The Waisman Laboratory
for Brain Imaging and Behavior

University of Wisconsin
SCHOOL OF MEDICINE
AND PUBLIC HEALTH

Lecture 1 Simplicial homology and persistent homology

Moo K. Chung
Department of Biostatistics and Medical Informatics
University of Wisconsin-Madison

https://github.com/laplcebeltrami/ISBI2023TDA

Acknowledgement

Zijian Chen, Vijay Anand D, Sixtus Dakurah, Soumya Das, Tananun Songdechakraiwut, Univ. of Wisconsin-Madison, US

Shih-Gu Huang, Anqi Qiu National University of Singapore, Singapore

Anass El Yaagoubi Bourakna, Hernando Ombao KAUST, Saudi Arabia

Hyekyung Lee, Dong Soo Lee Seoul National University, Korea

Grants: *NIH R01 EB022856, R01 EB028753, NSF DMS-2010778*

References

Gunnar Carlsson 2009, A User's Guide to Topological Data Analysis

Herbert Edelsbrunner and John L. Harer Computational Topology: An Introduction 2010, American Mathematical Society

Chung et al. 2020 Review: Toplogical distance and losses in brain networks arXiv:2102.08623

Matlab toolbox

PH-STAT

Statistical Inference on Persistent Homology

https://github.com/laplcebeltrami/PH-STAT

Most computation & data visualization in the tutorial is done through PH-STAT. Corresponding functions are color coded.

`WS_cluster.m` `PH_hodge_betti.m`

Topological Data Analysis

- Branch of data science that uses topology
- Study properties of data that remain <u>invariant</u> under continuous transformations
- Identify underlying patterns using topology

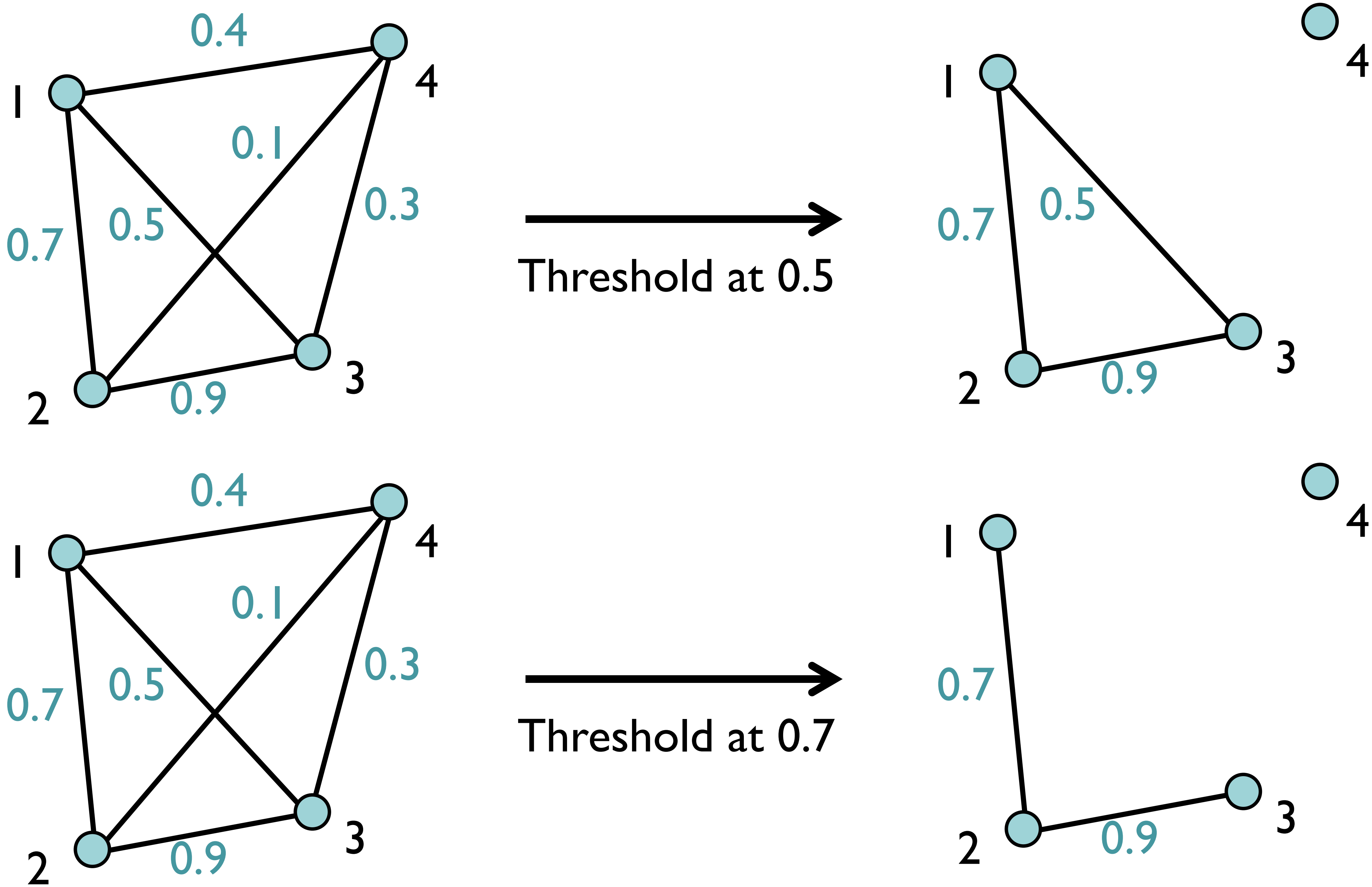
Persistent Homology

- Captures the topological features of data across different scales
- More persistent topological features → signal
- Less persistent topological features → noise
- Multiscale approach

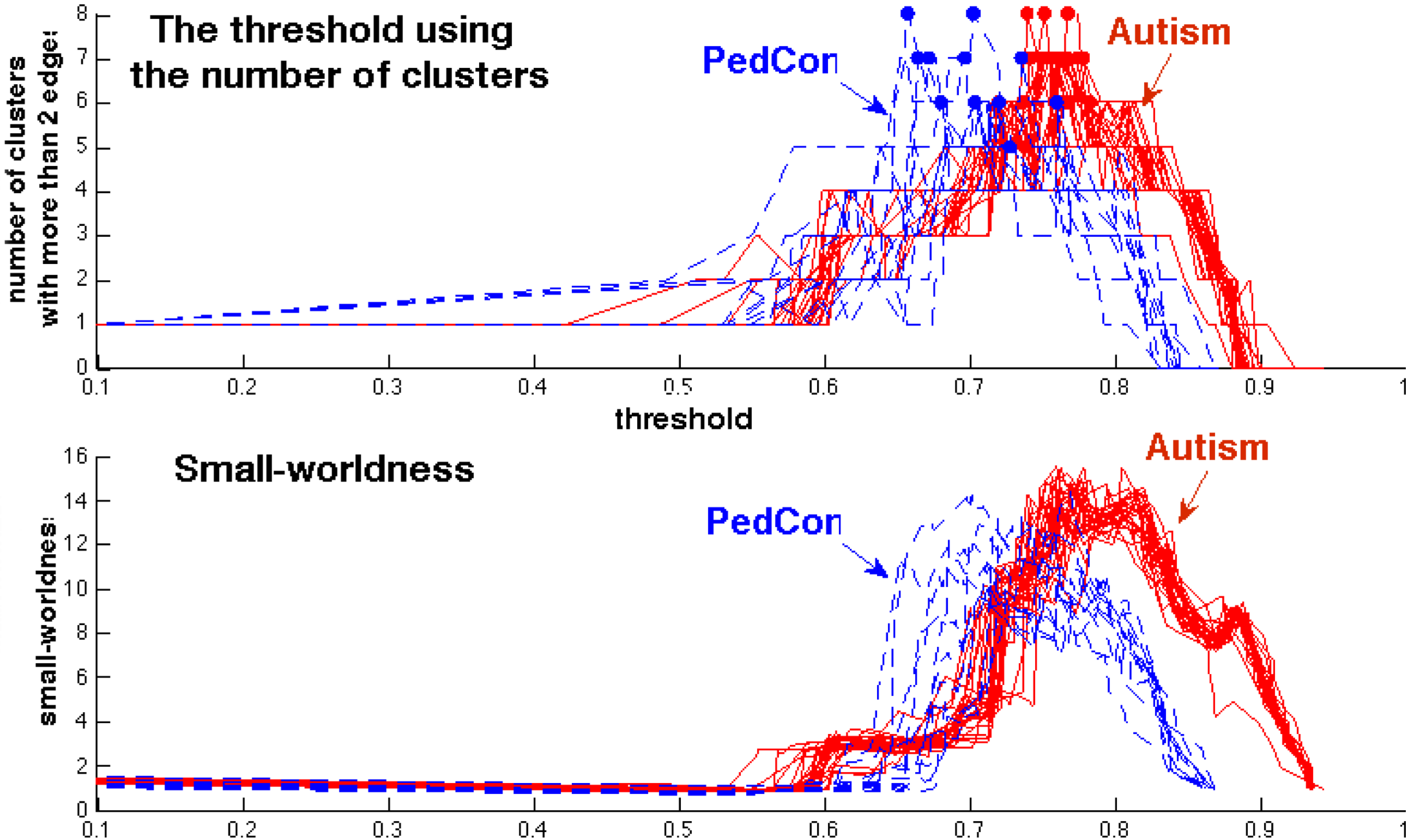
What is wrong with standard brain network analysis?

Edge weight ρ_{ij} between node *i* and *j*

→ Connectivity matrix $\rho = (\rho_{ij})$



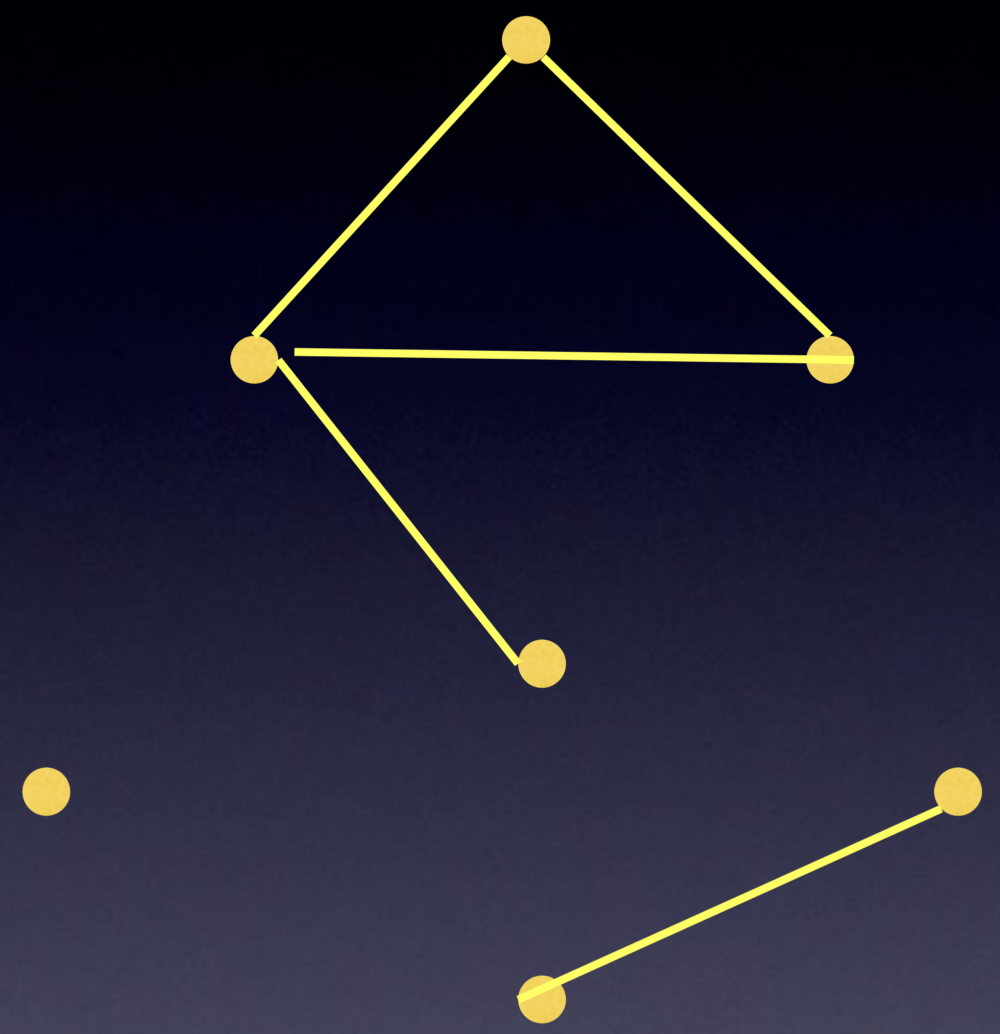
Single threshold often suboptimal → multiple thresholds



Lee et al. 2011. IEEE TMI 30:1154-1165

Betti numbers β_i

of i-dimensional holes/loops

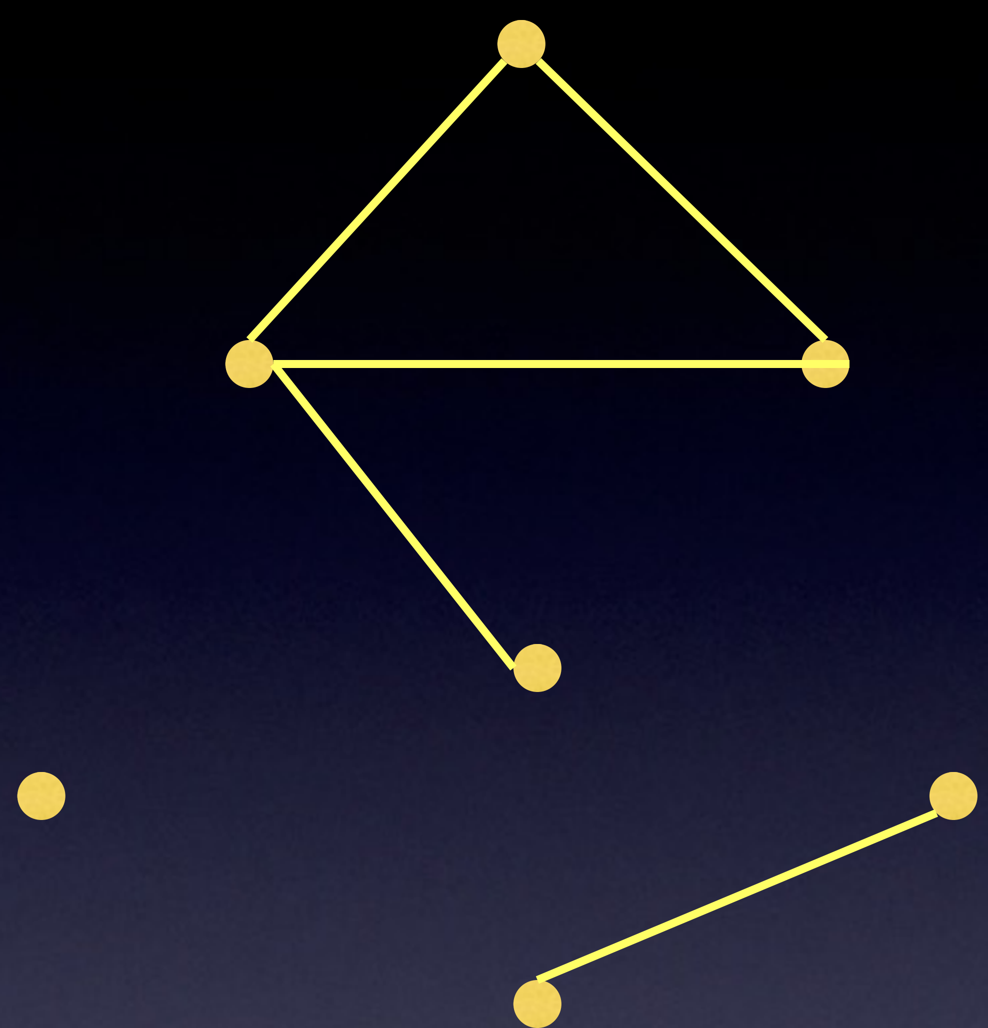


β_0 = # of connected components = 3

β_1 = # of cycles = 1

Euler characteristic: $\chi = 3 - 1 = 2$

Betti numbers β_i # of i-dimensional holes/loops



β_0 = # of connected components = 3

β_1 = # of 1D holes = 1

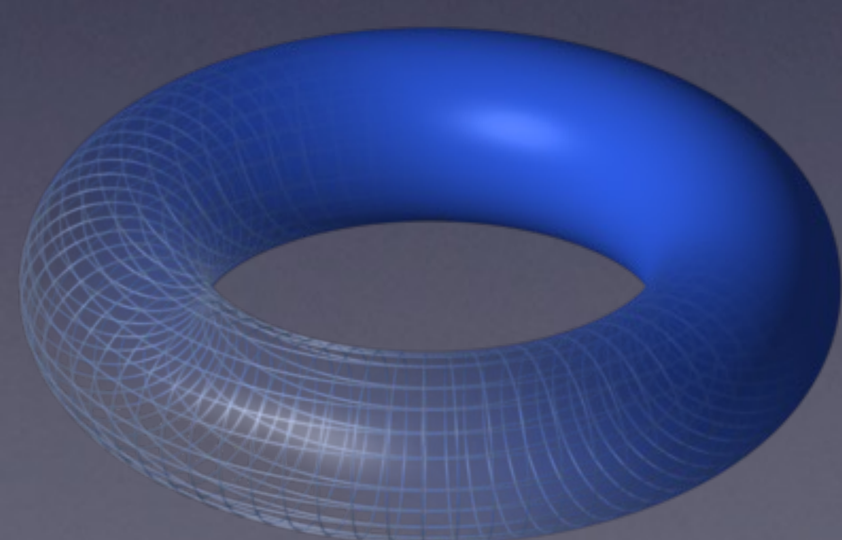
β_2 = # of 2D cavities =0

Betti-number representation:

(3,1,0,0,...)

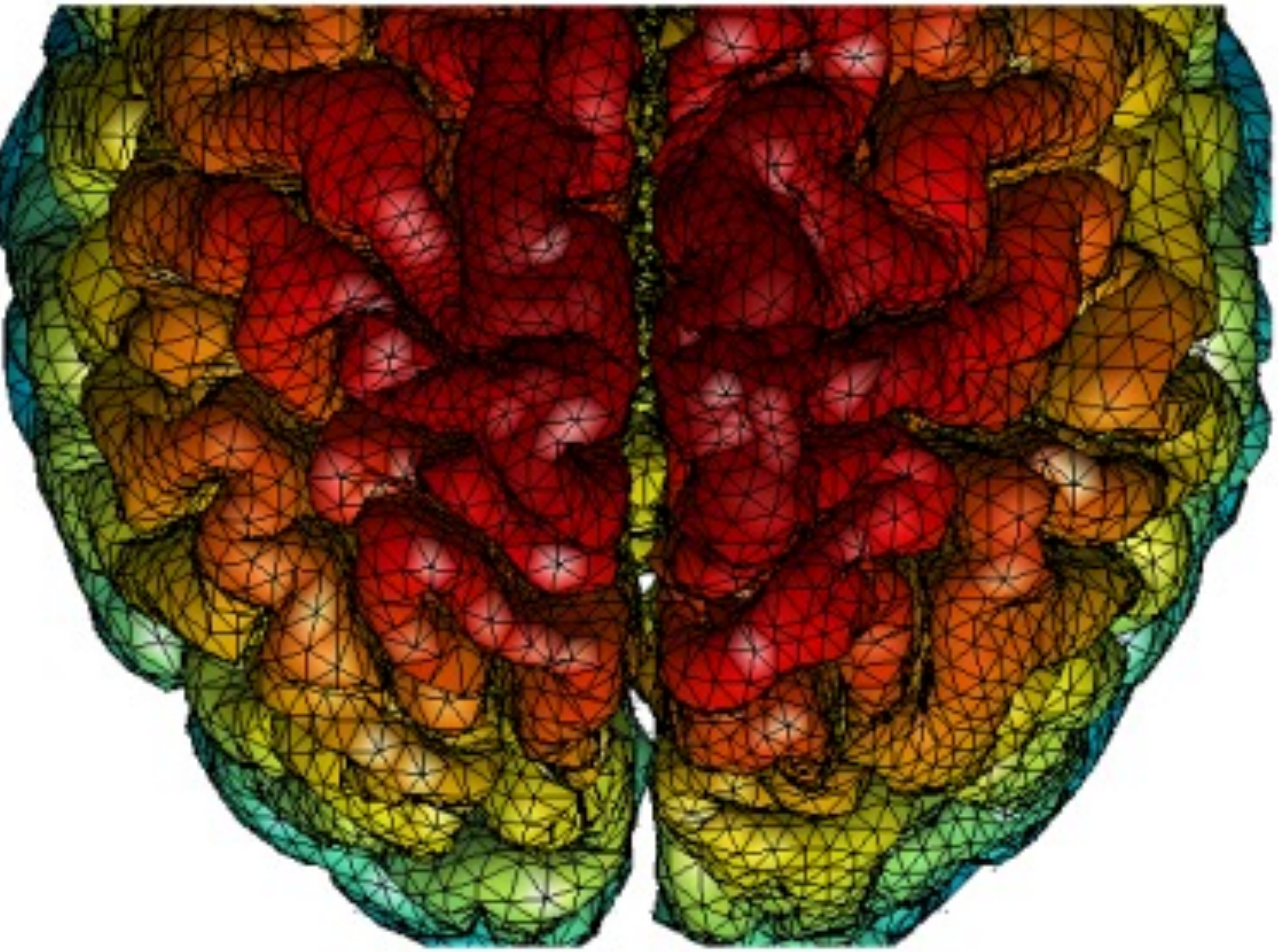
Euler characteristic:

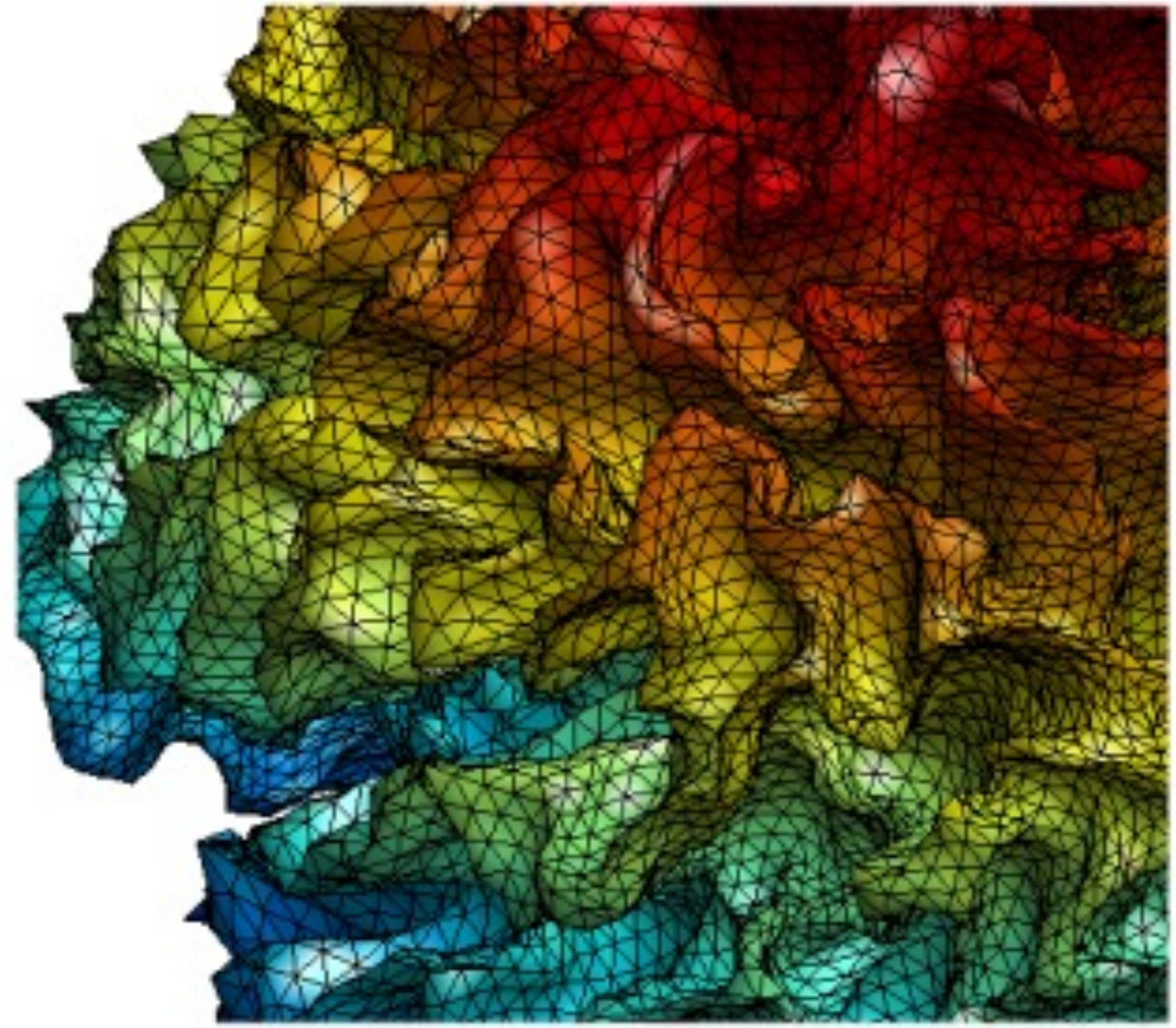
$$\chi = \beta_0 - \beta_1 = 2$$



$$\beta_0 = 1, \beta_1 = 2, \beta_2 = 1$$

(1,2,1,0,0,...)

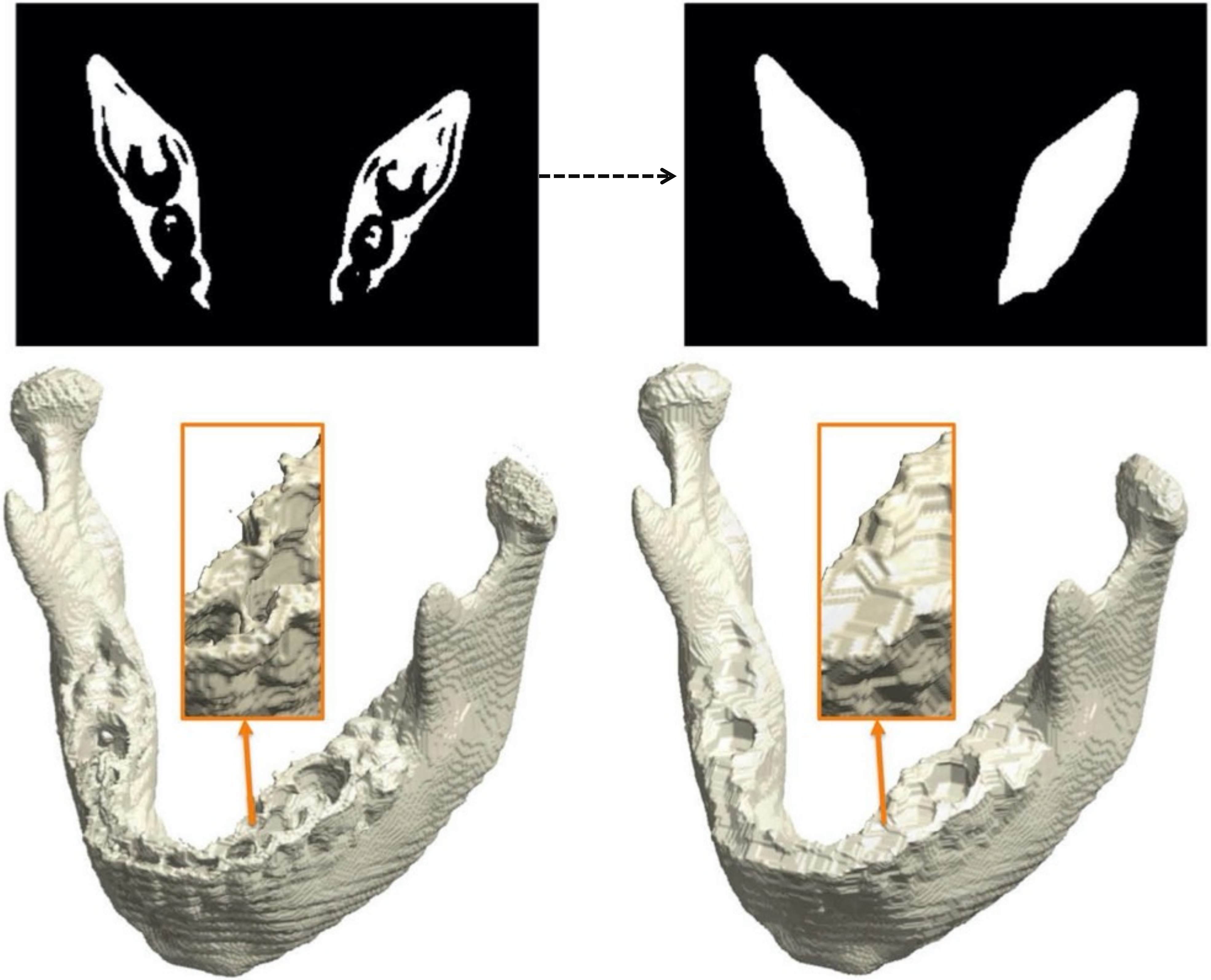




Euler characteristic of a surface mesh from SurfStat

$N - E + F = 2$ for a surface topologically equivalent to a sphere. For each triangle, there are three edges. Since two adjacent triangles share the same edge, the total number of edges is $E = 3F/2$. Hence, we have $F=2N - 4$ for a closed surface.

Topology correction in CT segmentation



Hole & handles corrected using Euler characteristic

Chung et al. 2015 Medical Image Analysis. 22:63-76

Keith Worsley's random field theory

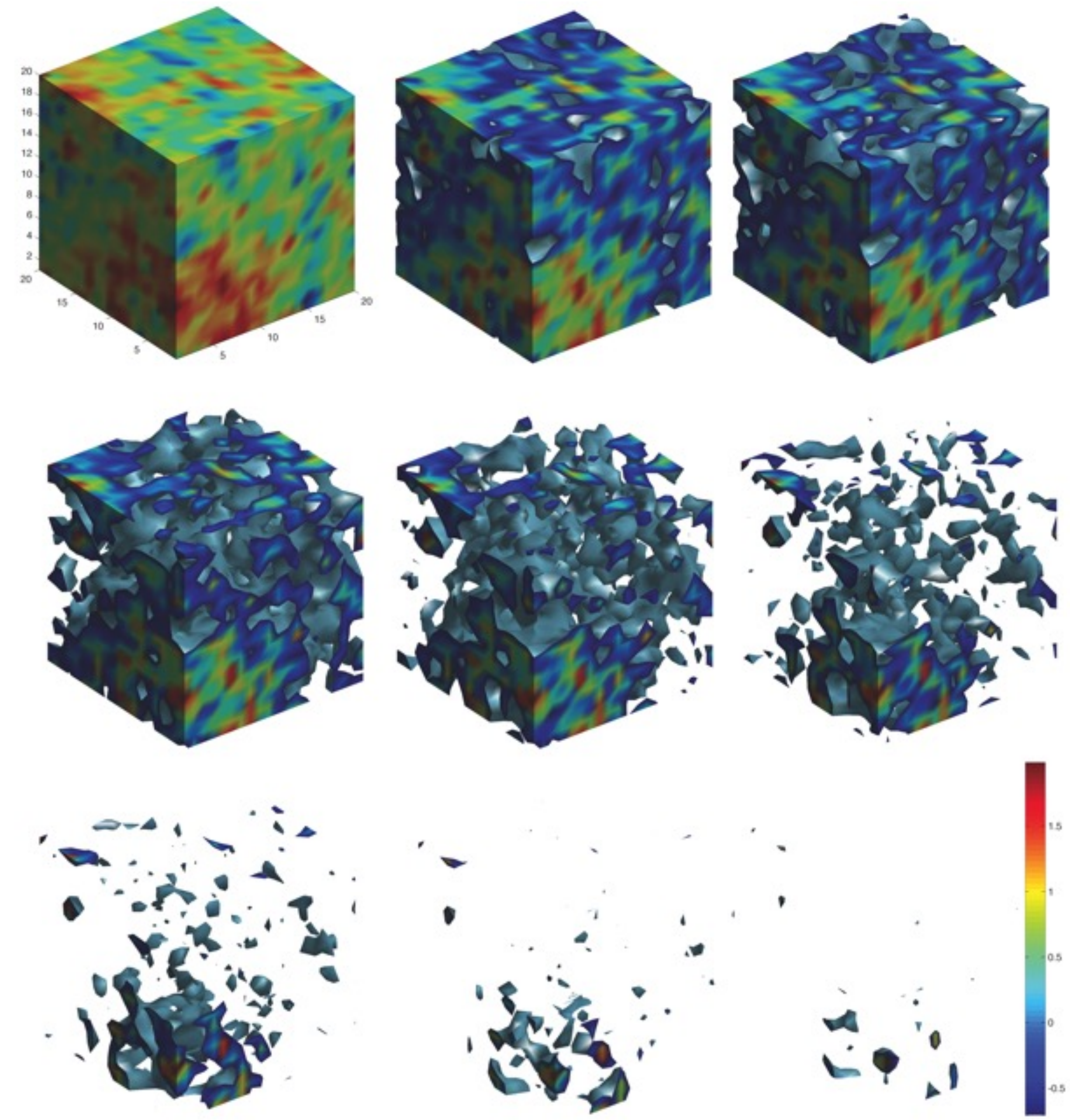
Random field

$$P\Big(\sup_{x\in\mathbb{M}} T(x) > h\Big)$$

$$A_h = \{x \in \mathbb{M} : T(x) > h\}$$

$$P\Big(\sup_{x\in\mathbb{M}} T(x) > h\Big) = \mathbb{E}\chi(A_h)$$

$$\chi(A_h) = \sum_j (-1)^j \beta_j(A_h)$$



Milor 1963 Morse theory

Adler, 1994 The geometry of random fields

Worsley et al., 1996 Human Brain Mapping

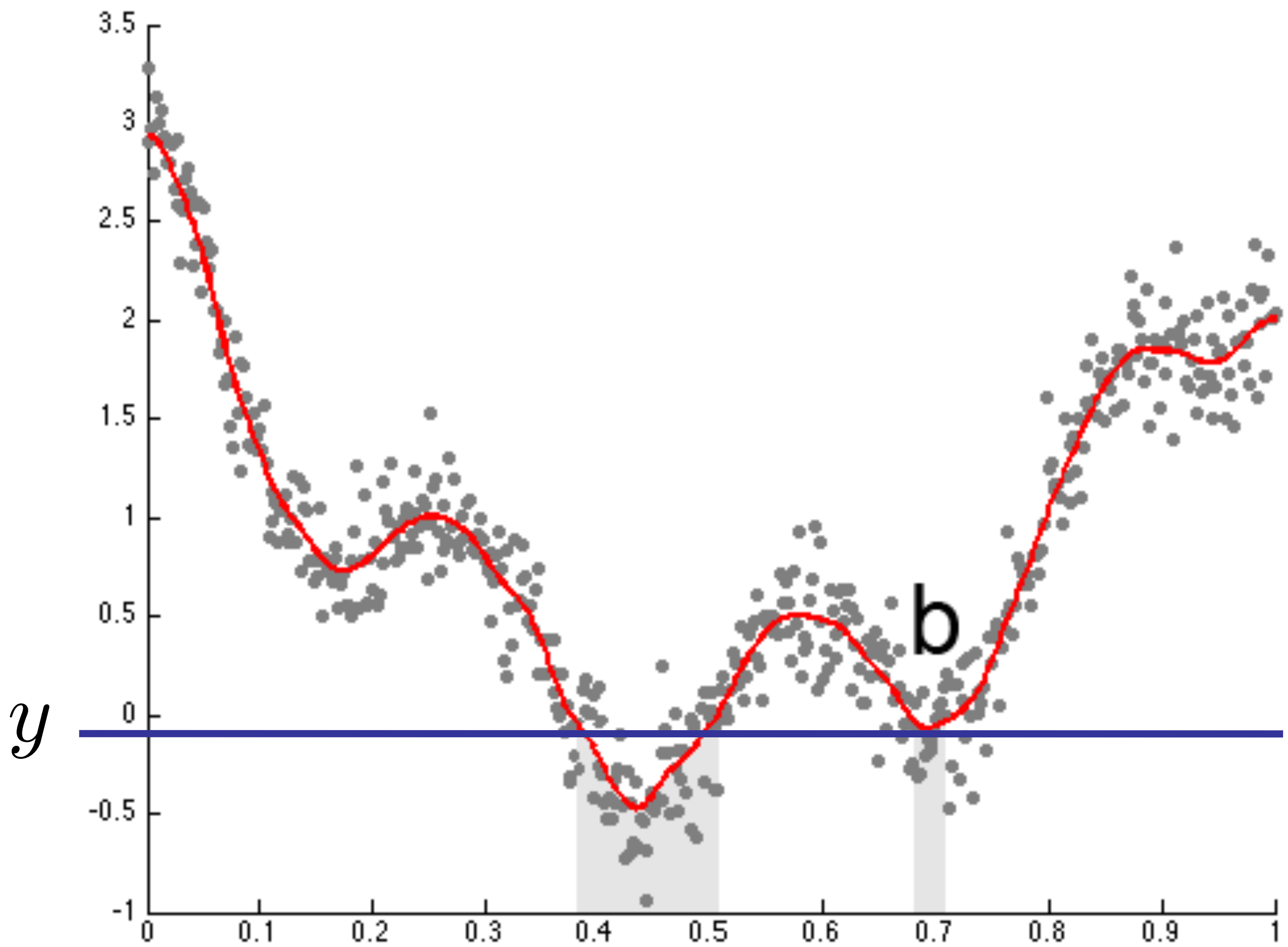
Morse Filtration

Chung et al., 2009 Information Processing in Medical Imaging (IPMI) 5636:386-397.

Morse theory for functional data

$$Y(t) = \mu(t) + \epsilon(t)$$

Unknown signal μ is assumed to be a Morse function: all critical values are unique.



