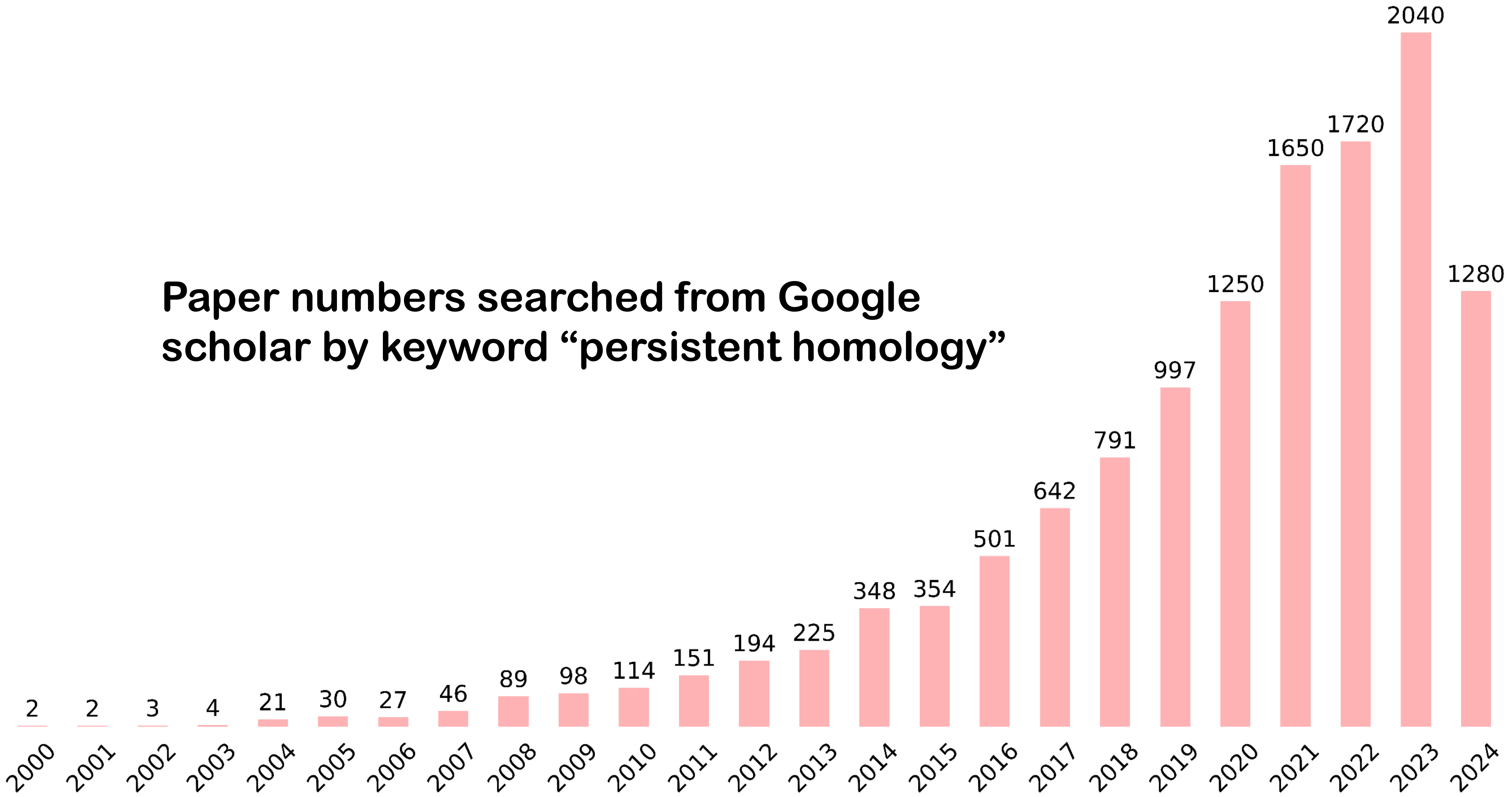
Persistent Homology: an overview

Xiang Liu

BIMSA

August 2, 2024

Persistent Homology



Paper numbers searched from Google scholar by keyword "persistent homology"

Size Function (0-D persistent homology)

DOI: 10.1017/S0004972700028574 • Corpus ID: 121731439

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A distance for similarity classes of submanifolds of a Euclidean space

Patrizio Frosini • Published in Bulletin of the Australian... 1 December 1990 • Mathematics

A distance is defined on the quotient of the set of submanifolds of a Euclidean space, with respect to similarity. It is then related to a previously defined function which captures the metric behaviour of paths. Collapse

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Size theory as a topological tool for computer vision

Patrizio Frosini, C. Landi • Published 1999 • Computer Science, Mathematics

TLDR The usefulness of such a theory in comparing shapes is high lighted by showing some examples and the robustness of Size Theory with respect to noise and occlusions is pointed out.

Abstract In this paper we give an outline of Size Theory and its main results The usefulness of such a theory in comparing shapes is high lighted by showing some examples The robustness of Size Theory with respect to noise and occlusions is pointed out In addition an algebraic approach to the theory is presented

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Home > Acta Applicandae Mathematica > Article

Size Functions from a Categorical Viewpoint

Published: July 2001

Volume 67, pages 225–235, (2001) Cite this article

Acta Applicandae Mathematica

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Persistent Homology

Topology Proceedings
Volume 24, Summer 1999, 503–532

1999

TOWARDS COMPUTING HOMOLOGY FROM FINITE APPROXIMATIONS

V. Robins

Abstract

We consider the problem of extrapolating the homology of a compact metric space from a finite point-set approximation. Our approach is based on inverse systems of ϵ-neighborhoods and inclusion maps. We show that the inclusion maps are necessary to identify topological features in an ϵ-neighborhood that persist in the limit as $\epsilon \to 0$. We outline a possible algorithm for computer implementation. As test examples, we present data for some iterated function system relatives of the Sierpinski triangle.

Computing Persistent Homology*

2004

Afra Zomorodian[1] and Gunnar Carlsson[2]

[1]Department of Computer Science, Stanford University,
Stanford, CA 94305, USA
afra@cs.stanford.edu

[2]Department of Mathematics, Stanford University,
Stanford, CA 94305, USA
gunnar@math.stanford.edu

Abstract. We show that the persistent homology of a filtered d-dimensional simplicial complex is simply the standard homology of a particular graded module over a polynomial ring. Our analysis establishes the existence of a simple description of persistent homology groups over arbitrary fields. It also enables us to derive a natural algorithm for computing persistent homology of spaces in arbitrary dimension over any field. This result generalizes and extends the previously known algorithm that was restricted to subcomplexes of $\mathbb{S}^3$ and $\mathbb{Z}_2$ coefficients. Finally, our study implies the lack of a simple classification over non-fields. Instead, we give an algorithm for computing individual persistent homology groups over an arbitrary principal ideal domain in any dimension.

