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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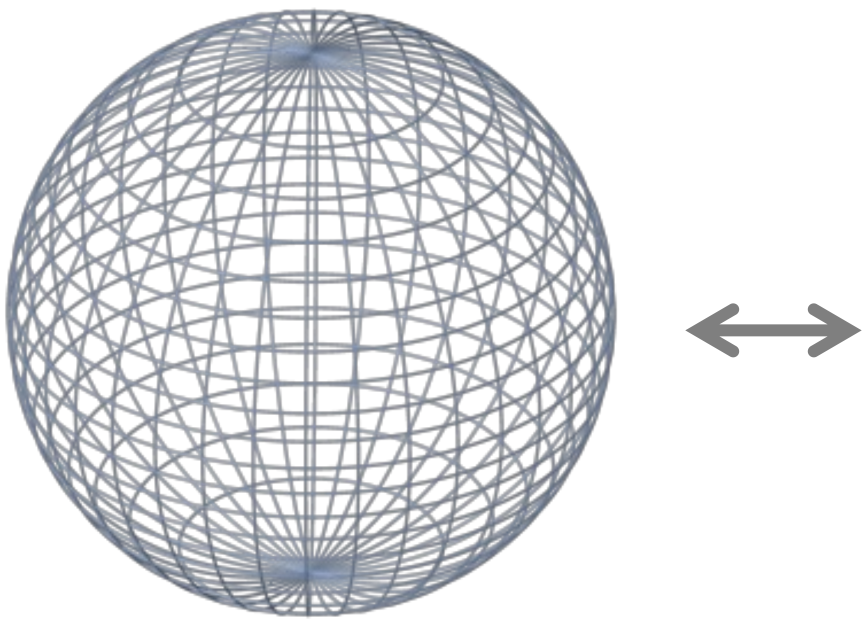
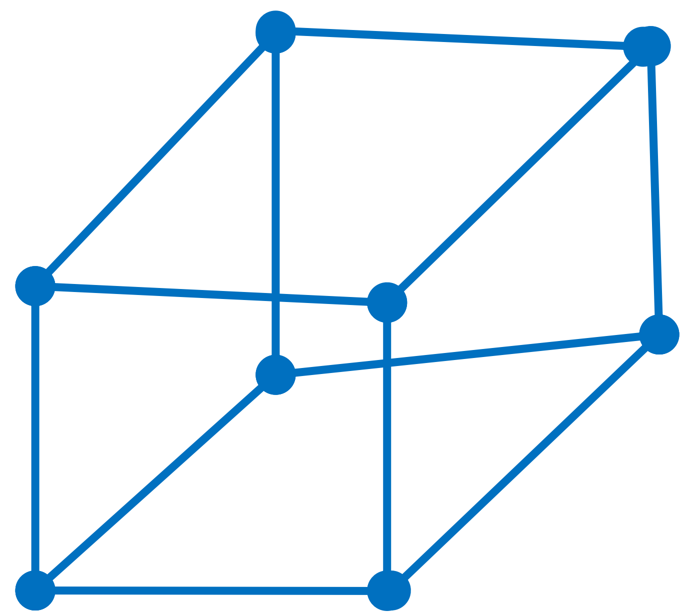
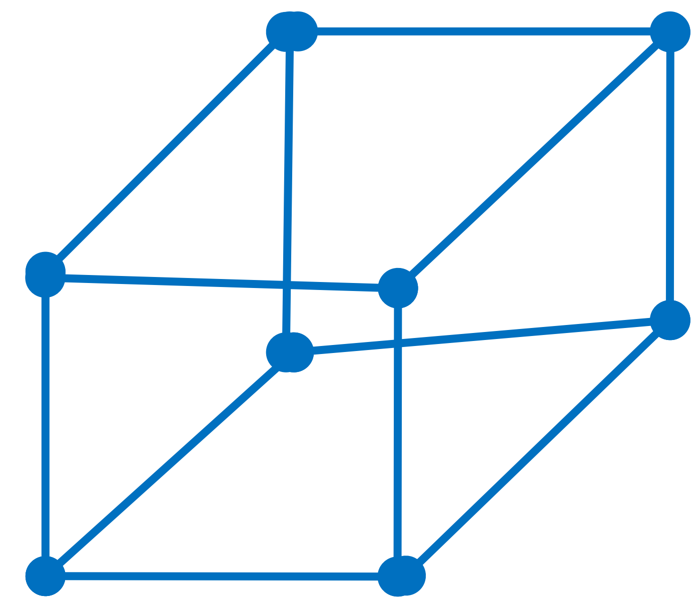
Euler characteristic

Topologically equivalent
Deformation-invariant







Sphere

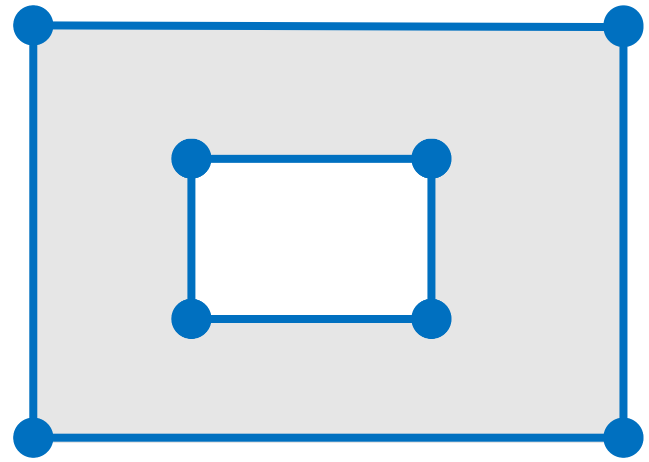
$$EC = N - E + F$$
$$= 8 - 12 + 6$$
$$= 2$$

Solid ball

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

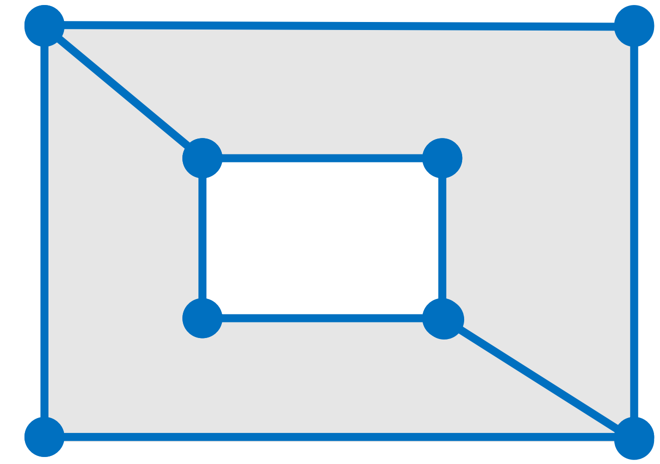
Computing Euler characteristic by parts

Cover an object with polyhedrons

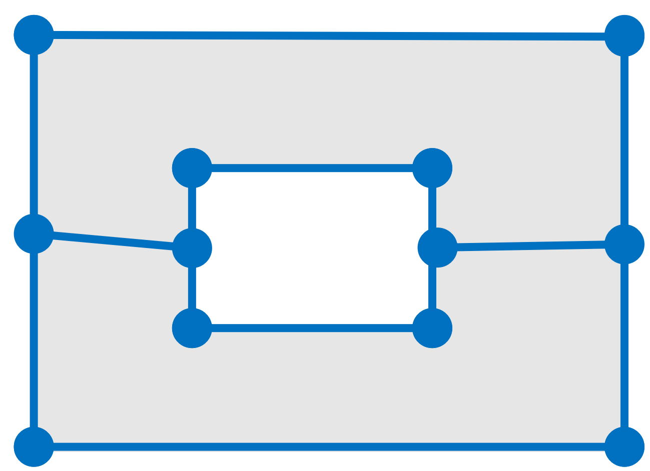


Incorrect computation

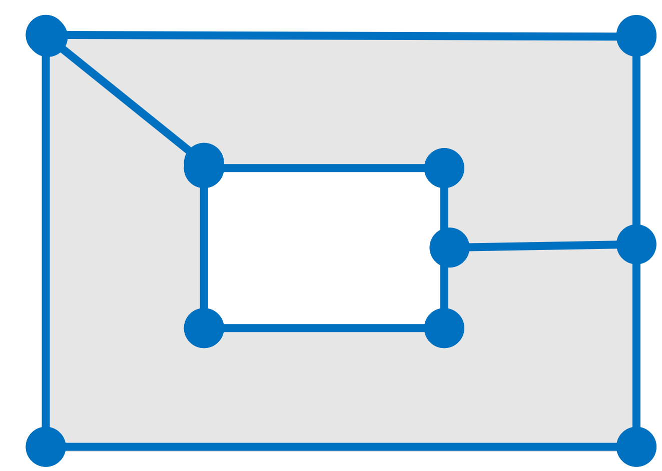
EC = N – E + F
=8 – 8 + 1
= 1



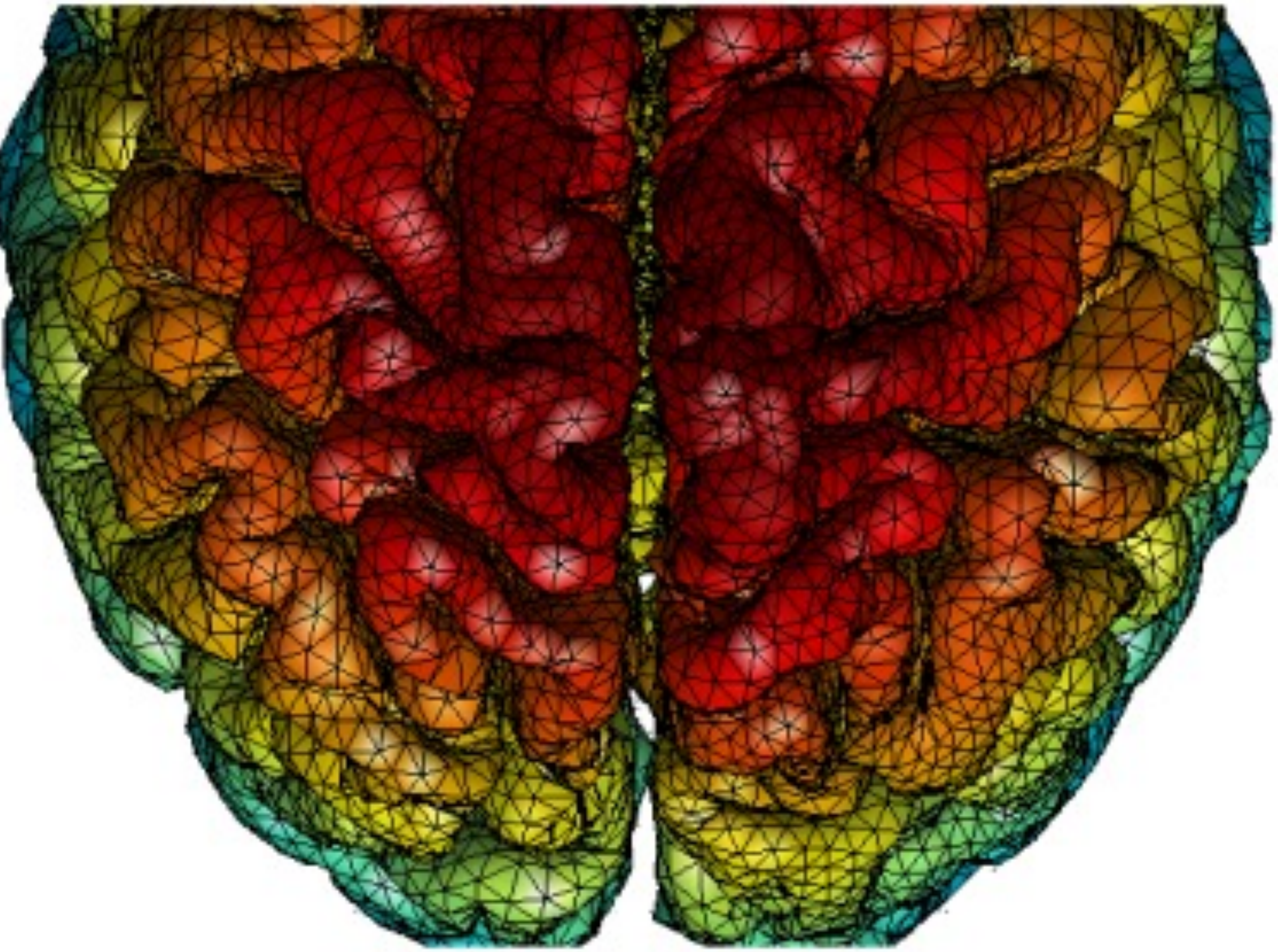
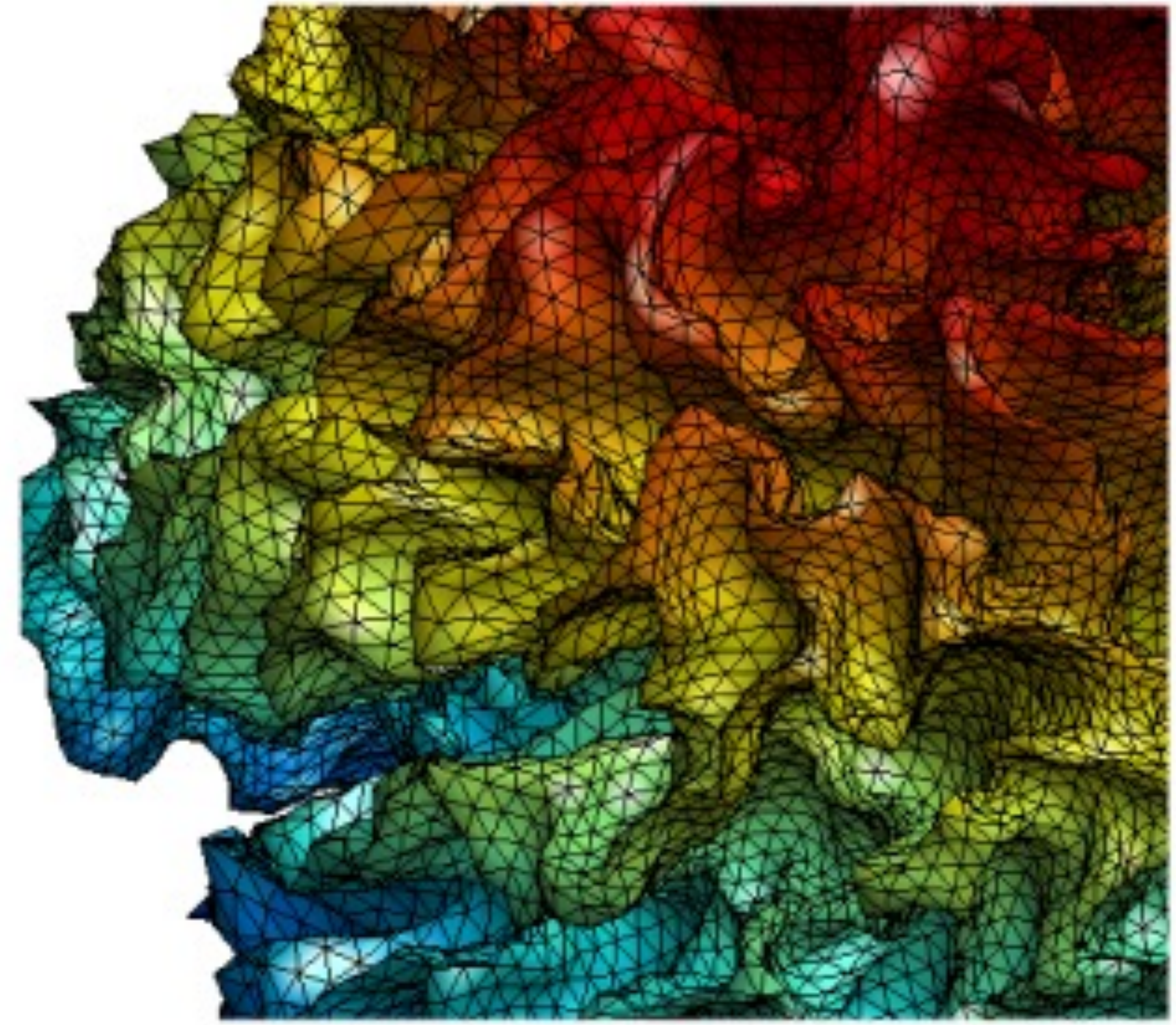
EC = N – E + F
= 8 – (8+2) + (1+1)
= 0



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



EC = N – E + F
=(8+2)–(8+4) +(1+1)
= 0

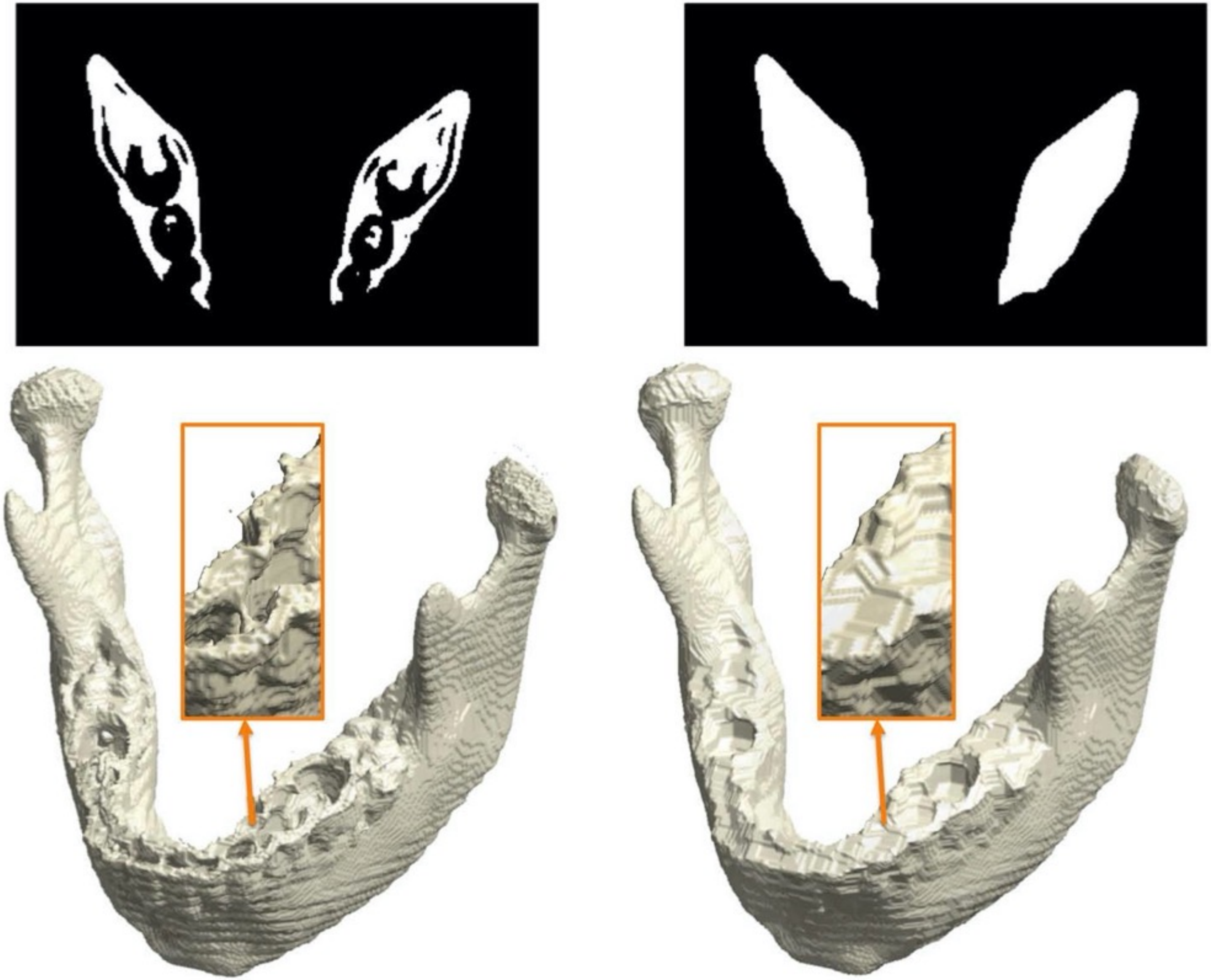
 

Euler characteristic of a surface mesh from SurfStat

$N - E + F = 2$ 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.

