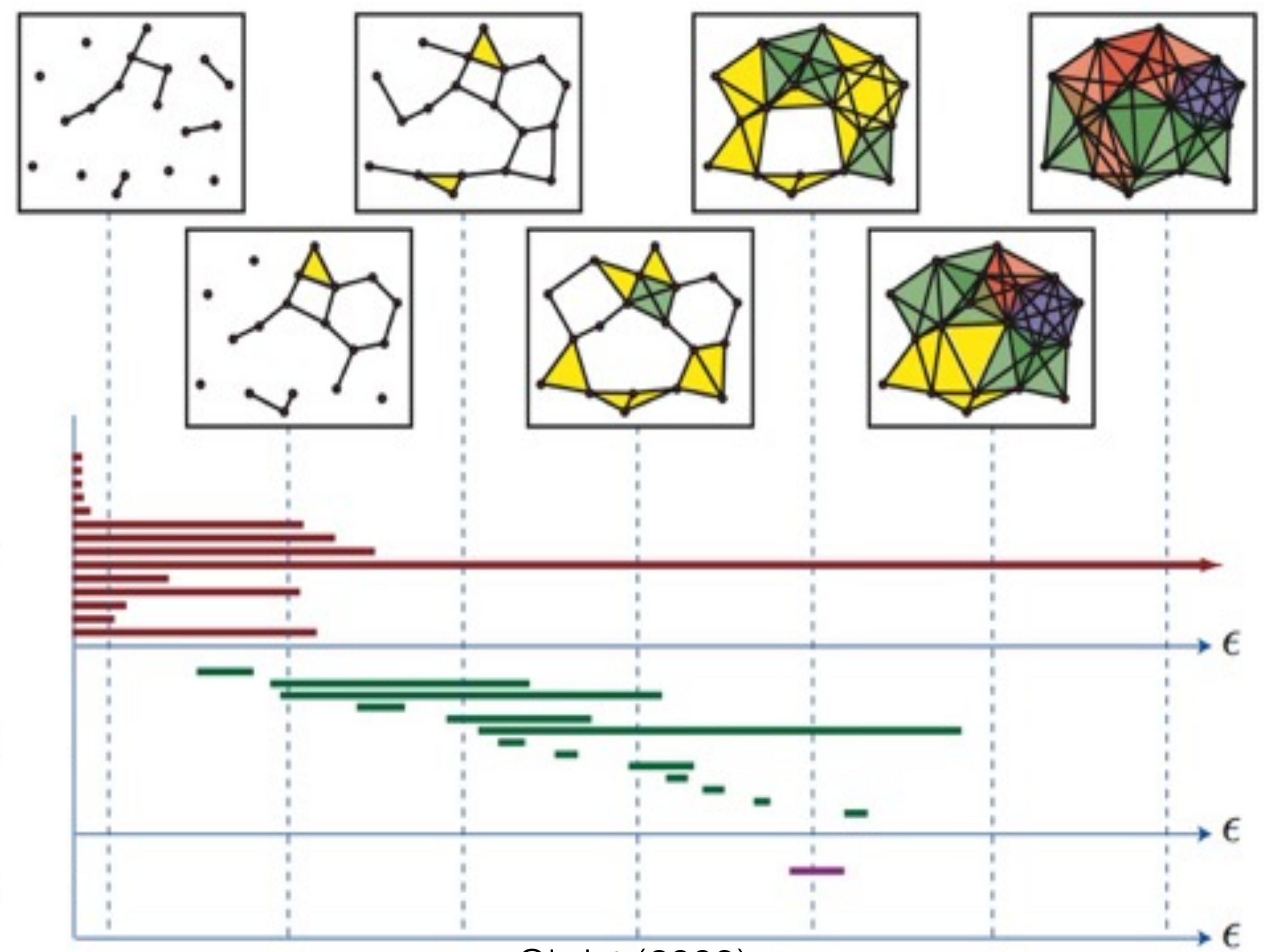
Topology and biology: Persistent homology of aggregation models

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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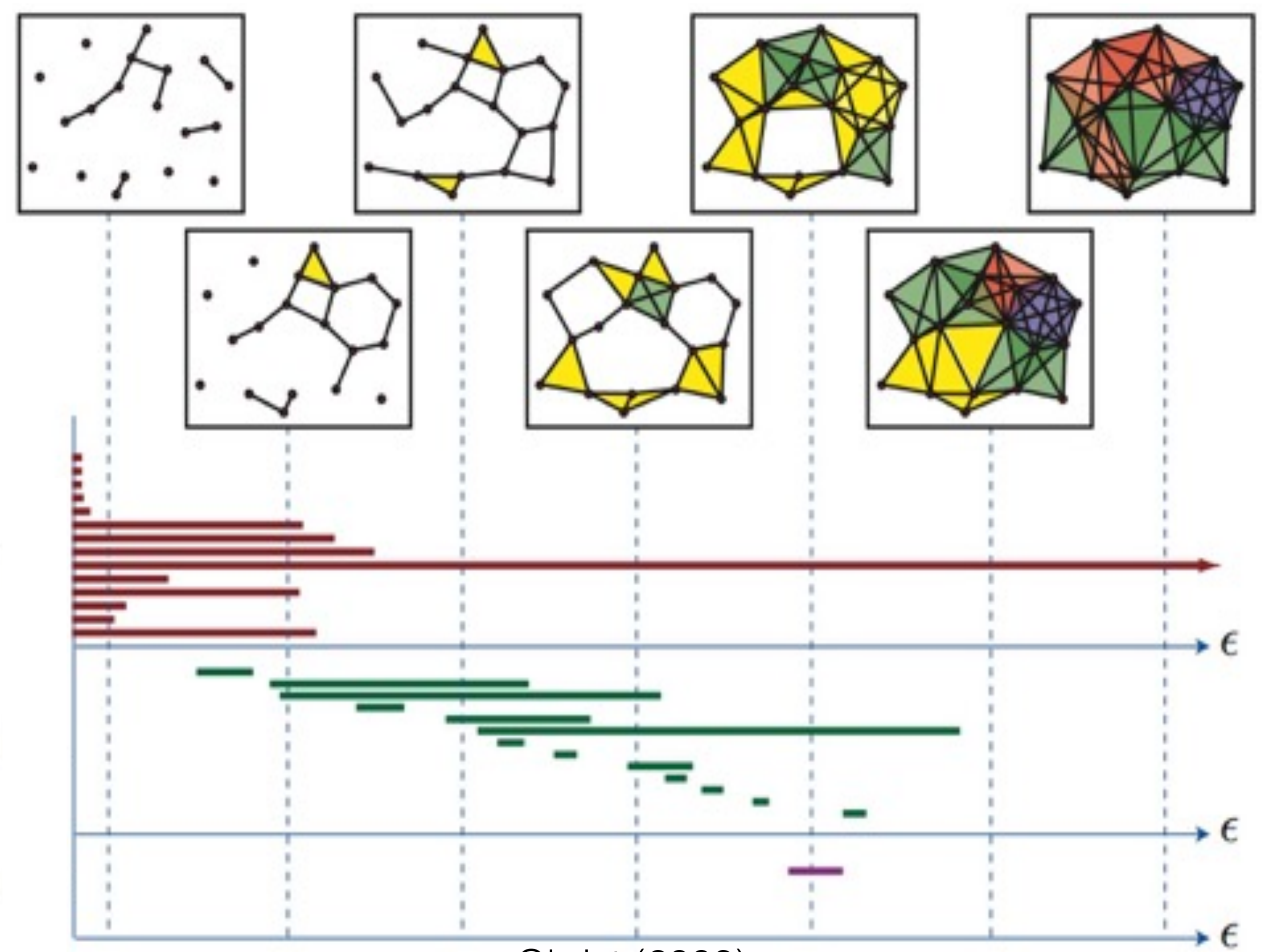


Ghrist (2008)

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?

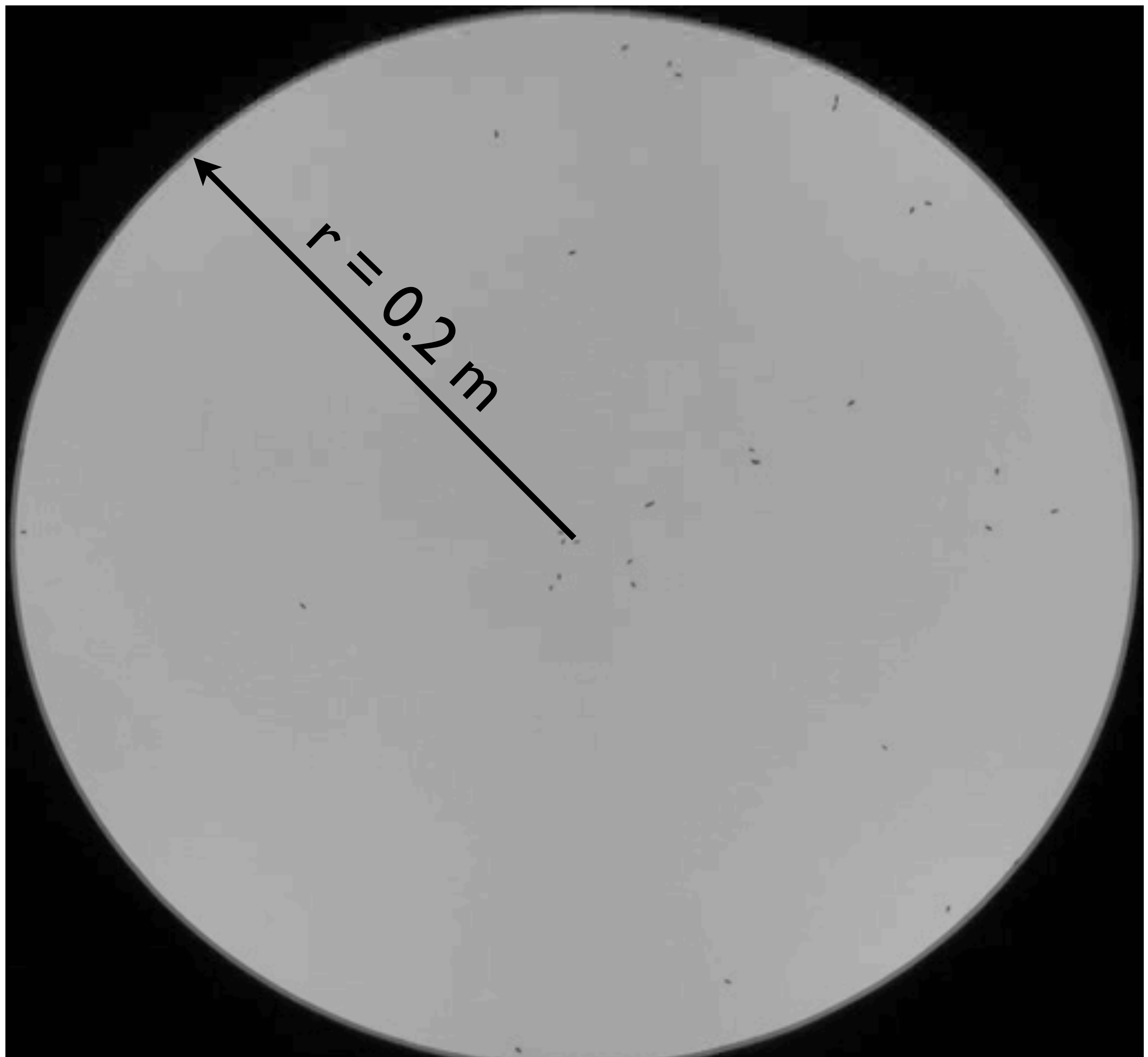
  3. How are individual and group behavior linked?

- Demonstrate utility of computational persistent homology in addressing #2 above

What is this group doing?

http://youtu.be/iRNqhi2ka9k

What is this group doing?



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 ...

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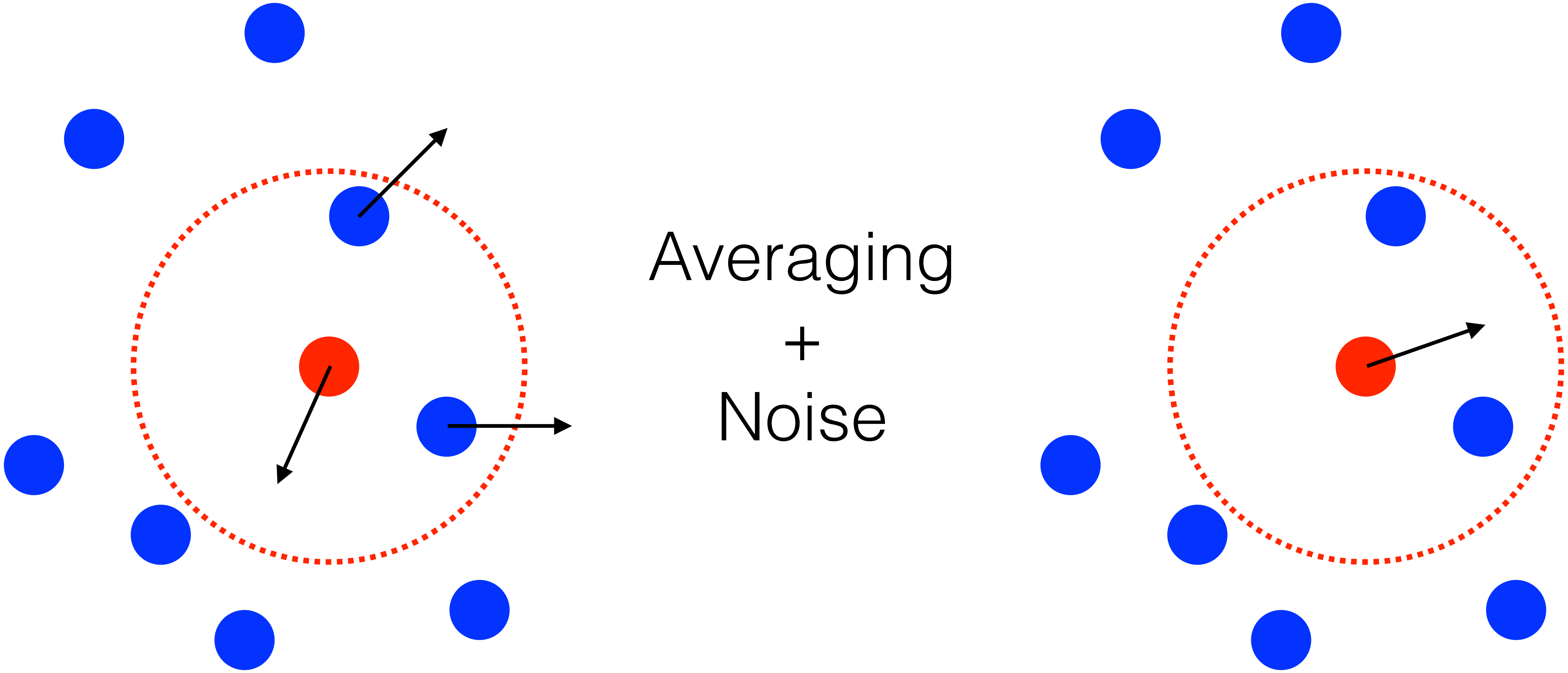
Example 1: Vicsek Model



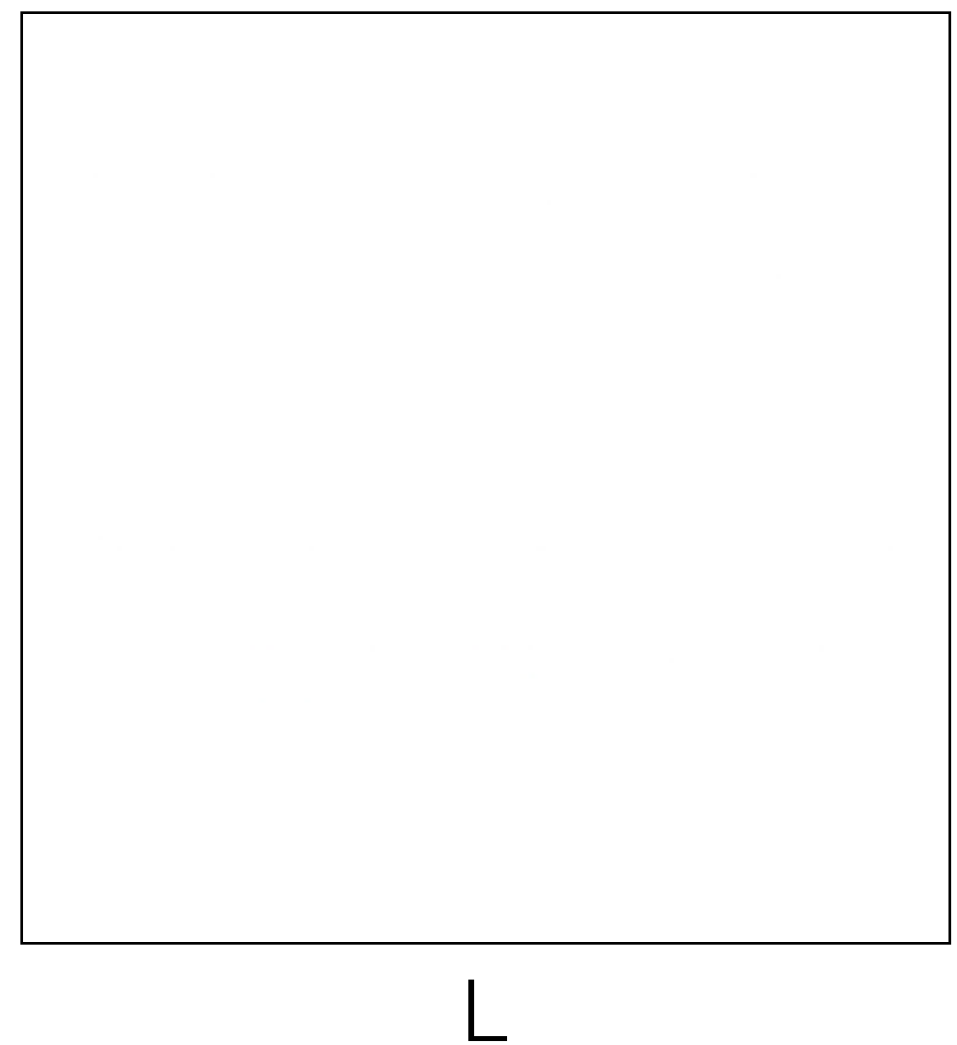
Example 1:
Vicsek Model

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

$$+ U(-\eta/2, \eta/2)$$

$$\mathbf{v}_i \quad \leftarrow \quad v_0(\cos\theta_i, \sin\theta_i)$$

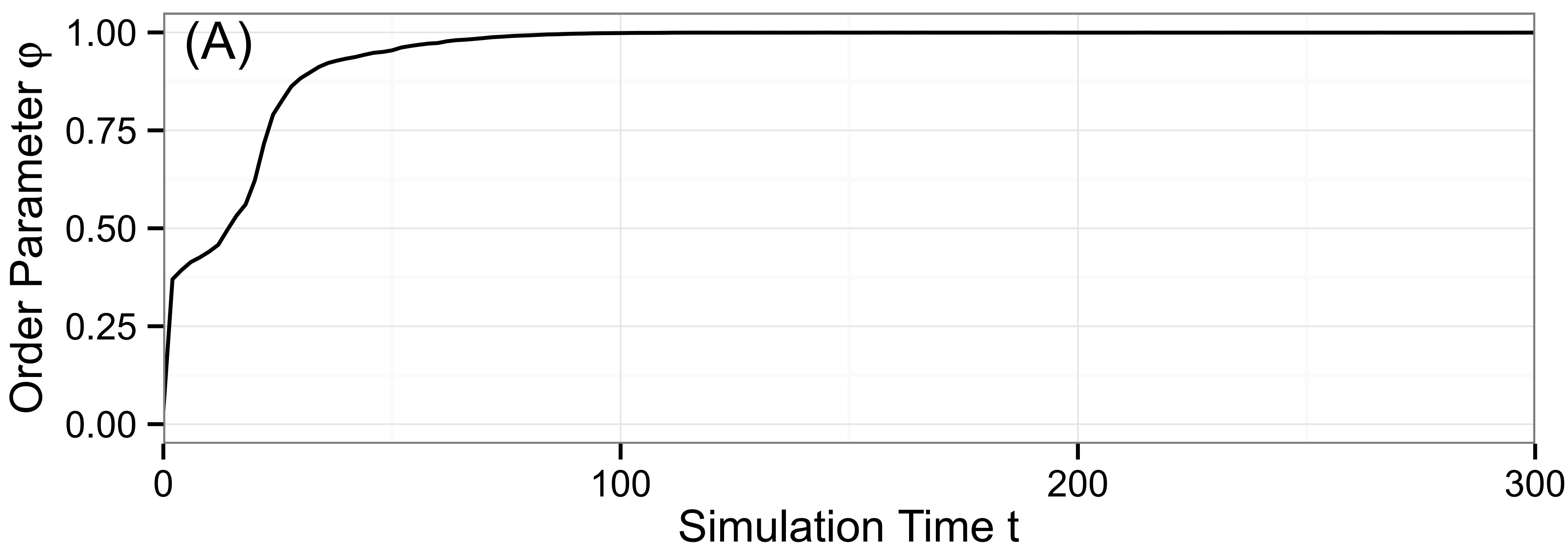
$$\mathbf{x}_i \quad \leftarrow \quad \mathbf{x}_i + \mathbf{v}_i \, \Delta t$$



http://youtu.be/jphRZV3oCaI

Example 1:
Vicsek Model

$$\varphi(t) = \frac{1}{N v_0} \left| \sum_{i=1}^{N} \mathbf{v}_i(t) \right|$$



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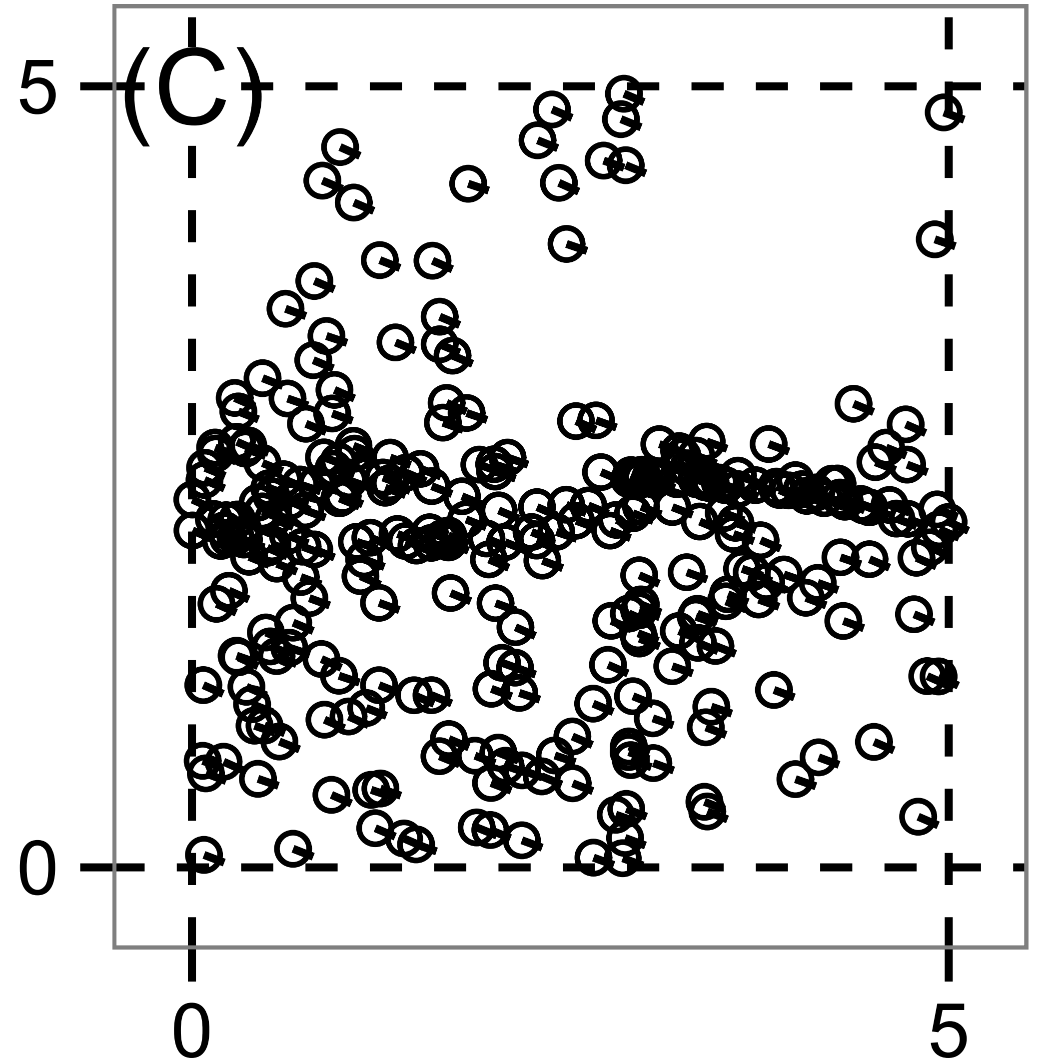