Home > Browse by Title > Proceedings > FOCS '00 > Topological persistence and simplification

2000

ARTICLE

Topological persistence and simplification

Authors: H. Edelsbrunner, D. Letscher, and A. Zomorodian | Authors Info & Claims

FOCS '00: Proceedings of the 41st Annual Symposium on Foundations of Computer Science • November 2000 • Page 454

Published: 12 November 2000 Publication History

63 0

Publisher Site

Home > Conferences > SOCG > Proceedings > SCG '93 > An incremental algorithm for Betti numbers of simplicial complexes

1993

ARTICLE | FREE ACCESS

An incremental algorithm for Betti numbers of simplicial complexes

Authors: Cecil Jose A. Delfinado and Herbert Edelsbrunner | Authors Info & Claims

SCG '93: Proceedings of the ninth annual symposium on Computational geometry • July 1993 • Pages 232 - 239
https://doi.org/10.1145/160985.161140

Published: 01 July 1993 Publication History   Check for updates

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Home > Conferences > SGP > Proceedings > SGP '04 > Persistence barcodes for shapes

2004

ARTICLE

Persistence barcodes for shapes

Authors: Gunnar Carlsson, Afra Zomorodian, Anne Collins, and Leonidas Guibas | Authors Info & Claims

SGP '04: Proceedings of the 2004 Eurographics/ACM SIGGRAPH symposium on Geometry processing • July 2004 • Pages 124 - 135
https://doi.org/10.1145/1057432.1057449

Published: 08 July 2004 Publication History   Check for updates

57 778

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Topological Data Analysis

Topological Invariant:

Homology Group

Homotopy Group

Cohomology Ring

Steenrod Module

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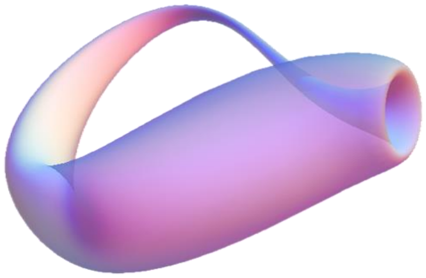


Klein bottle

Sphere

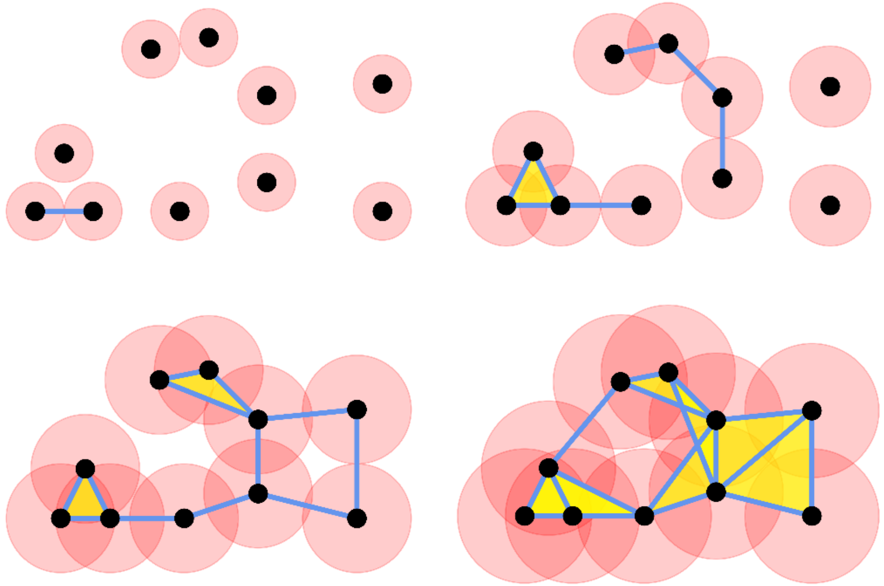
Torus

Double Torus

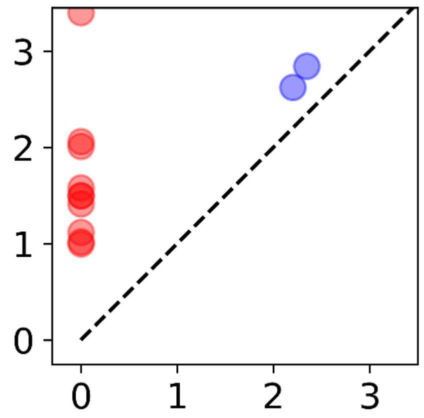
Knot

Möbius Strip

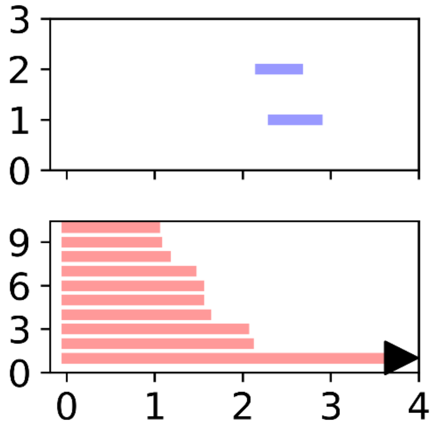
Persistent Homology



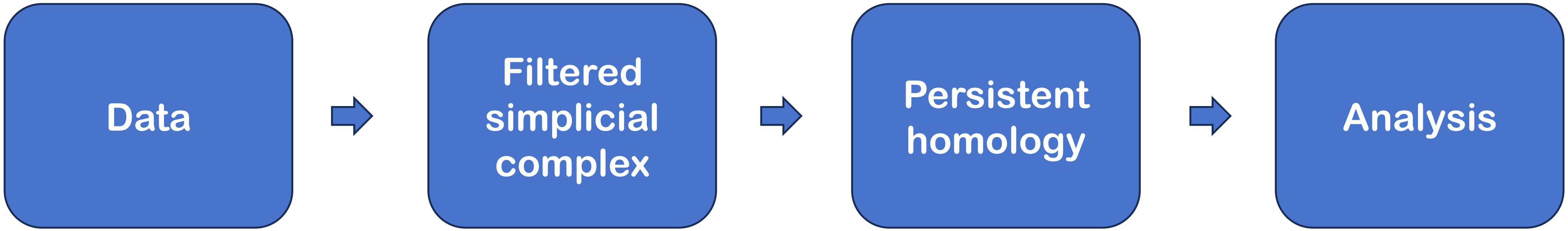
Persistent Diagram



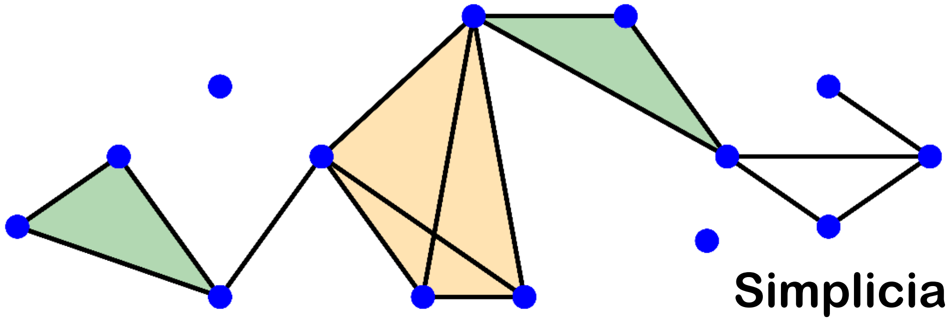
Persistent Barcode



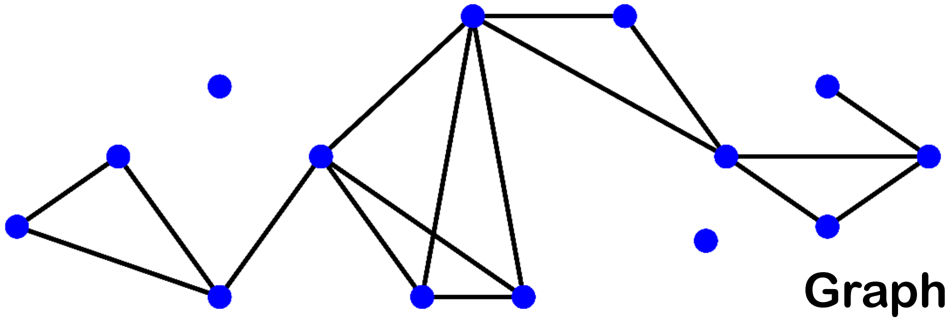
Basic workflow in TDA



Simplicial Complex



Simplicial complex



Graph

Perspective | Published: 04 October 2021

The physics of higher-order interactions in complex systems

Federico Battiston, Enrico Amico, Alain Barrat, Ginestra Bianconi, Guilherme Ferraz de Arruda, Benedetta Franceschiello, Iacopo Iacopini, Sonia Kéfi, Vito Latora, Yamir Moreno, Micah M. Murray, Tiago P. Peixoto, Francesco Vaccarino & Giovanni Petri

Nature Physics 17, 1093–1098 (2021) | Cite this article

Abstract

Complex networks have become the main paradigm for modelling the dynamics of interacting systems. However, networks are intrinsically limited to describing pairwise interactions, whereas real-world systems are often characterized by higher-order interactions involving groups of three or more units. Higher-order structures, such as hypergraphs and simplicial complexes, are therefore a better tool to map the real organization of many social, biological and man-made systems. Here, we highlight recent evidence of collective behaviours induced by higher-order interactions, and we outline three key challenges for the physics of higher-order systems.

