Topological Data Analysis

Persistence & Networks

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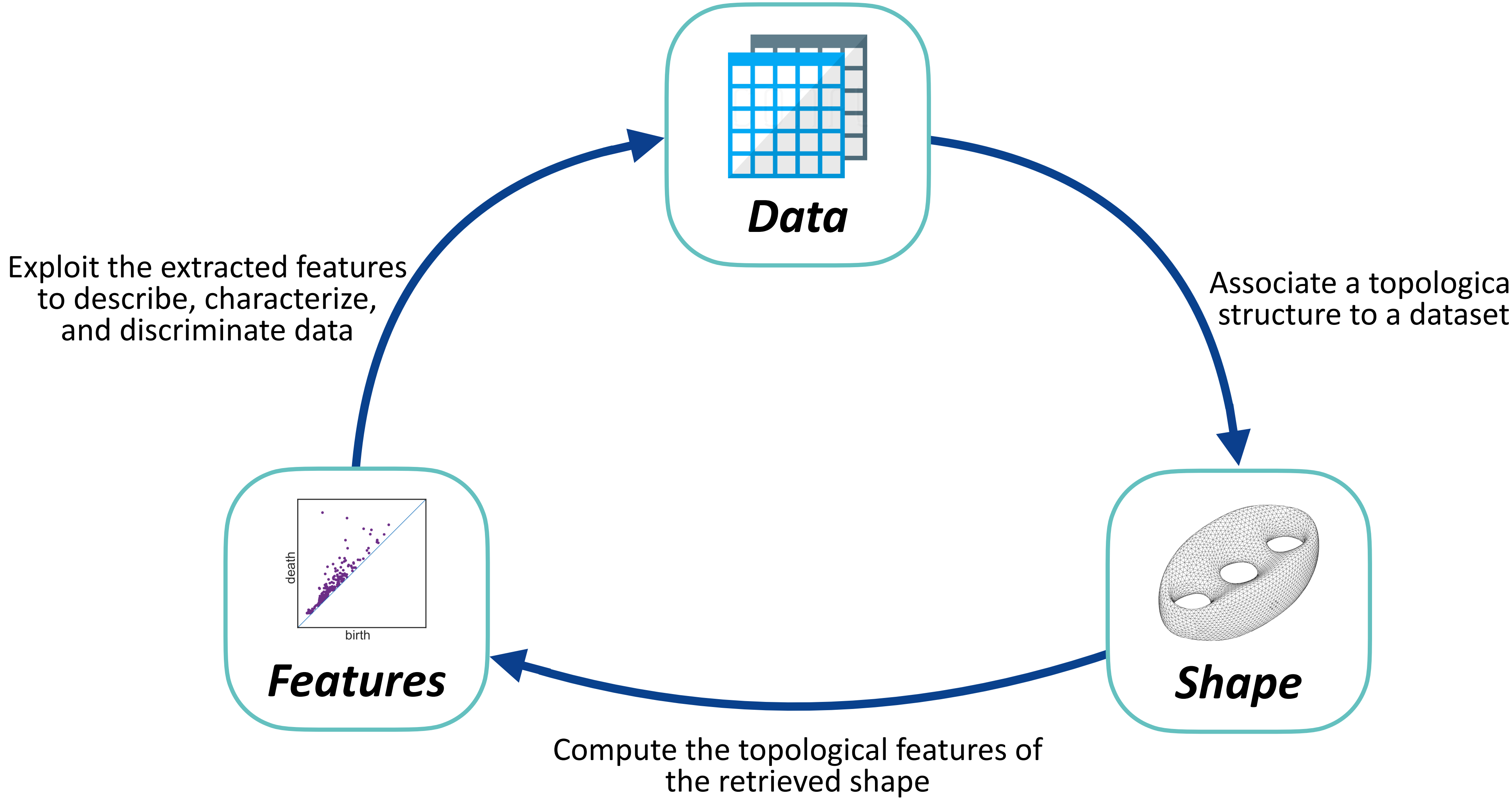
CNR - IMATI

Topological Data Analysis



Persistence and Complex Networks

- *A Primer on Complex Networks*
- *Homological Scaffolds*
- *Clique Community Persistence*

Persistence and Complex Networks

- ***A Primer on Complex Networks***
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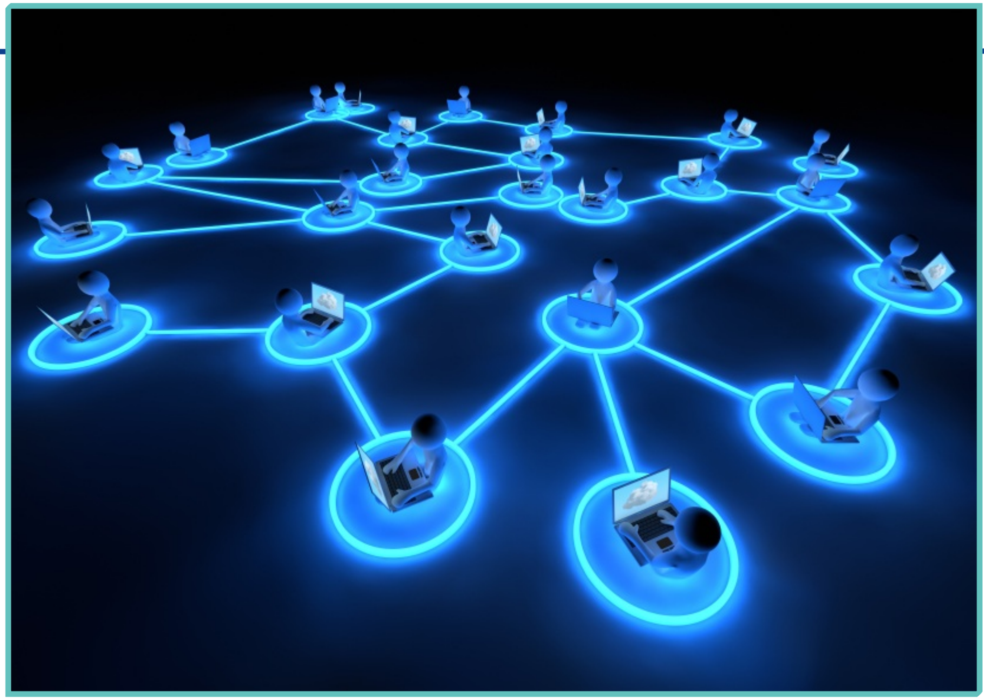
Persistence and Complex Networks

Networks:

*A **network** is a complex system consisting of **individuals or entities connected by specific ties** such as friendship, common interest, and shared knowledge*

E.g.