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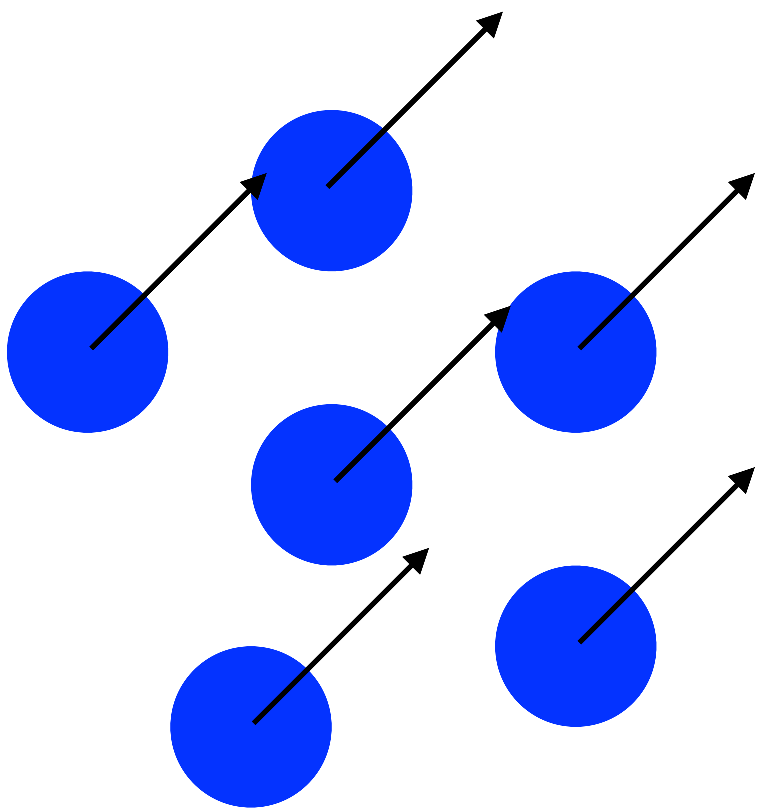
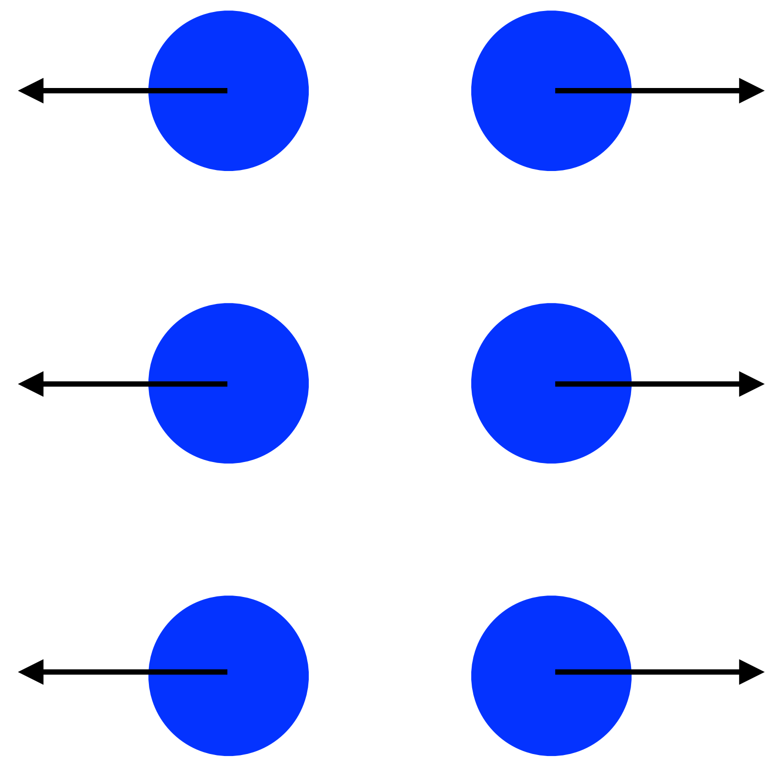
Vicsek Model



$\varphi = 1$



$\varphi = 0$

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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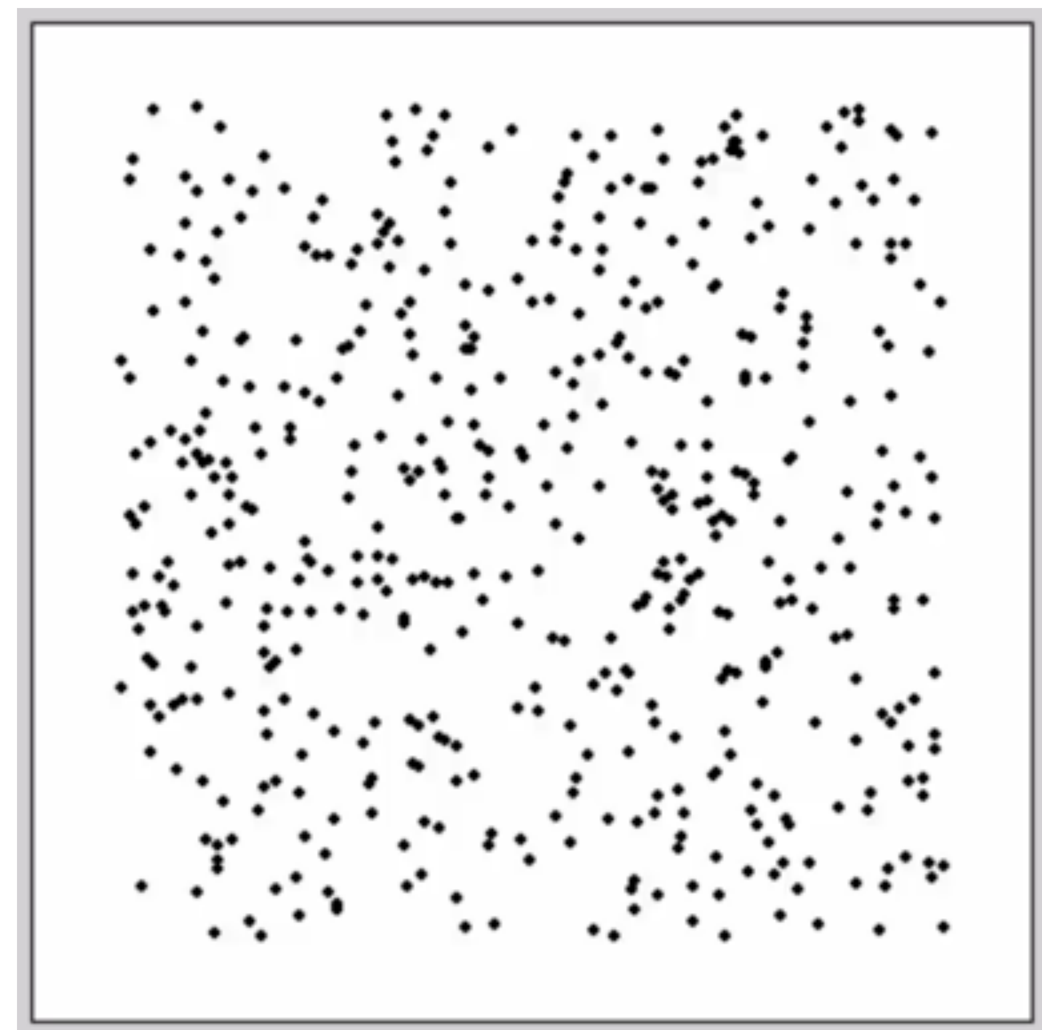
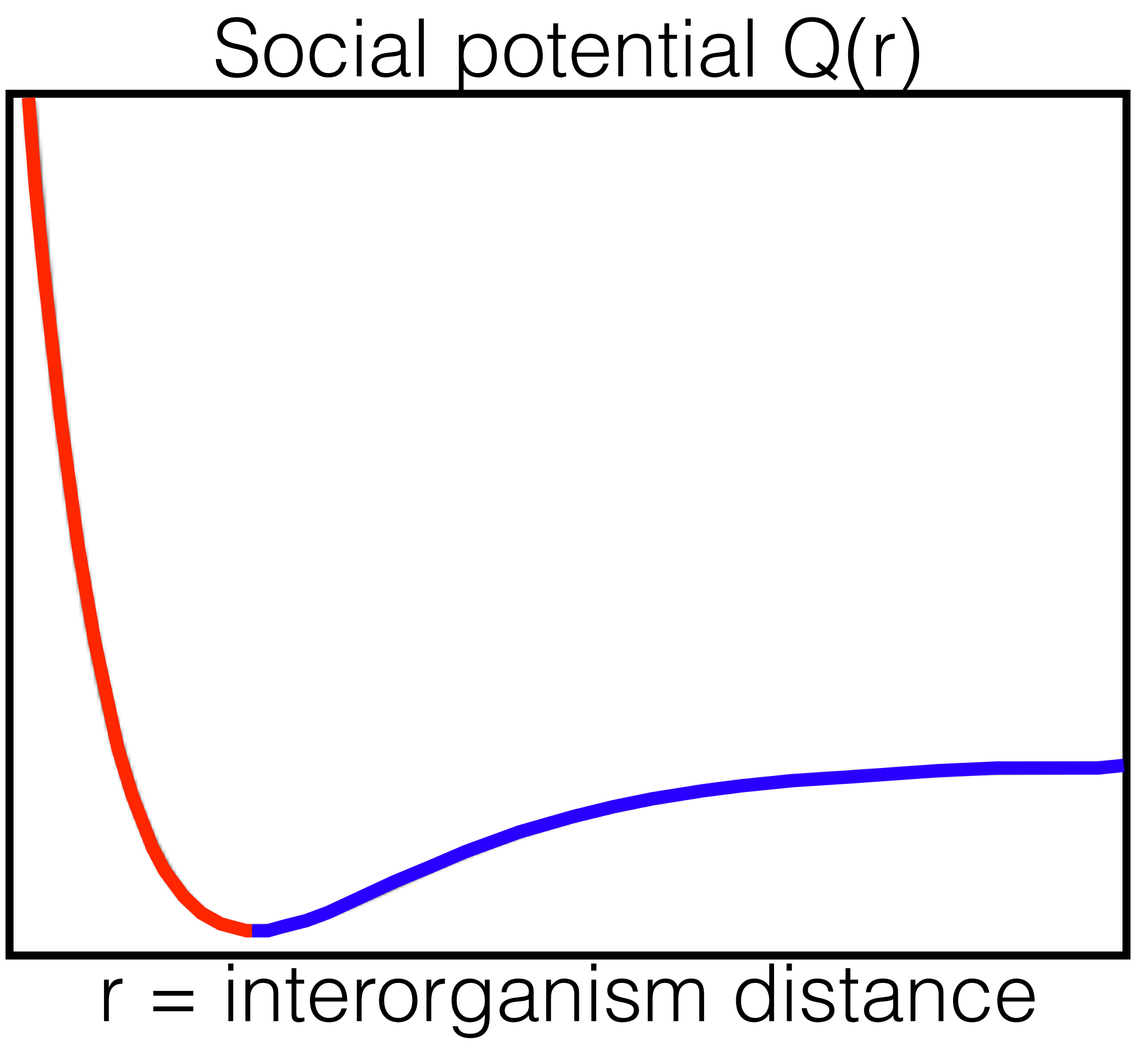
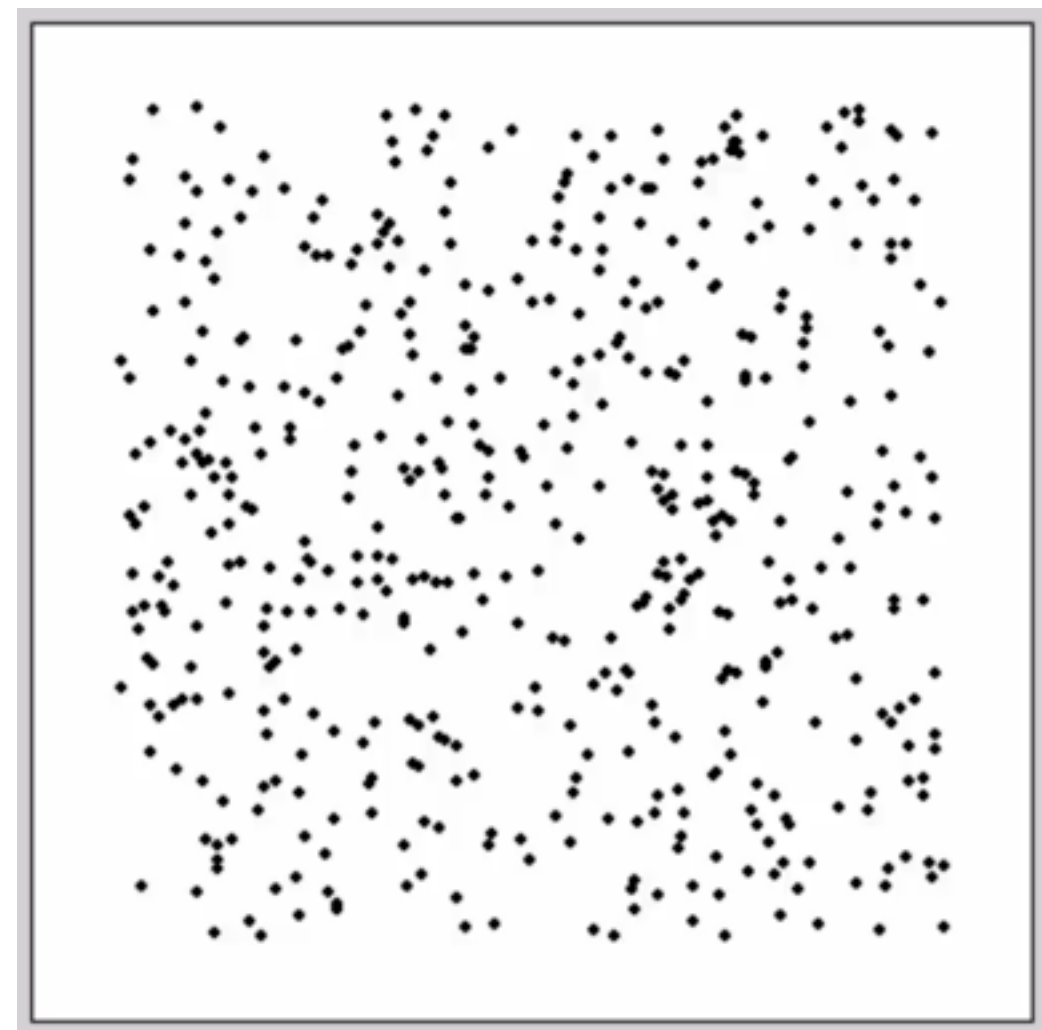
Example 2: D'Orsogna Model

$$
\begin{aligned}
\dot{\mathbf{x}}_i &= \mathbf{v}_i \\
m\dot{\mathbf{v}}_i &= \left(\alpha - \beta|\mathbf{v}_i|^2\right)\mathbf{v}_i - \nabla_i Q_i \\
Q_i &= \sum_{j\neq i} C_r e^{-|\mathbf{x}_i - \mathbf{x}_j|/L_r} \\
&\quad - C_a e^{-|\mathbf{x}_i - \mathbf{x}_j|/L_a}.
\end{aligned}
$$



Example 2:
D'Orsogna Model



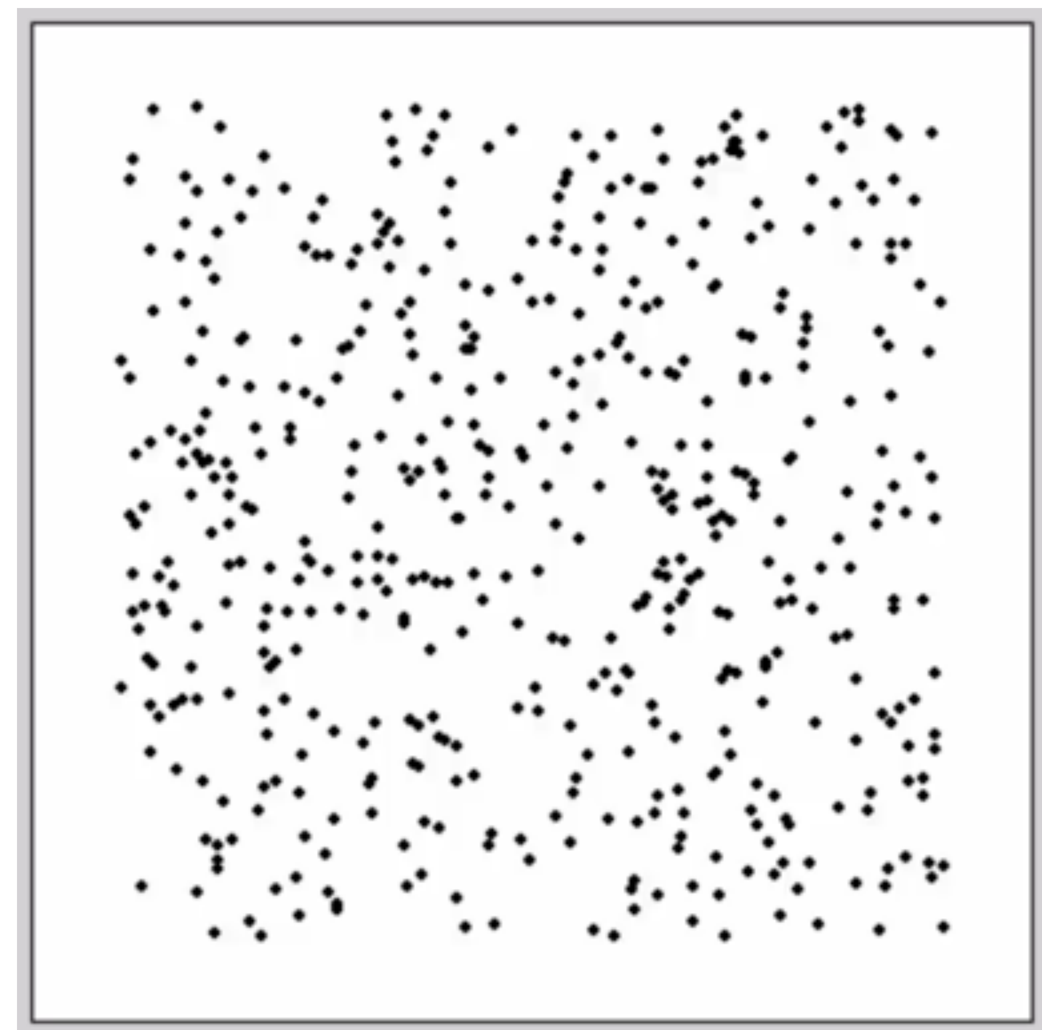


Example 2: D'Orsogna Model

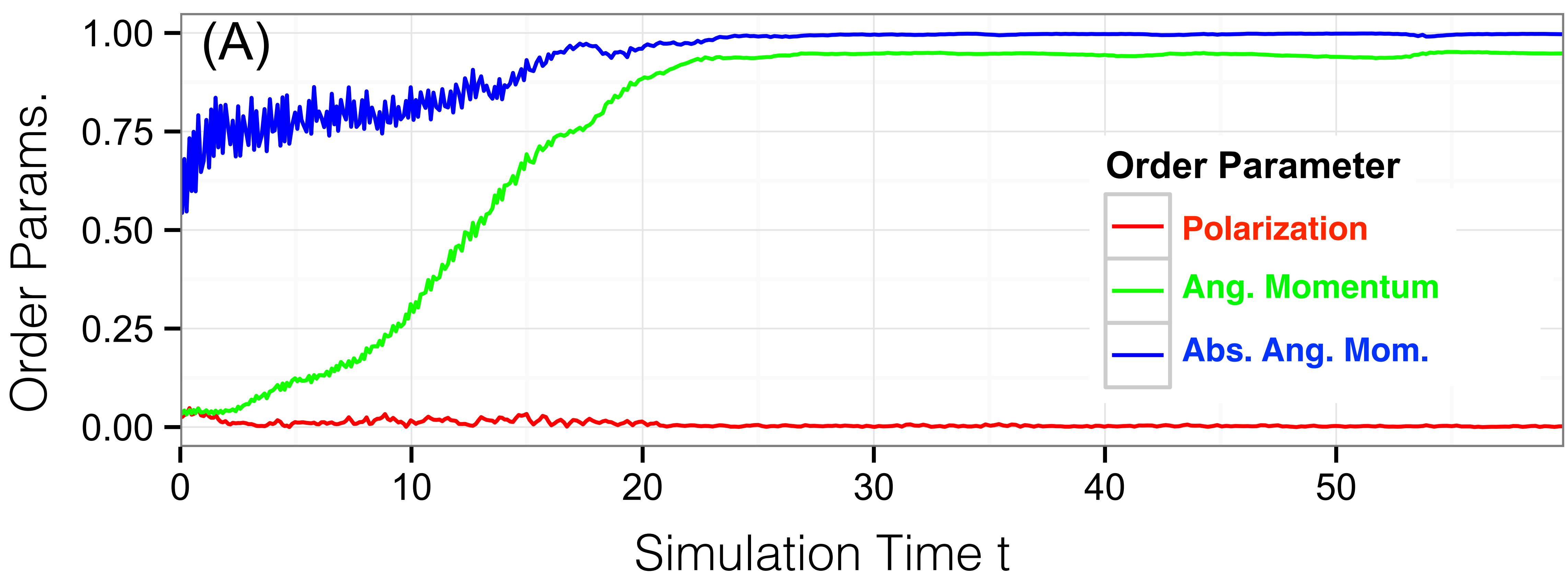
$$\dot{\mathbf{x}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = \left(\alpha - \beta|\mathbf{v}_i|^2\right)\mathbf{v}_i - \nabla_i Q_i$$

$$Q_i = \sum_{j \neq i} C_r e^{-|\mathbf{x}_i - \mathbf{x}_j|/L_r} - C_a e^{-|\mathbf{x}_i - \mathbf{x}_j|/L_a}.$$



Example 2: D'Orsogna Model



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 asses different scales
   - calculate persistent homology
5. Evolve in time
   - CROCKER plots

