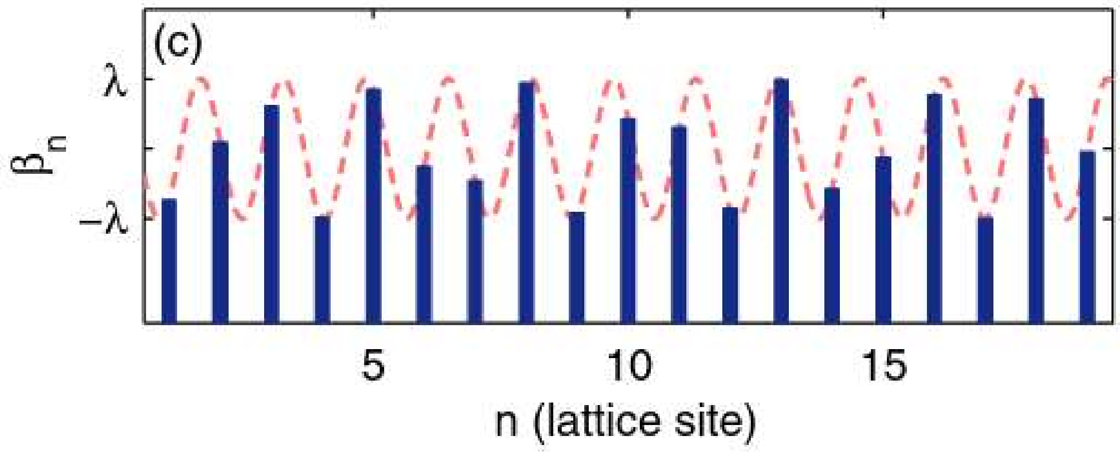


Leykam & Angelakis, APL Photonics 6, 030802 (2021); Park, Hwang, & Yang, Phys. Rev. B 105, 195115 (2022)

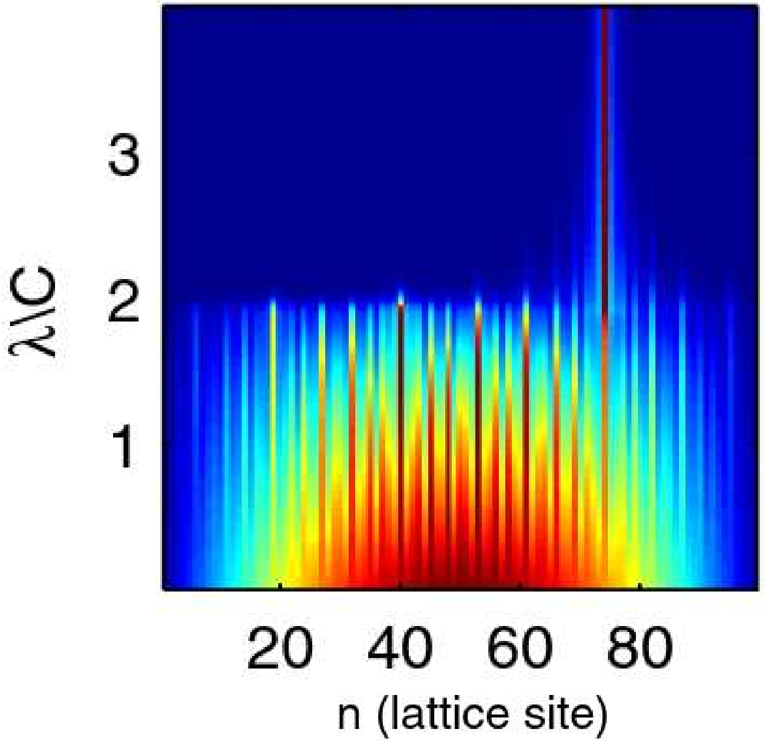
Aubry-Andre-Harper model

$$i\frac{\partial \psi_n}{\partial t}+[\beta_0+\lambda\cos(2\pi n\chi)]\psi_n+C(\psi_{n-1}+\psi_{n+1})=0,$$

Transition from extended to localized eigenstates at $\lambda/C = 2$



Ground state intensity



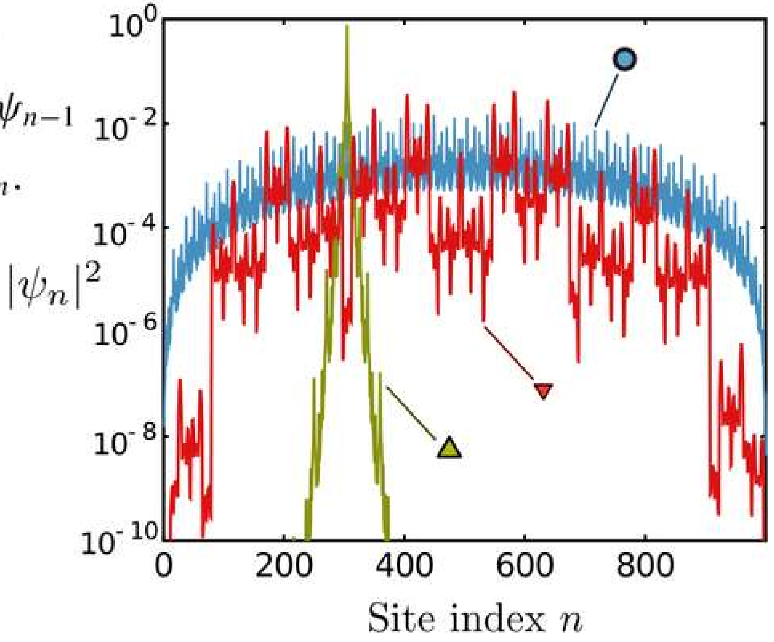
Harper, Proc. Phys. Soc. London A 68, 874 (1955)
Aubry & Andre, Ann. Israel Phys. Soc. 3, 133 (1980)
Lahini et al., Phys. Rev. Lett. 103, 013901 (2009)