- ***Social*** Networks
- ***Sensor*** Networks
- ***Biological*** Networks
- ***Collaborative*** Networks
- …

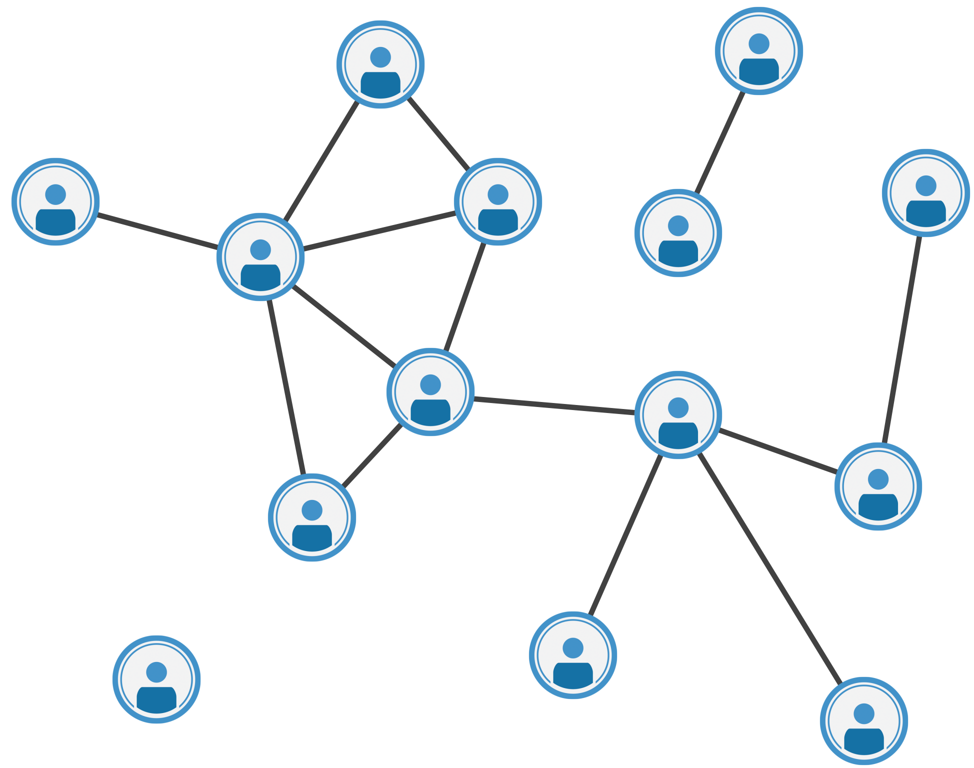


Persistence and Complex Networks

Representation:

A network can be represented by a *graph* ***G = (V, E)*** such that:

Nodes of V	⟺	*Entities or individuals*
Arcs of E		*Ties between entities*



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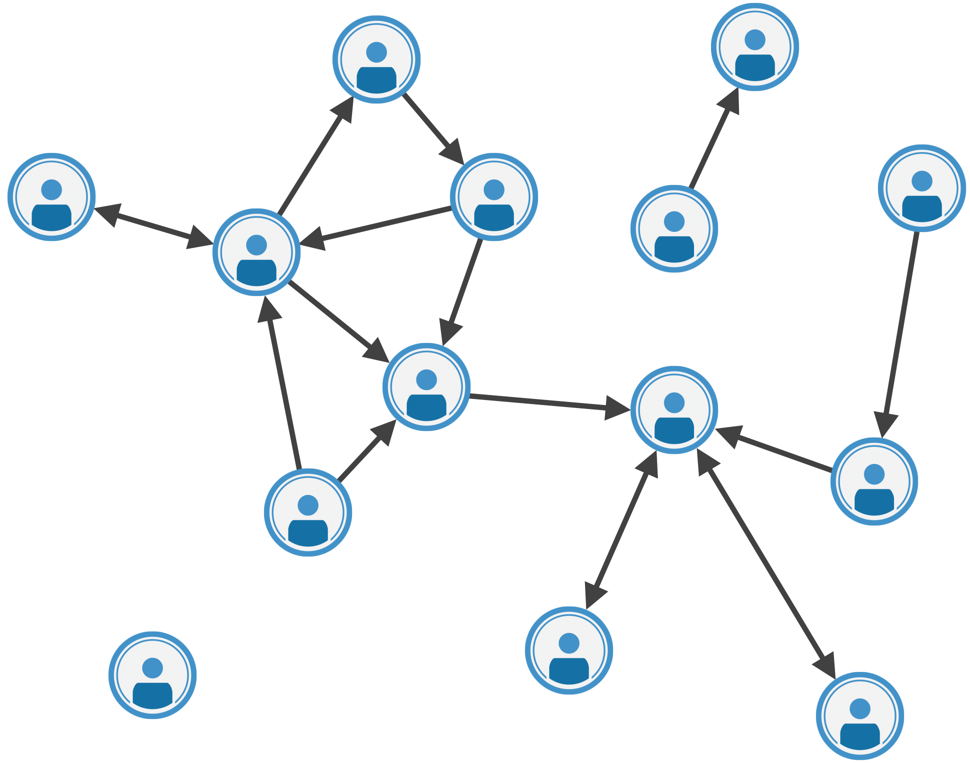
Arcs can be:

- ***Directed***
- ***Weighted***



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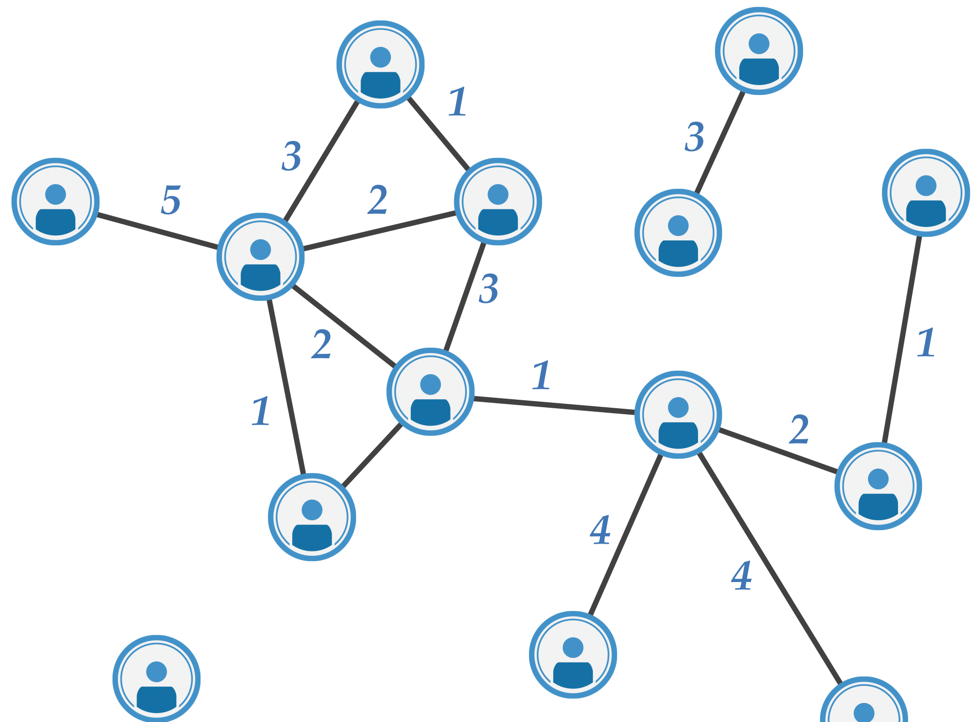

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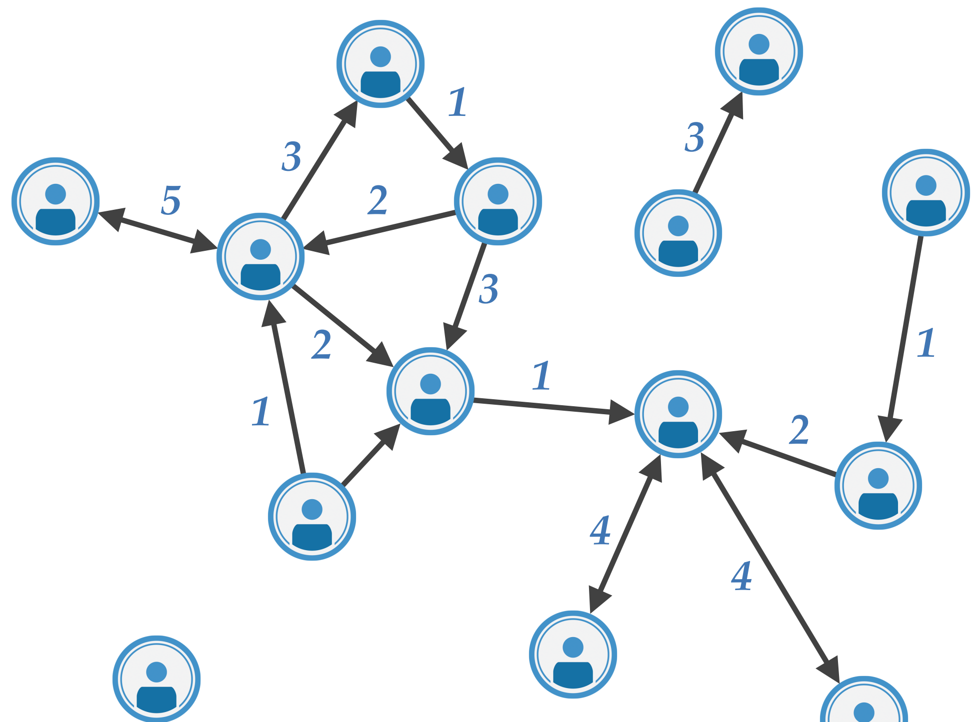
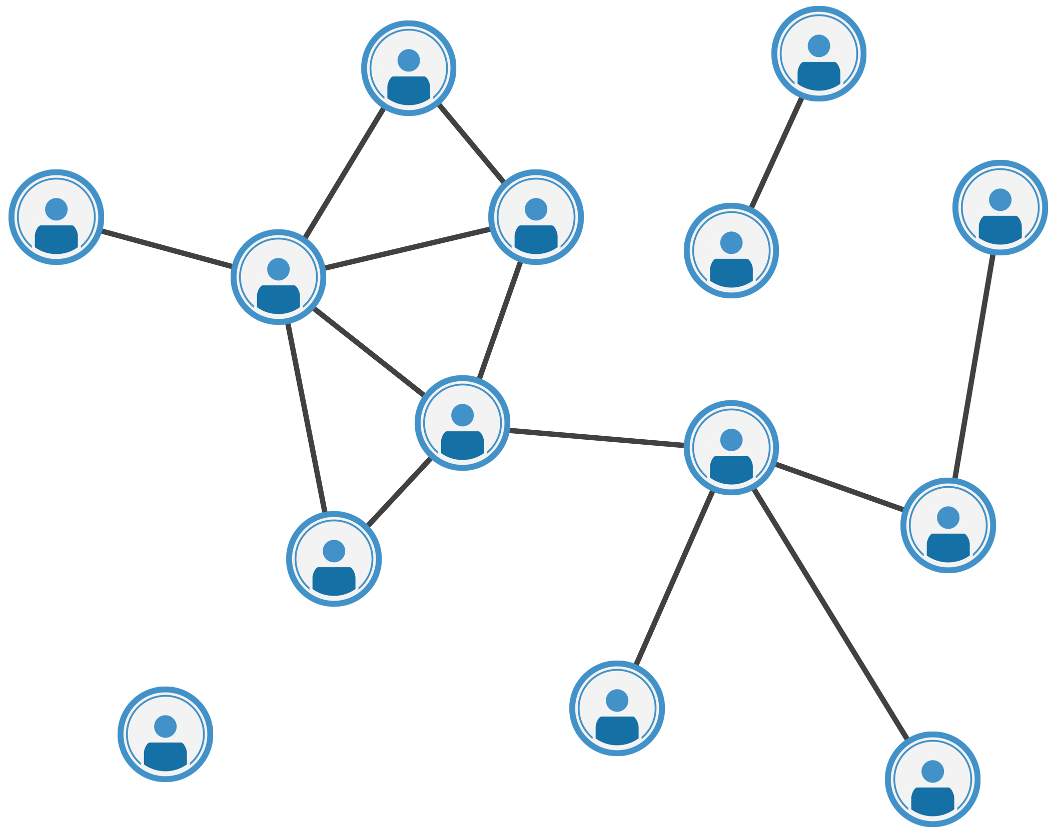