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 Euler characteristic

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

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

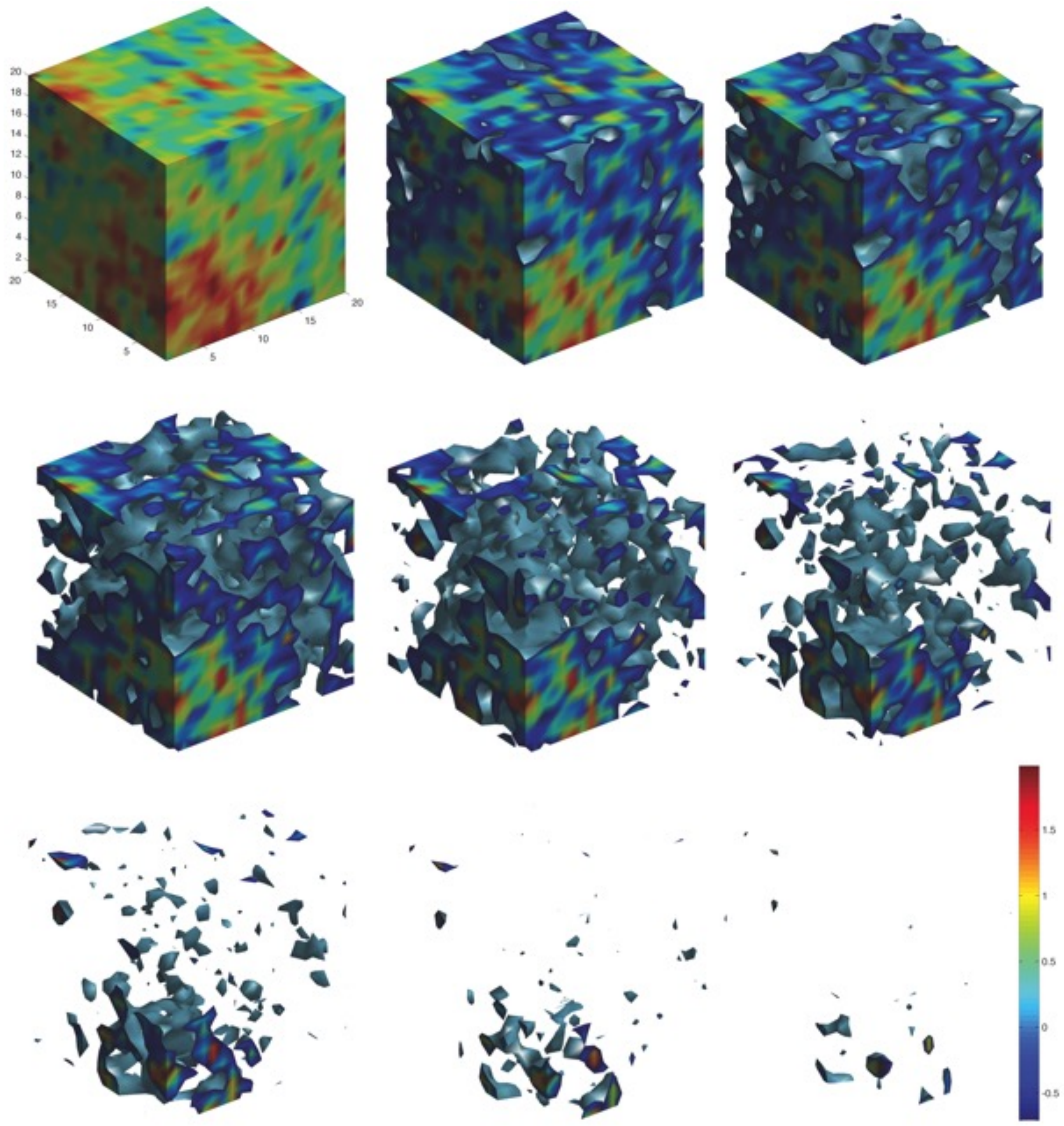
Random field, stochastic process

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

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

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

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



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

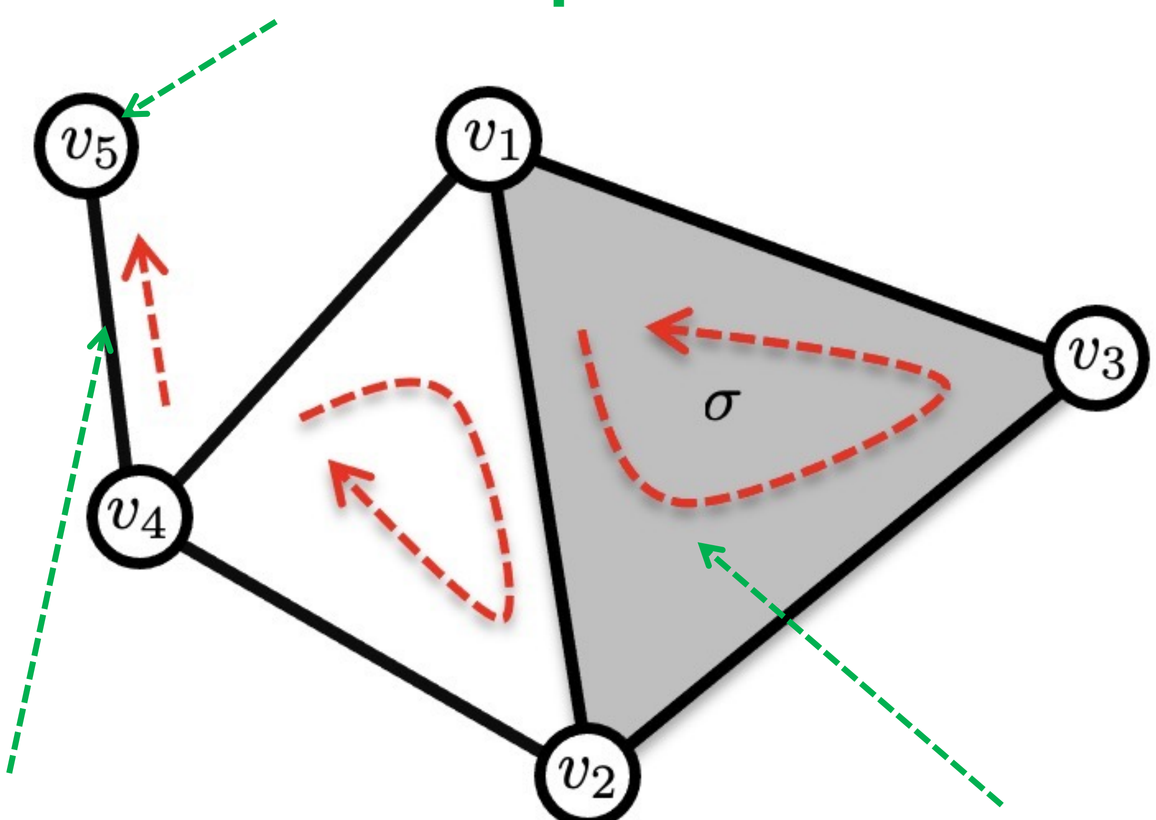
n-simplex

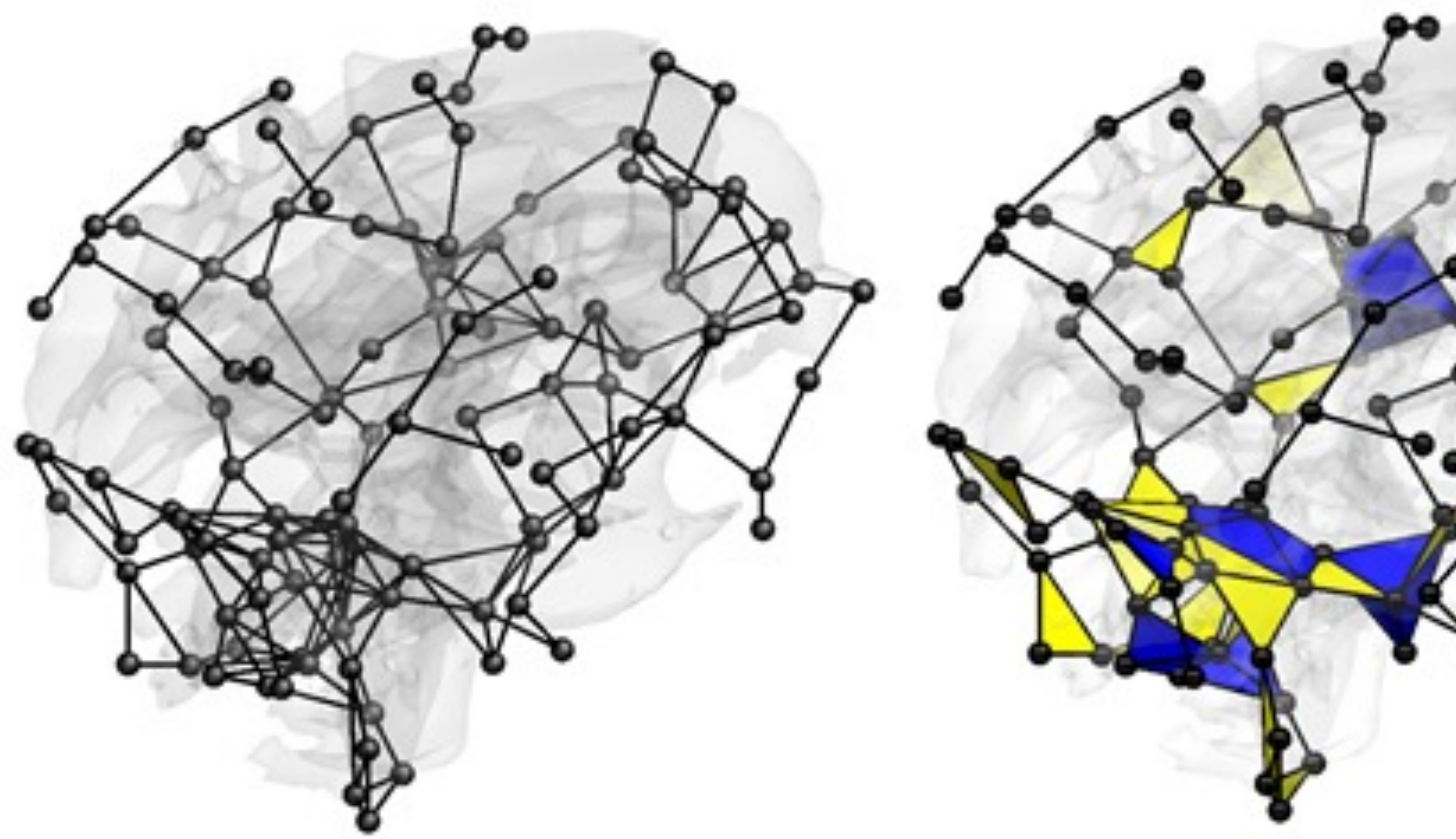
The basic building block of persistent homology

The smallest convex set containing *n+1* points

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

0-simplex $[v_5]$





1-simplex

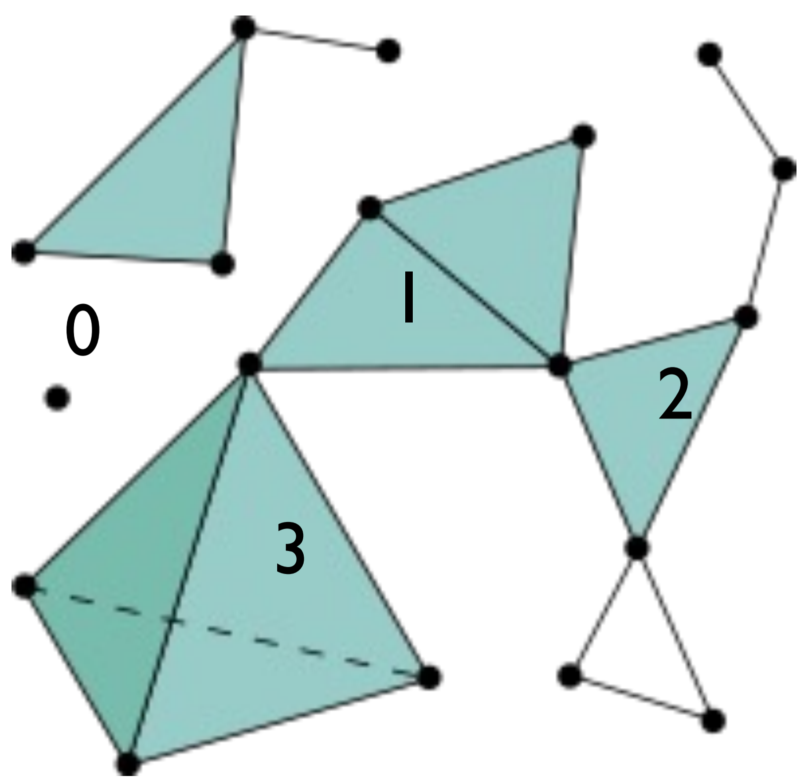
$[v_4, v_5] = -[v_5, v_4]$

2-simplex

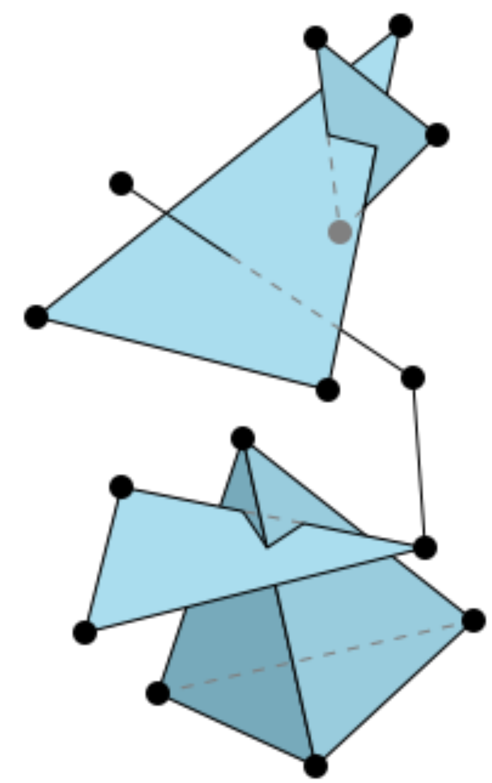
$\sigma = [v_1, v_2, v_3]$

Simplicial complex

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



Simplicial complex

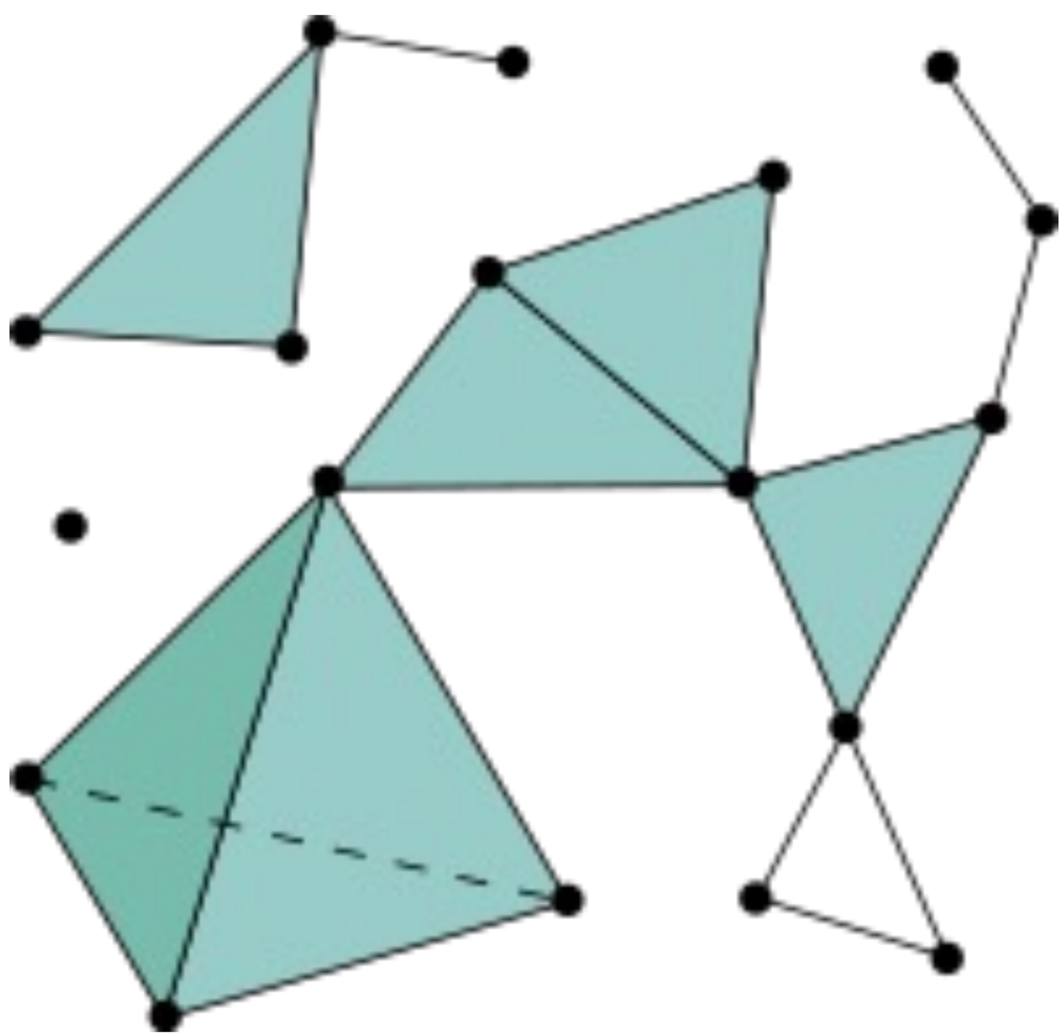


Not simplicial complex

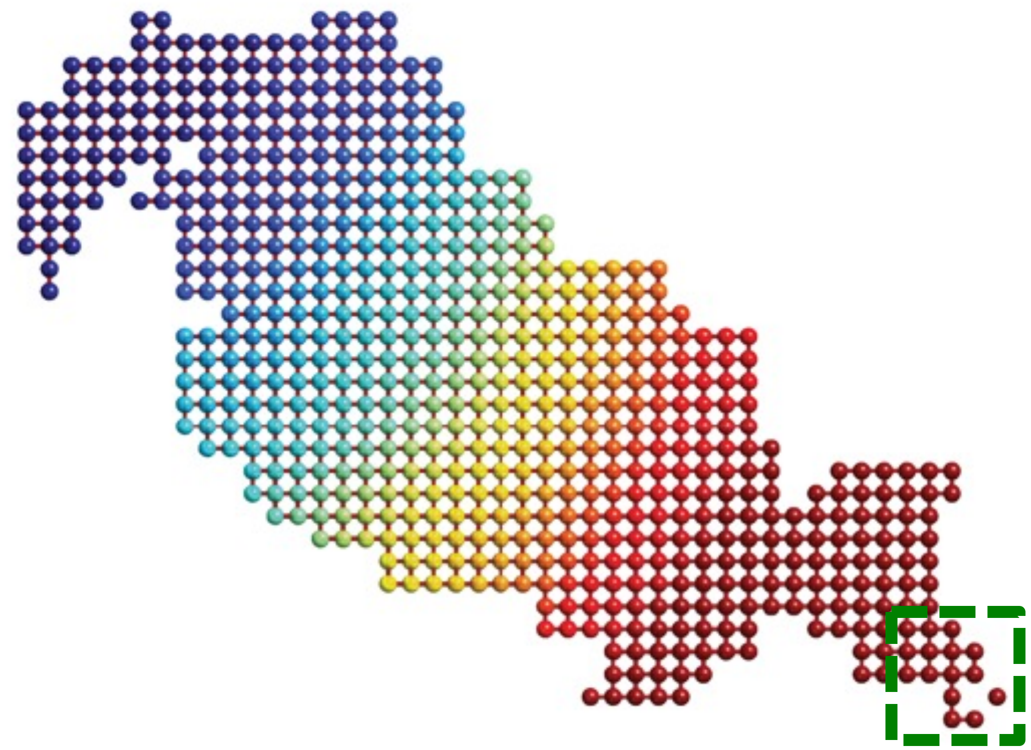
Ex. surface mesh, graphs (including hypergraphs), networks

k-skeleton

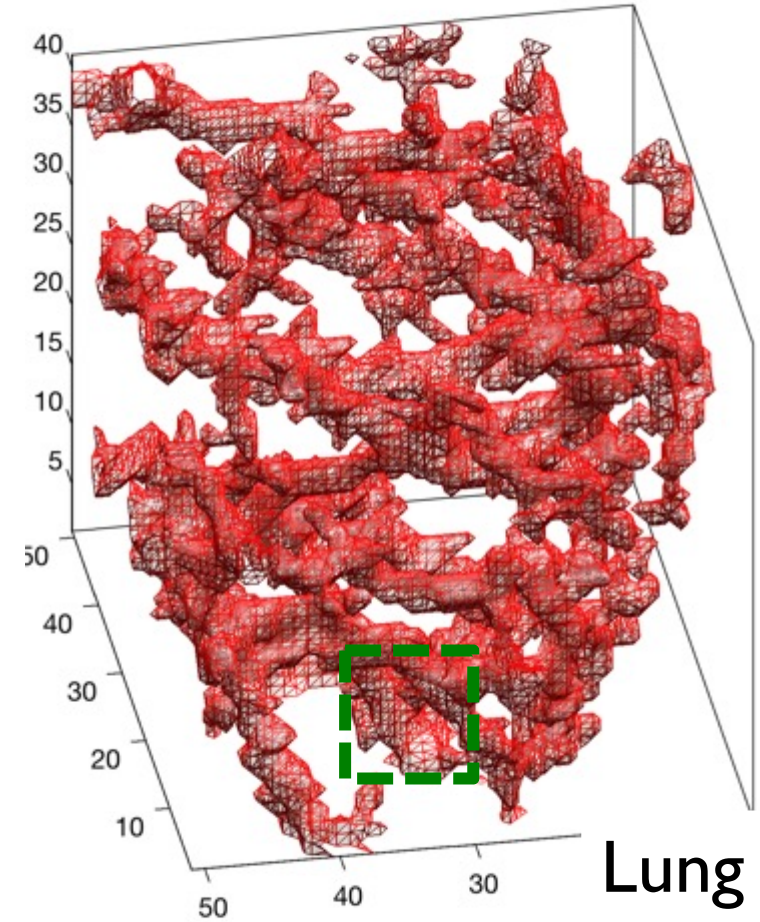
A simplicial complex consisting of points and line segments only → graphs & network



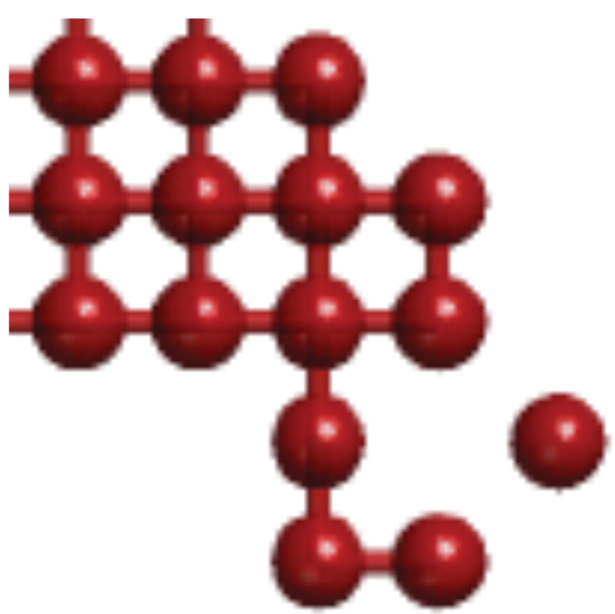
Cubical complex (2D or 3D images)



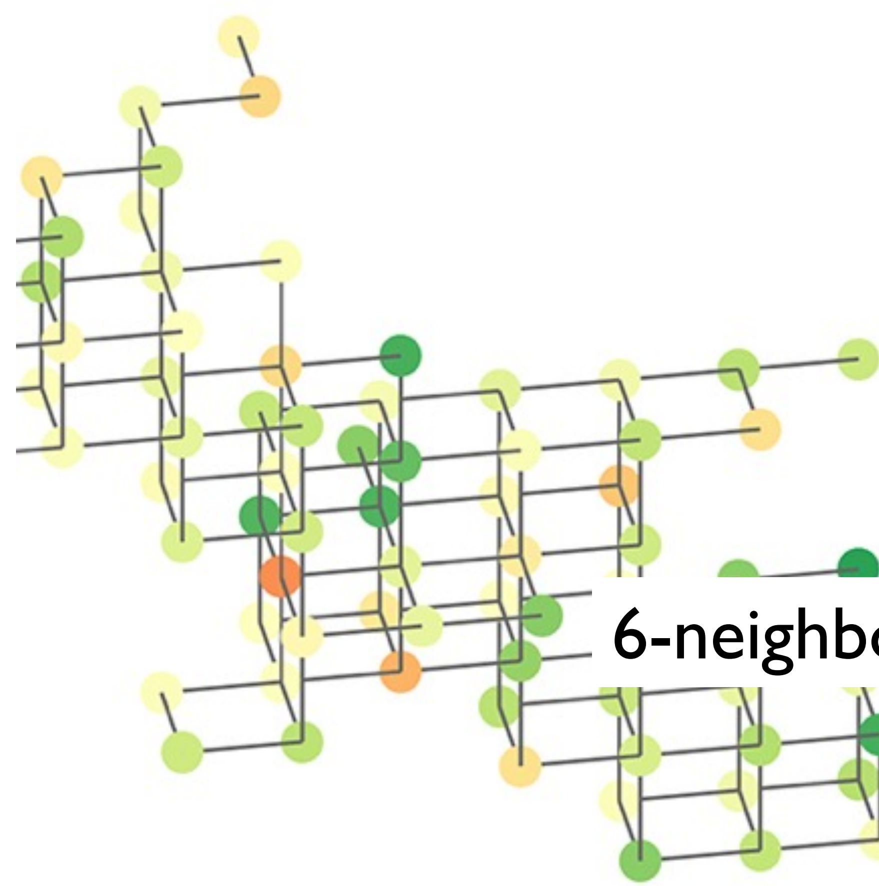
Left central gyrus



Lung blood vessel



4-neighbor connectivity



6-neighbor connectivity

Betti numbers β_i

of i-dimensional holes/loops

β_0 = # of connected components = 3

β_1 = # of cycles = 1

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

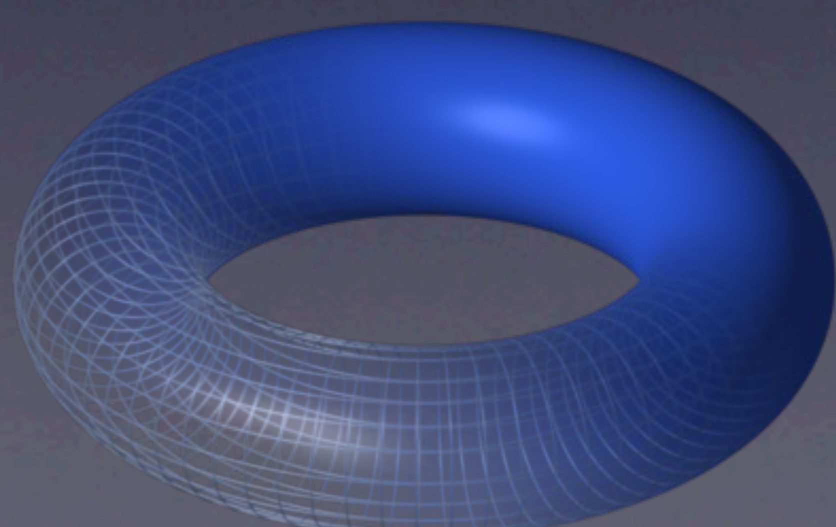
Betti numbers β_i # of i-dimensional holes/loops

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,...)

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

Morse Filtration

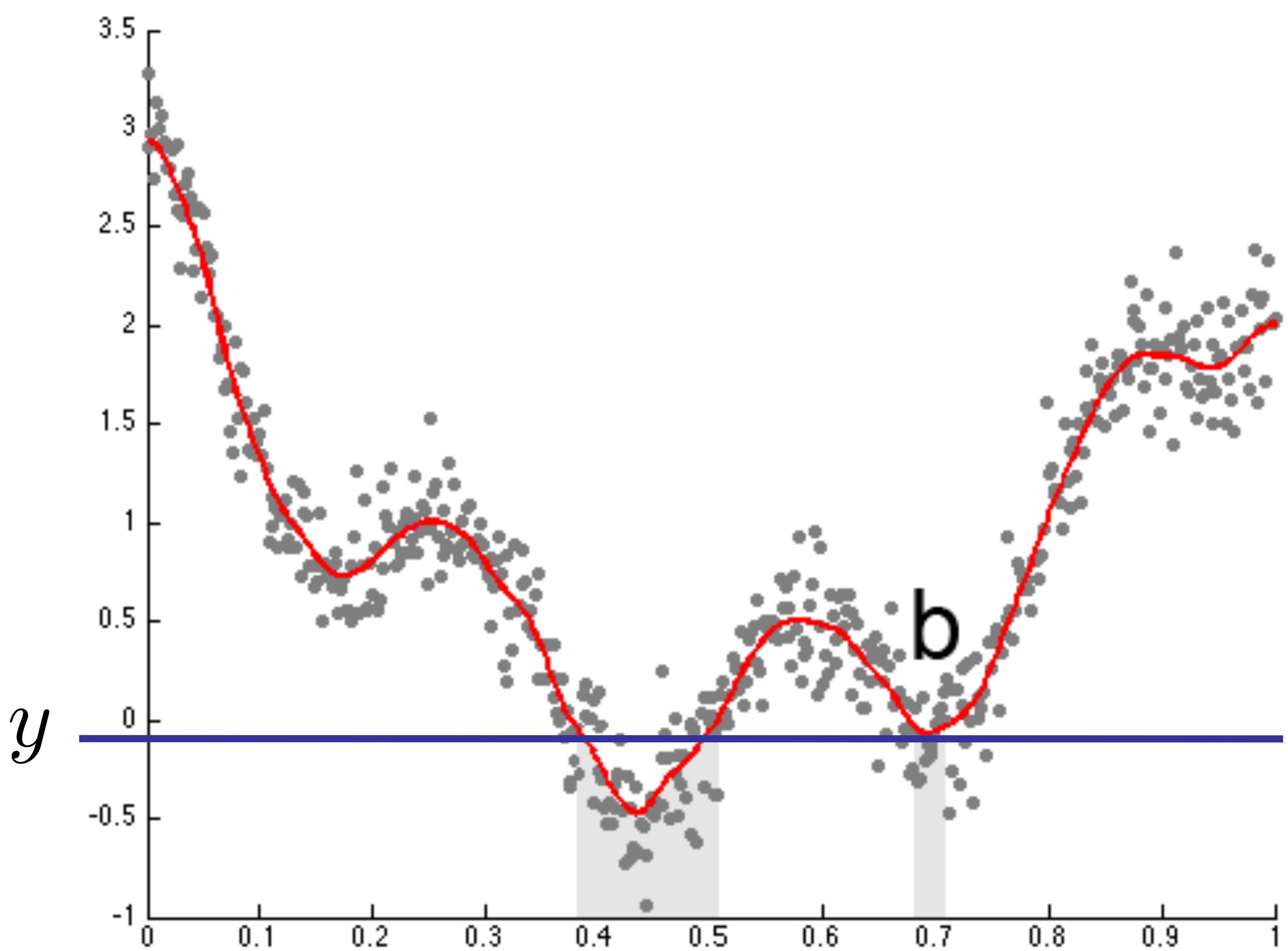
Most useful in functional and time series data