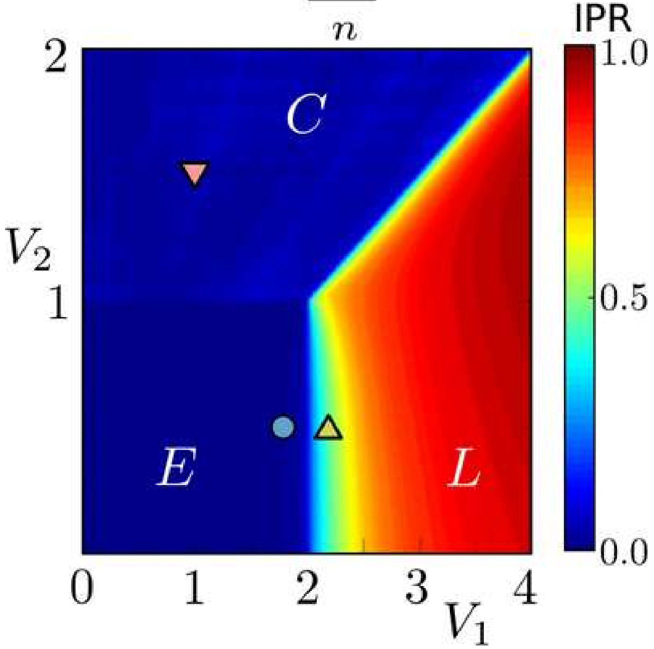
Generalized Aubry-Andre-Harper model

- Hosts critical phase (C) with fractal eigenstates
- Difficult to distinguish extended, critical phases using IPR

$$\mathrm{IPR} = \sum_n |\phi_n|^4$$

$$\left\{t + V_2 \cos\left[\left(n + \tfrac{1}{2}\right) Q + k\right]\right\} \psi_{n+1} + \left\{t + V_2 \cos\left[\left(n - \tfrac{1}{2}\right) Q + k\right]\right\} \psi_{n-1} + V_1 \cos(nQ + k + \phi)\psi_n = E\psi_n .$$