Persistence and Complex Networks

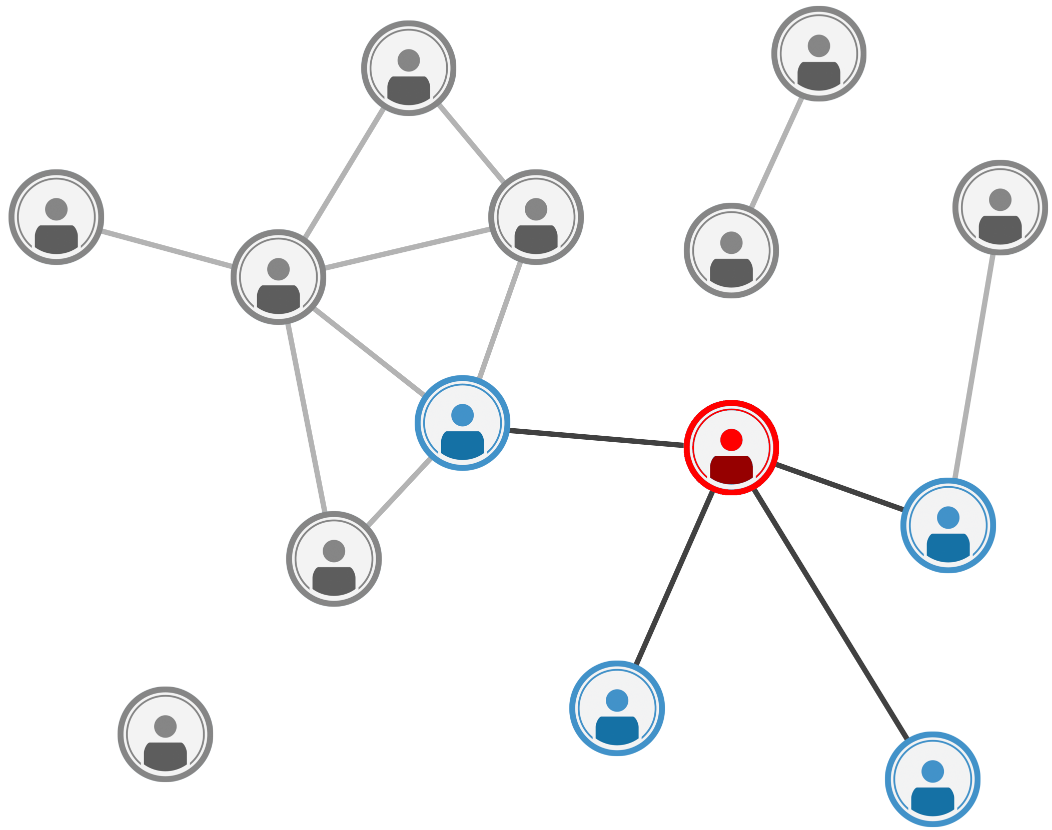
A Two-Level Analysis:



Persistence and Complex Networks

A Two-Level Analysis:

- ***Egocentric***
- *Sociocentric*



Persistence and Complex Networks

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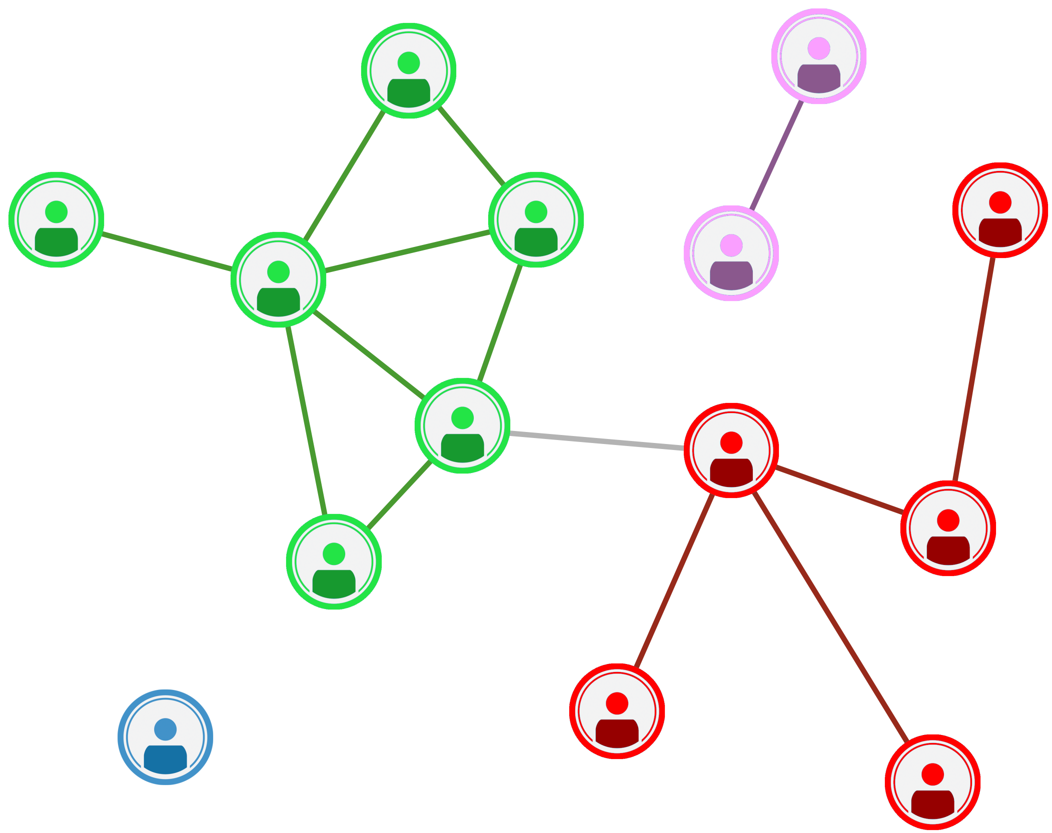
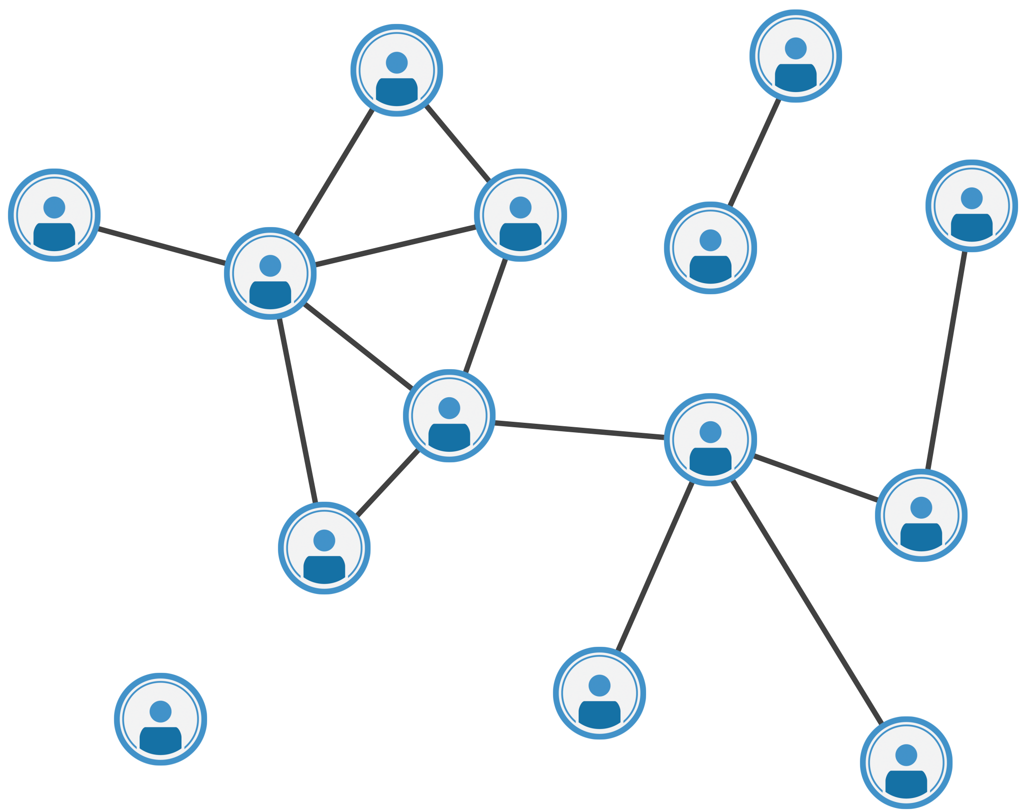