Morse theory for functional data

$$Y = \mu + \epsilon$$

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

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

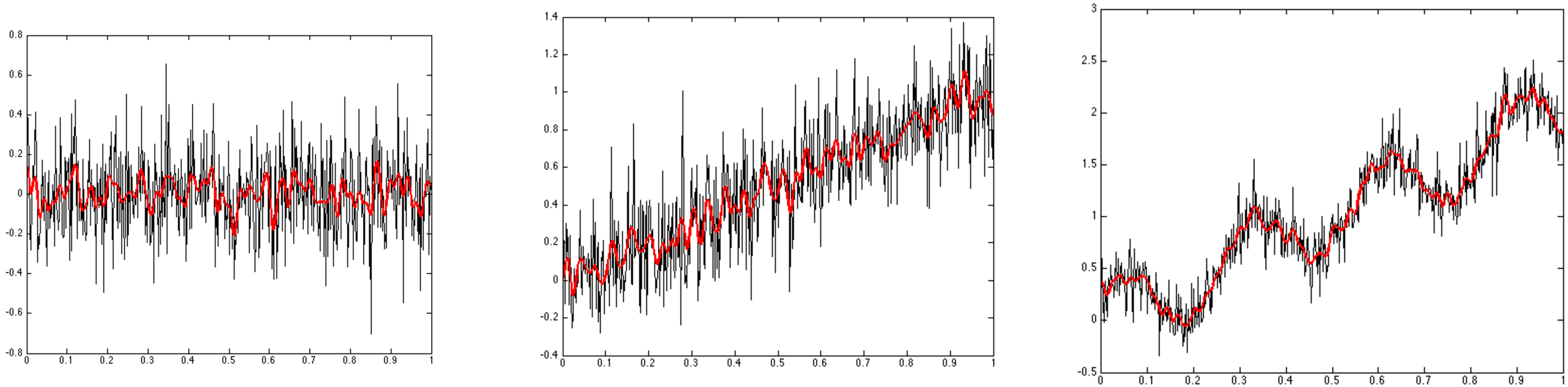


Sublevel set

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

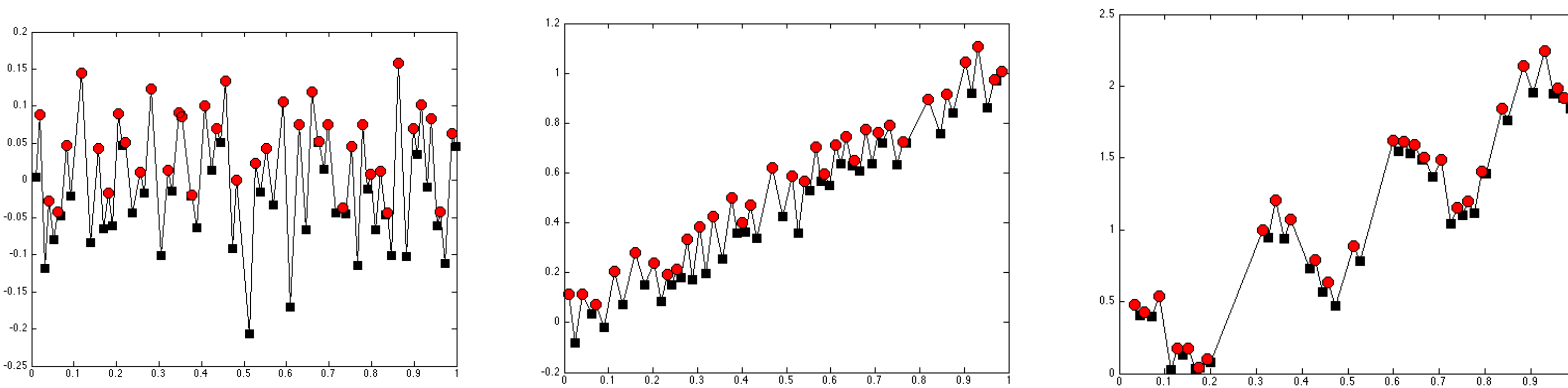
Number of connected components $\#R(y)$

Critical values capture the pattern of signal changes



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

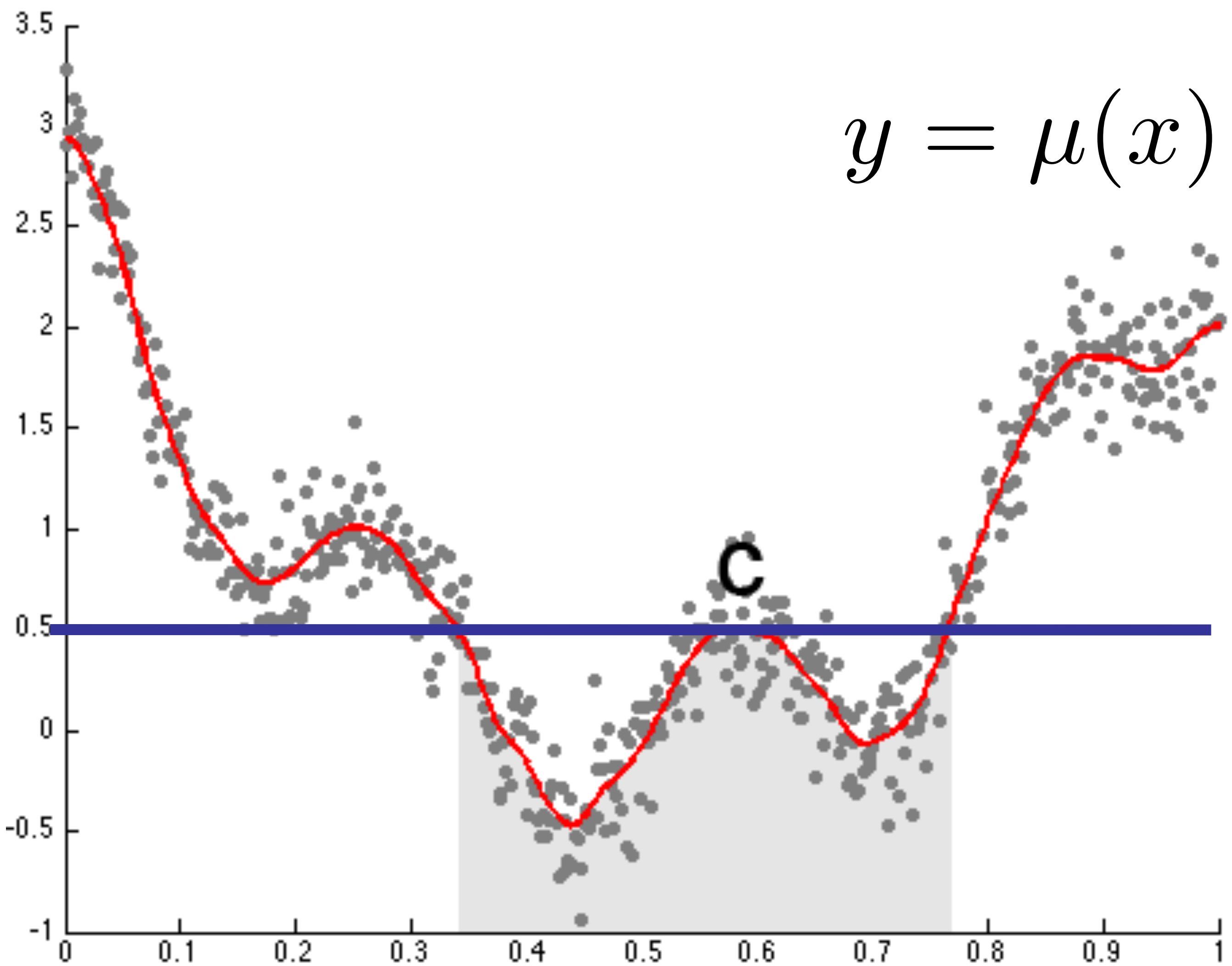
$$f(t) = t + e(t)$$



Morse filtration

Consider a sublevel set

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



For critical values

$$b < c$$

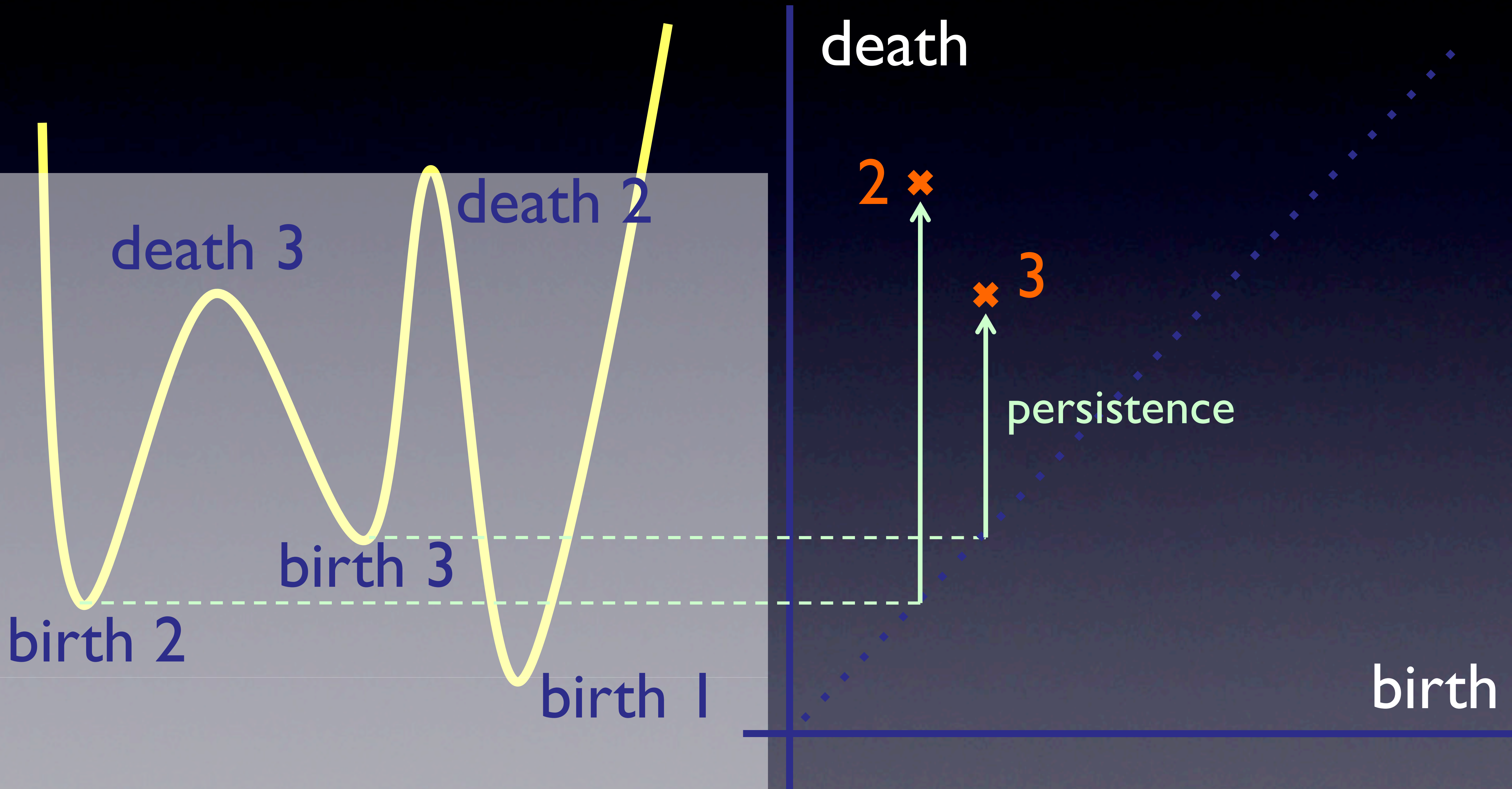
$$R(b) \subset R(c)$$

# 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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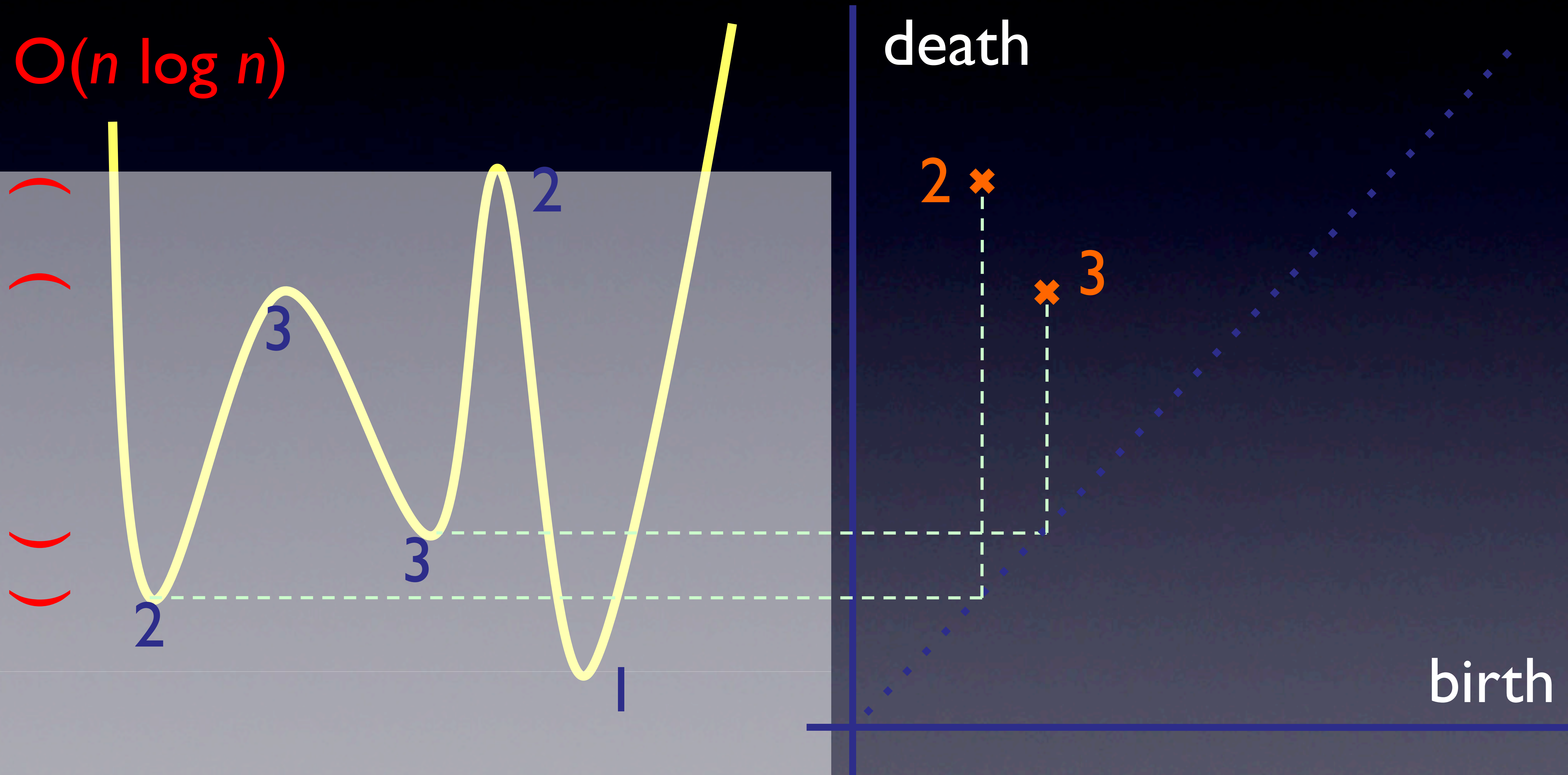
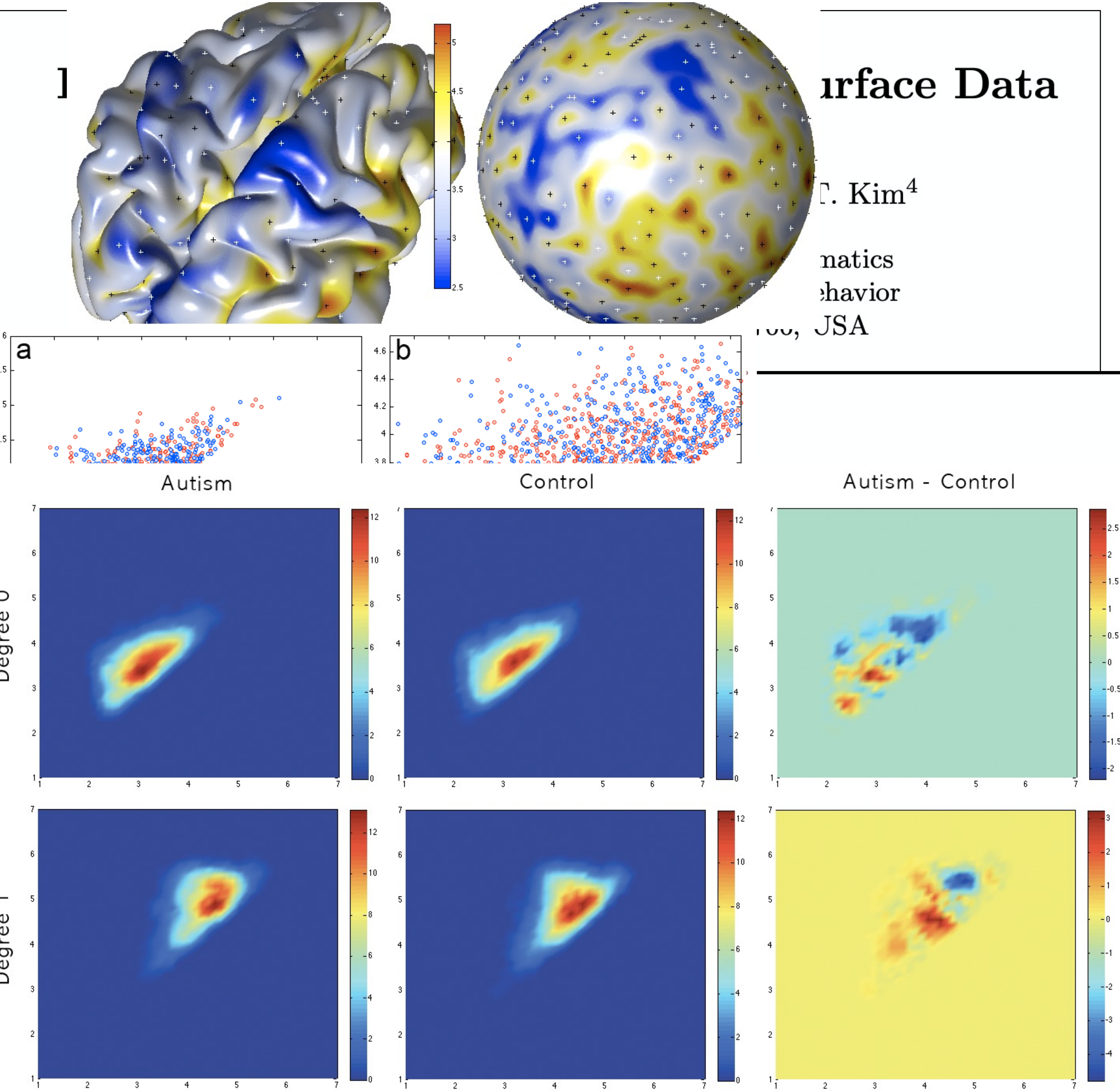
Persistence Diagram (PD)



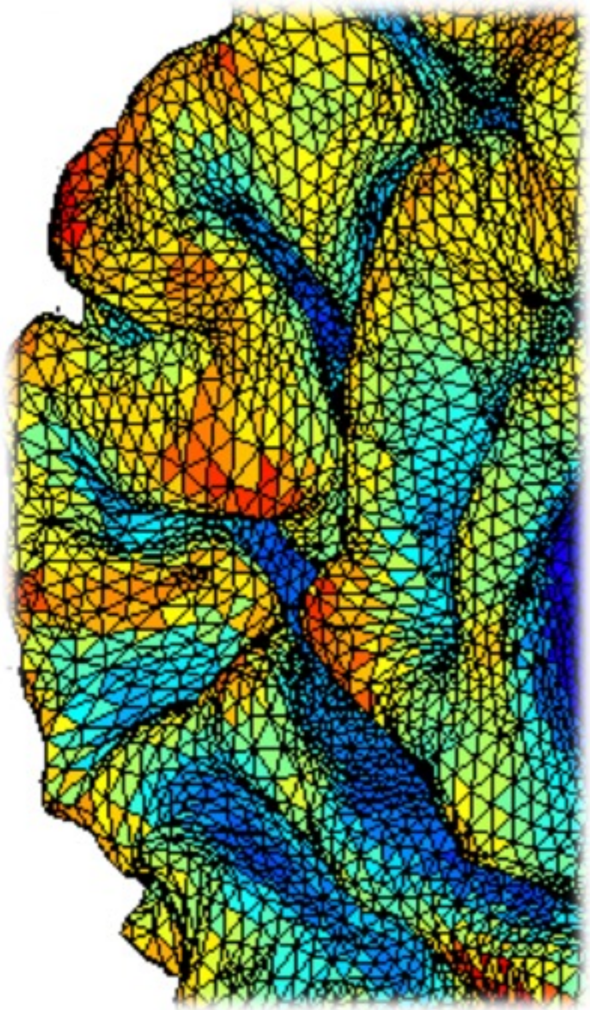
Pair the time of death with the time of the closest earlier birth

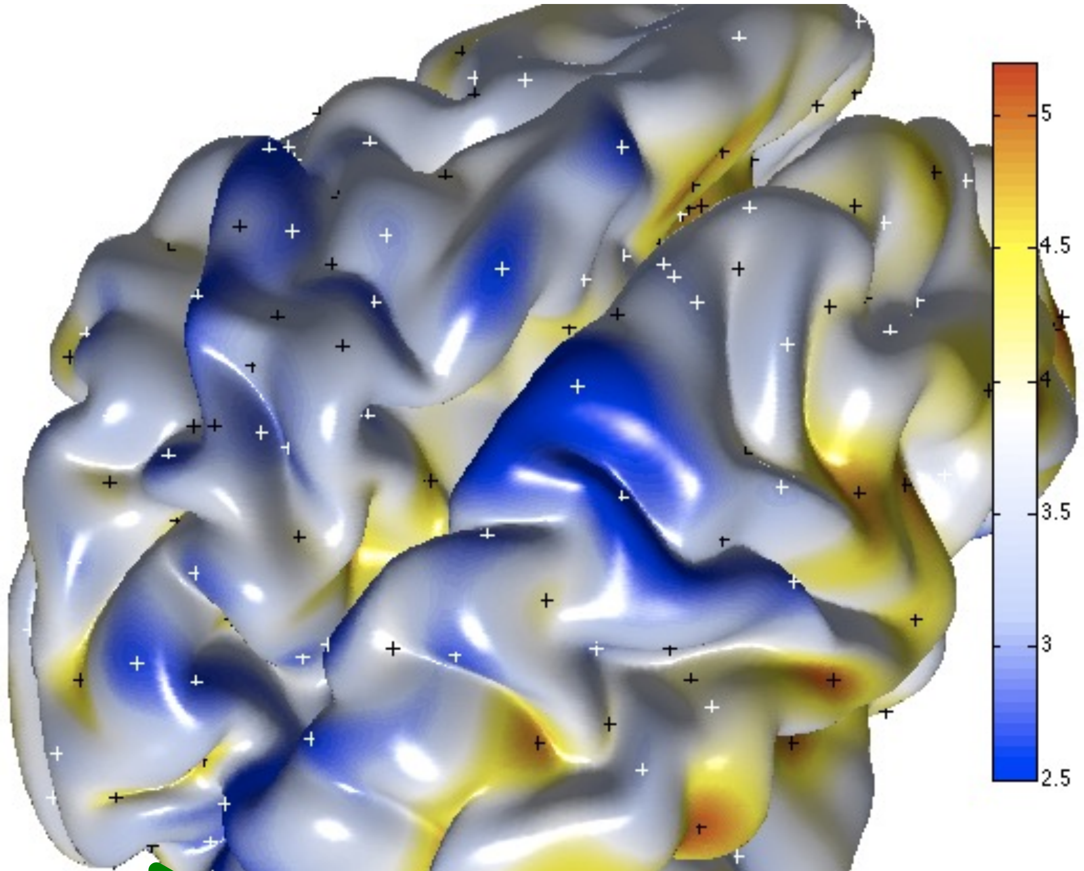


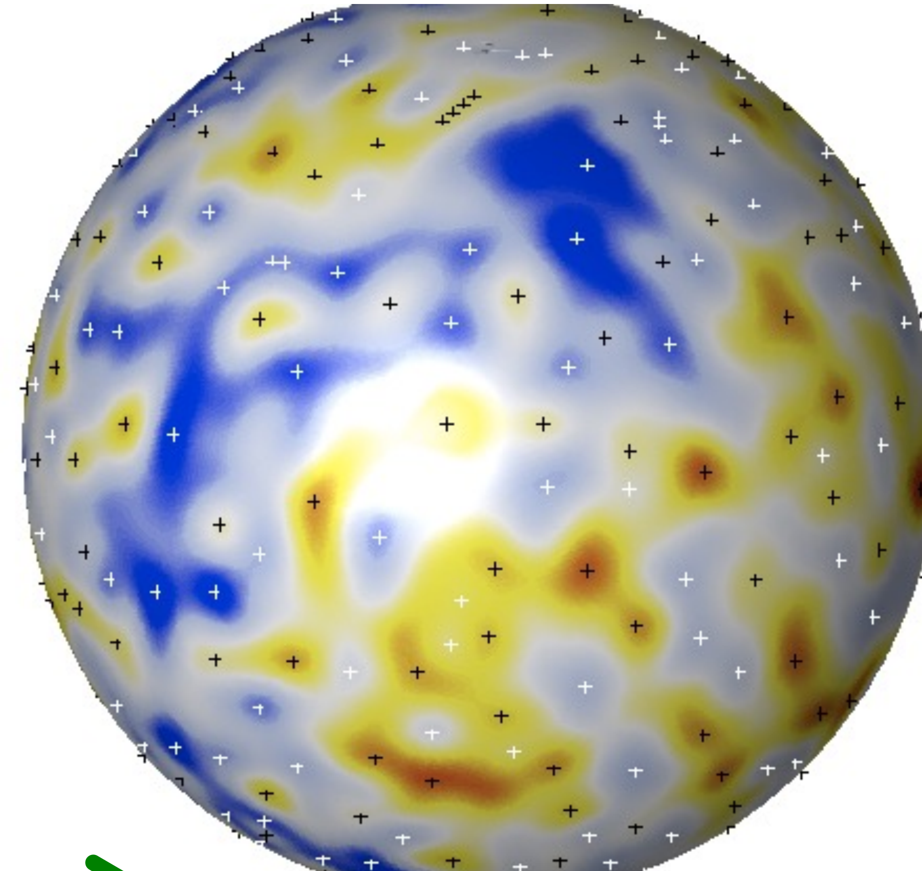
Chung et al., 2009
Information Processing in Medical Imaging (IPMI) 5636:386-397.