The big picture: Study data via topology

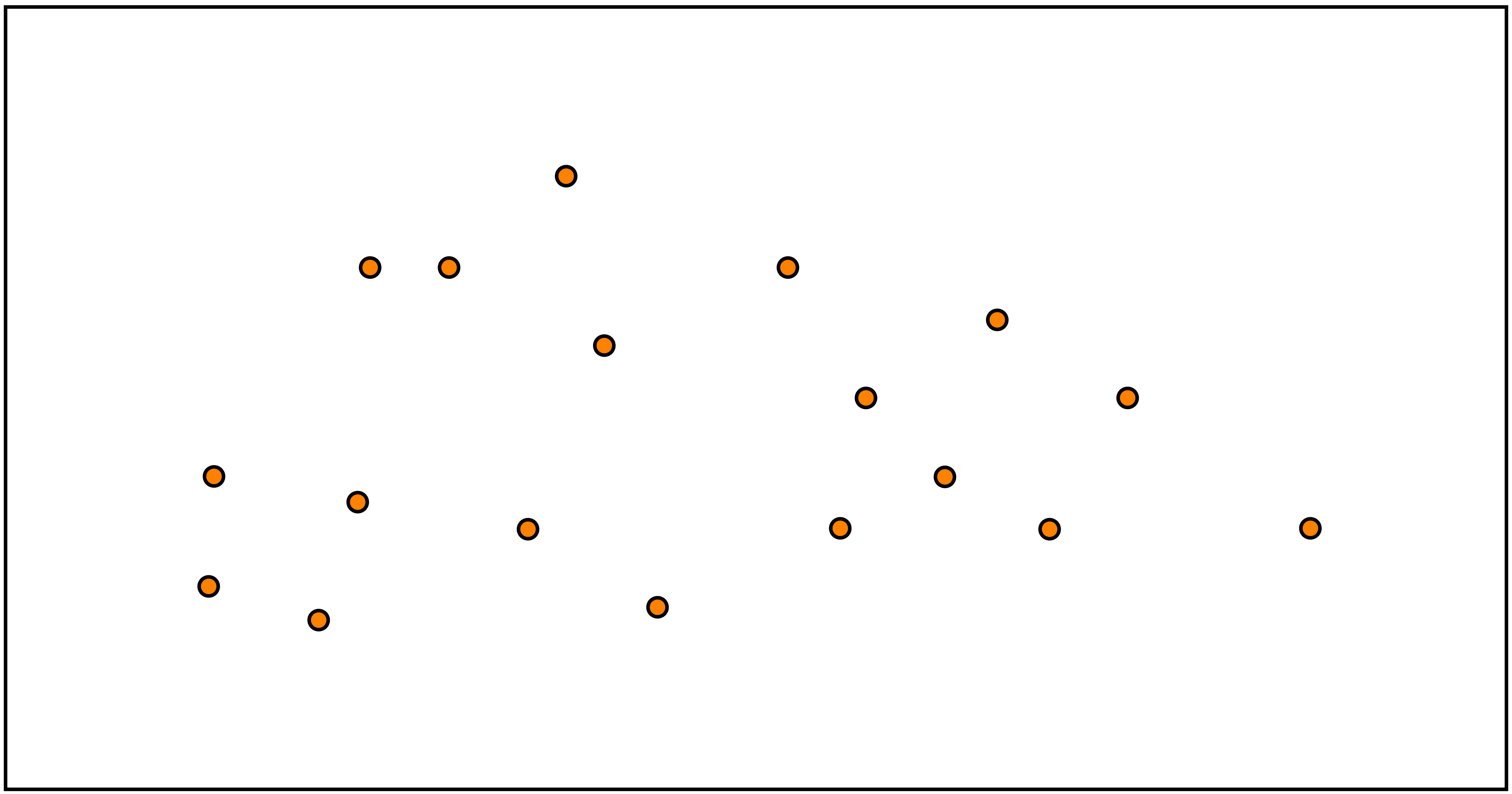
1. Computing persistent homology
   A. Zomorodian, G. Carlsson. Disc. & Comp. Geom. (2005)

2. Barcodes: The persistent topology of data
   R. Ghrist. Bull. Am. Math. Soc. (2008)

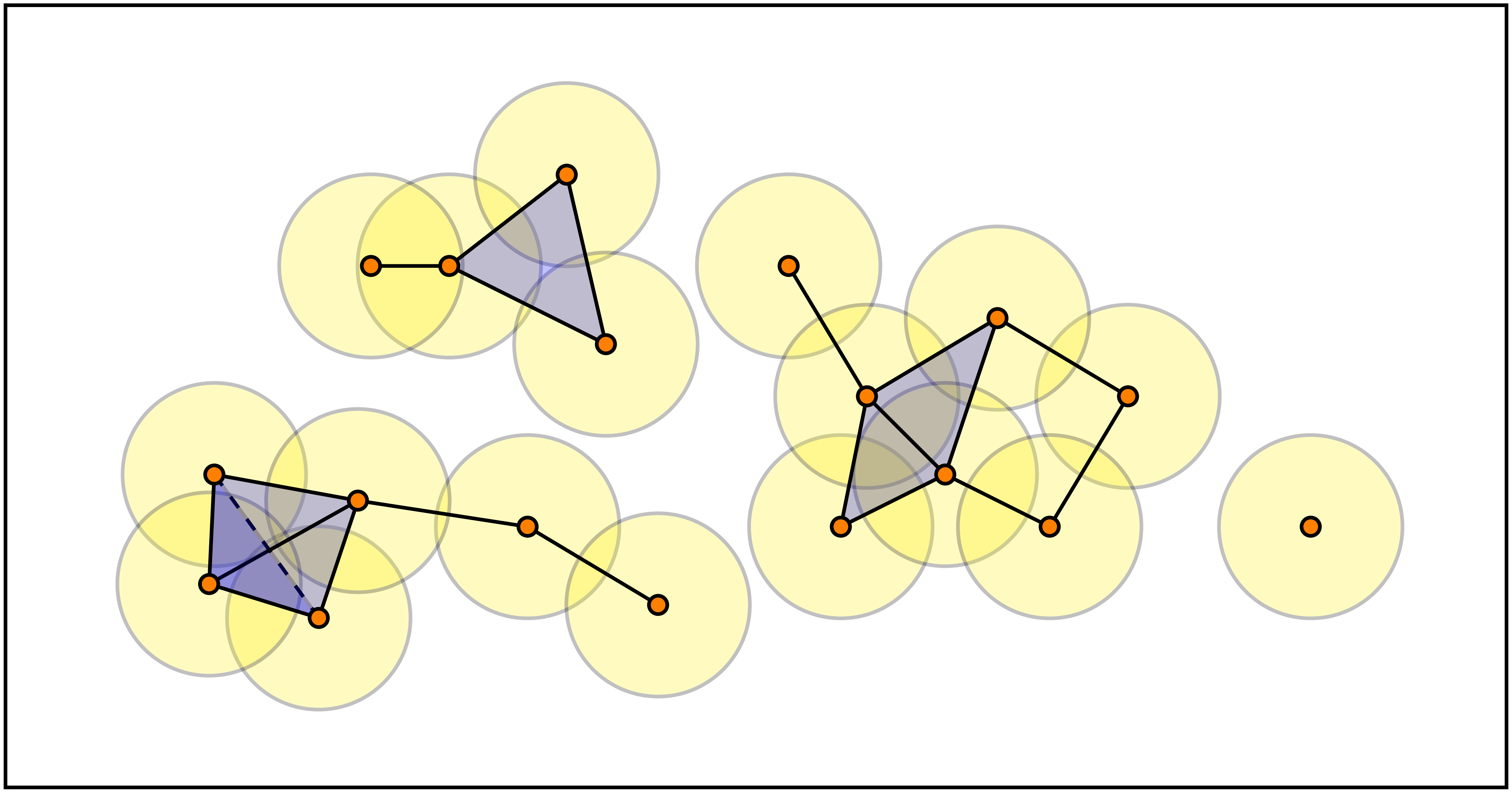
3. Persistent homology: A Survey
   H. Edelsbrunner, J. Harer. Contemp. Math. (2008)

4. Topology and Data
   G. Carlsson. Bull. Am. Math. Soc. (2009)

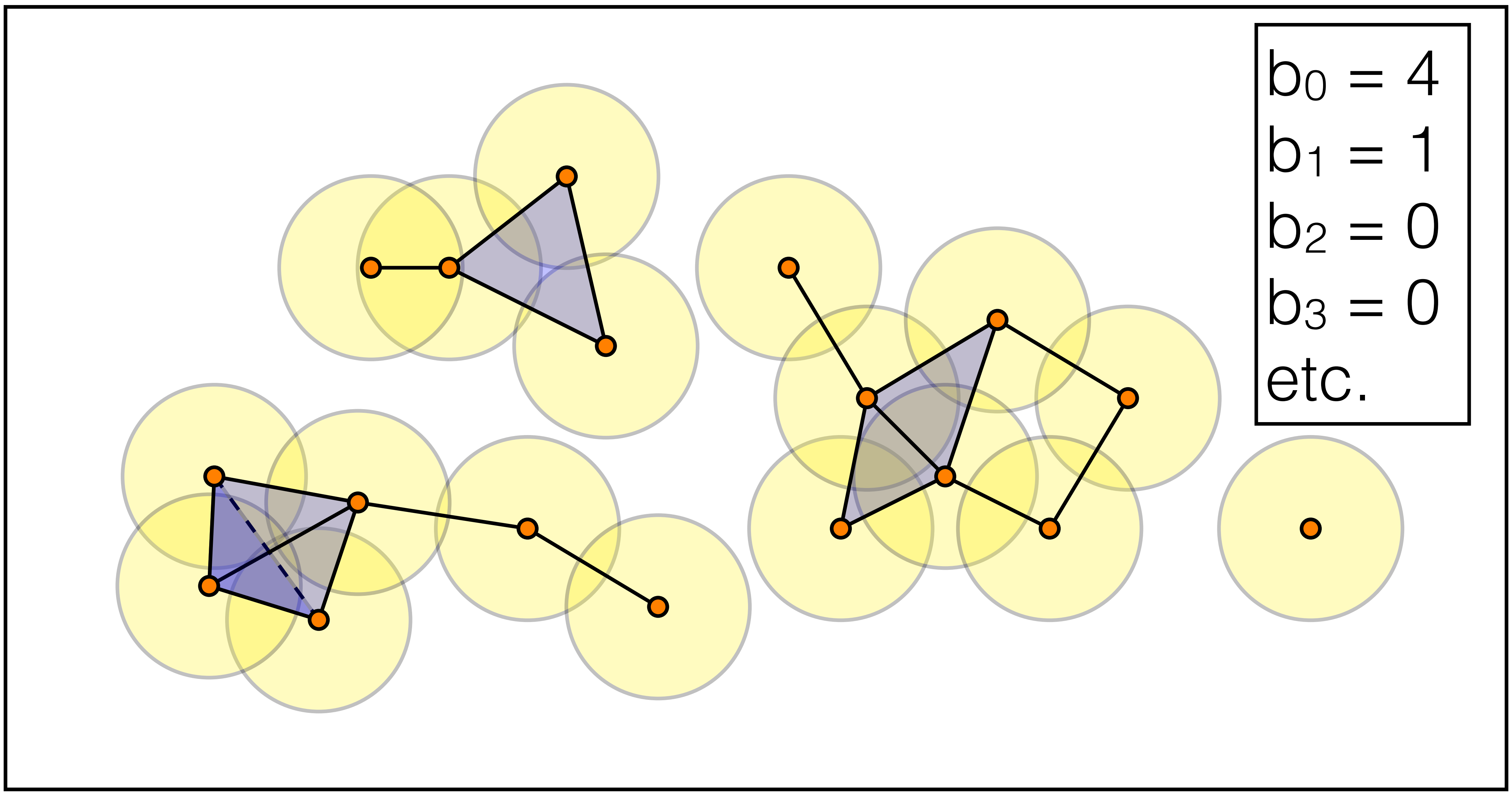
Step 1:
Envision data as point cloud



Step 2:
Build simplicial complex

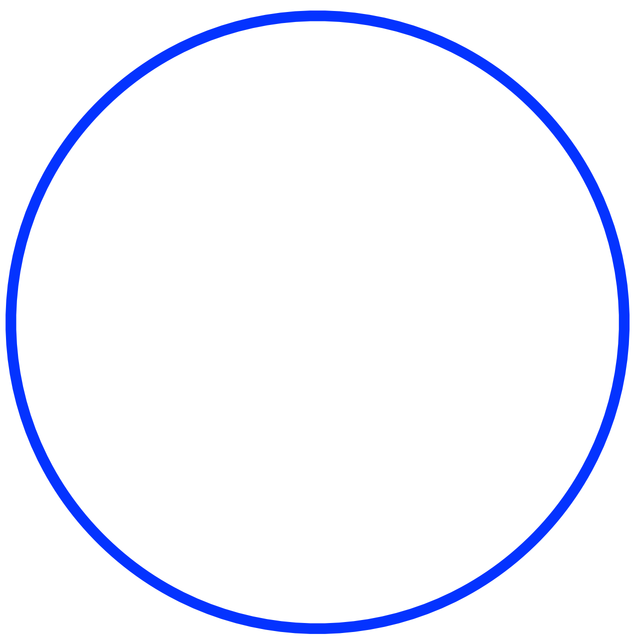


Step 3:
Calculate Betti numbers



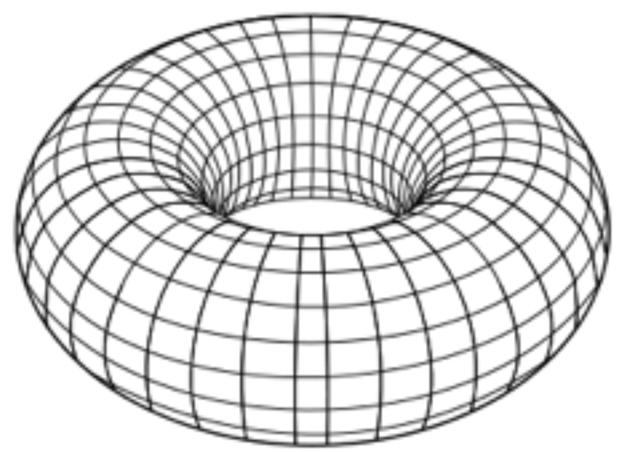
Step 3:
Calculate Betti numbers

Circle



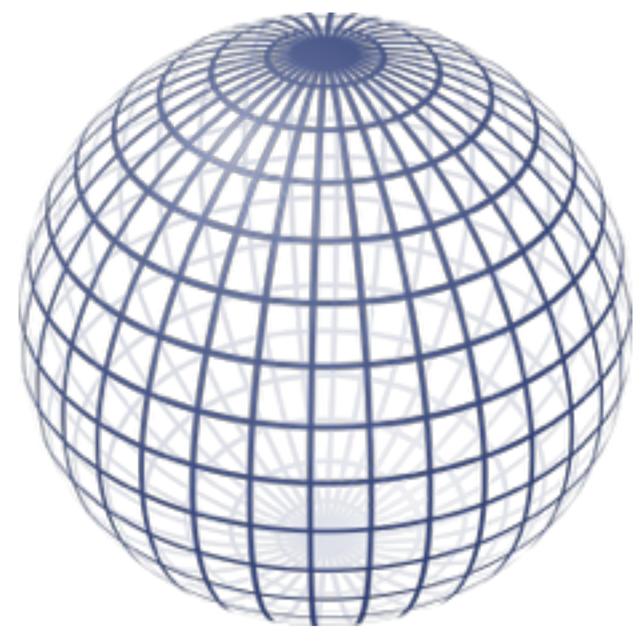
b=(1,1,0,0,...)

Two-Torus



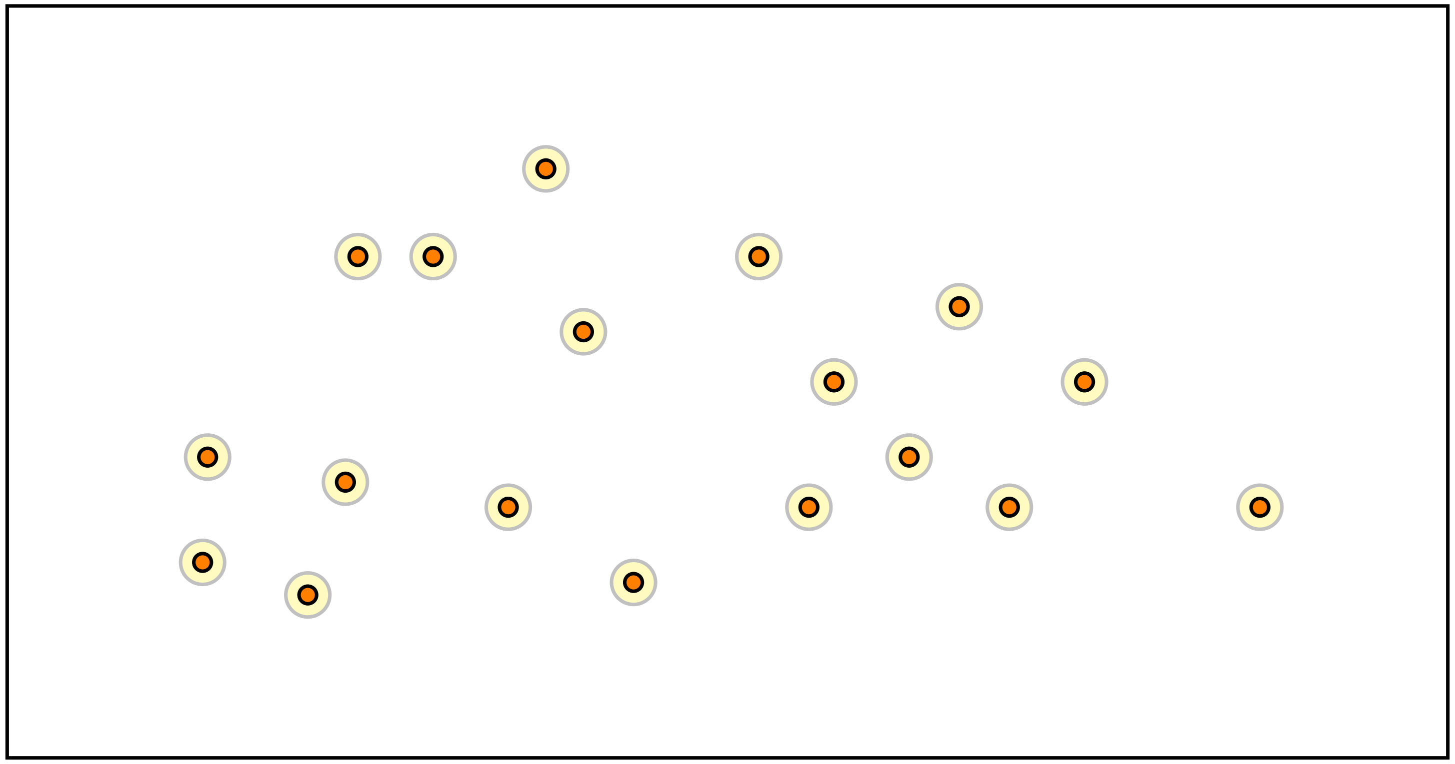
b=(1,2,1,0,...)

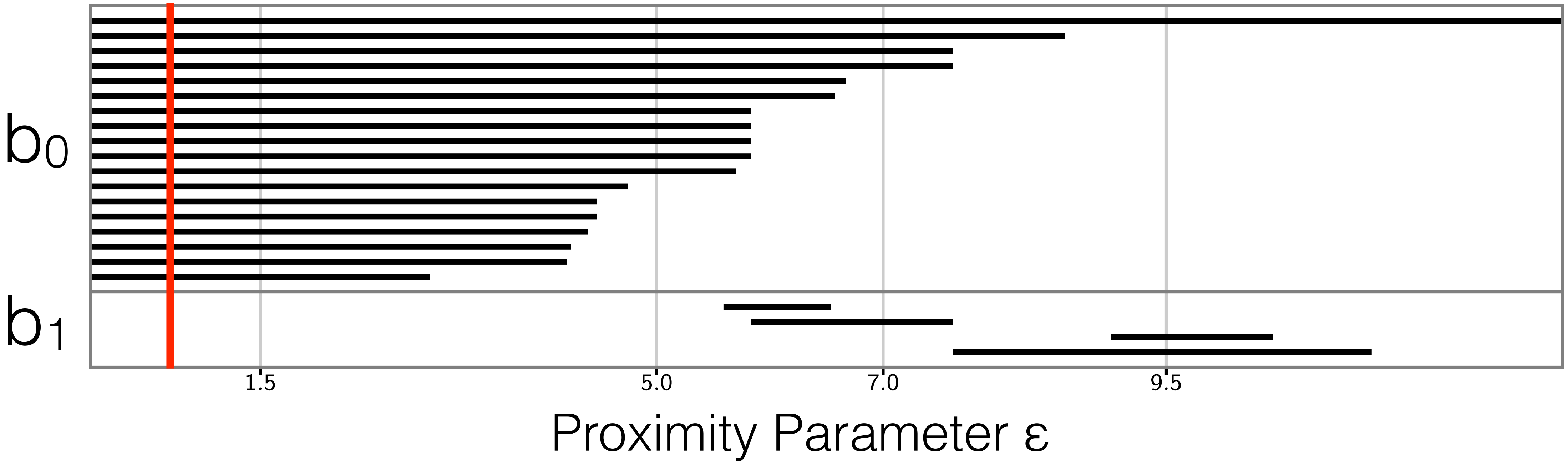
Two-Sphere



b=(1,0,1,0,...)

