Finding shape and structure in data: geometry and topology in the natural sciences

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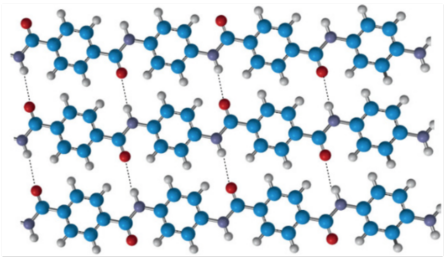
The Shape Of Nature

In physics:

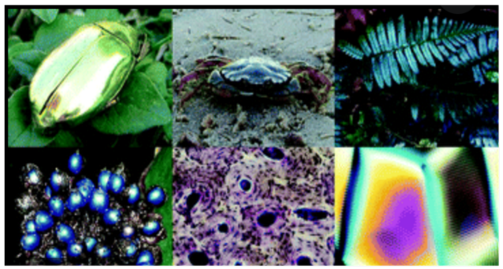
- **Matter** is any substance that has mass and occupies space by having volume.
- **Shape** describes the spatial distribution of **matter** within a body.



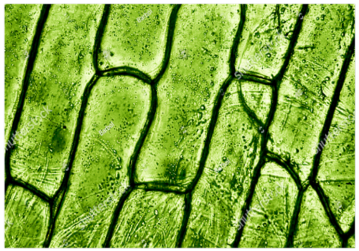
molecular arrangements

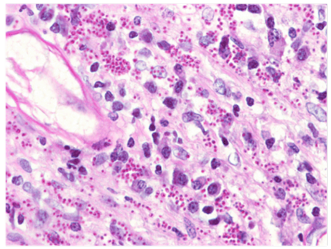
schools and swarms

materials



organisms



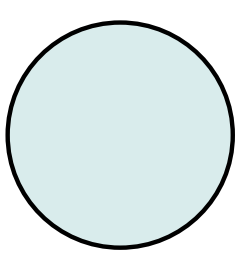


biological tissues

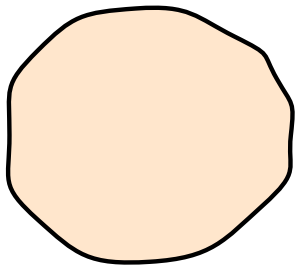
"To model nature, we must model the evolution of shape"

Geometry and Topology: The Mathematics of Shape

- **Geometry** studies shapes with measurements such as distances, angles, and curvature.
- **Topology** study properties of shapes that remain the same after continuously deforming them.
- Together, they model how shapes exist, transform, and relate, from molecules to spacetime curvature.



Geometric shape

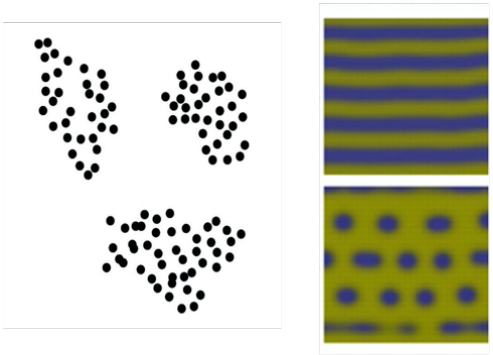


Topological deformation

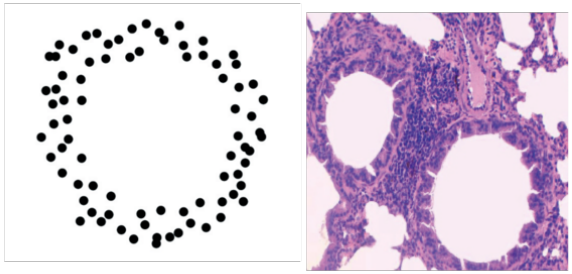
Shape is not static, its **evolution** encodes structure and dynamics across physics, chemistry, and biology.