F. Liu, S. Ghosh, and Y. D.Chong, Phys. Rev. B 91, 014108 (2015)

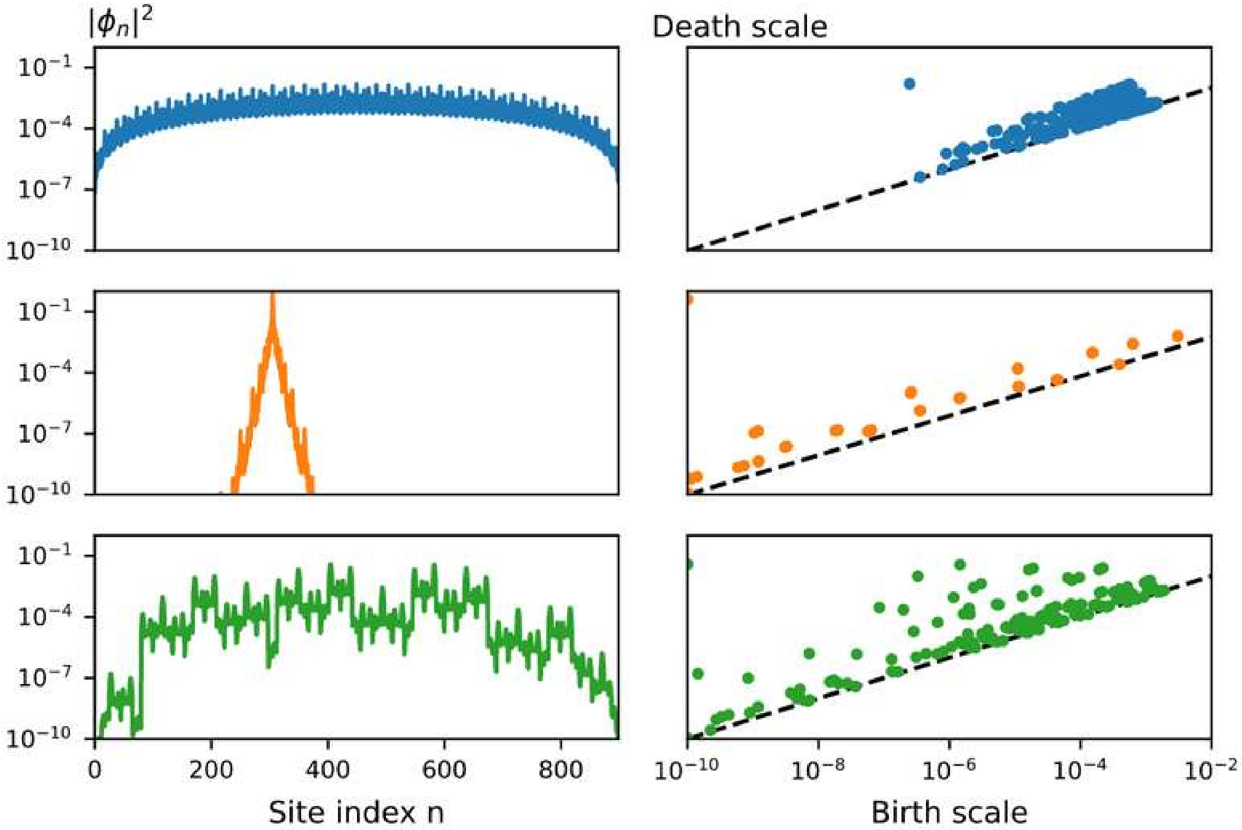
Persistent homology of AAH eigenstates

Ground states have different structure of local maxima, minima

Extended phase

Localized phase

Critical phase

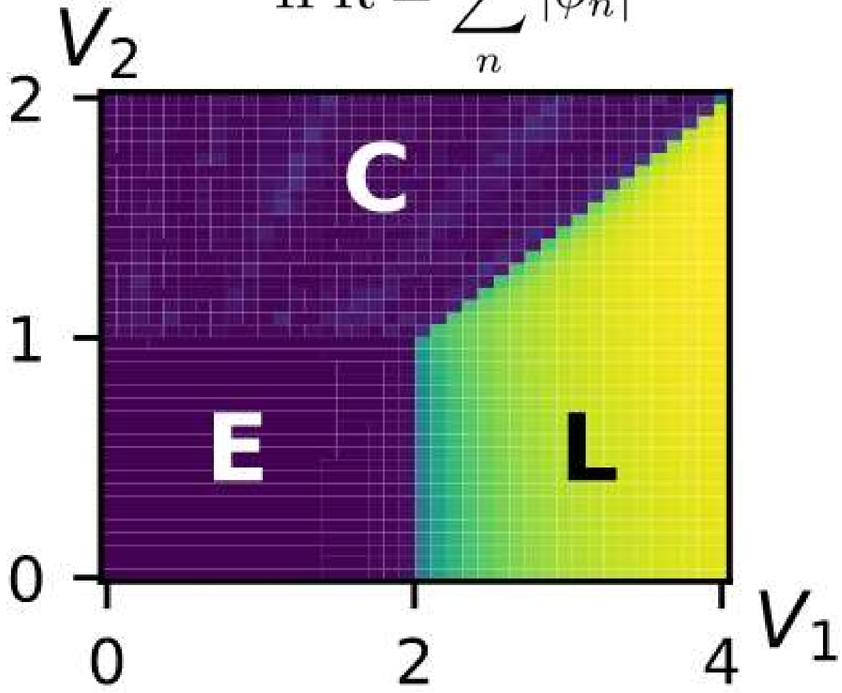


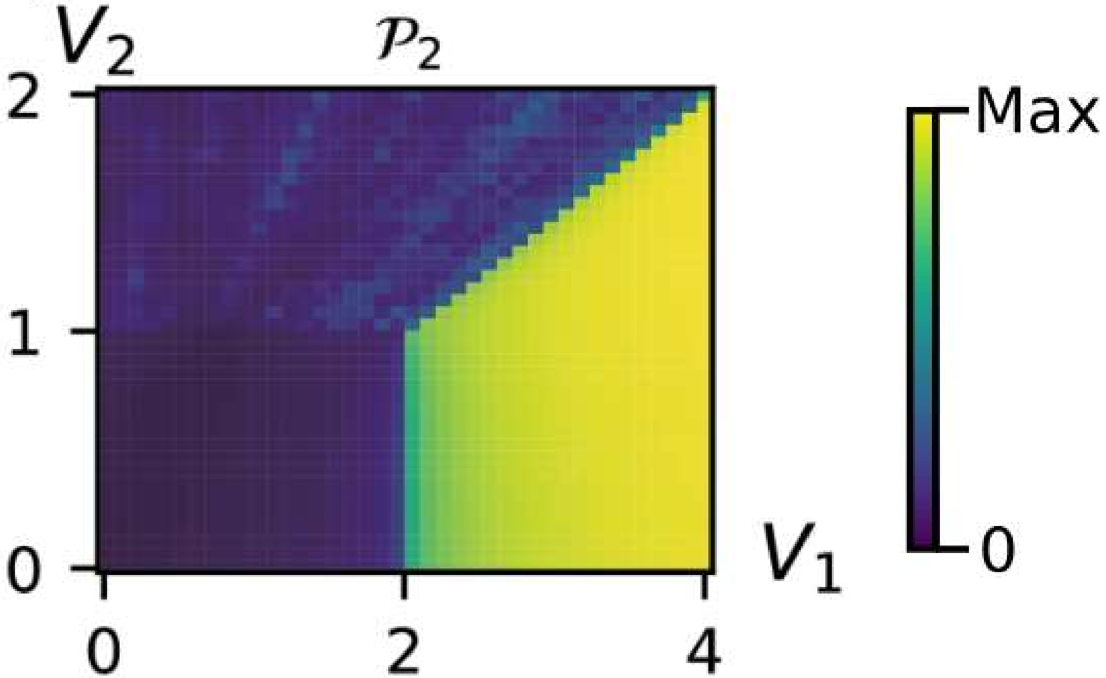
Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

Phase diagrams: Standard measures vs TDA

Persistence diagram norm: $\mathcal{P}_p(D) = \left(\sum_{(b,d)\in D} |d-b|^p \right)^{1/p}$