Step 4:
Find persistent homology





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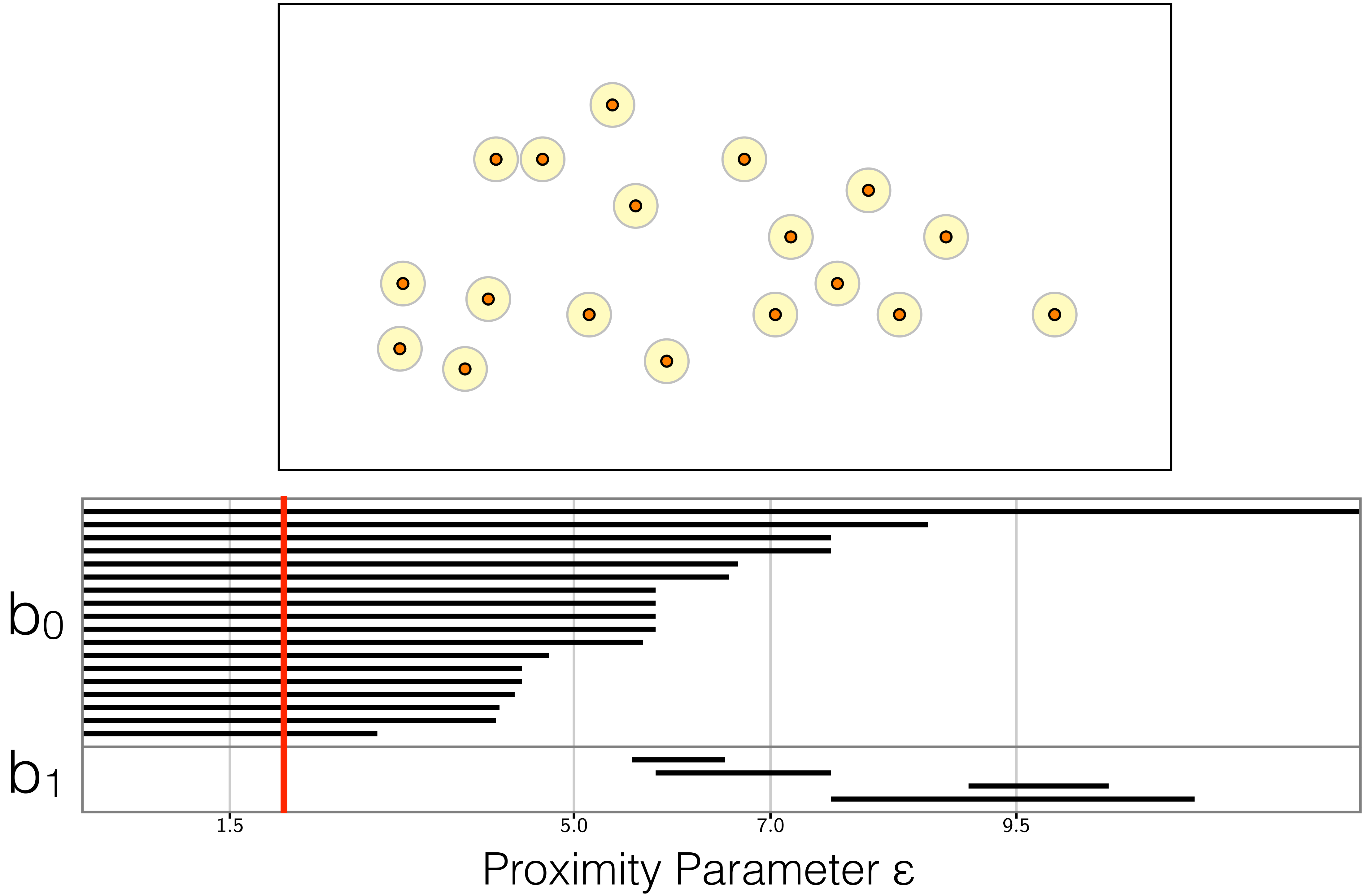

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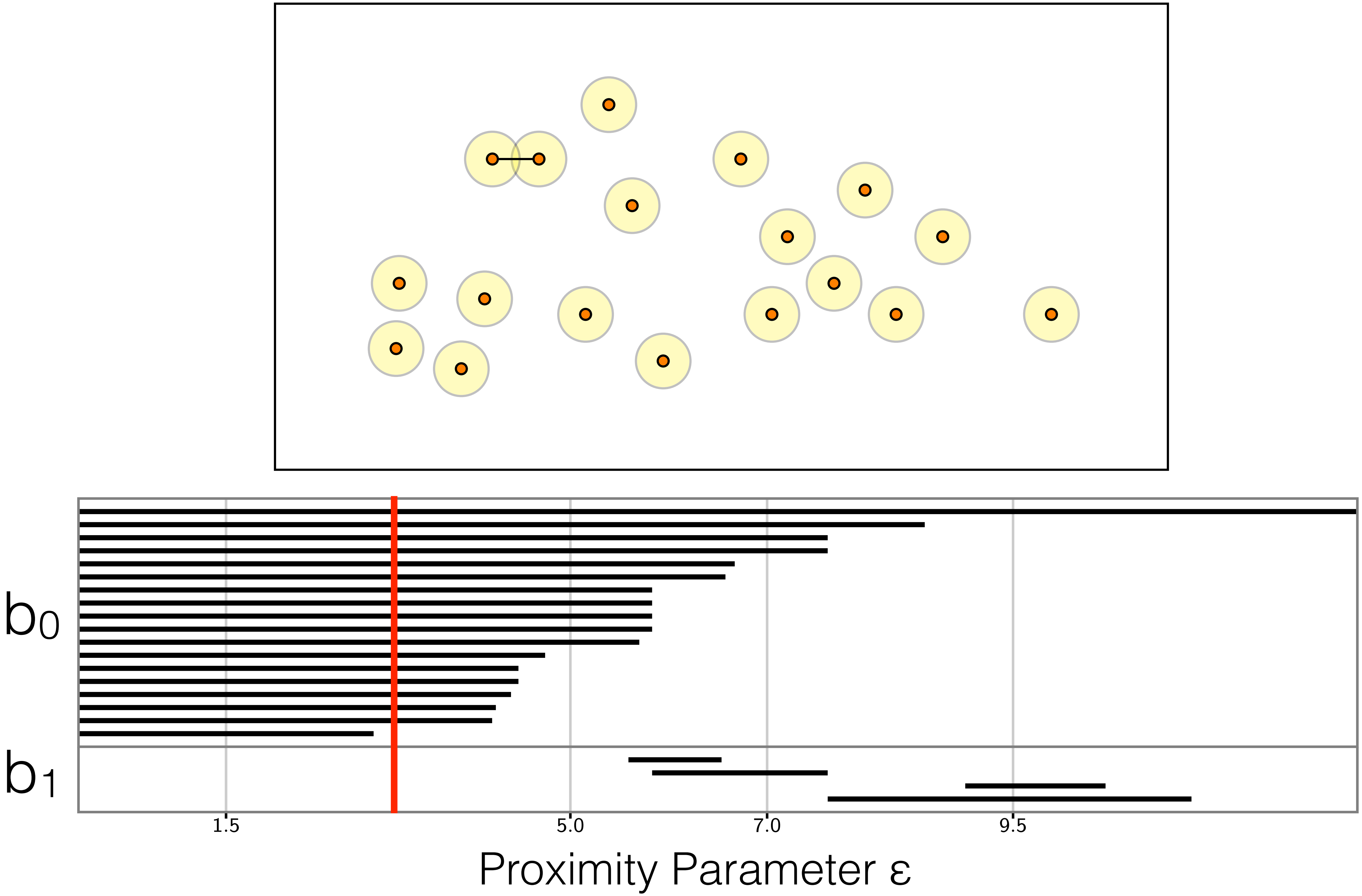
Find persistent homology



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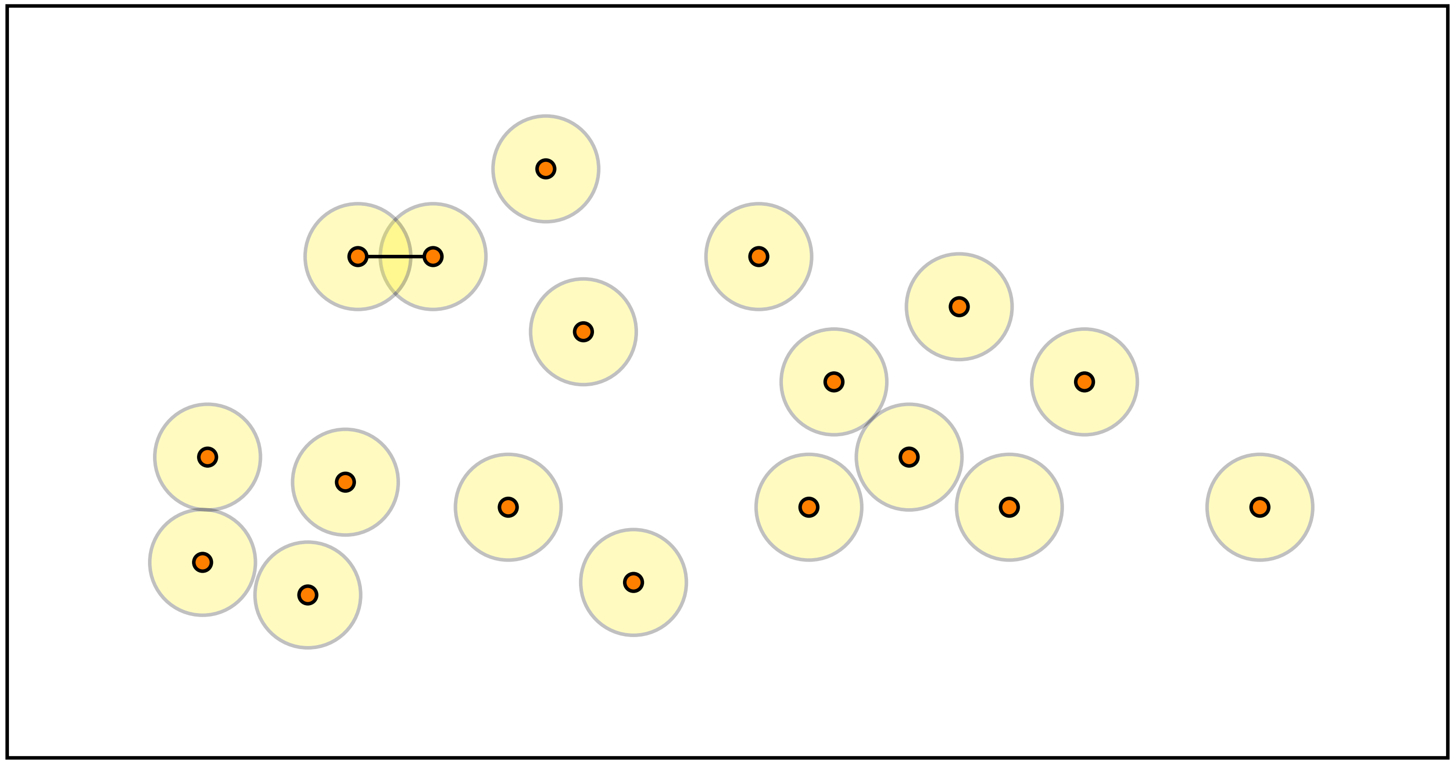

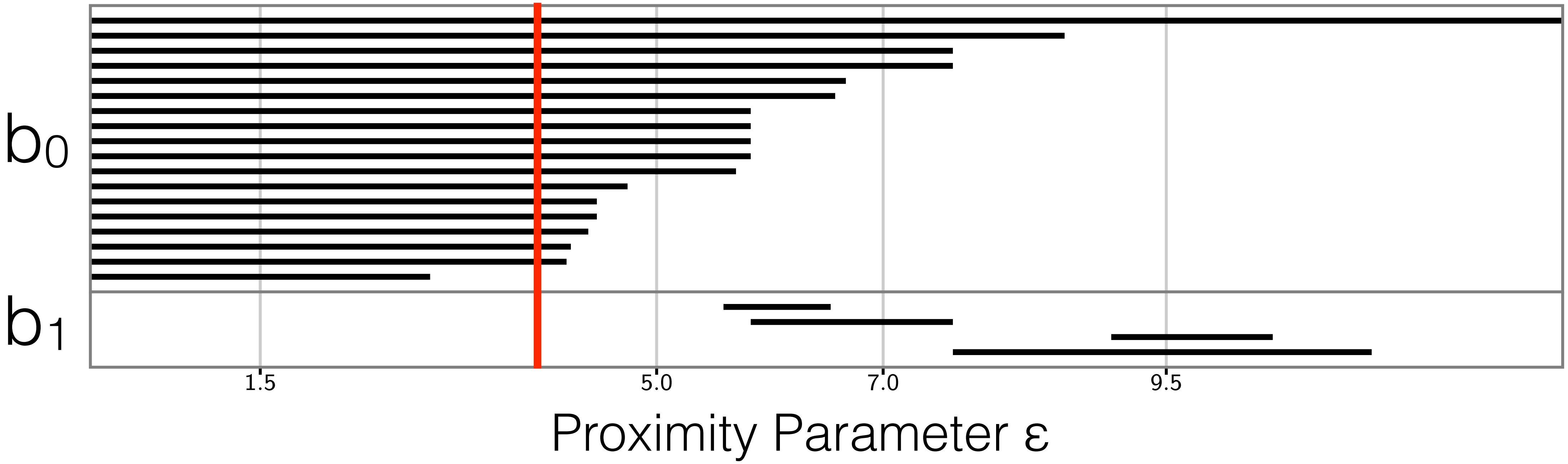

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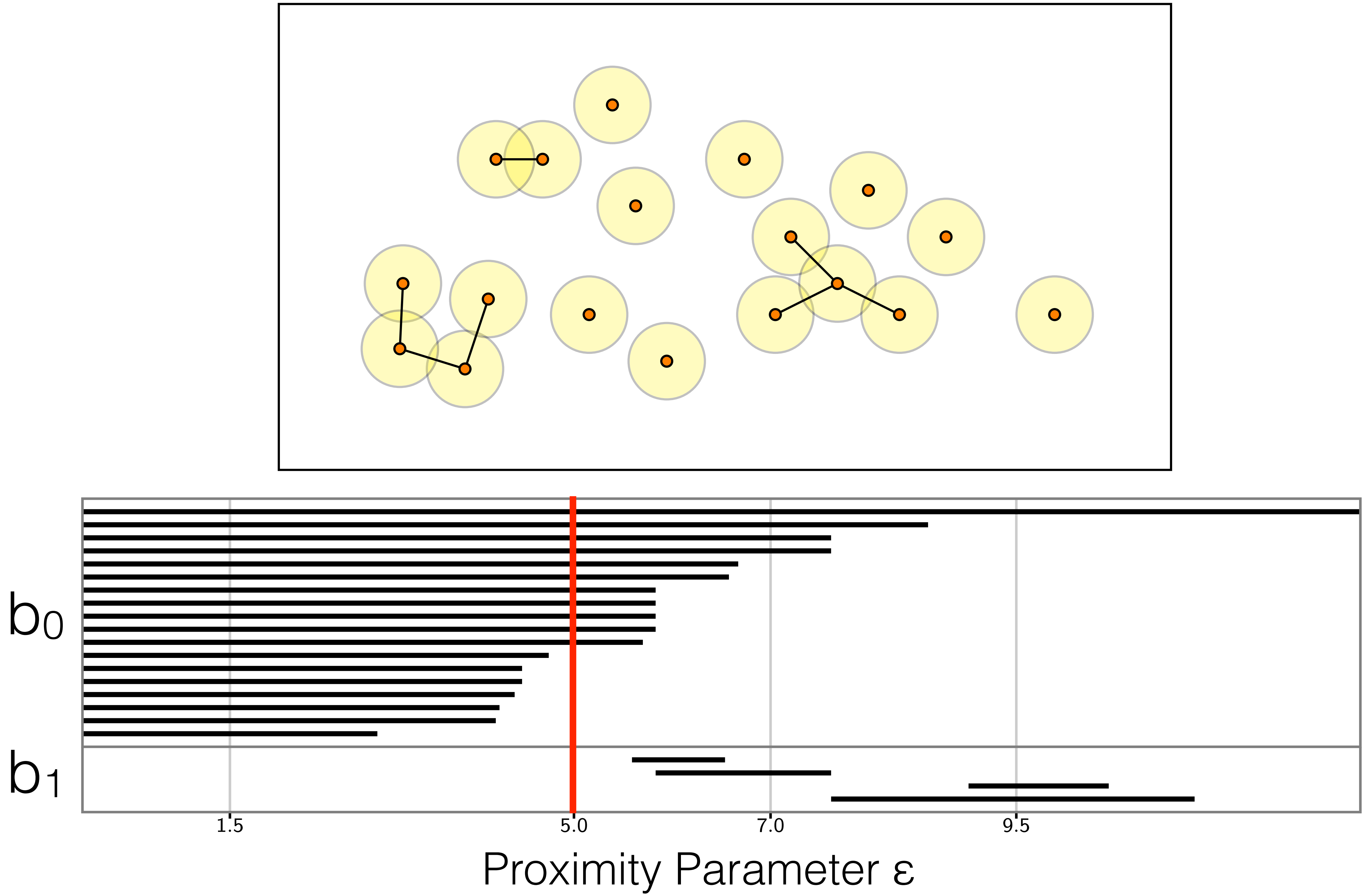

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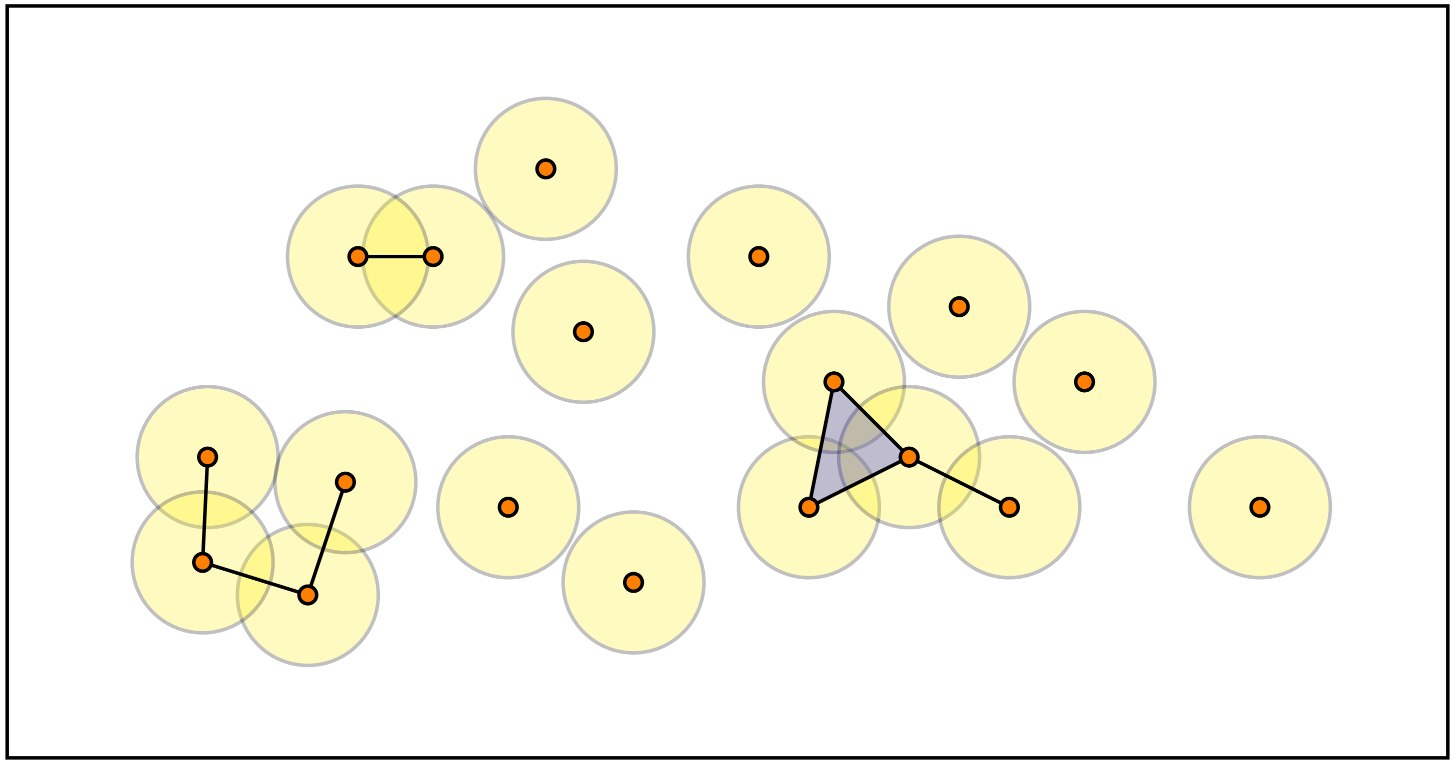

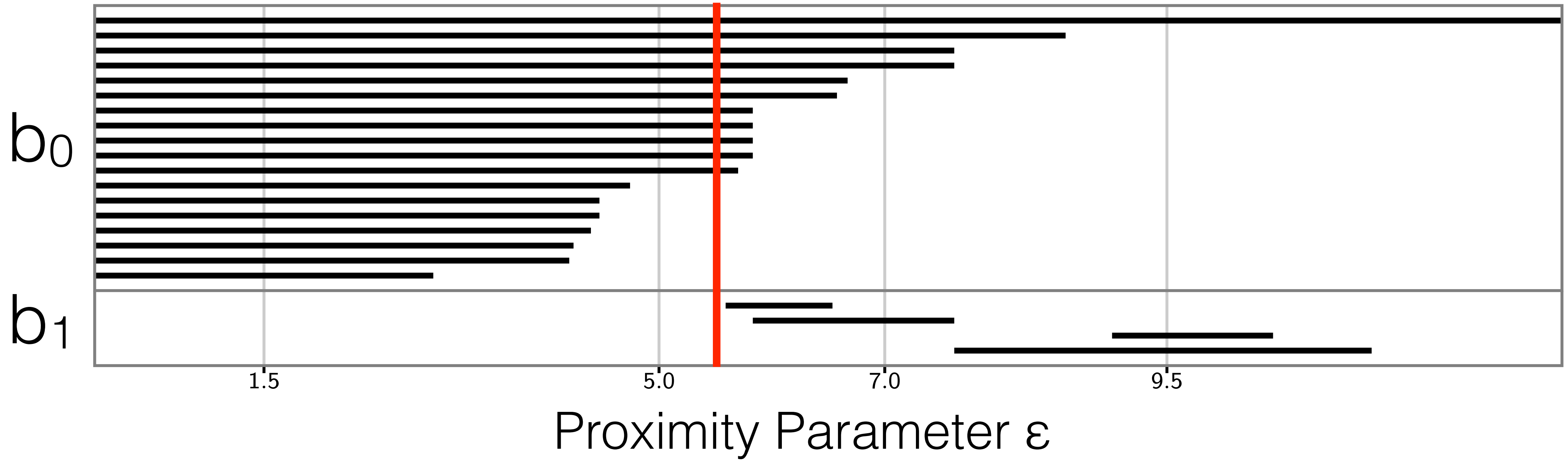

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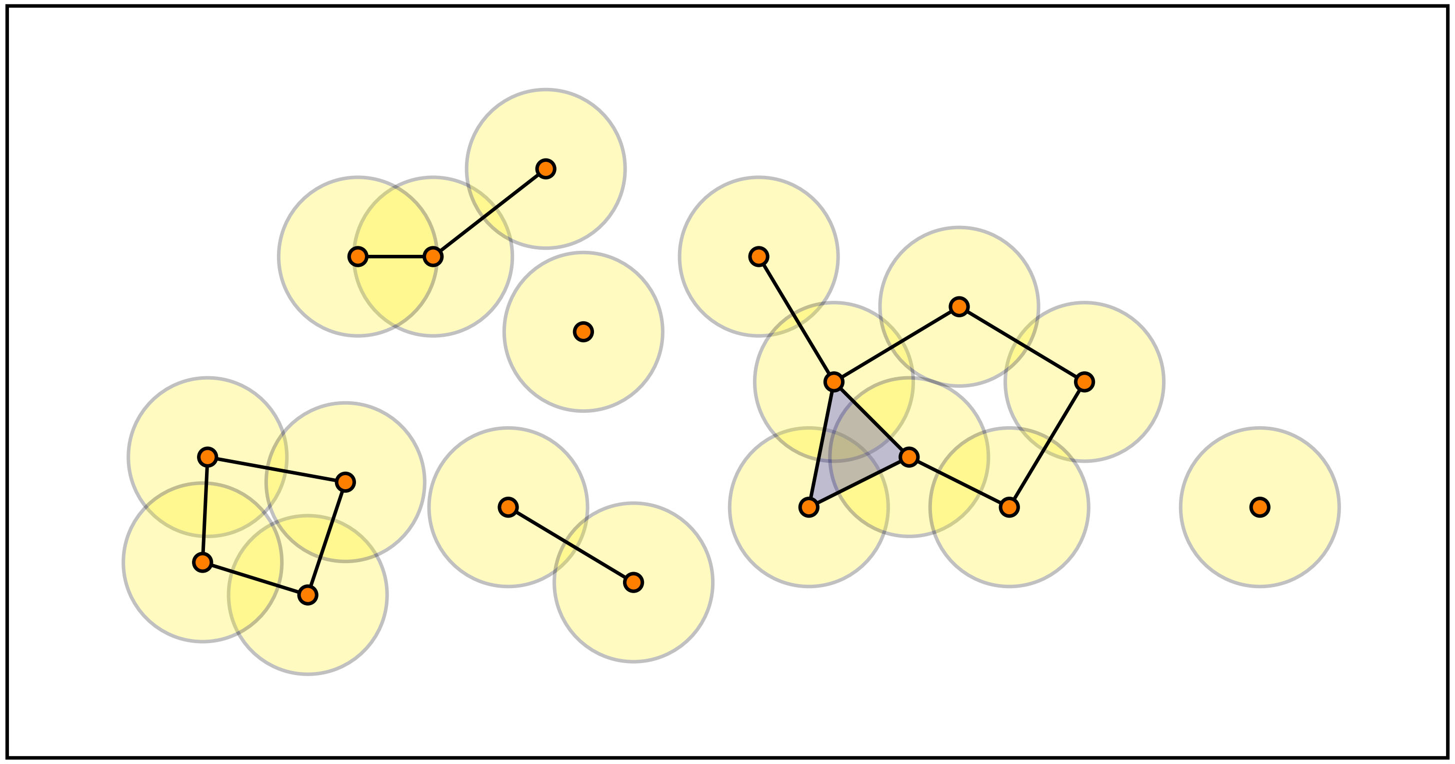