Sublevel set

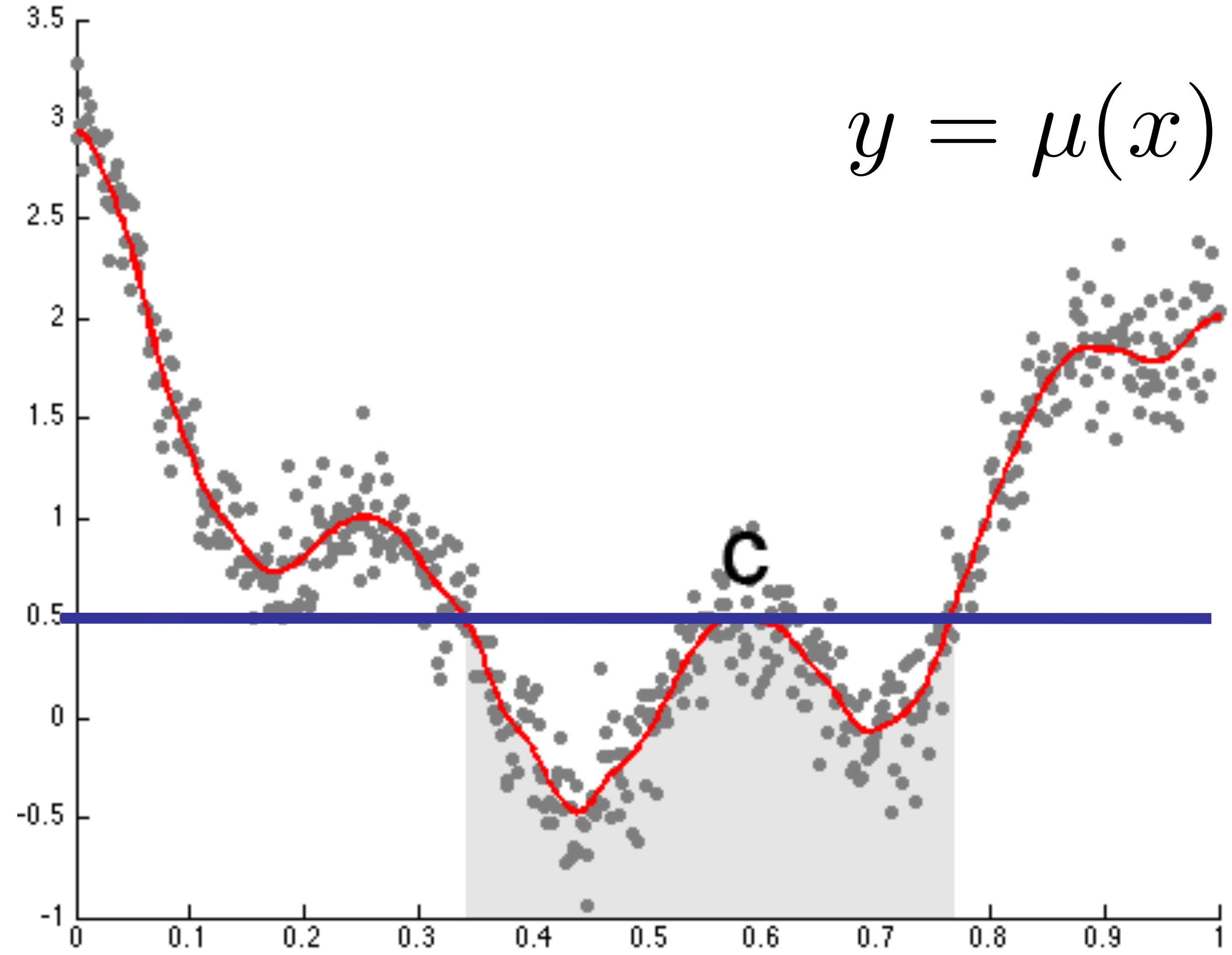
$$R_y = \{t : \mu(t) \leq y\}$$

The topology of sublevel set is characterized by Betti-0 number only

Morse filtration

Sublevel set

$$R_y = \{t : \mu(t) \leq y\}$$



Morse filtration

$$R_b \subset R_c$$

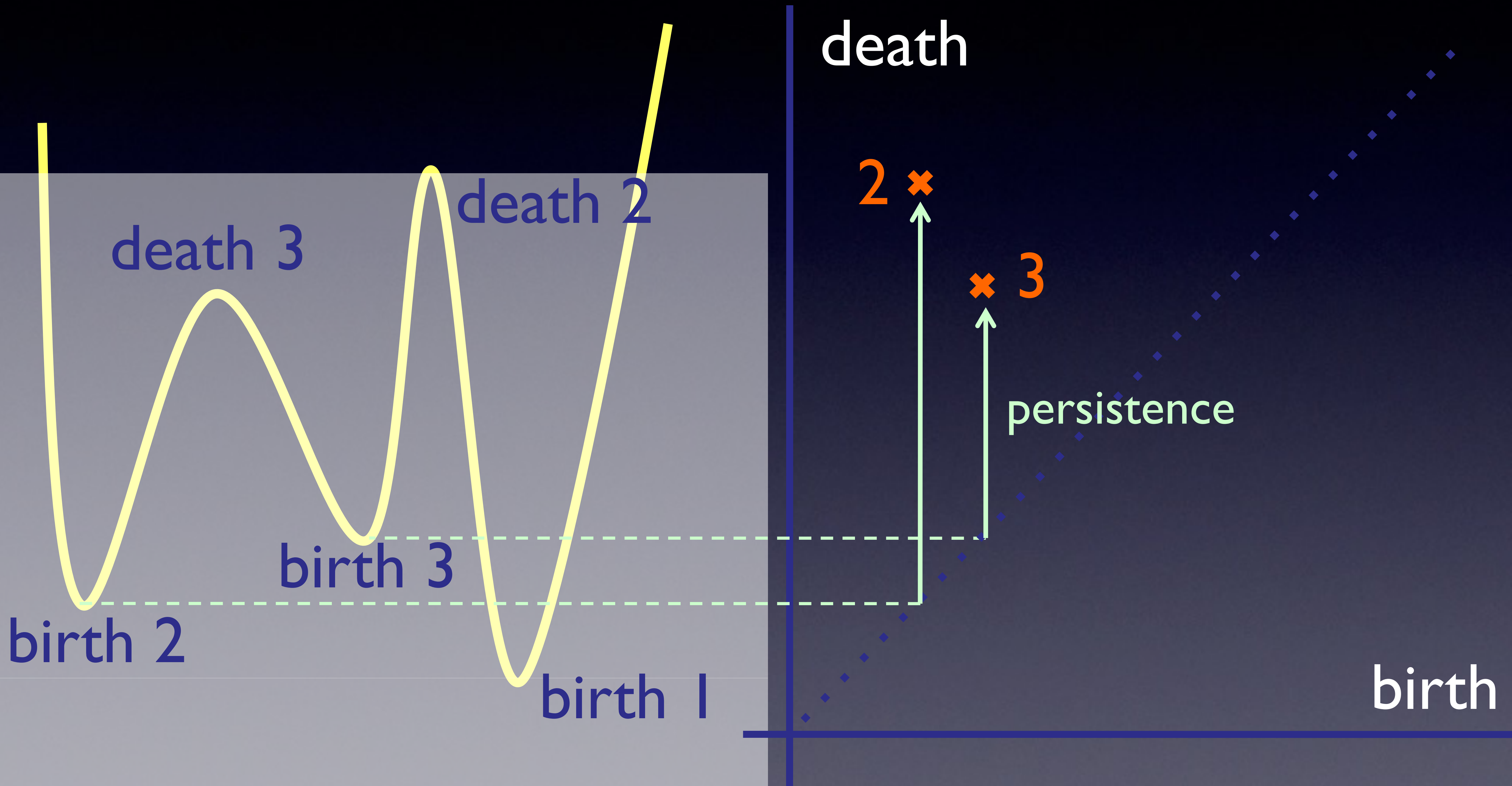
Component dies at c

$$\beta_0(R_c) = \beta_0(R_b) - 1$$

PH_morse1D.m

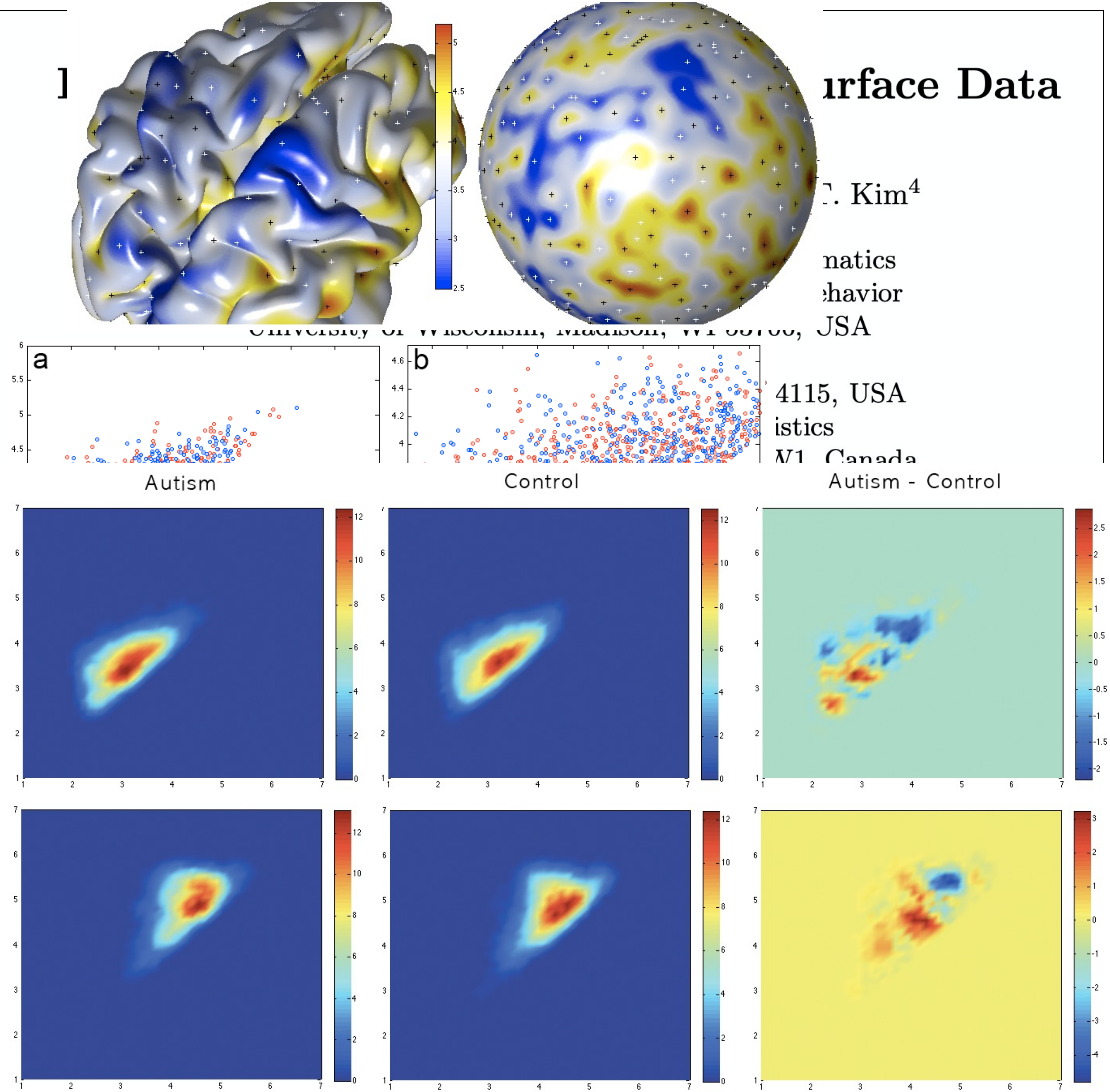
Persistence Diagram (PD)

O(n log n)



Elder's rule:

Pair the time of death with the time of the closest earlier birth.



Chung et al., 2009
Information Processing in Medical Imaging (IPMI) 5636:386-397.

First TDA paper in medical imaging

Boundary matrix

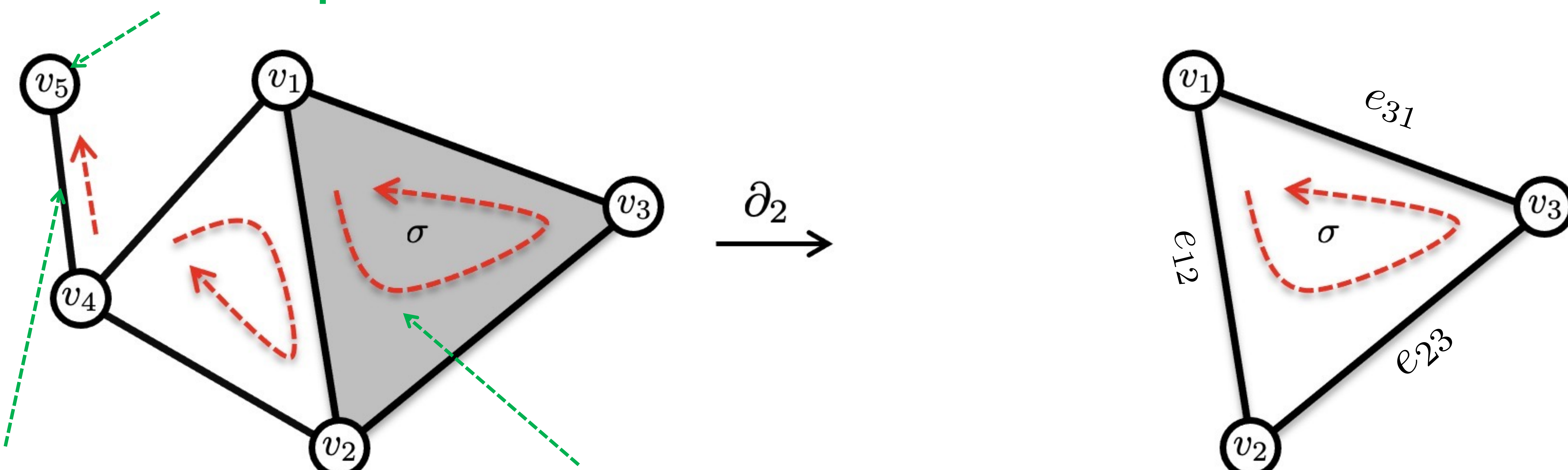
n-simplex

The basic building block of persistent homology

The smallest convex set containing *n*+*1* points

$$\sum_{i=0}^{n} x_i = 1, x_i \geq 0$$

0-simplex $[v_5]$



1-simplex

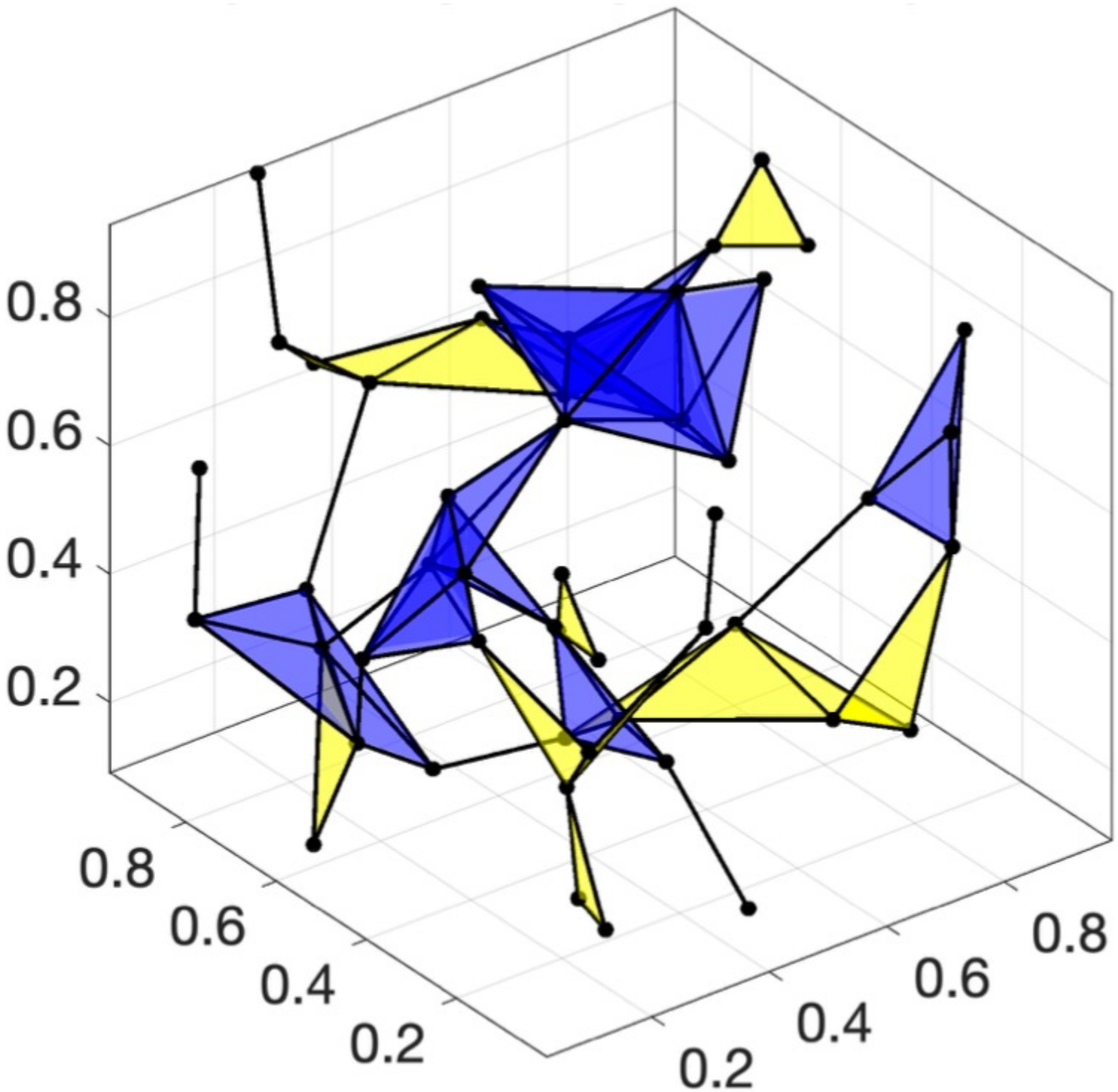
$[v_4, v_5] = -[v_5, v_4]$

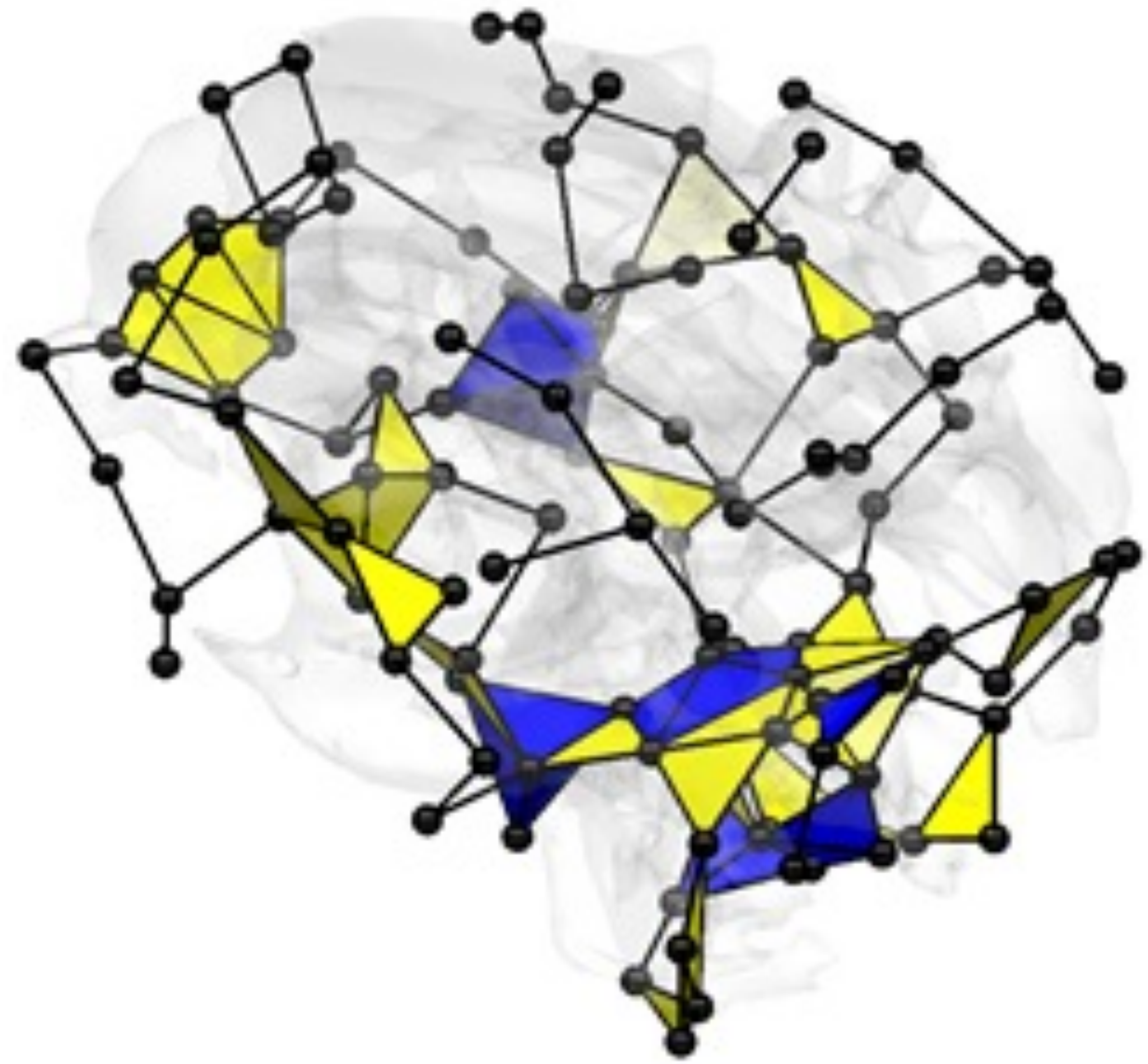
2-simplex

$\sigma = [v_1, v_2, v_3]$

Simplicial complex

A simplicial complex is a set composed of points, line segments, triangles, and their n-dimensional counterparts.



