The Waisman Laboratory for Brain Imaging and Behavior

University of Wisconsin SCHOOL OF MEDICINE AND PUBLIC HEALTH

# Lecture 1 Simplicial homology and persistent homology


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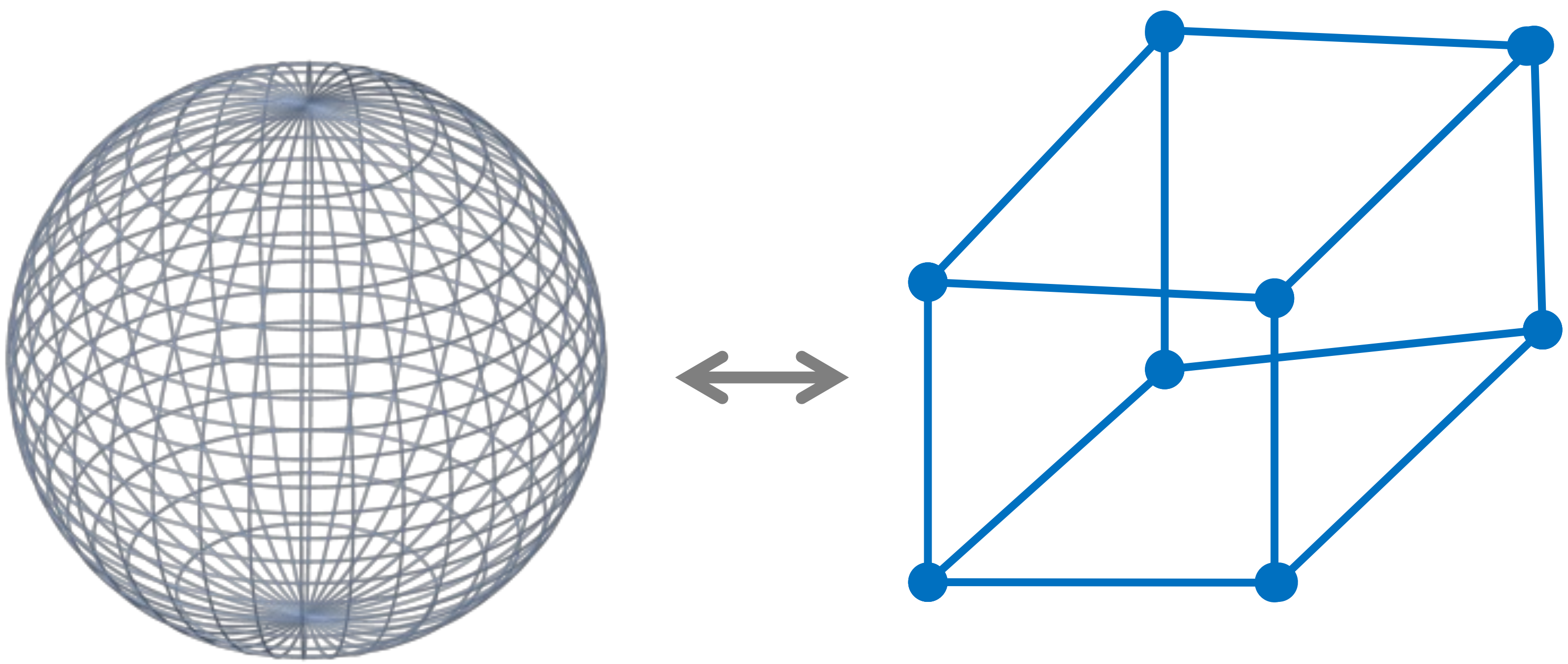
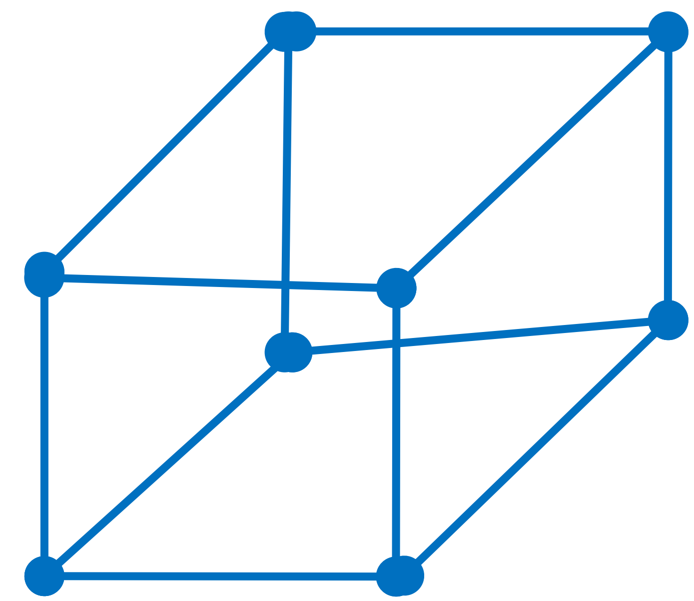
# Euler characteristic

Topologically equivalent
Deformation-invariant



Sphere

$$EC = N - E + F$$
$$= 8 - 12 + 6$$
$$= 2$$



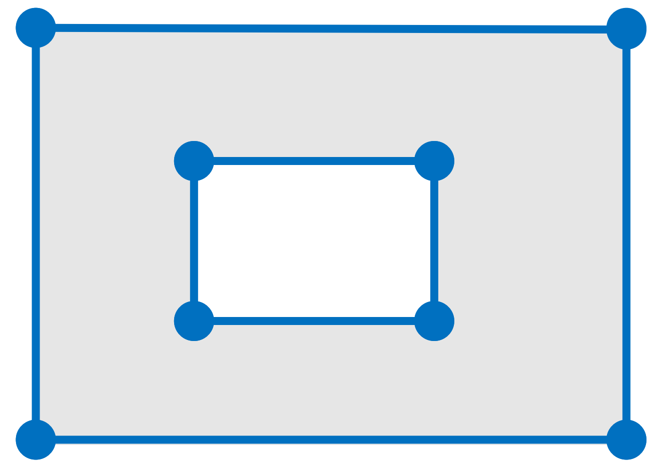
Solid ball

$$EC = N - E + F - V$$
$$= 8 - 12 + 6 - 1$$
$$= 1$$

# Computing Euler characteristic by parts

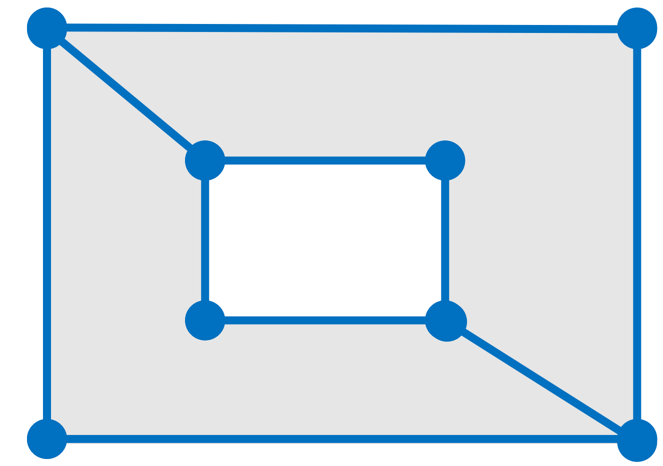


Cover an object with polyhedrons

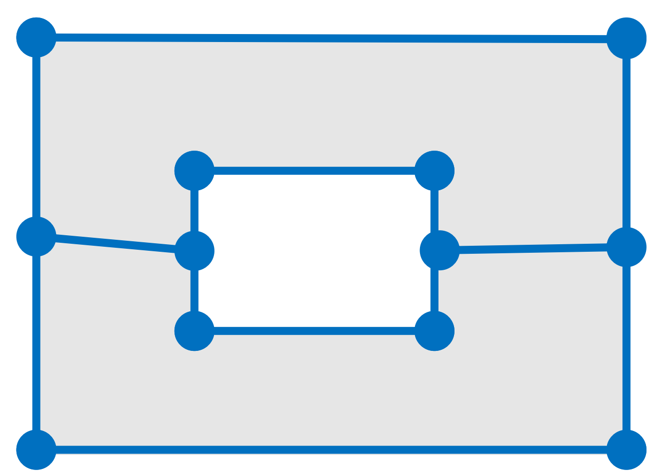


Incorrect computation

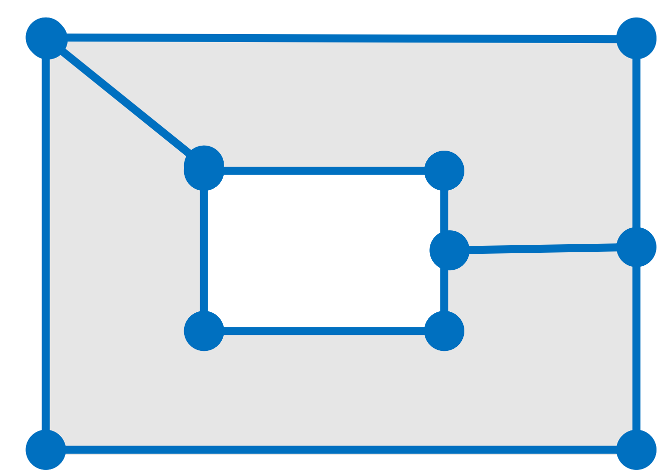
$$EC = N - E + F$$
$$= 8 - 8 + 1$$
$$= 1$$



$$EC = N - E + F$$
$$= 8 - (8+2) + (1+1)$$
$$= 0$$



$$EC = N - E + F$$
$$= (8+4) - (8+6) + (1+1)$$
$$= 0$$



$$EC = N - E + F$$
$$= (8+2) - (8+4) + (1+1)$$
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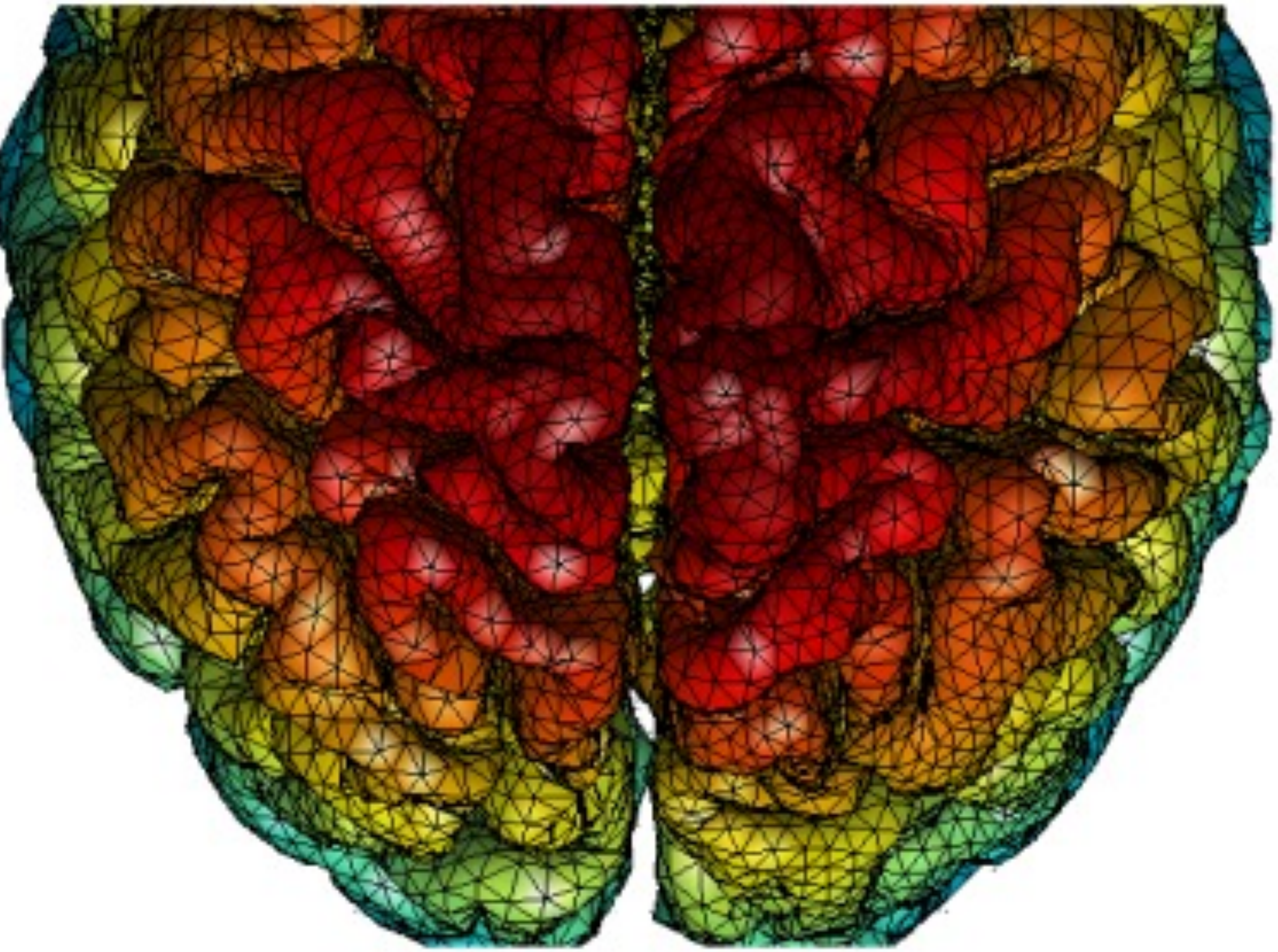
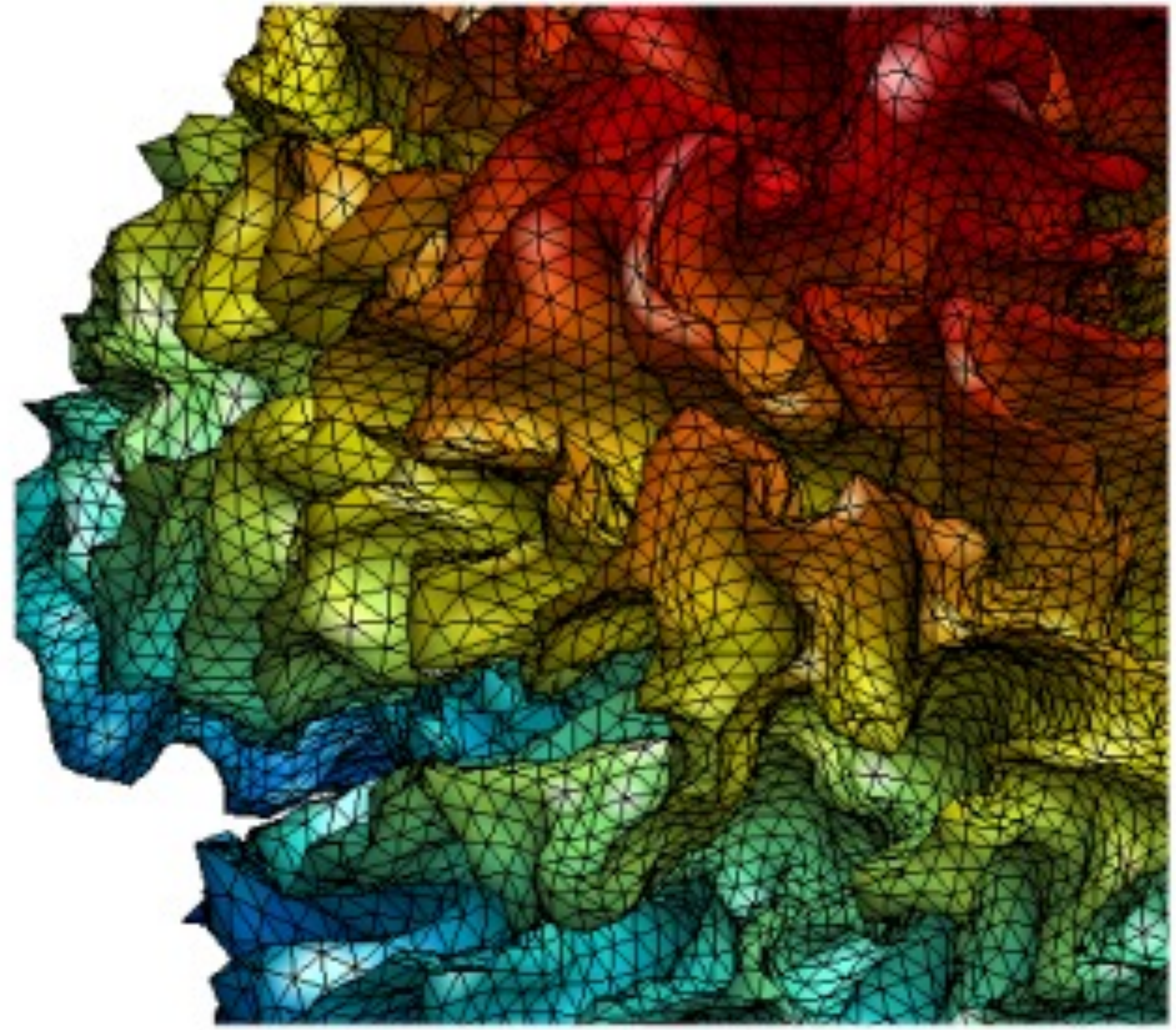


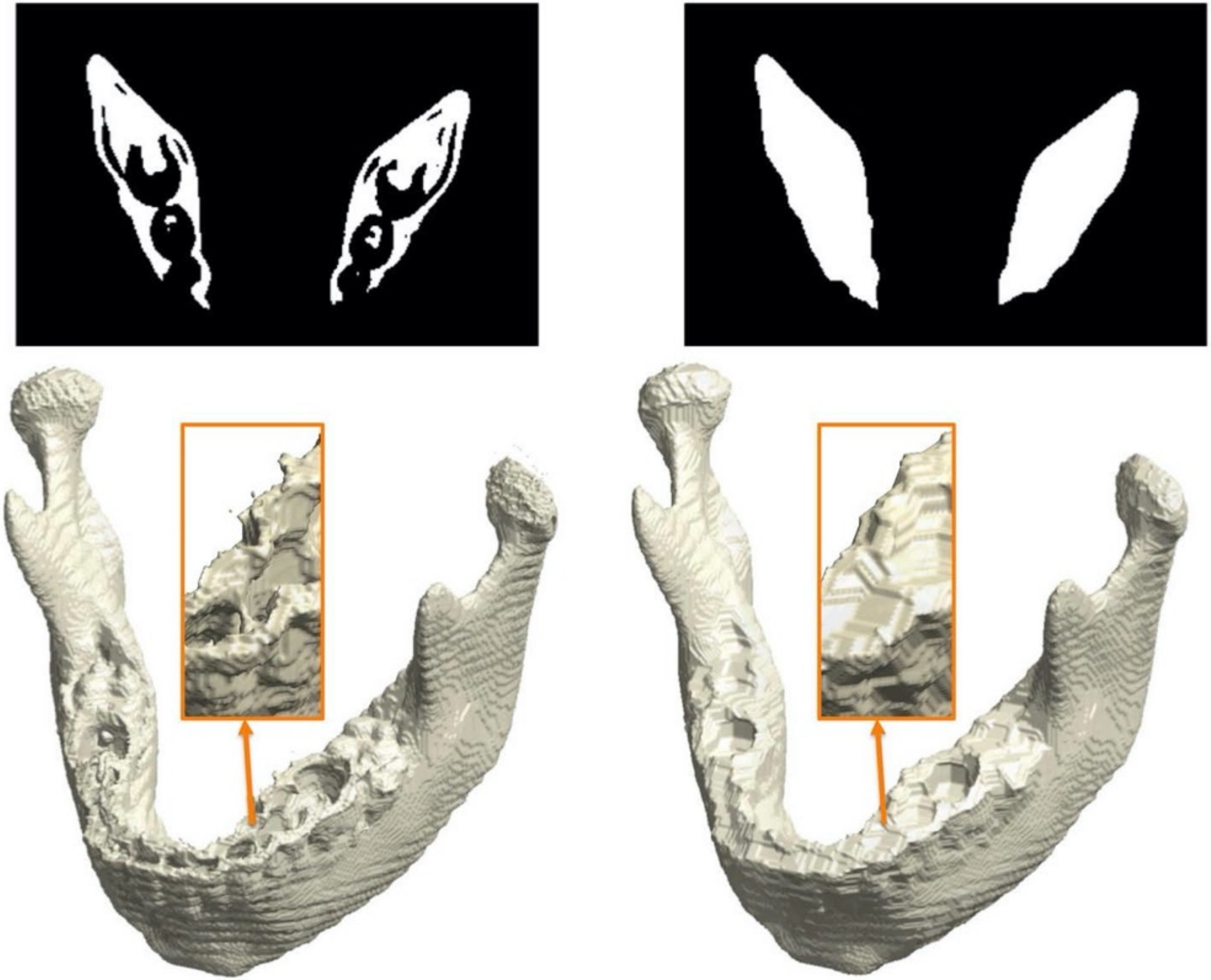


# Euler characteristic of a surface mesh from SurfStat

$N - E + F = 2$ 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.