$\mathrm{IPR} = \sum_n |\phi_n|^4$



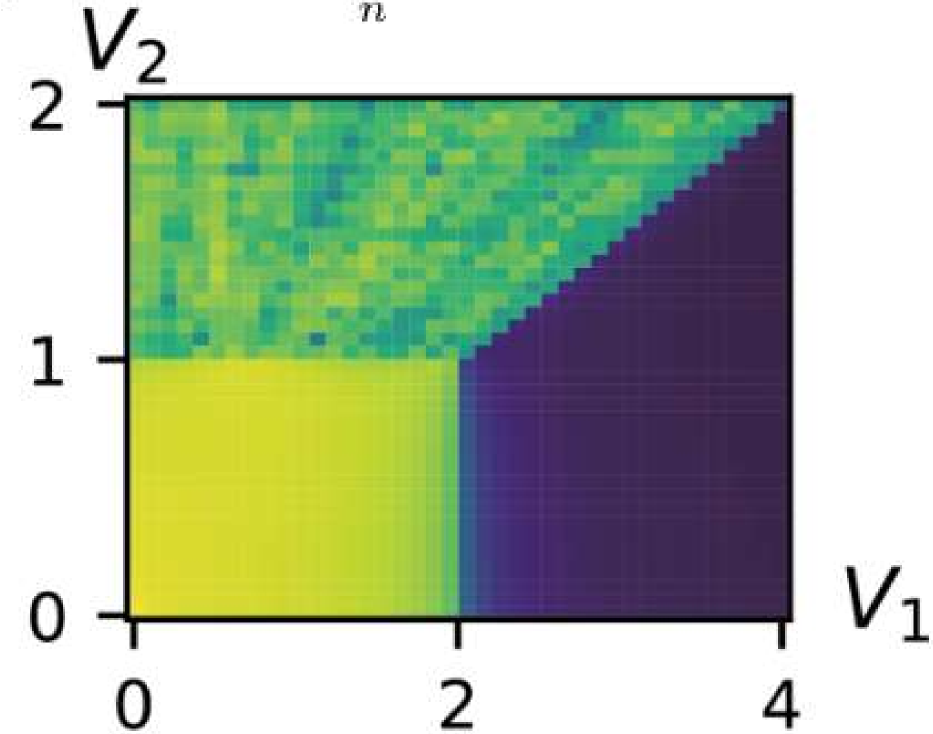


Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

Phase diagrams: Standard measures vs TDA

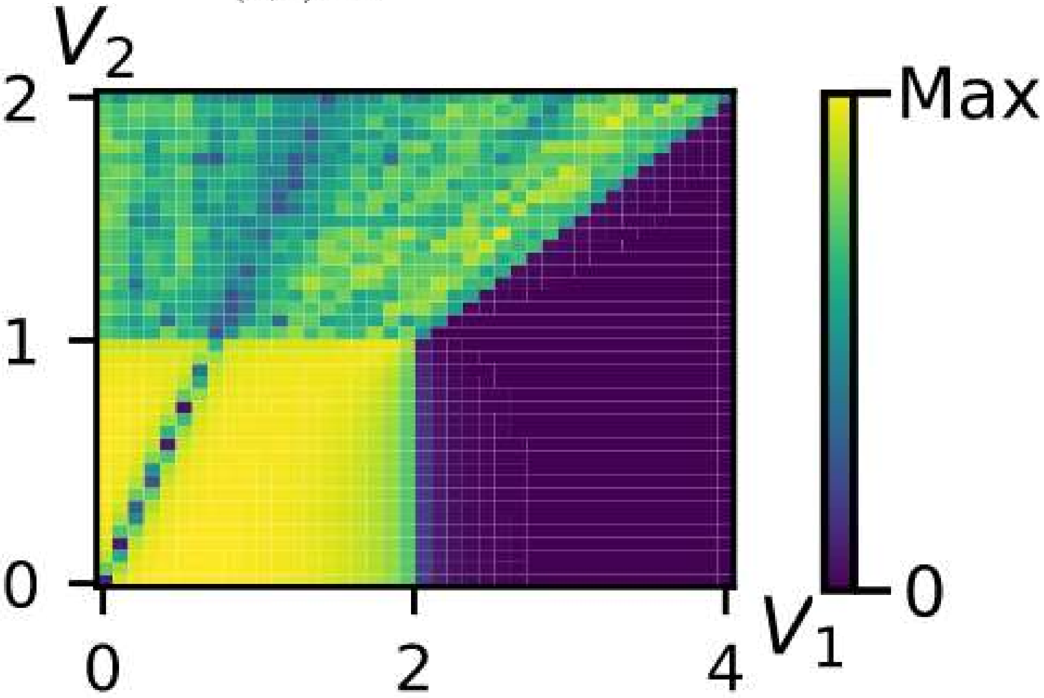
Eigenstate entropy

$$S = -\sum_n |\phi_n|^2 \ln |\phi_n|^2$$



Persistence diagram entropy

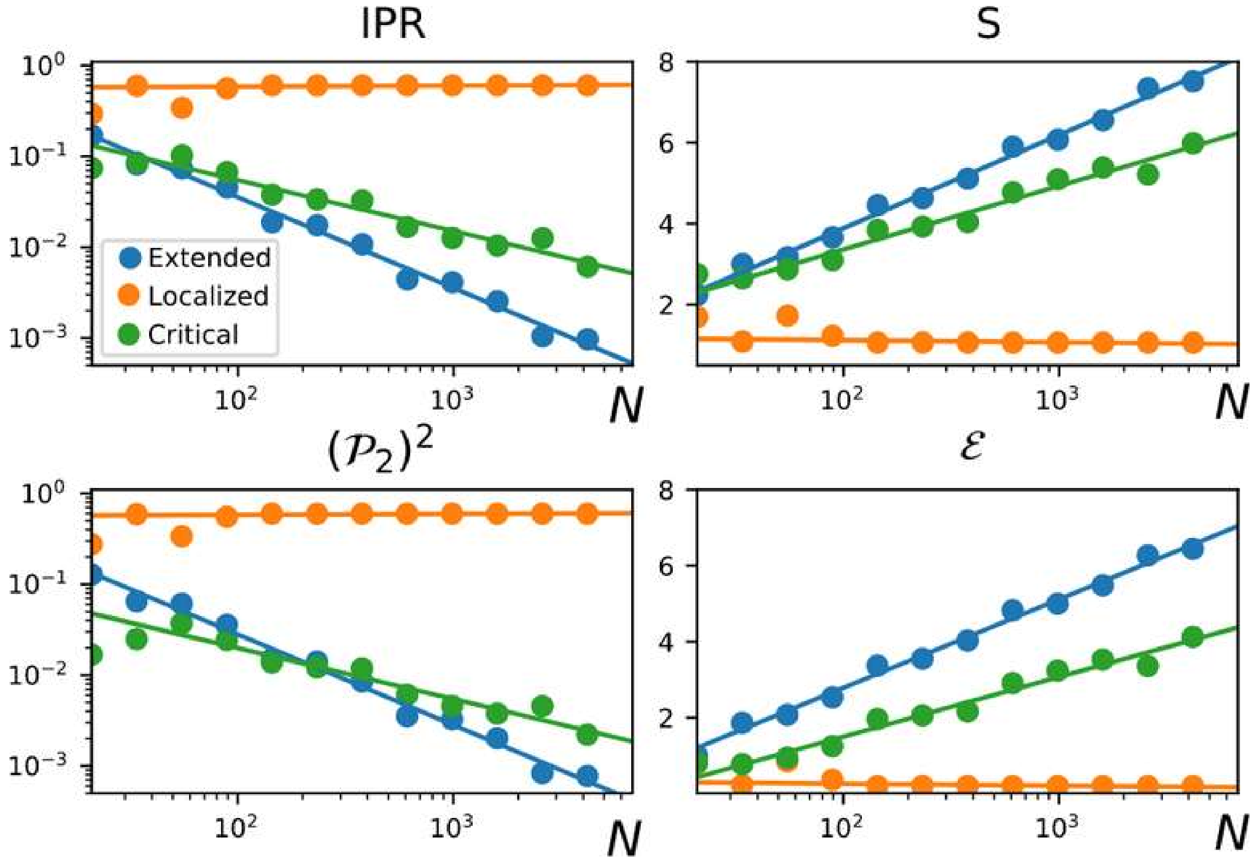
$$\mathcal{E}(D) = - \sum_{(b,d)\in D} \frac{|d-b|}{\mathcal{S}(D)} \log\left(\frac{|d-b|}{\mathcal{S}(D)}\right),$$