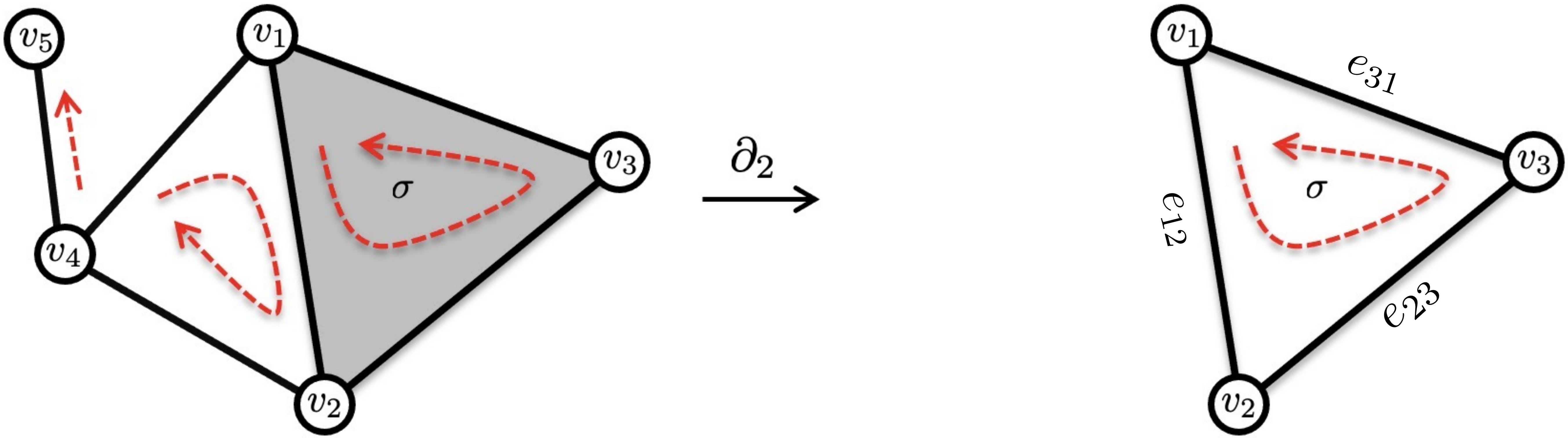


PH_rips.m

Boundary operators ∂_k

∂_k Removes the filled-in interior of *k*-simplexes

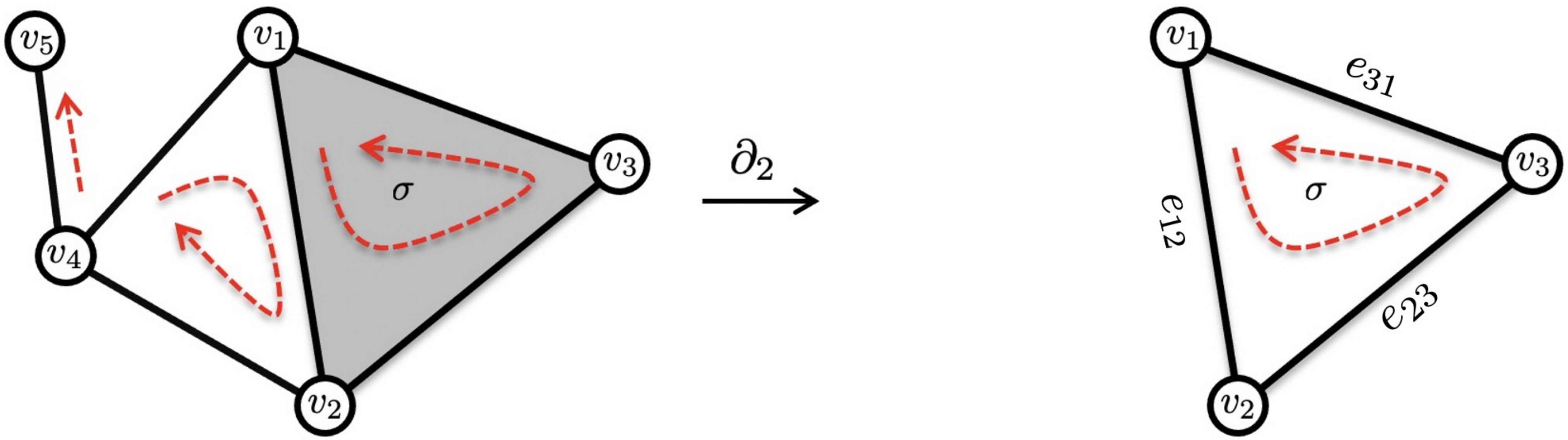
$\partial_k : C_k \to C_{k-1}$



$$\partial_2 \sigma = [v_1, v_2] + [v_2, v_3] + [v_3, v_1]$$

$$\partial_1 \partial_2 \sigma = v_2 - v_1 + v_3 - v_2 + v_1 - v_3 = 0$$

Boundary matrix ∂_0

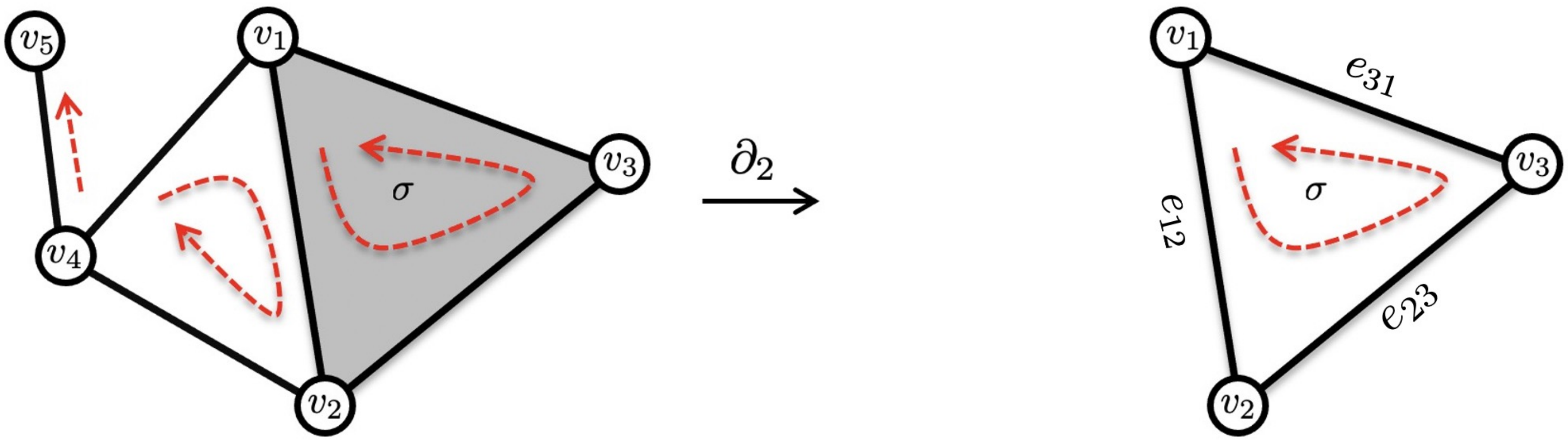


$$\boldsymbol{\partial}_0 = \begin{array}{c c} & \begin{array}{ccccc} v_1 & v_2 & v_3 & v_4 & v_5 \end{array} \\ 0 & \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

PH_boundary.m

Boundary matrix

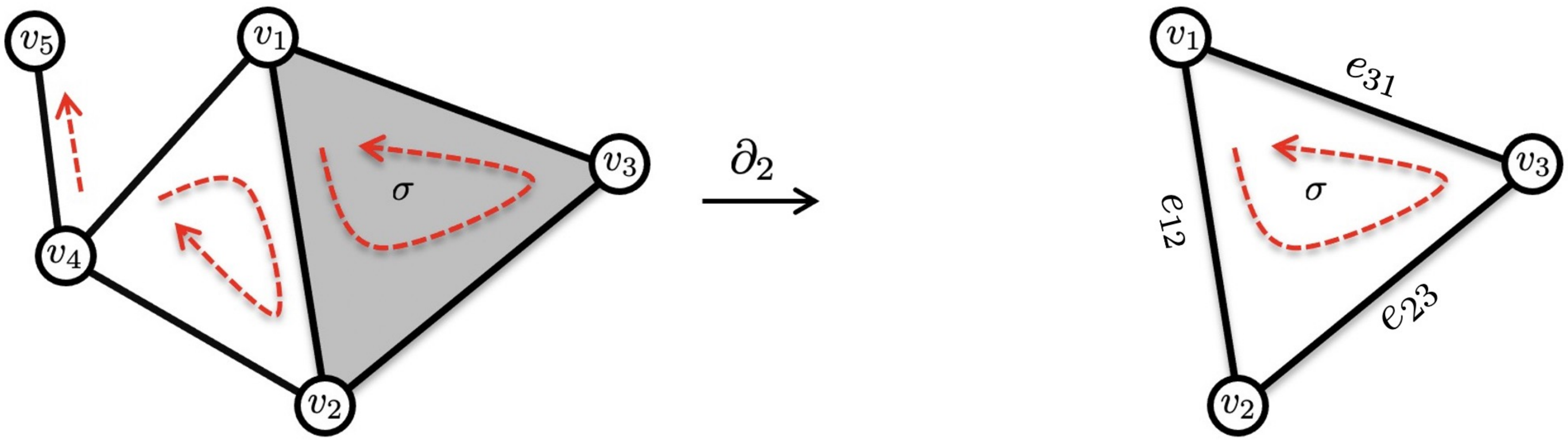
∂_1



$$\partial_1 \partial_2 \sigma = v_2 - v_1 + v_3 - v_2 + v_1 - v_3 = 0$$

$$\boldsymbol{\partial}_1 = \begin{array}{c c} & \begin{array}{cccccc} & & \sigma & & & \\ e_{12} & e_{23} & e_{31} & e_{24} & e_{41} & e_{45} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{array} & \begin{pmatrix} -1 & 0 & 1 & 0 & 1 & 0 \\ 1 & -1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

Boundary matrix ∂_2



$$\partial_2 \sigma = [v_1, v_2] + [v_2, v_3] + [v_3, v_1]$$

$$\boldsymbol{\partial}_2 = \begin{array}{c c} & \sigma \\ \begin{array}{c} e_{12} \\ e_{23} \\ e_{31} \\ e_{24} \\ e_{41} \\ e_{45} \end{array} & \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{array}$$

PH_boundary.m

Boundary matrix ∂_k

(*i*,*j*)-th entry = 1 if $\tau_i \subset \sigma_j$

Sign depends on the orientation of τ_i

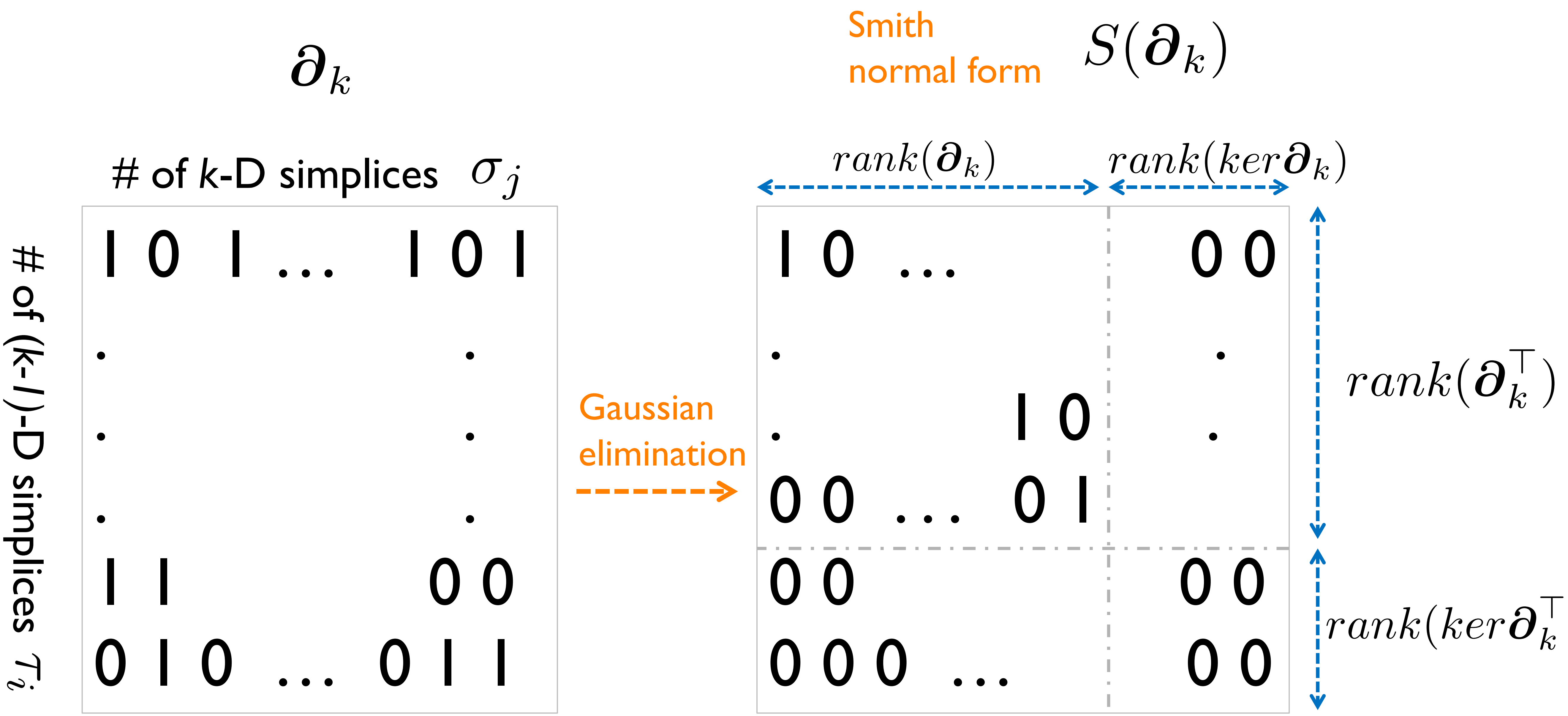
of *k*-dimensional simplices σ_j

of (*k*-*1*)-dimensional simplices τ_i

$$
\partial_k = \begin{bmatrix}
1 & 0 & 1 & \dots & 1 & 0 & 1 \\
\cdot & & & & \cdot & & \\
\cdot & & & & \cdot & & \\
\cdot & & & & \cdot & & \\
1 & 1 & & & & 0 & 0 \\
0 & 1 & 0 & \dots & 0 & 1 & -1
\end{bmatrix}
$$

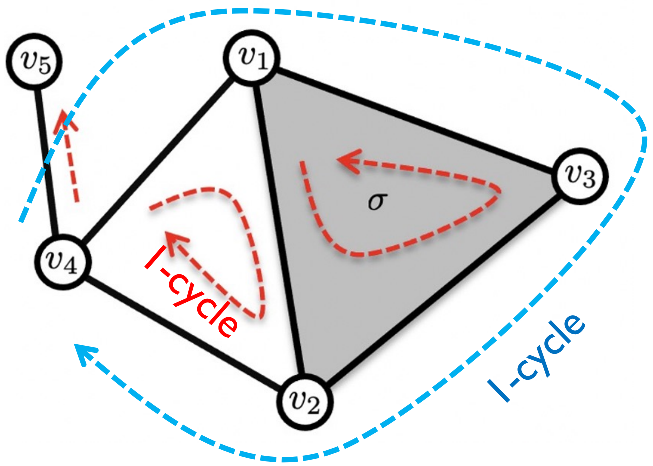
PH_boundary.m

Rank nullity theorem for boundary matrix



$$\beta_k = rank(ker\boldsymbol{\partial}_k) - rank(\boldsymbol{\partial}_{k+1})$$

Computing Betti numbers through boundary matrices



$$\mathcal{S}(\boldsymbol{\partial}_1) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{S}(\boldsymbol{\partial}_2) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\beta_0 = rank(ker\boldsymbol{\partial}_0) - rank(\boldsymbol{\partial}_1) \quad = 5\text{-}4$$

$$\beta_1 = rank(ker\boldsymbol{\partial}_1) - rank(\boldsymbol{\partial}_2) \quad = 2\text{-}1$$

PH_boundary_betti.m

k-th Hodge Laplacian

PH_hodge.m

$$\Delta_k = \partial_{k+1}\partial_{k+1}^\top + \partial_k^\top \partial_k$$

0th Hodge Laplacian
Graph Laplacian

# of nodes

$$\Delta_0 = \boxed{\partial_1 \partial_1^\top}$$

# of nodes

1st Hodge Laplacian

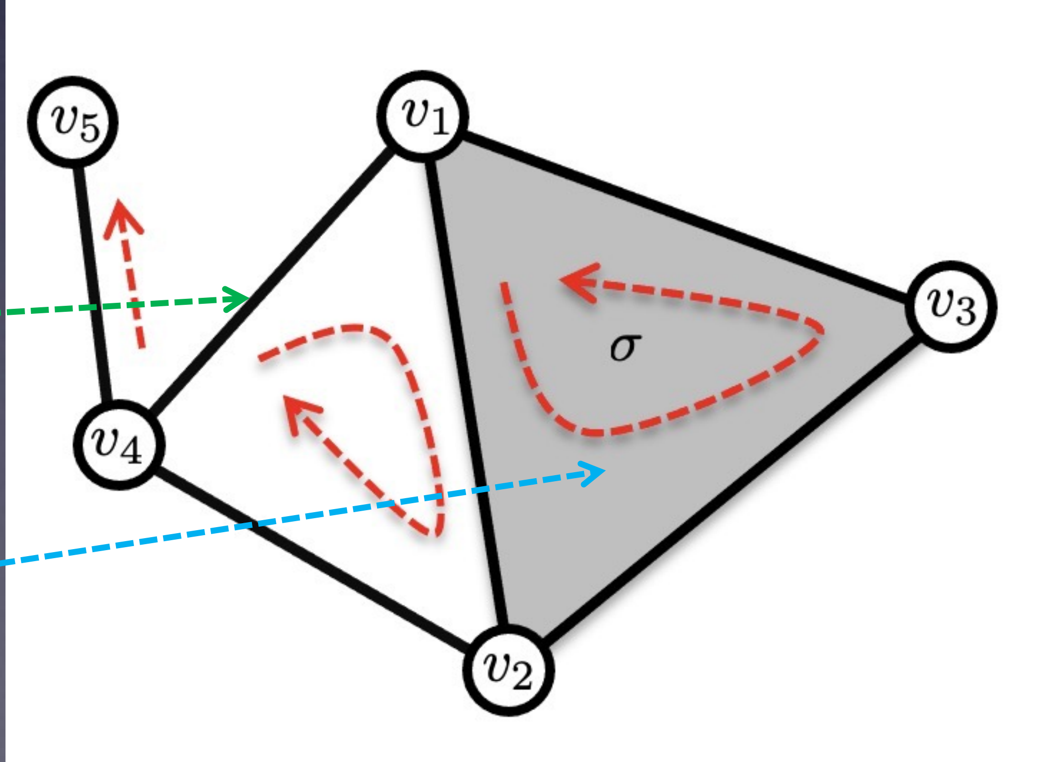
# of edges

# of edges

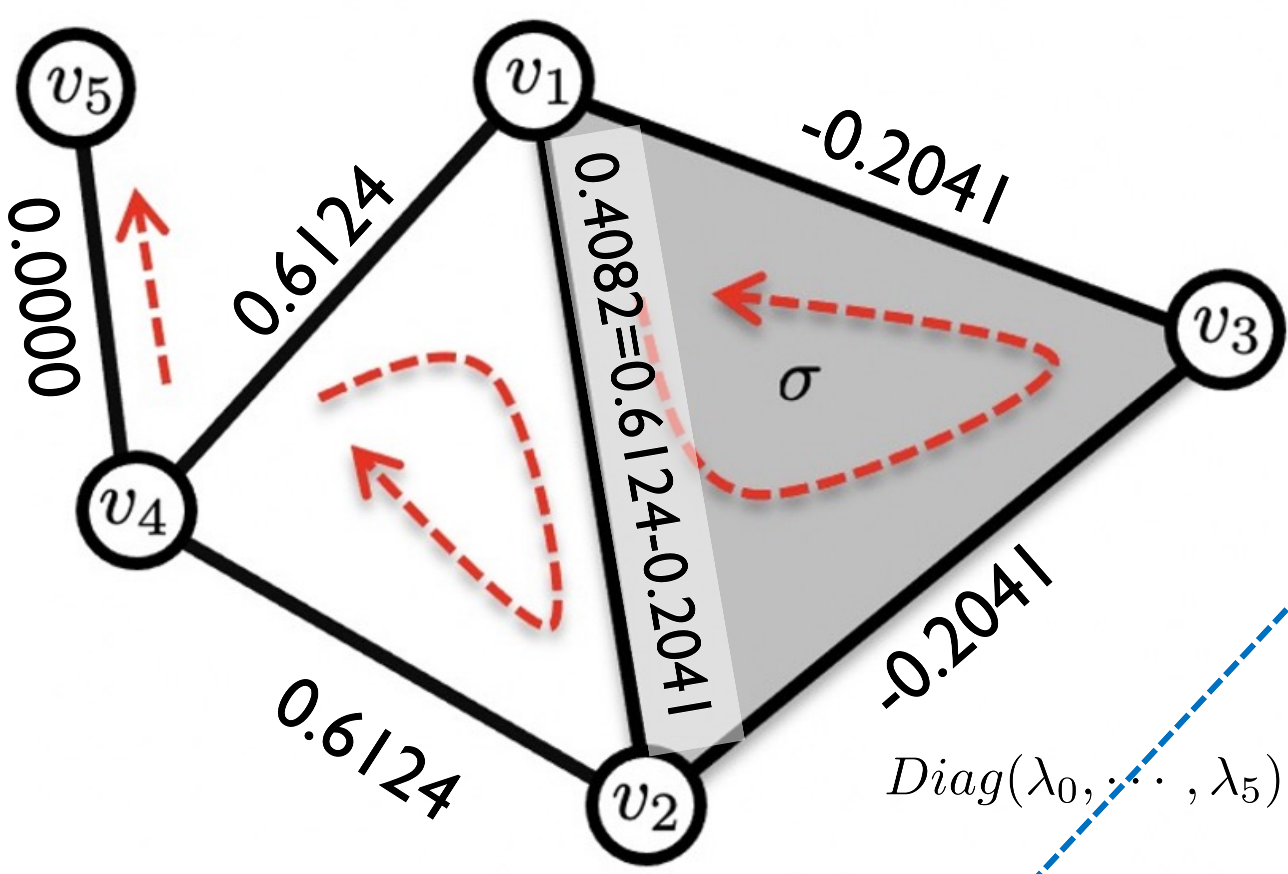
$$\Delta_1 = \boxed{\partial_2 \partial_2^\top} + \boxed{\partial_1^\top \partial_1}$$