Persistence and Complex Networks

Who is the most important individual?



Persistence and Complex Networks

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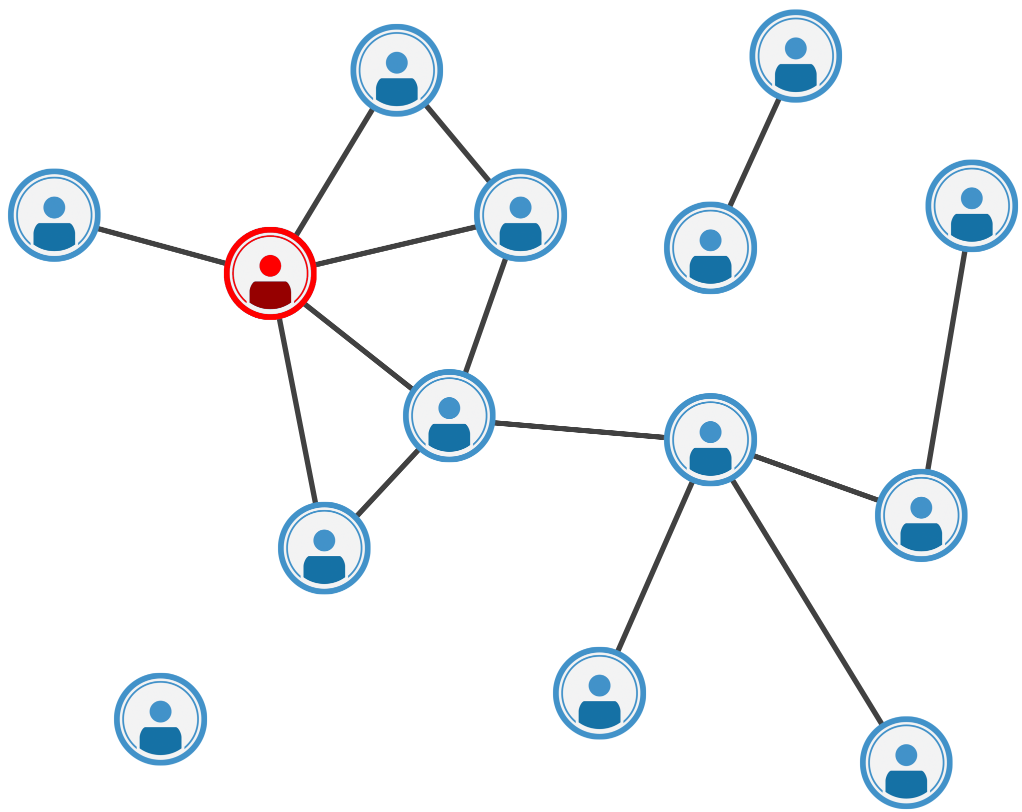

Persistence and Complex Networks

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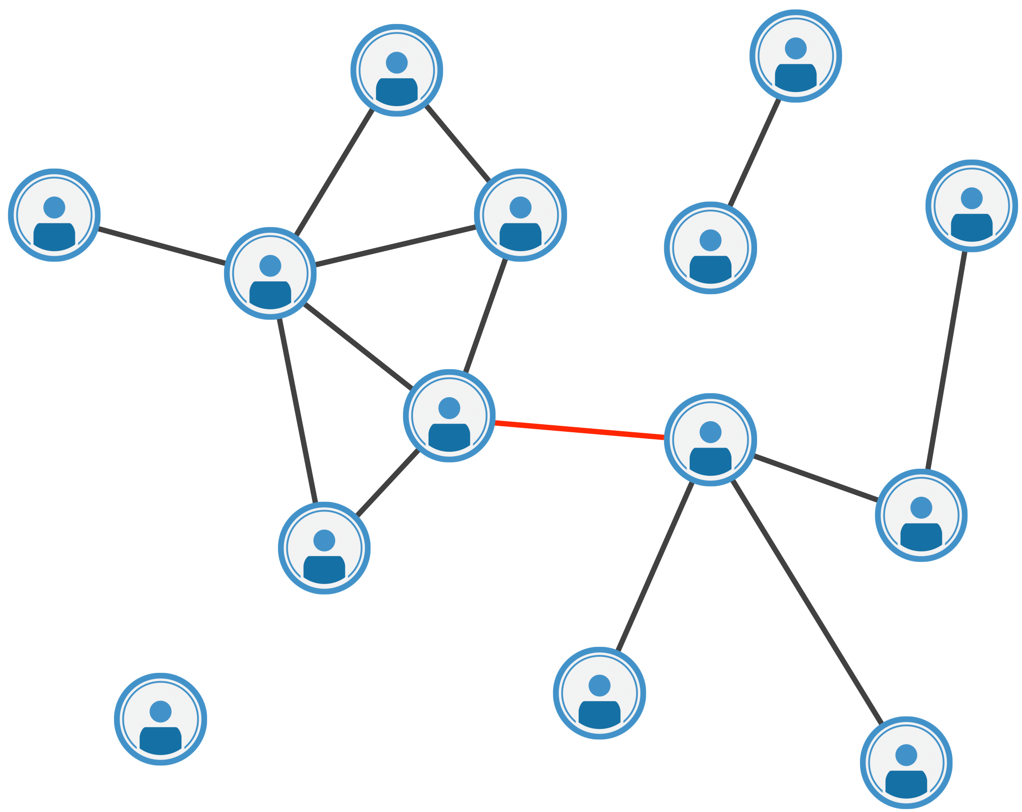