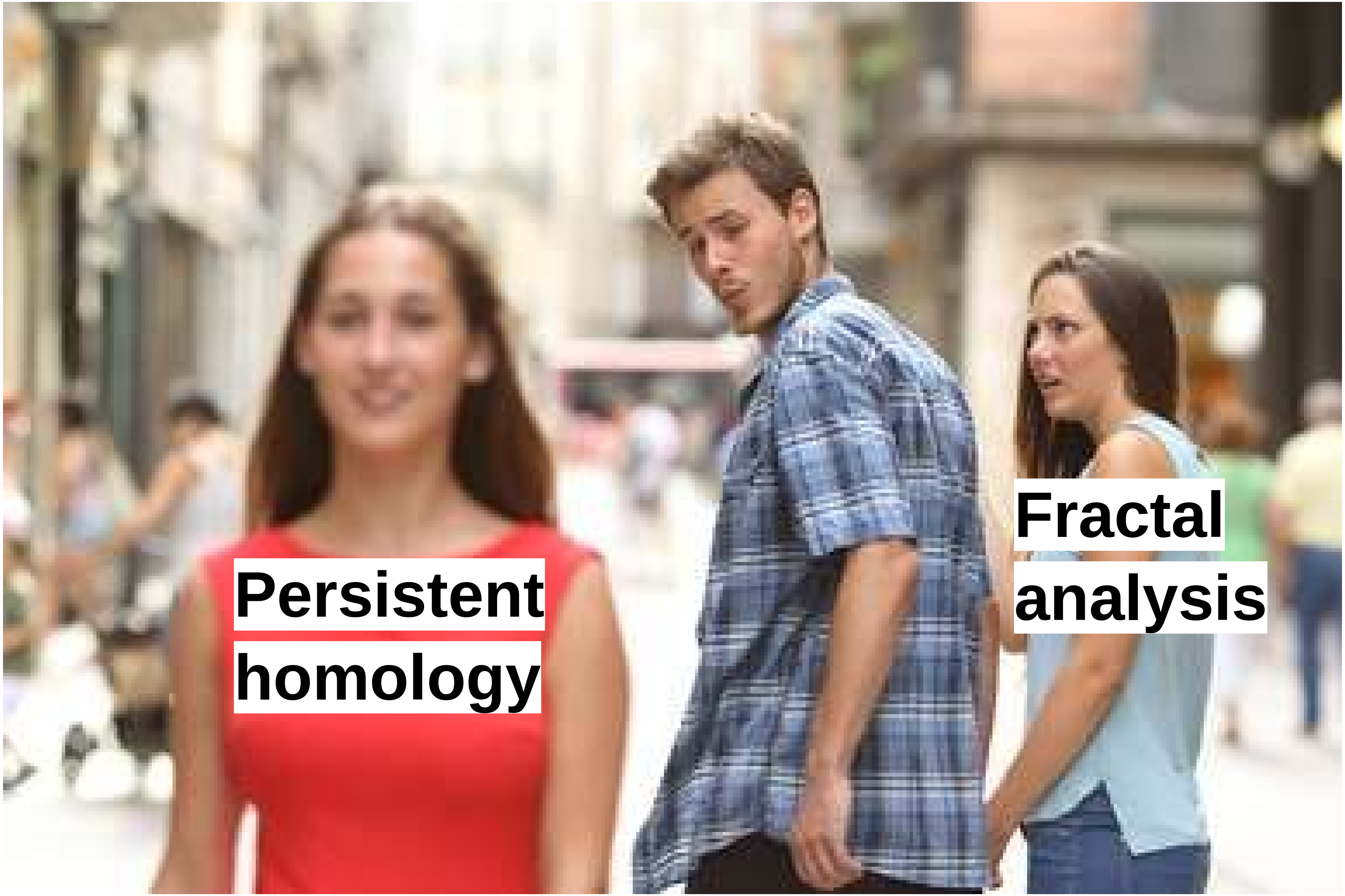
Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

Fractal analysis

Persistent homology reproduces correct fractal dimensions



Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)


Persistent homology
Fractal analysis

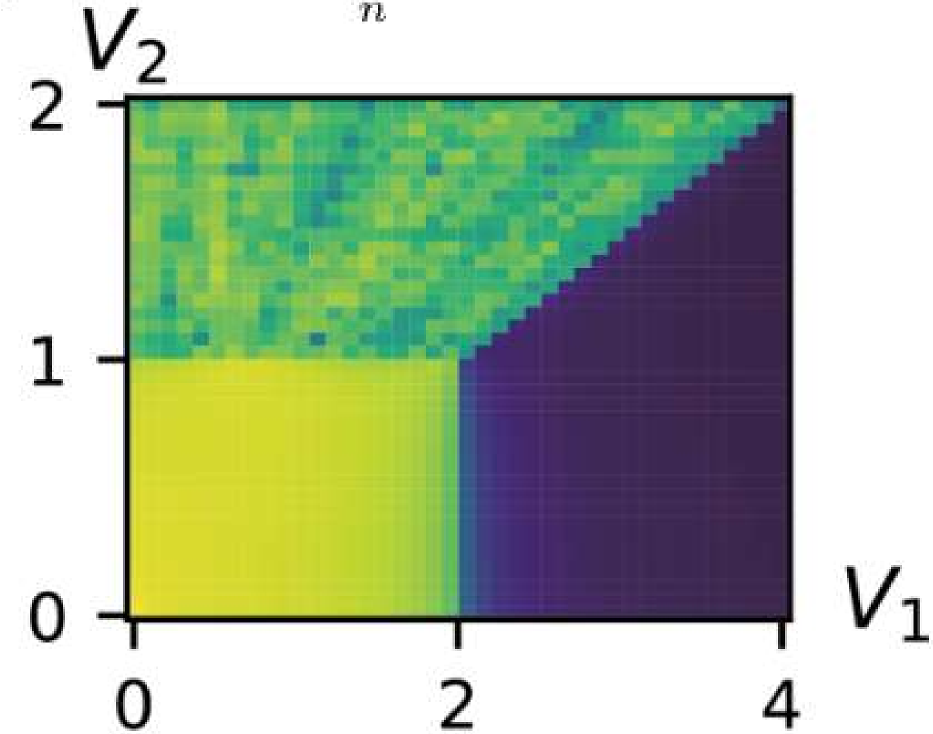
Phase diagrams: Standard measures vs TDA

