Topology and biology: Persistent homology of aggregation models

Chad Topaz, Lori Ziegelmeier, Tom Halverson
Macalester College

Ghrist (2008)
If I can do applied topology, YOU can do applied topology

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Macalester College

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The big picture

• Questions about biological aggregations (and maybe agent-based systems in general?)

  1. How does each individual behave?

  2. How does the group behave?

  3. How are individual and group behavior linked?

• Demonstrate utility of computational persistent homology in addressing #2 above
What is this group doing?

http://youtu.be/iRNqhi2ka9k
What is this group doing?

\[ r = 0.2 \text{ m} \]
What is this group doing?
Aggregation Models
Example 1: Vicsek Model

Novel type of phase transition in a system of self-driven particles
T Vicsek, A Czirók, E Ben-Jacob, I Cohen, O Shochet - Physical review letters, 1995 - APS

Abstract A simple model with a novel type of dynamics is introduced in order to investigate the emergence of self-ordered motion in systems of particles with biologically motivated interaction. In our model particles are driven with a constant absolute velocity and at each ...
Example 1: Vicsek Model

Averaging + Noise
Example 1: Vicsek Model

\[ \theta_i \leftarrow \frac{1}{N} \sum_{|\mathbf{x}_i - \mathbf{x}_j| \leq R} \theta_j \]

\[ + U(-\eta/2, \eta/2) \]

\[ \mathbf{v}_i \leftarrow v_0(\cos \theta_i, \sin \theta_i) \]

\[ \mathbf{x}_i \leftarrow \mathbf{x}_i + \mathbf{v}_i \Delta t \]

http://youtu.be/jphRZV3oCal
Example 1: Vicsek Model

\[ \phi(t) = \frac{1}{Nv_0} \left| \sum_{i=1}^{N} v_i(t) \right| \]
Example 1: Vicsek Model

\[ \varphi(t) = \frac{1}{Nv_0} \left| \sum_{i=1}^{N} \mathbf{v}_i(t) \right| \]
Example 1:
Vicsek Model

$\varphi = 1$

$\varphi = 0$
Example 2: D’Orsogna Model

Self-propelled particles with soft-core interactions: patterns, stability, and collapse
MR D’Orsogna, YL Chuang, AL Bertozzi, LS Chayes - Physical review letters, 2006 - APS
Abstract Understanding collective properties of driven particle systems is significant for naturally occurring aggregates and because the knowledge gained can be used as building blocks for the design of artificial ones. We model self-propelling biological or artificial ...

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Example 2: D’Orsogna Model

\[
\begin{align*}
\dot{x}_i &= v_i \\
\dot{m}v_i &= (\alpha - \beta |v_i|^2) v_i - \nabla_i Q_i \\
Q_i &= \sum_{j \neq i} C_r e^{-|x_i - x_j|/L_r} - C_a e^{-|x_i - x_j|/L_a}.
\end{align*}
\]
Example 2: D’Orsogna Model

Social potential $Q(r)$

$r = \text{interorganism distance}$
Example 2: D’Orsogna Model

\[
\dot{x}_i = v_i
\]

\[
m\dot{v}_i = (\alpha - \beta |v_i|^2) v_i - \nabla_i Q_i
\]

\[
Q_i = \sum_{j \neq i} C_r e^{-|x_i - x_j|/L_r} - C_a e^{-|x_i - x_j|/L_a}
\]
Example 2:
D’Orsogna Model

Order Parameters

- \( b_0 \geq 5 \)
- \( b_1 = 0 \)
- \( b_1 \geq 5 \)
- \( b_1 = 1 \)
- \( b_1 = 2 \)

Order Parameter

- Polarization
- Angular Momentum
- Abs. Angular Mom.
Persistent Homology
The big picture: Study data via topology

1. Envision data as high dimensional point cloud
   - *e.g.*, position-velocity for one simulation snapshot
2. Create connections between proximate points
   - build simplicial complex
3. Determine topological structure of complex
   - calculate Betti numbers (measure # holes)
4. Vary proximity parameter to assess different scales
   - calculate persistent homology
5. Evolve in time
   - CROCKER plots
The big picture: Study data via topology