By checking the Euler characteristic of the binary volume of a mandible, holes in the binary volume can be detected. This process is necessary to make the mandible binary volume to be topologically equivalent to a solid sphere.

# Topology correction in segmentation



Hole & handles corrected using <u>Euler characteristic</u>

<u>*Chung et al. 2015 Medical Image Analysis.* 22:63-76</u>

# Geometry to Topology

Gauss–Bonnet theorem The integral of the Gauss curvature on a 2D Riemannian manifold I $2\pi\chi(\mathcal{M})$, where $\chi(\mathcal{M})$ is the Euler characteristic of $\mathcal{M}$.

# Keith Worsley's random field theory

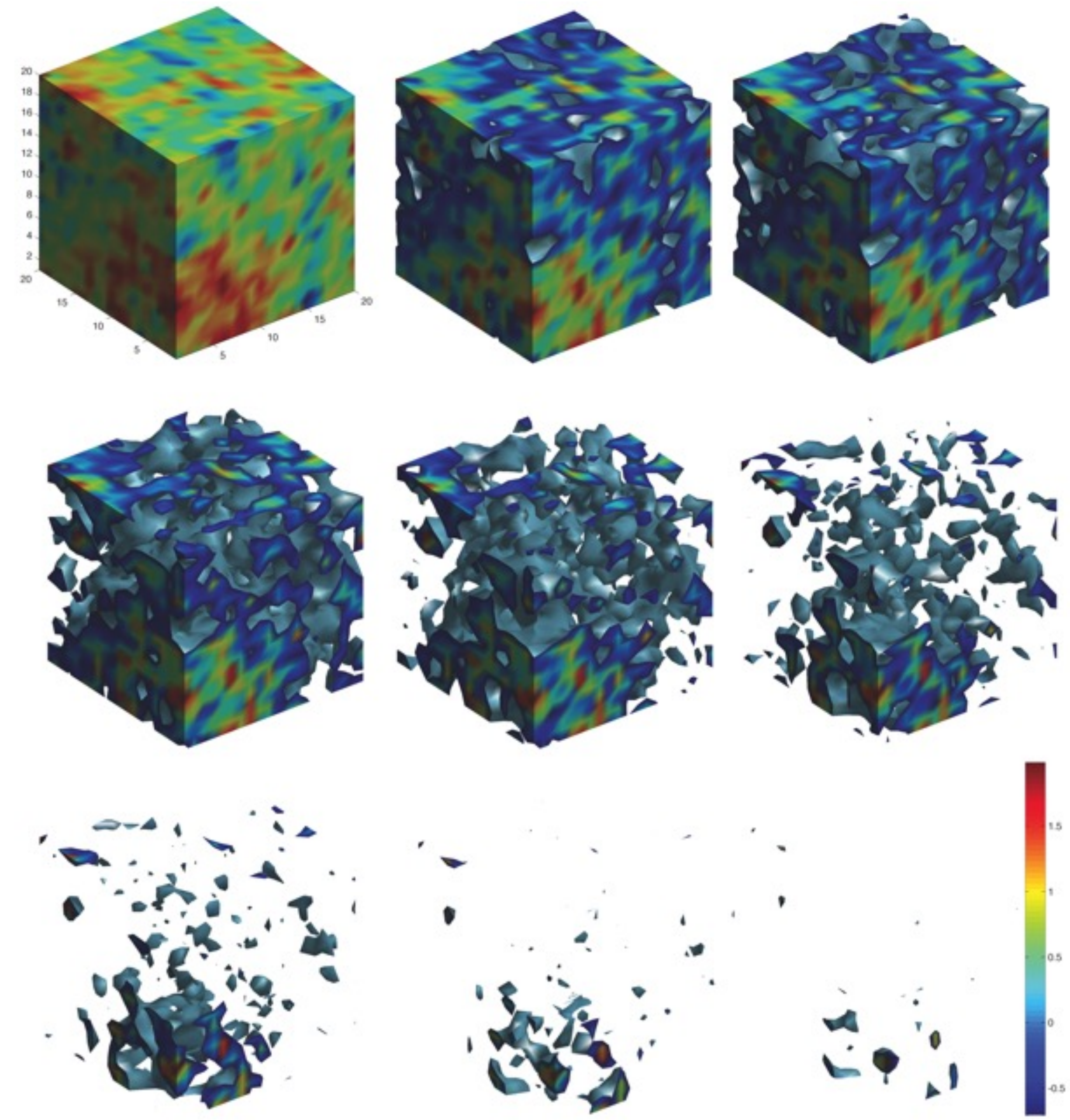
Random field, stochastic process

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

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

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

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



*Milor 1963 Morse theory*

*Adler, 1994 The geometry of random fields*

*Worsley et al., 1996 Human Brain Mapping*

# Matlab toolbox

## PH-STAT

Statistical Inference on Persistent Homology

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

# 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 <u>across different scales</u>
- More <u>persistent</u> topological features → signal
- Less <u>persistent</u> topological features → noise
- <u>Multiscale</u> approach

## *References*


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

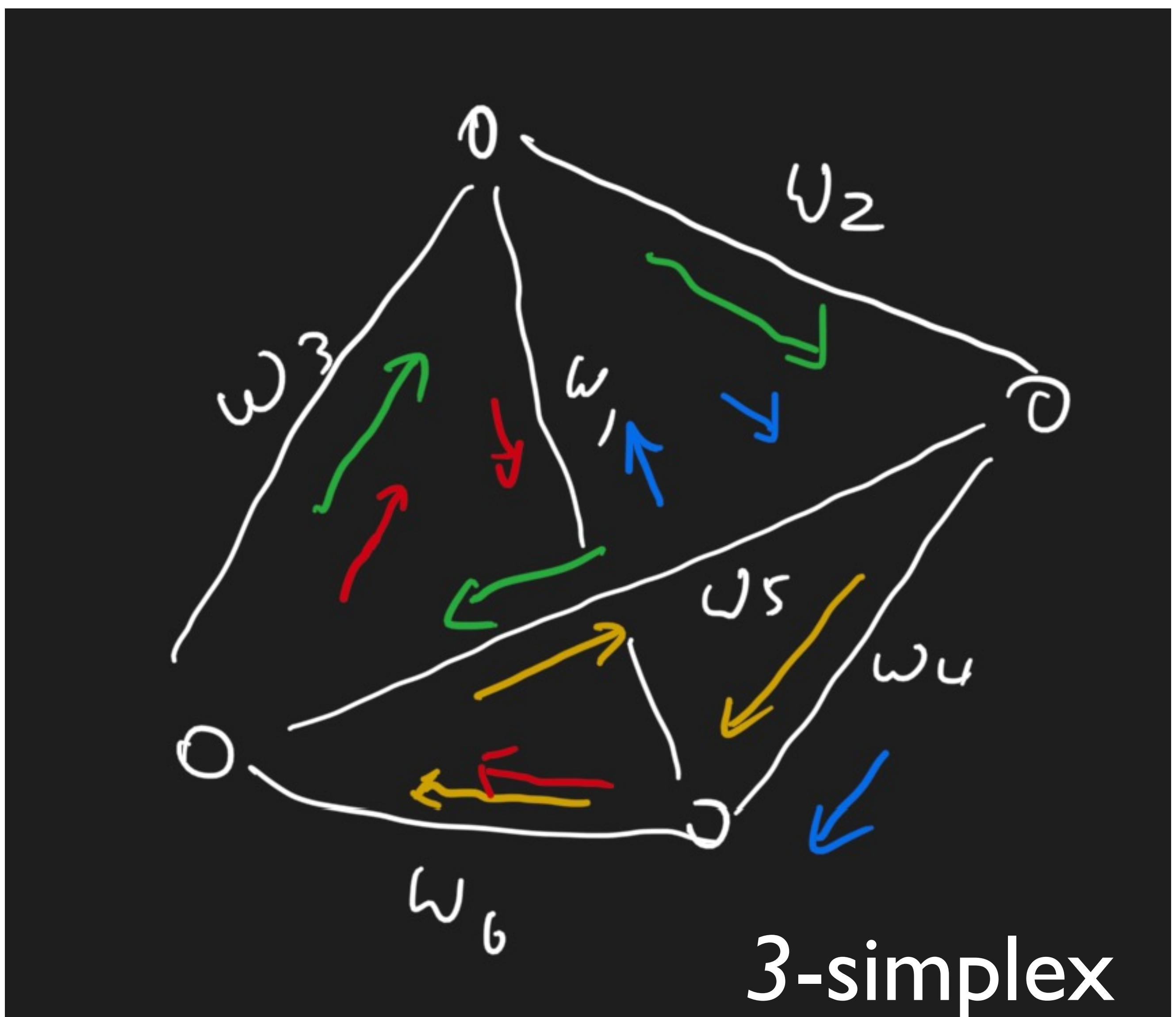
Herbert Edelsbrunner and John L. Harer Computational Topology: An Introduction 2010, American Mathematical Society

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

# *n*-simplex

The basic building block of persistent homology

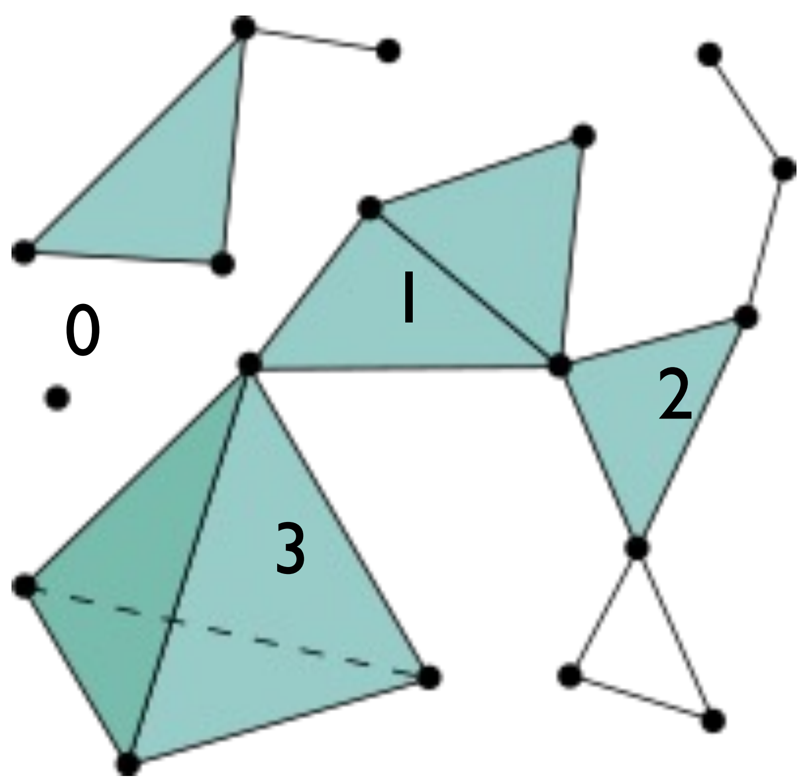
The smallest convex set containing *n+1* points



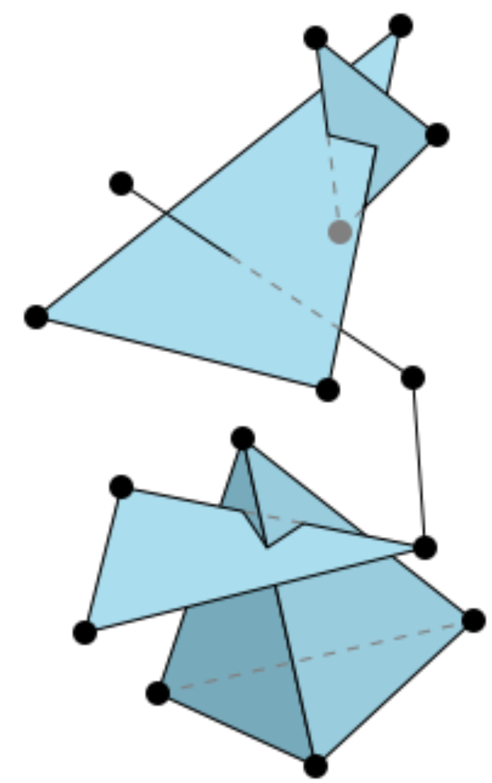

$$\sum_{i=0}^{n} x_i = 1, x_i \geq 0$$

# Simplicial complex

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




Simplicial complex

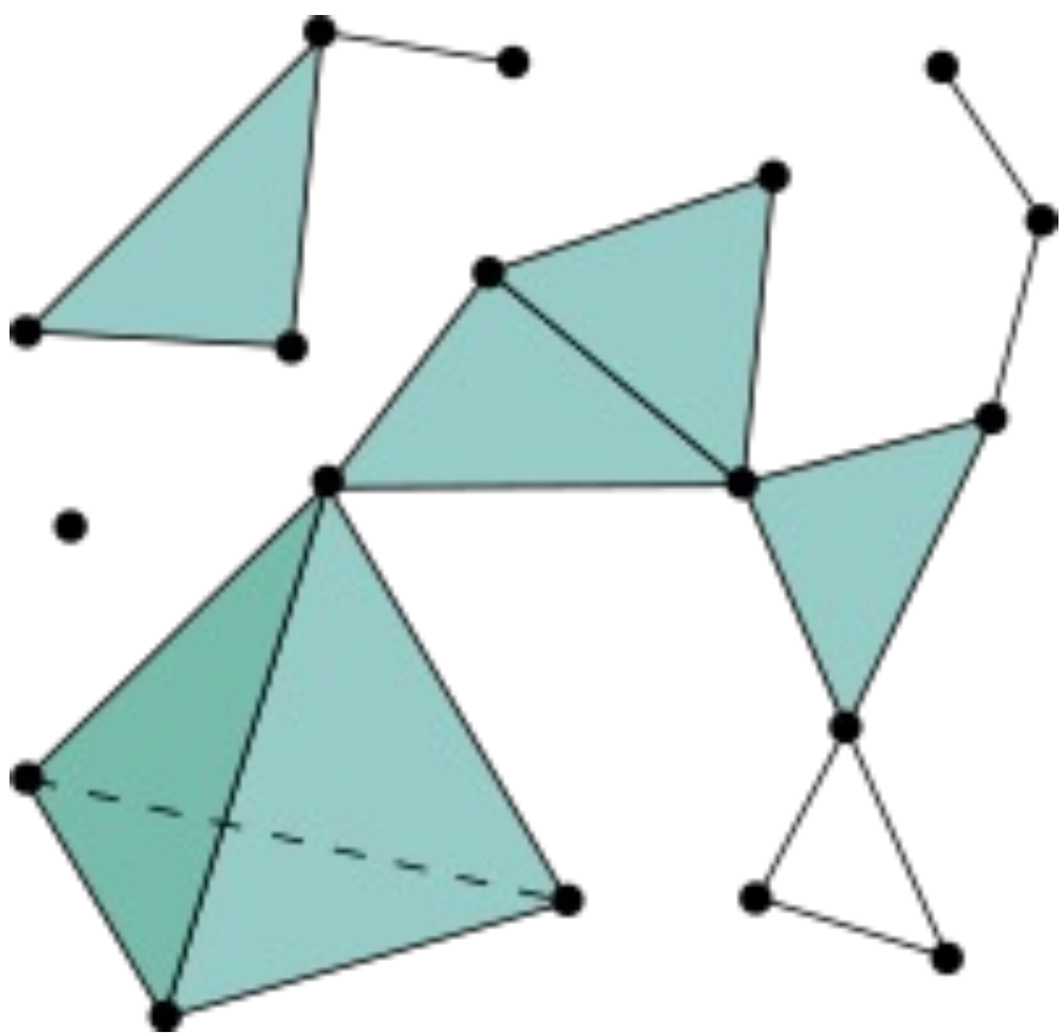


Not simplicial complex

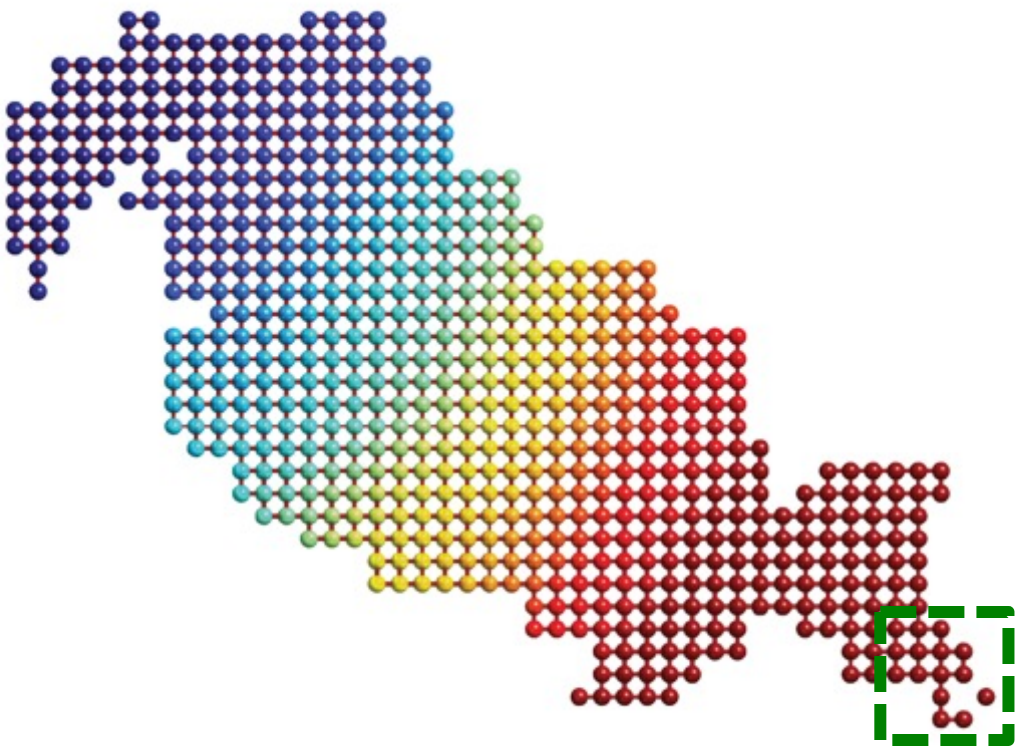
*Ex.* surface mesh, graphs (including hypergraphs), networks

# k-skeleton

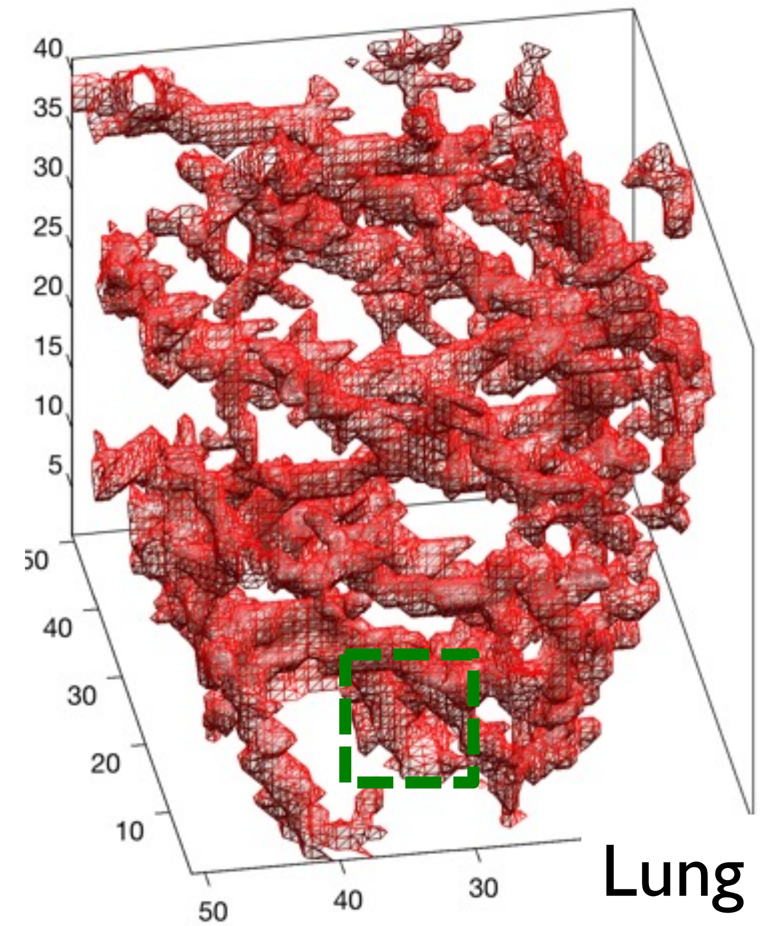
A simplicial complex consisting of points and line segments only → graphs & network