# of edges

# of edges



Eigenvectors of Hodge Laplacian



$$\Delta_1 = \boldsymbol{\partial}_2 \boldsymbol{\partial}_2^\top + \boldsymbol{\partial}_1^\top \boldsymbol{\partial}_1$$

$$ker \Delta_1$$

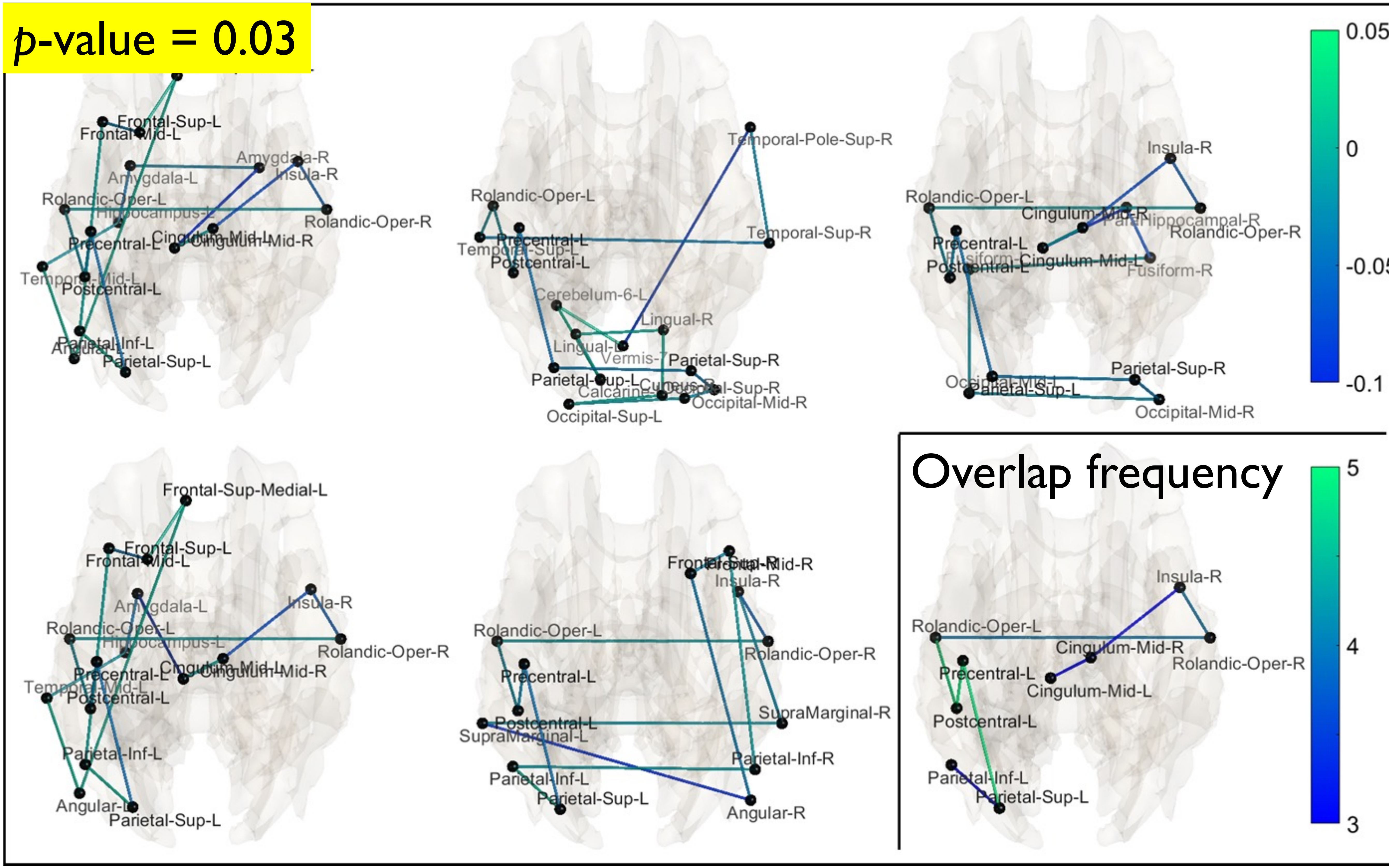
span

$$Diag(\lambda_0, \cdots, \lambda_5) = \begin{pmatrix} \boxed{0.0000} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.8299 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.6889 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.4812 \end{pmatrix}$$

$$(\mathbf{f}_0, \cdots, \mathbf{f}_5) = \begin{pmatrix} 0.4082 & -0.0000 & 0.0000 & 0.5774 & 0.7071 & -0.0000 \\ -0.2041 & 0.1993 & -0.5765 & 0.5774 & -0.3536 & 0.3578 \\ -0.2041 & -0.1993 & 0.5765 & 0.5774 & -0.3536 & -0.3578 \\ 0.6124 & -0.4325 & 0.1793 & -0.0000 & -0.3536 & 0.5299 \\ 0.6124 & 0.4325 & -0.1793 & -0.0000 & -0.3536 & -0.5299 \\ 0.0000 & -0.7392 & -0.5207 & 0.0000 & 0.0000 & -0.4271 \end{pmatrix}$$

Basis vector for cycles

Five biggest cycle differences (male – female) in HCP



Anand et al. 2023, IEEE TMI in press arXiv:2110.14599

Rips filtrations

Rips filtration

Metric space

$$\mathcal{X} = (V, w) \quad w = (w_{ij})$$

Node set

Metric

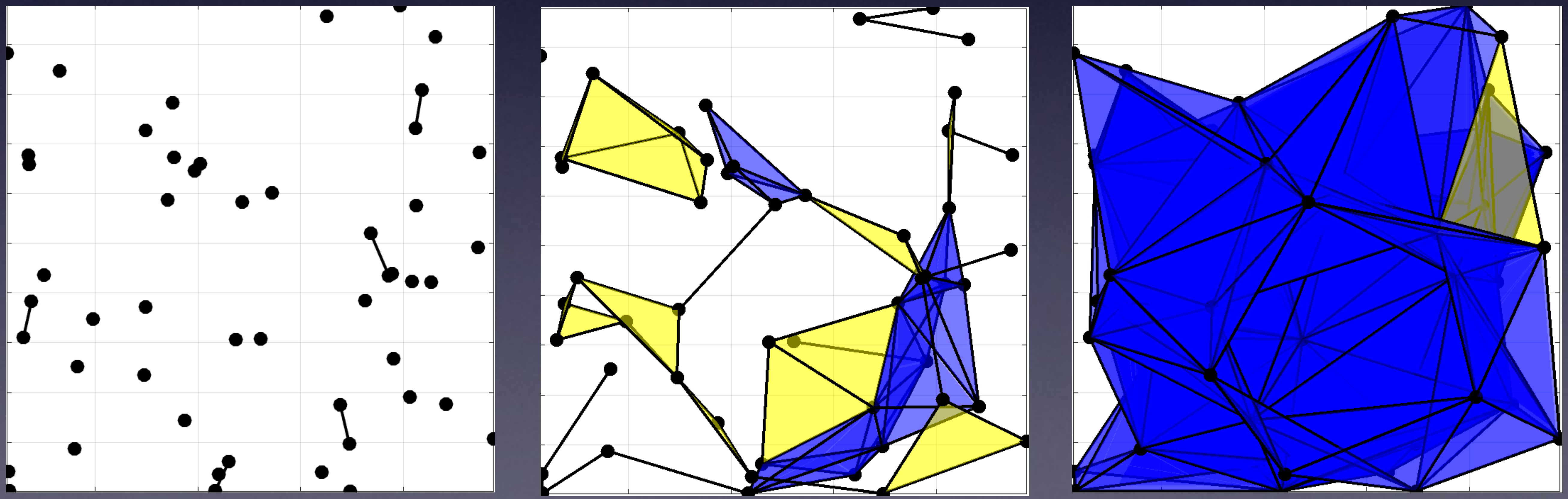
$$w_{ik} < w_{ij} + w_{jk}$$

Rips filtration

$$\mathcal{X}_{\epsilon_0} \subset \mathcal{X}_{\epsilon_1} \subset \mathcal{X}_{\epsilon_2} \subset \cdots$$

for filtration values

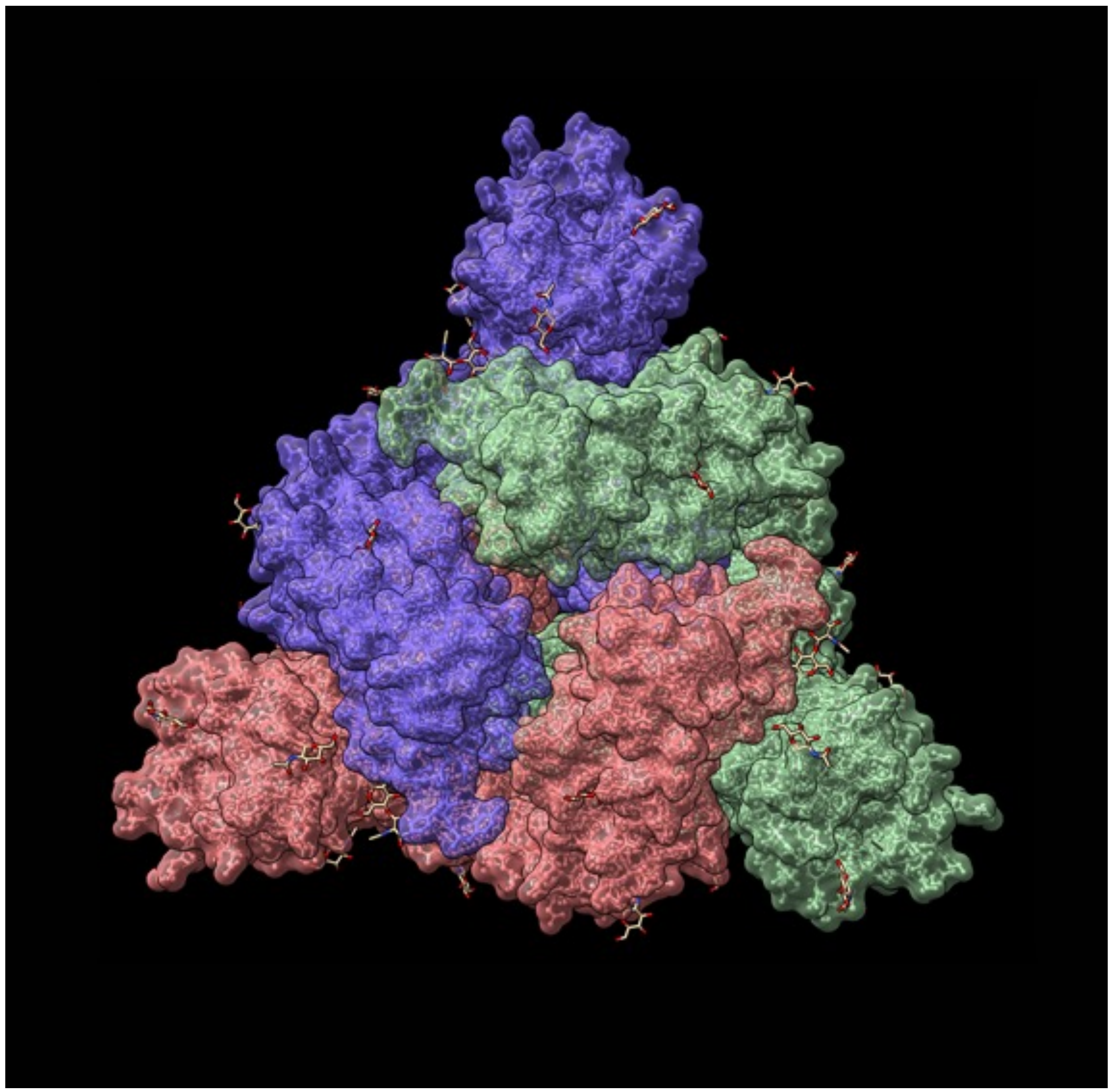
$$\epsilon_0 < \epsilon_1 < \epsilon_2 < \cdots$$

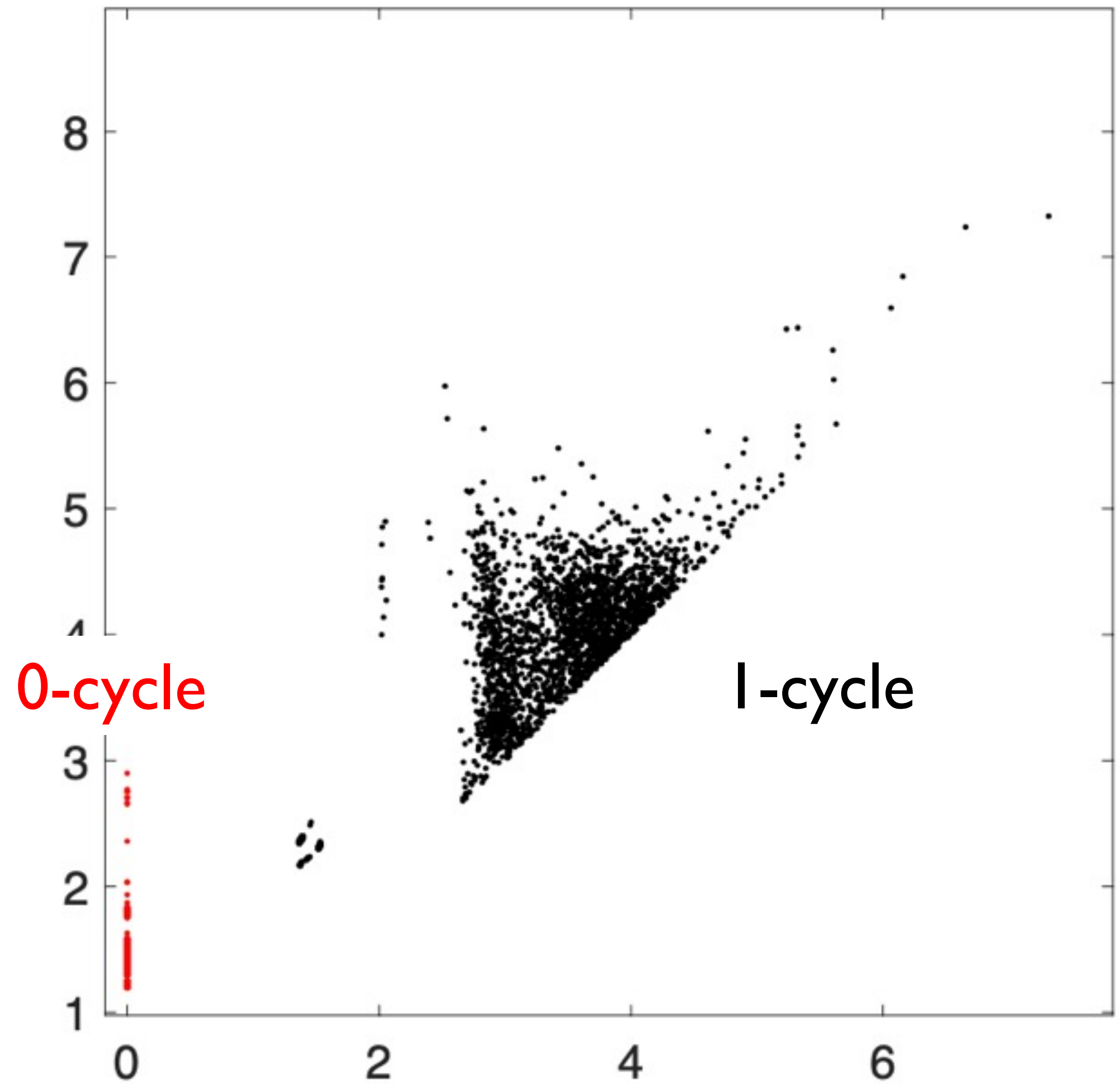


$\epsilon = 0.1$ $\epsilon = 0.3$ $\epsilon = 0.5$

Persistence Diagram (PD) of a protein molecule

Rips filtration on distance between 8000 atoms

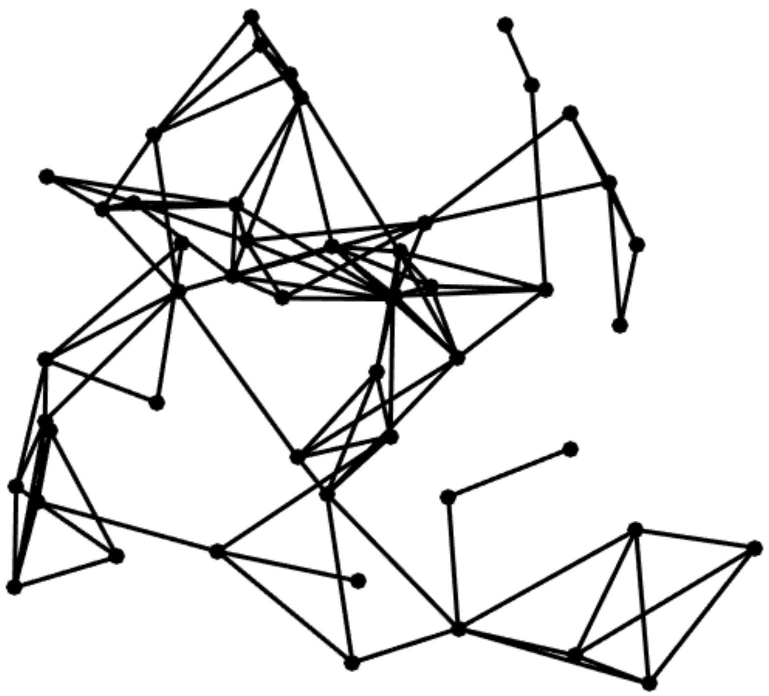




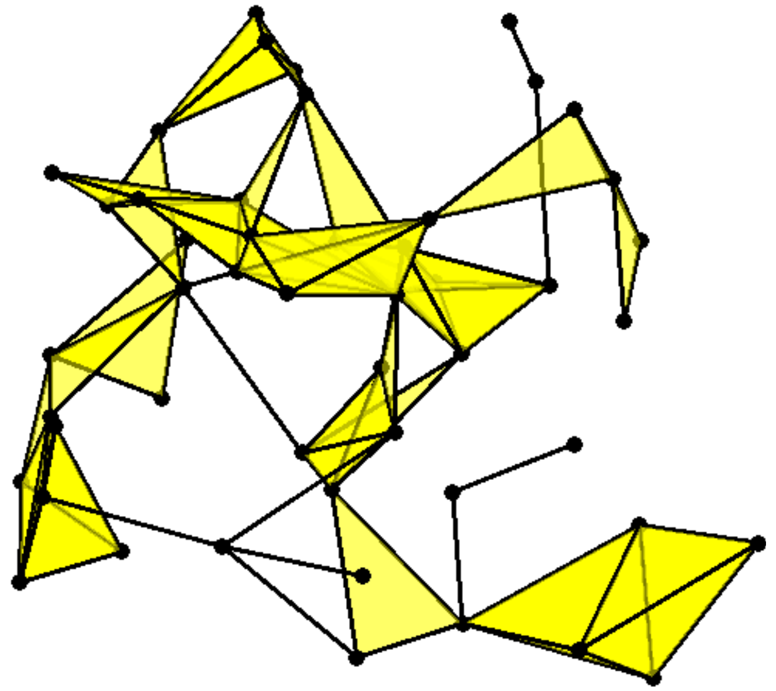
Extremely slow computation → Simply use graph filtration

k-skeleton

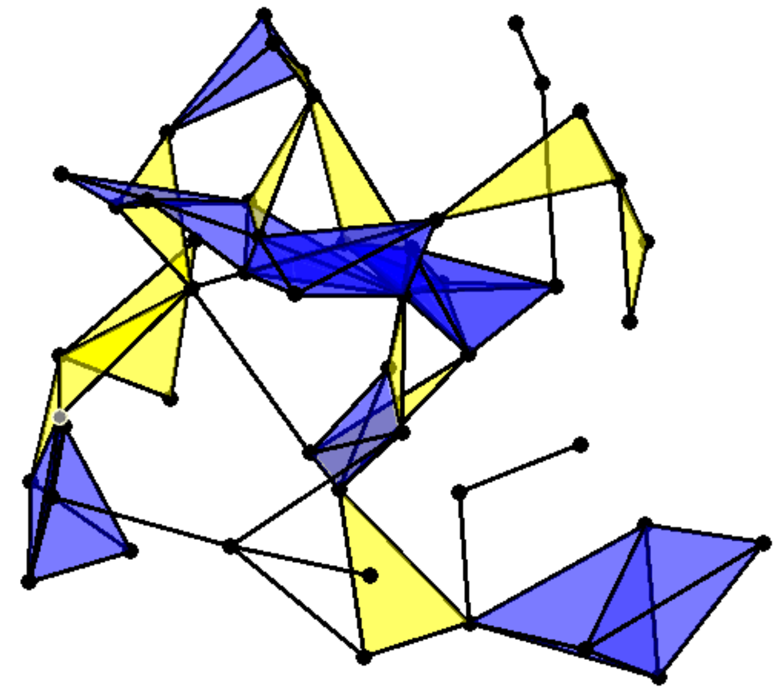
A simplicial complex consisting of up to k-simplices



1-skeleton



2-skeleton



3-skeleton

PH_rips.m

Graph filtrations

Baseline filtration for brain networks introduced in

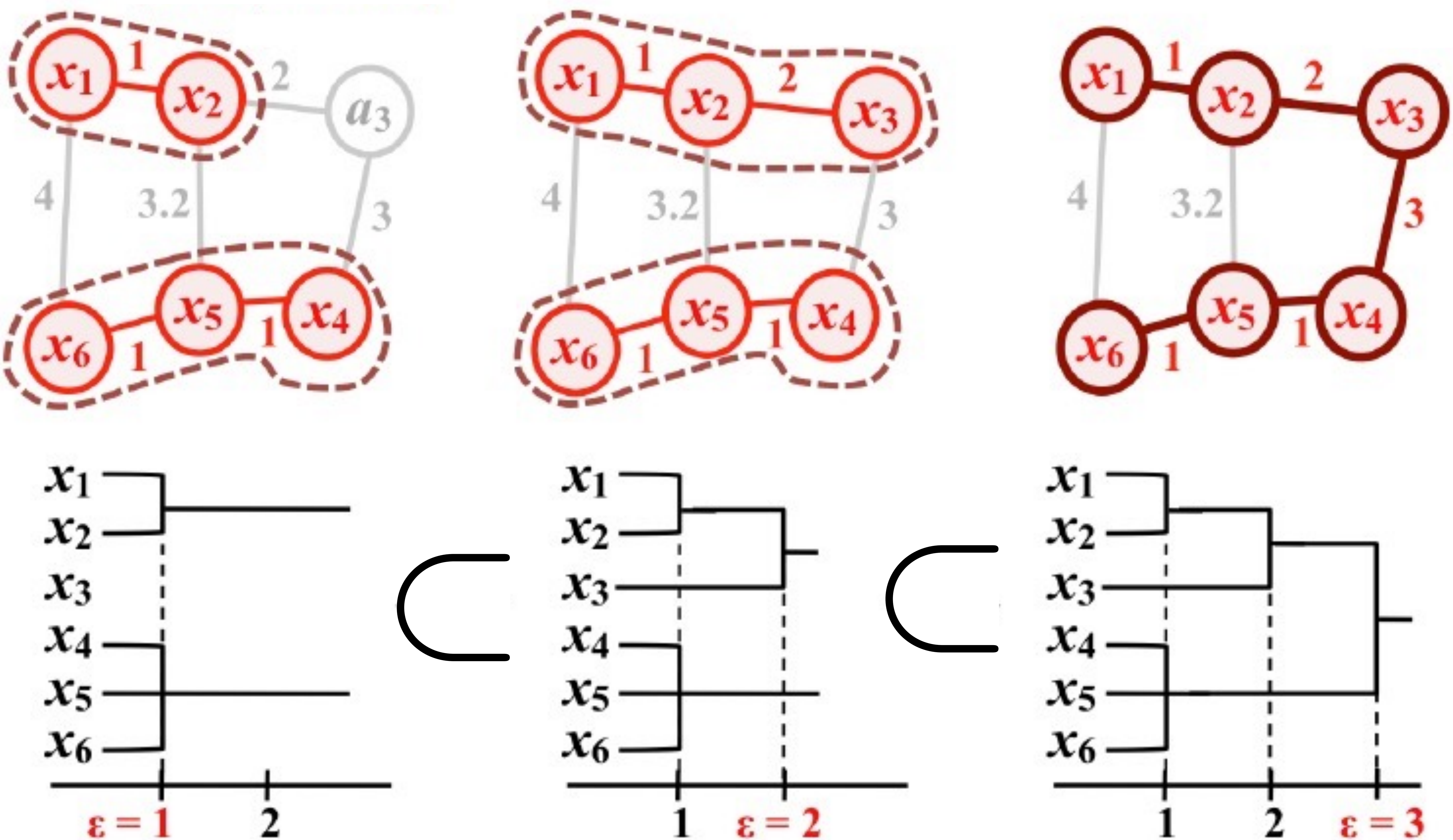
Lee et al. 2011 ISBI
Lee et al. 2011 MICCAI 302-309
Lee et al. 2012 IEEE Transactions on Medical Imaging 31:2267-2277

Graph filtration (filtration on 1-skeleton)

Rips filtration is computationally expensive:
For n-nodes, $O(n^{3k+3})$ for the k-th Betti number.