Topological Properties

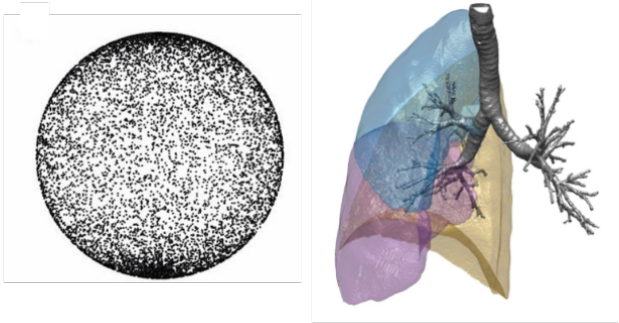
"Holes"



clusters/components



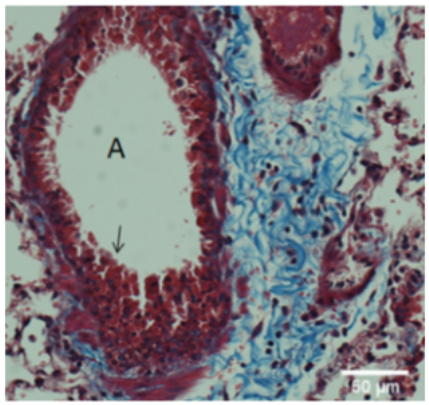
loops/holes

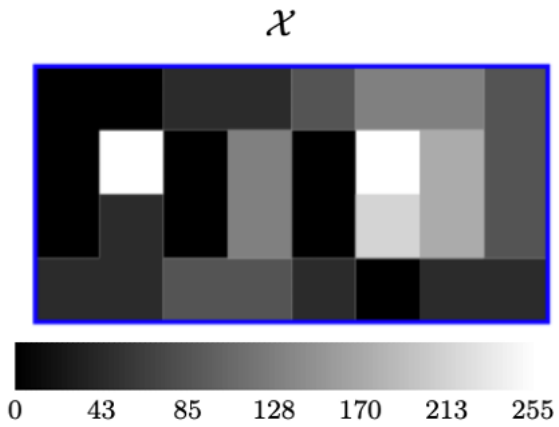


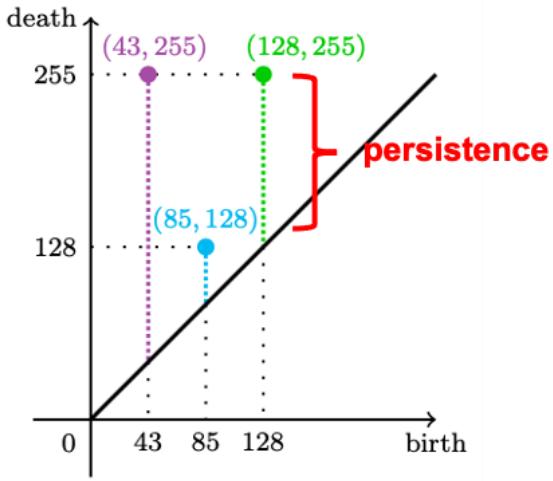
voids

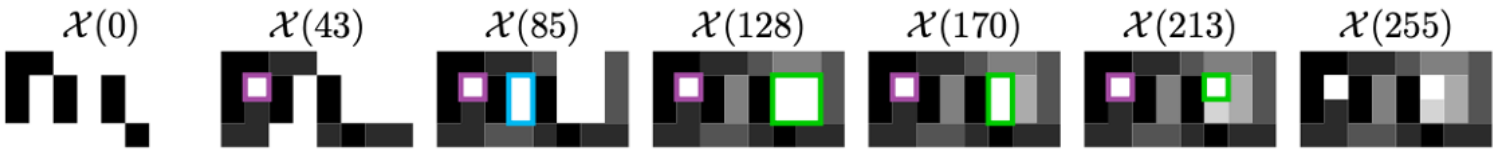
Detecting topological features at scales

Persistent Homology









Comparing Persistence Diagrams

- The **bottleneck distance** measures how far two persistence diagrams differ by looking at the *largest shift* needed to match their points.