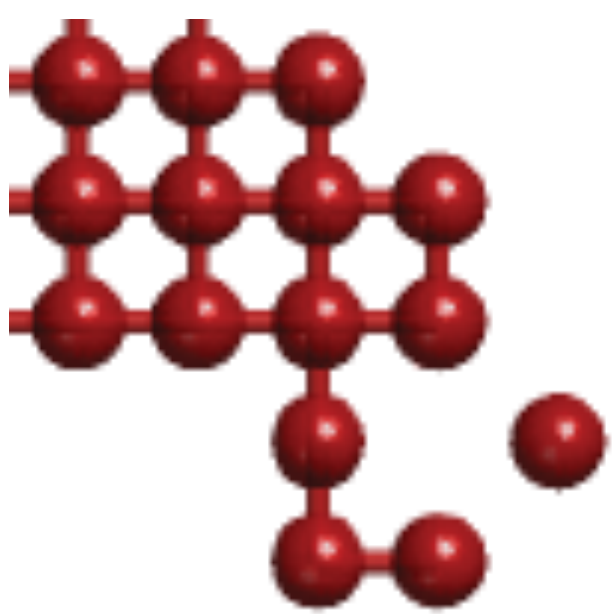
# Cubical complex (2D or 3D images)



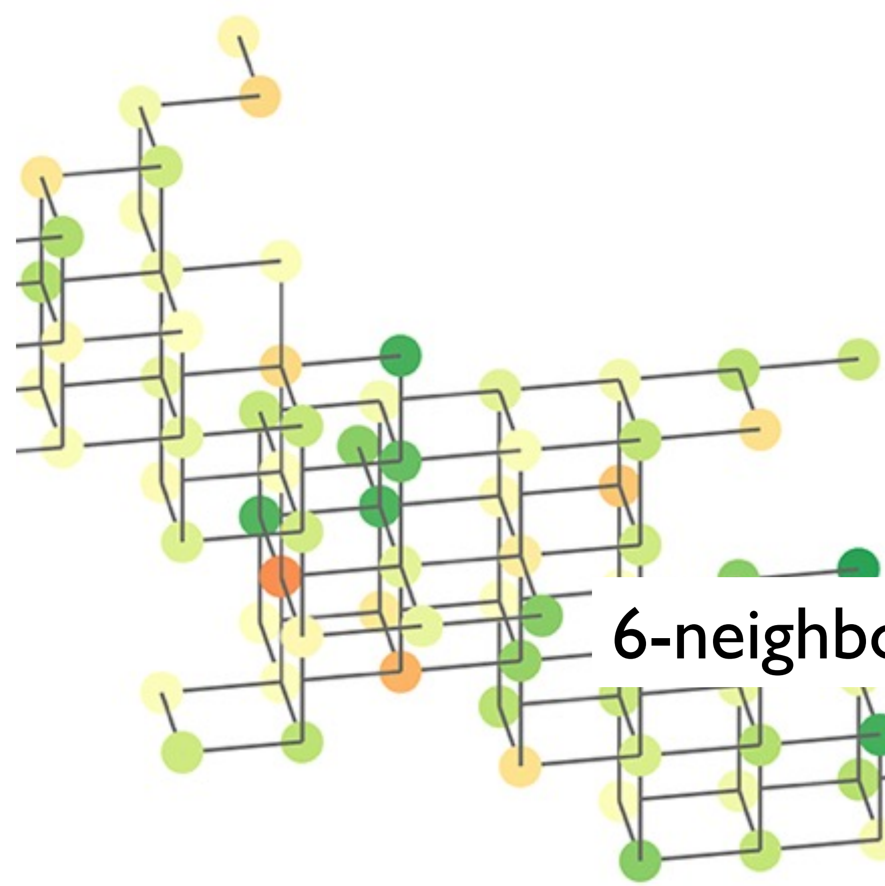
Left central gyrus




Lung blood vessel



4-neighbor connectivity



6-neighbor connectivity

# Betti numbers $\beta_i$

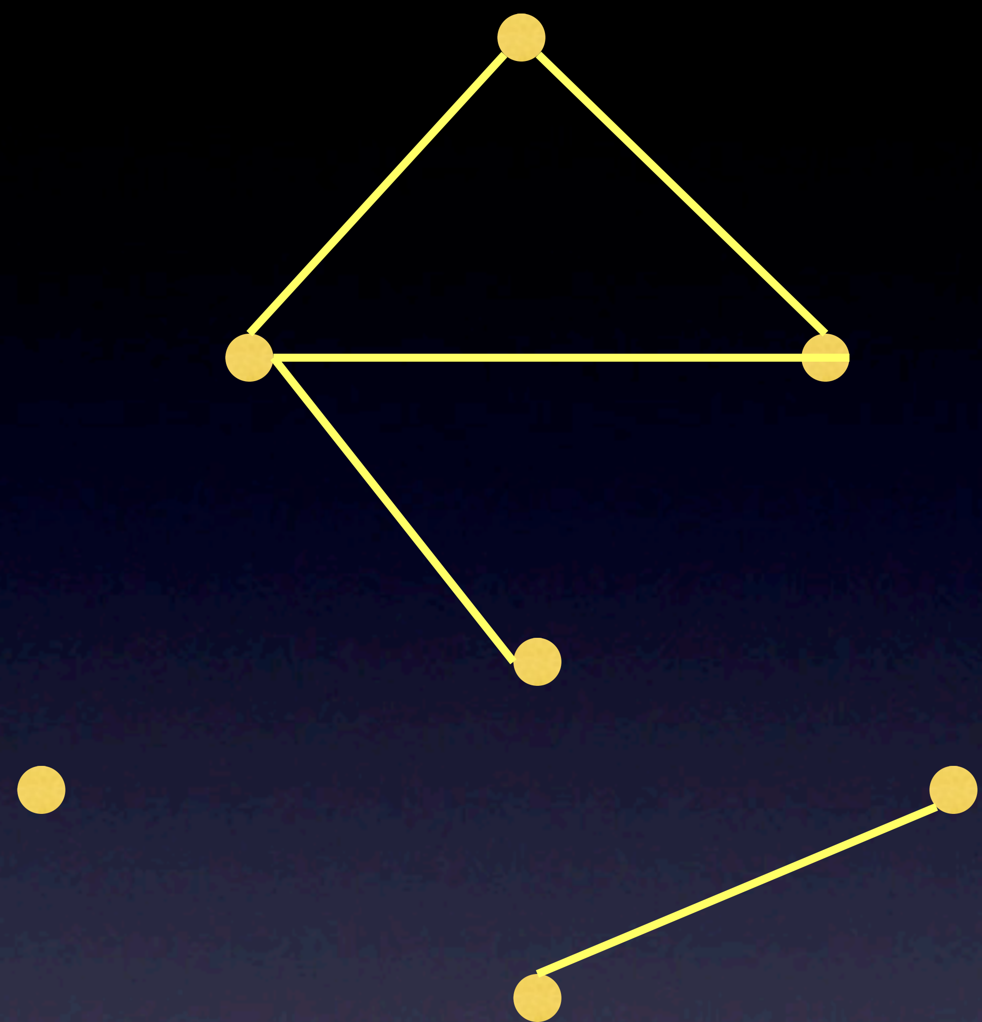
\# of i-dimensional holes/loops

$\beta_0$ = # of connected components = 3

$\beta_1$ = # of cycles = 1

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

# Betti numbers $\beta_i$ # of i-dimensional holes/loops



$\beta_0$ = # of connected components = 3

$\beta_1$ = # of 1D holes = 1

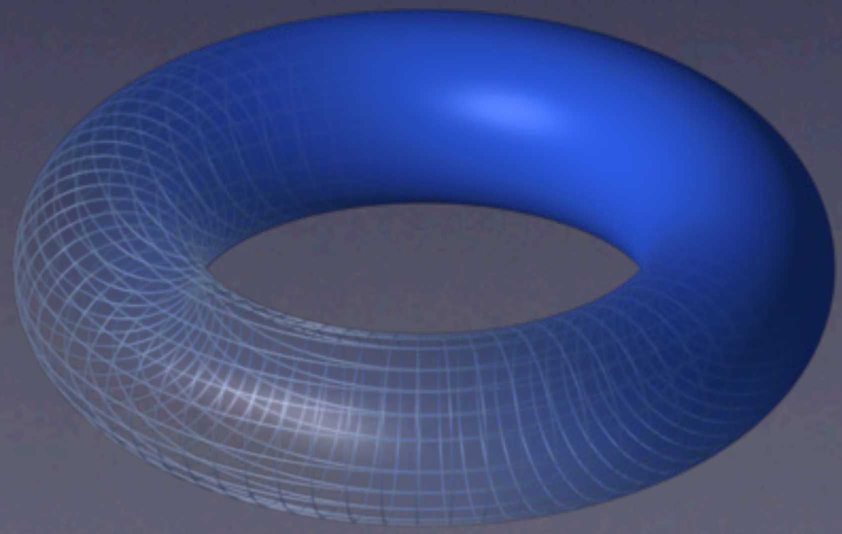
$\beta_2$ = # of 2D cavities =0

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,...)

# Filtration

$$\mathcal{G}_1 \subset \mathcal{G}_2 \subset \mathcal{G}_3 \subset \cdots$$

Sequence of nested objects or vector spaces

Extract persistent homological features

Persistent diagram, barcodes

Hiearchical nestness does not imply robustness

$$\mathcal{G}_1 \subset \mathcal{G}_2 \subset \mathcal{G}_3 \subset \cdots$$

Sequence of nested objects or vector spaces

To have robustness, you need monotone feature

$$\beta_i(\mathcal{G}_1) < \beta_i(\mathcal{G}_2) < \beta_i(\mathcal{G}_3) < \cdots$$

# Morse Filtration

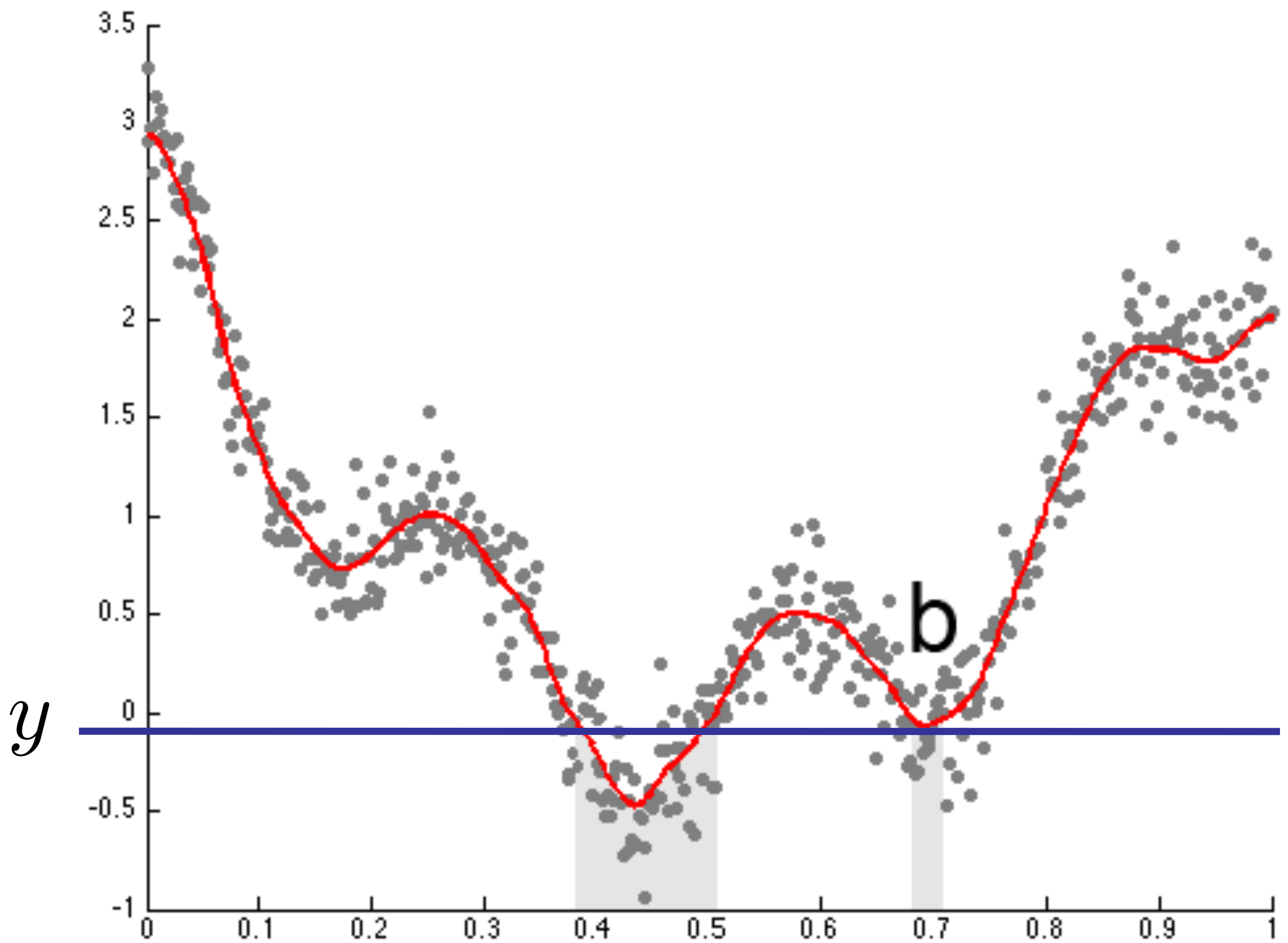
Most useful in functional and time series data

# Morse theory for functional data

$$Y = \mu + \epsilon$$

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

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

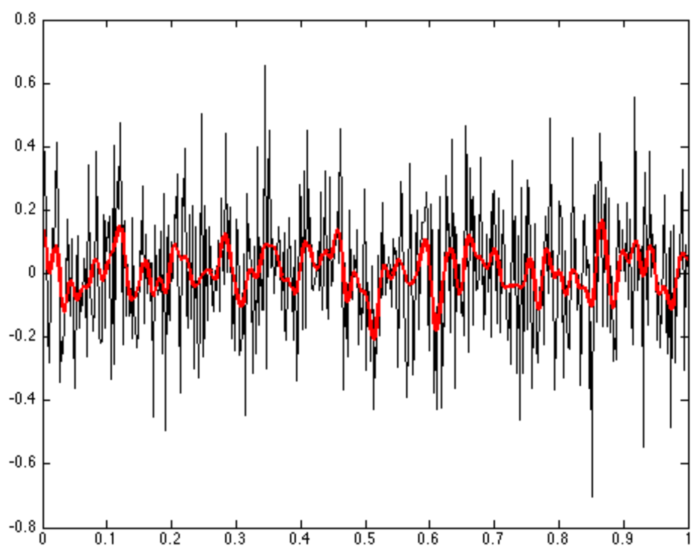
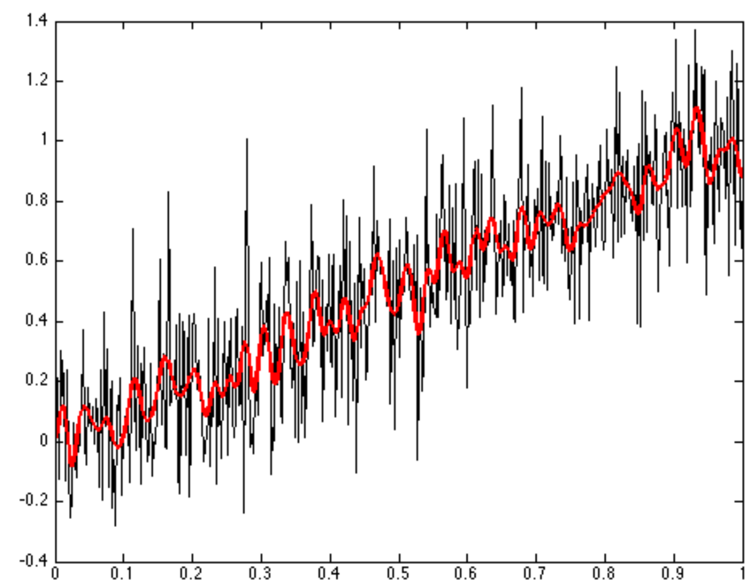
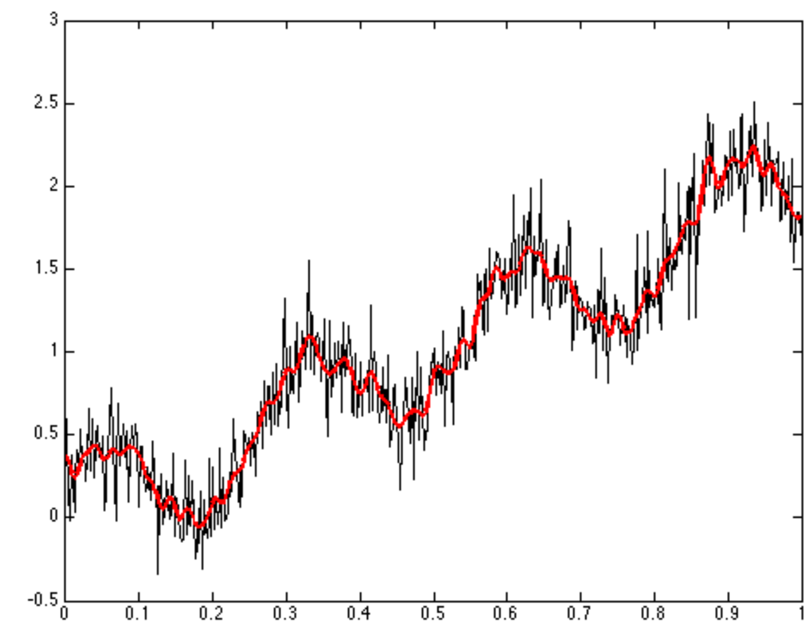



Sublevel set

$$R(y) = \mu^{-1}(-\infty, y]$$

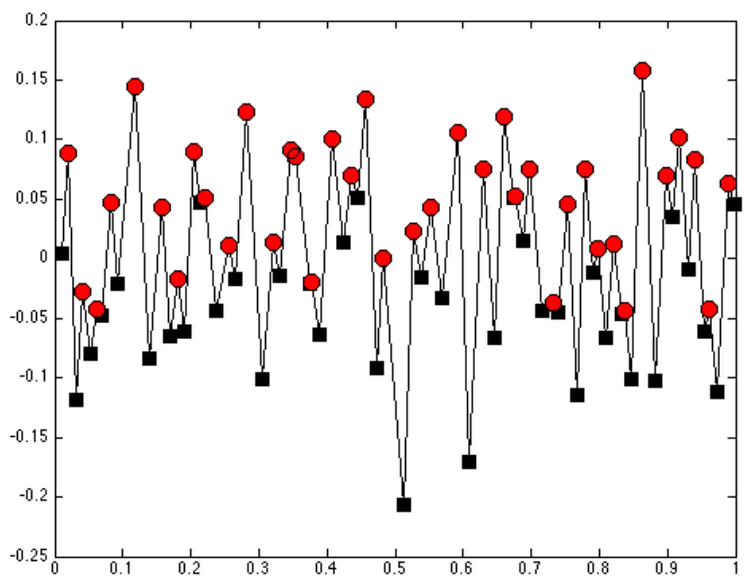
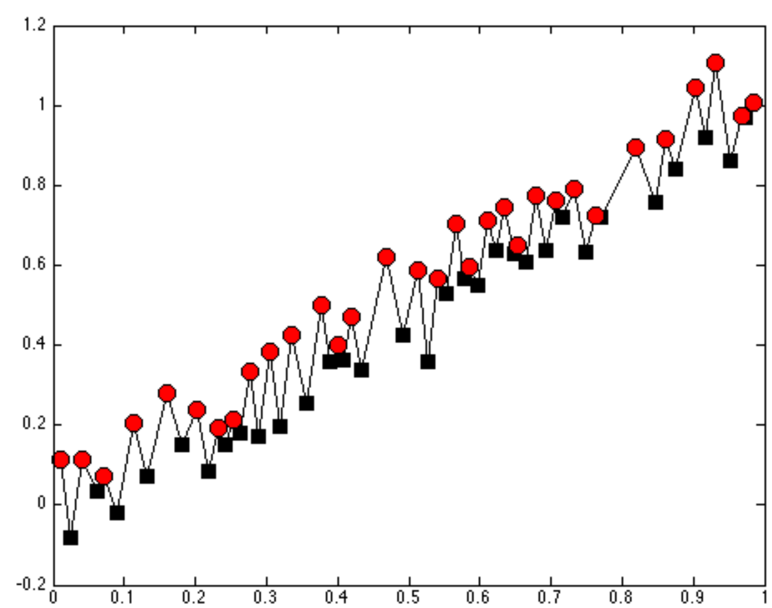
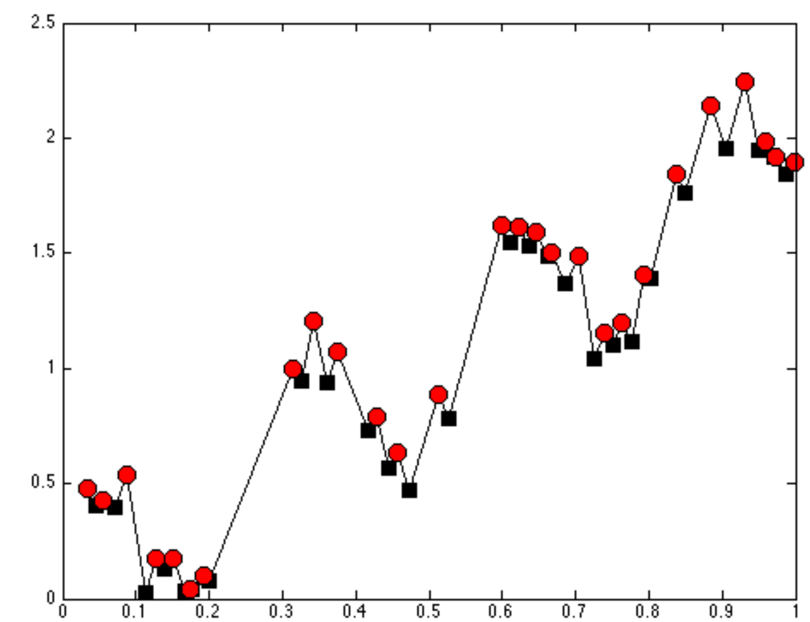
Number of connected components $\#R(y)$