1. Computing persistent homology

2. Barcodes: The persistent topology of data

3. Persistent homology: A Survey

4. Topology and Data
Step 1:
Envision data as point cloud
Step 2: Build simplicial complex
Step 3: Calculate Betti numbers

\[ b_0 = 4 \]
\[ b_1 = 1 \]
\[ b_2 = 0 \]
\[ b_3 = 0 \]
etc.
Step 3: Calculate Betti numbers

Circle: $b=(1,1,0,0,...)$

Two-Torus: $b=(1,2,1,0,...)$

Two-Sphere: $b=(1,0,1,0,...)$
Step 4:
Find persistent homology

Proximity Parameter $\varepsilon$
Step 4: Find persistent homology

Proximity Parameter $\varepsilon$

$b_0$

$b_1$

Proximity Parameter $\varepsilon$
Step 4: Find persistent homology

Proximity Parameter $\epsilon$
Step 4:
Find persistent homology

Proximity Parameter $\varepsilon$

Graph showing the persistence diagram with bars for $b_0$ and $b_1$.
Step 4: Find persistent homology

Proximity Parameter $\varepsilon$

$\varepsilon = 1.5, 5.0, 7.0, 9.5$

$\beta_0, \beta_1$
Step 4: Find persistent homology

Proximity Parameter \( \varepsilon \)

- \( b_0 \)
- \( b_1 \)

Proximity Parameter \( \varepsilon \)
Step 4:
Find persistent homology

Proximity Parameter \( \varepsilon \)

Proximity Parameter values are given as follows:

- \( b_0 \) values: 1.5, 5.0, 7.0, 9.5
- \( b_1 \) values: 1.5, 5.0, 7.0, 9.5

The diagram illustrates the persistent homology with the proximity parameter values.
Step 4:
Find persistent homology

Proximity Parameter

$\varepsilon$
Step 4: Find persistent homology

Proximity Parameter $\varepsilon$

$[1.5, 5.0, 7.0, 9.5]$
Step 4: Find persistent homology

Proximity Parameter $\epsilon$

Proximities $b_0$ and $b_1$
Step 4:
Find persistent homology

Proximity Parameter

Proximity Parameter $\epsilon$
Step 4: Find persistent homology

Proximity Parameter $\varepsilon$

$b_0$ and $b_1$
Step 4: Find persistent homology

Proximity Parameter \( \varepsilon \)

\[ b_0 \]
\[ b_1 \]

Proximity Parameter Parameter

1.5 5.0 7.0 9.5
Step 4: Find persistent homology

Proximity Parameter $\varepsilon$

$\beta_0, \beta_1$
Step 4:
Find persistent homology
Step 4:
Find persistent homology

Proximity Parameter $\varepsilon$

$\beta_0$
Step 4:
Find persistent homology
Step 4: Find persistent homology
Step 5: Evolve in time (CROCKER)

Contour Realization Of Computed K-dimensional-hole Evolution in the Rips complex
Step 5: Evolve in time (CROCKER)
Step 5: Evolve in time (CROCKER)

Contour Realization Of Computed K-dimensional-hole Evolution in the Rips complex

Contour Plot of $b_0(\varepsilon, t)$
Results
Vicsek Model
Initial Condition

Three-torus $T^3$
$b = (1,3,3,1,0,...)$
Vicsek Model
Long Term Behaviors

Clusters?

Loose alignment?

Strong alignment?
- Intermittent clustering
- Loss of two topol. circles
- $b = (2 - 4, 1, \ldots)$
- One group
- Two persistent topol. circles
- $b = (1, 2, 1, \ldots)$
- One group, one rogue
- Two persistent topol. circles
- $b = (1, 2, 0, \ldots)$
- Hole in the data
D’Orsogna Model Simulations Snapshots

(A) $t = 5$ (early)
(B) $t = 23$ (middle)
(C) $t = 34$ (late)
- 1 - 2 groups
- 2 topol. circles
- $b = (2, 2, ...)$
In four dimensional $\mathbf{x} - \mathbf{v}$ space, #1 and #3 are closer than #1 and #2.
- 1 - 2 groups
- 2 topol. circles
- \( b = (2, 2, \ldots) \)
Conclusions

1. Persistent homology computations
   • reveal dynamics missed by order parameters
   • distinguish dynamics missed when OP do not
   • recognize similarity when OP do not
   • useful when manual examination of data is hard

2. Non-topologists can do persistent homology

3. Non-topologists SHOULD do persistent homology