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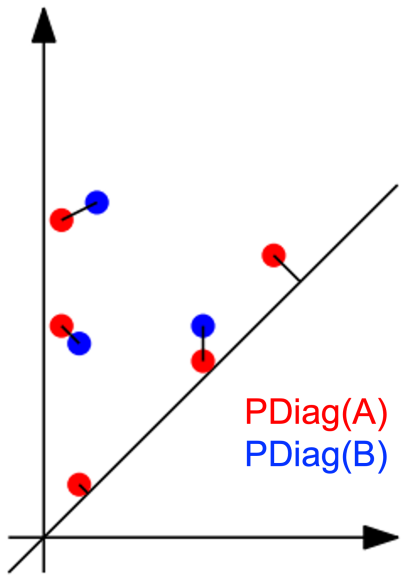
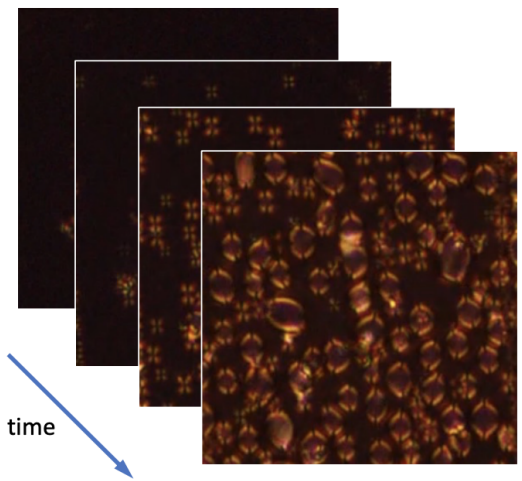
Smaller $W_\infty \Rightarrow$ diagrams (and shapes) are more similar



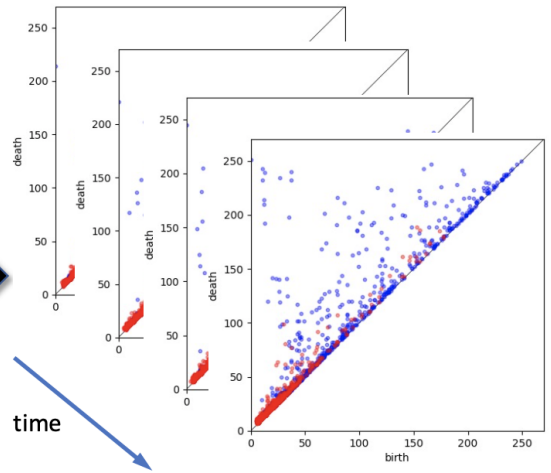
Maximum distance among matched pairs (the "bottleneck")

Case study: soft matter dynamics

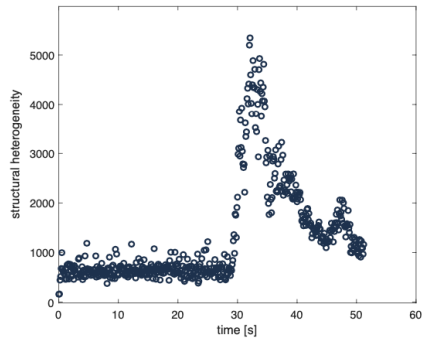
- Topological data analysis of phase transition videos
- Statistical analysis of topological features
- Unsupervised learning using topological features