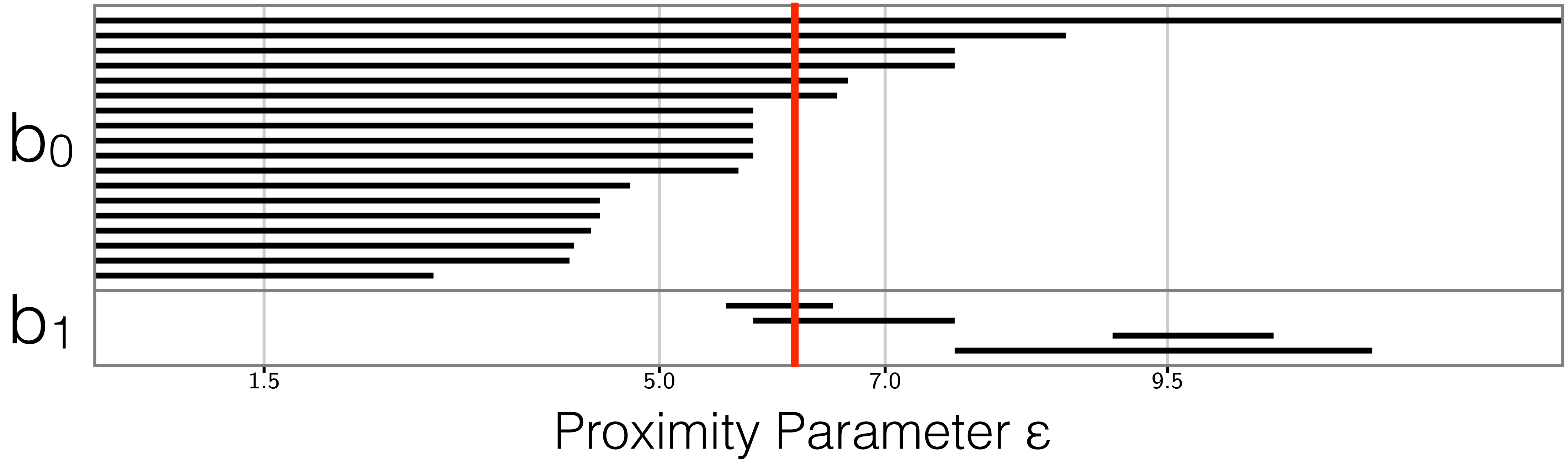

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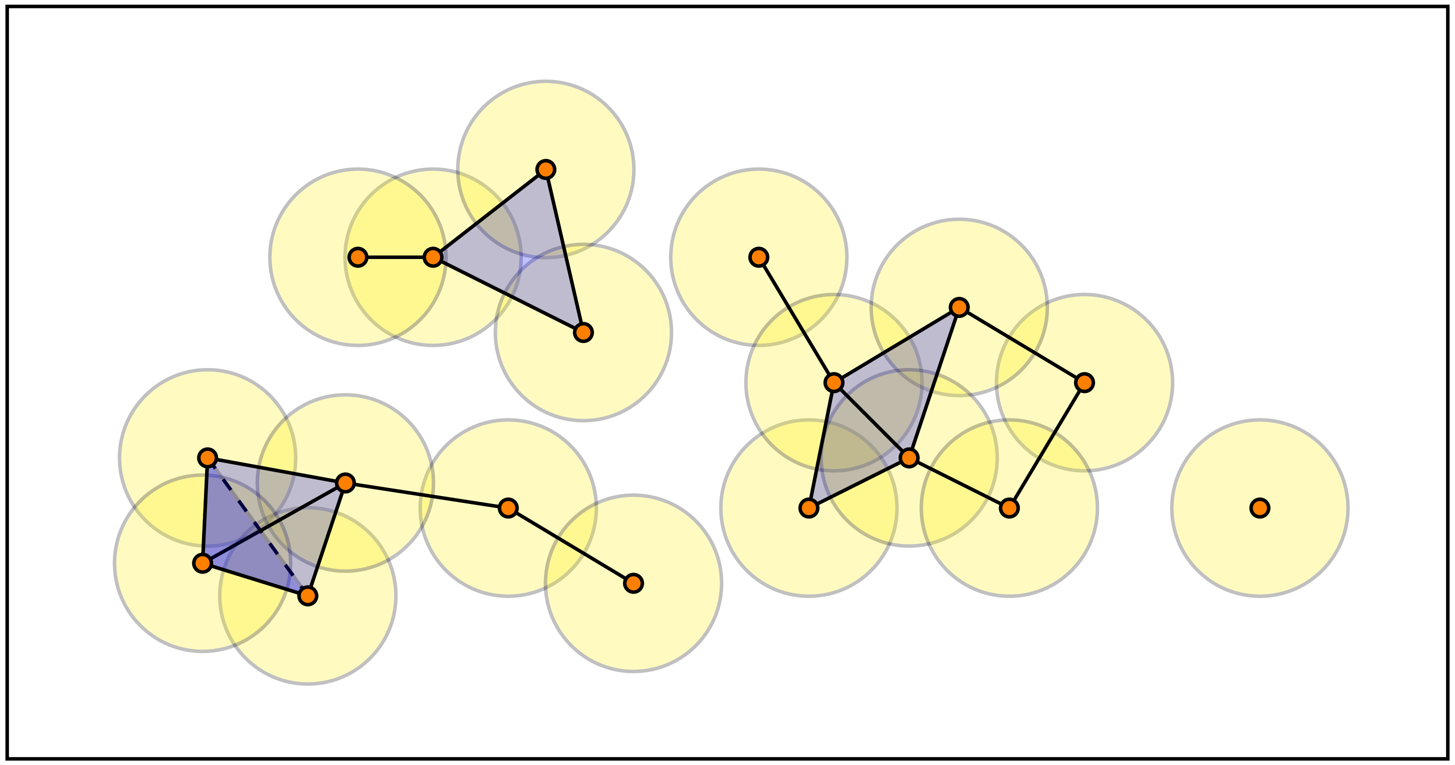

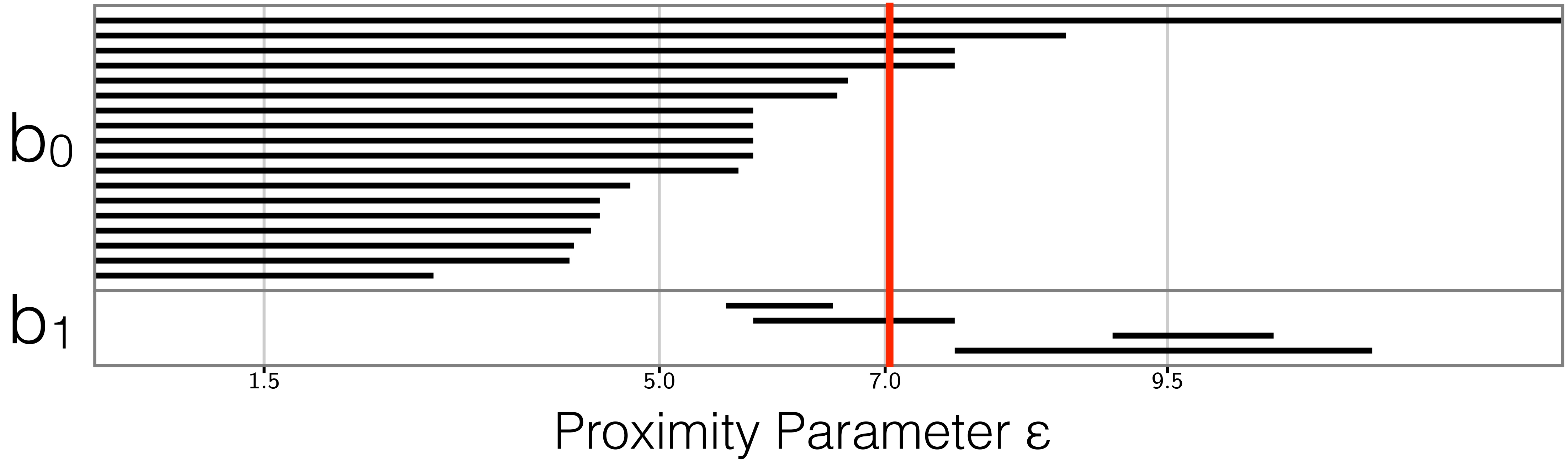

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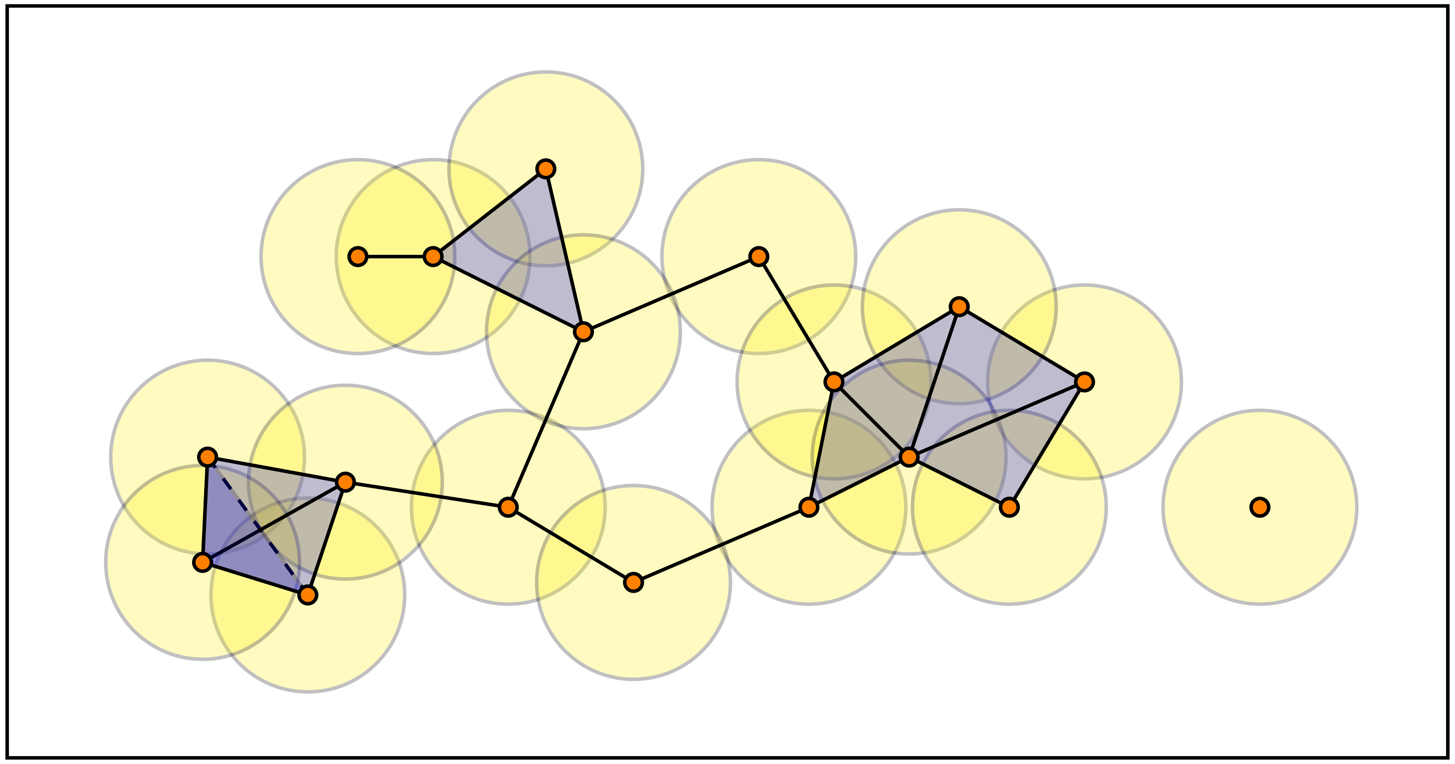

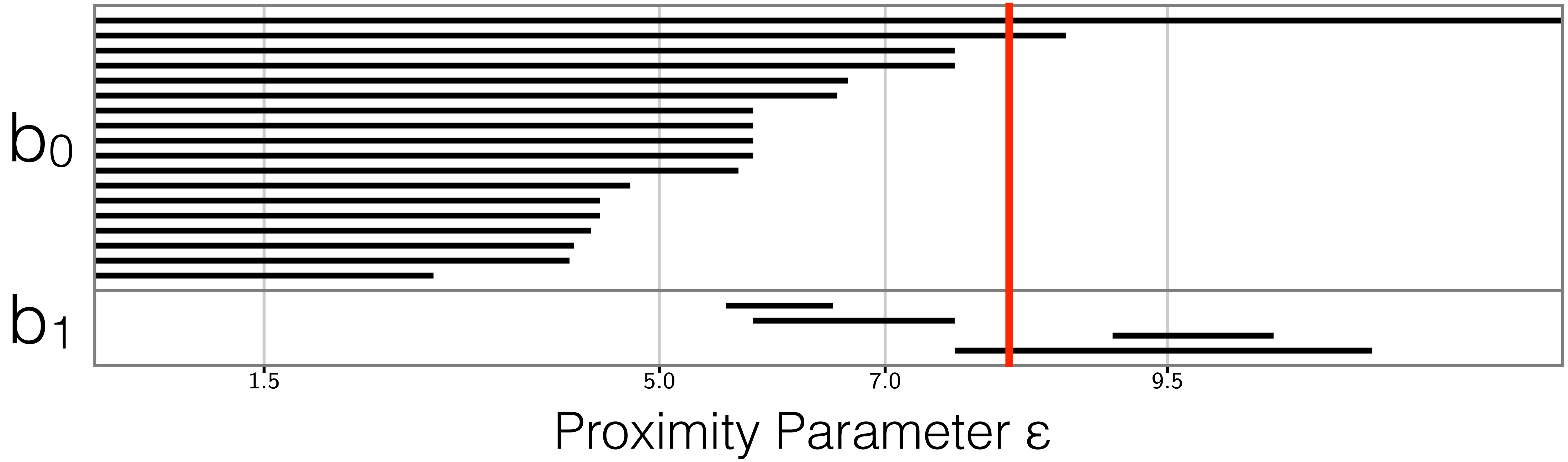

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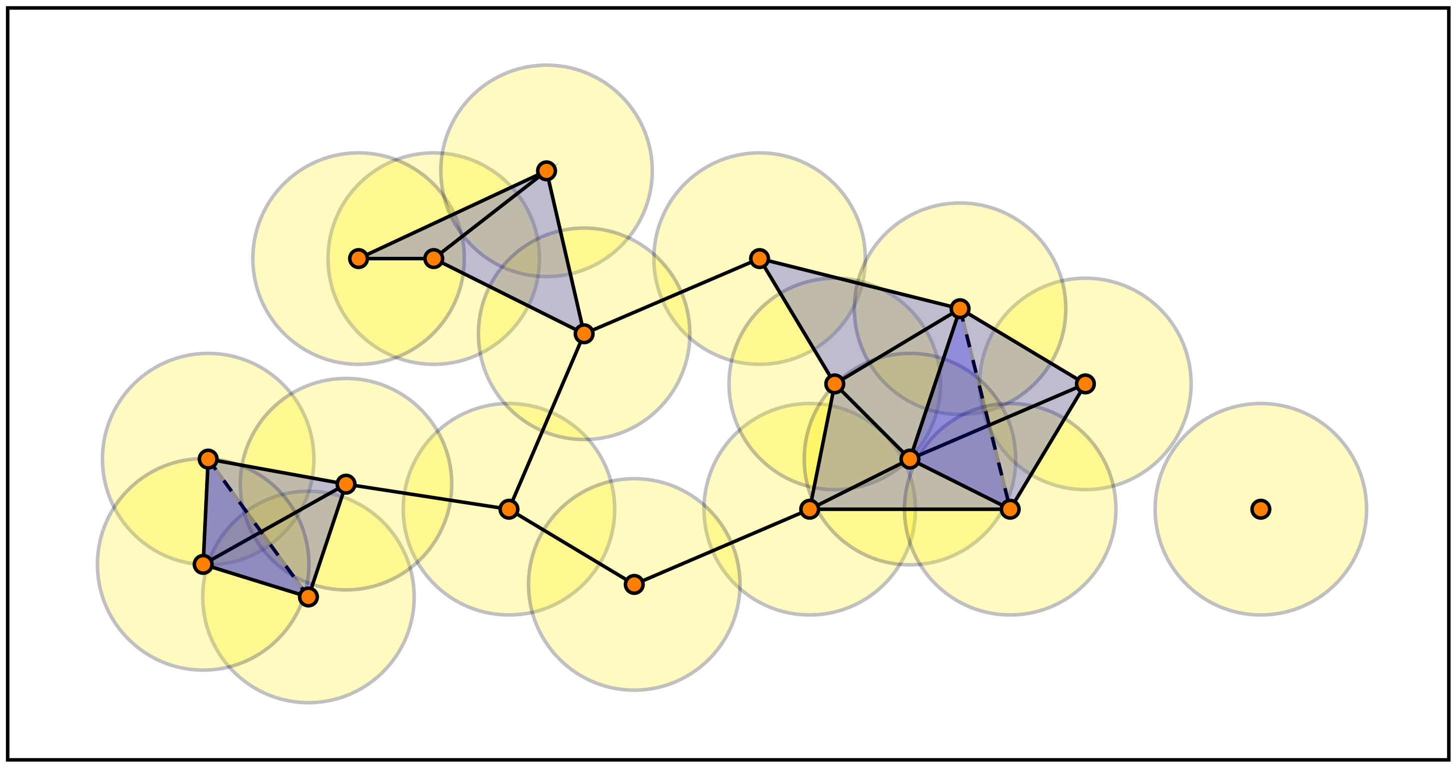
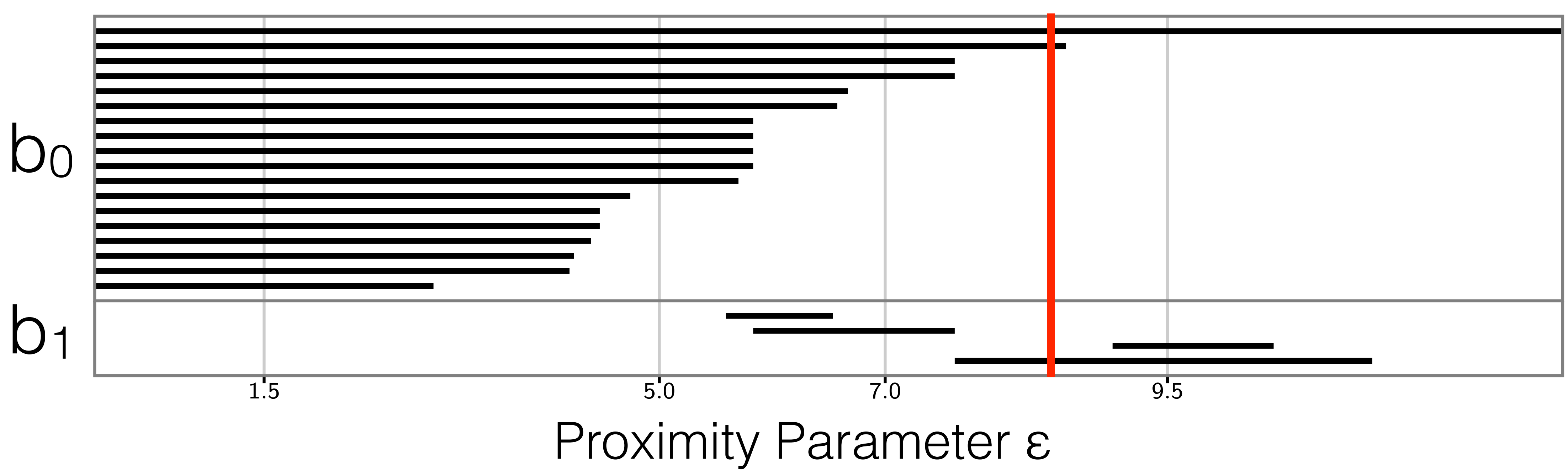
Find persistent homology





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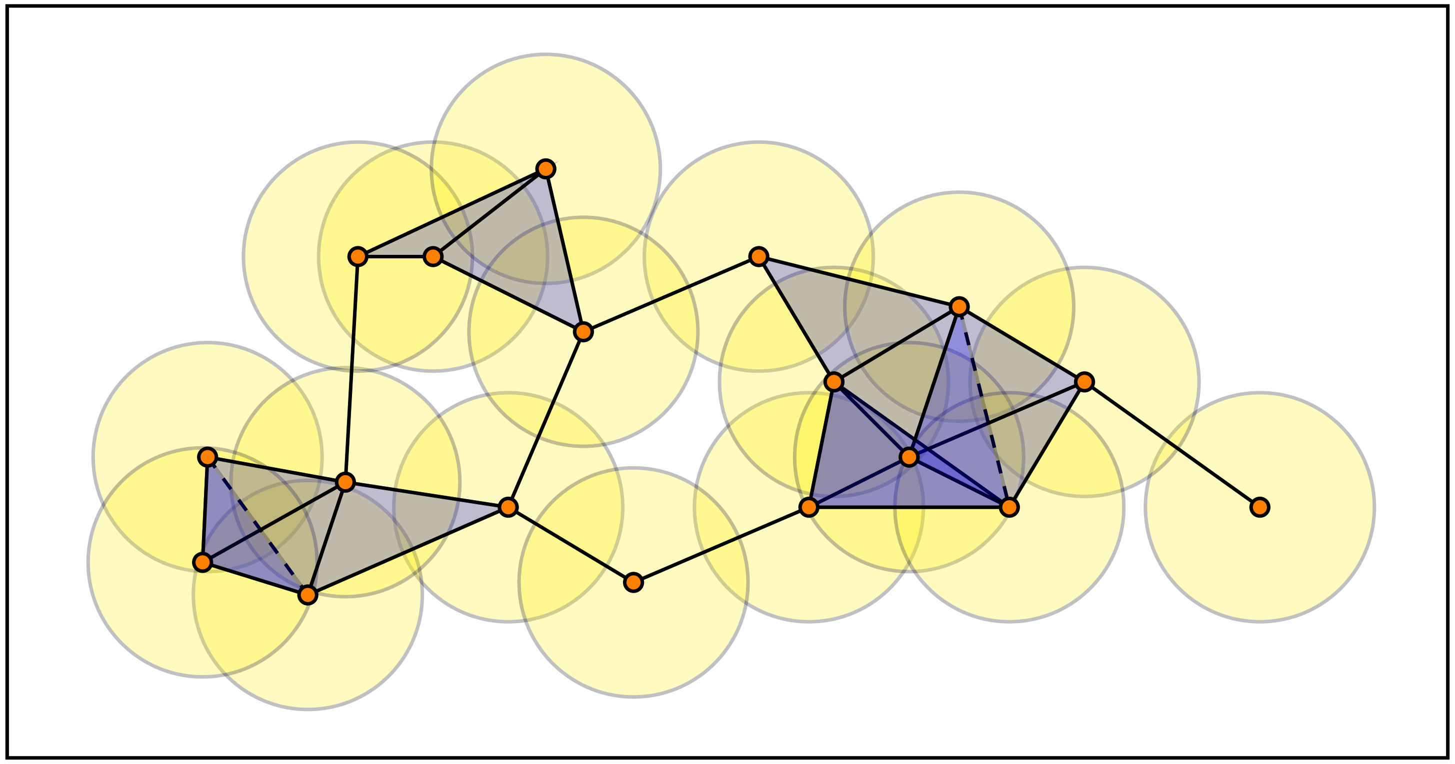