# Critical values capture the pattern of signal changes

$$f(t) = e(t)$$

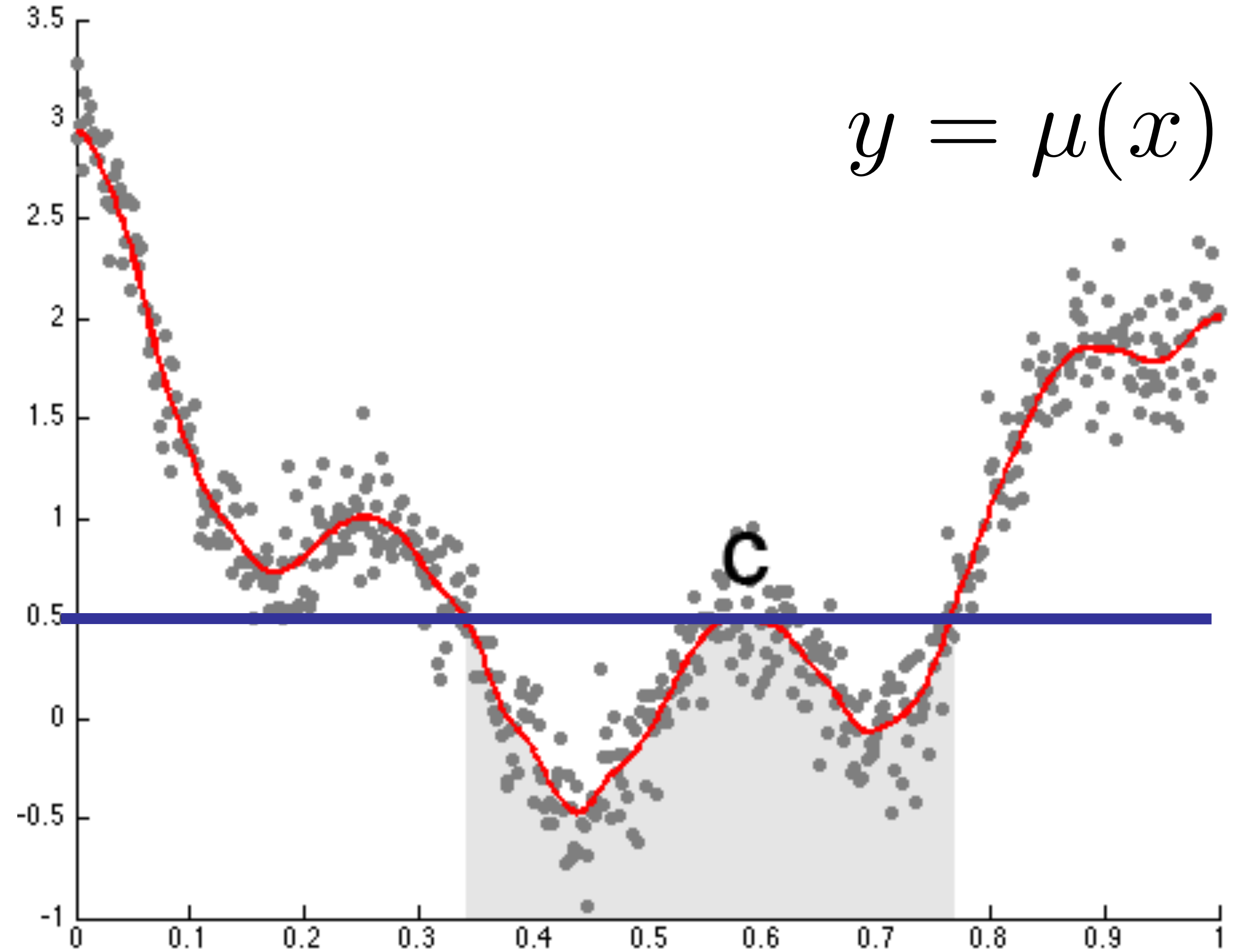
$$f(t) = t + e(t)$$

# Morse filtration

Consider a sublevel set

$$R(y) = \mu^{-1}(-\infty, y]$$




For critical values

$$b < c$$

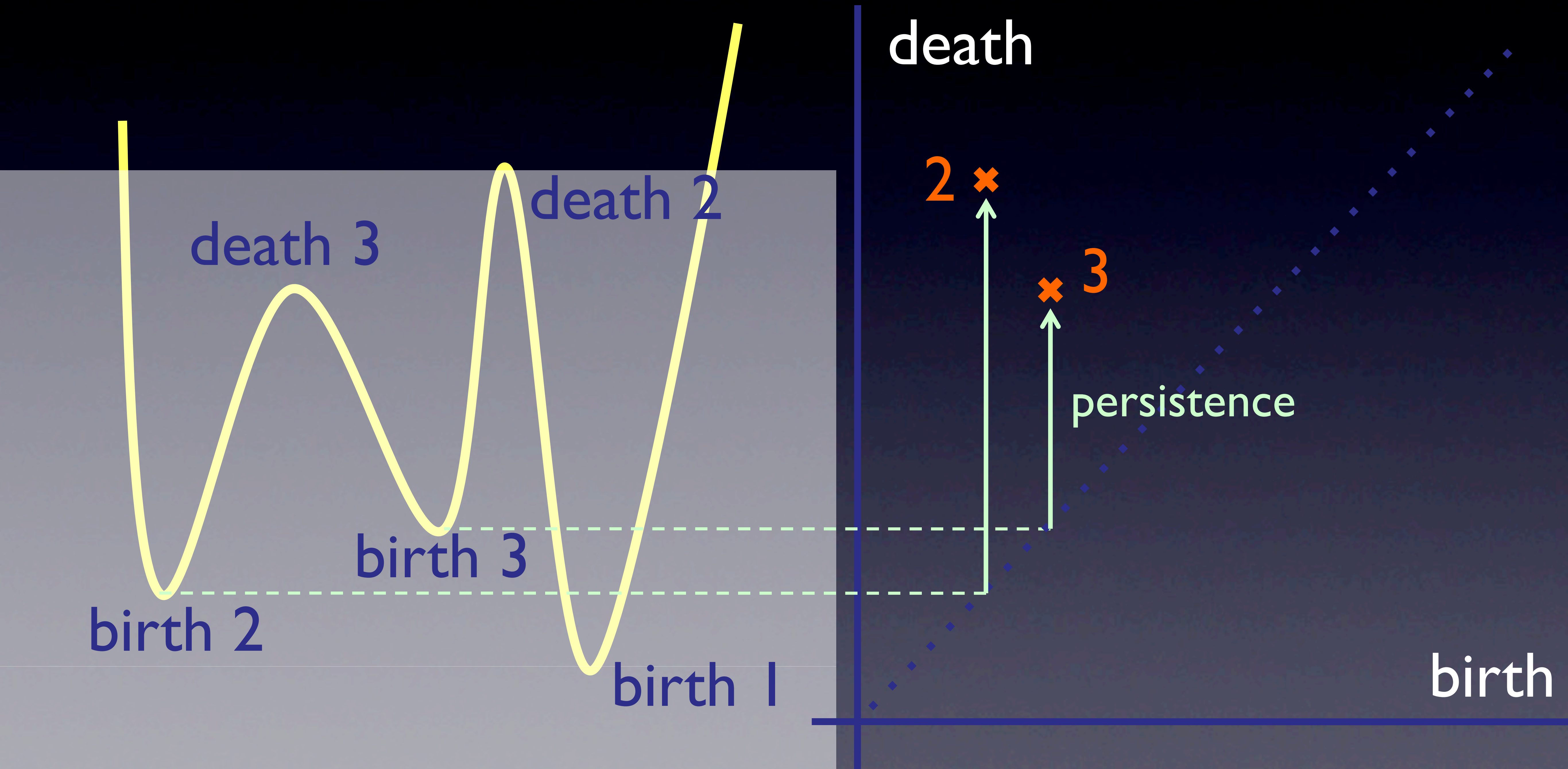
$$R(b) \subset R(c)$$

# of connected components

$$\#R(b) = \#R(c) - 1$$

# Persistence Diagram (PD)

$O(n \log n)$




Pair the time of death with the time of the closest earlier birth.
Birth 1 is paired to infinity or ignored.

# Pairing Brackets

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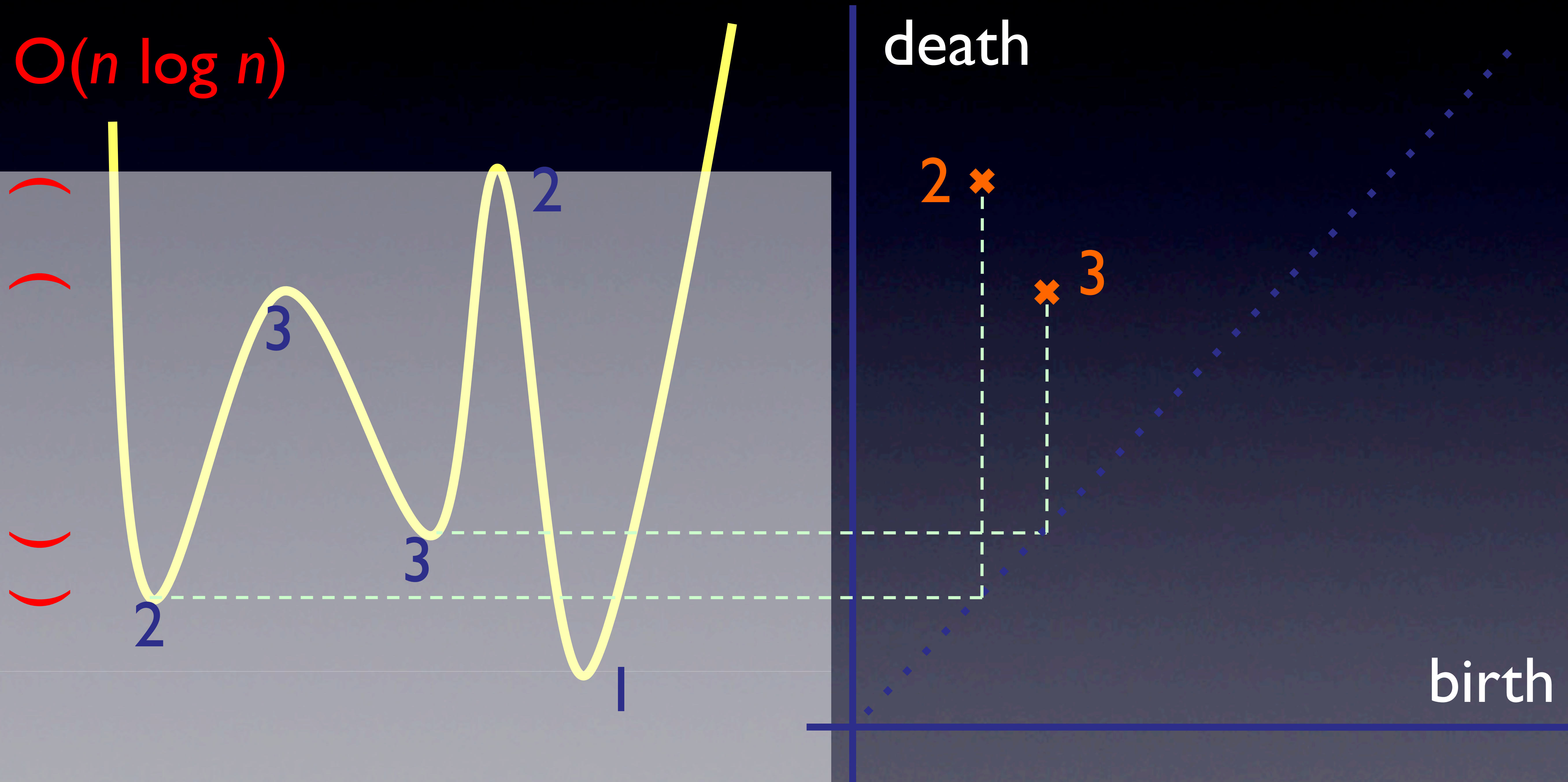
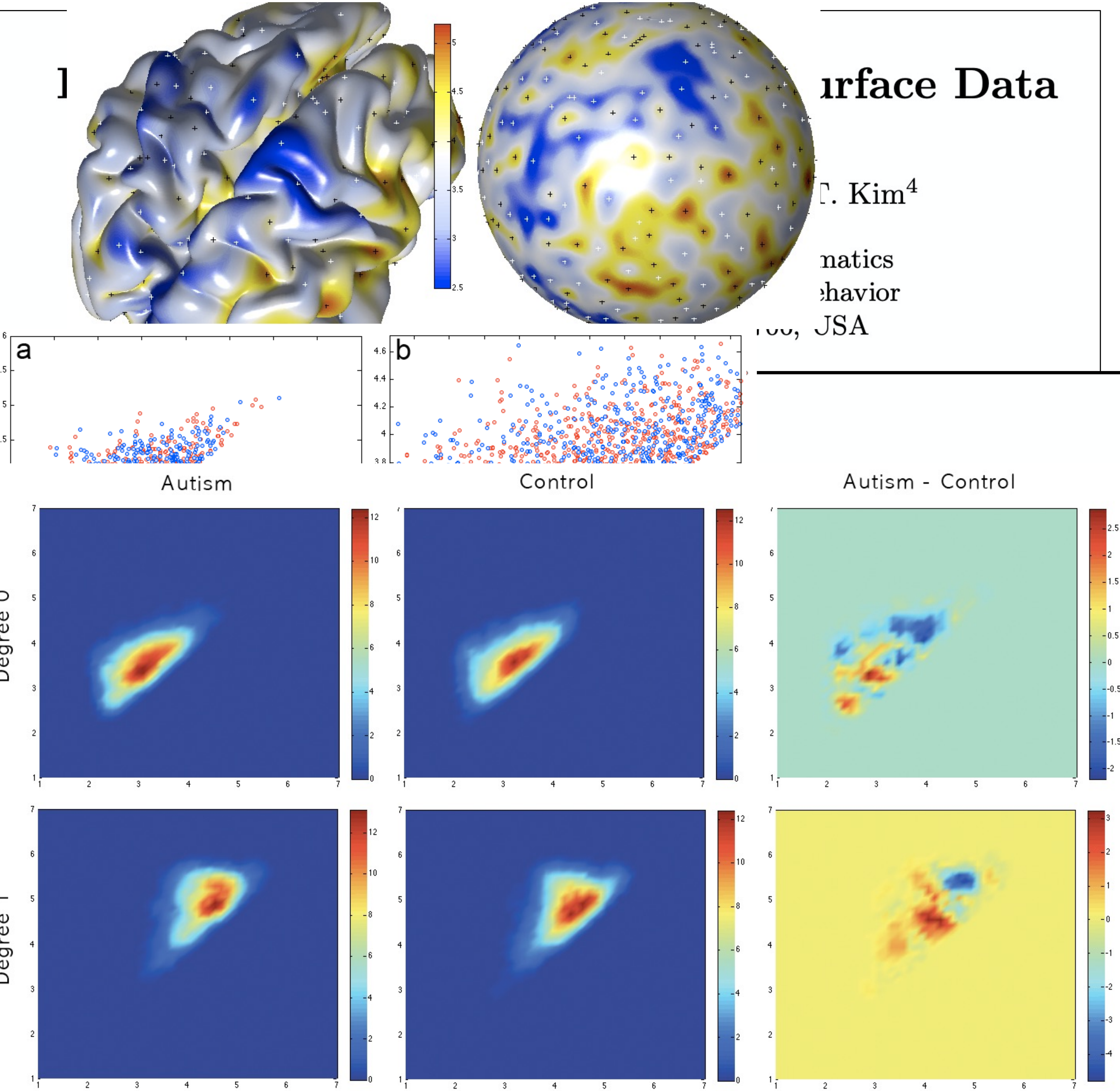
# Persistence Diagram (PD)