Article | Open access | Published: 23 March 2023

Higher-order interactions shape collective dynamics differently in hypergraphs and simplicial complexes

Yuanzhao Zhang, Maxime Lucas & Federico Battiston

Nature Communications 14, Article number: 1605 (2023) | Cite this article

Abstract

Higher-order networks have emerged as a powerful framework to model complex systems and their collective behavior. Going beyond pairwise interactions, they encode structured relations among arbitrary numbers of units through representations such as simplicial complexes and hypergraphs. So far, the choice between simplicial complexes and hypergraphs has often been motivated by technical convenience. Here, using synchronization as an example, we demonstrate that the effects of higher-order interactions are highly representation-dependent. In particular, higher-order interactions typically enhance synchronization in hypergraphs but have the opposite effect in simplicial complexes. We provide theoretical insight by linking the synchronizability of different

Article | Open access | Published: 18 June 2024

Reconstructing higher-order interactions in coupled dynamical systems

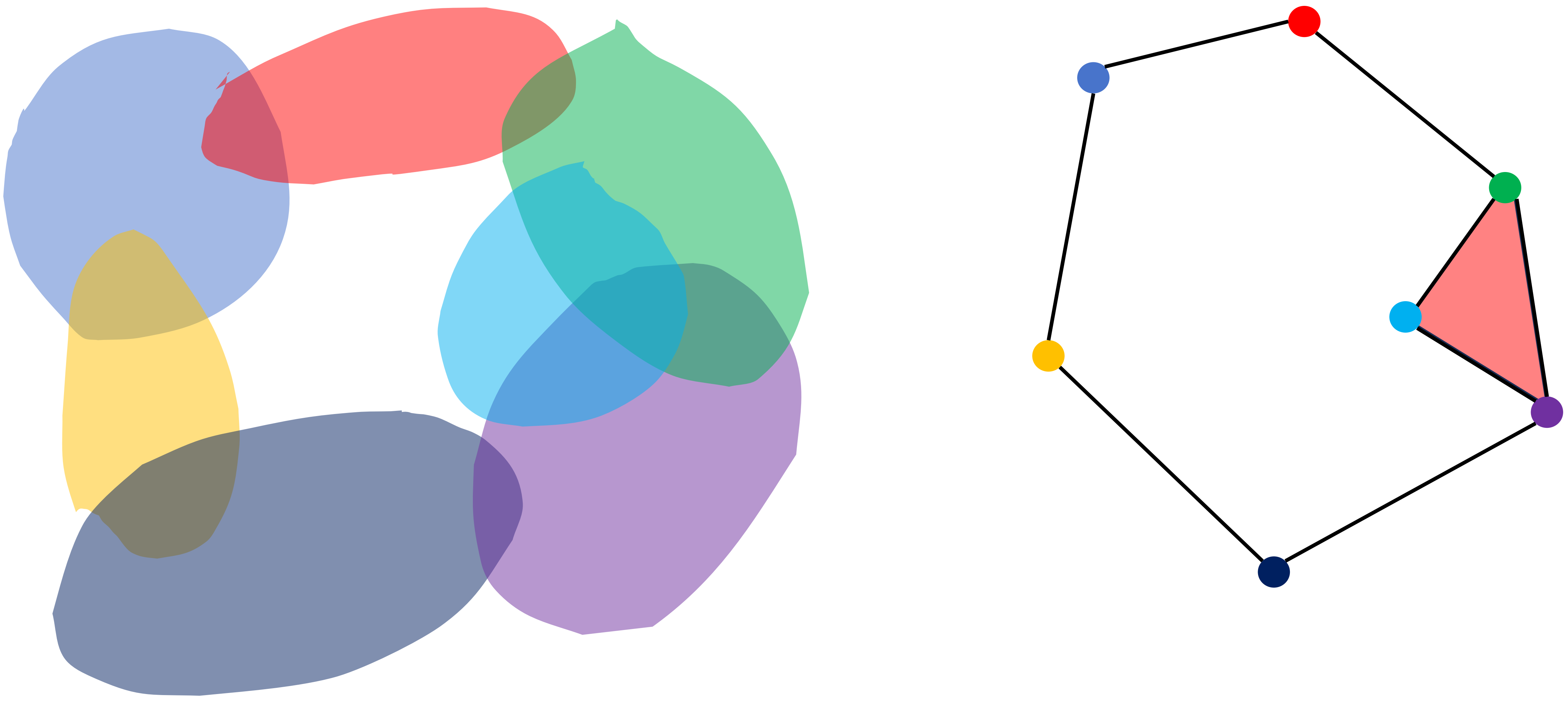
Federico Malizia, Alessandra Corso, Lucia Valentina Gambuzza, Giovanni Russo, Vito Latora & Mattia Frasc

Nature Communications 15, Article number: 5184 (2024) | Cite this article

Abstract

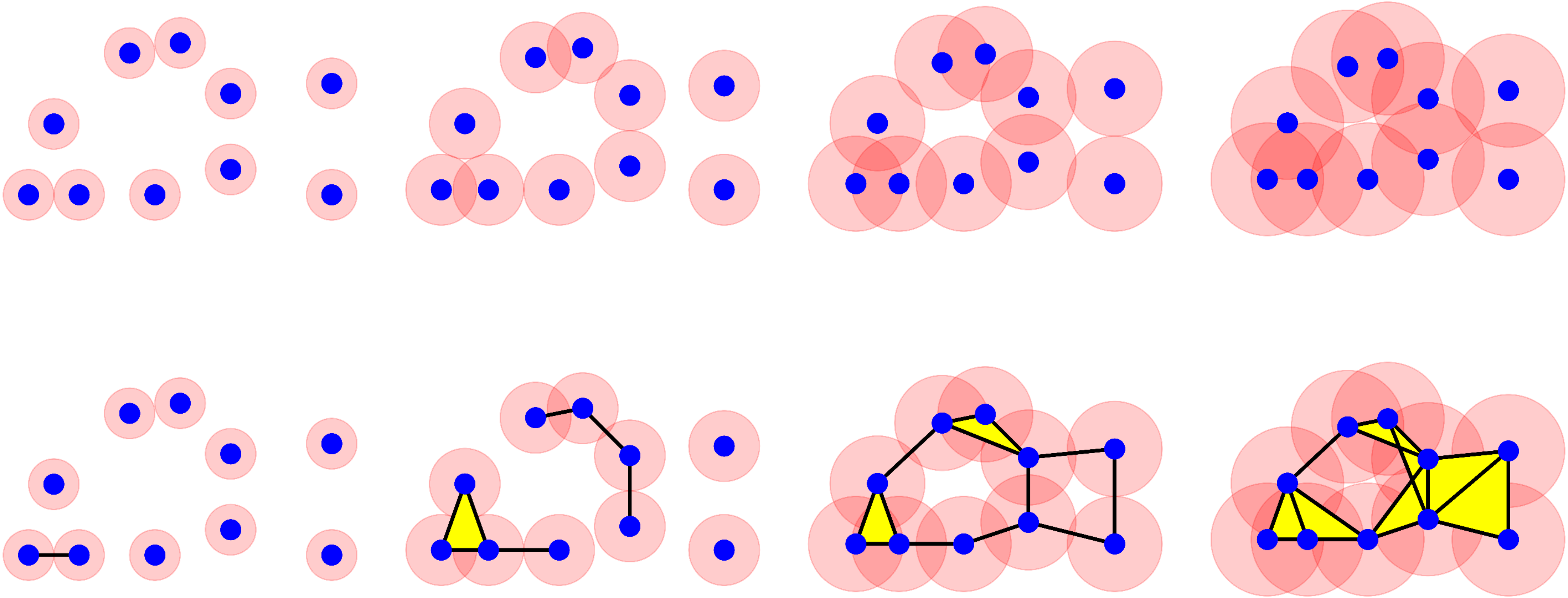
Higher-order interactions play a key role for the operation and function of a complex system. However, how to identify them is still an open problem. Here, we propose a method to fully reconstruct the structural connectivity of a system of coupled dynamical units, identifying both pairwise and higher-order interactions from the system time evolution. Our method works for any dynamics, and allows the reconstruction of both hypergraphs and simplicial complexes, either undirected or directed, unweighted or weighted. With two concrete applications, we show how the method can help understanding the complexity of bacterial systems, or the microscopic mechanisms of interaction underlying coupled chaotic oscillators.