First persistent homology study applied to medical imaging

Persistent homology on cortical manifolds



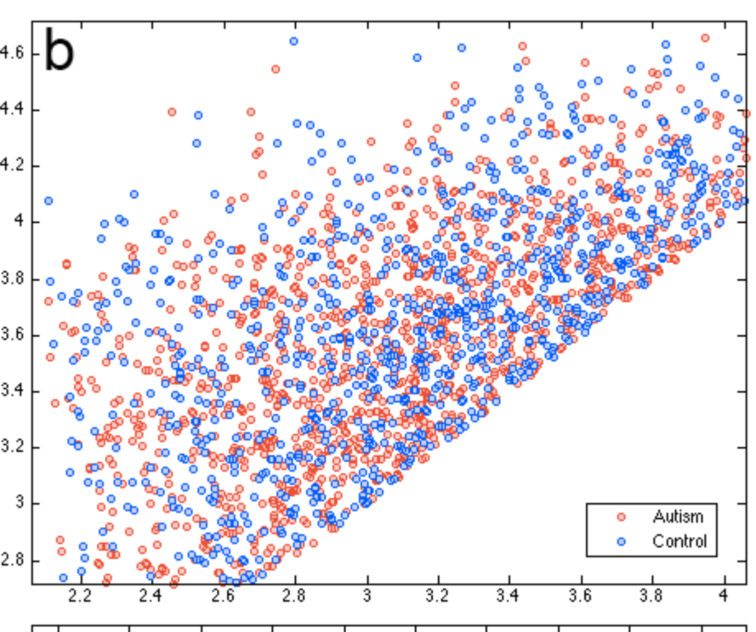




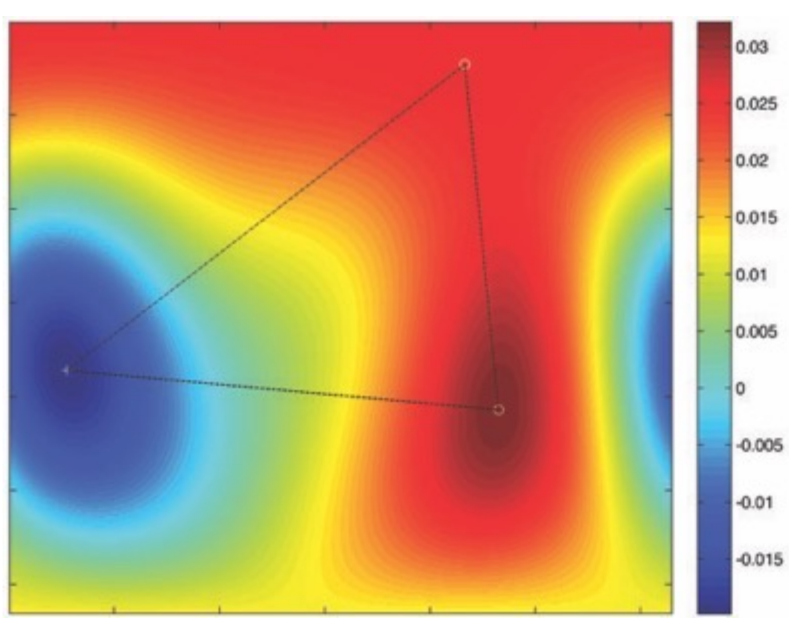
Heat kernel smoothing

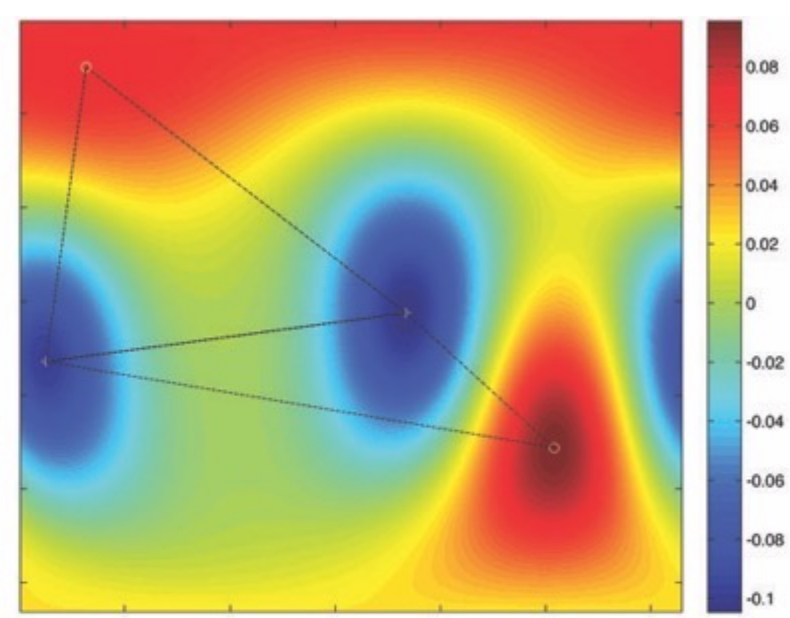
Flattening

(Delaunay) Triangulation



PD

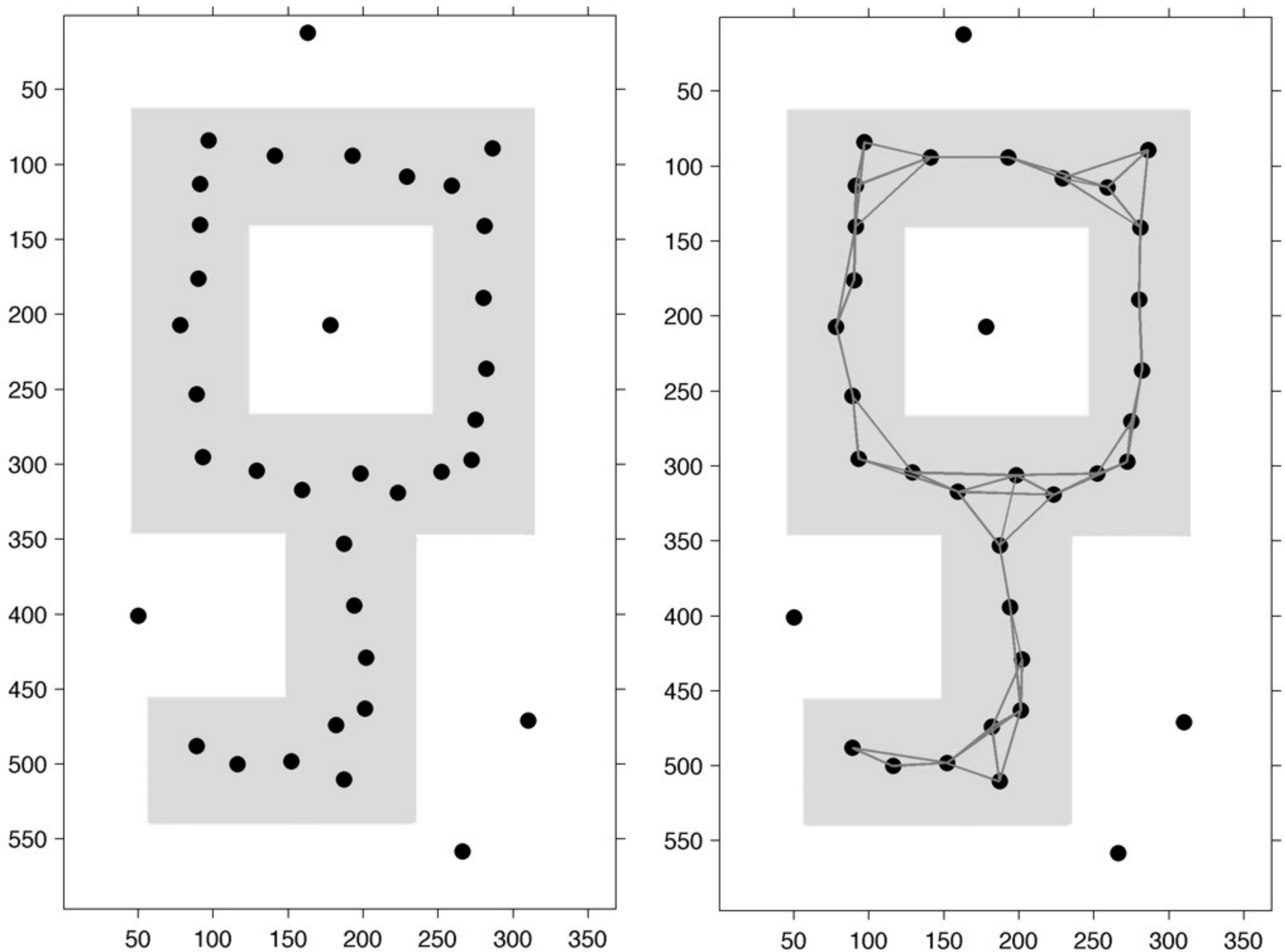




Rips filtrations

1-skeleton of point cloud data

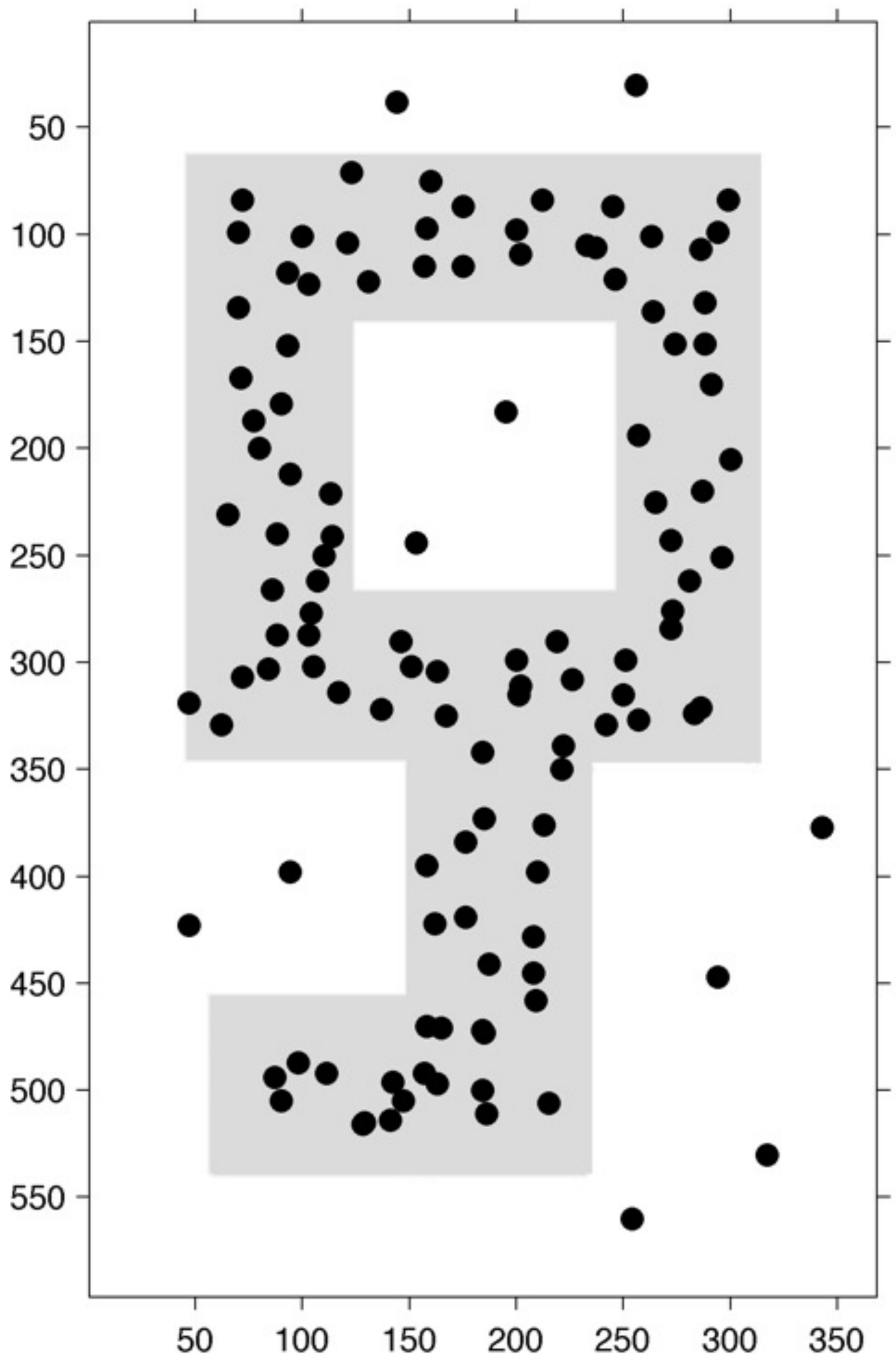
ε = 70mm

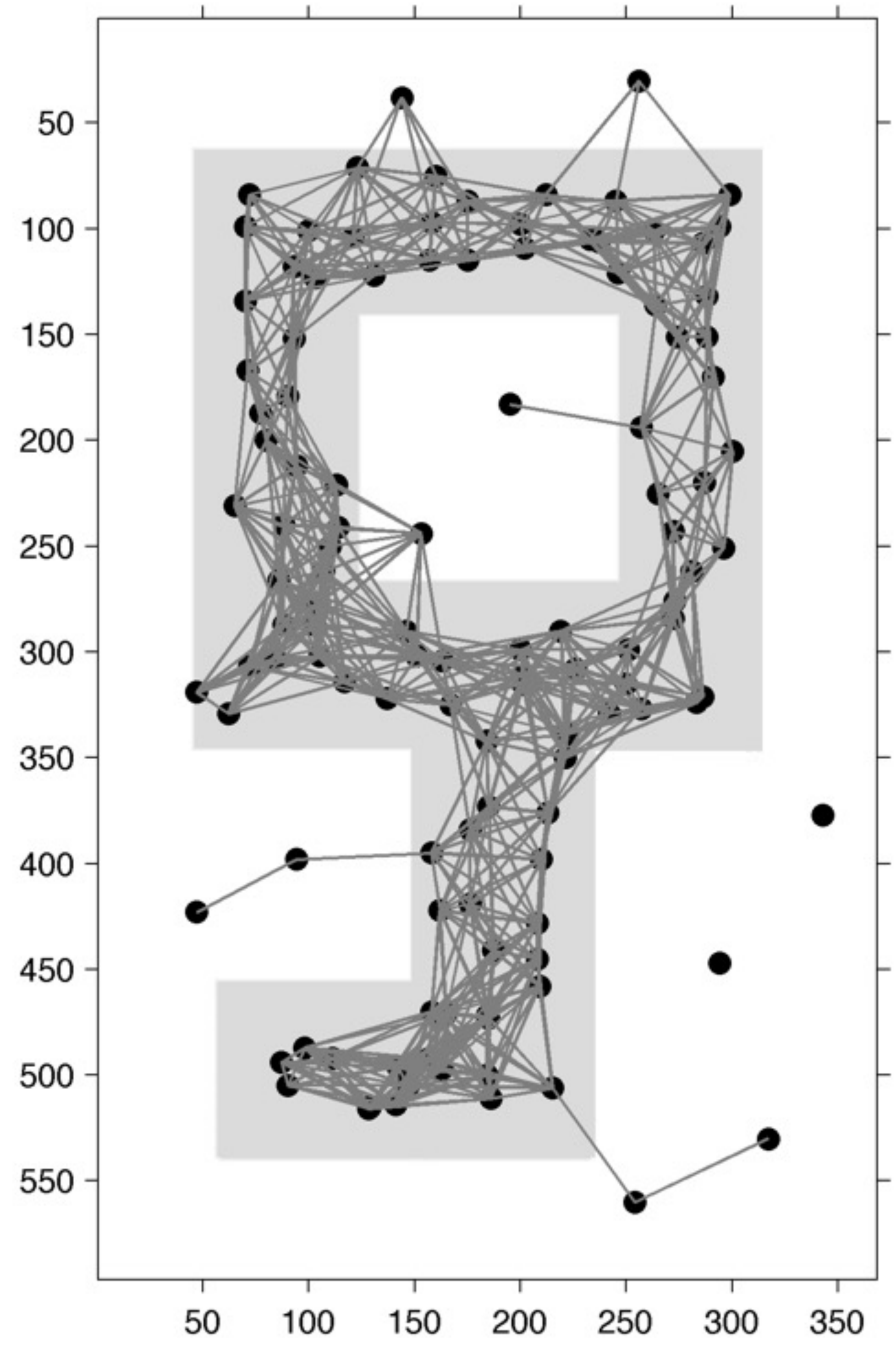


Recovering underlying topology

1-skeleton of point cloud data

ε = 70mm

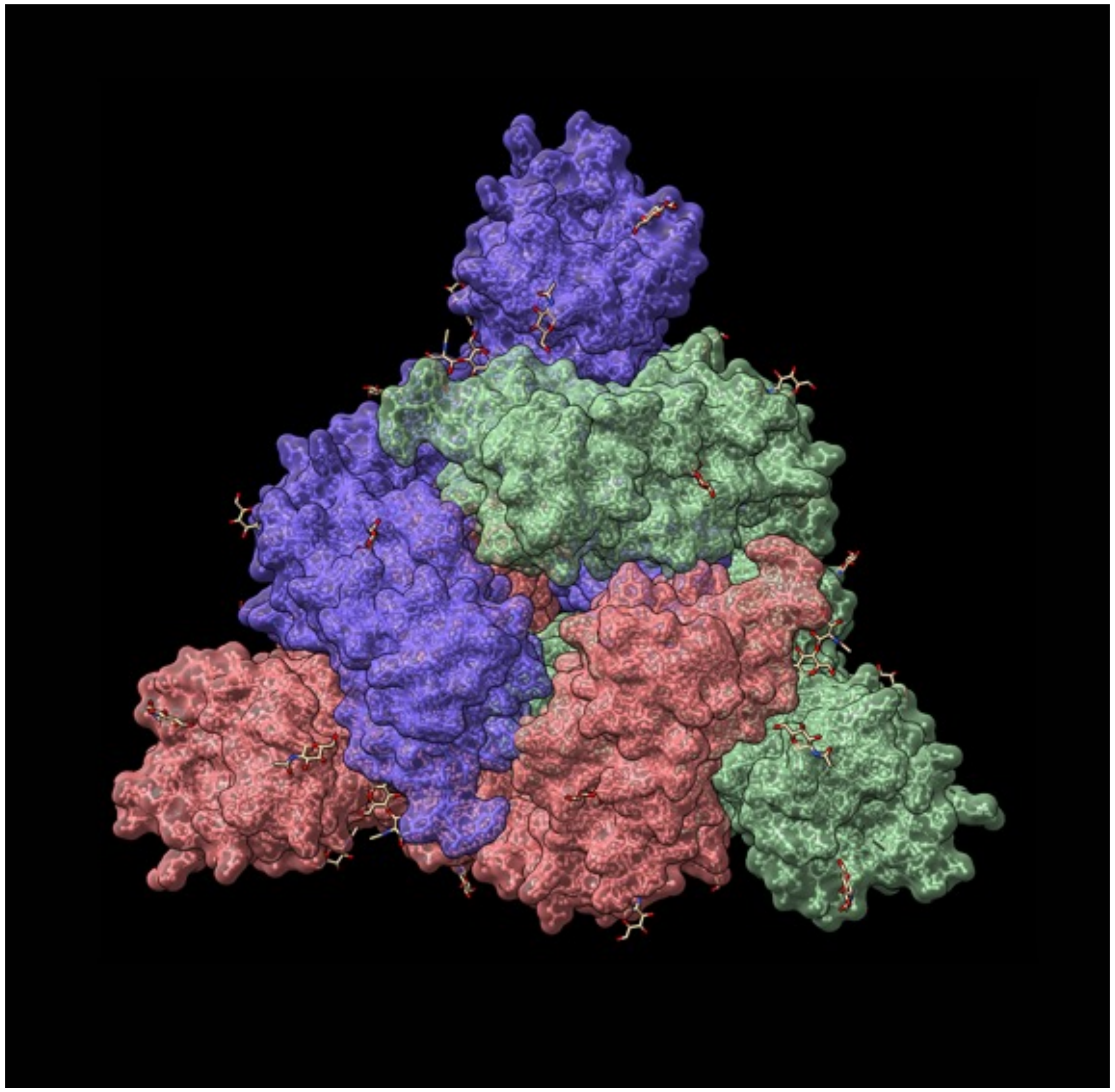


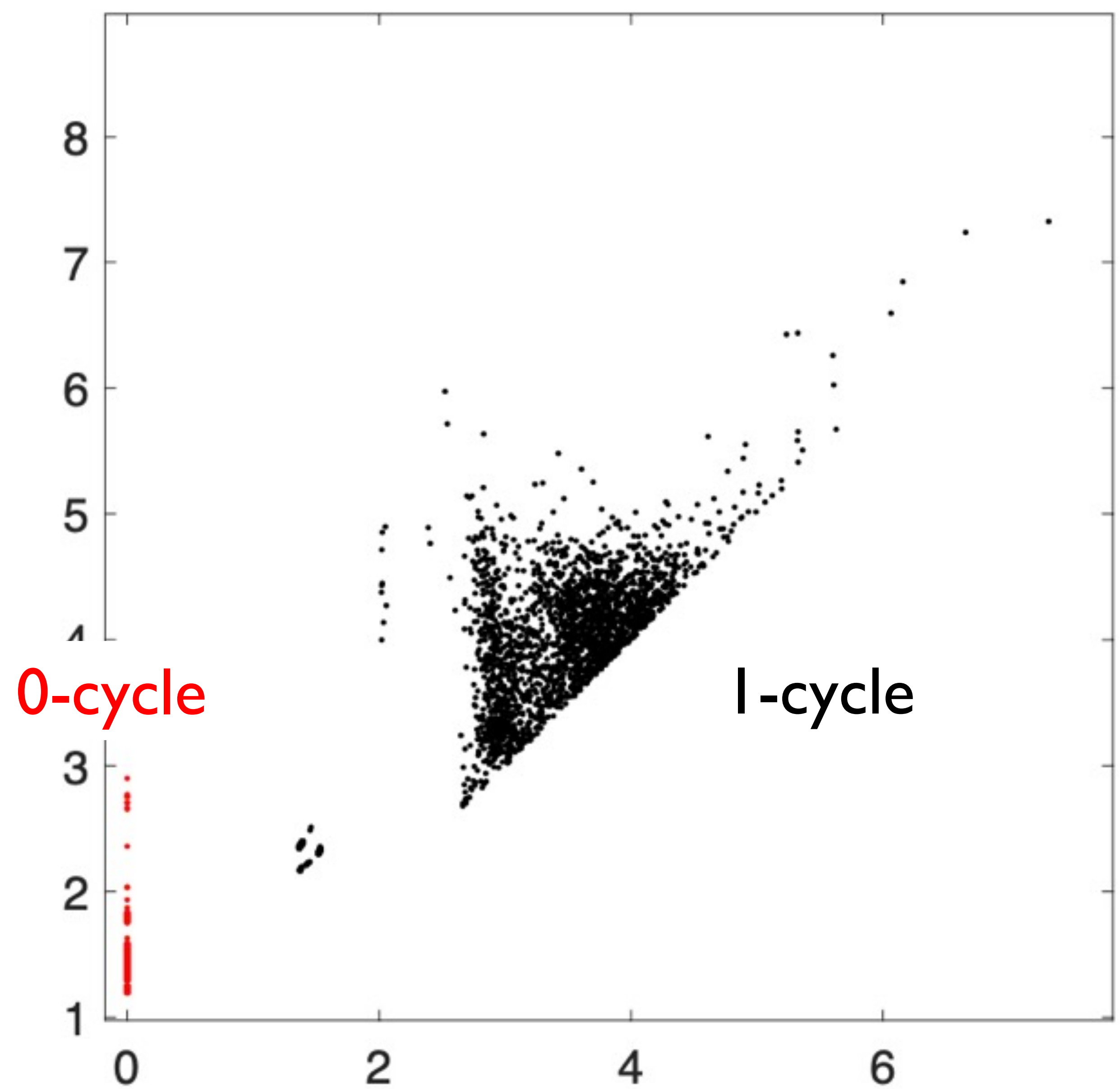


Better approach: perform kernel smoothing and then Morse filtration

Persistence Diagram (PD) of a protein molecule

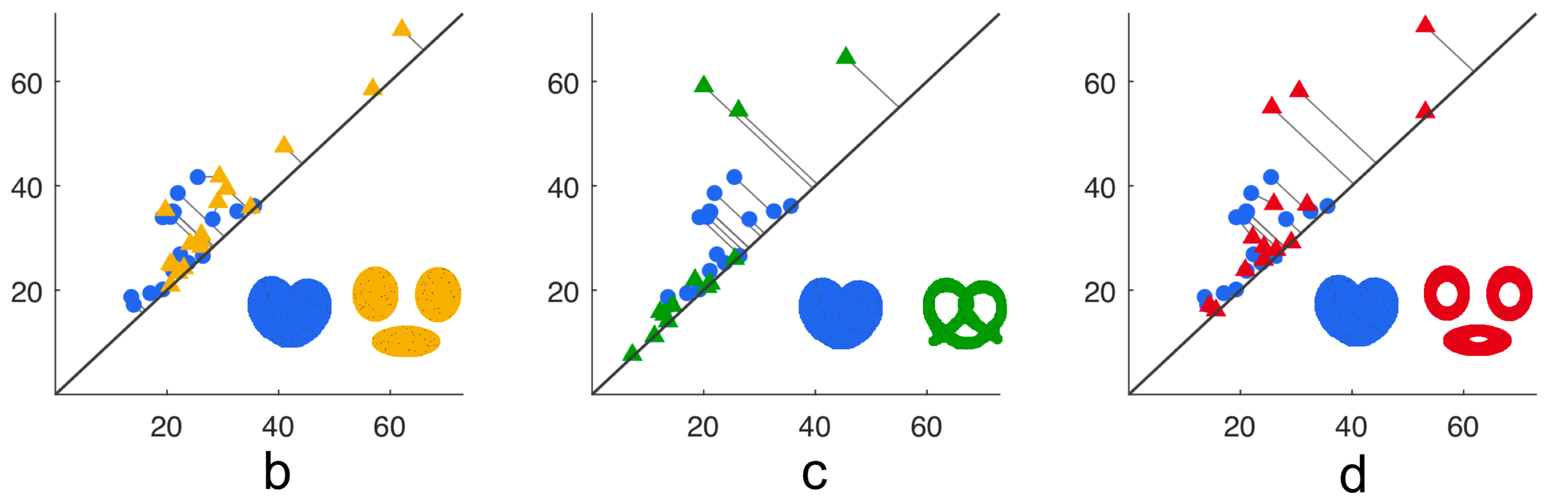
Rips filtration on distance between 8000 atoms