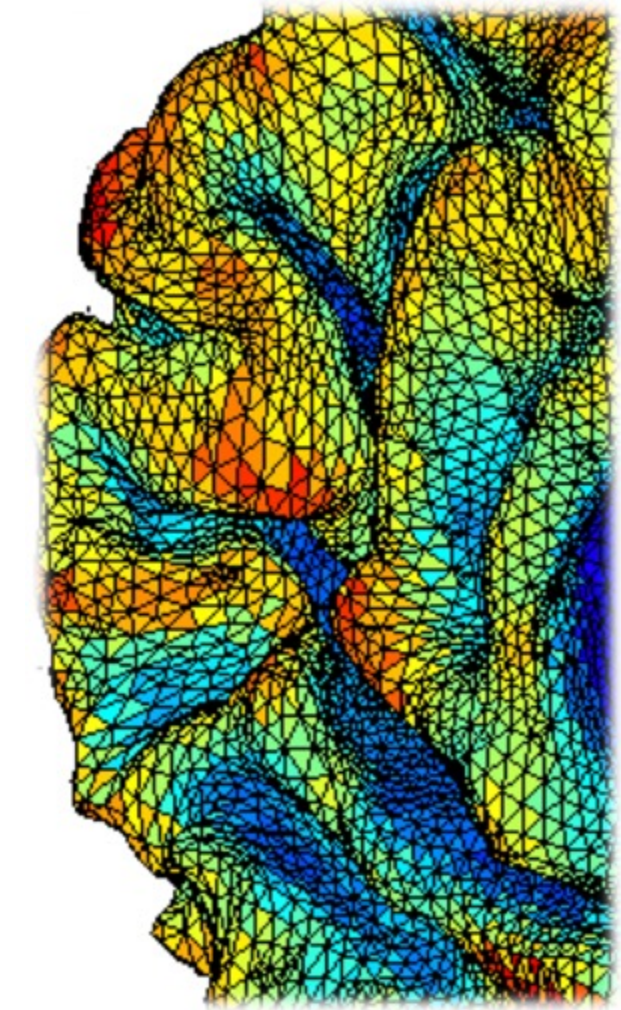

Pair the time of death with the time of the closest earlier birth

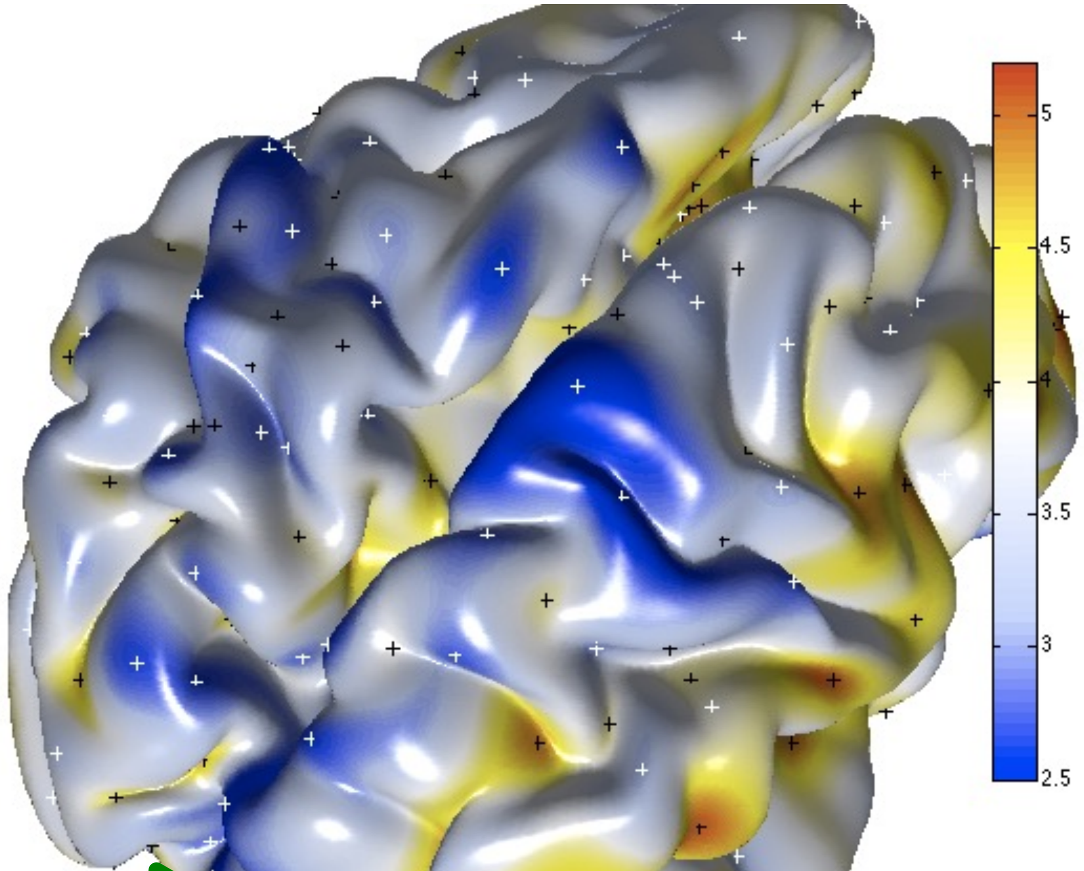


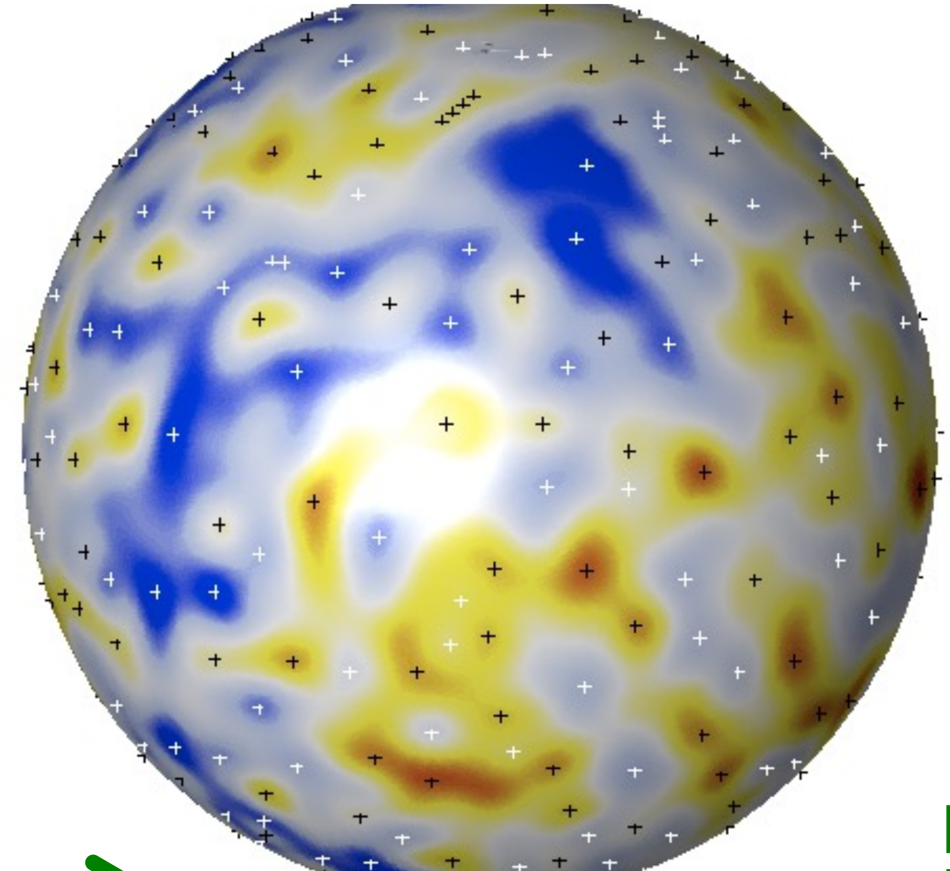

*Chung et al., 2009*
*Information Processing in Medical Imaging (IPMI) 5636:386-397.*