Nerve Complex

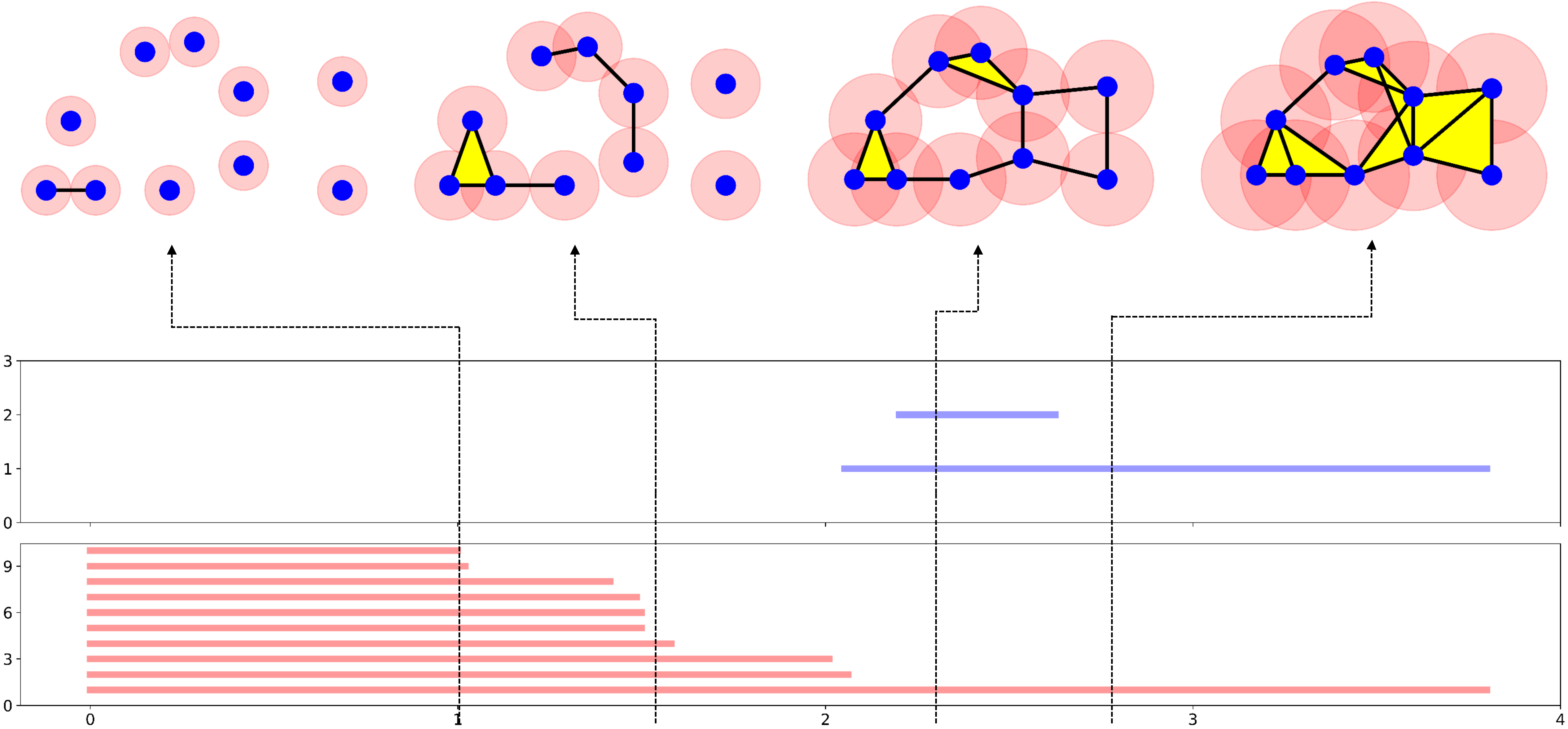


Filtered Simplicial Complex

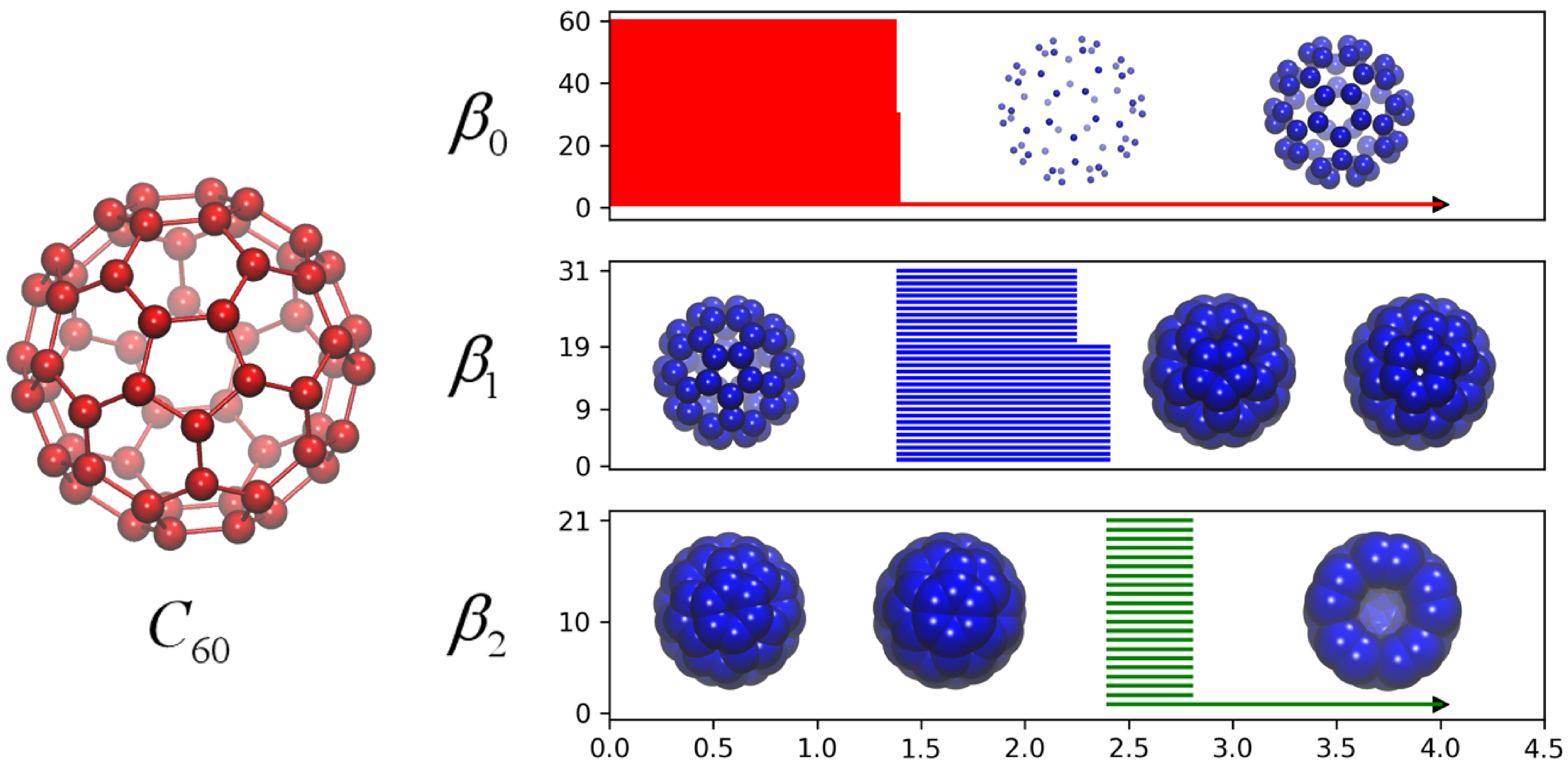
Cech Complex, Vietoris-Rips Complex, Alpha Complex, ……