Persistence and Complex Networks

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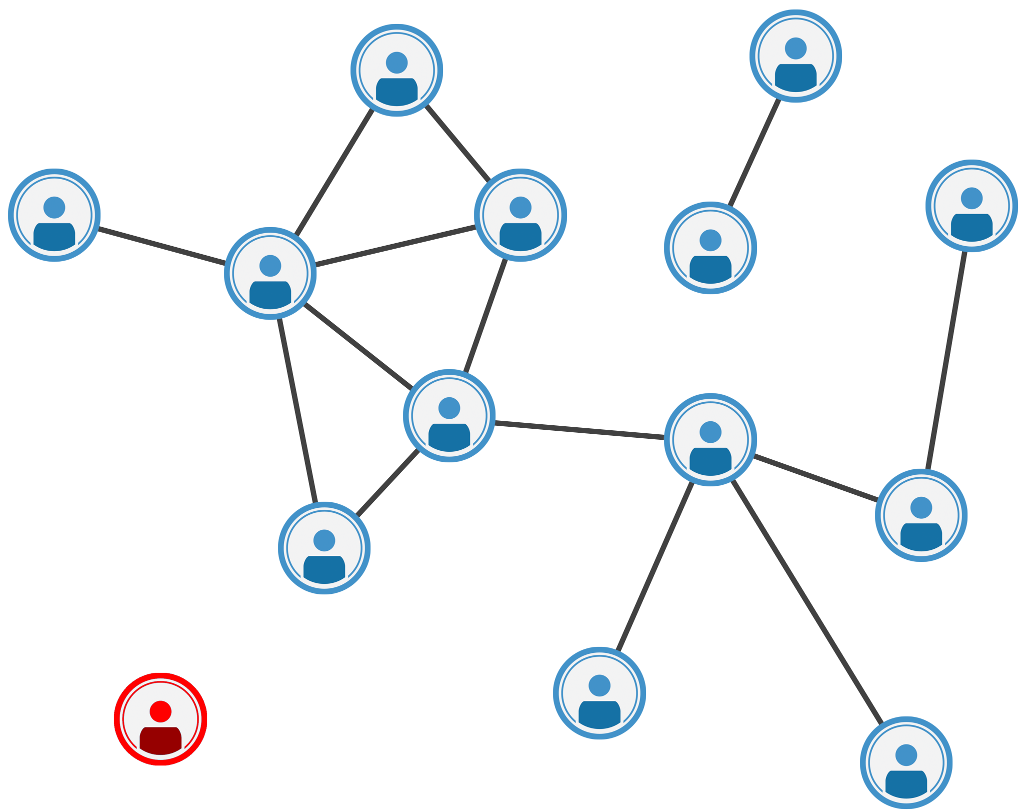


Persistence and Complex Networks

Centrality Measures:

Different criteria to underline **different roles**:

- *Key players*
- *Brokers*
- *Bridges*
- *Isolated*
- ...

Definition:

*A centrality measure is a function $F : V \longrightarrow \mathbb{R}$ assigning to each node a "**centrality**" value:*

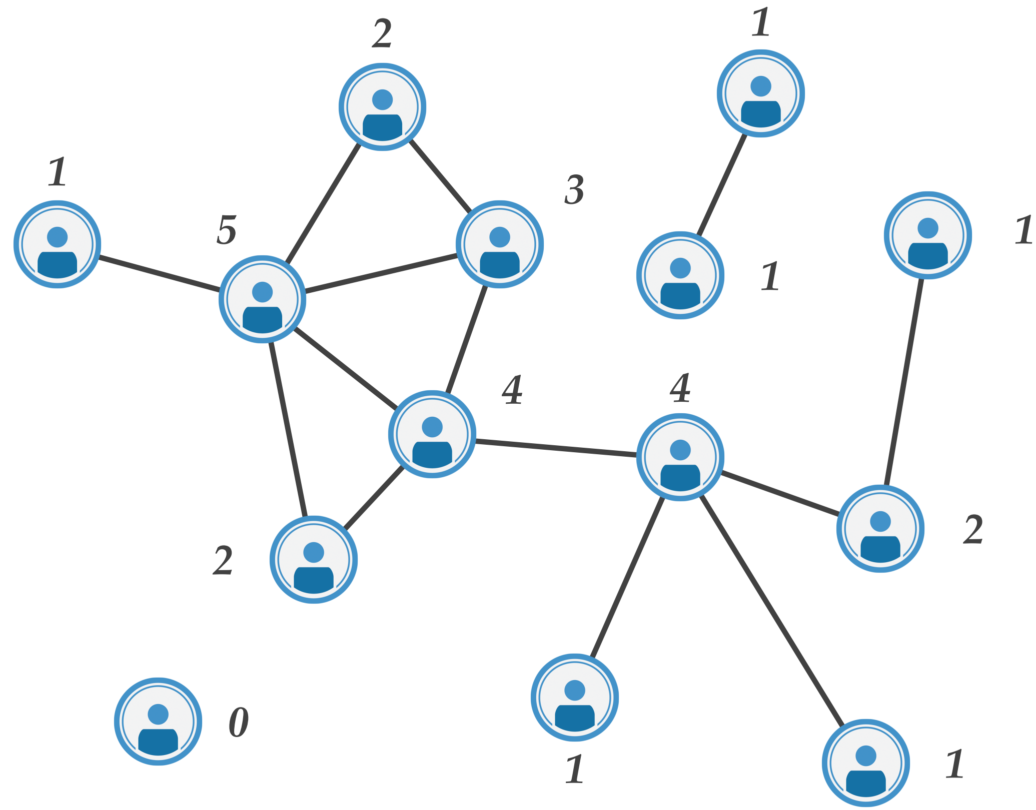
- ***Degree** centrality*
- ***Betweenness** centrality*
- ***Closeness** centrality*
- ***Eigenvector** centrality*
- ***Erdös** distance*