For 1-skeleton, graph filtration is $O(n \log n)$ for both 0-th and 1-st Betti number.

Graph filtration=single linkage clustering



Lee et al. 2011 MICCAI 302-309

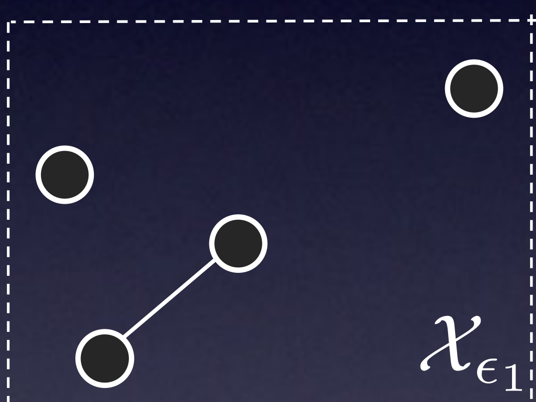
Rips filtration vs. graph filtration

Metric space

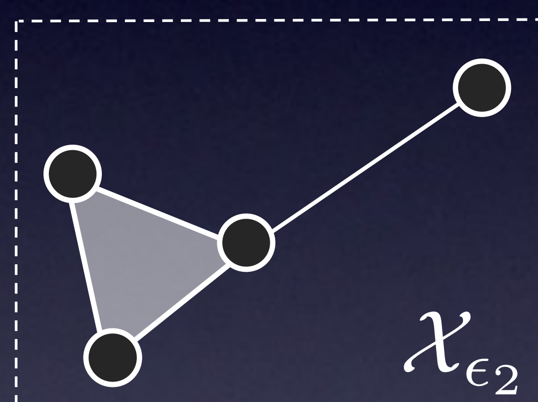
$$\mathcal{X} = (V, w) \quad w = (w_{ij})$$

Node set — Metric

Rips complex = Simplicial complex



$\subset$



Rips filtration

$$\mathcal{X}_{\epsilon_0} \subset \mathcal{X}_{\epsilon_1} \subset \mathcal{X}_{\epsilon_2} \subset \cdots$$

for increased radius

$$\epsilon_0 < \epsilon_1 < \epsilon_2 < \cdots$$

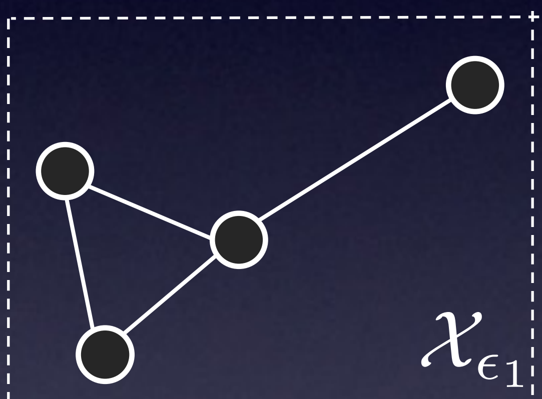
PH_rips.m

Weighted graph

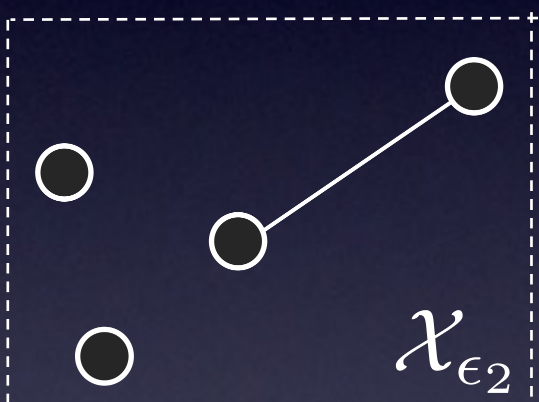
$$\mathcal{X} = (V, w) \quad w = (w_{ij})$$

Node set — Edge weight

Binary graph: 1-skeleton



$\supset$



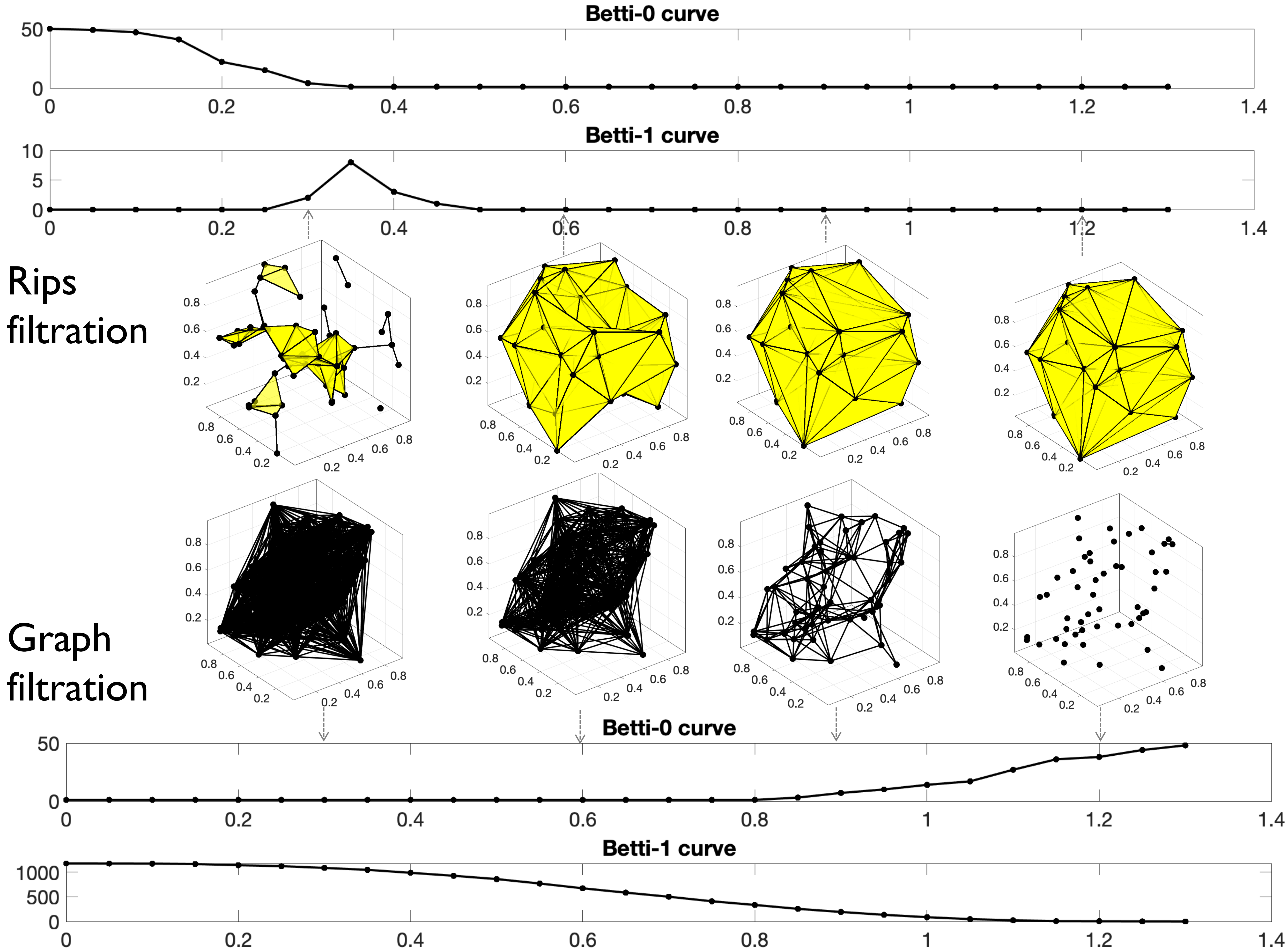
Graph filtration

$$\mathcal{X}_{\epsilon_0} \supset \mathcal{X}_{\epsilon_1} \supset \mathcal{X}_{\epsilon_2} \supset \cdots$$

for increased edge weights

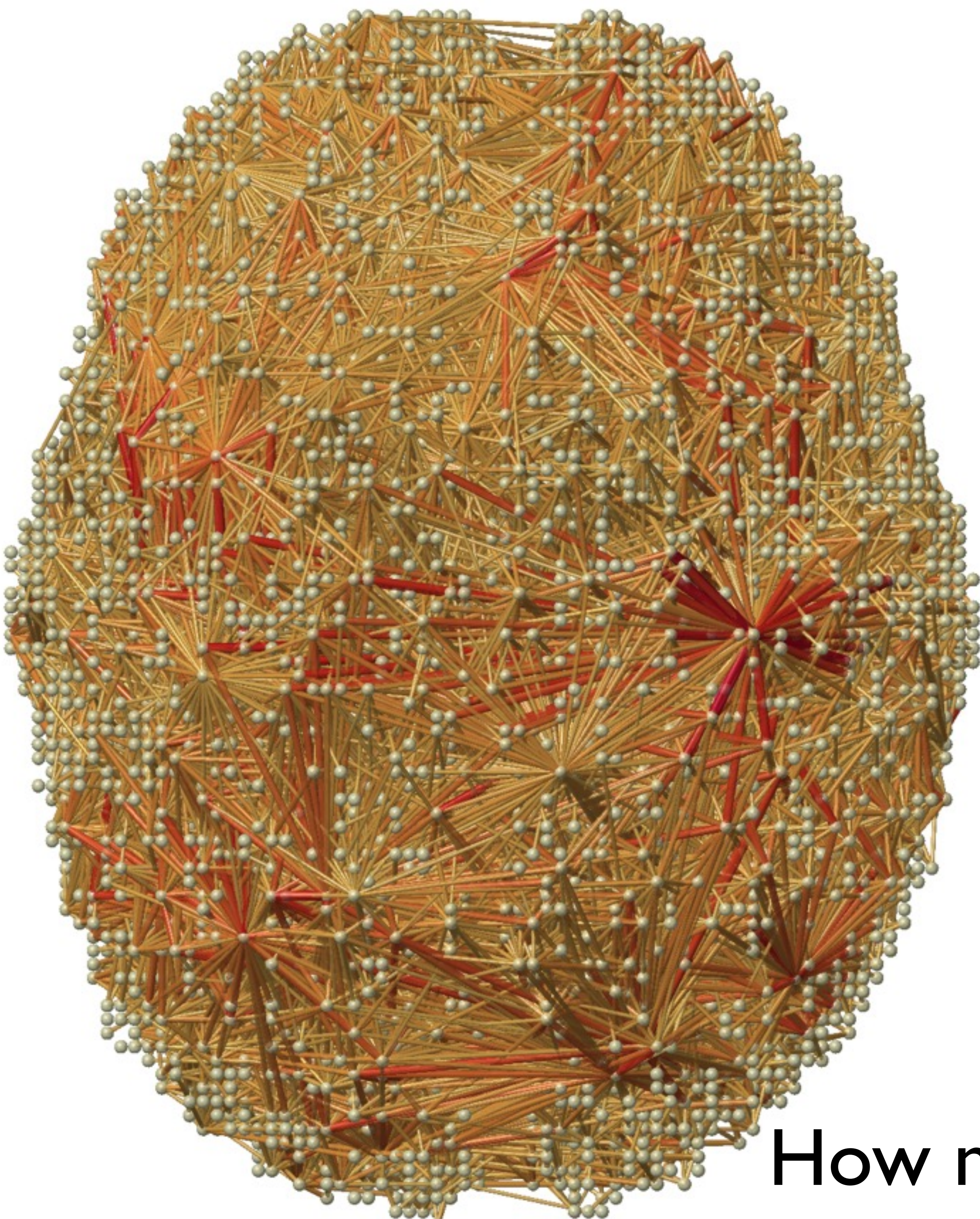
$$\epsilon_0 < \epsilon_1 < \epsilon_2 < \cdots$$

PH_graph.m



Betti-0 curve
Betti-1 curve
Rips filtration
Graph filtration
Betti-0 curve
Betti-1 curve

How to compute the number of cycles in big network data?



How many cycles in the network?

Fast computation of Betti curves

Computation of β_0: Many existing algorithms. Can use a built-in function in MATLAB.

```
[beta_0, S] = graphconncomp(adj)
```

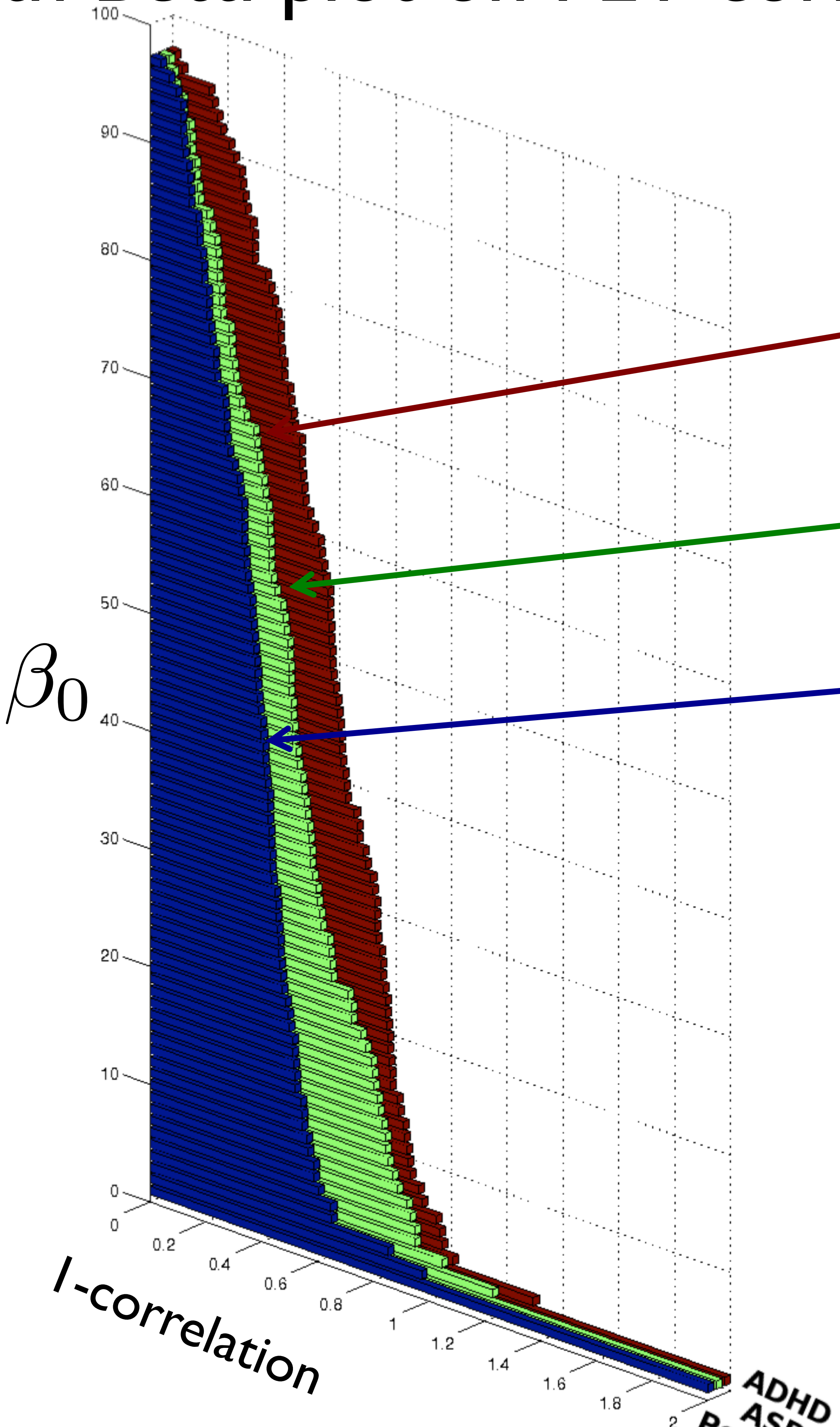
Computation of β_1: As a function of β_0

$$\beta_1 = \beta_0 - p + q$$

```
q=sum(sum(adj))/2;
beta_1 = beta_0 – p + q;
```

PH_betti.m

0-th Betti plot on PET correlation network



24 attention deficit hyperactivity disorder (ADHD) children

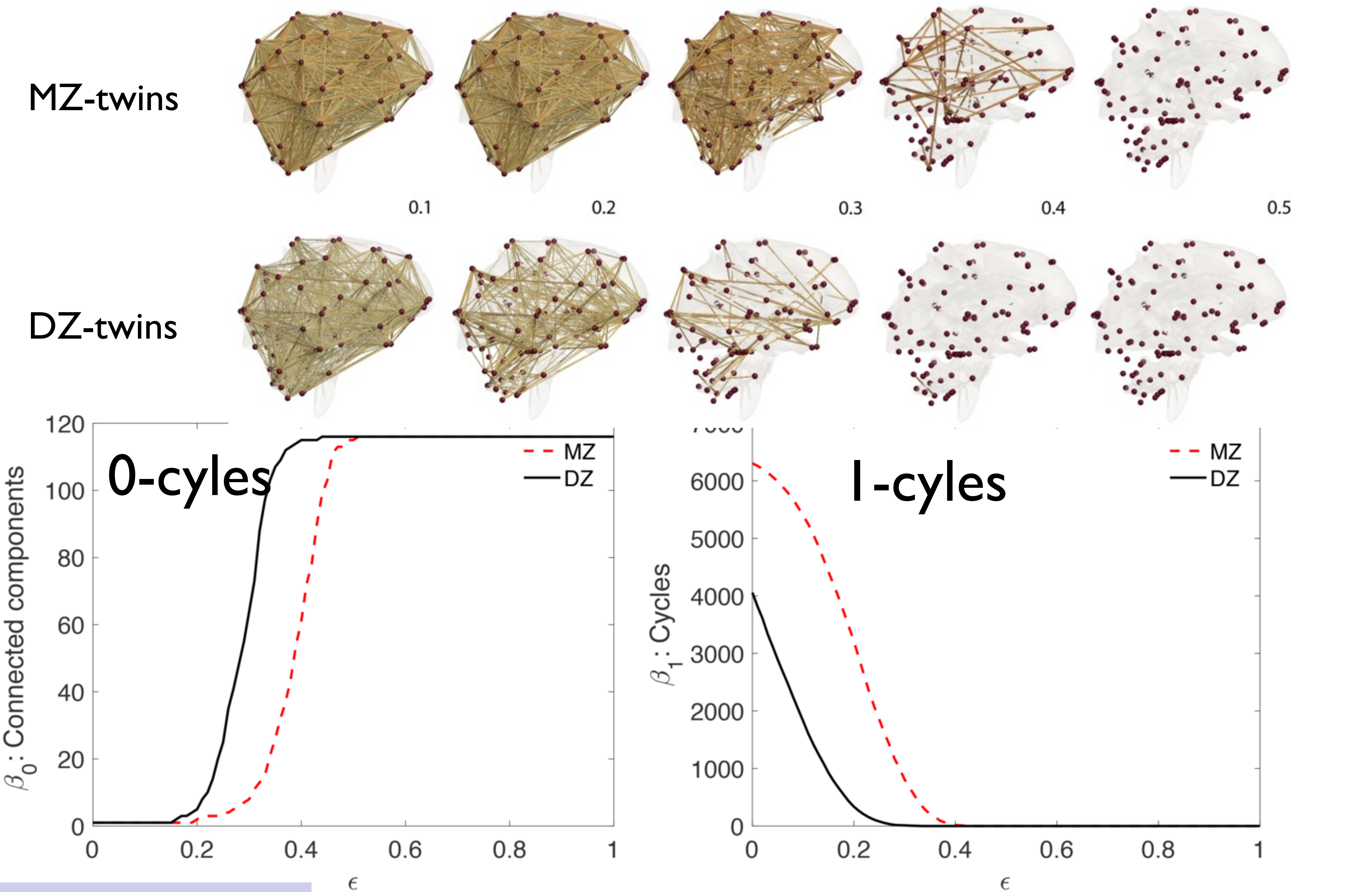
26 autism spectrum disorder (ASD) children