Persistent Homology

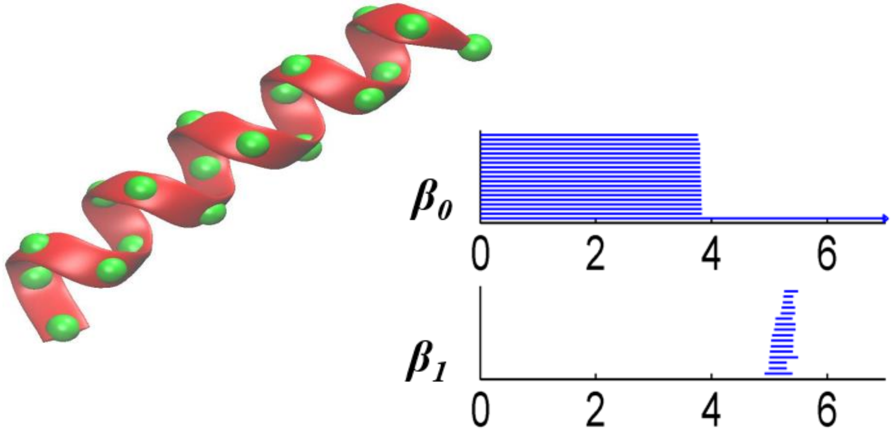


Persistent homology for C60 analysis

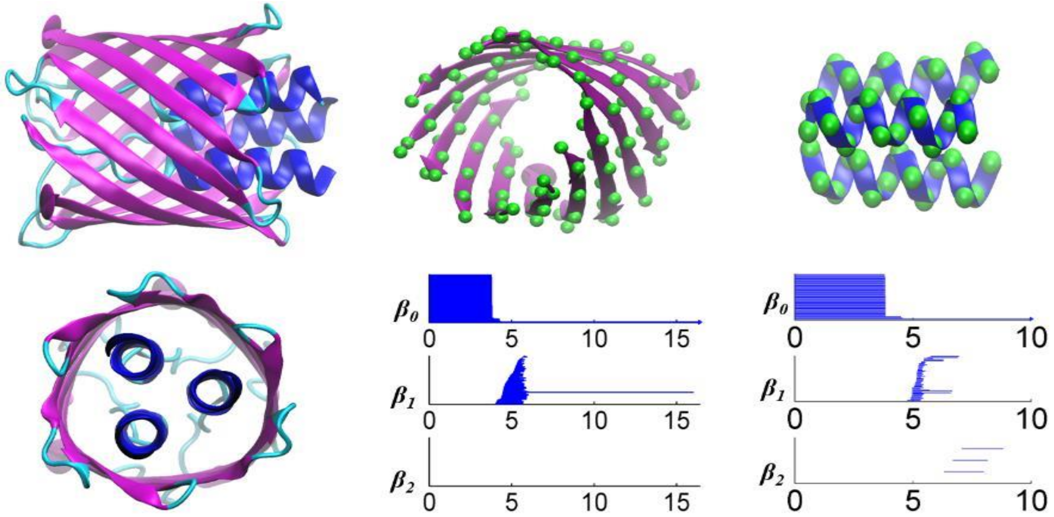


Persistent homology for Biomolecule analysis

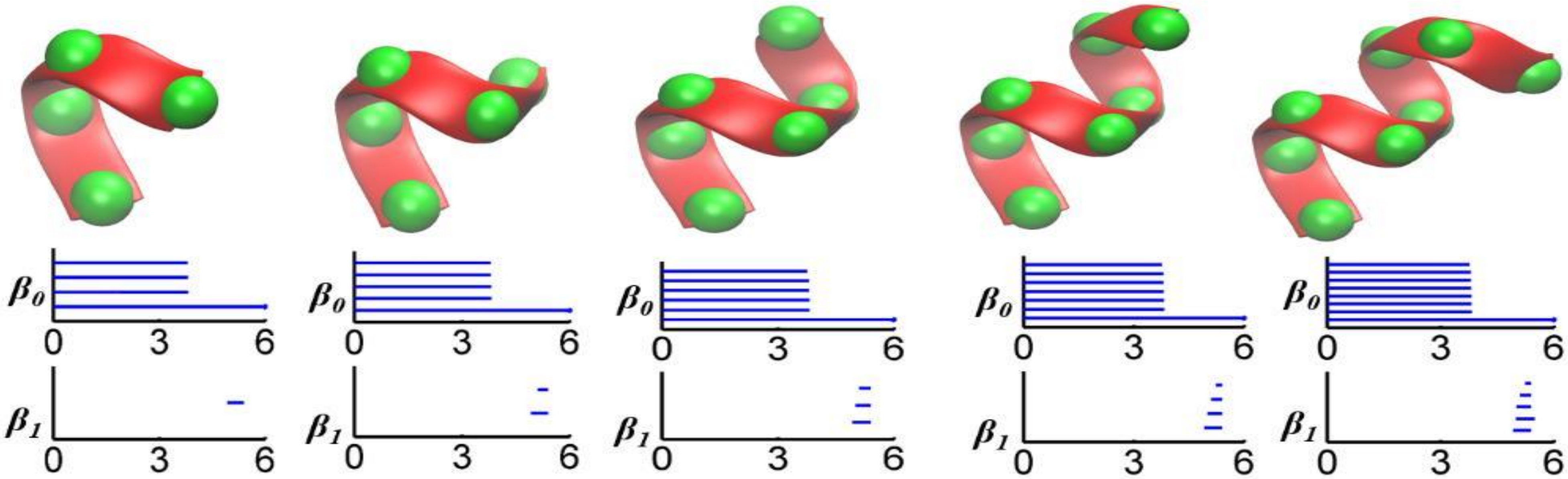
alpha helix



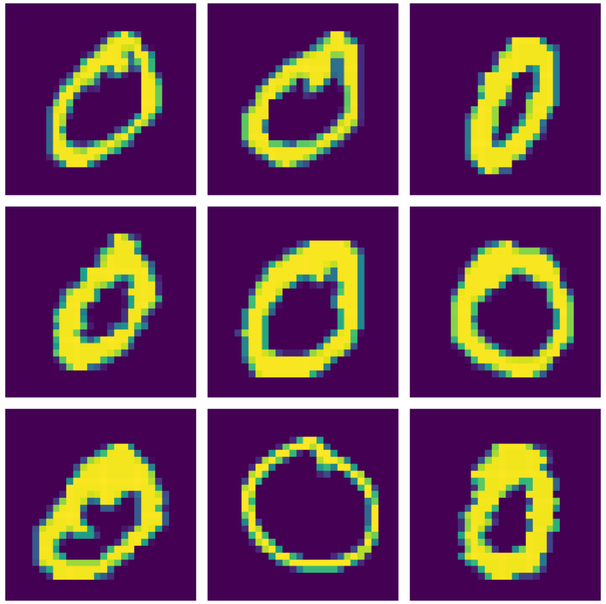
beta barrel



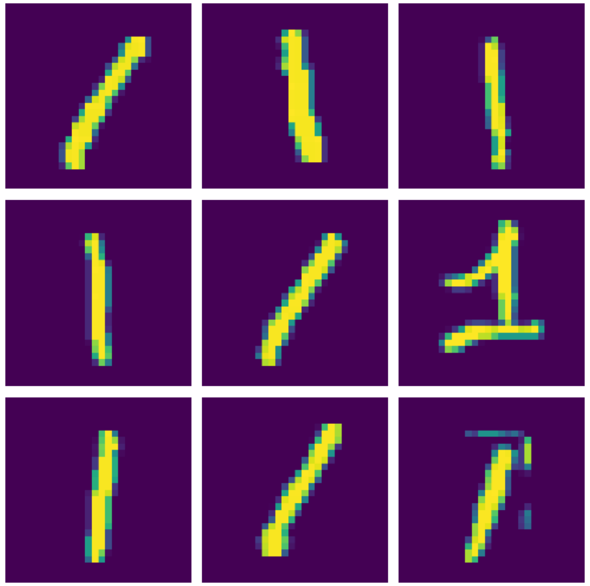
Slicing method