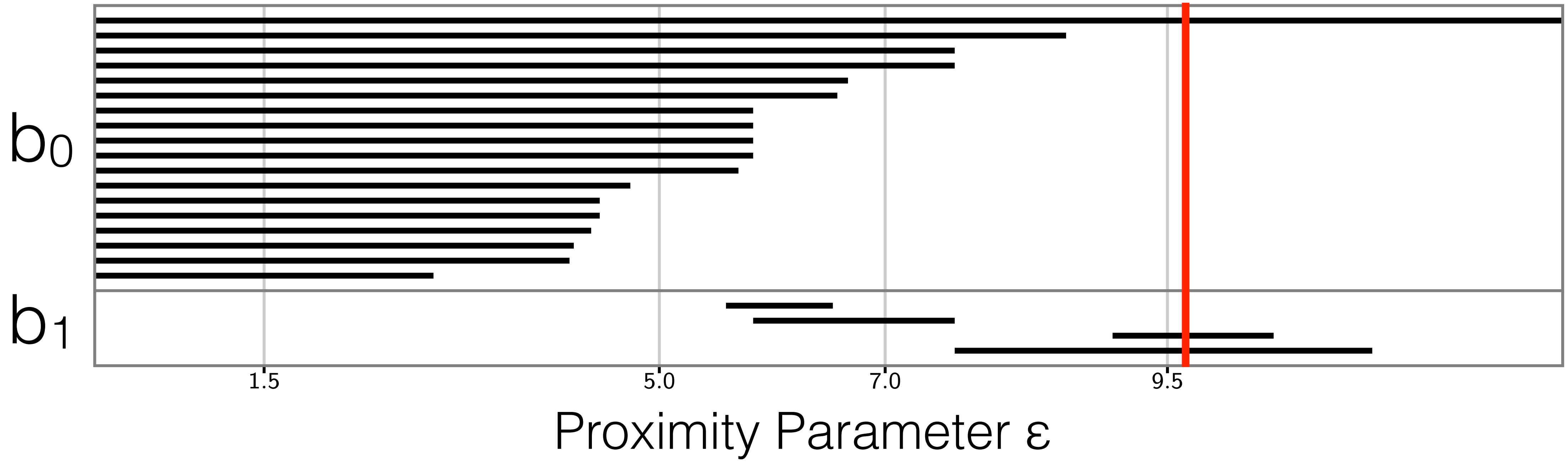

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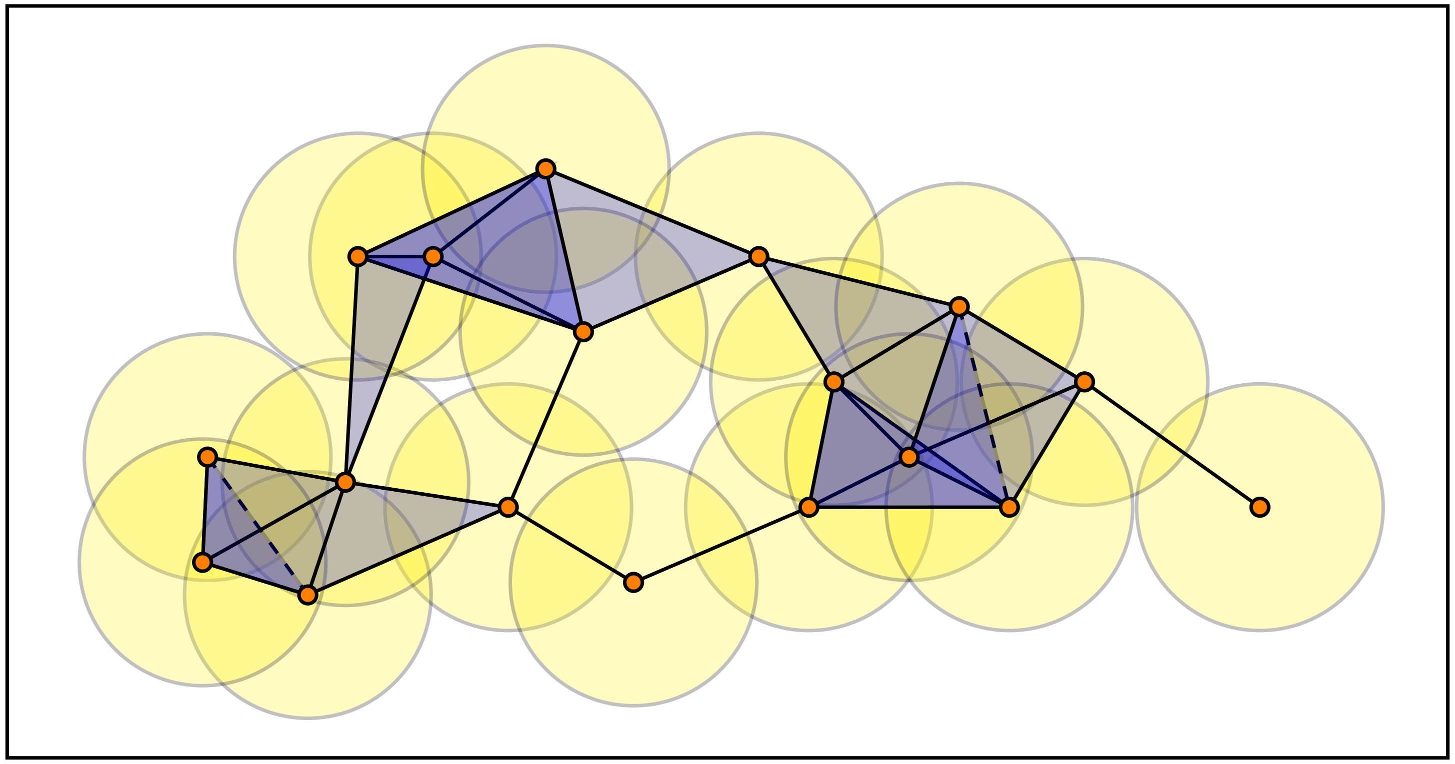

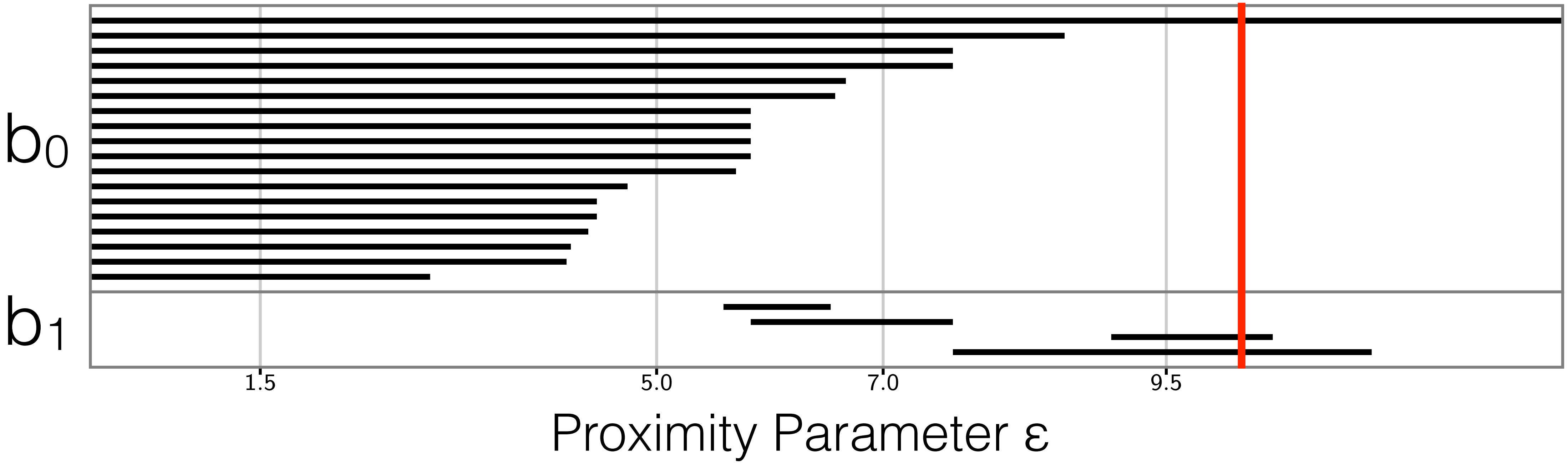

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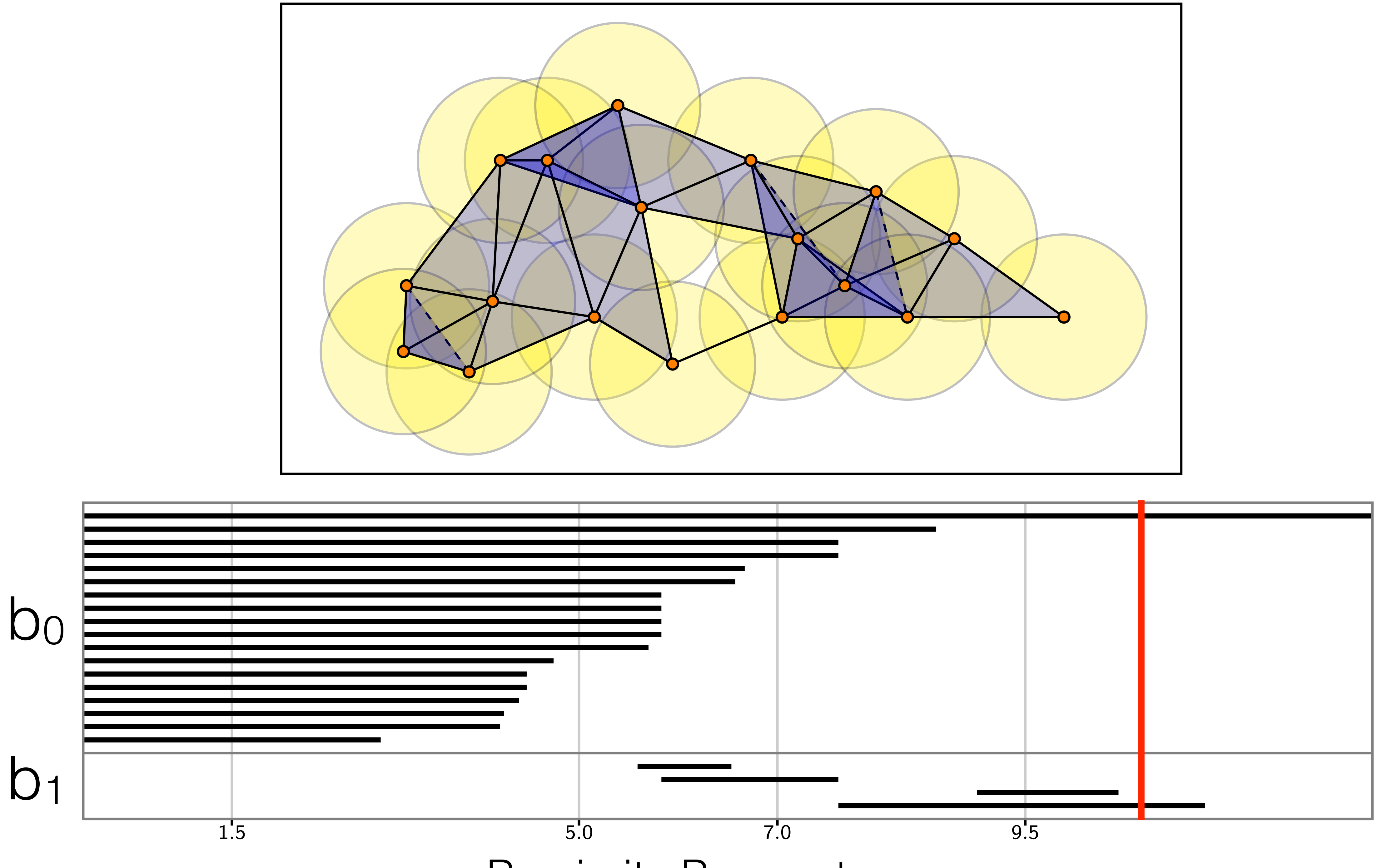

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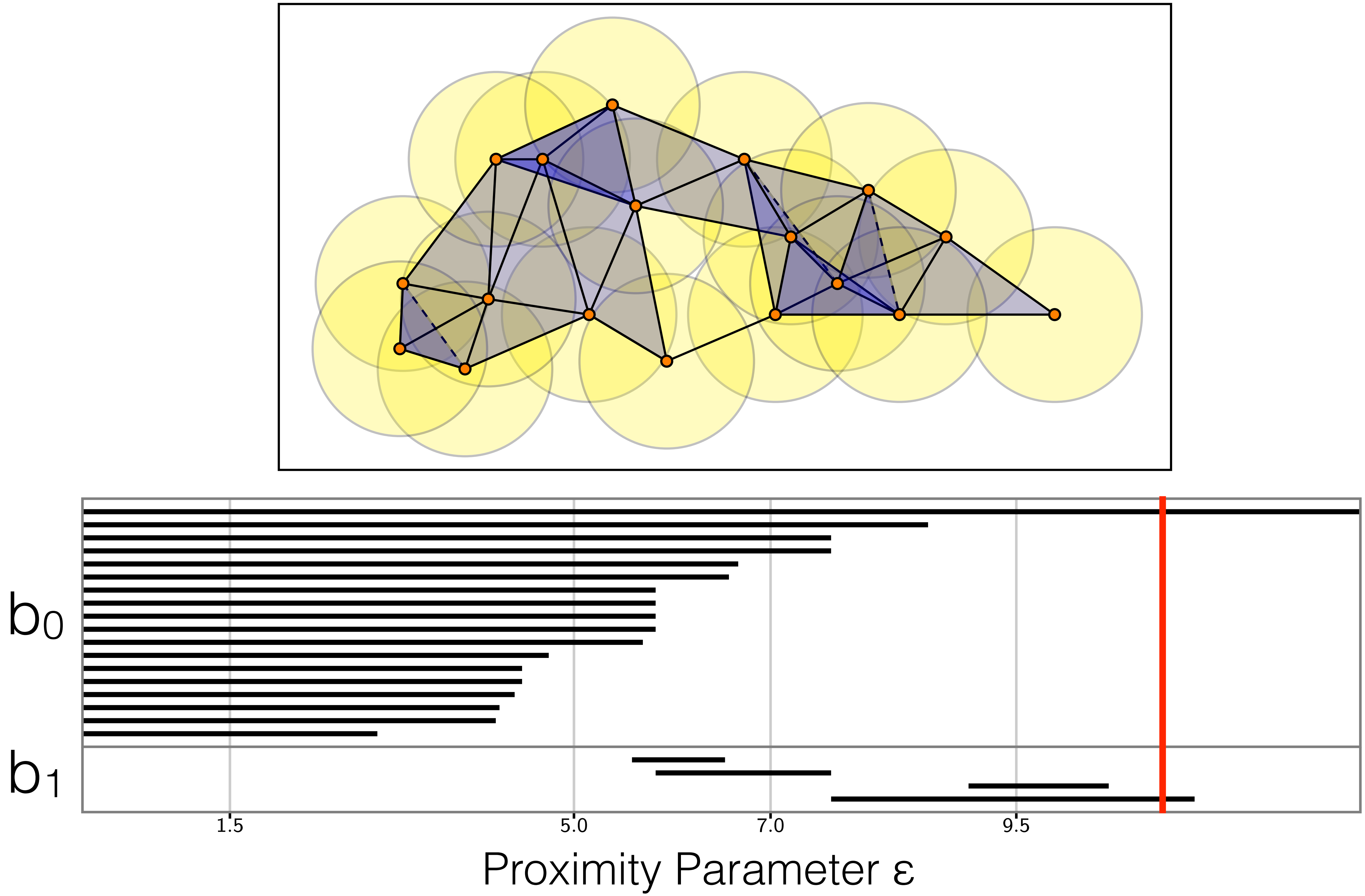

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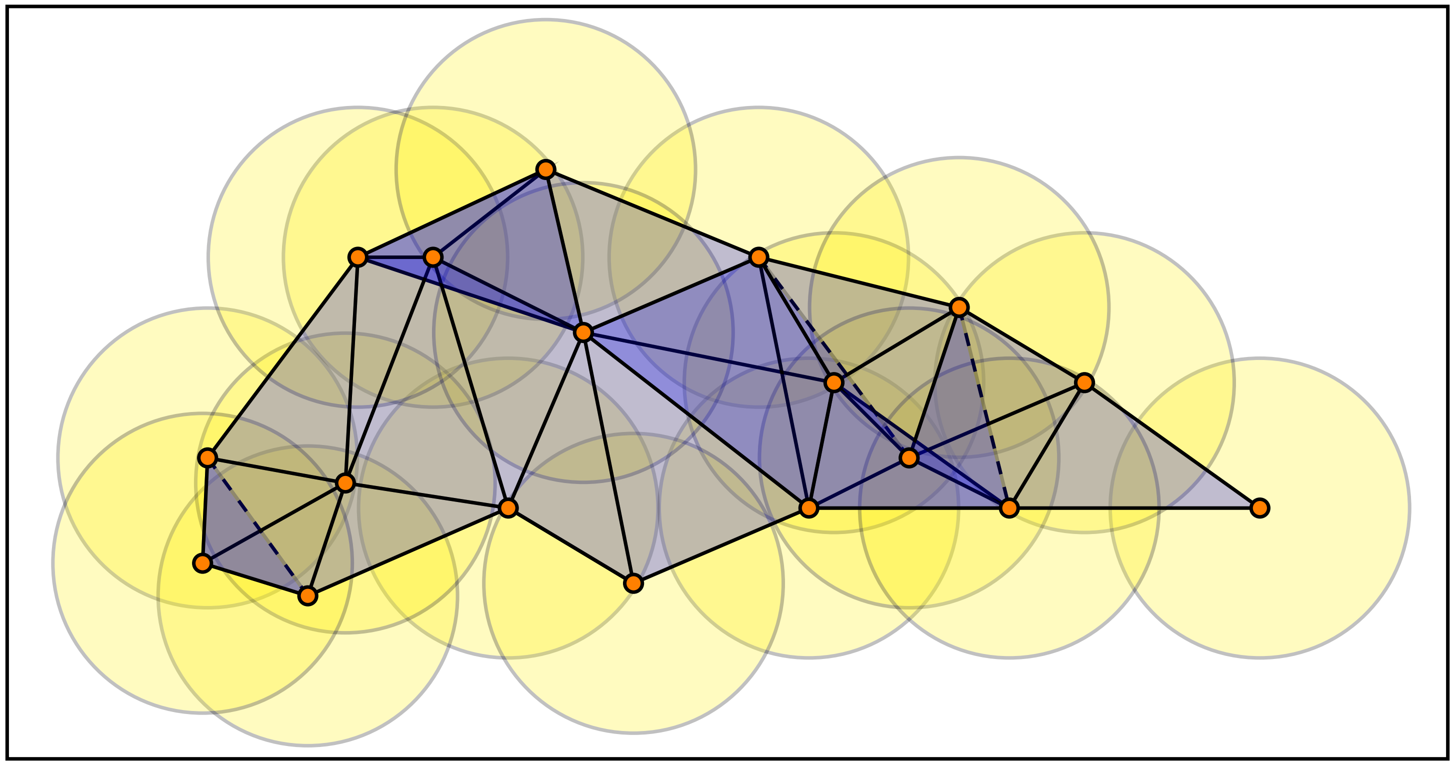

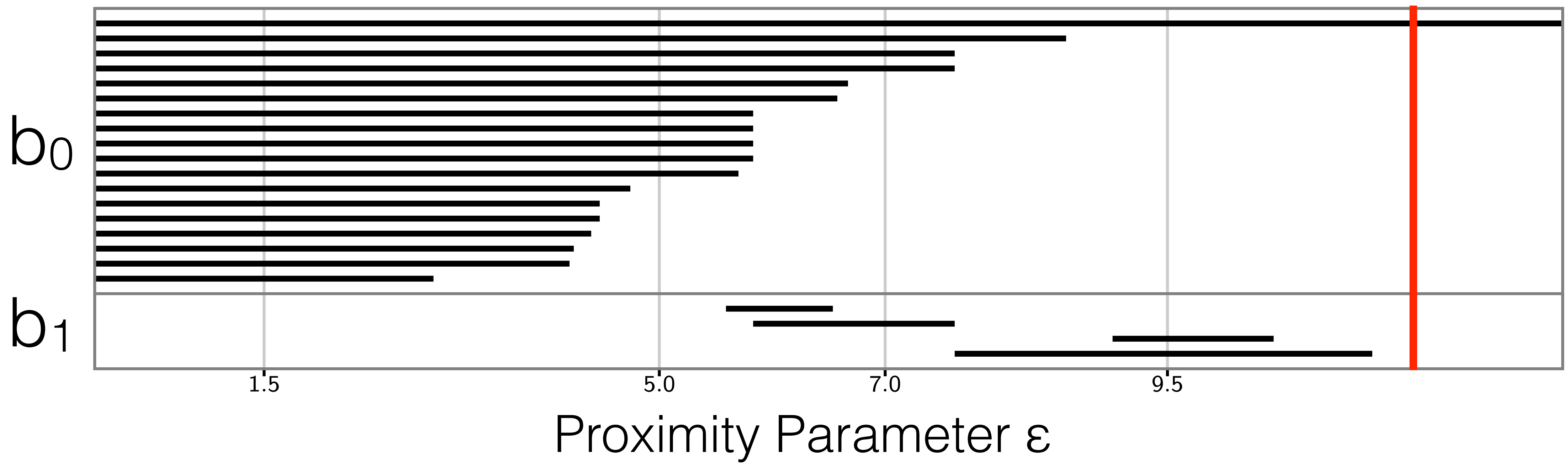

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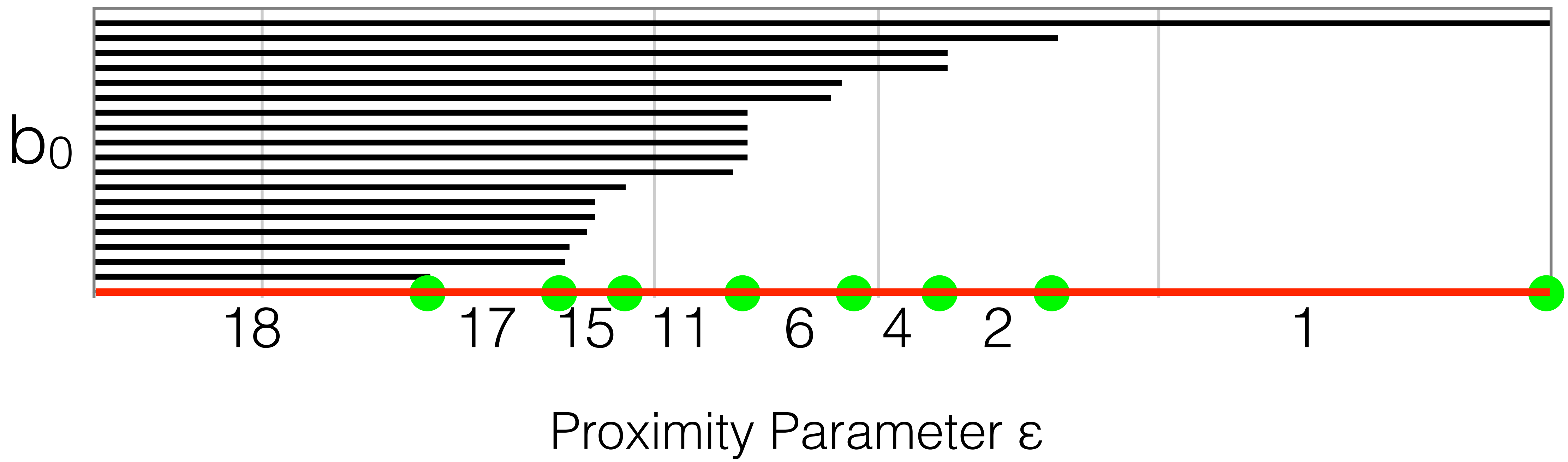
Find persistent homology



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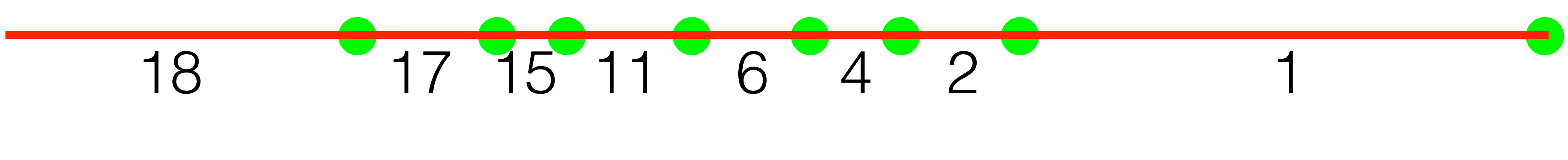