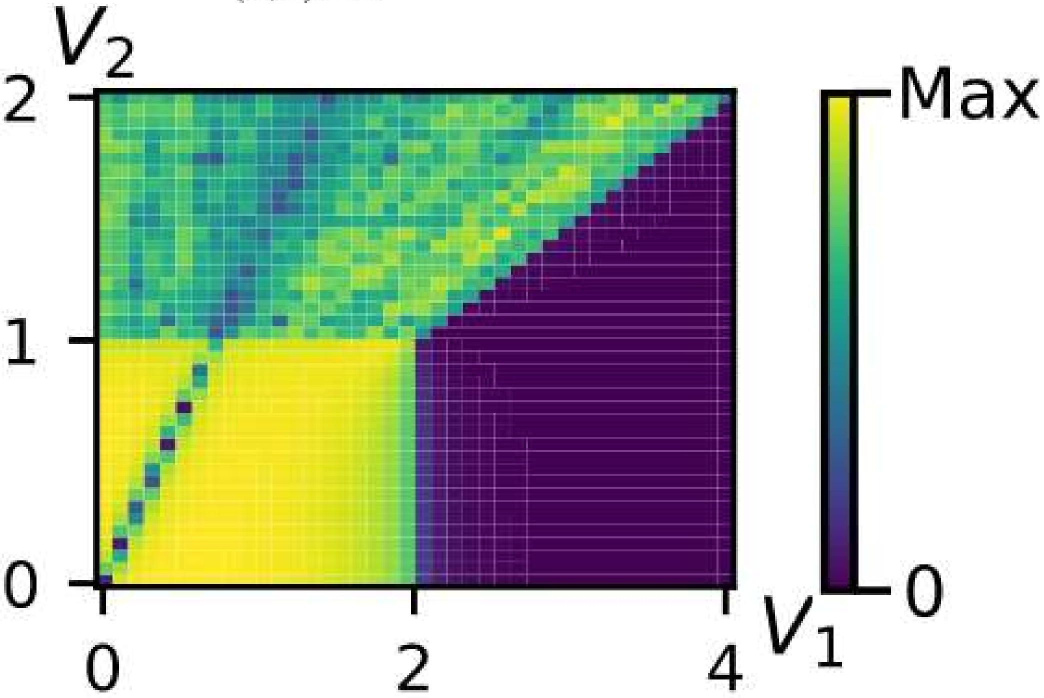
Eigenstate entropy

$$S = -\sum_n |\phi_n|^2 \ln |\phi_n|^2$$

Persistence diagram entropy

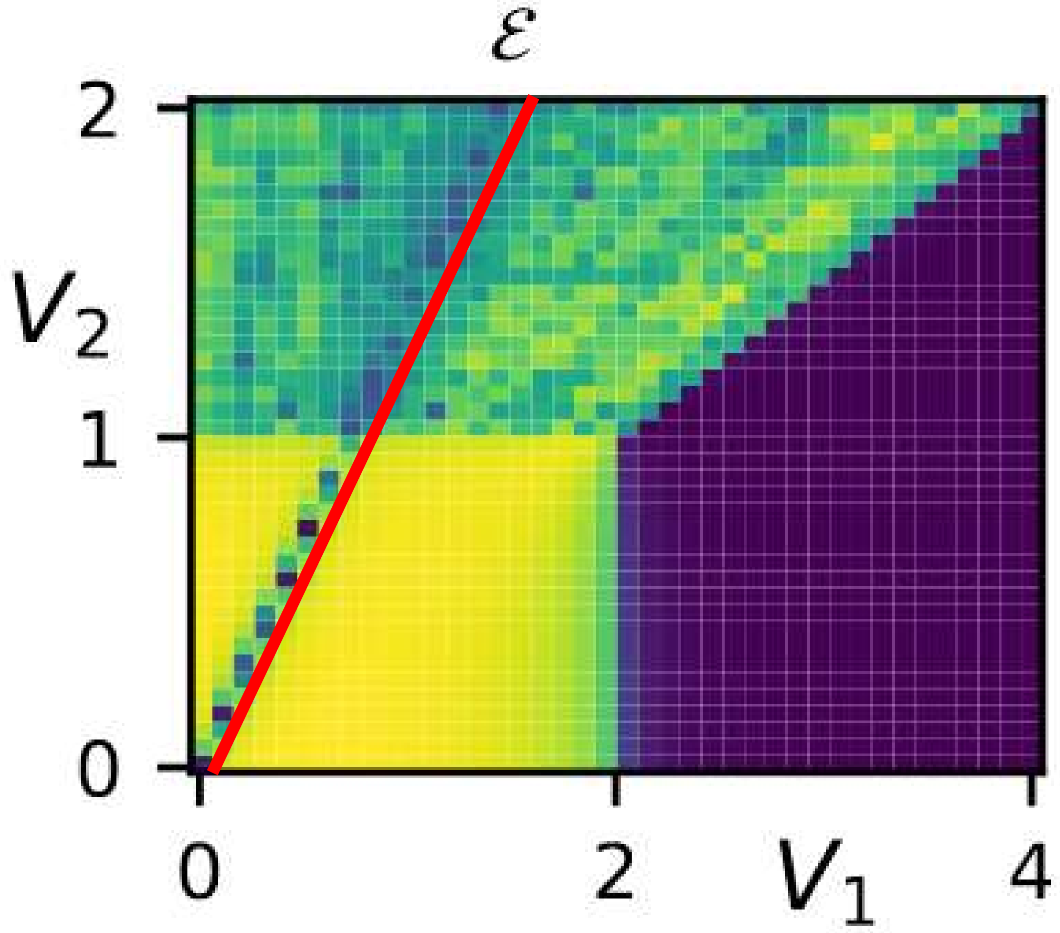
$$\mathcal{E}(D) = -\sum_{(b,d)\in D} \frac{|d-b|}{\mathcal{S}(D)} \log\left(\frac{|d-b|}{\mathcal{S}(D)}\right),$$





Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

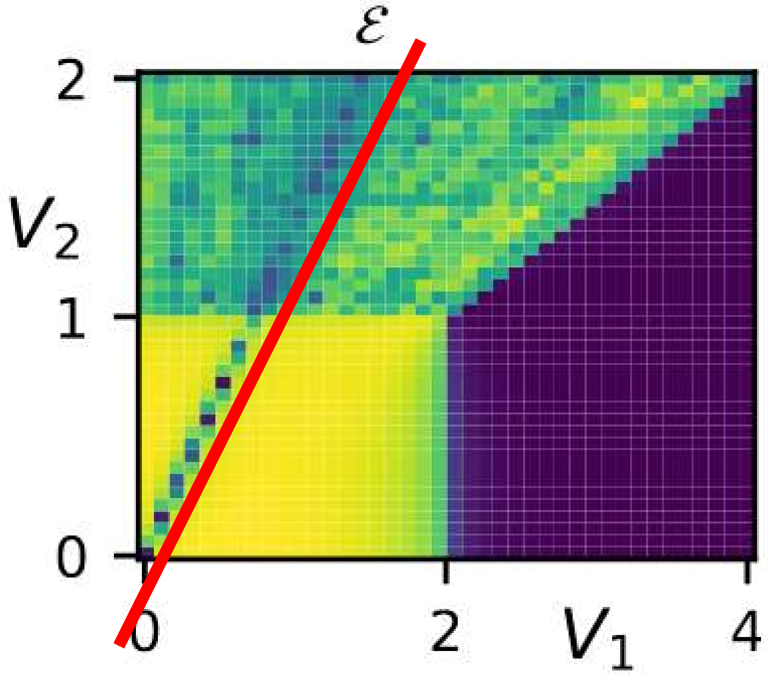
Persistent entropy detects an anomaly!

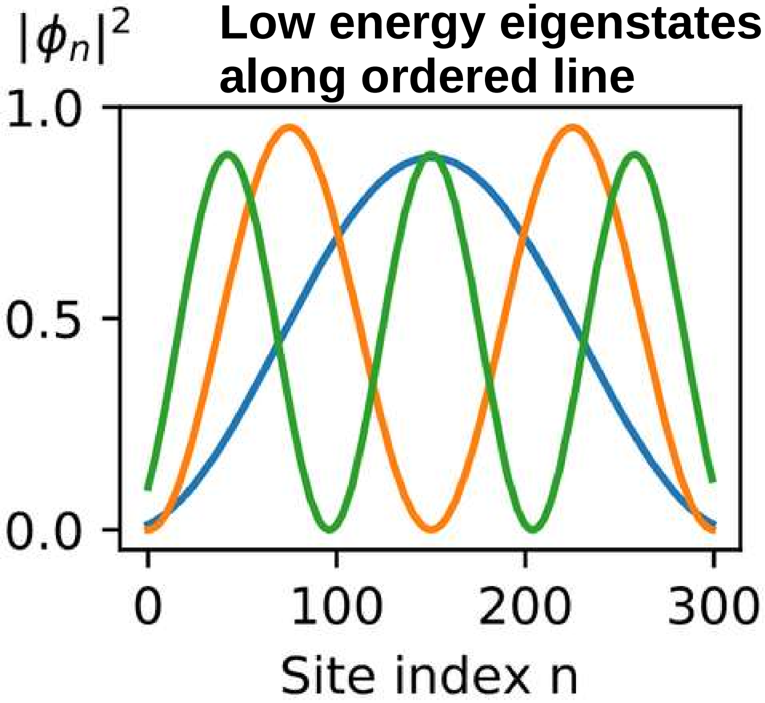


Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

Persistent entropy detects an anomaly!

- Potential transparent to low energy wavepackets if $V_1 = 2V_2 \cos(Q/2)$
- Standard measures do not distinguish between order and disorder





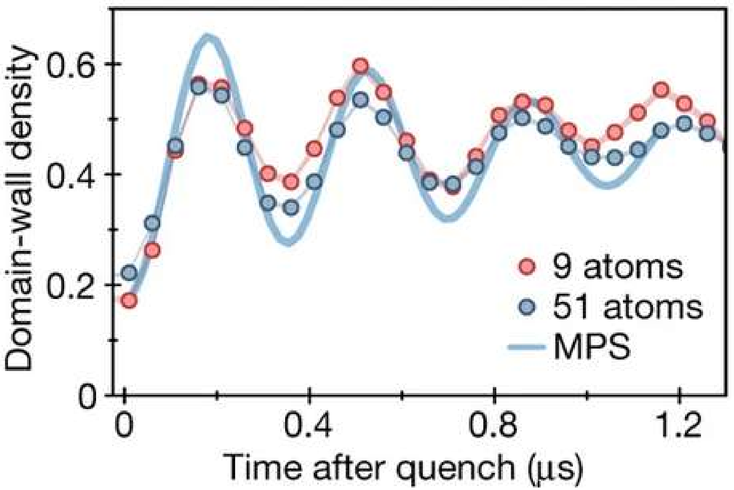
Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