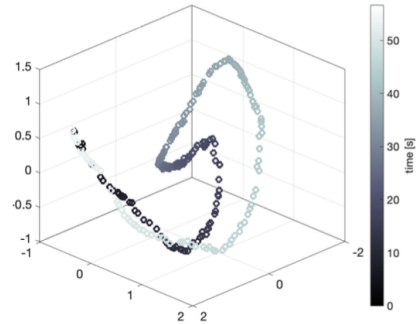
Time-dependent observations



Time-dependent topological descriptors

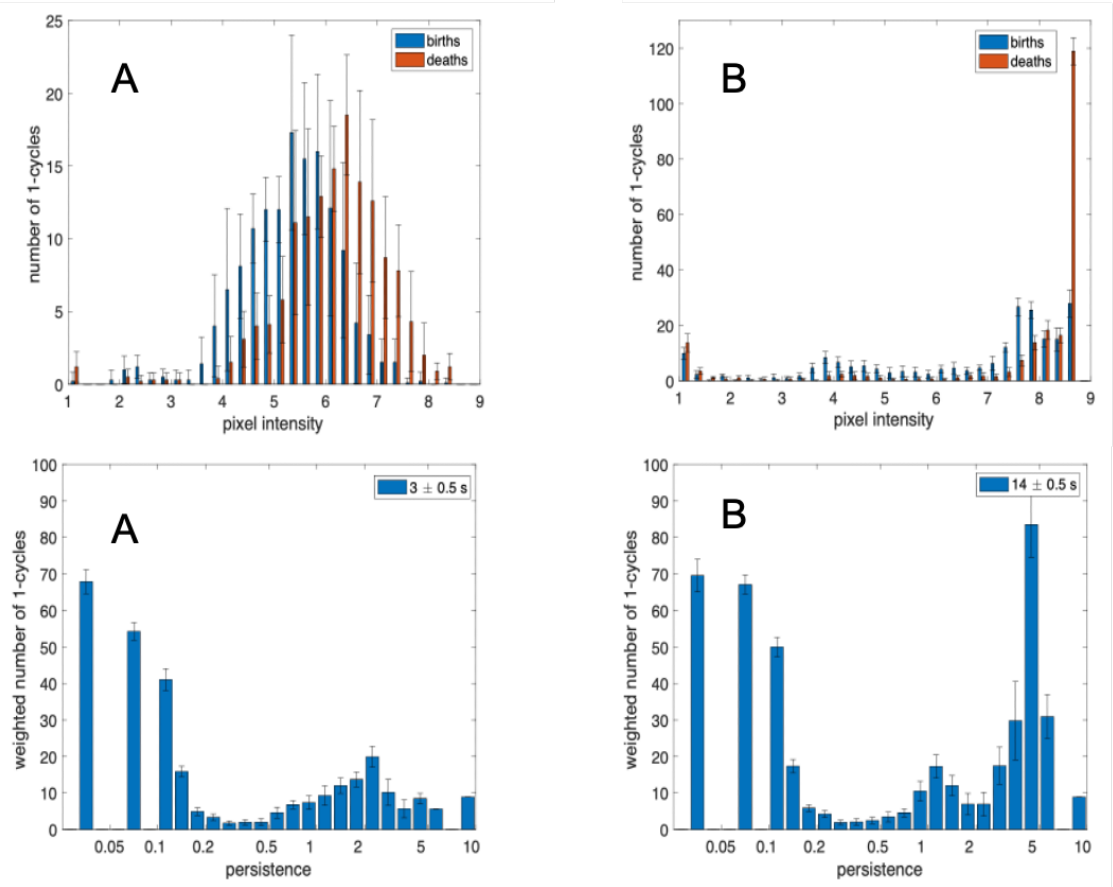


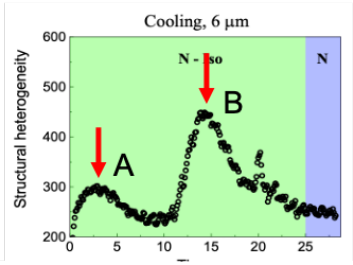
Structural heterogeneity

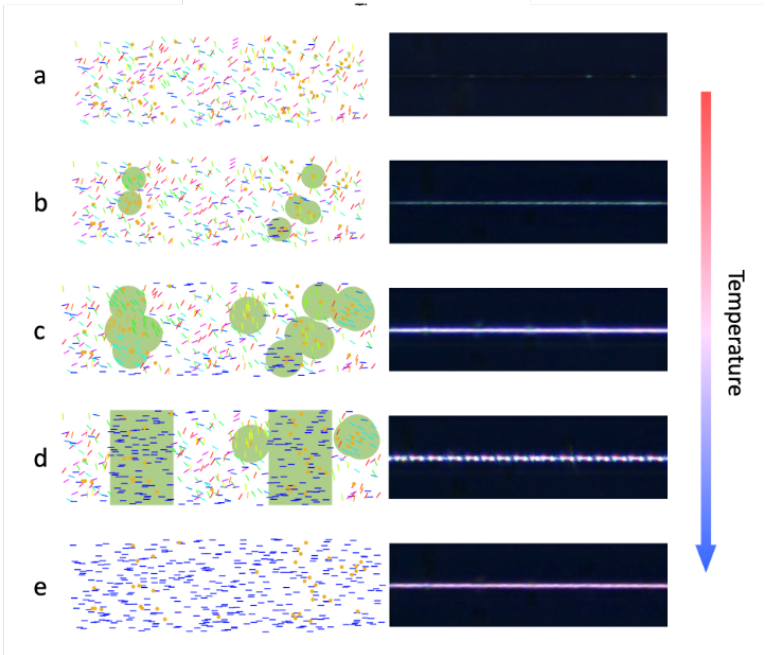


Topological pathway

Statistical analysis of topological features







TDA in Data Science: Current Work and Future Directions

Current Applications

- Feature extraction of molecular systems
- Theoretical and image analyis of phase transition
- Brain morphology
- Image analysis in healthcare data
- Climate regime characterisation
- Reaction-difussion systems

Potential Directions

- Topological evolution of weather patterns
- Biological Morphogenesis
- Collective cell movement
- Chemical kinetics
- Morphological transitions in glaciers, rivers, and coastlines
- Structure-activity of the brain and artificial neural networks

Thank you!