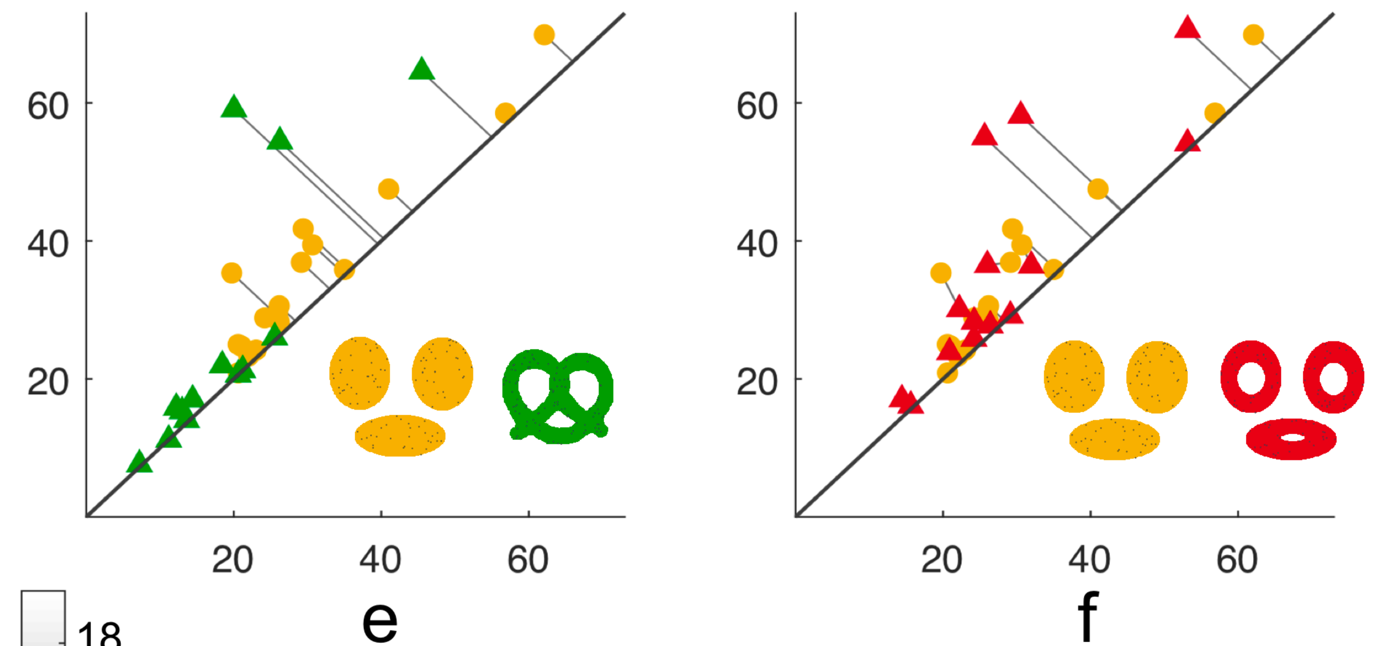


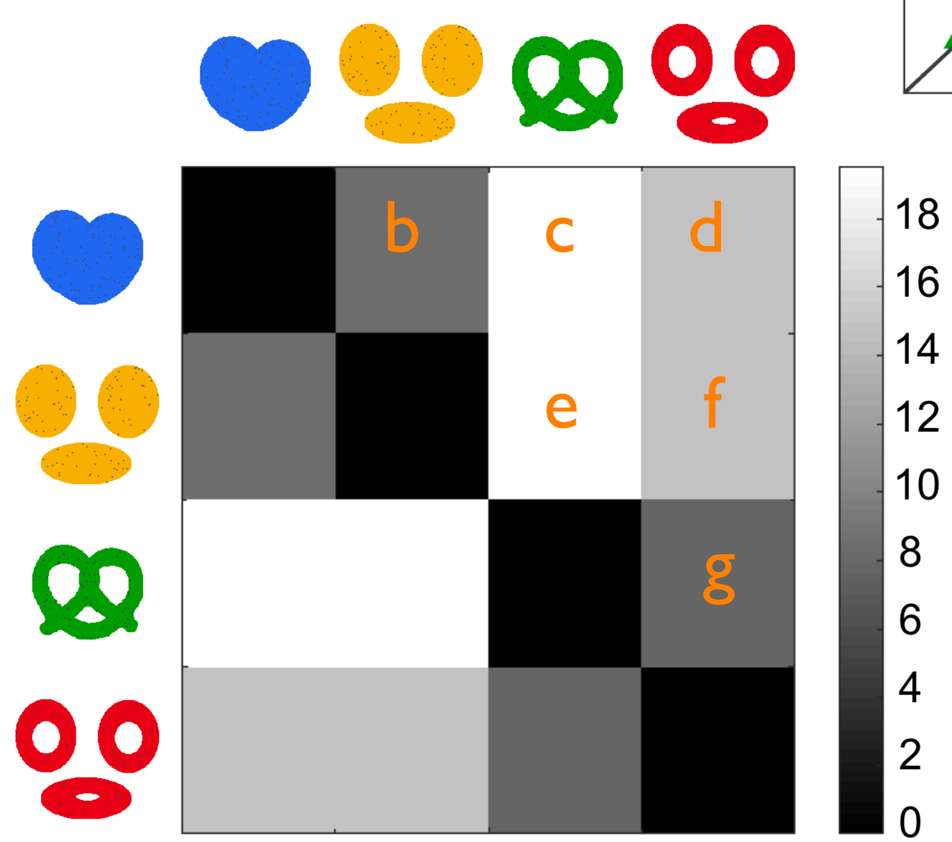
Extremely slow computation → Simply use graph filtration

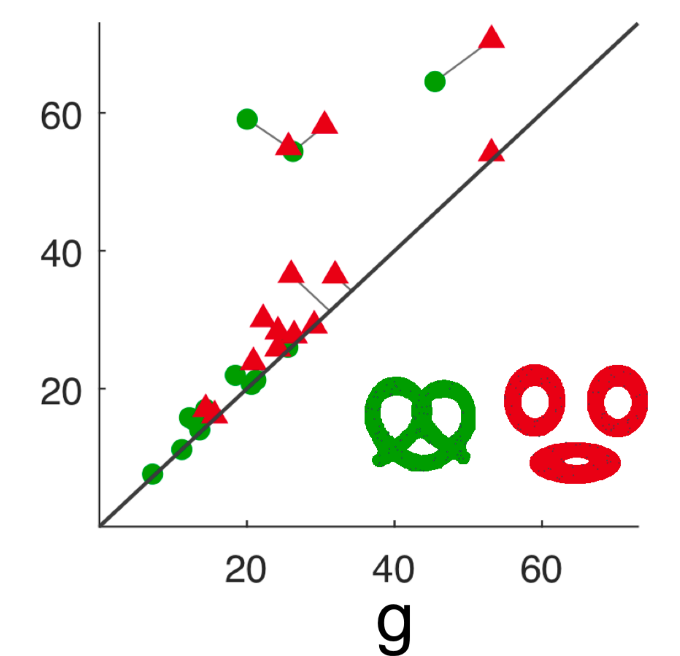
Bottleneck distance



For definition, simply read the assigned reading PDF



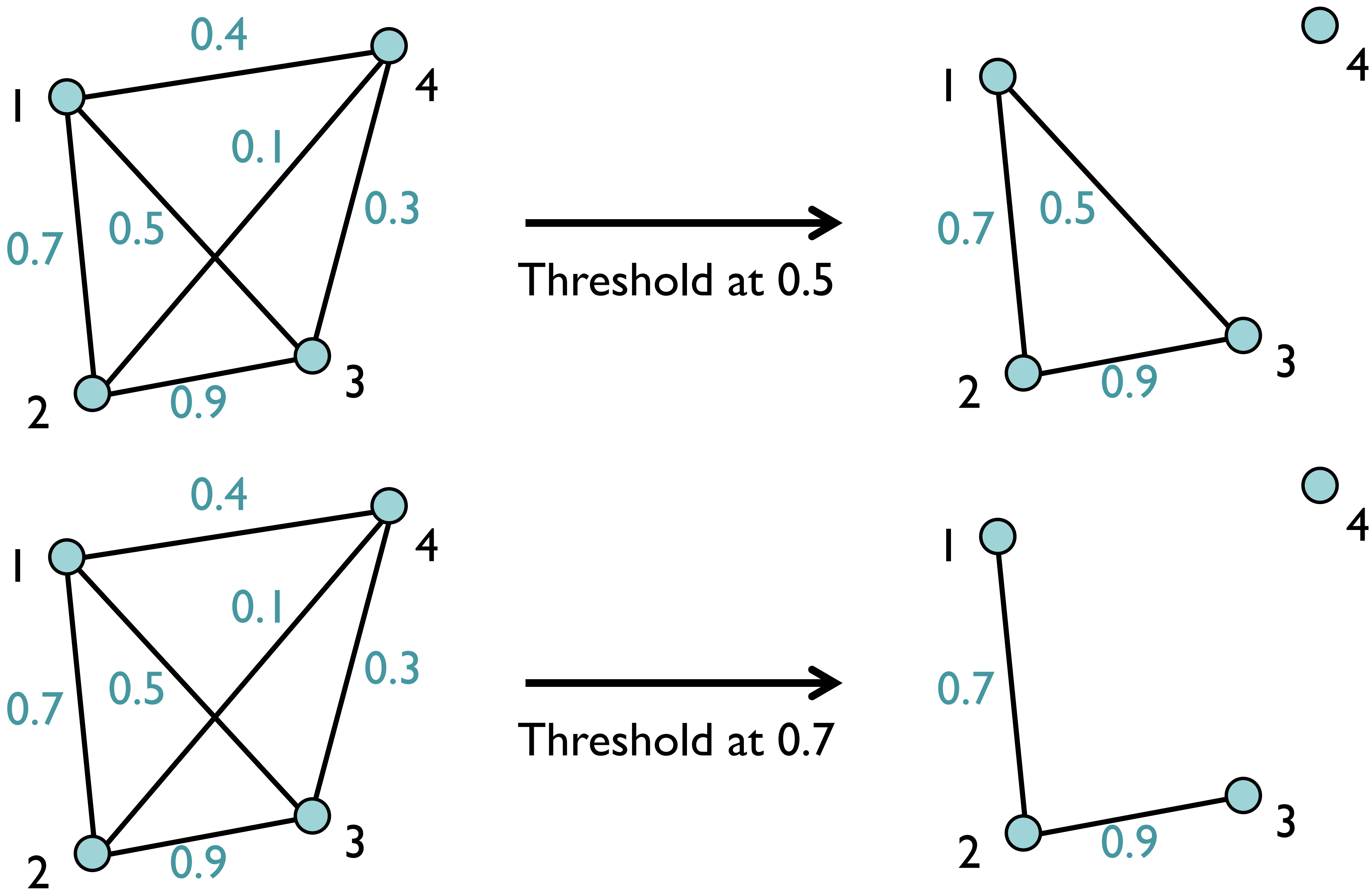




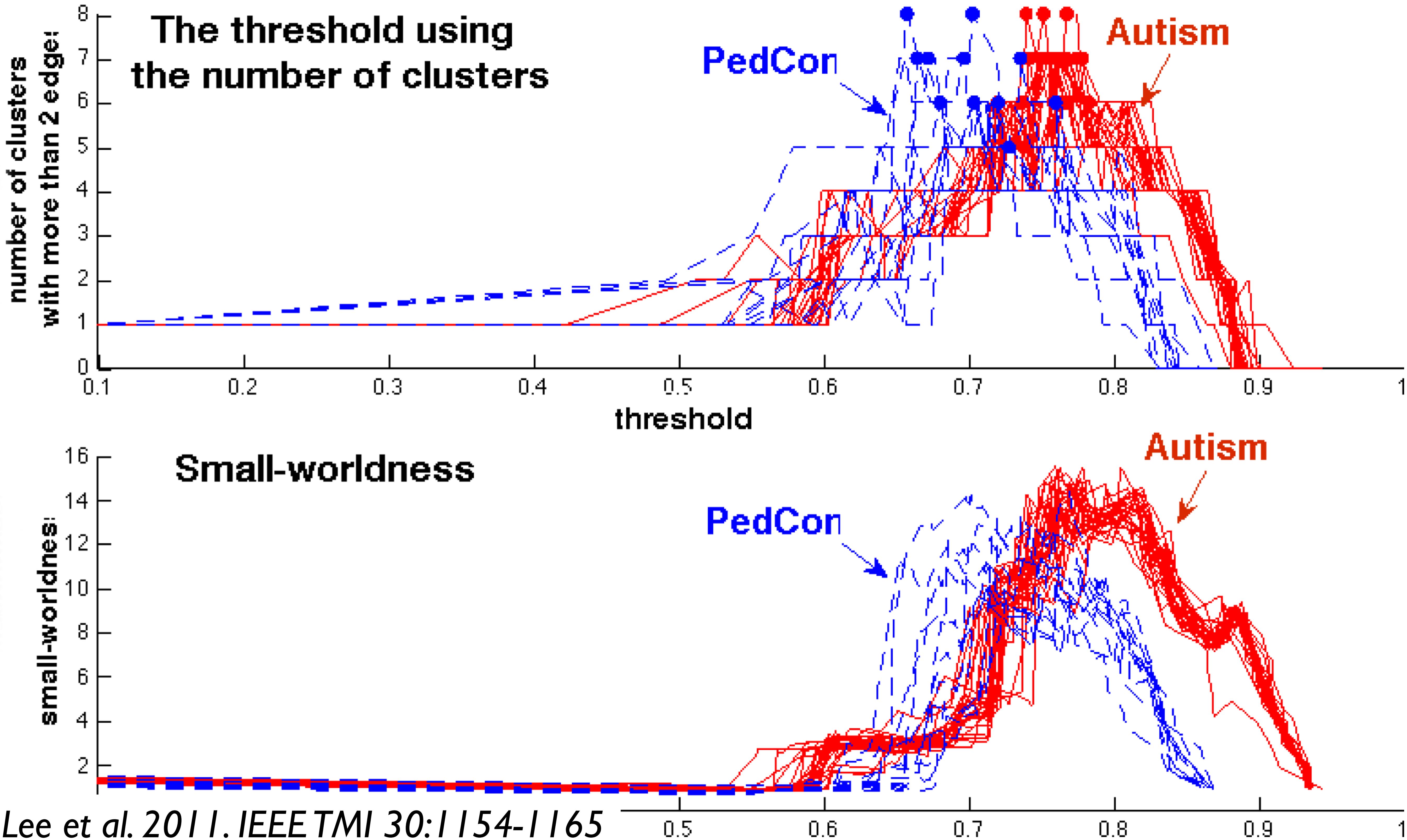
What is wrong with the arbitrary thresholding?

Edge weight ρ_{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

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

Weighted graph

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

Node set — Edge weight

Rips complex = Simplicial complex

Binary graph: 1-skeleton

Rips filtration

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

for increased radius

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

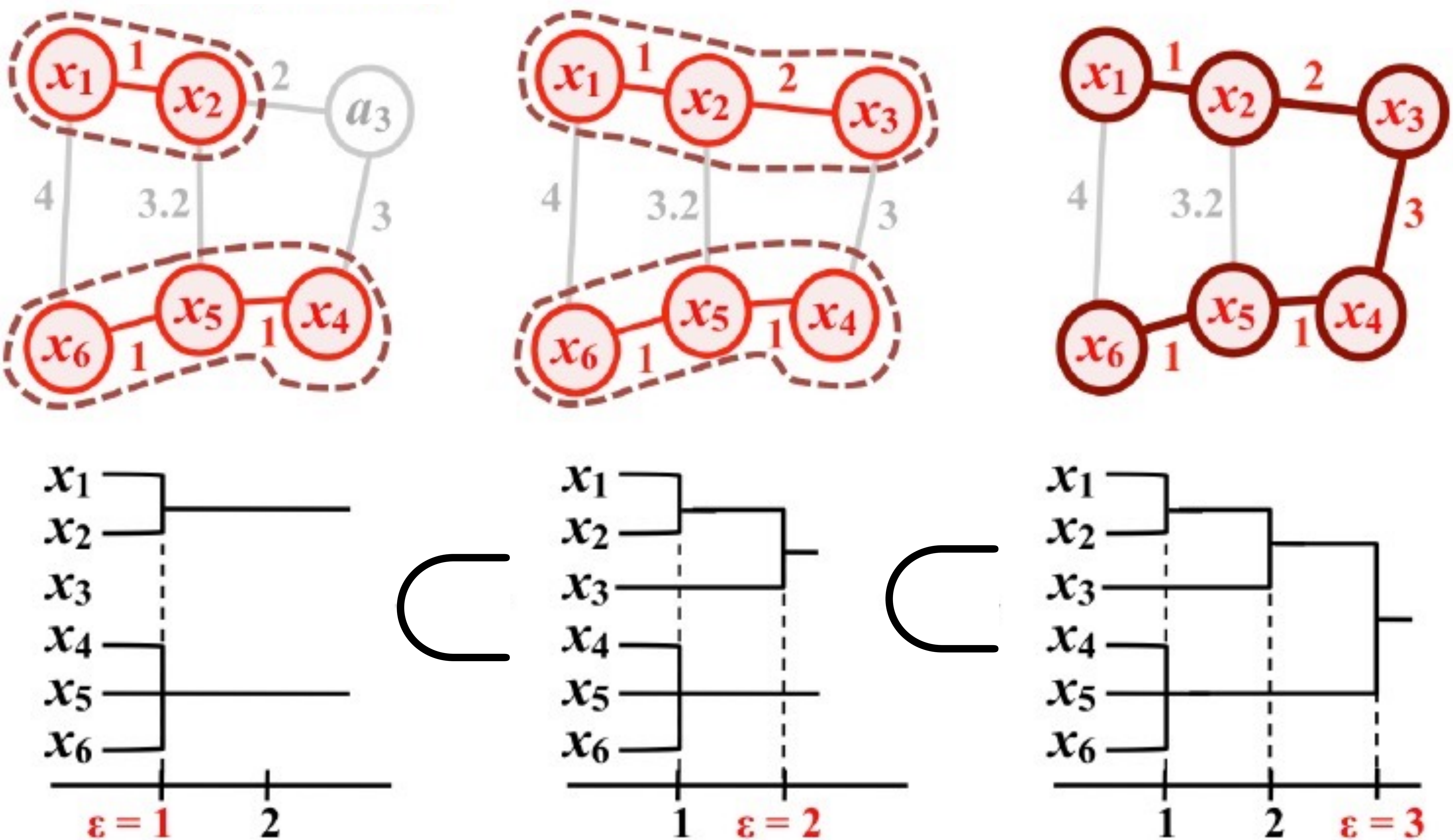
Graph filtration

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

for increased edge weights

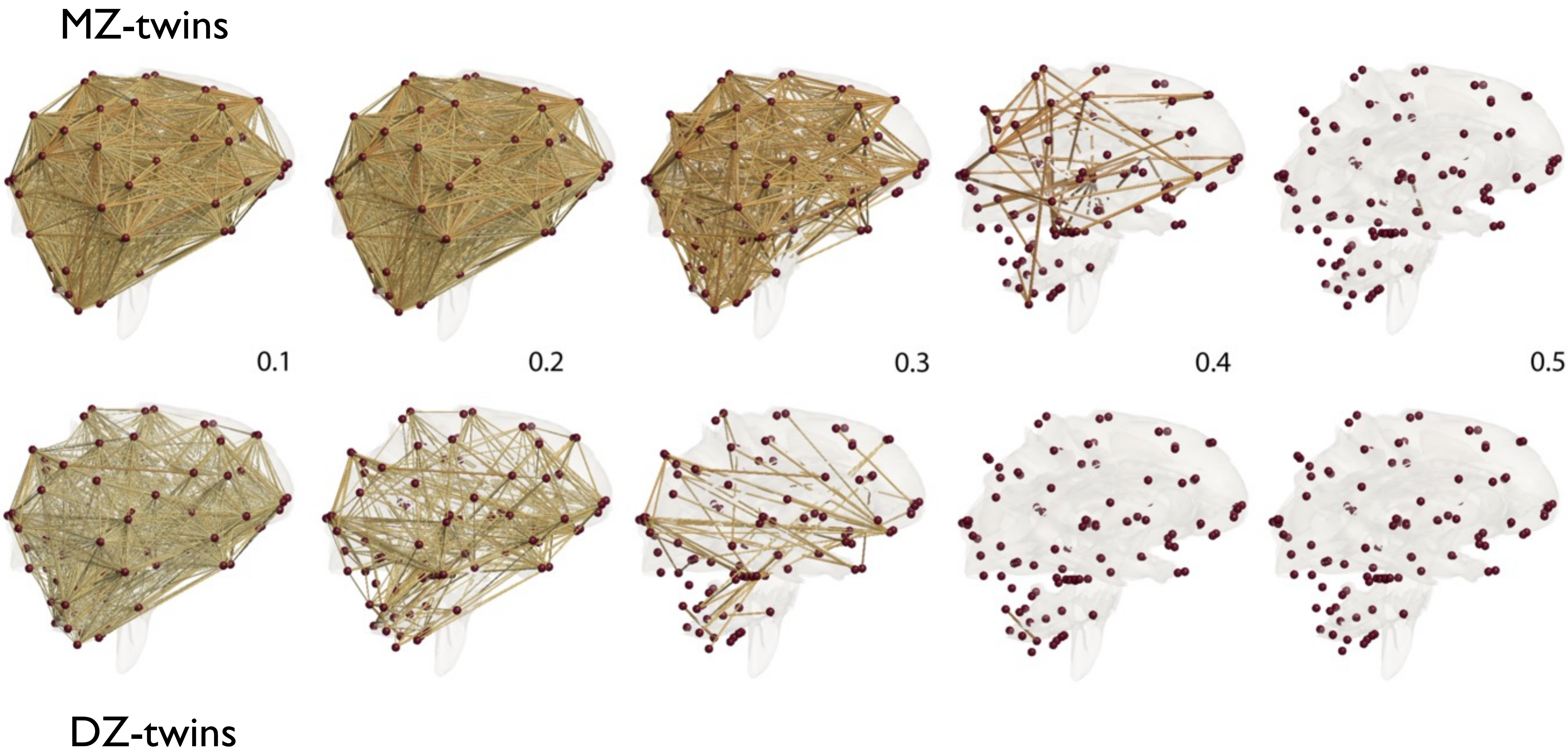
$$\epsilon_0 < \epsilon_1 < \epsilon_2 < \cdots$$

Graph filtration=single linkage clustering



<u>*Lee et al. 2011 MICCAI 302-309*</u>

Graph filtrations on resting-state fMRI

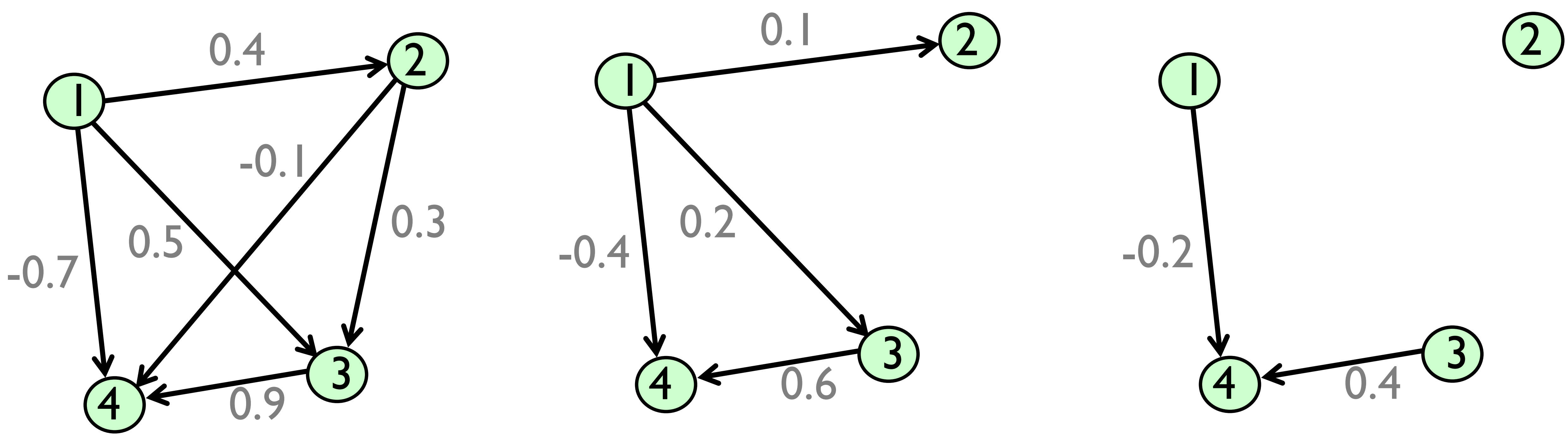


Graph filtration (filtration on 1-skeleton)

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.