*First persistent homology study applied to medical imaging*

# Persistent homology on cortical manifolds



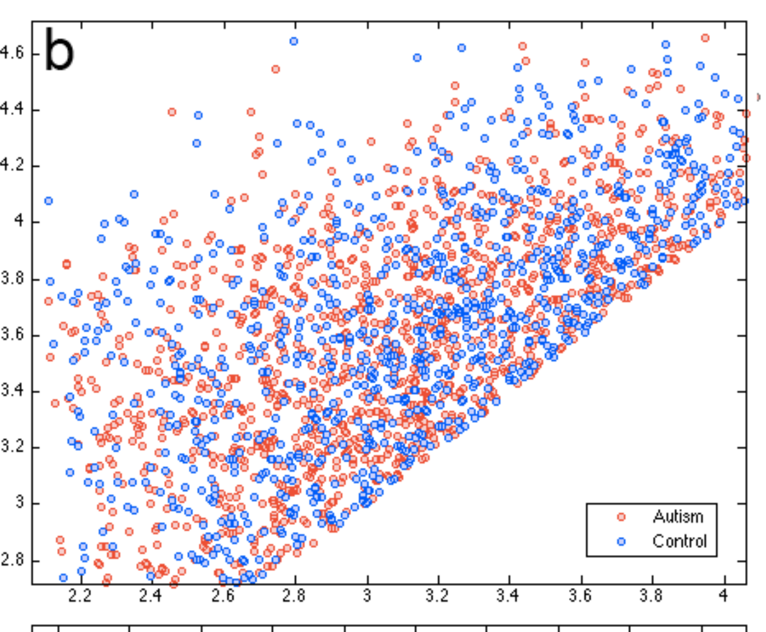




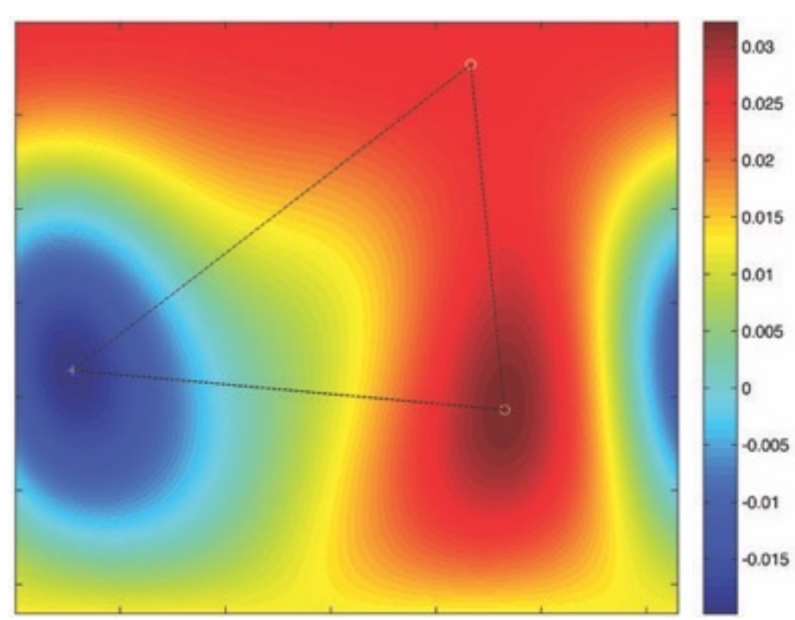
Heat kernel smoothing

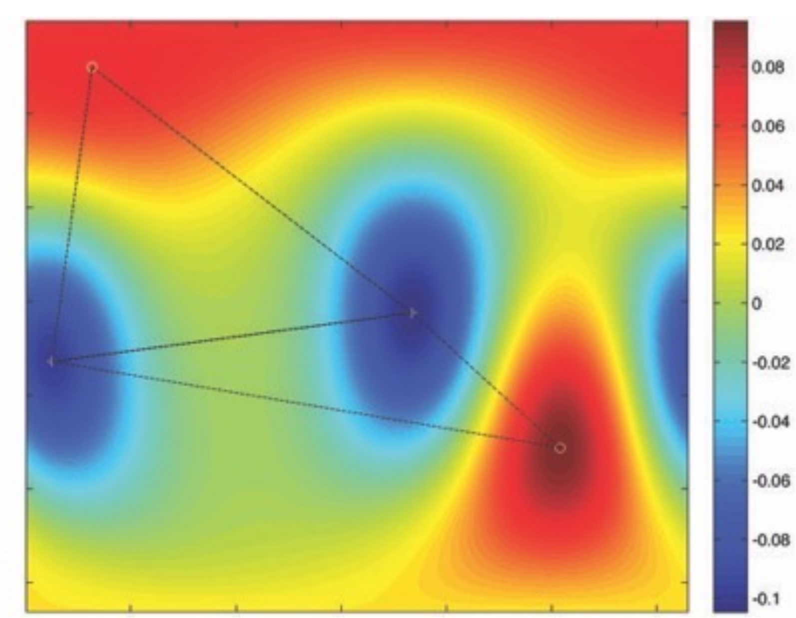
Flattening

(Delaunay) Triangulation




PD

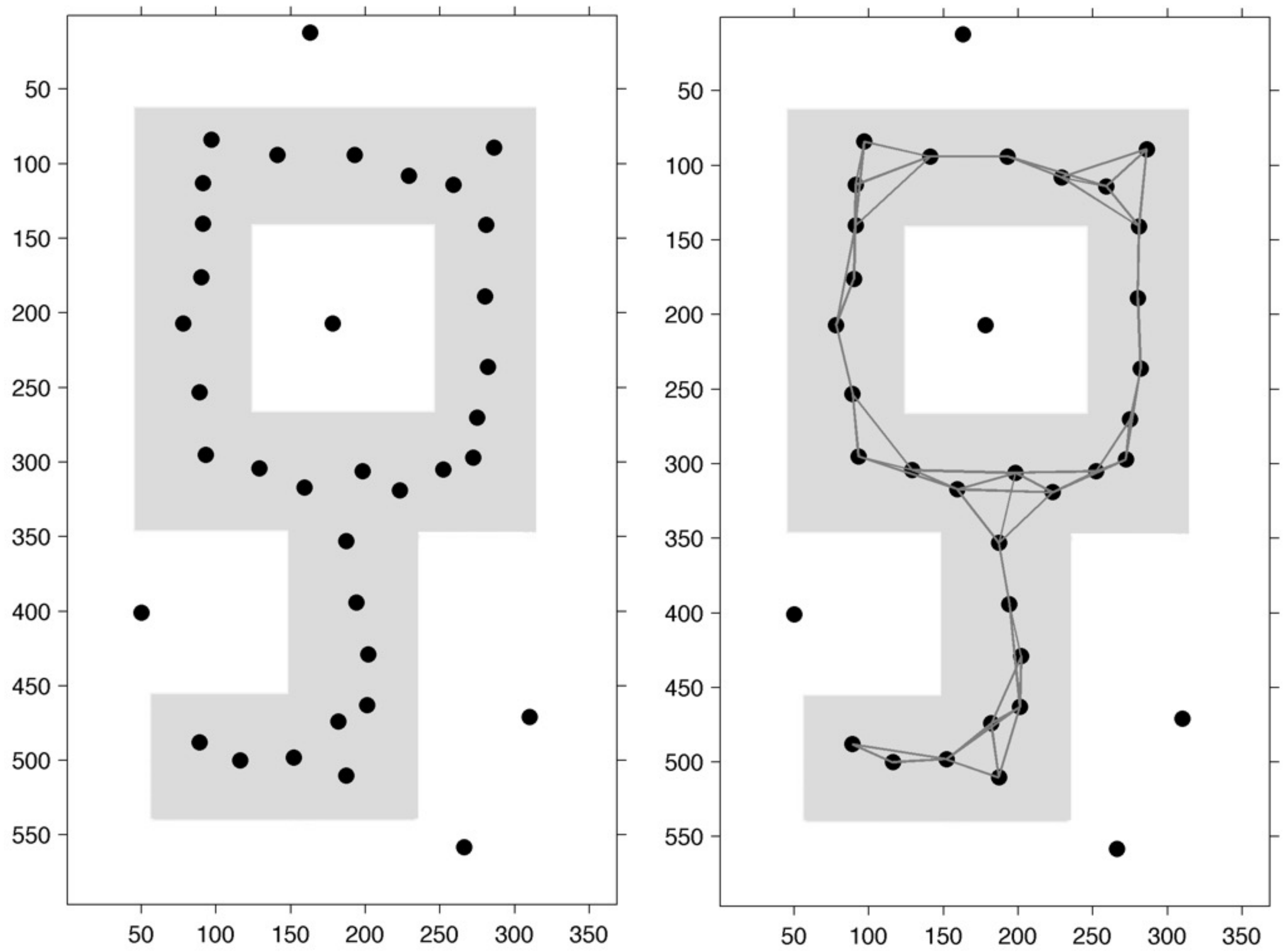




# Rips filtrations

# 1-skeleton of point cloud data

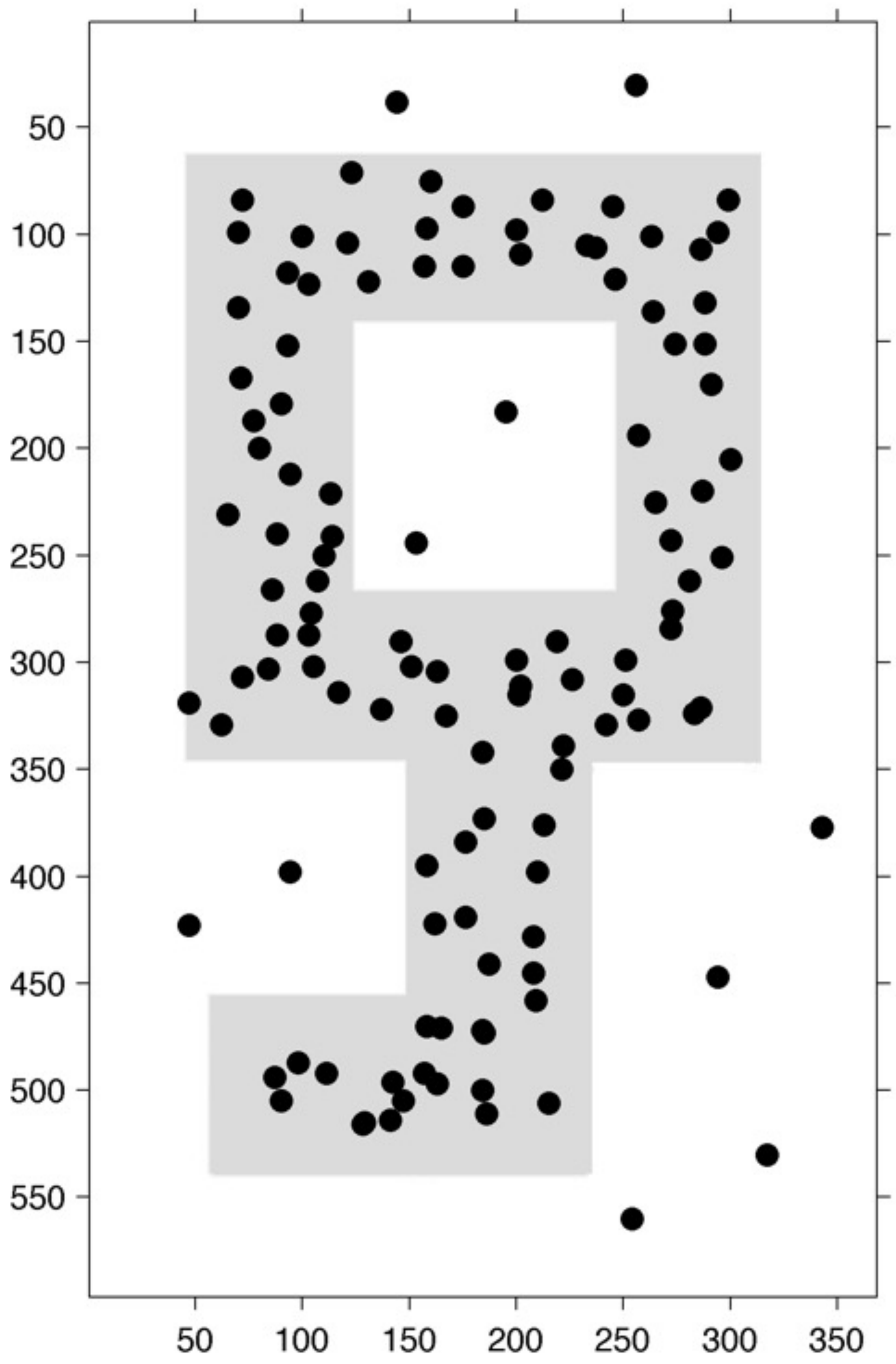
ε = 70mm

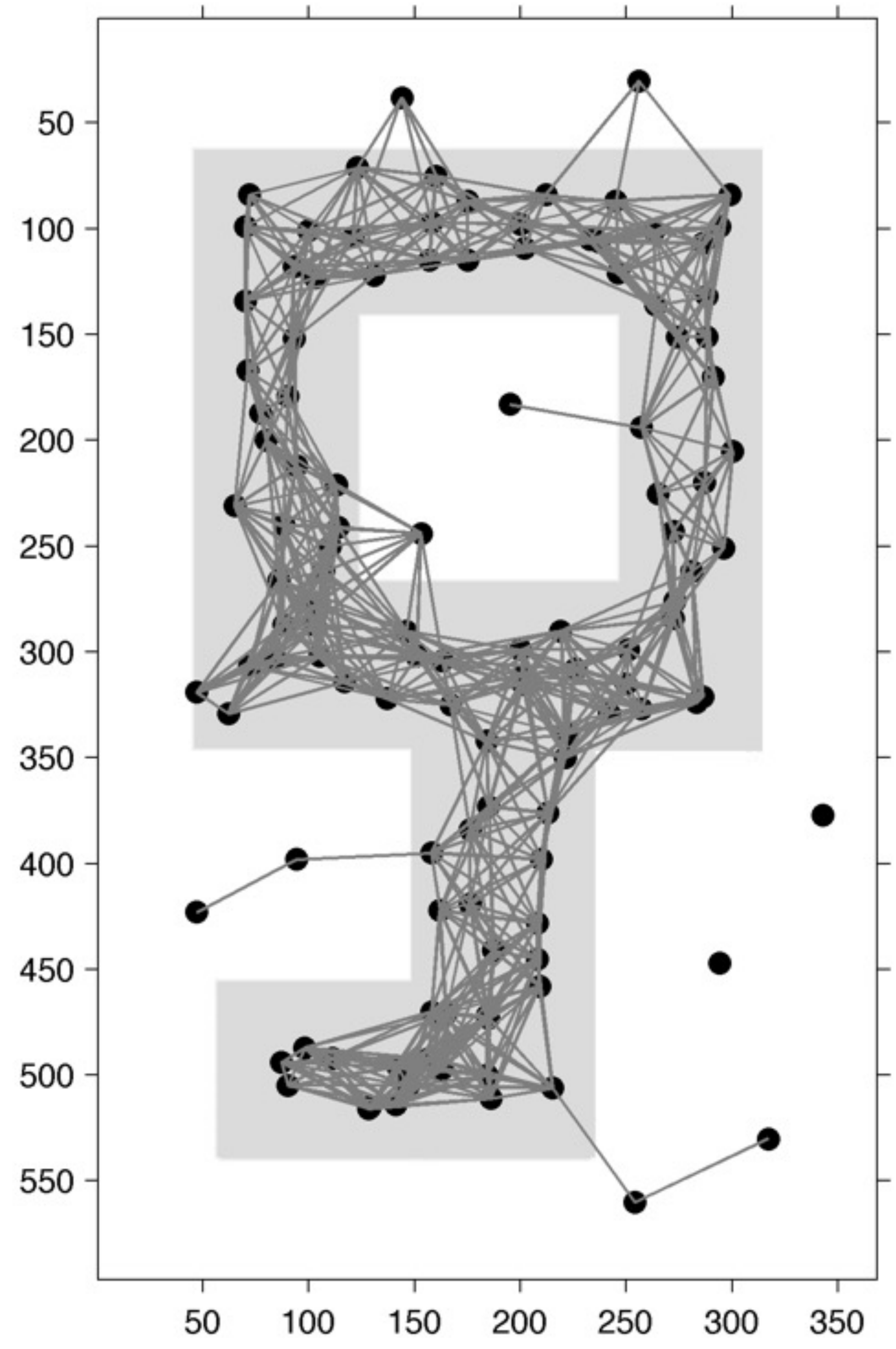



Recovering underlying topology

# 1-skeleton of point cloud data

ε = 70mm

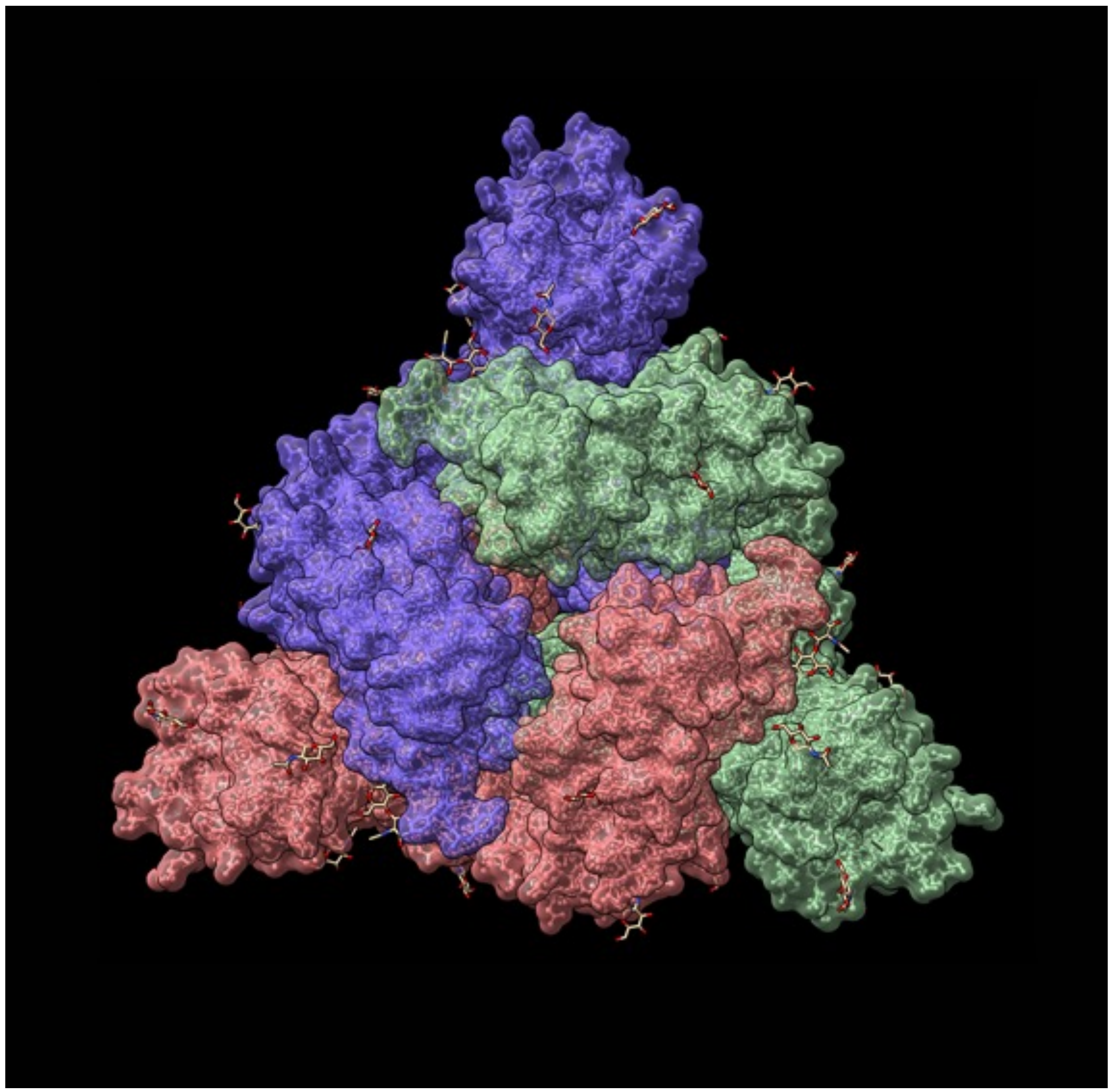


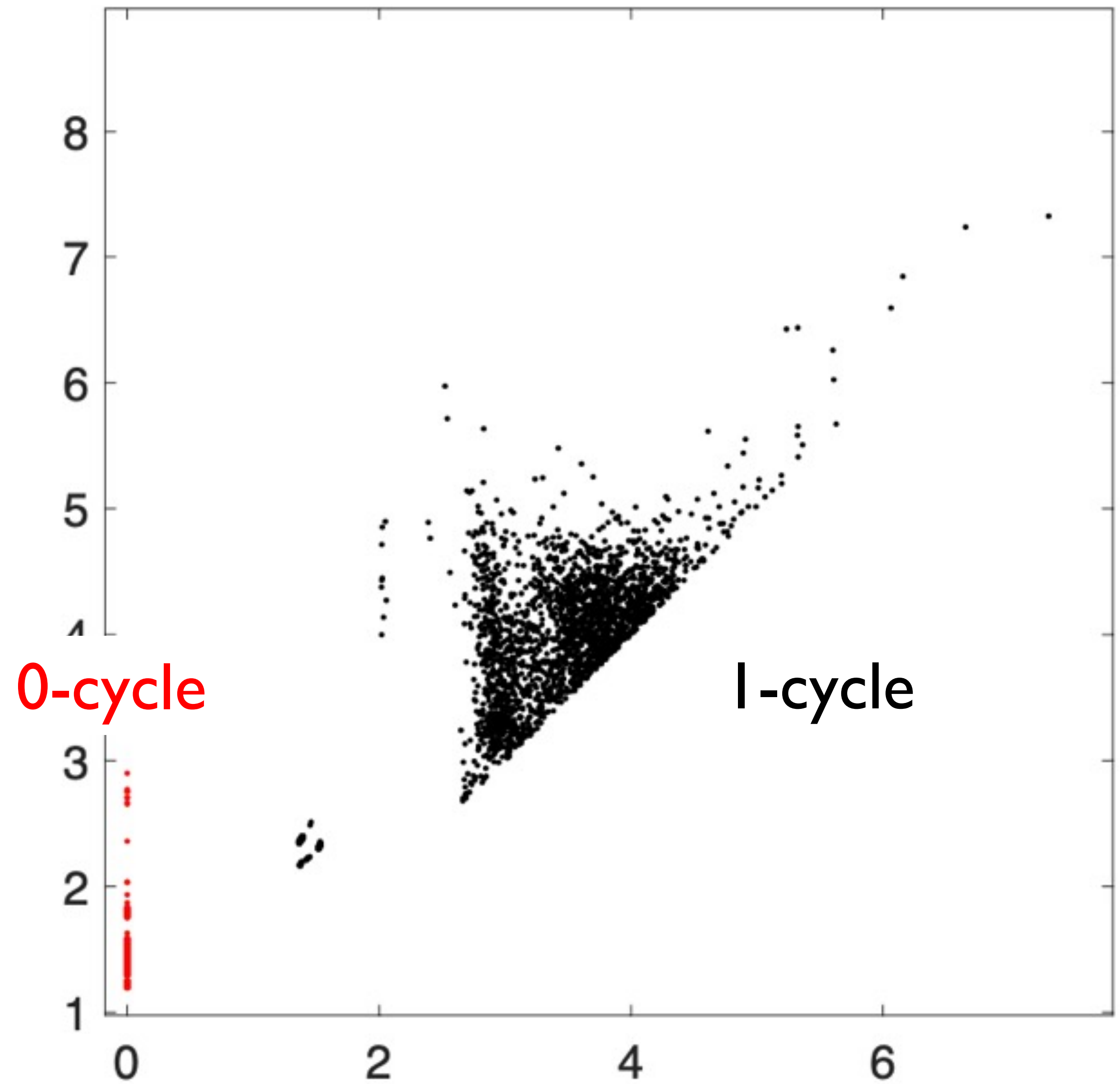




Better approach: perform kernel smoothing and then Morse filtration

# Persistence Diagram (PD) of a protein molecule

Rips filtration on distance between 8000 atoms

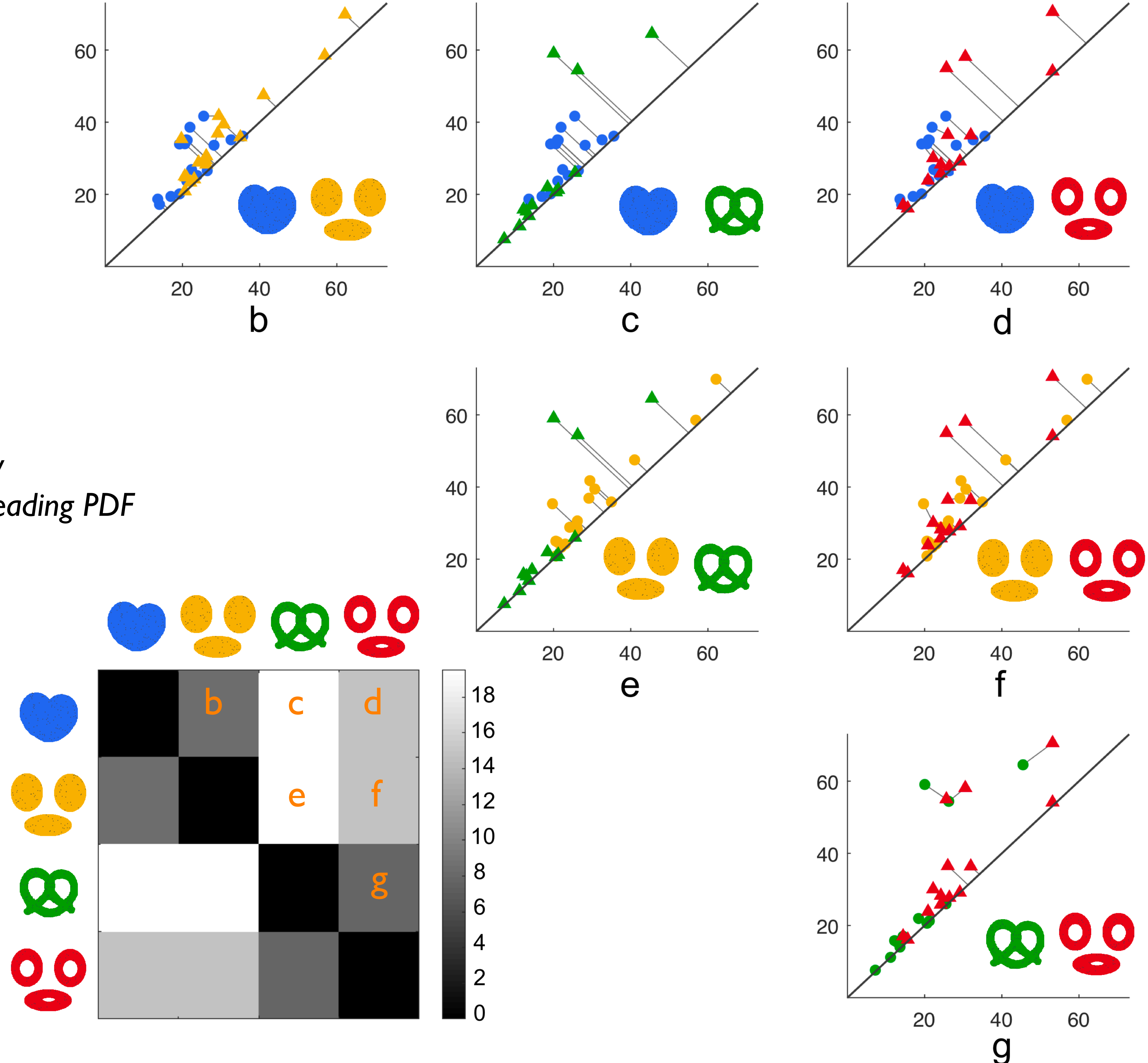





Extremely slow computation → Simply use graph filtration

# Bottleneck distance

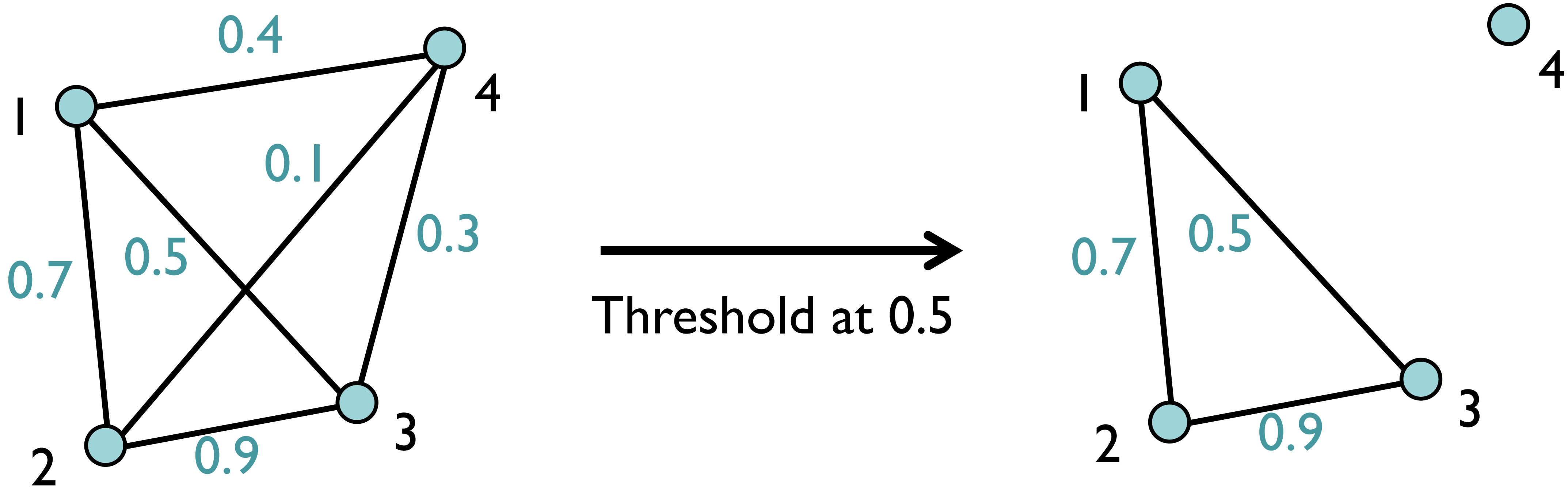
*For definition, simply read the assigned reading PDF*

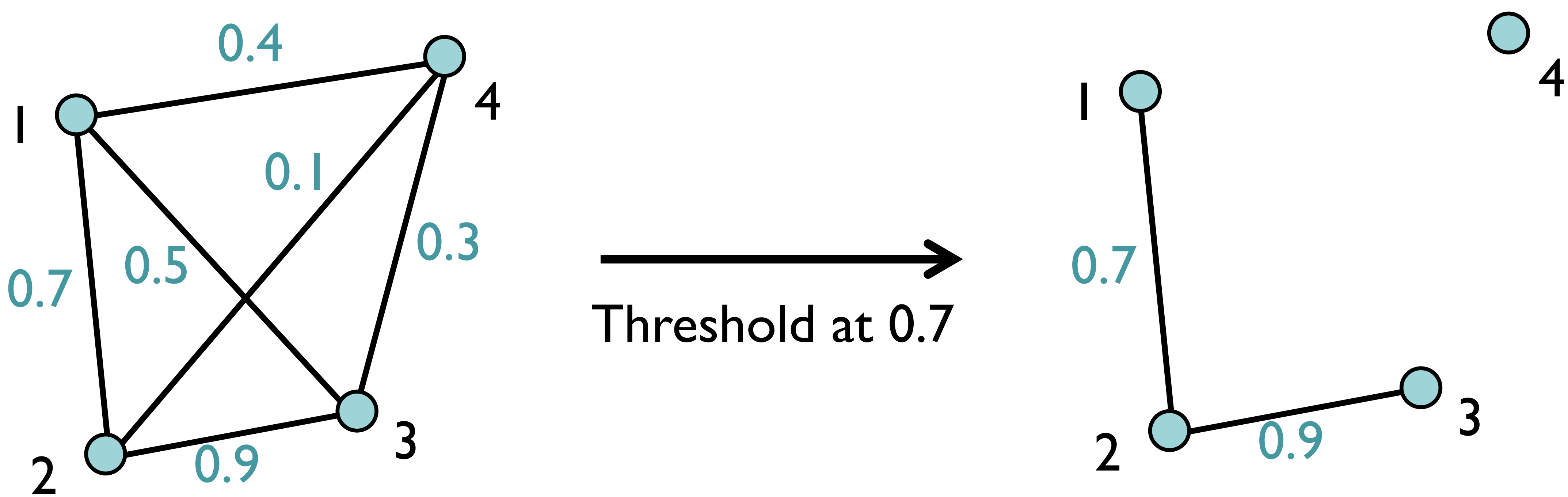


# What is wrong with the arbitrary thresholding?

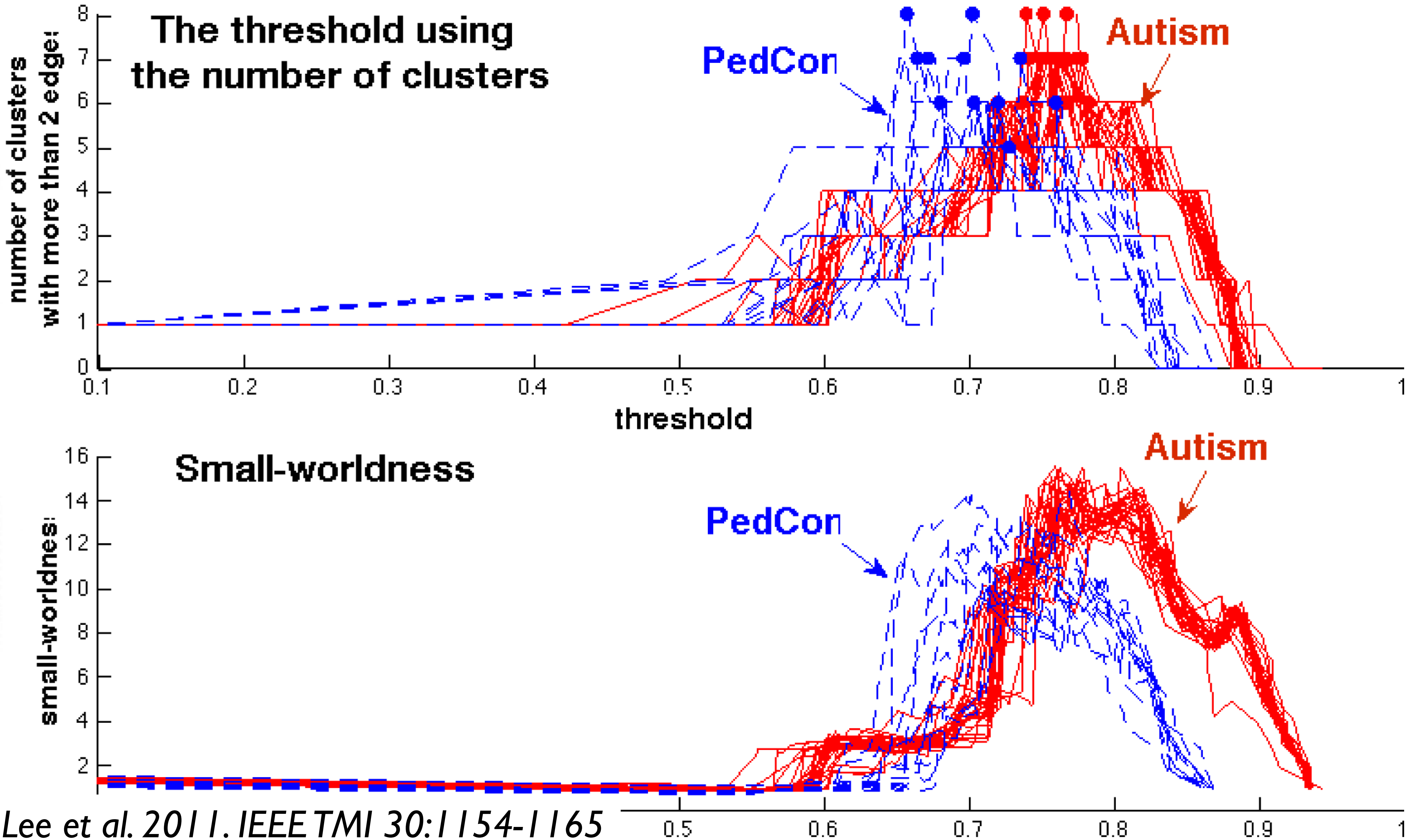
Edge weight $\rho_{ij}$ between node *i* and *j*