11 pediatric control subjects

PH_betti.m

Lee et al. (2011) ISBI

Genetic effect on Betti curves of rs-fMRI network

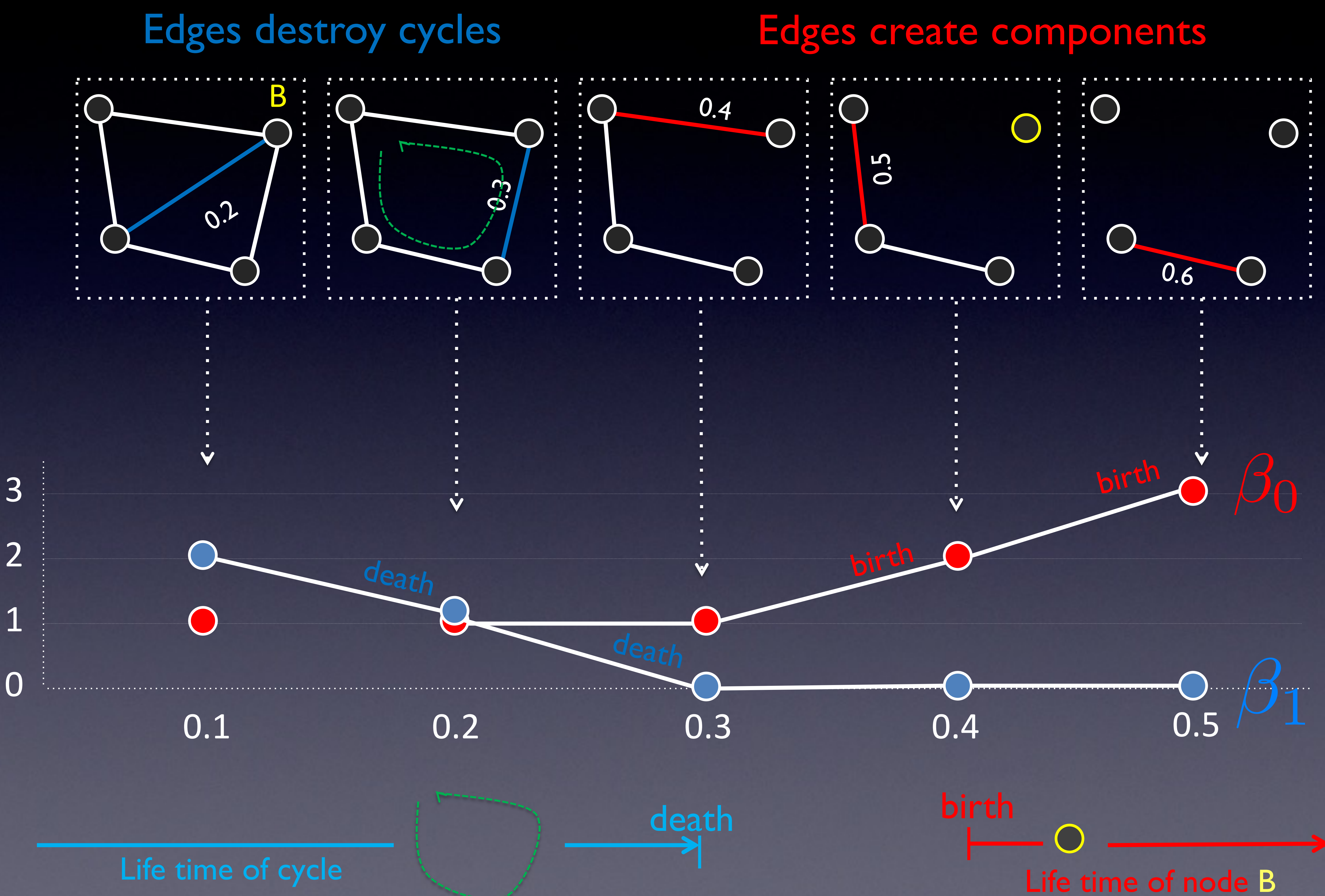


PH_betti.m

Chung et al. 2019 Network Neuroscience 3:674-694

Birth and death decomposition

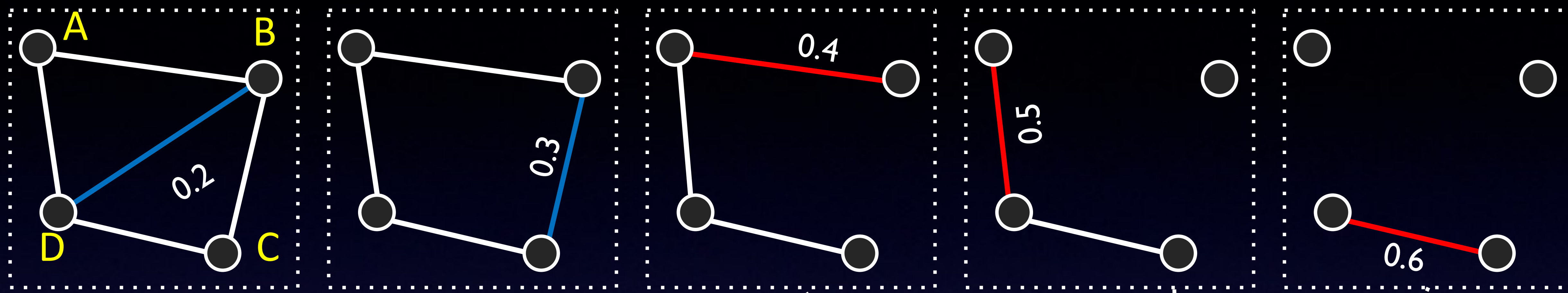
Persistence = Life time (death – birth) of a feature



Theorem Birth & death sets partition the edge set

E_1 Edges destroy cycles

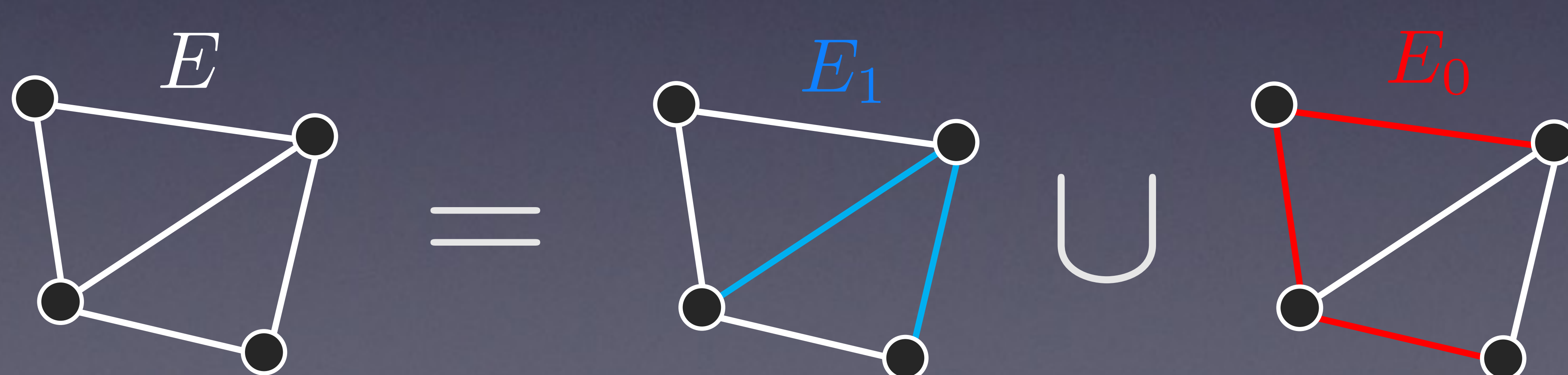
E_0 Edges create components



$$\#(E_1) = 1 + \frac{|V|(|V|-3)}{2}$$

$$\#(E_0) = |V| - 1$$

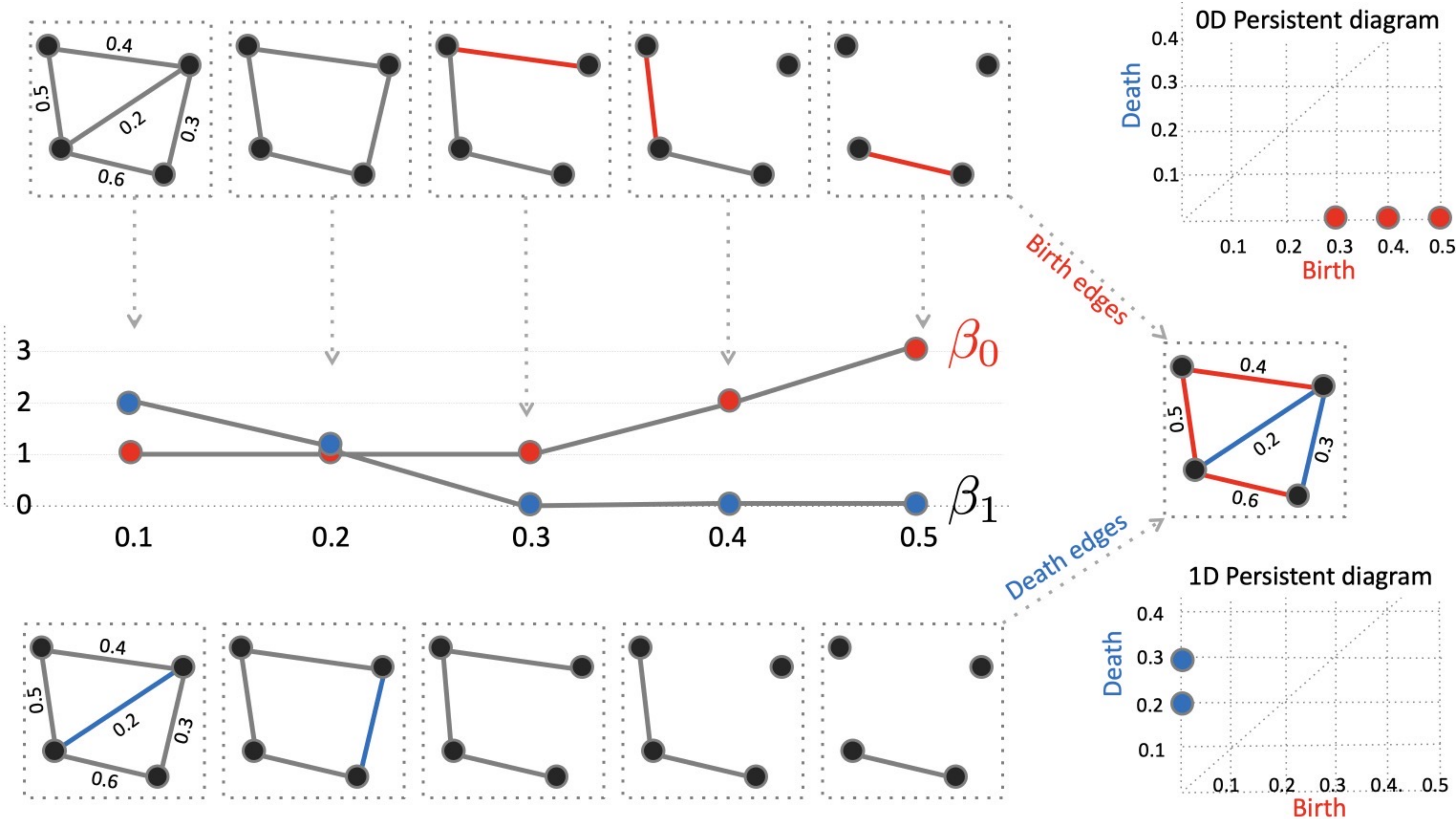
$$\#(E) = \frac{|V|(|V|-1)}{2}$$



Maximum spanning tree

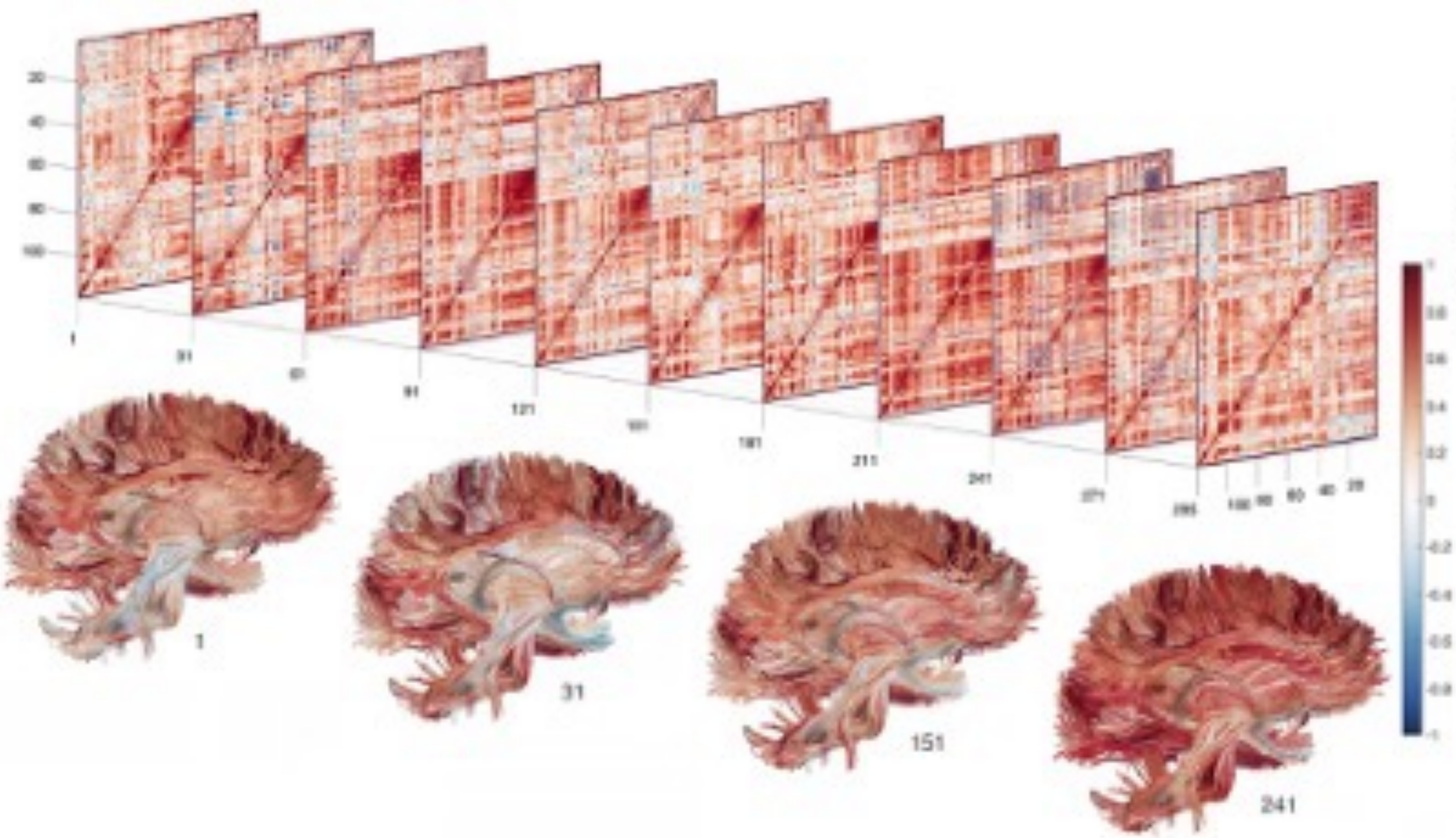
$O(|E| \log |V|)$

Songdechakraiwut & Chung 2020 arXiv: 2012.00675

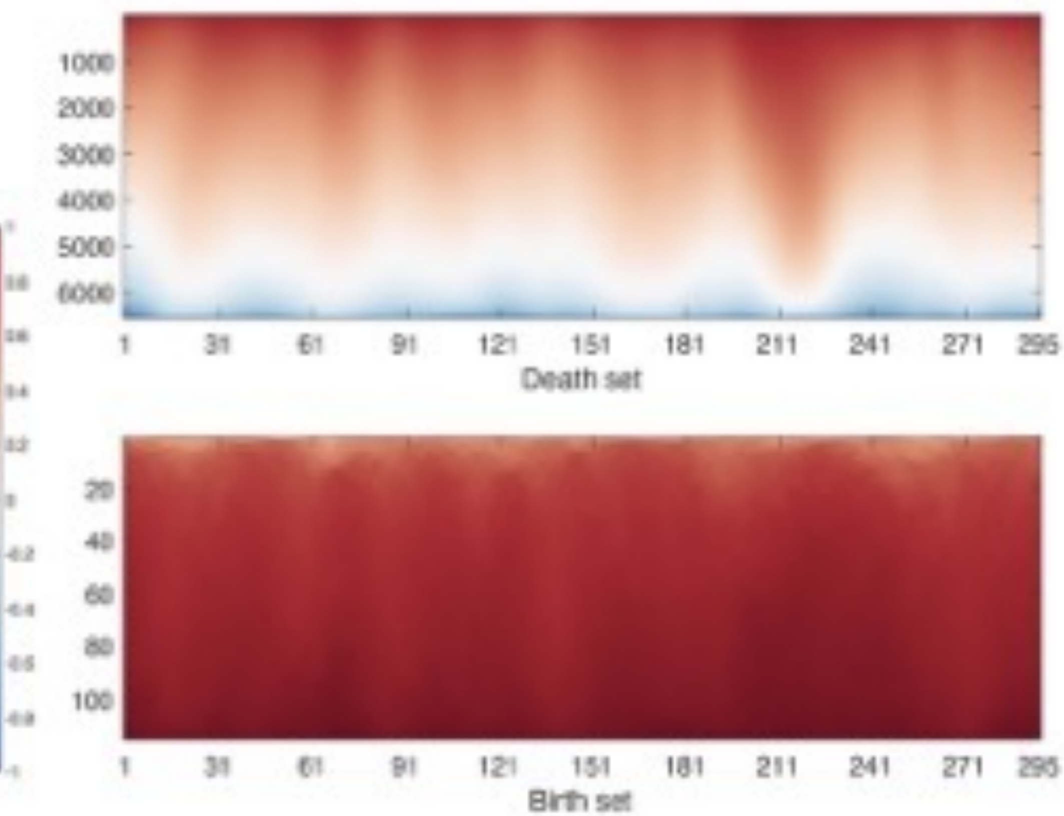


0D Persistent diagram
Death
Birth
0.1
0.2
0.3
0.4.
0.5
Birth edges
Death edges
β_0
β_1
1D Persistent diagram

Dynamically changing correlation network from rs-fMRI



Dynamically changing birth-death sets



WS_decompose.m

Topological inference

2-Wasserstein distance between persistent diagrams

Random variables: $X \sim f_1 \quad Y \sim f_2$

2-Wasserstein distance: $\mathcal{D}(X, Y) = \big(\inf \mathbb{E}\|X - Y\|^2\big)^{1/2}$

Persistent diagrams

$$P_1 = \{x_1, \cdots, x_q\} \subset \mathbb{R}^2 \qquad P_2 = \{y_1, \cdots, y_q\} \in \mathbb{R}^2$$

Empirical distributions

$$f_1(x) = \frac{1}{q}\sum_{i=1}^{q}\delta(x - x_i) \qquad f_2(y) = \frac{1}{q}\sum_{i=1}^{q}\delta(y - y_i)$$

$$\mathcal{D}(P_1, P_2) = \inf_{\psi: P_1 \to P_2}\Big(\sum_{x \in P_1}\|x - \psi(x)\|^2\Big)^{1/2}$$