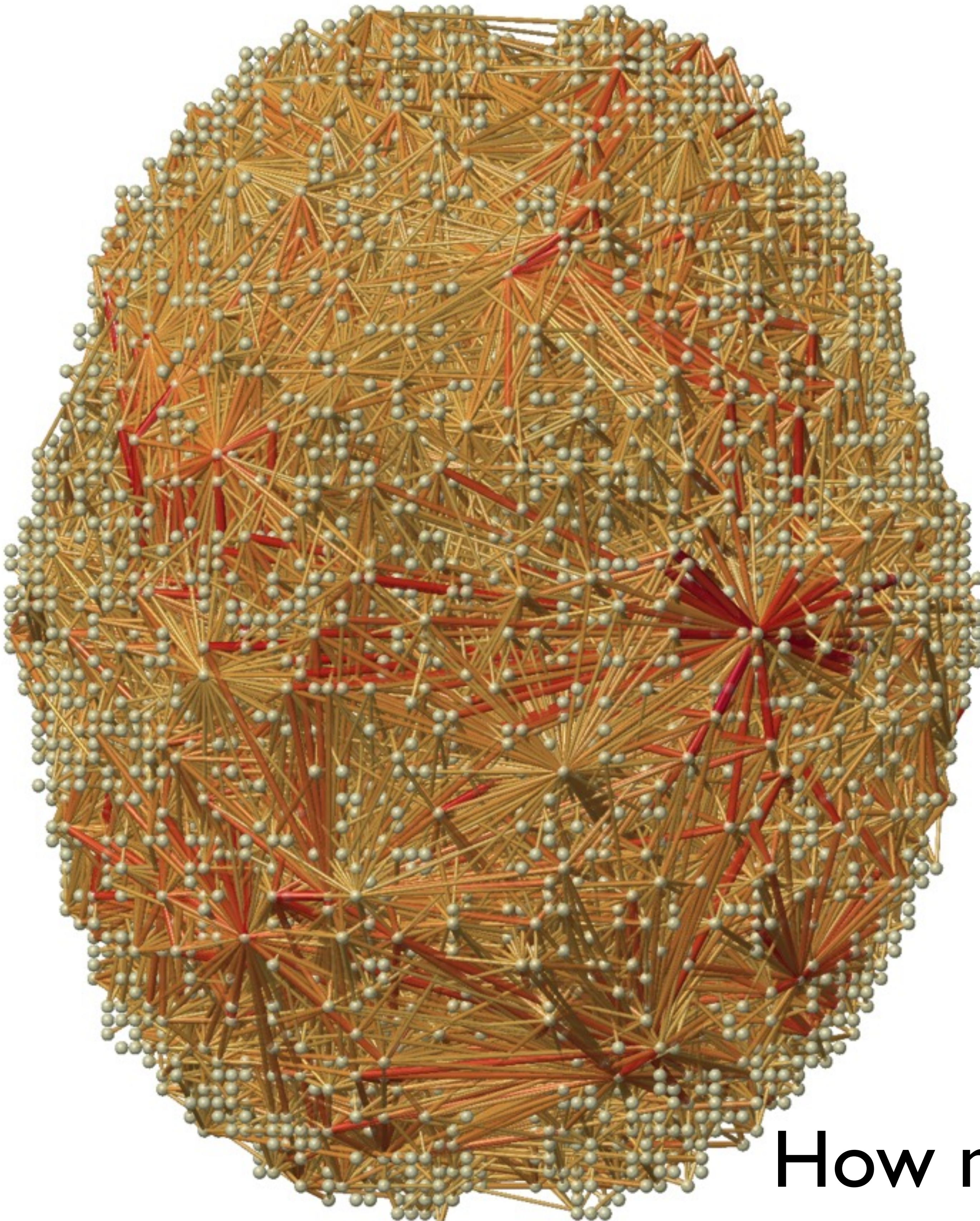
Graph filtration on directed graphs

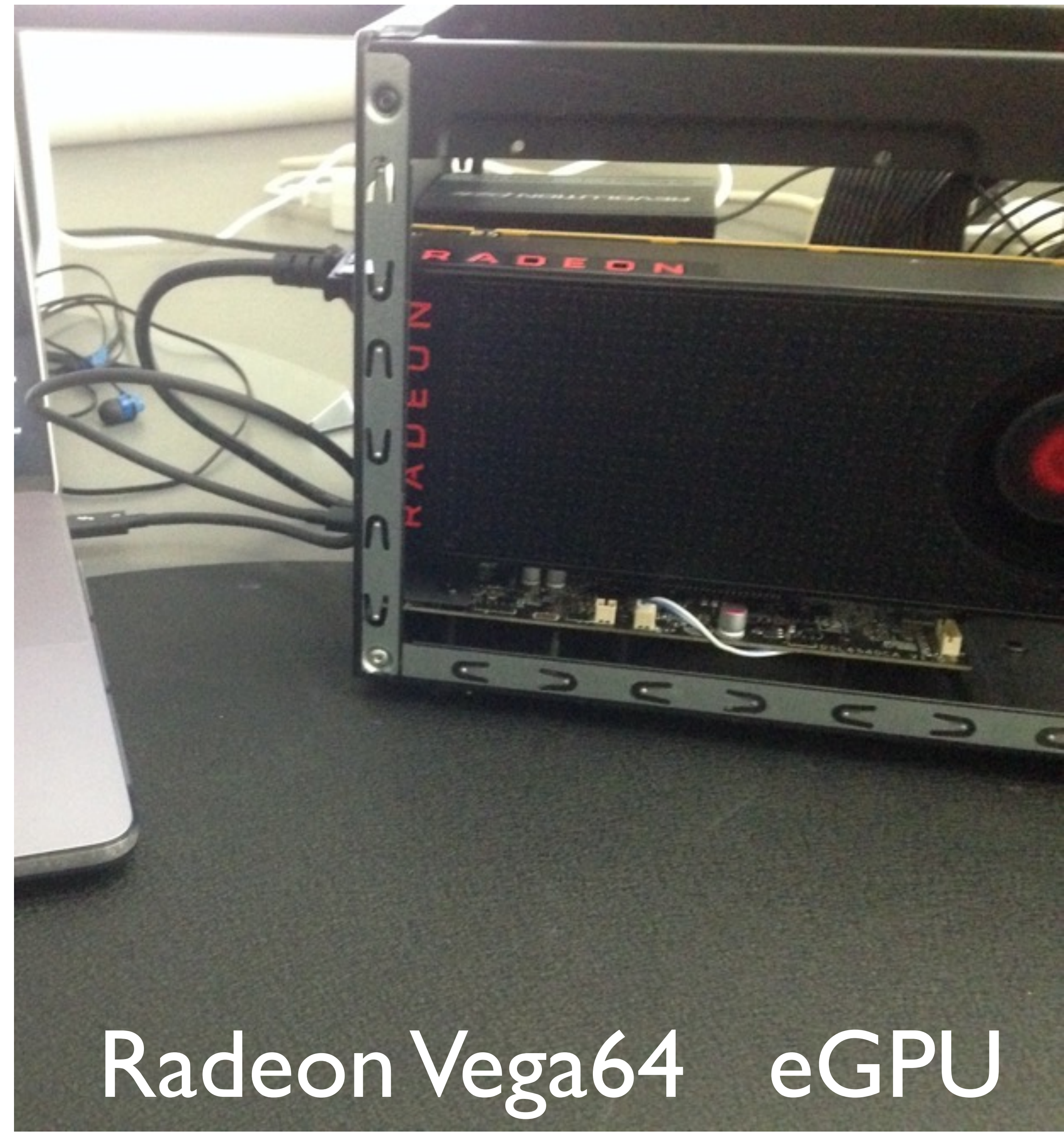


$$G(0) \supset G(0.3) \supset G(0.5)$$

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?

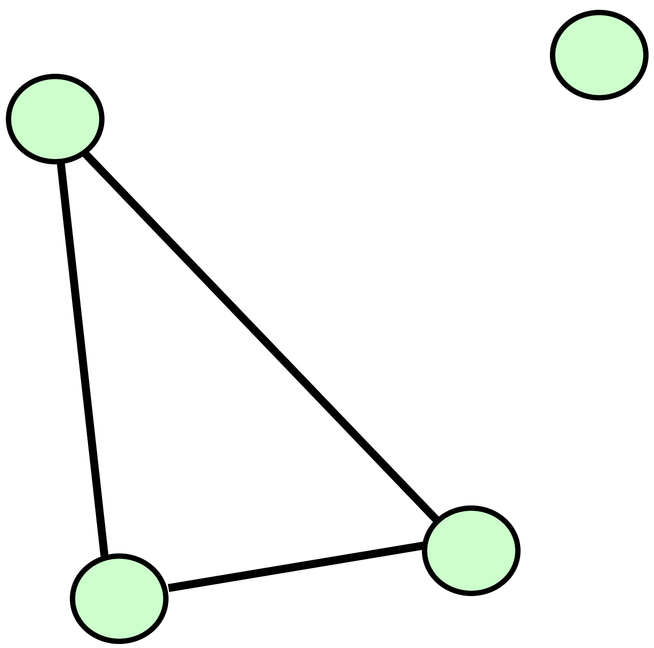
Betti numbers

Monotonicity of Betti-0 plot

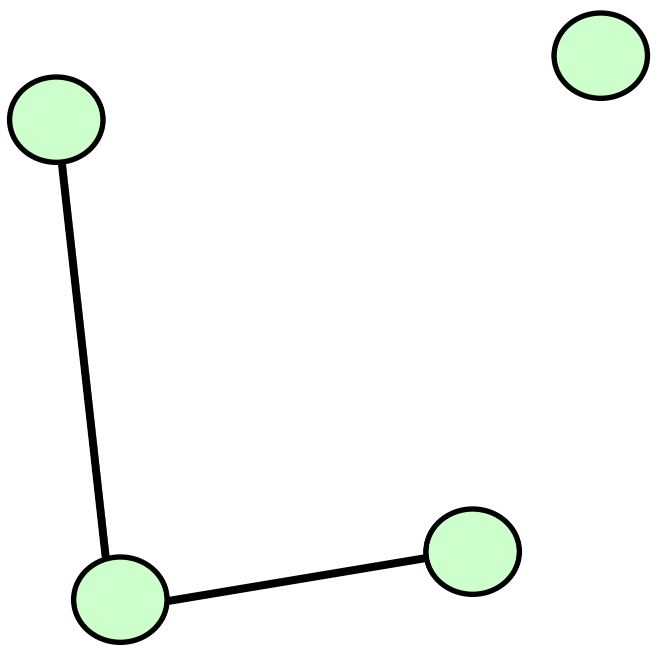
Monotonicity of β_0

The deletion of edge increases the the number of connected components by at most 1.
β_0 increases by 0 or 1.

Case 1

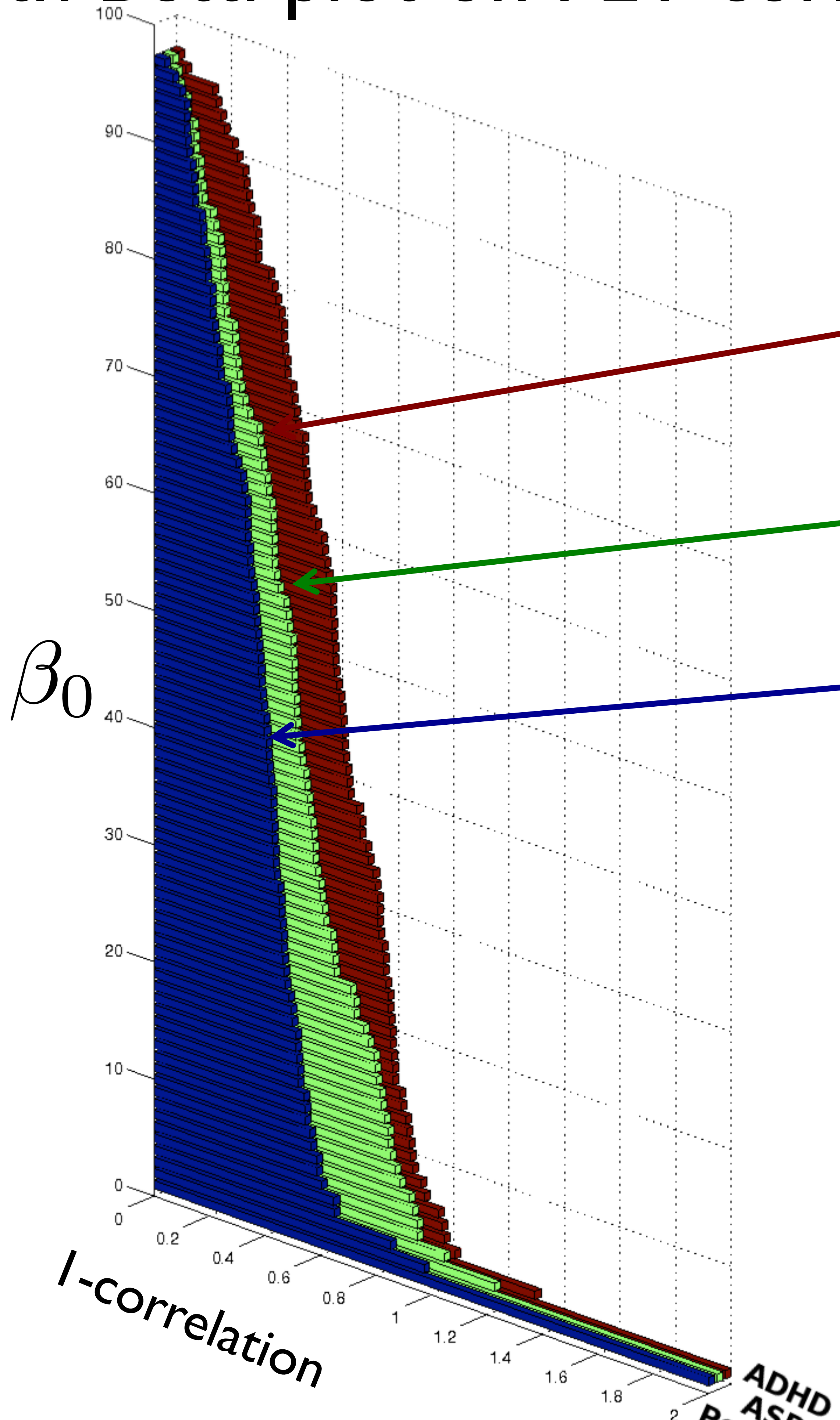


Case 2



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 β_1:

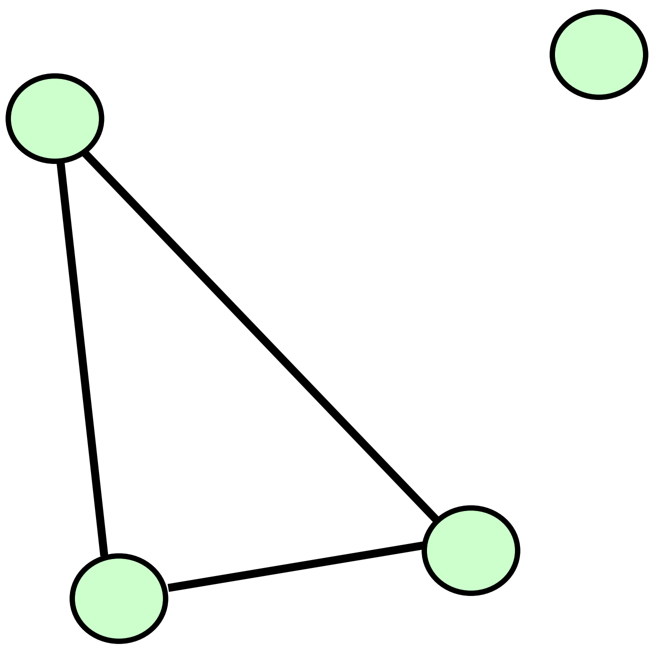
The deletion of edge (in the filtration download) decreases the the number of cycles by at most 1. β_1 decreases by 0 or 1.

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



$\beta_0 = 2$

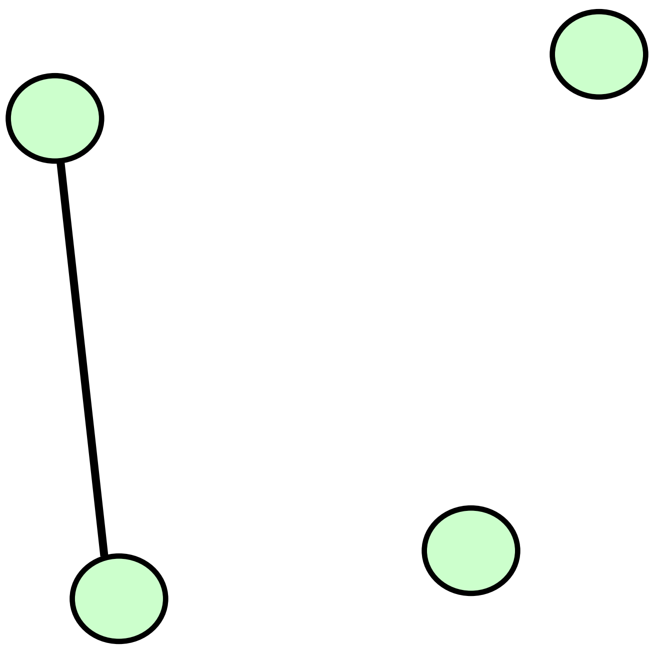
$\beta_1 = 1$

$$\beta_0 - \beta_1 = 1$$

$p = 4$

$q = 3$

$$p - q = 1$$



$\beta_0 = 3$

$\beta_1 = 0$

$$\beta_0 - \beta_1 = 3$$

$p = 4$

$q = 1$

$$p - q = 3$$

Computation of Betti-plots in practice

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

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

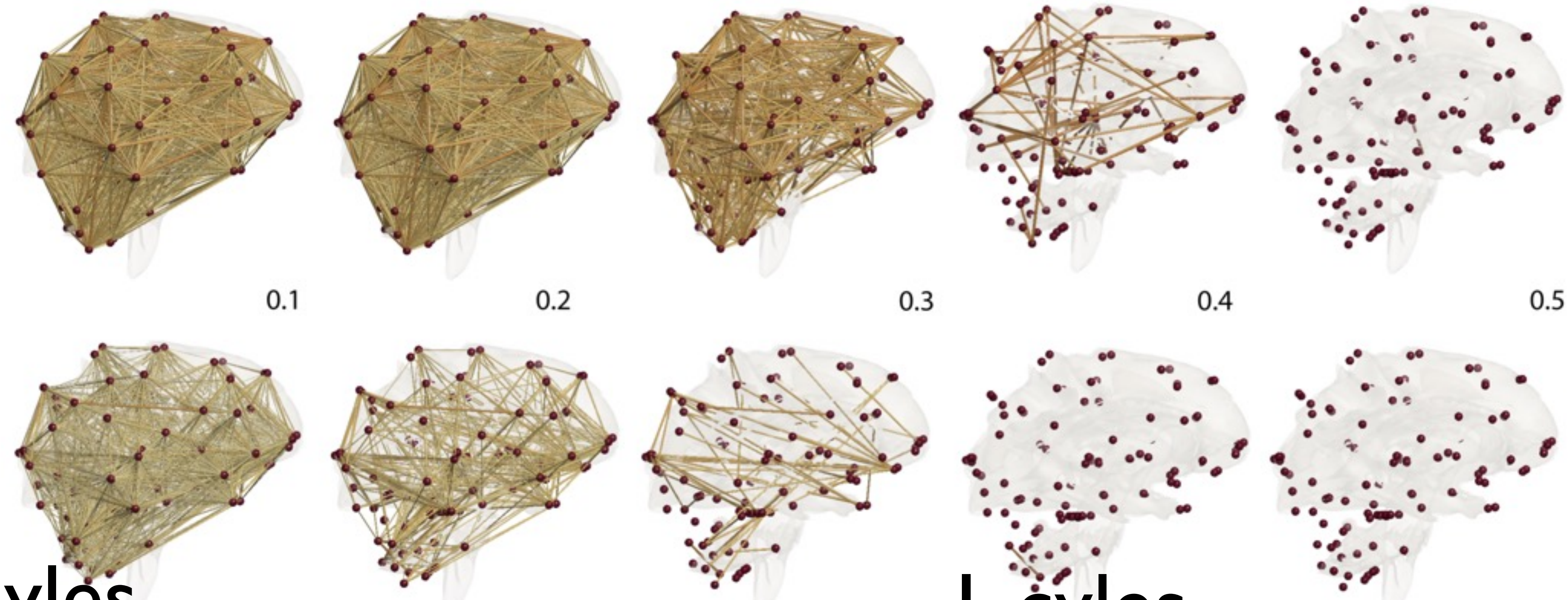
Computation of β_1: As a function of β_0

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

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

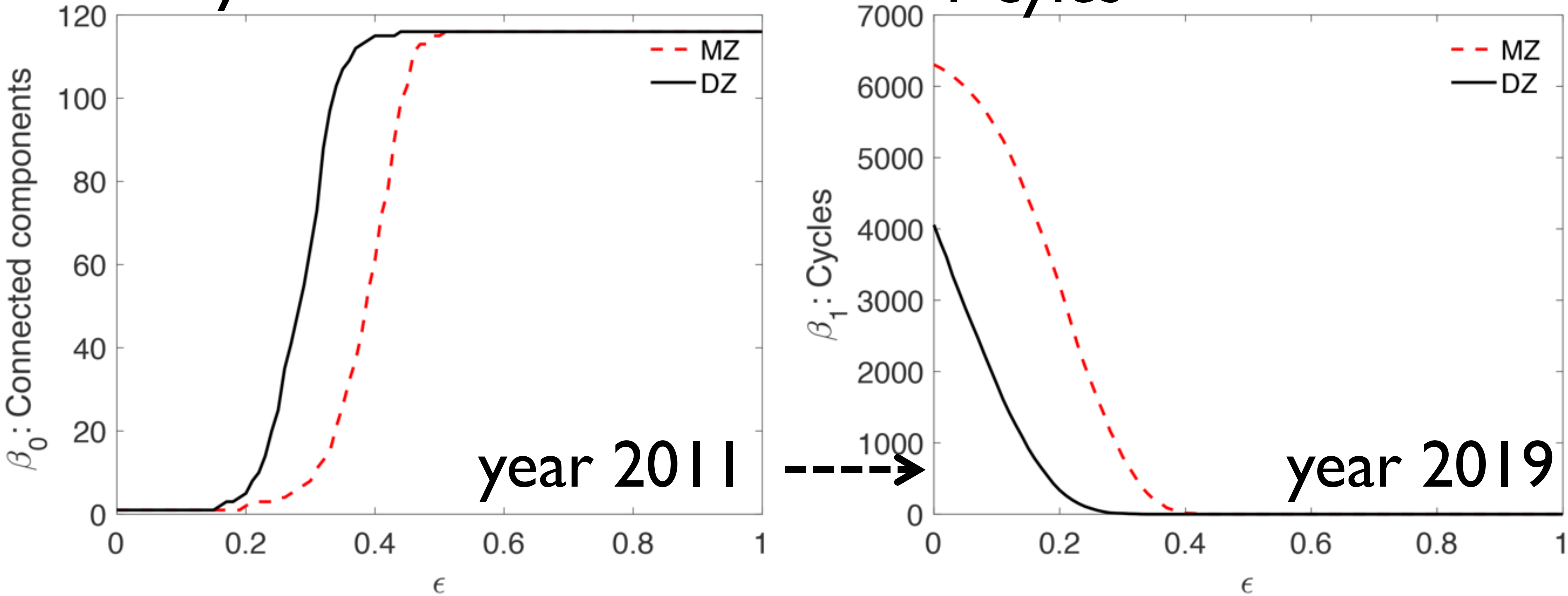
This is not efficient. Need an incremental algorithm that updates as we delete one edge at a time.