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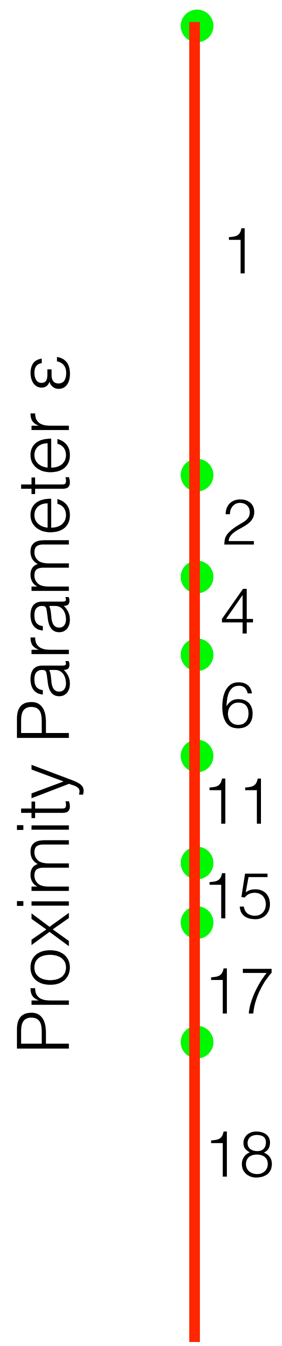
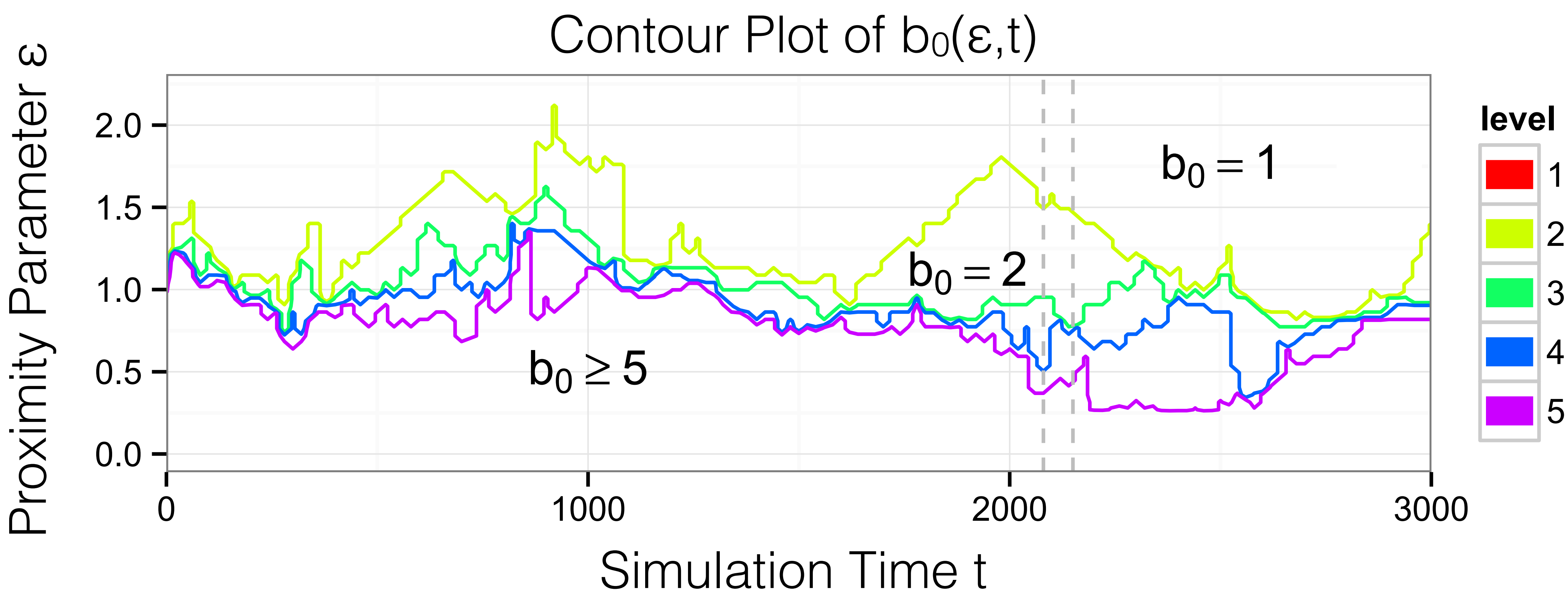


Step 5:
Evolve in time (CROCKER)

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



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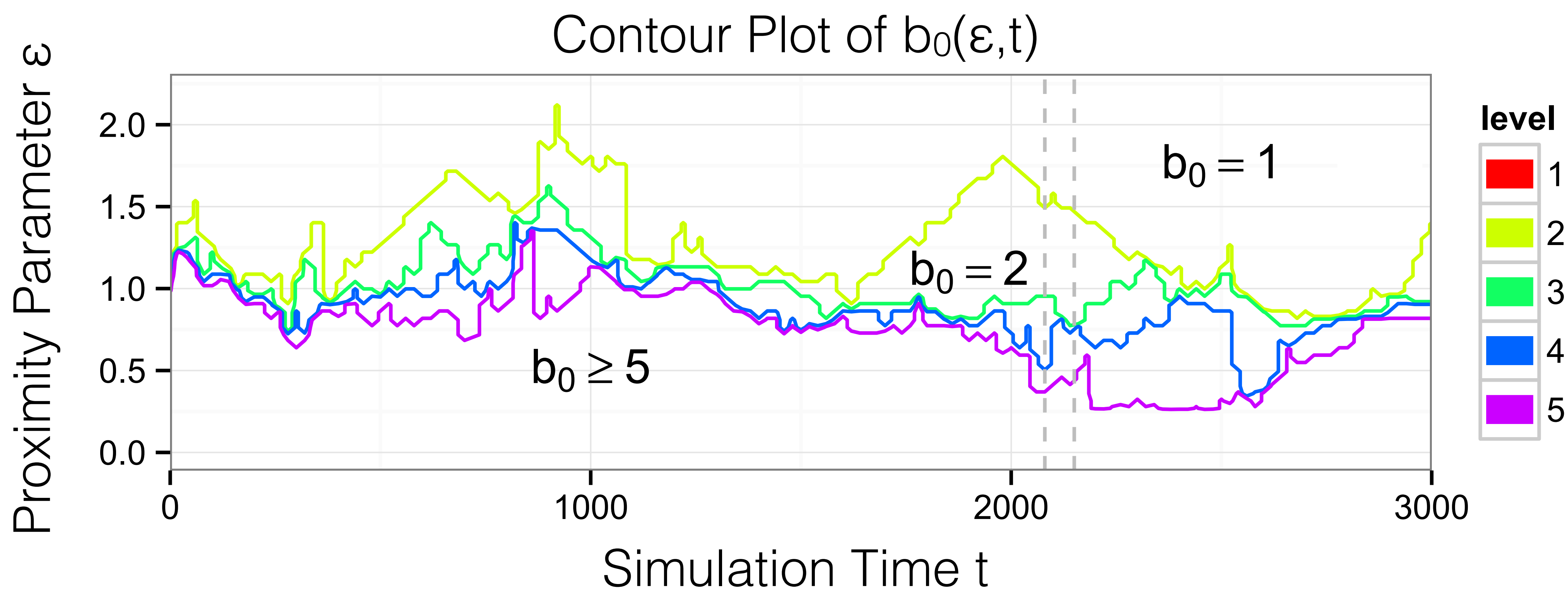
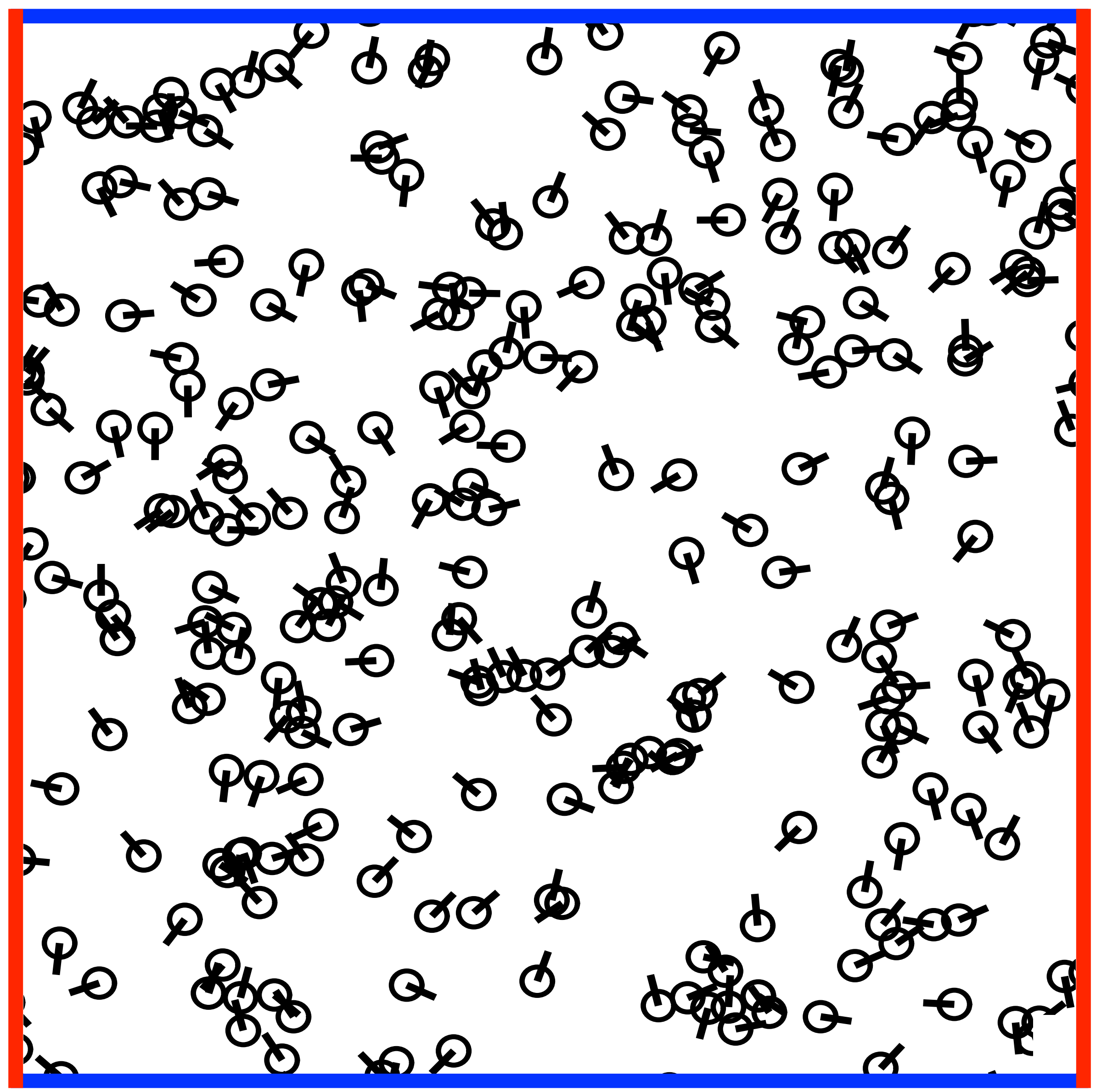


Results

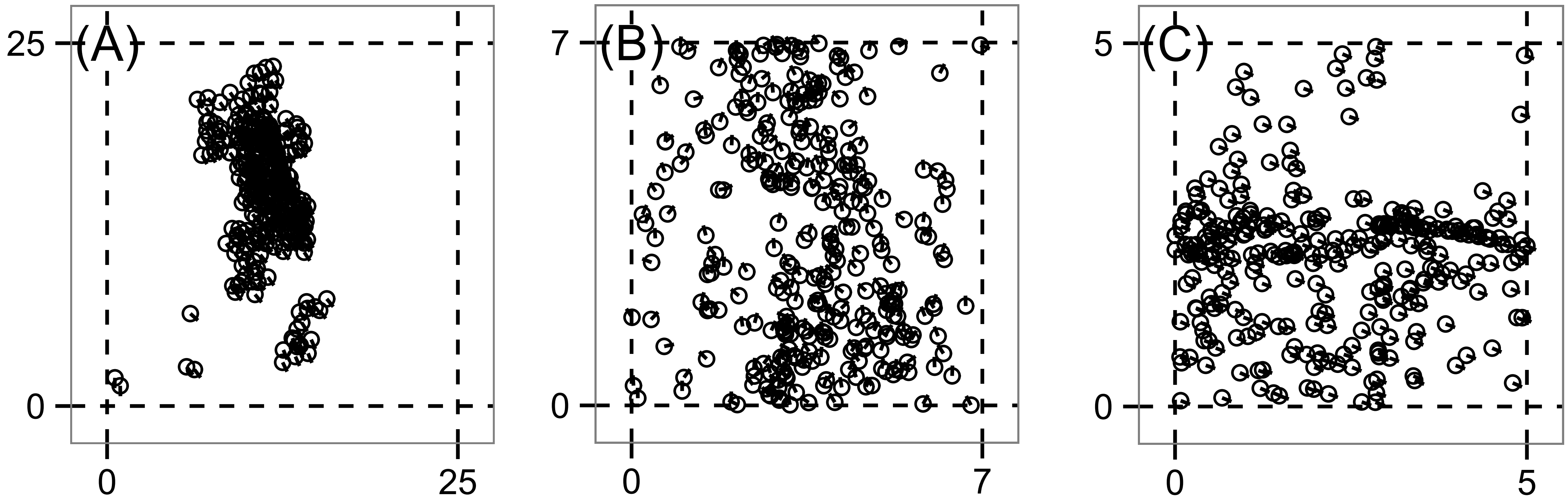
Vicsek Model
Initial Condition



Three-torus T^3

$b = (1,3,3,1,0,\ldots)$

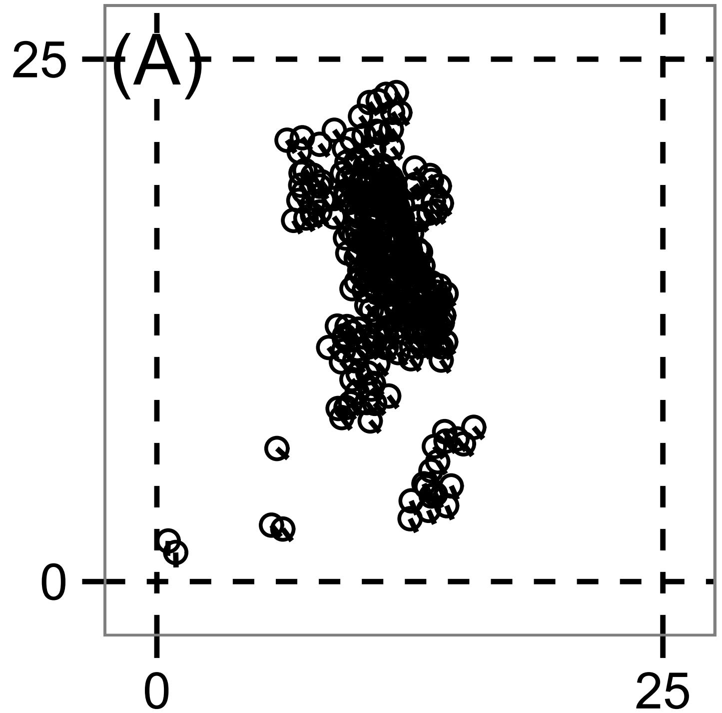
Vicsek Model
Long Term Behaviors



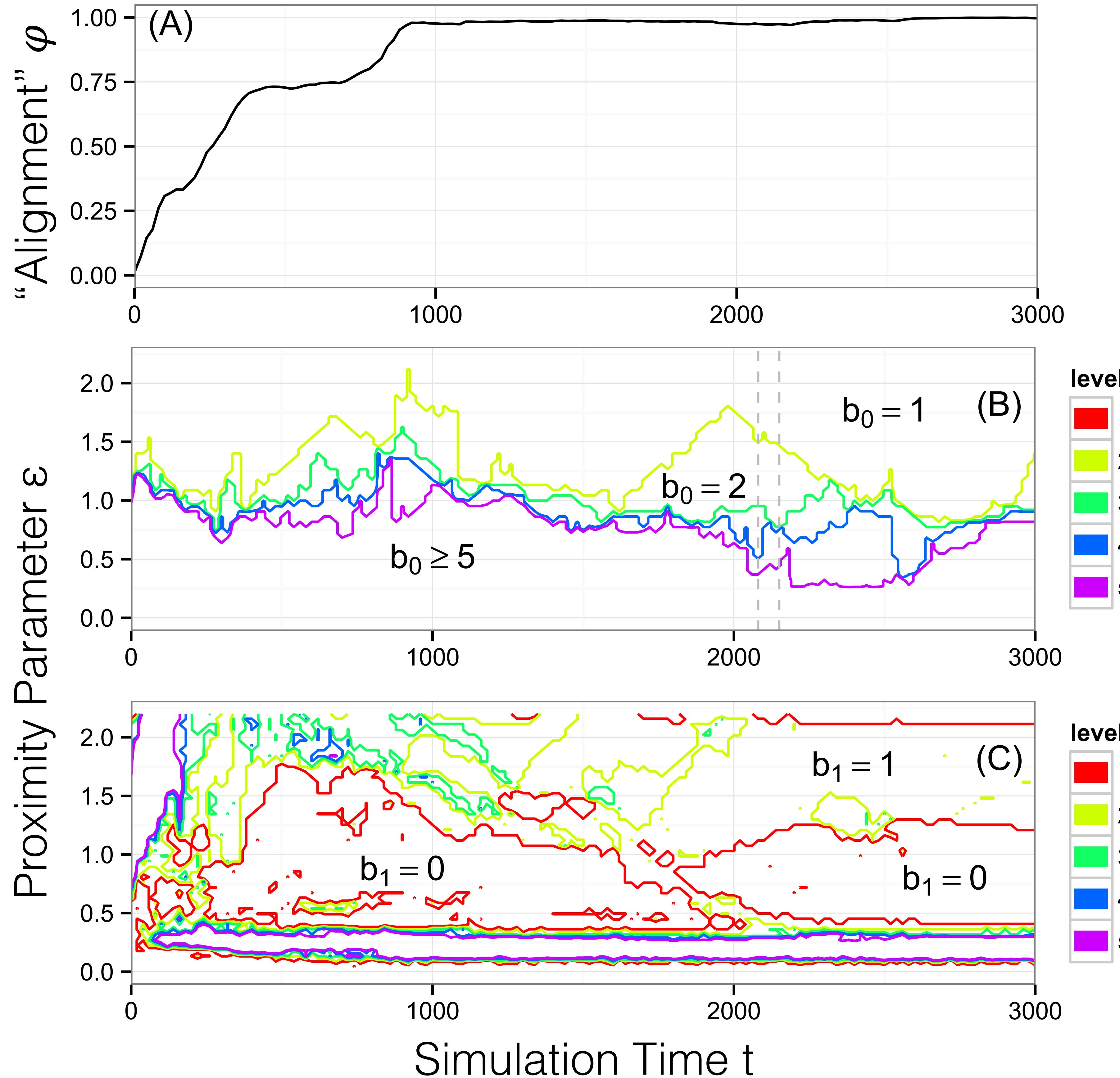
Clusters?

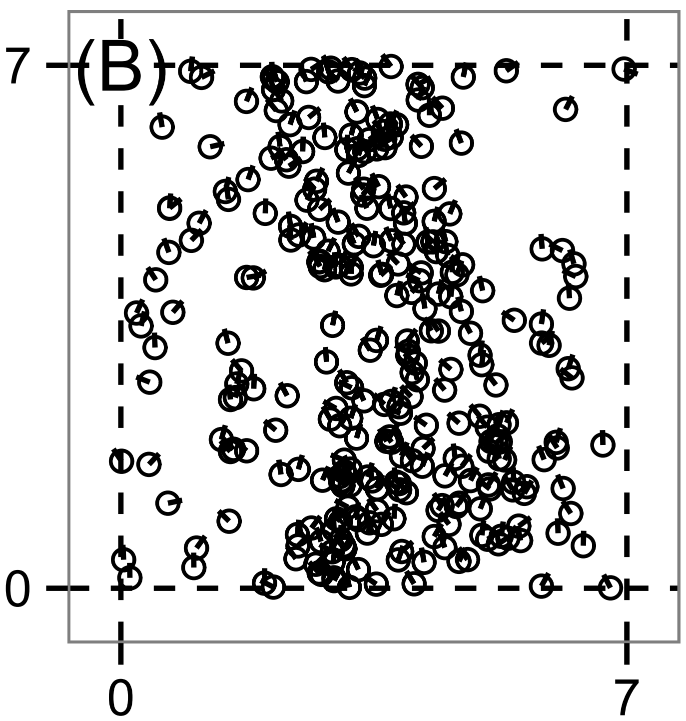
Loose alignment?

Strong alignment?

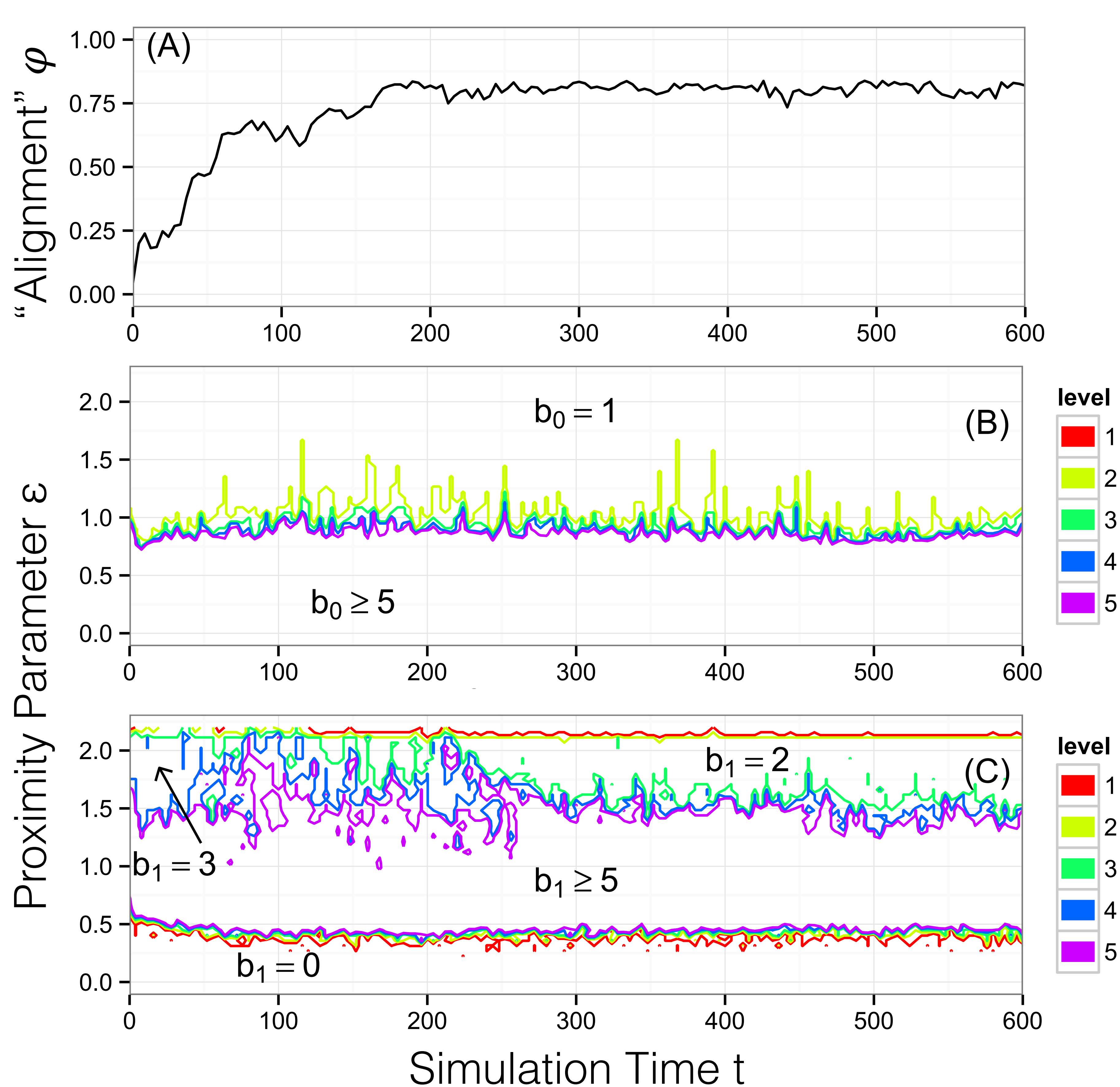


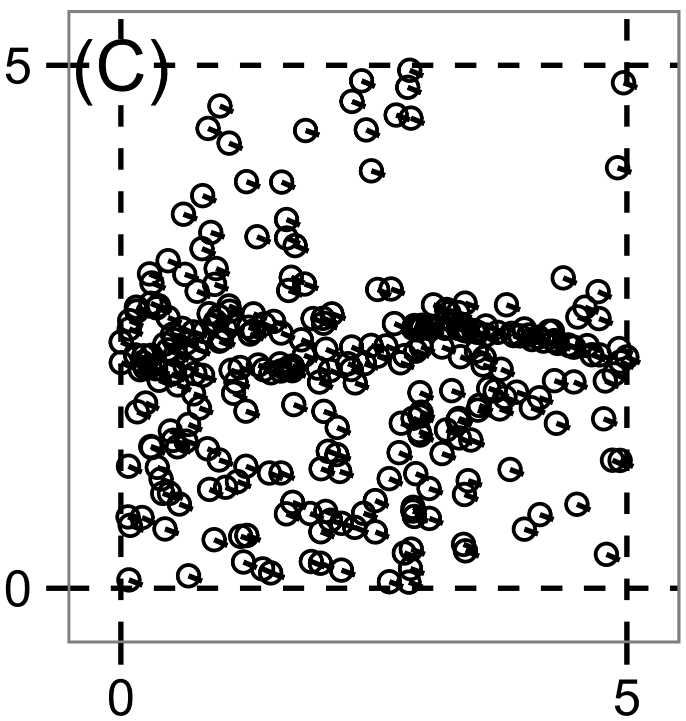
- Intermittent clustering
- Loss of two topol. circles
- b = (2 - 4, 1, …)