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



# *Single threshold often suboptimal → TDA-based network analysis*




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

# Graph filtrations

Baseline filtration for brain networks first introduced in

Lee et al. 2011 MICCAI 302-309

Lee et al. 2012 IEEE Transactions on Medical Imaging 31:2267-2277

# Rips filtration vs. graph filtration

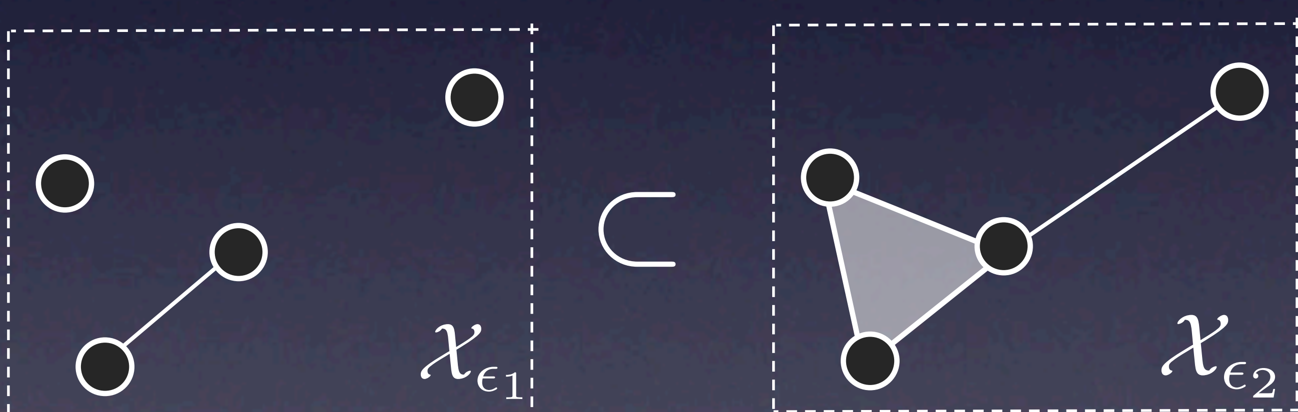
Metric space

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

Node set — Metric

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

Rips complex = Simplicial complex




## Rips filtration

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

for increased radius

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

Weighted graph

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

Node set — Edge weight

Binary graph: 1-skeleton

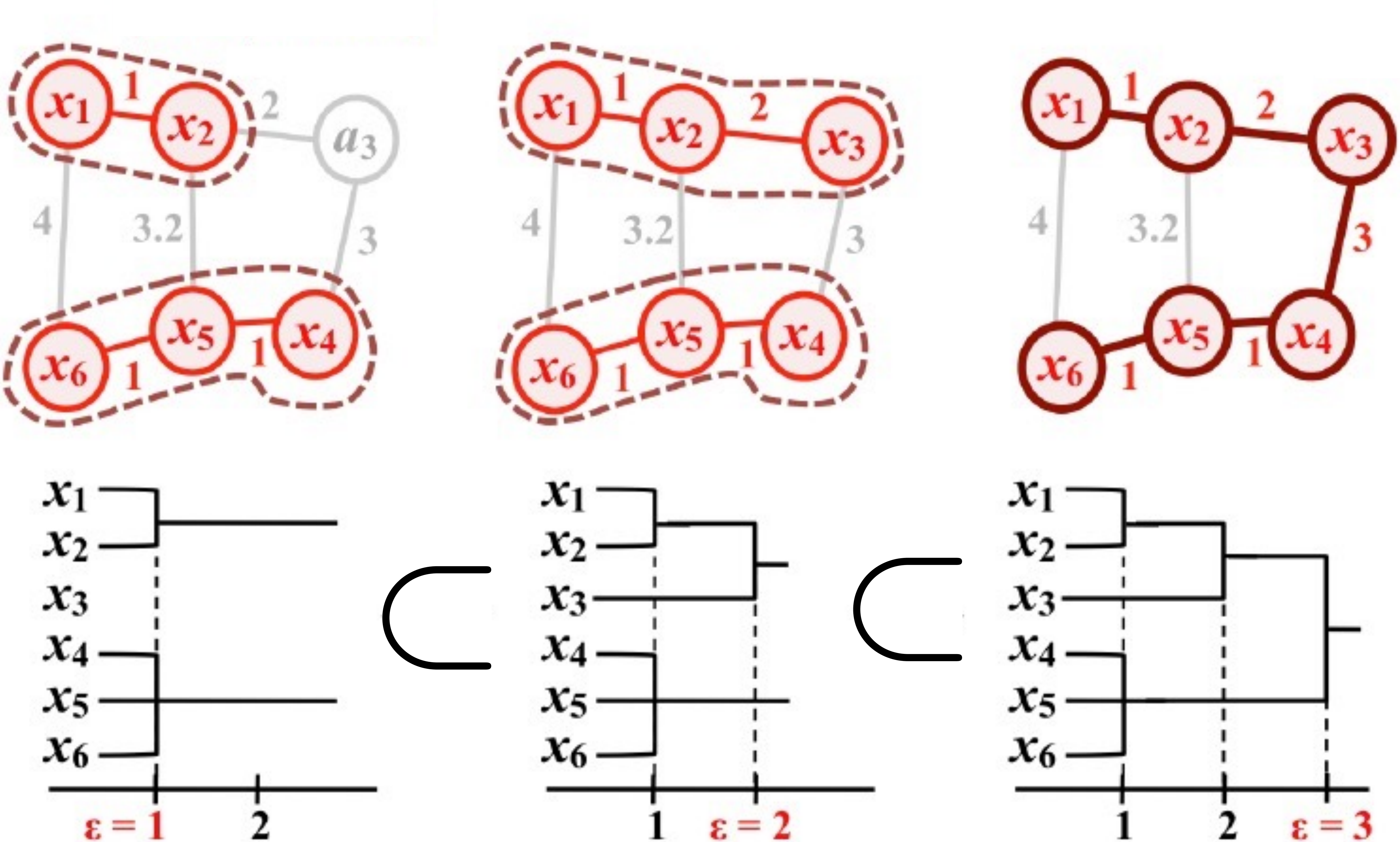

## Graph filtration

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

for increased edge weights

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

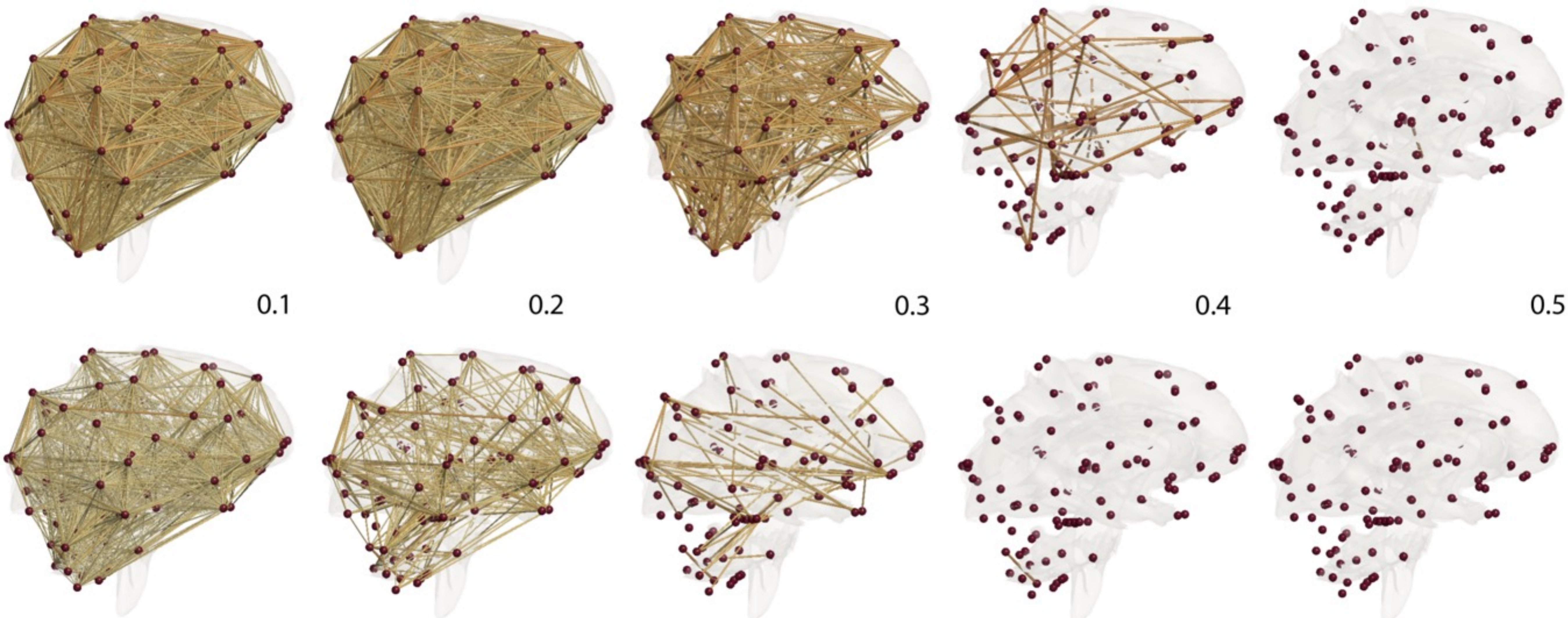
# Graph filtration=single linkage clustering




Lee et al. 2011 MICCAI 302-309

# Graph filtrations on resting-state fMRI

MZ-twins




DZ-twins

# Advantage of 1-skeleton over Rips-complex

Easy biological interpretation

Betti numbers are monotone over filtration

Robustness

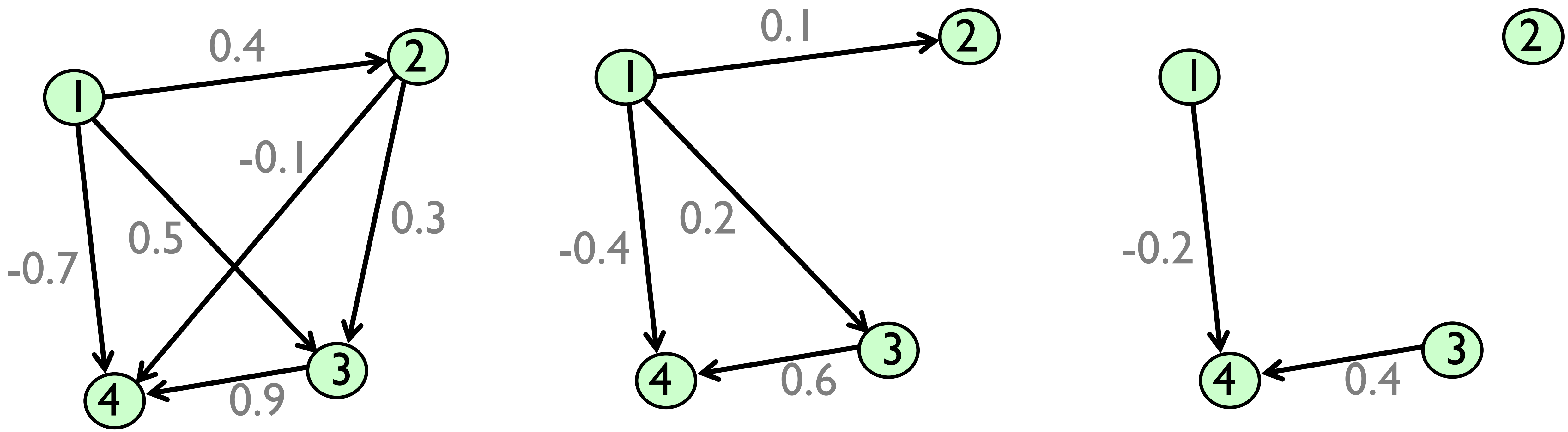
Easier statistical inference

# 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.

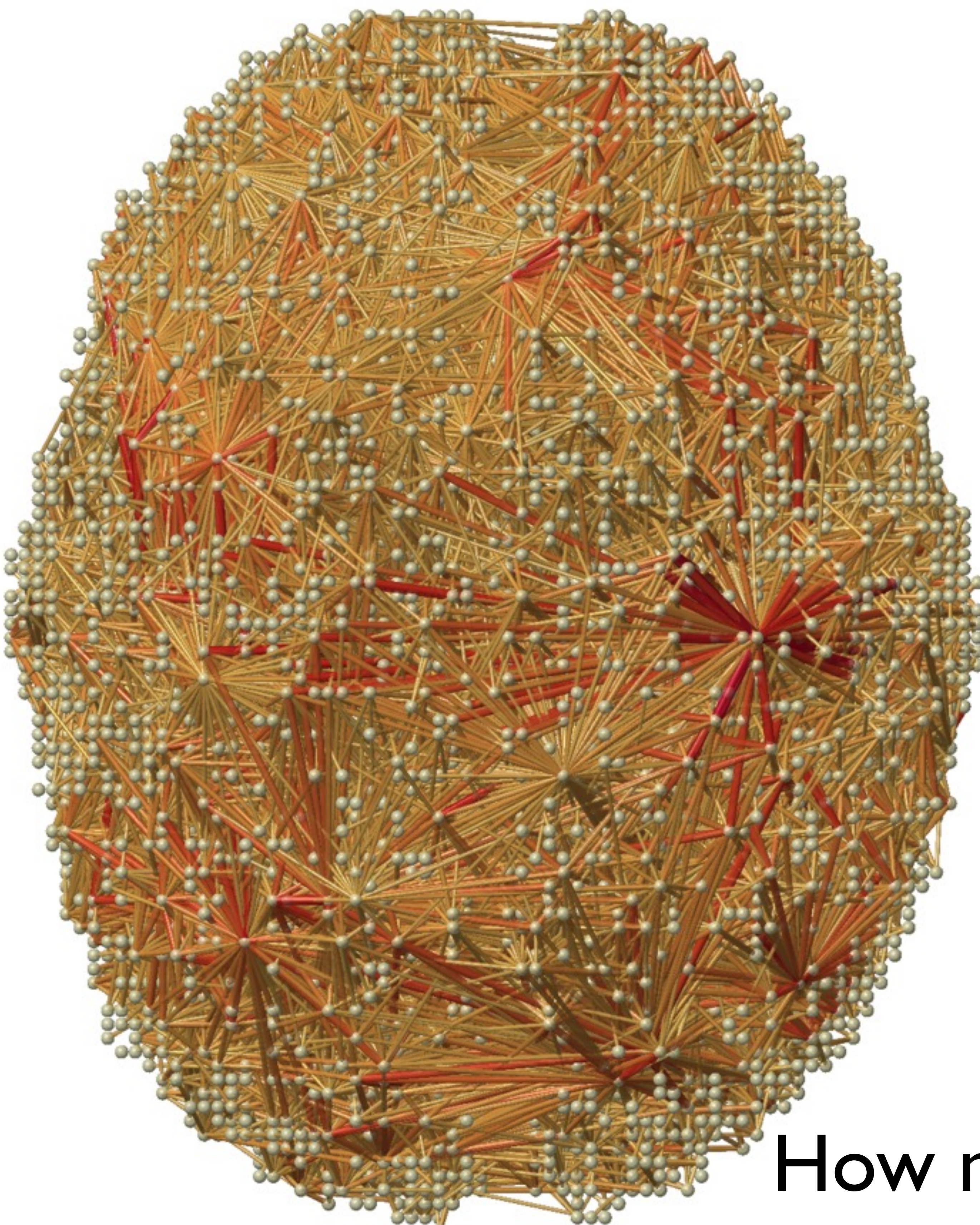
# Graph filtration on directed graphs

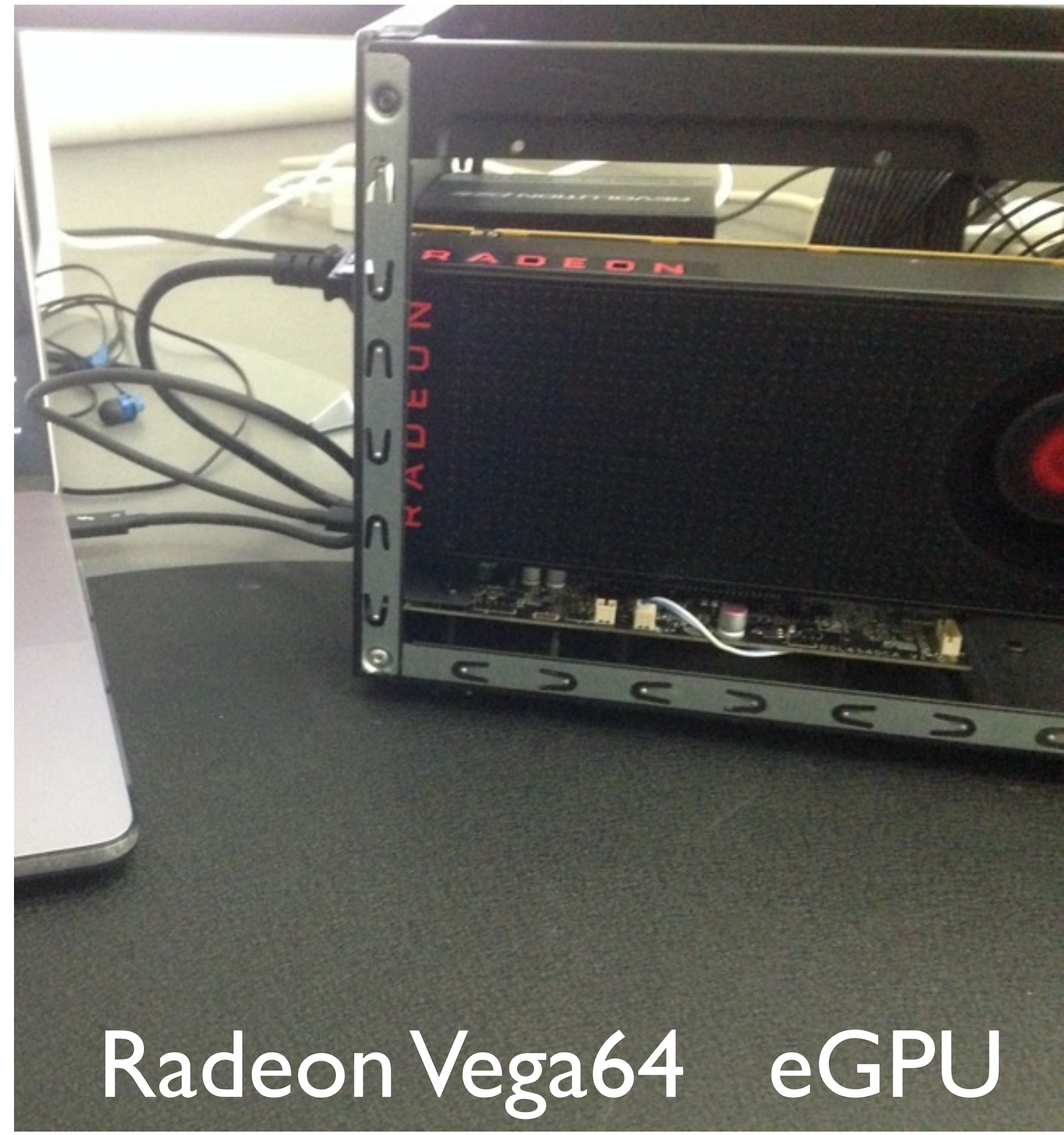



$$G(0) \supset G(0.3) \supset G(0.5)$$

Building persistent homology on directed graphs is not trivial and important → Research project

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






How many cycles in the network?