Betti-plots in 116 nodes network



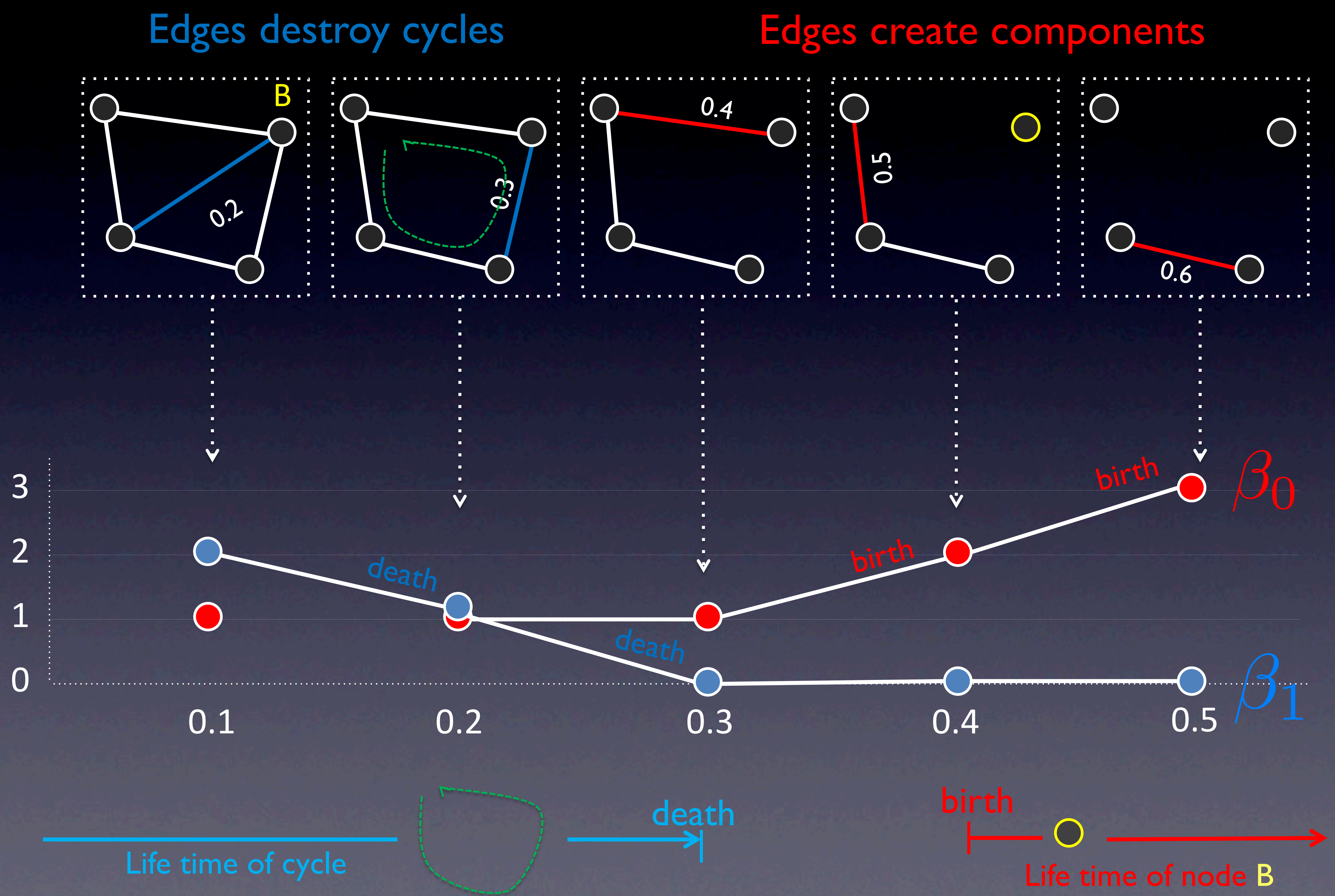
0-cyles

1-cyles



Birth and death decomposition

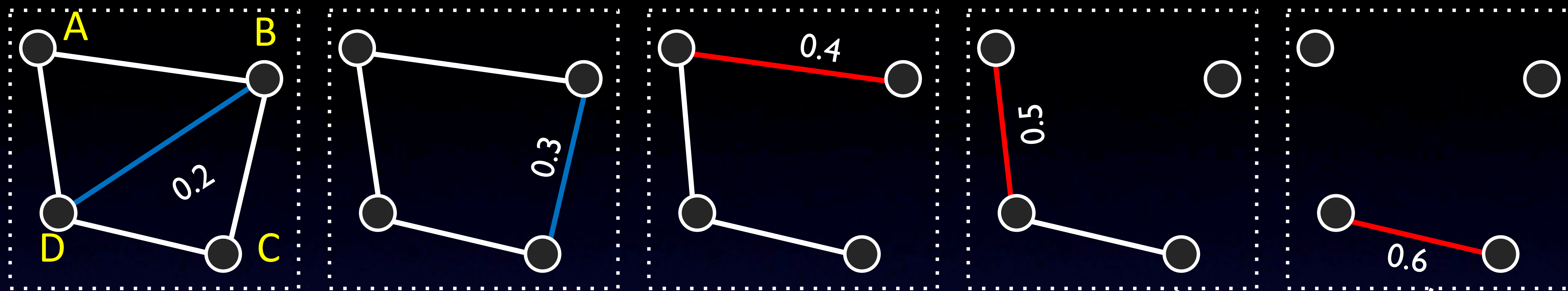
Persistence = Life time (death – birth) of a feature



Theorem *Birth & death sets partition* the edge set

E_1 Edges destroy cycles

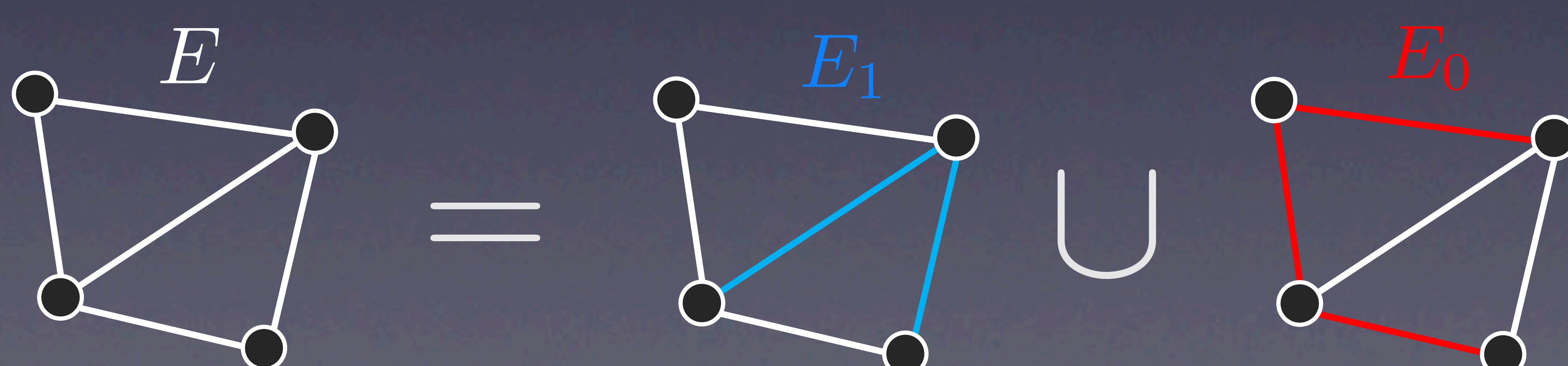
E_0 Edges create components



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

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

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



Maximum spanning tree

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

Songdechakraiwut & Chung 2020 arXiv: 2012.00675

Hodge Laplacian

Multiplicity of eigenvalues

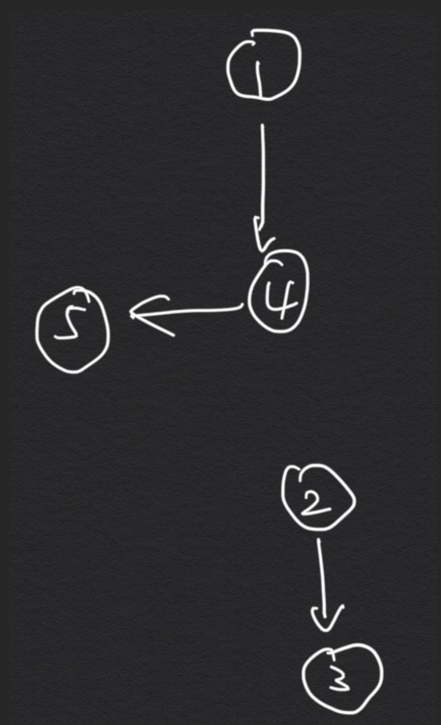
Multiplicity m of eigenvalue λ :

$$L\mathbf{v}_1 = \lambda\mathbf{v}_1, \cdots, L\mathbf{v}_m = \lambda\mathbf{v}_m$$

Theorem: The multiplicity of eigenvalue $\lambda_0 = 0$ is the number of connected components: 0-th Betti number β_0.

Equivalently $\beta_0 = p - rank(L)$

Multiplicity of eigenvalues



$$
\begin{array}{c|ccccc}
 & 1 & 4 & 5 & 2 & 3 \\
\hline
1 & 1 & -1 & 0 & 0 & 0 \\
4 & -1 & 2 & -1 & 0 & 0 \\
5 & 0 & -1 & 1 & 0 & 0 \\
2 & 0 & 0 & 0 & 1 & -1 \\
3 & 0 & 0 & 0 & -1 & 1
\end{array}
$$

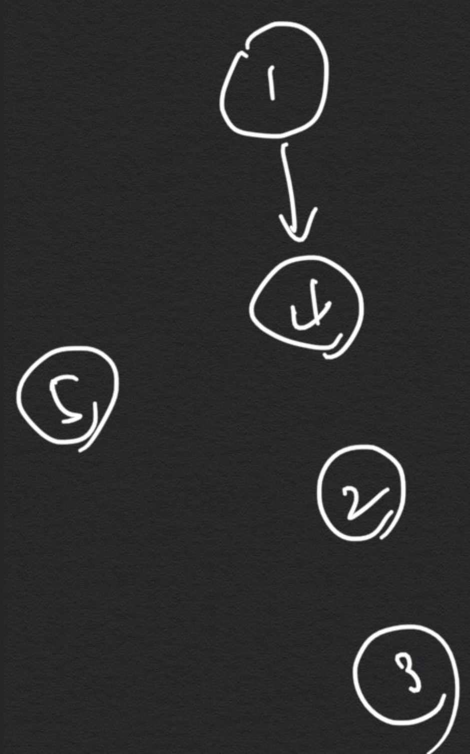
```
>>  [F, D] = eig(L)

F =
         0   -0.5774   -0.7071         0    0.4082
         0   -0.5774    0.0000         0   -0.8165
         0   -0.5774    0.7071         0    0.4082
   -0.7071         0         0   -0.7071         0
   -0.7071         0         0    0.7071         0

D =
         0         0         0         0         0
         0    0.0000         0         0         0
         0         0    1.0000         0         0
         0         0         0    2.0000         0
         0         0         0         0    3.0000
```

$rank(L) = 3$ $\beta_0 = 2$

Theorem: $\beta_0 = p - rank(L)$

Proof. $$rank(L) = rank(MM^\top) = rank(M^\top)$$

$$kerL = \{\sigma : L\sigma = 0\} = \{\sigma : M^\top\sigma = 0\}$$



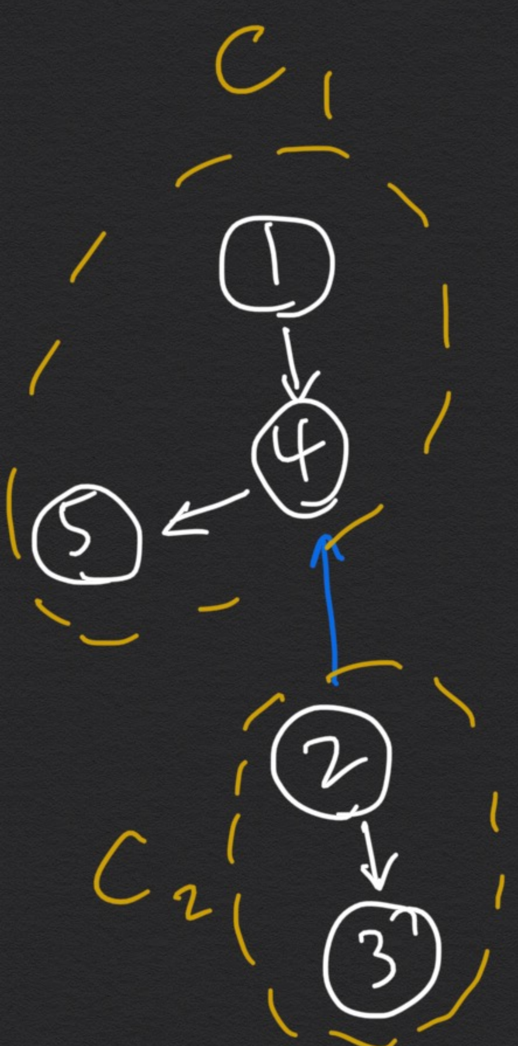
M	...	14	....
1		-1	
5			
4		1	
2			
3			

$$rank(kerL) = 4$$
$$rank(L) = 1$$

$$\sigma = [a, a, b, c, d]^\top$$

Graph with 2 disconnected components

$$kerL = \{\sigma : L\sigma = 0\} = \{\sigma : M^\top \sigma = 0\}$$



M	14 15 45	24	23	12 13 25 34 35
1 5 4	C_1	0 0	0	0
2 3	0	0 0	C_2	0

$$\sigma = [a, a, a, b, b]^\top$$

$$rank(kerL) = \beta_0 = 2$$

$$rank(L) = p - 2$$

Rank-nullity theorem for graph Laplacian

$$kerL = \{\sigma : L\sigma = 0\} = \{\sigma : M^\top \sigma = 0\}$$

$$imgL = \{L\sigma : \sigma \in \mathbb{R}^p\}$$

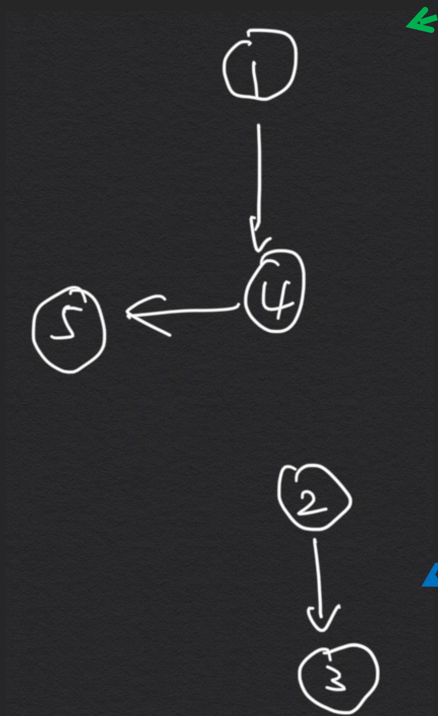
$$rank(imgL) + rank(kerL) = p$$

$rank(L)$ β_0

How to find the connected components?

$$ker L = \{\sigma : L\sigma = 0\} = \{\sigma : M^\top \sigma = 0\}$$

The kernel space is spanned by the eigenvectors corresponding to zero eigenvalue




```
>>  [F, D] = eig(L)

F =
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        0   -0.5774    0.0000         0   -0.8165
        0   -0.5774    0.7071         0    0.4082
  -0.7071         0         0   -0.7071         0
  -0.7071         0         0    0.7071         0

D =
        0         0         0         0         0
        0    0.0000         0         0         0
        0         0    1.0000         0         0
        0         0         0    2.0000         0
        0         0         0         0    3.0000
```
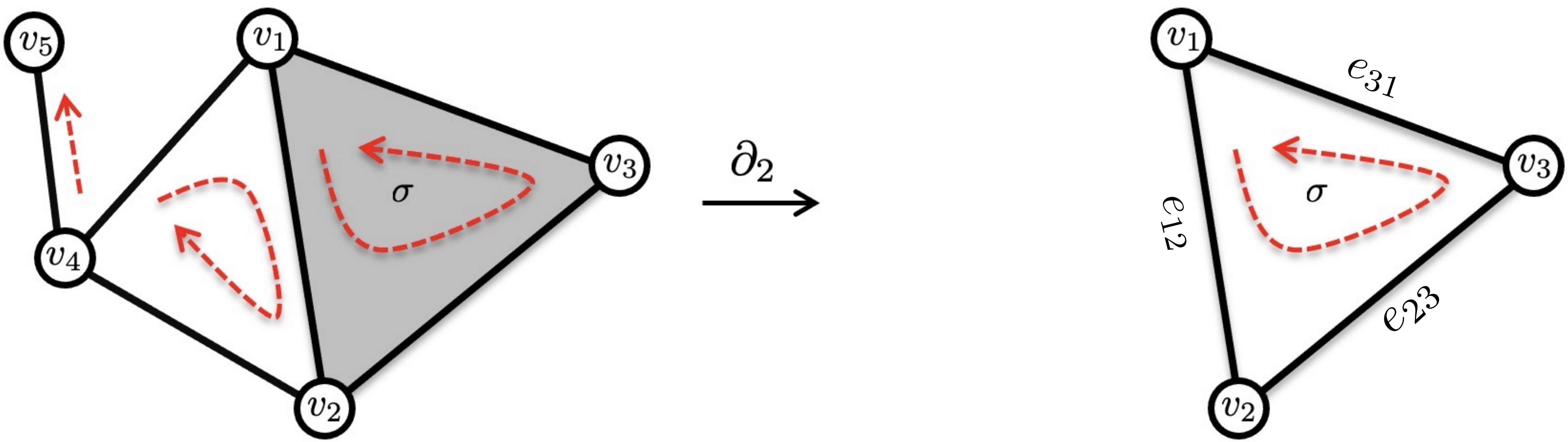

Boundary operators ∂_k

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

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



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

$$\partial_1 \partial_2 \sigma = 0$$

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

Theorem. $\partial_{k-1} \partial_k \sigma = 0$

Example. Boundary of boundary of a filled-in tetrahedron = edges

→ Does the sum of edges vanish?

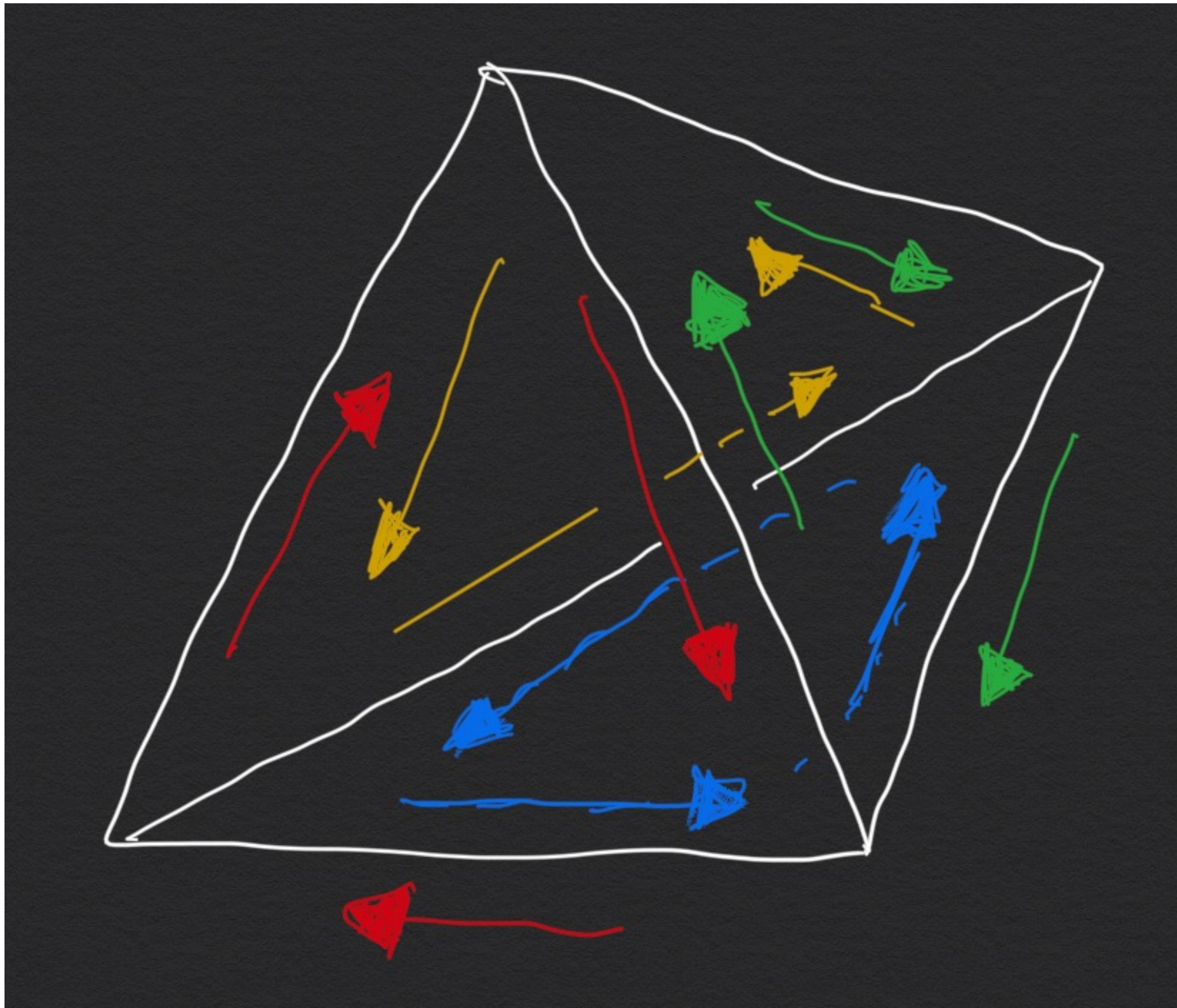
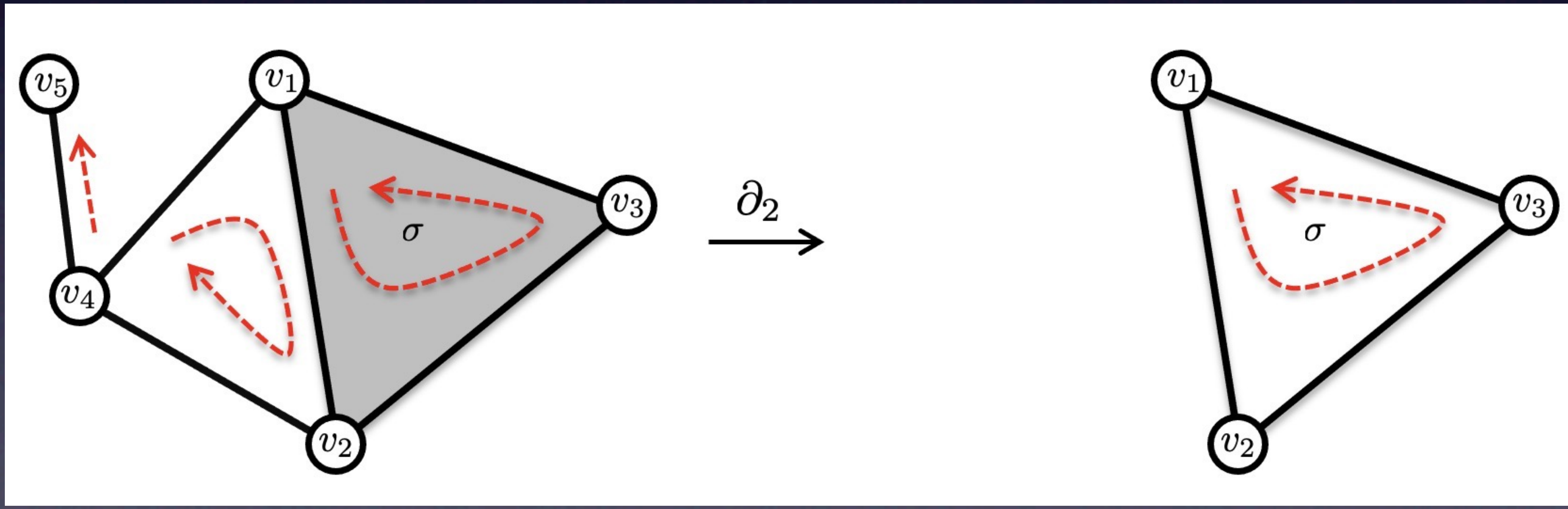


Image of boundary operator

$$img\ \partial_{k+1} = \{\partial_{k+1}\sigma : \sigma \in C_{k+1}\}$$

collection of *k*-boundaries

$\partial_2\sigma = [v_1, v_2] + [v_2, v_3] + [v_3, v_1]$ is 1-boundary



Kernel of boundary operator

$$ker\ \partial_k = \{\sigma \in C_k : \partial_k \sigma = 0\}$$

collection of *k*-cycles

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

$$\partial_2 \sigma = [v_1, v_2] + [v_2, v_3] + [v_3, v_1]$$ is 1-cycle

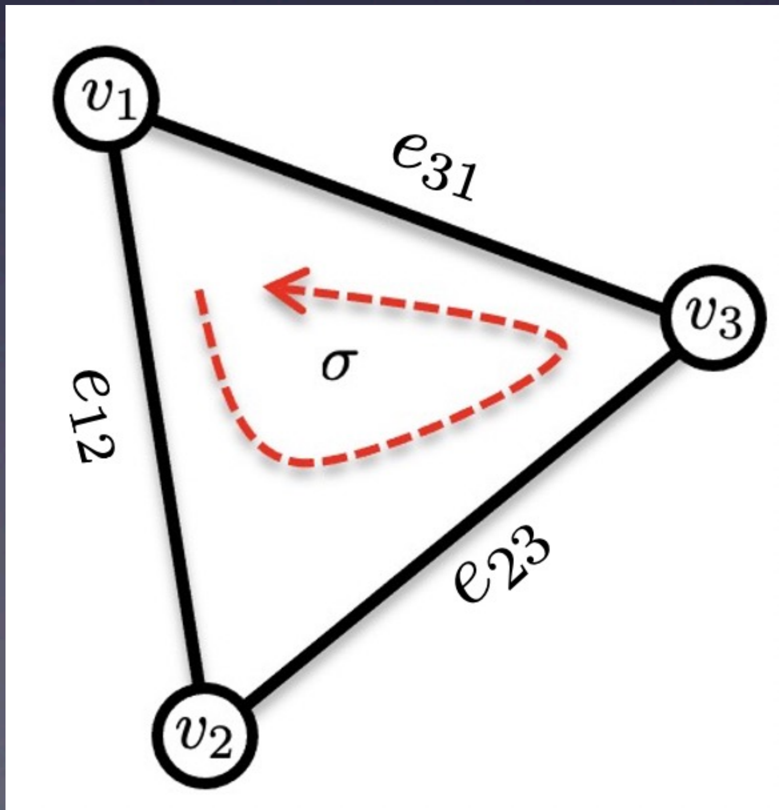


Image of boundary operator

From theorem $\partial_k \partial_{k+1} \sigma = 0$

boundary $\partial_{k+1}\sigma$ is always a cycle.

$$ker\partial_k \supset img\partial_{k+1}$$

Set of cycles Set of boundaries

Quotient space:

$$H_k = ker\partial_k / img\partial_{k+1}$$

$$\beta_k = rank(ker\partial_k) - rank(img\partial_{k+1})$$

Total number of algebraically independent cycles (# of basis).