Assignment problem: Hungarian algorithm

$\mathcal{O}(q^3)$

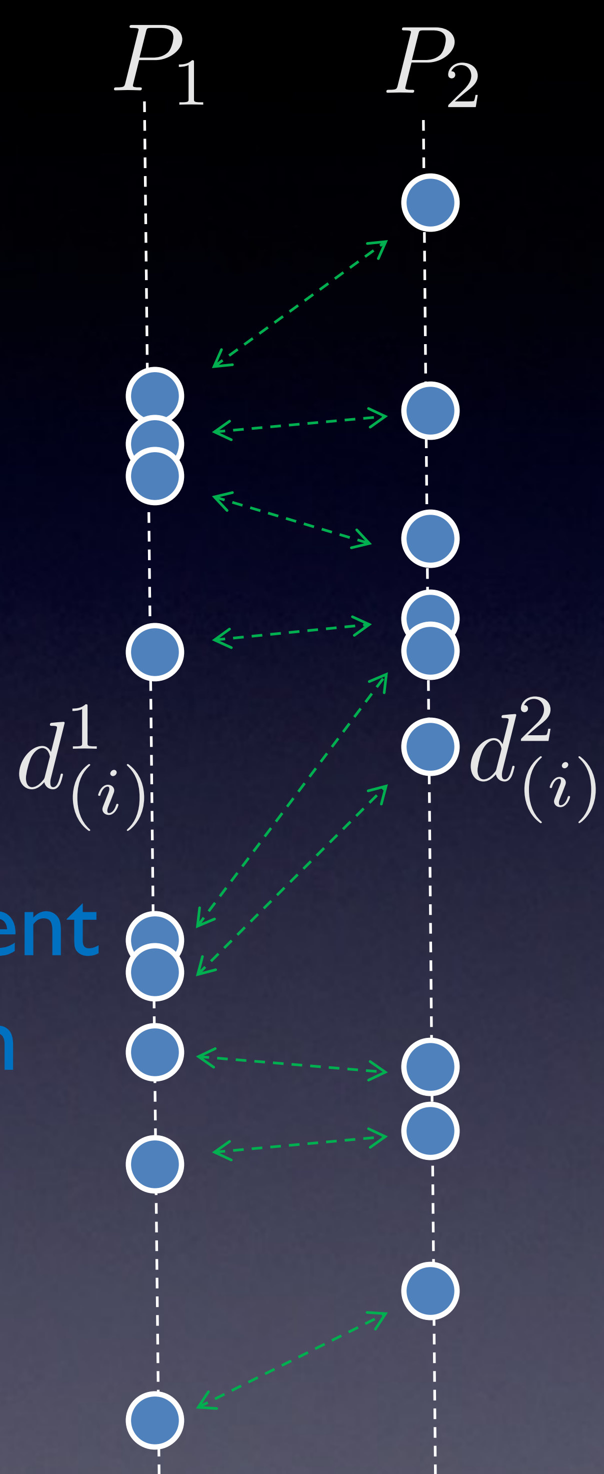
Graph filtration

$\mathcal{O}(q \log q)$

Wasserstein distance for graph filtrations

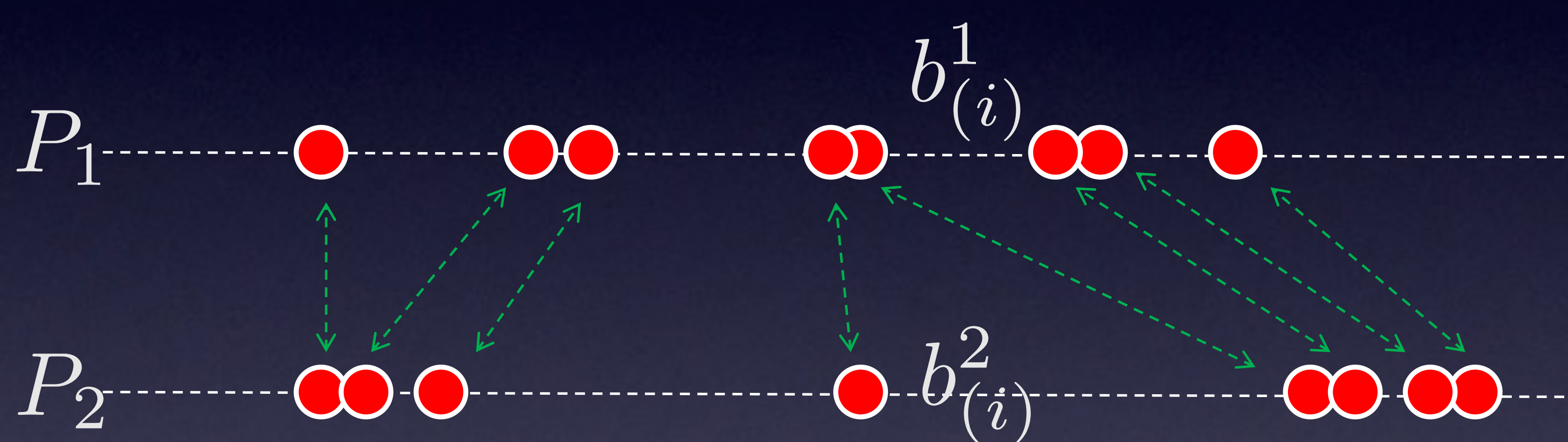
WS_pdist2.m

H_1 1D persistent diagram



$$\mathcal{D}_1(P_1, P_2)^2 = \sum_i (d^1_{(i)} - d^2_{(i)})^2$$

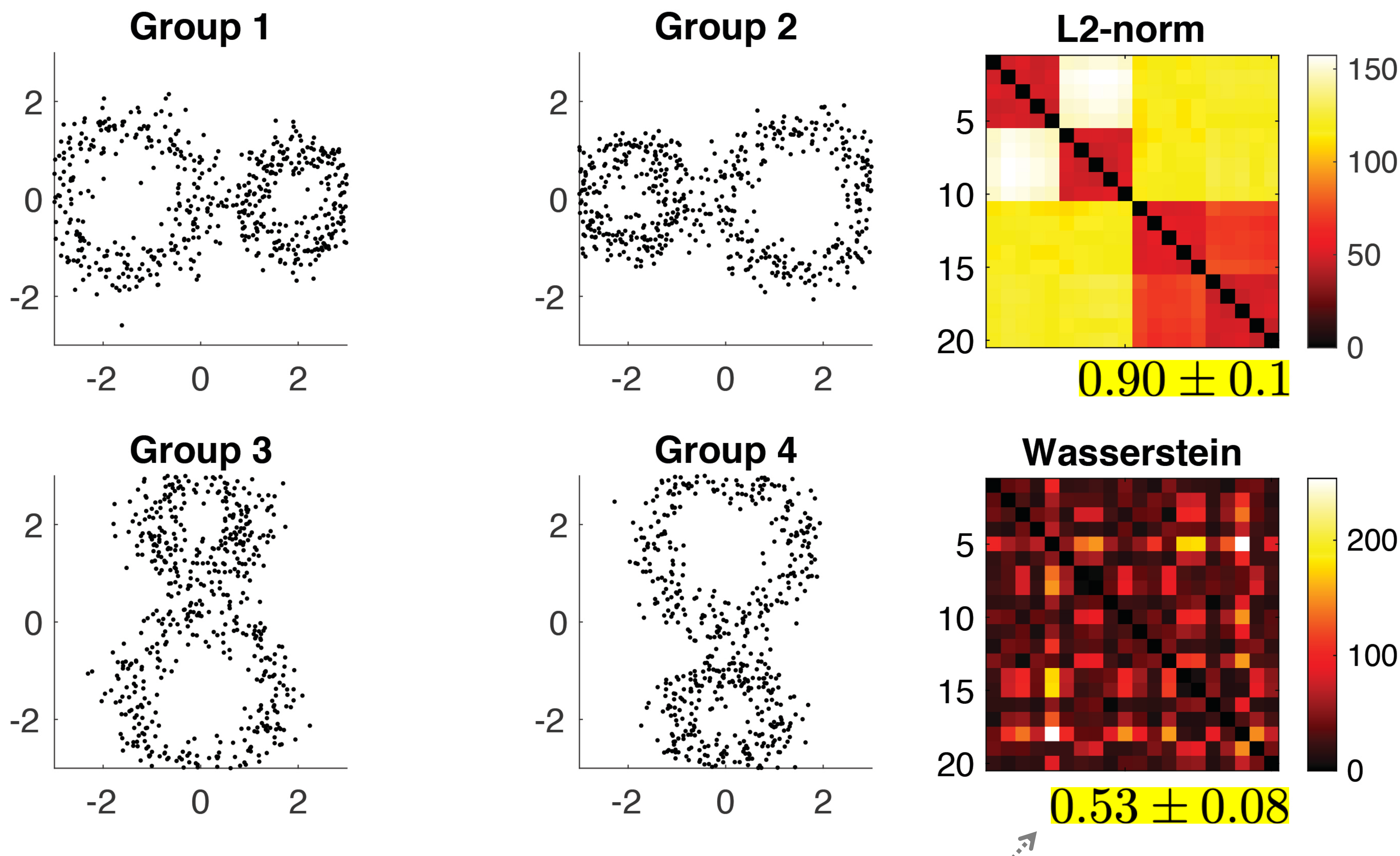
H_0 0D persistent diagram



$$\mathcal{D}_0(P_1, P_2)^2 = \sum_i (b^1_{(i)} - b^2_{(i)})^2$$

Songdechakraiwu & Chung 2023
Annals of Applied Statistics 17:403-433

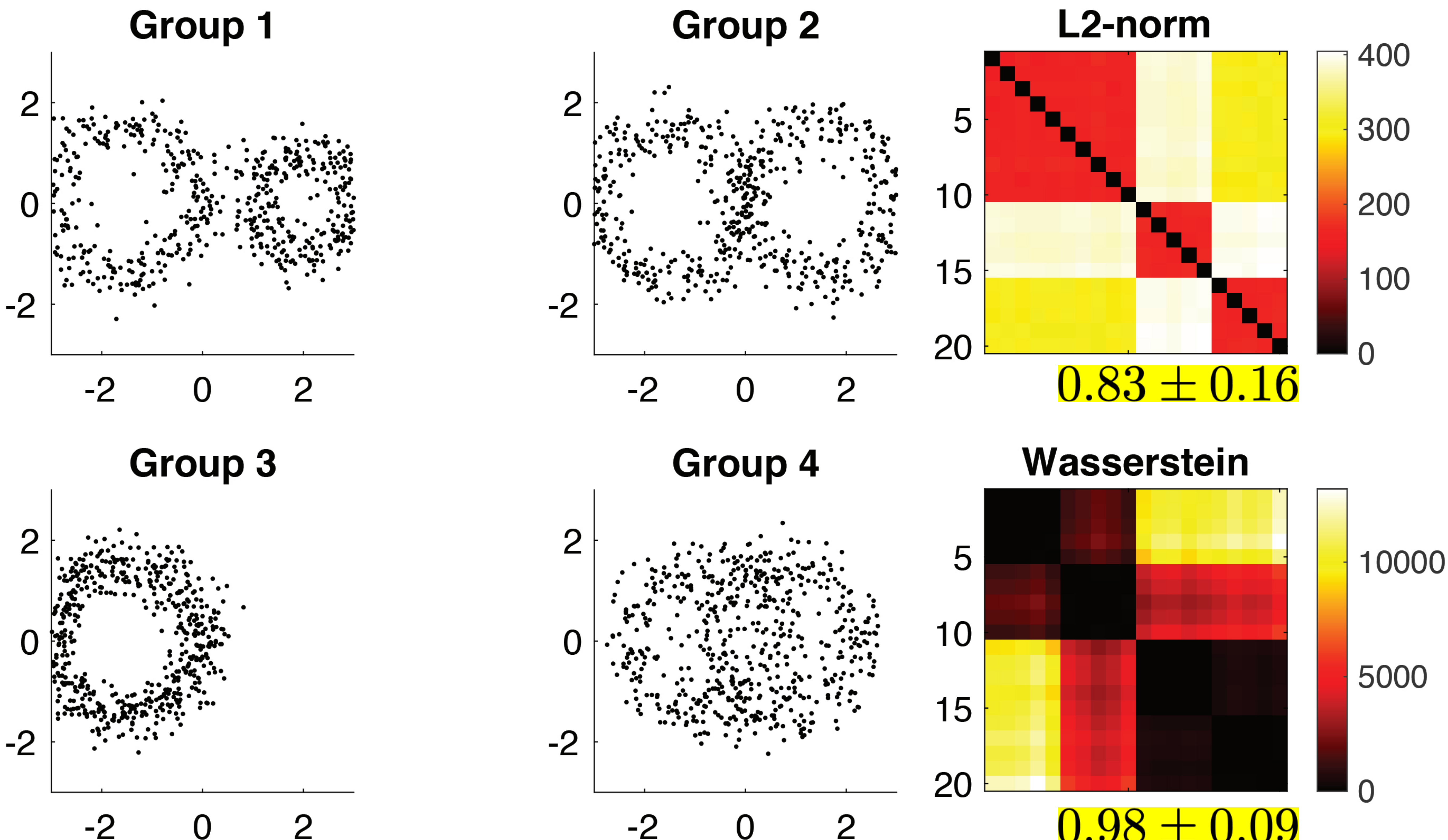
Topologically invariant patterns



Clustering accuracy

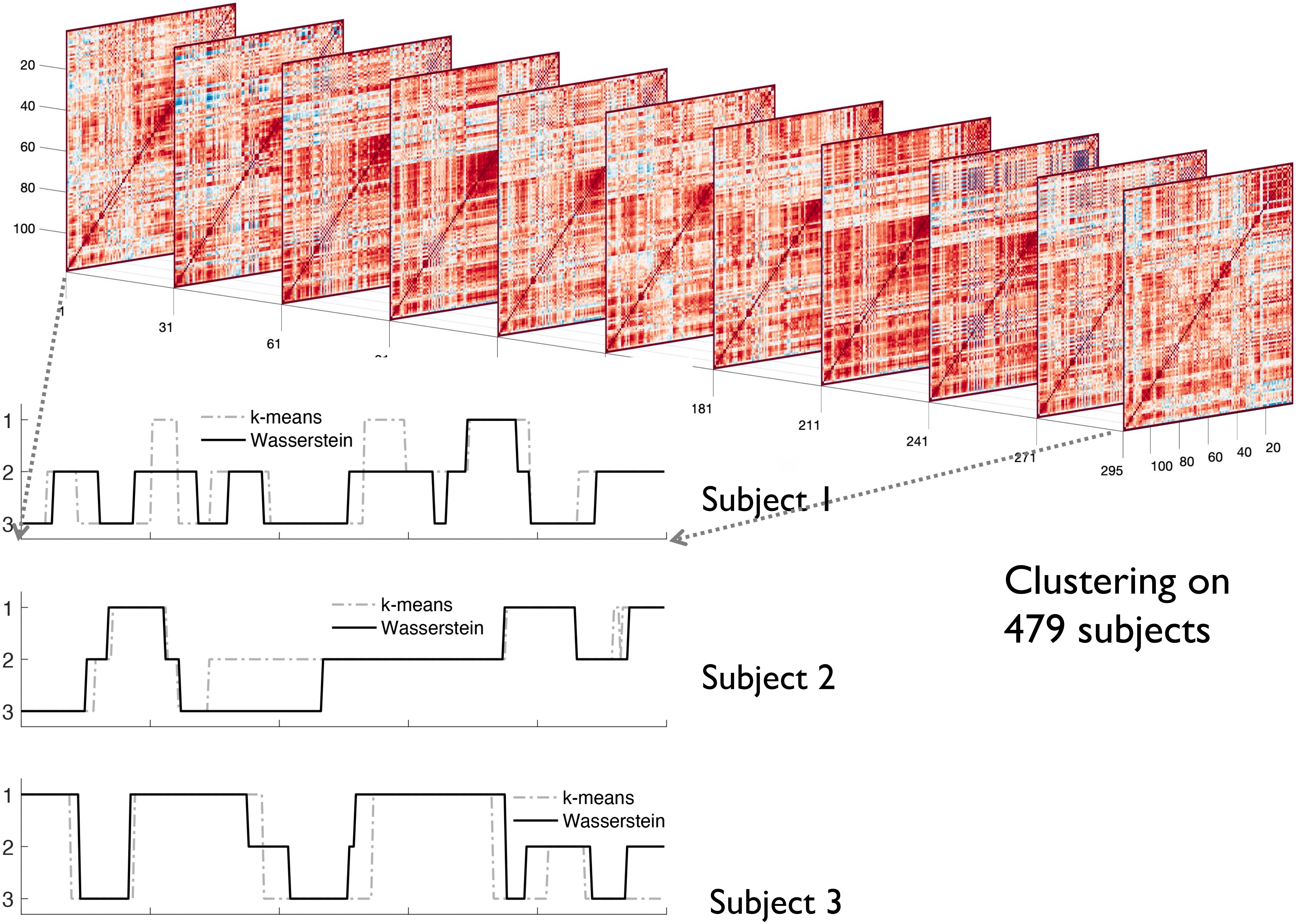
WS_cluster.m

Topologically different patterns

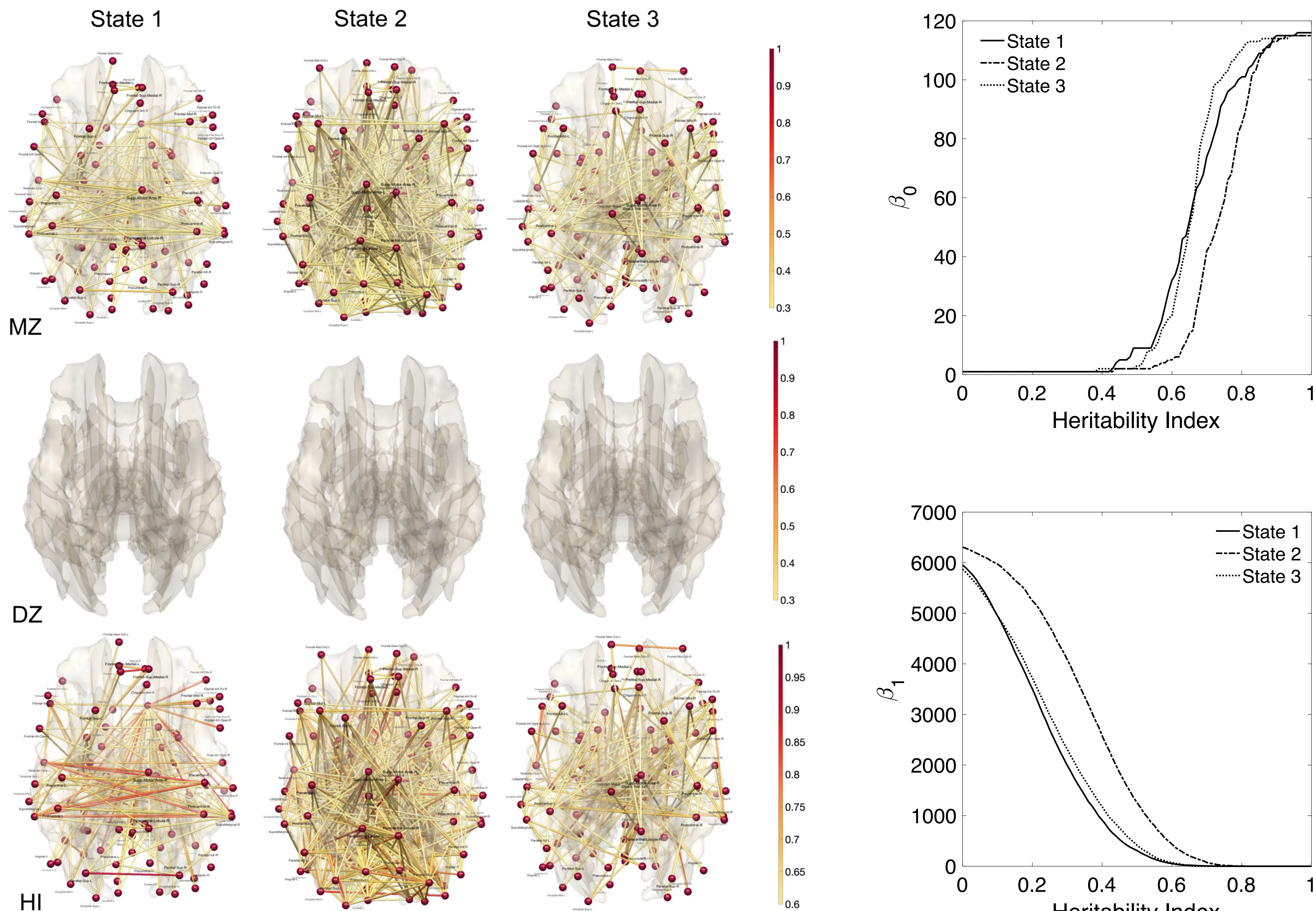


WS_cluster.m

Clustering accuracy


20
40
60
80
100
1
31
61
181
211
241
271
295
100
80
60
40
20
k-means
Wasserstein
Subject 1
Subject 2
Subject 3
Clustering on 479 subjects

Heritability of state-space of rs-fMRI brain network



ISBI 2023 April 18-21 2023
Catagena de Indias, Colombia

Invited Session: Wasserstein Distance in Biomedical Imaging