Persistent homology for handwriting numbers



[[0.93, inf]]
[[0.98, inf]]
[[0.98, inf]]
[[0.98, inf]]
[[0.91, inf]]
[[0.95, inf]]
[[0.85, inf]]
[[1.00, inf]]
[[0.99, inf]]



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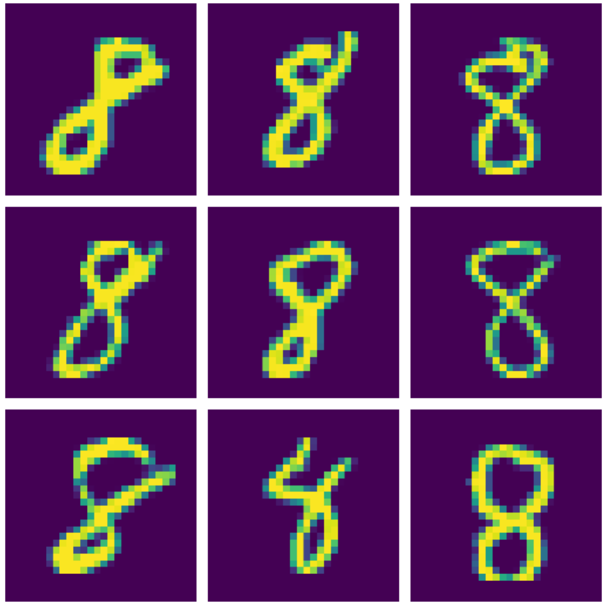
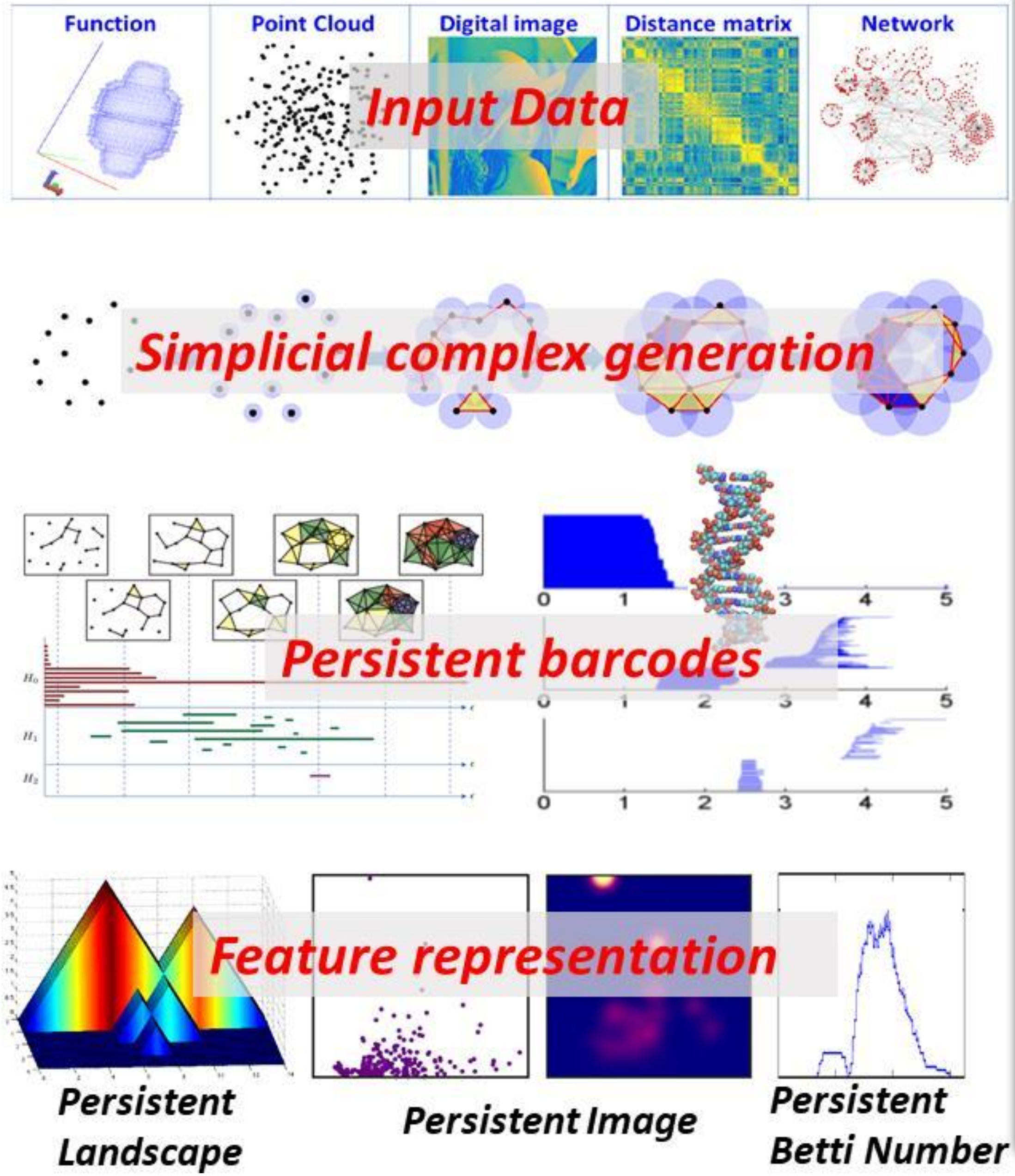
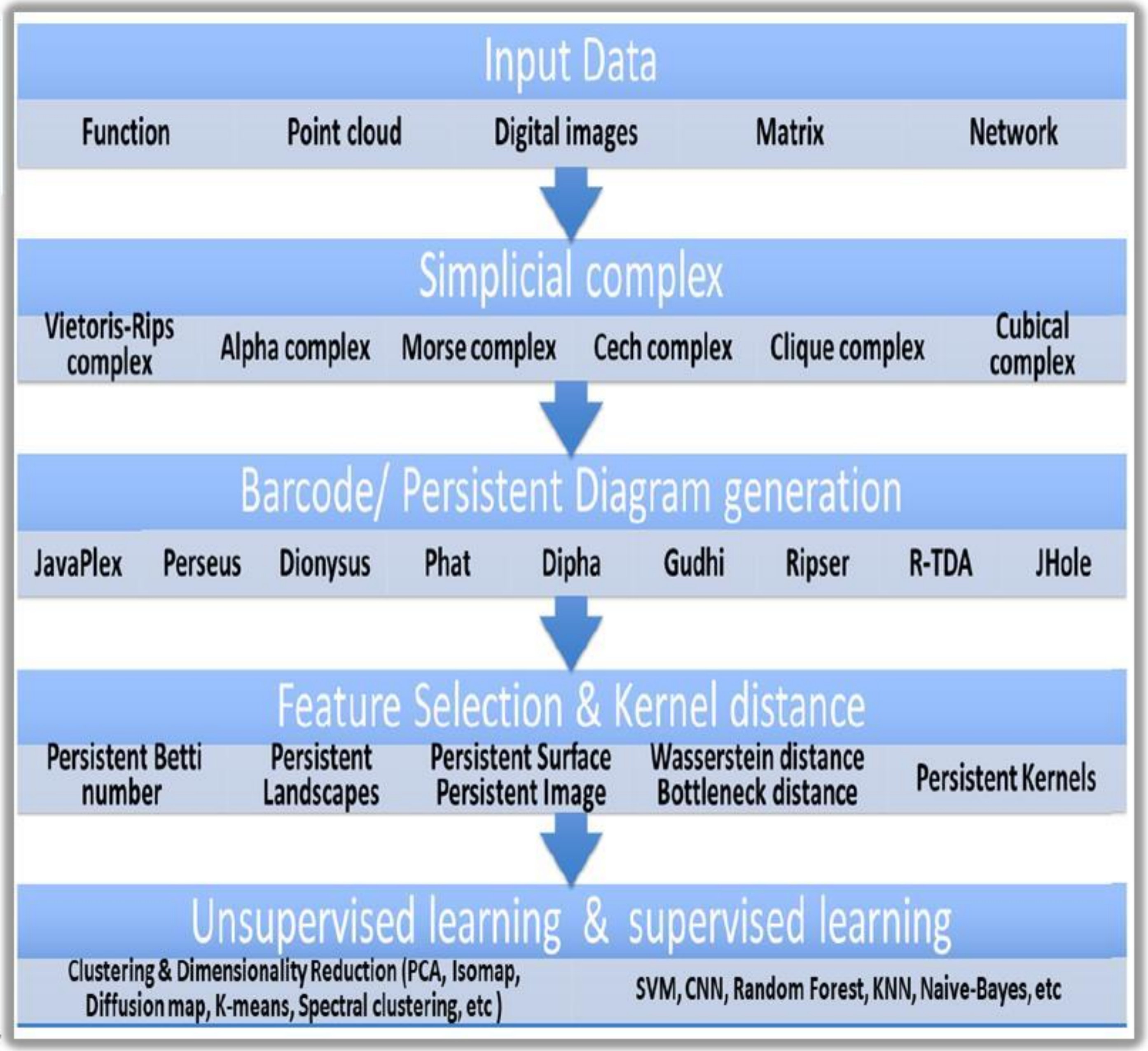