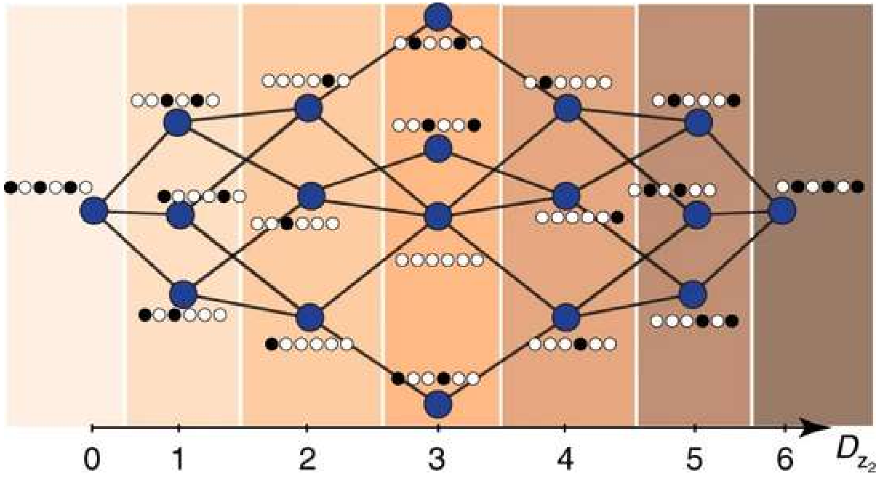
- Our results show how **topological data analysis** and **persistent homology** can **uncover novel features** of complicated quantum systems
- After the “ordered line” was **discovered numerically** using persistent homology, **we obtained an analytical explanation** by re-examining the tight binding Hamiltonian
- Persistent homology gives a **new tool** for theoretical analysis and **model building**

Y. He, S. Xia, D. G. Angelakis, D. Song, Z. Chen, D. Leykam, Phys. Rev. B 106, 054210 (2022)

Outlook: Many-body quantum dynamics

- Many-body quantum dynamics ~ high-dimensional Fock state graph
- Persistent oscillations due to “quantum scars”
- Can TDA characterise the “shape” of many-body quantum dynamics?





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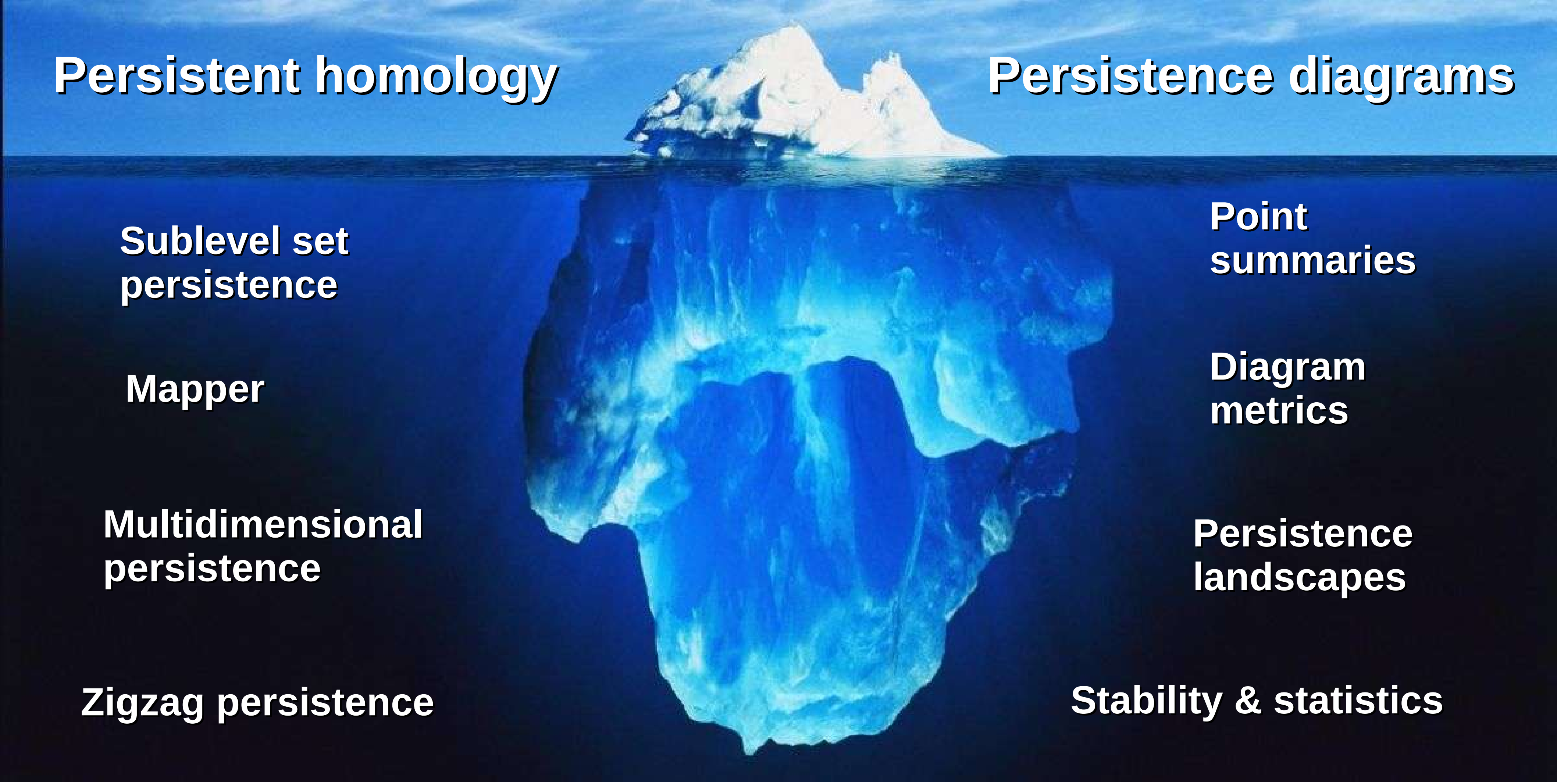

Reviews: Murugan & Robertson, arXiv:1904.11044; Carlsson, Nature Rev. Phys. 2, 697 (2020)
Leykam & Angelakis, arXiv:2206.15075

Summary

- Topological Data Analysis: promising techniques for physics
- Reveals scale-dependent topological features of complex systems

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Reviews

J. Murugan and D. Robertson, arXiv:1904.11044

G. Carlsson, Nature Rev. Phys. 2, 697 (2020)

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