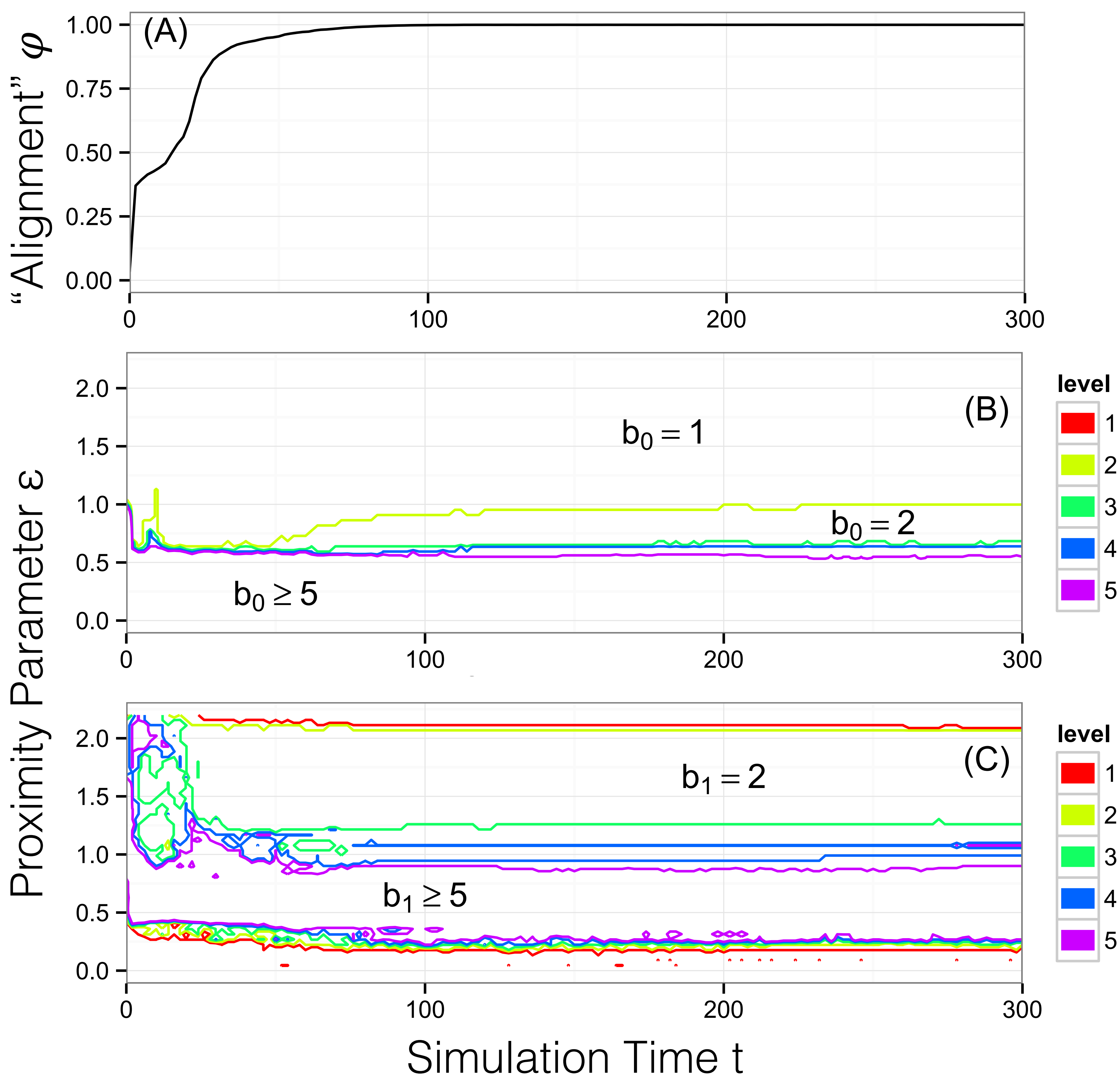


- One group
- Two persistent topol. circles
- b = (1, 2, 1, …)

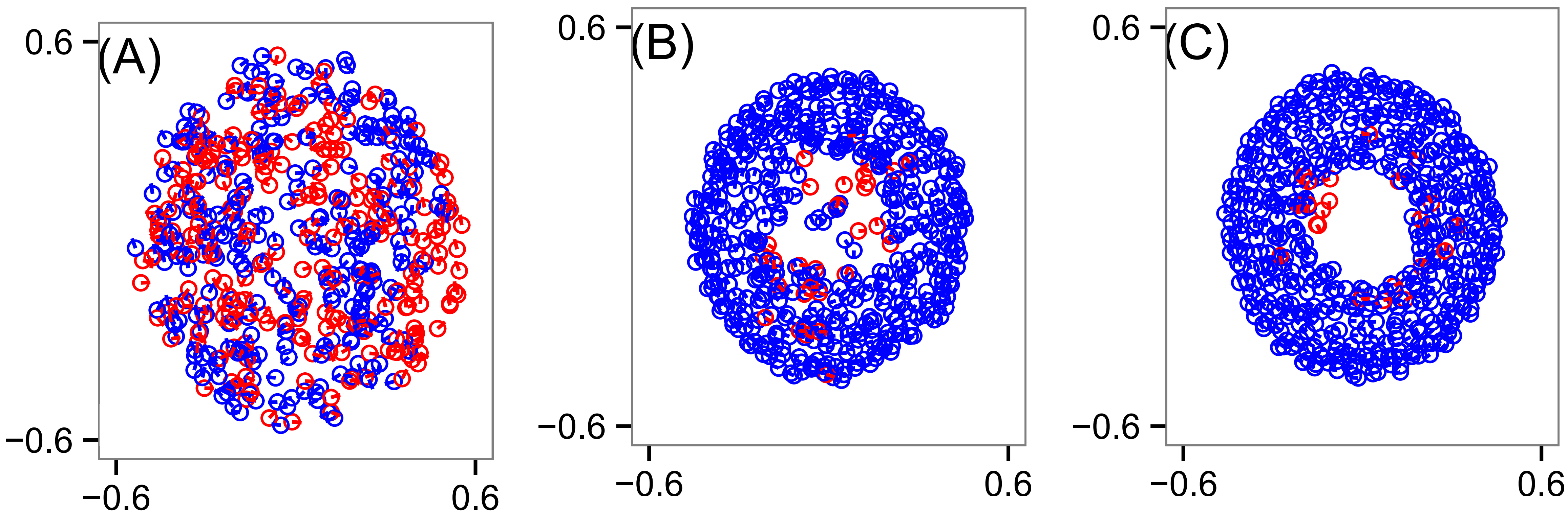




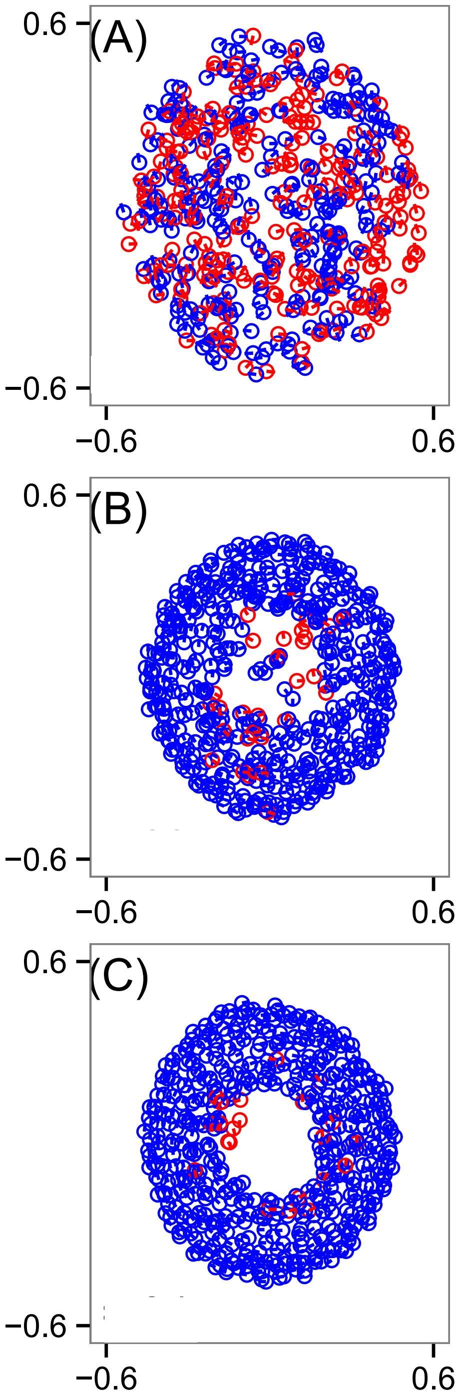
- One group, one rogue
- Two persistent topol. circles
- b = (1, 2, 0, …)
- Hole in the data



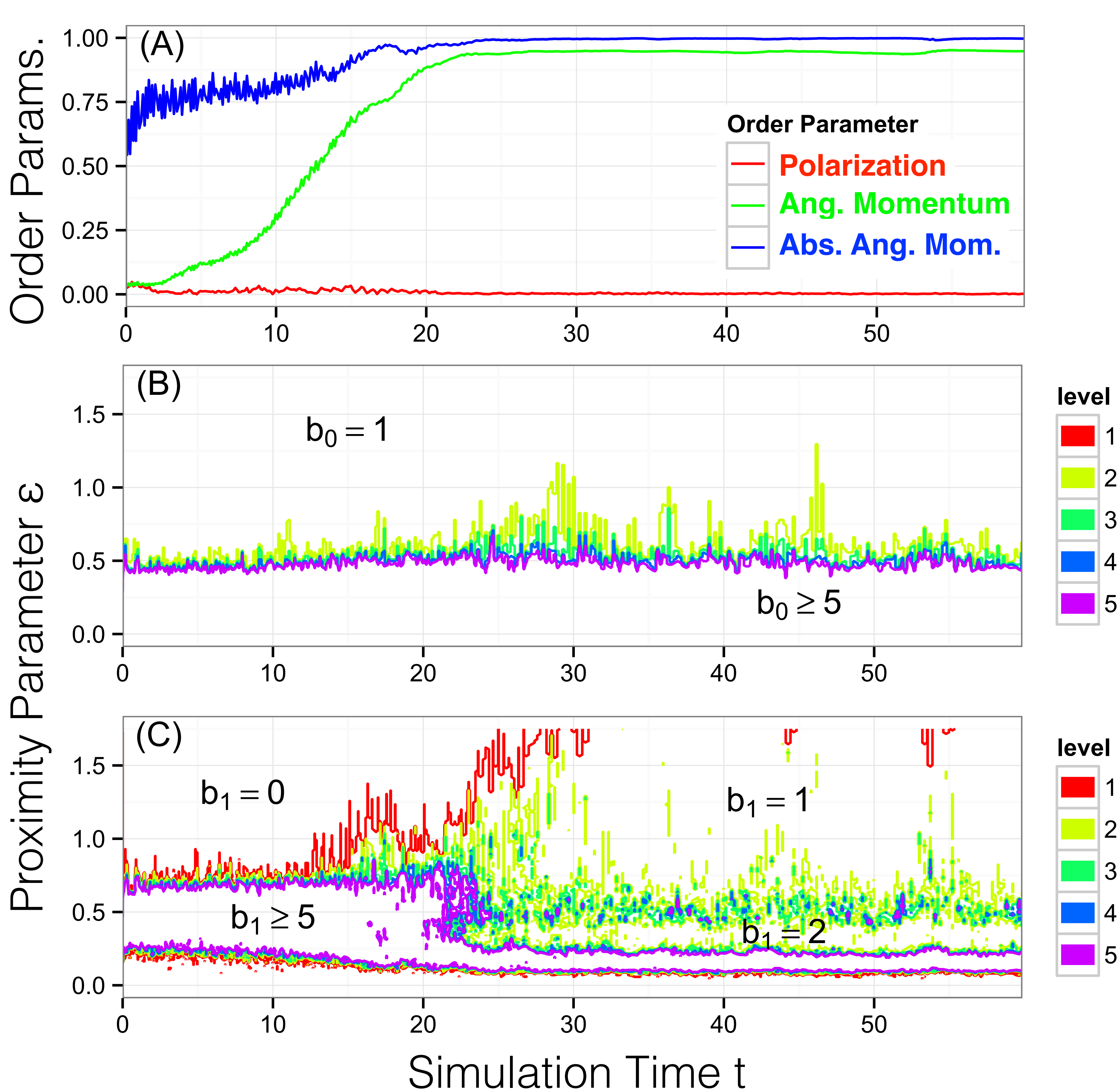
D'Orsogna Model Simulation Snapshots

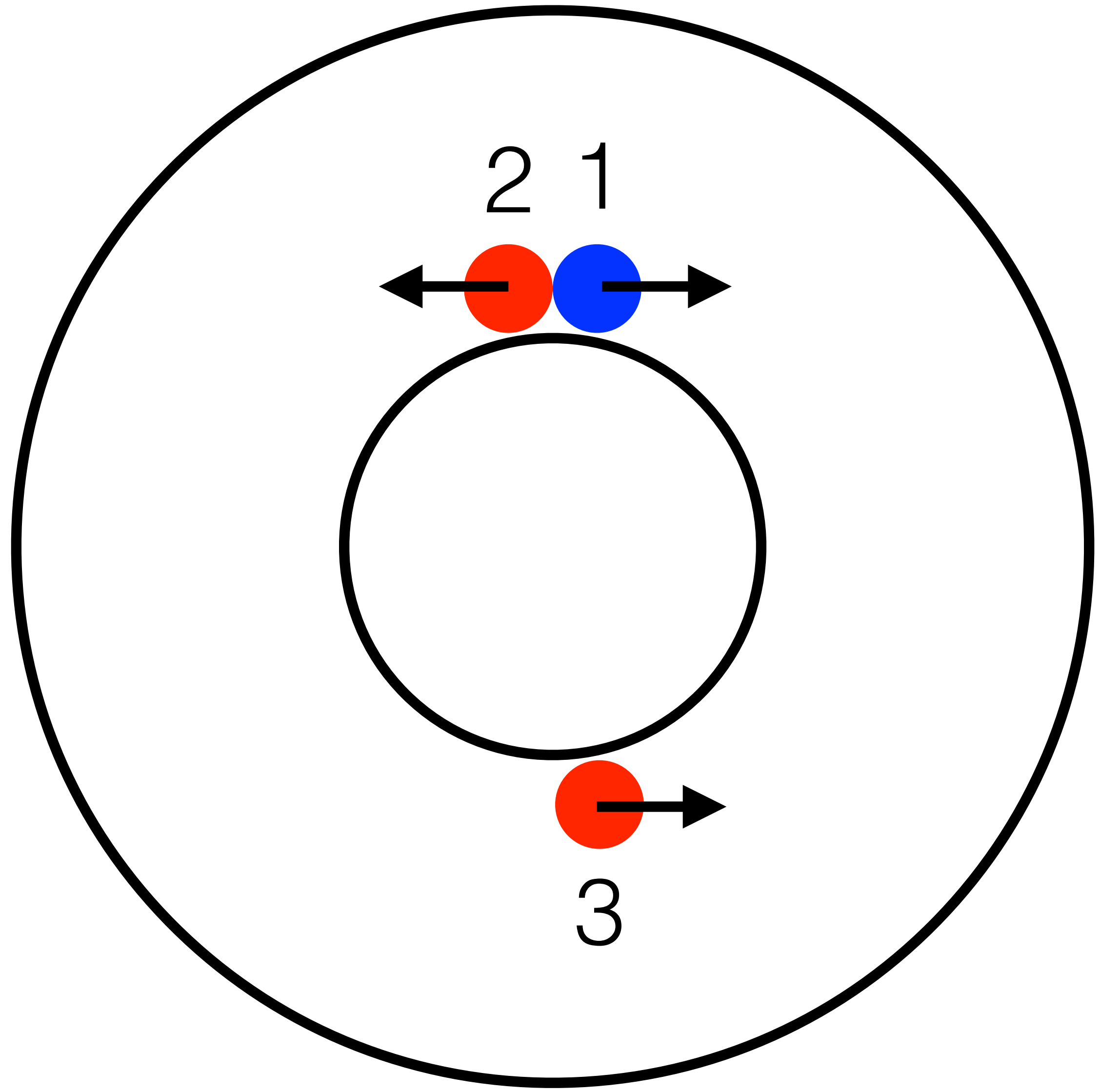


t = 5 (early) | t = 23 (middle) | t = 34 (late)

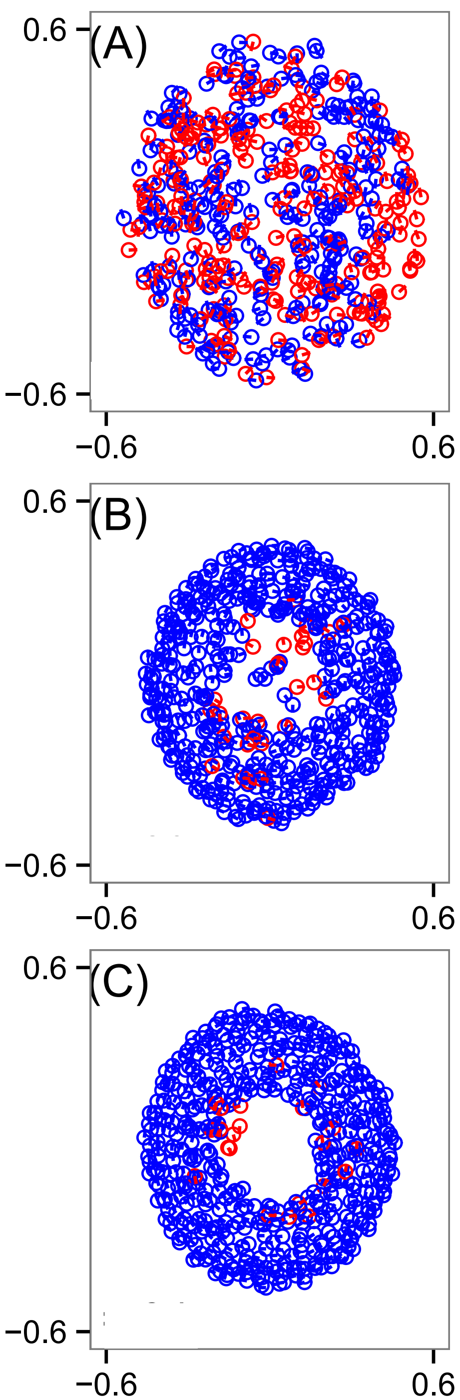


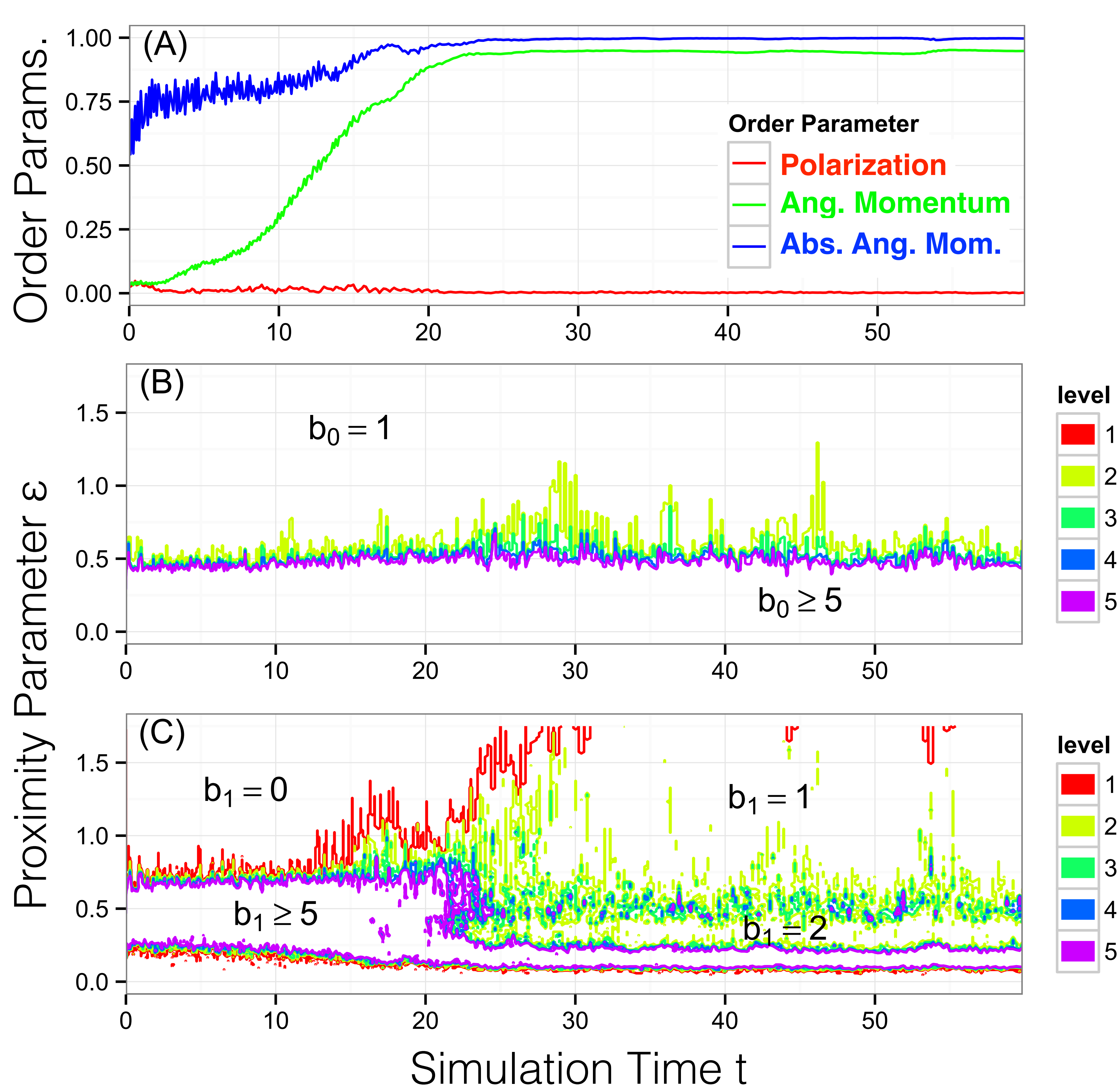
- 1 - 2 groups
- 2 topol. circles
- b = (2, 2, …)





In four dimensional **x** - **v** space, #1 and #3 are closer than #1 and #2.





- 1 - 2 groups
- 2 topol. circles
- b = (2, 2, …)

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