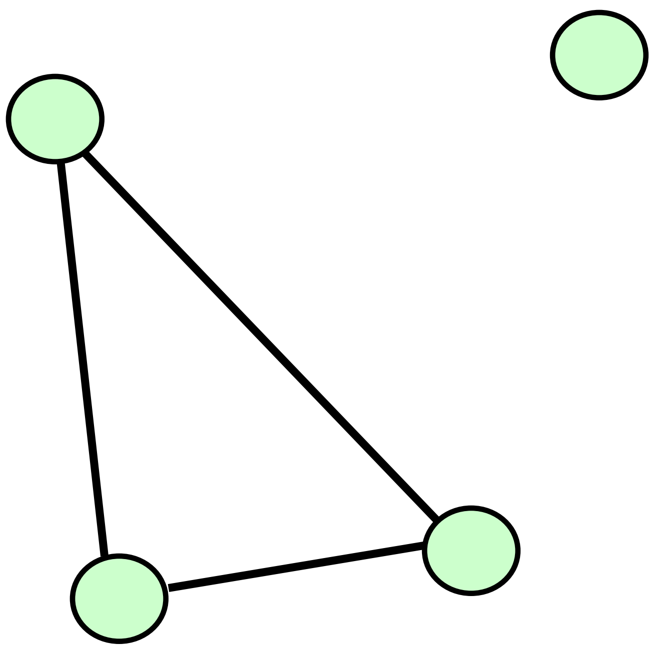
# Betti numbers

# Monotonicity of Betti-0 plot

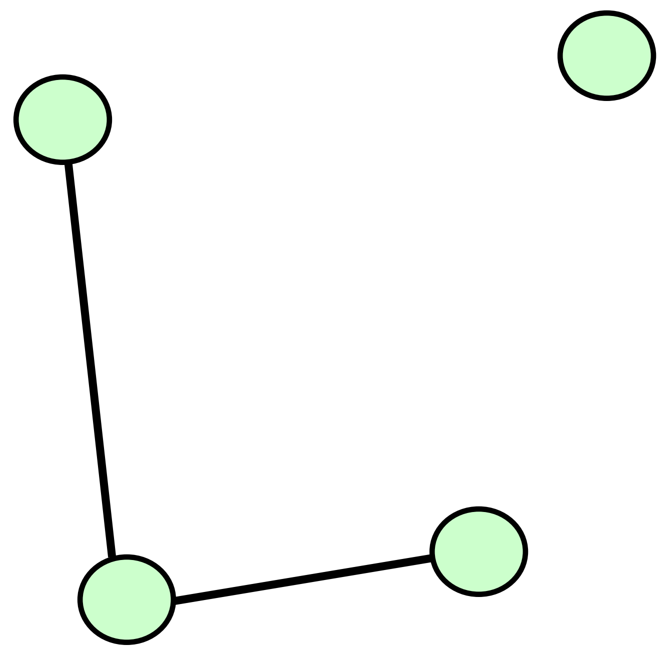
Monotonicity of $\beta_0$

The deletion of edge increases the the number of connected components by at most 1.
$\beta_0$ increases by 0 or 1.

Case 1

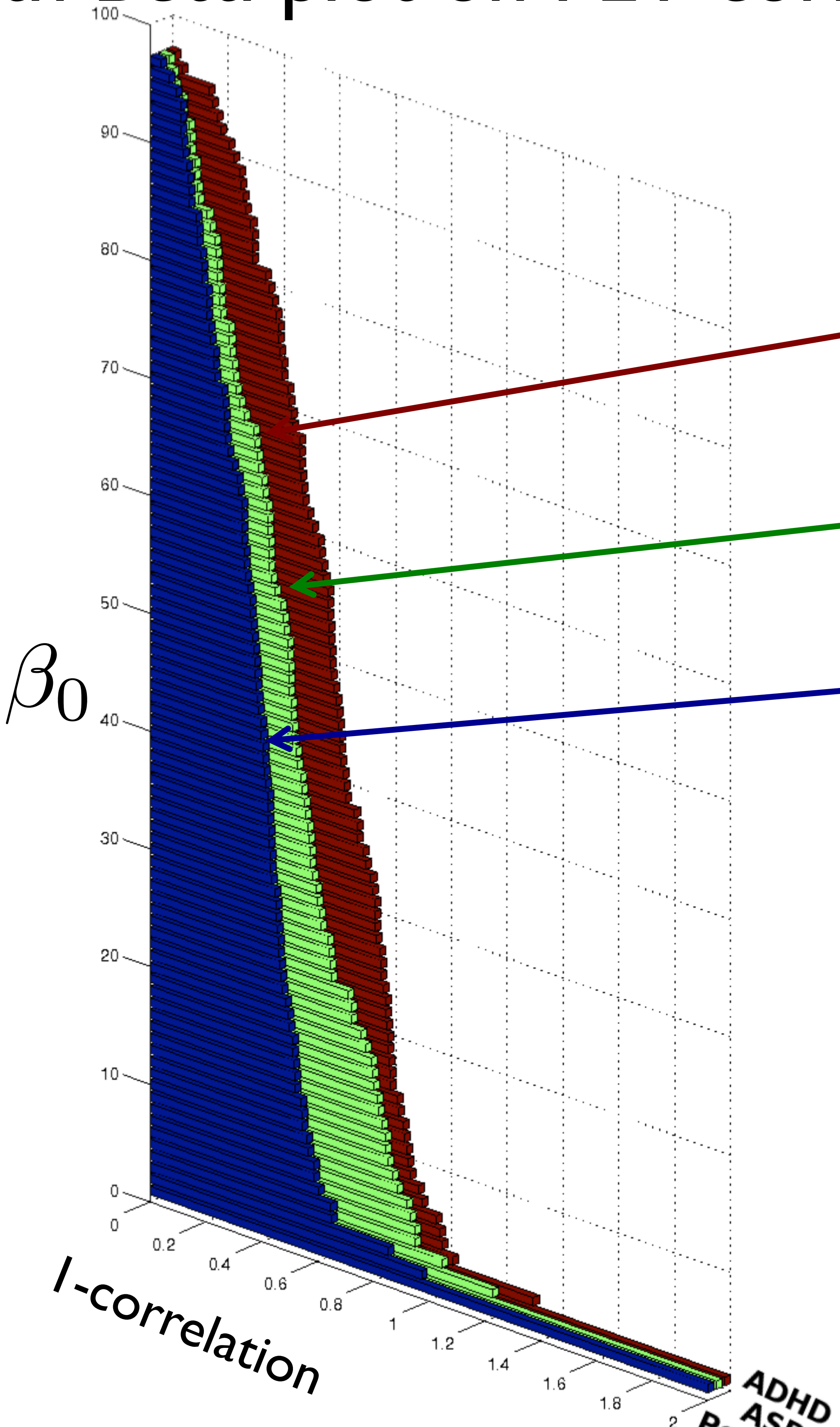


Case 2



*Proof:* *Chung et al. 2019 Network Neuroscience*

# 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

*Lee et al. (2011) ISBI*

# Monotonicity of Betti-1 plot

Monotonicity of $\beta_1$:

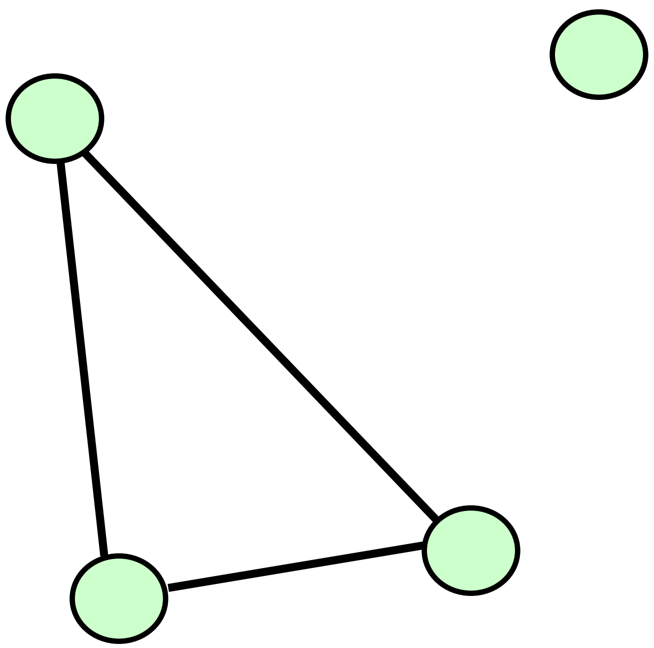
The deletion of edge (in the filtration download) decreases the the number of cycles by at most 1.
$\beta_1$ decreases by 0 or 1.

Euler characteristic for 1-skeleton:

$$\chi = \beta_0 - \beta_1 = \underset{\text{nodes}}{p} - \underset{\text{edges}}{q}$$

$$\underset{-1,\,0}{\beta_1} = \underset{0,\,+1}{\beta_0} - \underset{\text{fixed}}{p} + \underset{-1}{q}$$

# How Betti numbers change over downward graph filtration



$\beta_0 = 2$

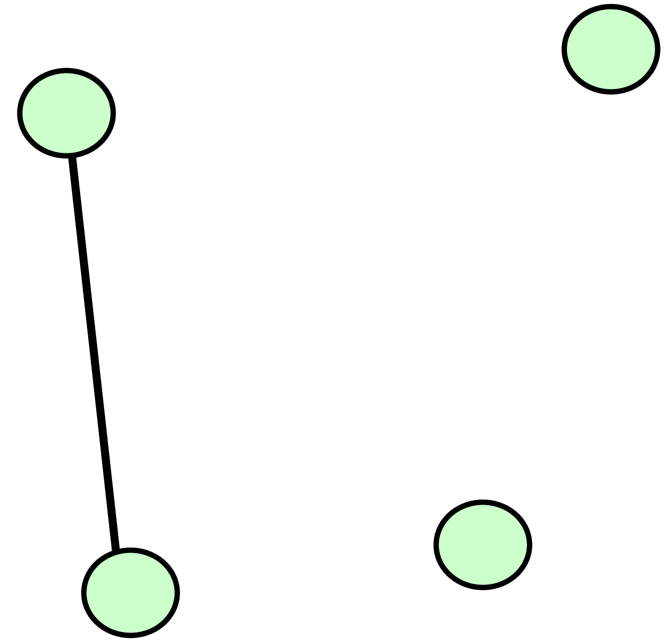
$\beta_1 = 1$

$$\beta_0 - \beta_1 = 1$$

$p = 4$

$q = 3$

$$p - q = 1$$



$\beta_0 = 3$

$\beta_1 = 0$

$$\beta_0 - \beta_1 = 3$$

$p = 4$

$q = 1$

$$p - q = 3$$

# Computation of Betti-plots in practice

Computation of $\beta_0$: Many existing algorithms. Can use a built-in function in MATLAB.

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

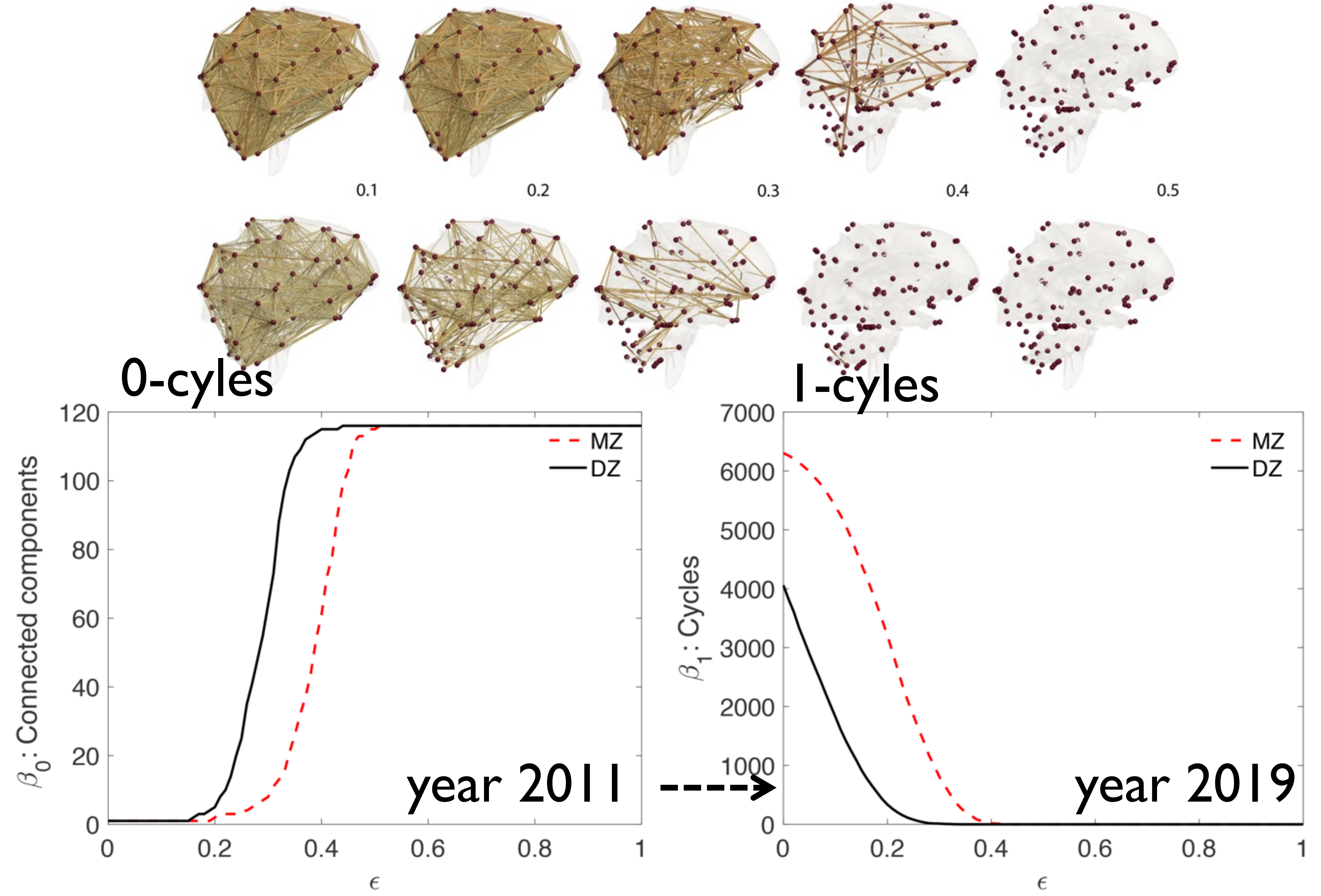
Computation of $\beta_1$: As a function of $\beta_0$

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

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

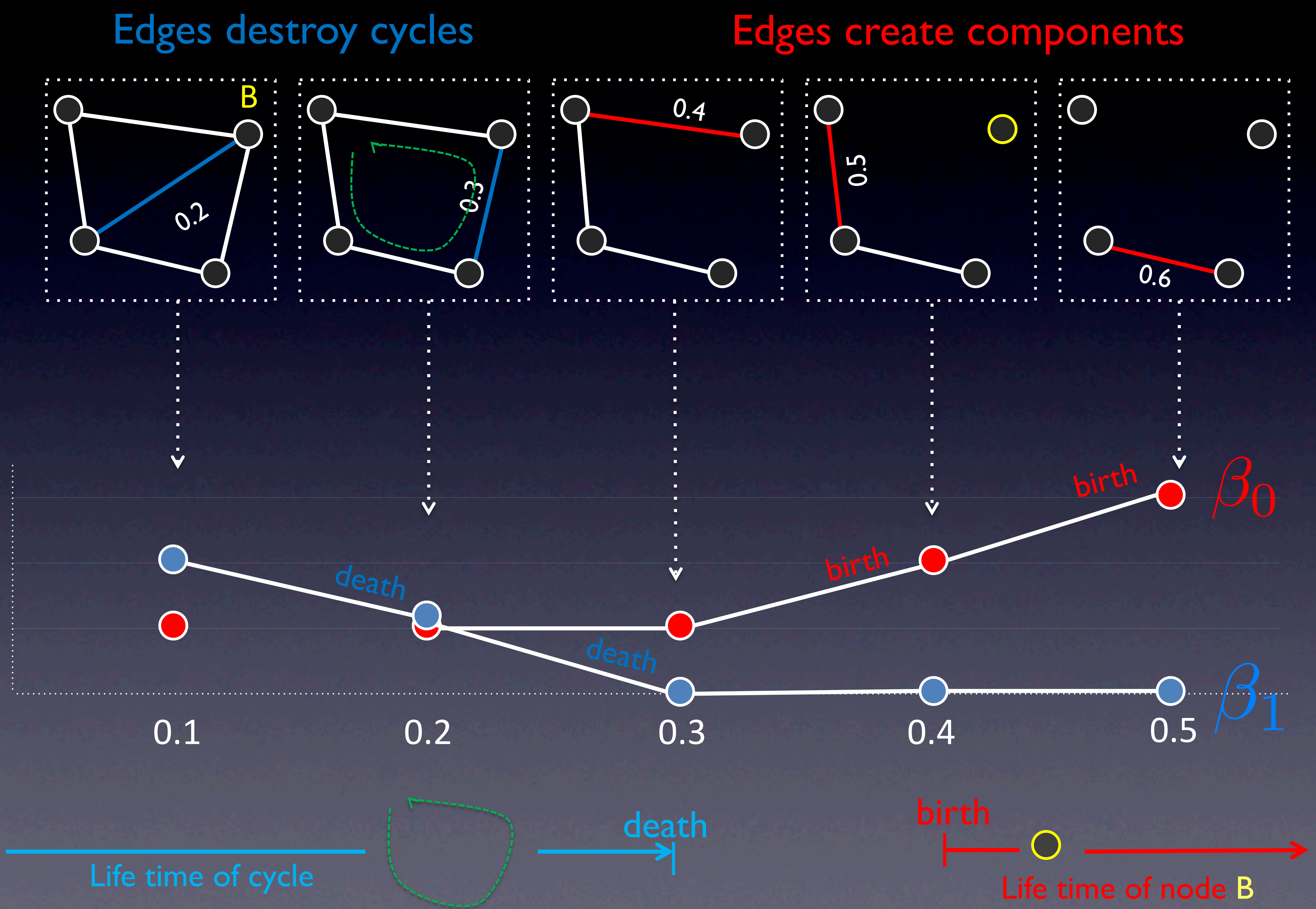
*<u>This is not efficient</u>*. Need an incremental algorithm that updates as we delete one edge at a time.

# Betti-plots in 116 nodes network



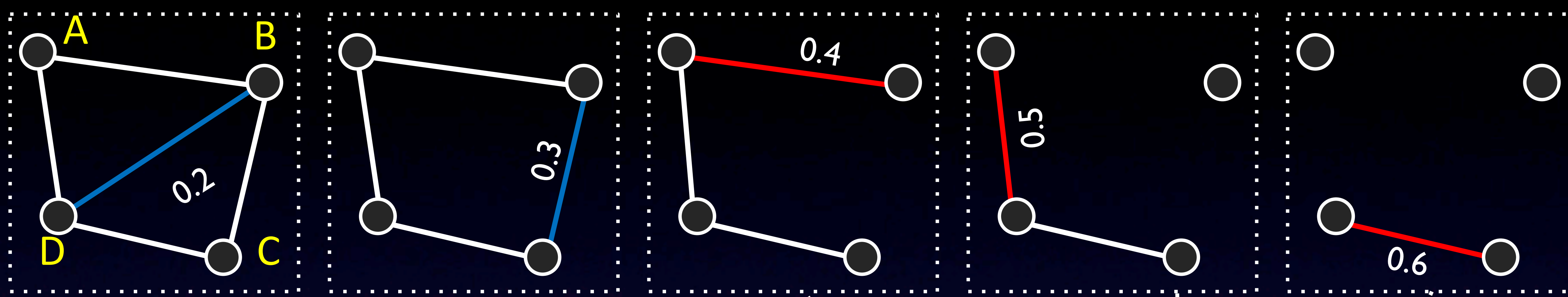
# Birth and death decomposition

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



# *Theorem* Birth & death sets partition the edge set

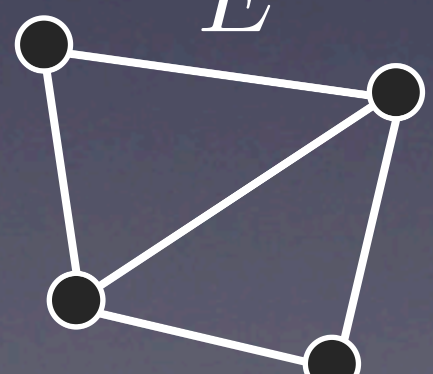
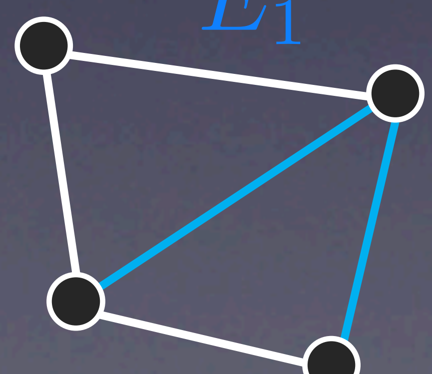
$E_1$ Edges destroy cycles $\qquad$ $E_0$ Edges create components




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

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

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

$E$  $=$ $E_1$  $\cup$ $E_0$ 

Maximum spanning tree

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

Songdechakraiwut & Chung 2020 arXiv: 2012.00675