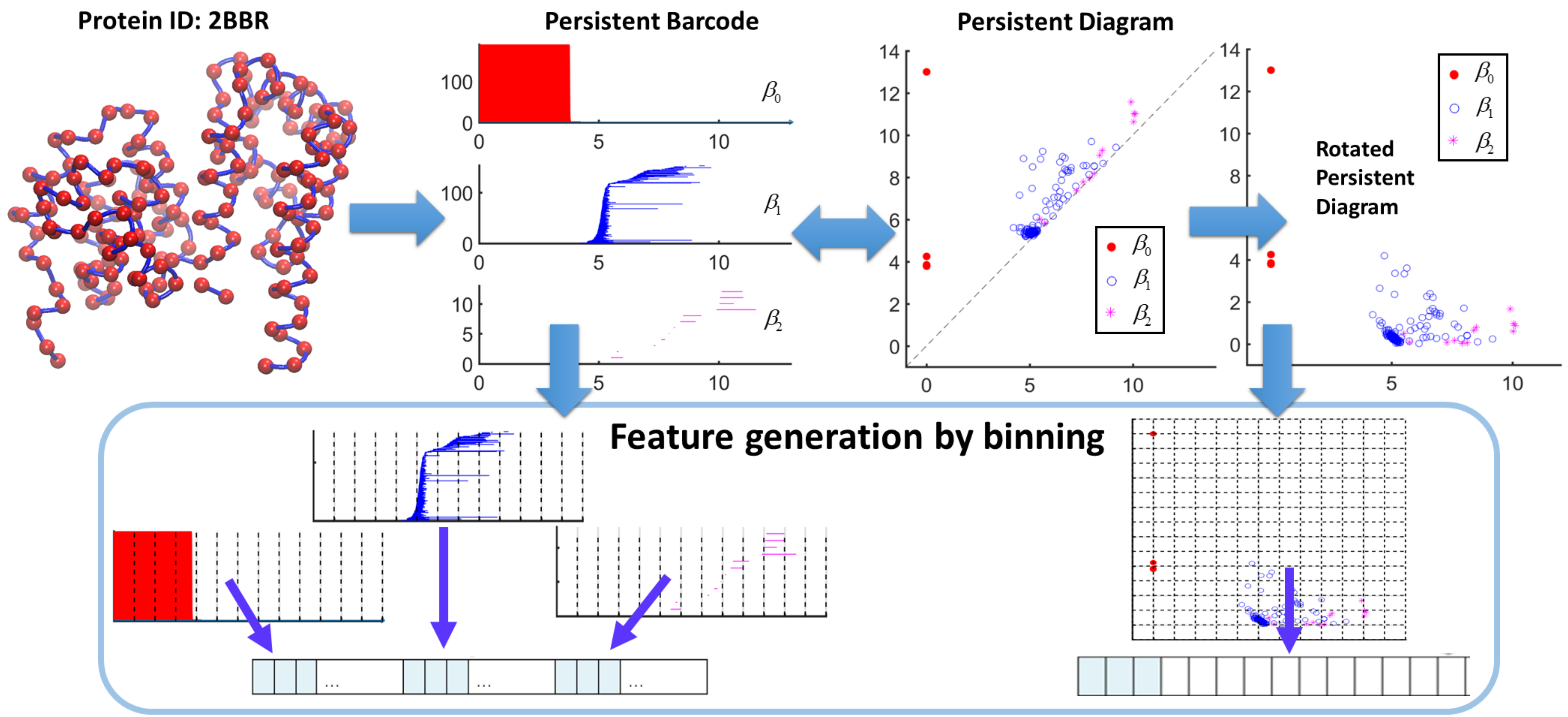
[[0.80, inf], [0.97, inf]]
[[0.58, inf], [0.58, inf]]
[[0.74, inf], [0.53, inf]]
[[0.93, inf], [0.86, inf]]
[[0.72, inf], [0.6, inf]]
[[0.71, inf], [0.68, inf]]
[[0.81, inf], [0.63, inf]]
[[0.94, inf], [0.4, inf]]
[[0.87, inf], [0.81, inf]]