Lee et al. 2014 (MICCAI 8675:297-304)

Boundary matrix = incidence matrix ∂_k

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

Sign depends on the orientation of τ_i

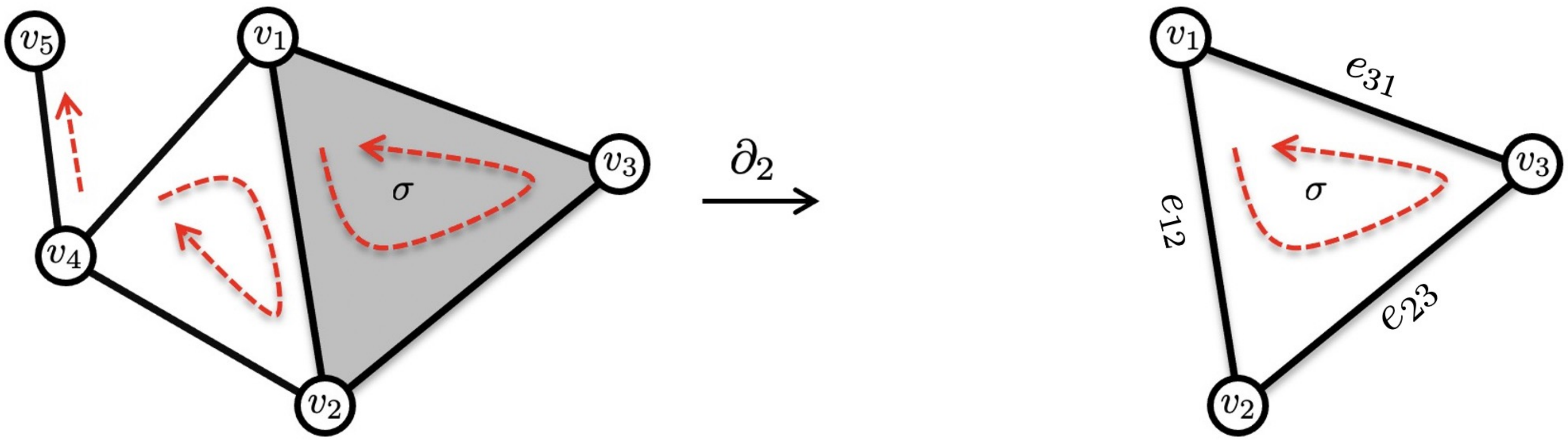
of *k*-dimensional simplices σ_j

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

$$\begin{array}{cccccccc}
1 & 0 & 1 & \dots & & 1 & 0 & 1 \\
\cdot & & & & & & \cdot & \\
\cdot & & & & & & \cdot & \\
\cdot & & & & & & \cdot & \\
1 & 1 & & & & & 0 & 0 \\
0 & 1 & 0 & \dots & & 0 & 1 & -1
\end{array}$$

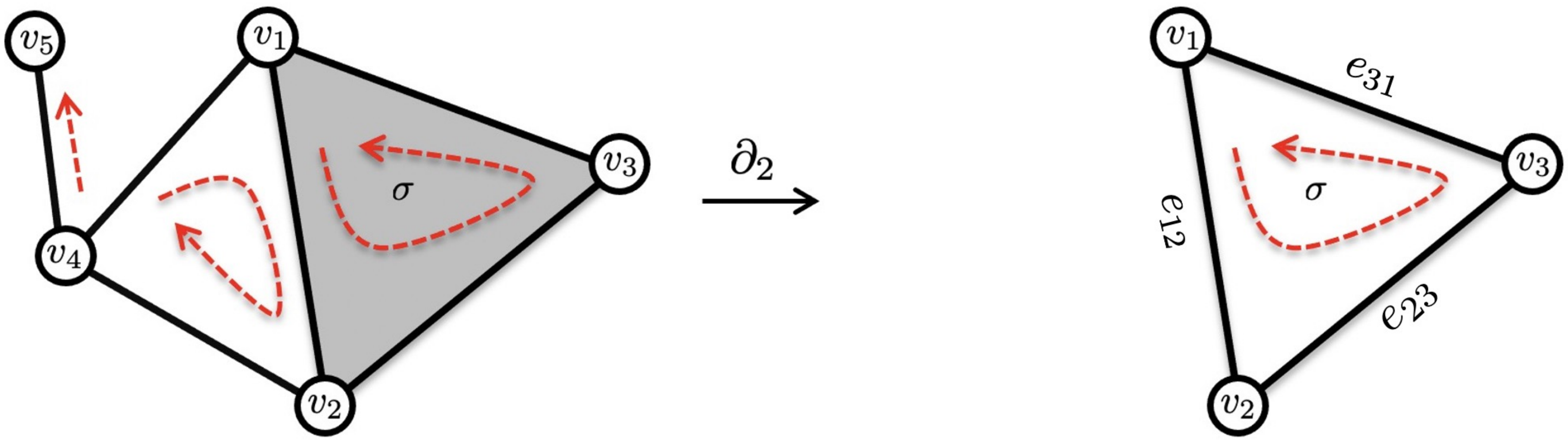
∂_k

Boundary matrix ∂_0



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

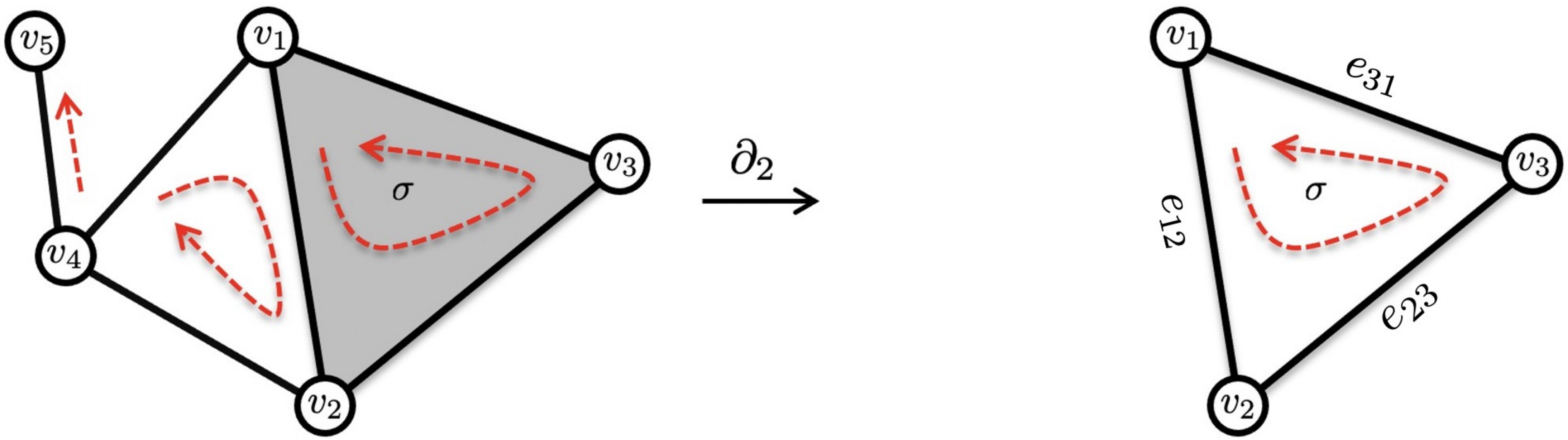
Boundary matrix ∂_1



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

$$\partial_1 = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{array} \begin{array}{c} \begin{array}{cccccc} e_{12} & e_{23} & e_{31} & e_{24} & e_{41} & e_{45} \end{array} \\ \begin{pmatrix} -1 & 0 & 1 & 0 & 1 & 0 \\ 1 & -1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

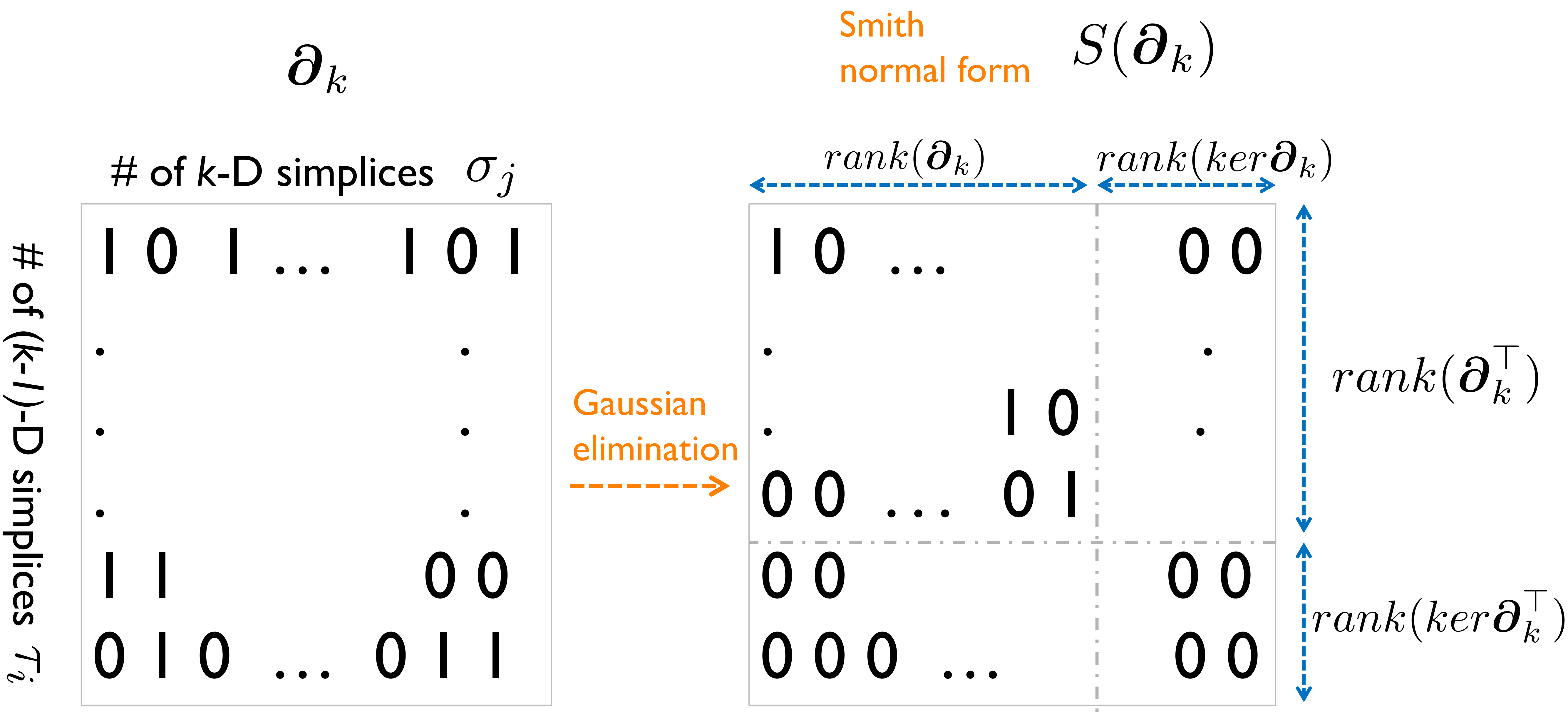
Boundary matrix ∂_2



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

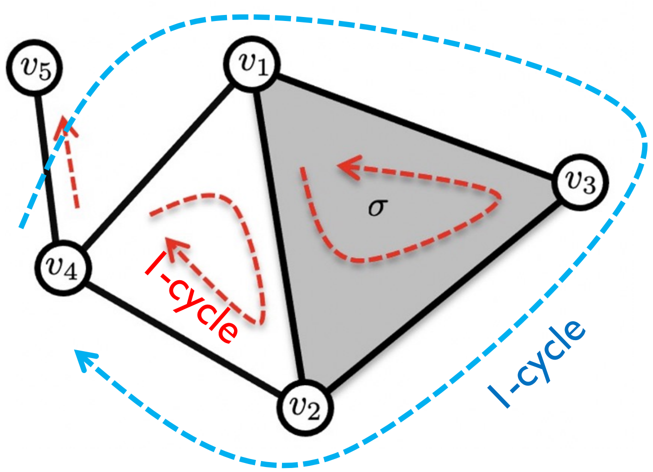
$$\boldsymbol{\partial}_2 = \begin{array}{c} \\ e_{12} \\ e_{23} \\ e_{31} \\ e_{24} \\ e_{41} \\ e_{45} \end{array} \begin{array}{c} \sigma \\ \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{array}$$

Rank nullity theorem for boundary matrix



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

Computing Betti numbers



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

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

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

Far simpler approach given in [*Chung et al. 2019 Network Neuroscience 3:674-694*]

k-th Hodge Laplacian

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

0th Hodge Laplacian
Graph Laplacian

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

\# of nodes

\# of nodes

~~1st Hodge Laplacian~~ $\cancel{\Delta_1 = \partial_2\partial_2^\top + \partial_1^\top\partial_1}$

\# of edges

\# of edges

1st Hodge Laplacian for graphs: $\Delta_1 = \boxed{\partial_1^\top \partial_1}$

k-th Hodge Laplacian

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

0th Hodge Laplacian
Graph Laplacian

# of nodes

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

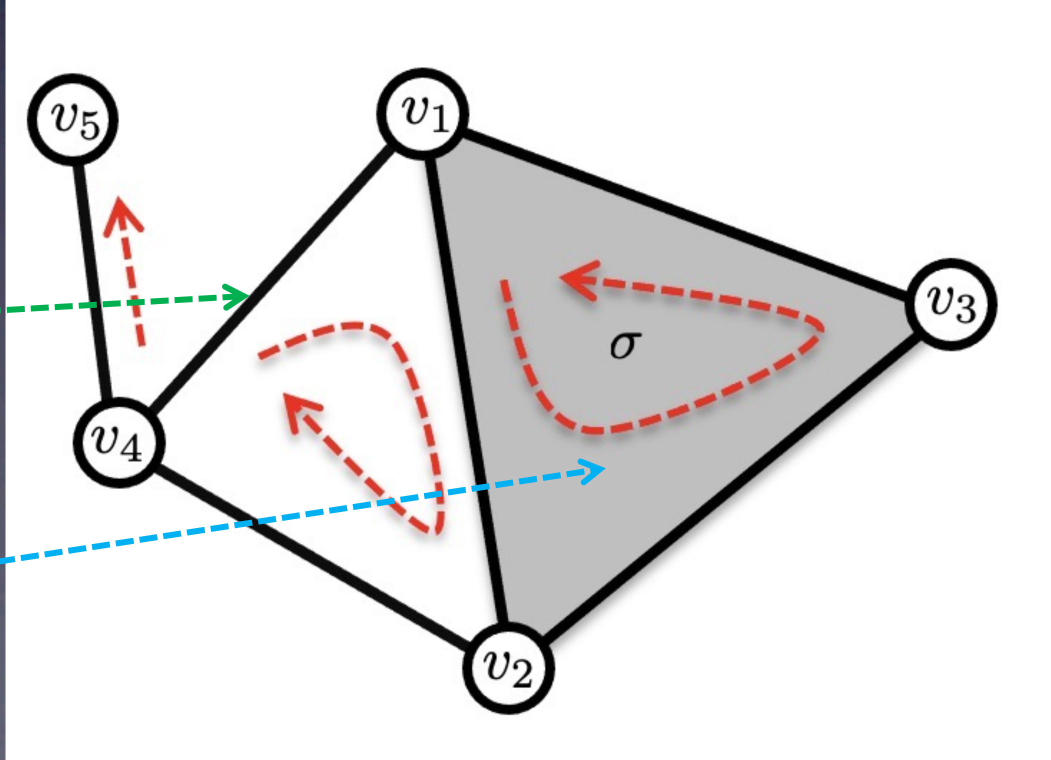
# of nodes

1st Hodge Laplacian

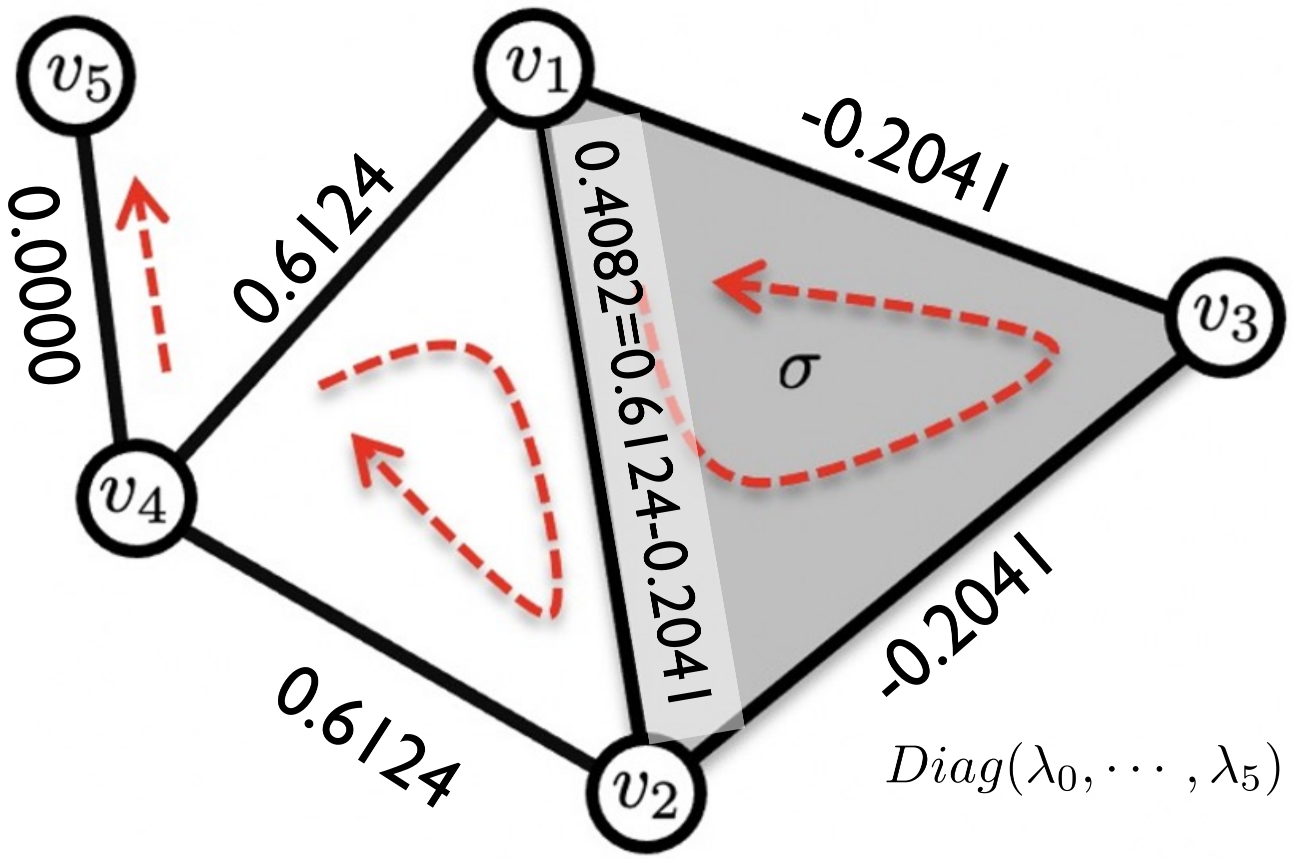
# of edges   # of edges

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

# of edges   # of edges



Eigenvectors of Hodge Laplacian of zero eigenvalue



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

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

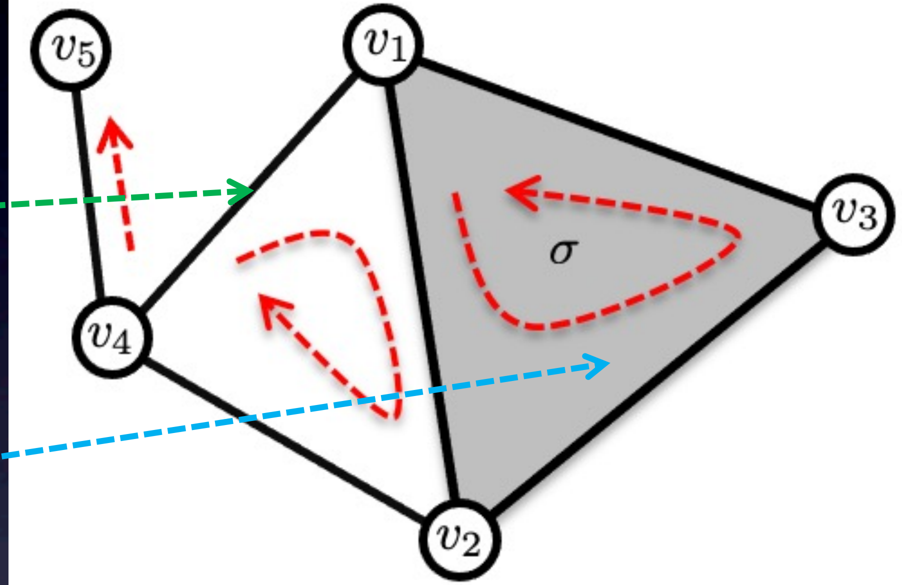
1st Hodge Laplacian for graphs

1st Hodge Laplacian for 2-simplex

\# of edges   # of edges

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

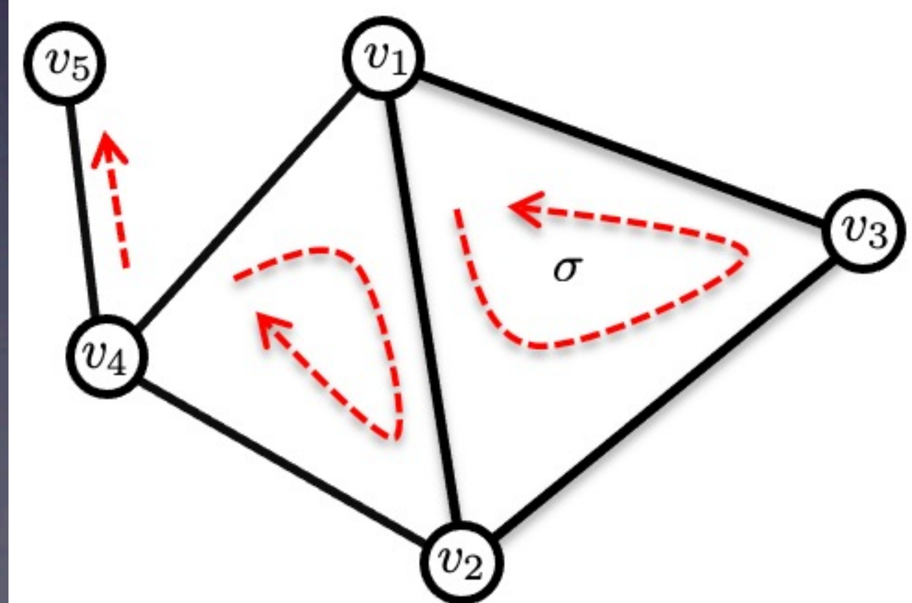
\# of edges   # of edges



\# of edges

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

\# of edges



vector representation of 1-cycles

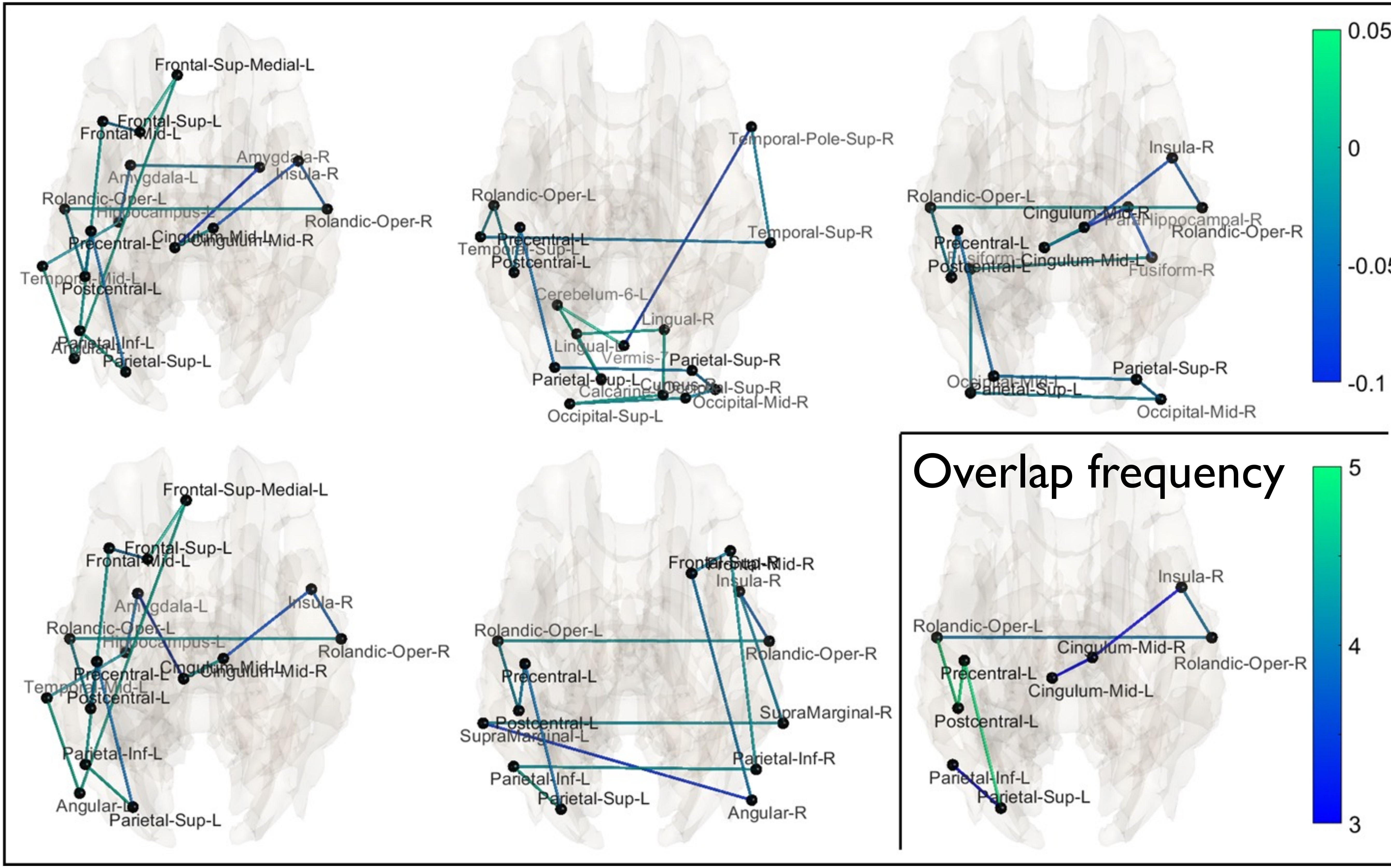
$$cycle = \sum_{i<j} a_{ij} e_{ij}$$

$$\begin{array}{cc} & \beta_1 \\ \text{\# of edges} & \begin{bmatrix} 2.3 & \dots & 1.39 \\ . & & . \\ . & & . \\ . & & . \\ -1.4 & \dots & 0 \end{bmatrix} \end{array} \xrightarrow{\text{Gaussian elimination}} \begin{array}{cc} & \beta_1 \\ \text{\# of edges} & \begin{bmatrix} 1 & 0\dots & & 0 \\ 1 & 0 & . & 0 \\ 0 & 1 & . & 0 \\ 0 & 1 & . & 1 \\ 1. & \dots & 0 & 1 \end{bmatrix} \end{array}$$

Linearly independent columns

More meaningful representation

Five biggest cycle differences (male – female) in HCP



Anand et al. 2021, IEEE TMI arXiv:2110.14599

p-value = 0.03