Persistent homology based machine learning





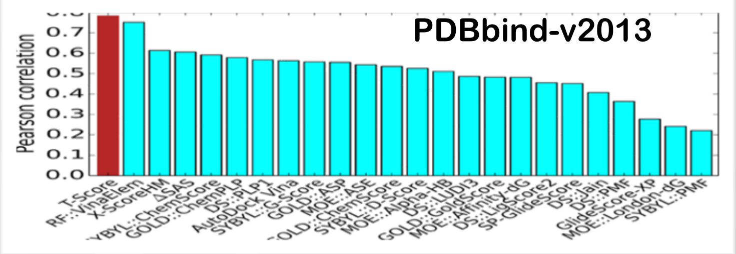
Persistent homology based features

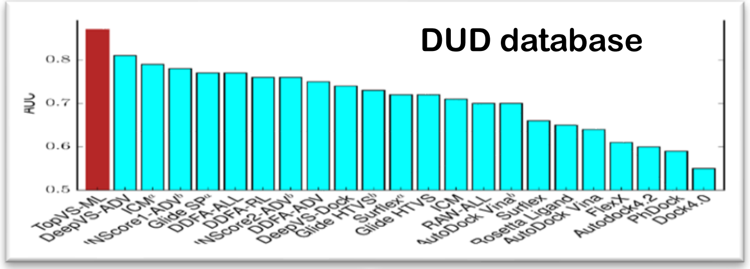


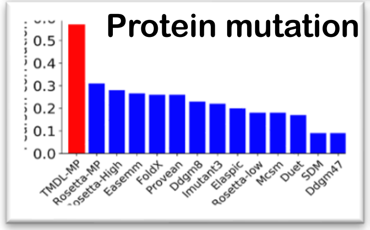
Recent Progress of TDA based drug design

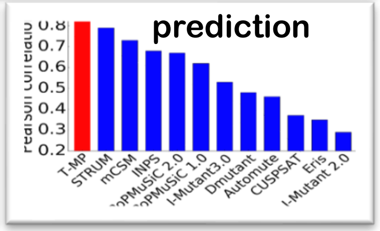
Prof Wei Team's performance using TDA-based learning models

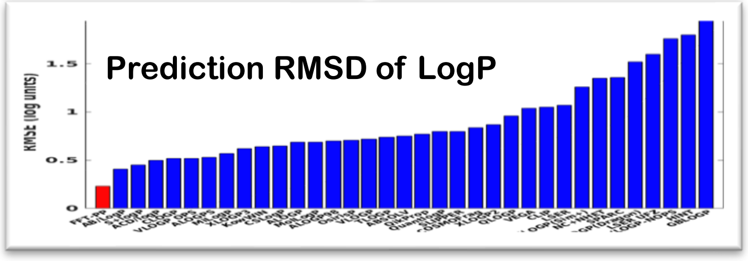
Drug design and discovery











D3R Grand Challenge

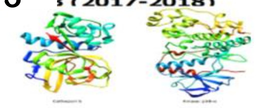
D3R Grand Challenge 2

Stage 1
Pose Predictions (partials)
Scoring (partials)
Free Energy Set 1 (partials)
Free Energy Set 2 (partials)

Stage 2
Scoring (partials)
Free Energy Set 1 (partials)
Free Energy Set 2 (partials)

D3R Grand Challenge 3

Wei Team's ... (2017-2018)



Pose Prediction
Cathepsin Stage 1A
Pose Predictions (partials)
Cathepsin Stage 1B
Pose Prediction

Affinity Rankings excluding Kds > 10 μM
Cathepsin Stage 1
Scoring (partials)
Free Energy Set
Cathepsin Stage 2
Scoring (partials)
Free Energy Set
VEGFR2
Scoring (partials)
JAK2 SC2
Scoring (partials)
p38-α
Scoring
JAK2 SC3
Scoring
Free Energy Set
TIE2
Scoring
Free Energy Set 2
ABL1
Scoring (partials)

Active / Inactive Classification
VEGFR2
Scoring (partials)
JAK2 SC2
Scoring (partials)
p38-α
Scoring (partials)
JAK2 SC3
Scoring
Free Energy Set
TIE2
Scoring (partials)
ABL1
Scoring (partials)

Affinity Rankings for Cocrystalized Ligands
Cathepsin Stage 1
Scoring (partials)
Free Energy Set
Cathepsin Stage 2
Scoring (partials)
Free Energy Set

D3R Grand Challenge 4

Pose Predictions
BACE Stage 1A
Pose Predictions (Partials)
BACE Stage 1B
Pose Predictions (Partials)

Affinity Predictions
Cathepsin Stage 1
Combined Ligand and Structure Based Scoring
Ligand Based Scoring (No participation)
Structure Based Scoring
Free Energy Set

Dr. Kaifu Gao Dr. D Nguyen

BACE Stage 1
Combined Ligand and Structure (No participation)
Ligand Based Scoring (Partials) (No participation)
Structure Based Scoring (Partials)(No participation)
Free Energy Set (No participation)

BACE Stage 2
Combined Ligand and Structure
Ligand Based Scoring (No participation)
Structure Based Scoring (Partials)
Free Energy Set

SARS-COV2 Analysis

Mutations Strengthened SARS-CoV-2 Infectivity

Jiahui Chen[1], Rui Wang[1], Menglun Wang[1] and Guo-Wei Wei[1,2,3]

1 - Department of Mathematics, Michigan State University, MI 48824, USA
2 - Department of Electrical and Computer Engineering, Michigan State University, MI 48824, USA
3 - Department of Biochemistry and Molecular Biology, Michigan State University, MI 48824, USA

Correspondence to Guo-Wei Wei: wei@math.msu.edu
https://doi.org/10.1016/j.jmb.2020.07.009
Edited by Anna Panchenko

Received 4 June 2020
Accepted 17 July 2020

Abstract

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infectivity is a major concern in coronavirus disease 2019 (COVID-19) prevention and economic reopening. However, rigorous determination of SARS-CoV-2 infectivity is very difficult owing to its continuous evolution with over 10,000 single nucleotide polymorphisms (SNP) variants in many subtypes. We employ an algebraic topology-based machine learning model to quantitatively evaluate the binding free energy changes of SARS-CoV-2 spike glycoprotein (S protein) and host angiotensin-converting enzyme 2 receptor following mutations. We reveal that the SARS-CoV-2 virus becomes more infectious. Three out of six SARS-CoV-2 subtypes have become slightly more infectious, while the other three subtypes have significantly strengthened their infectivity. We also find that SARS-CoV-2 is slightly more infectious than SARS-CoV according to computed S protein-angiotensin-converting enzyme 2 binding free energy changes. Based on a systematic evaluation of all possible 3686 future mutations on the S protein receptor-binding domain, we show that most likely future mutations will make SARS-CoV-2 more infectious. Combining sequence alignment, probability analysis, and binding free energy calculation, we predict that a few residues on the receptor-binding motif, i.e., 452, 489, 500, 501, and 505, have high chances to mutate into significantly more infectious COVID-19 strains.

Mutations at 501 and 452 in prevailing SARS-Cov-2 variants

Alpha : N501Y
Beta : K417N, E484K, N501Y
Gamma : K417T, E484K, N501Y
Delta : L452R, T478K
Epsilon : L452R
Kappa : L452R, E484Q
Omicron : N501,...

They predicts key mutation sites in prevailing variants

Thank You!