Persistence and Complex Networks

Degree Centrality:

Given a node v of G = (V, E),

$$D(v) := \#\{u \in V \,|\, (u, v) \in E\}$$

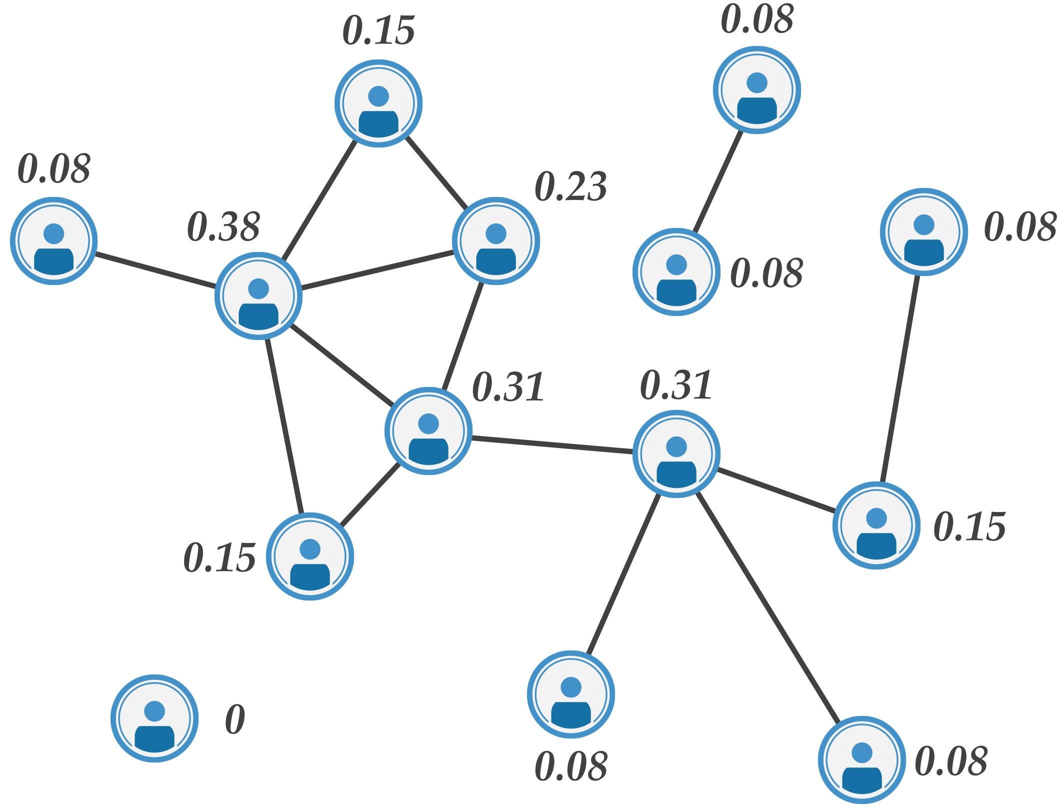


Persistence and Complex Networks

Degree Centrality:

Given a node v of G = (V, E),

$$D(v) := \frac{\#\{u \in V \mid (u,v) \in E\}}{\#V - 1}$$



Persistence and Complex Networks

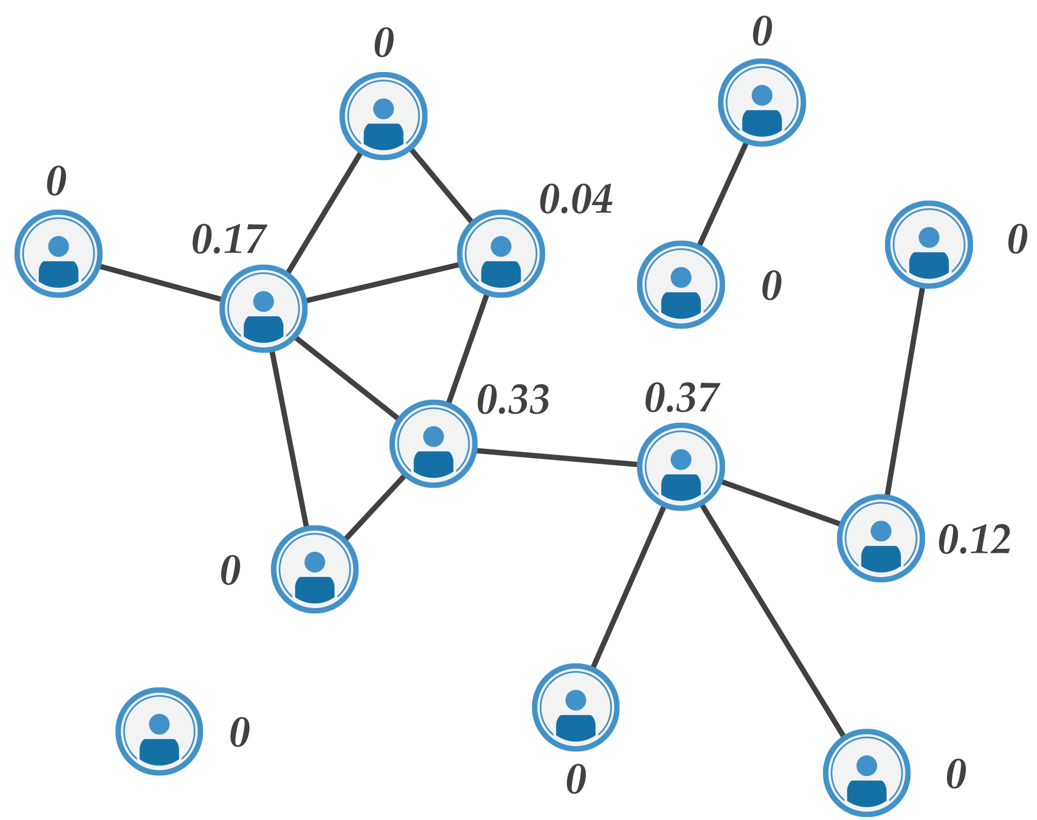
Betweenness Centrality:

Given a node v of G = (V, E),

$$B(v) := \sum_{s \neq v \neq t} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

where:

- σ_{st} is the number of ***shortest paths from s to t***
- $\sigma_{st}(v)$ is the number of those paths ***passing through v***

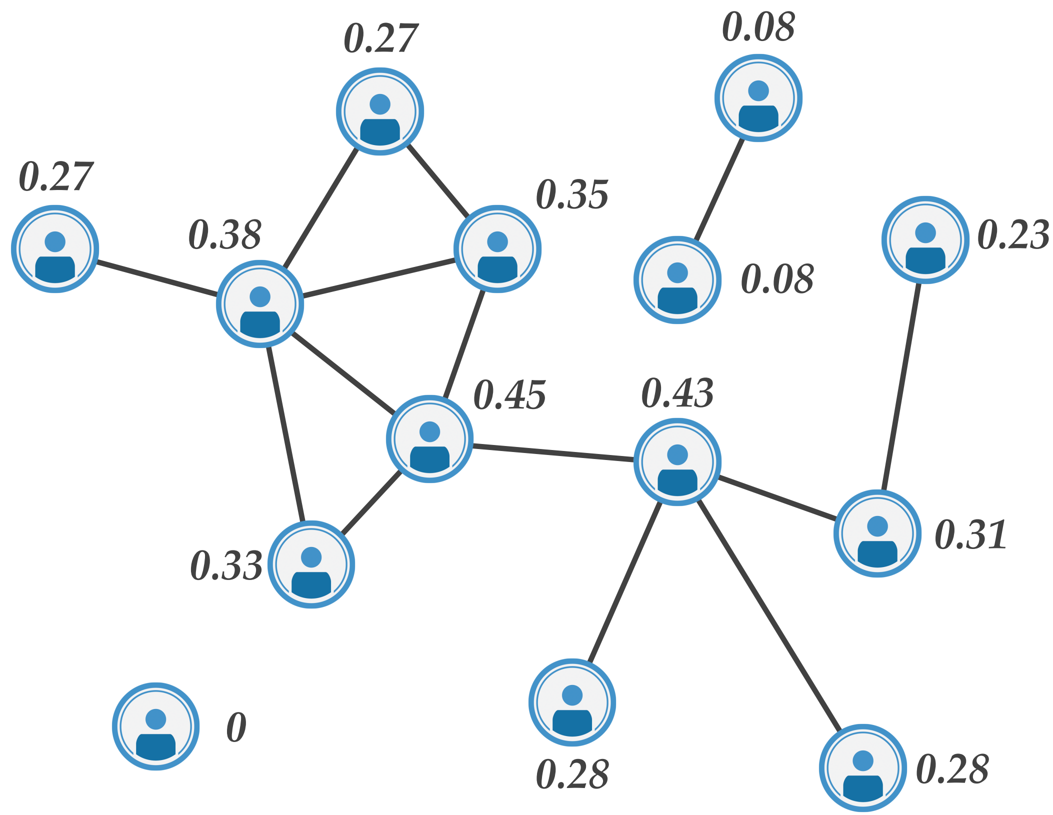


Persistence and Complex Networks

Closeness Centrality:

Given a node v of G = (V, E),

$$C(v) := \frac{\#V - 1}{\sum_{u\in V} d(u, v)}$$



Persistence and Complex Networks

Eigenvector Centrality:

Given a node v of G = (V, E),

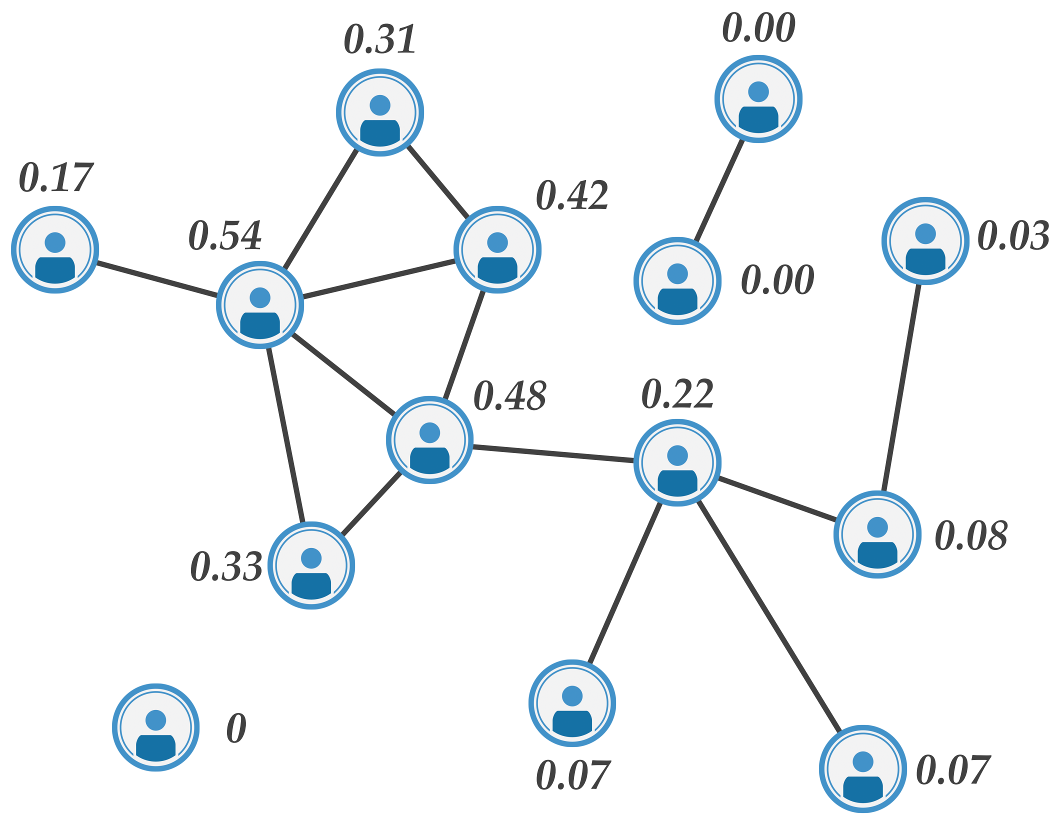
$$x_v := \frac{1}{\lambda} \sum_{u \in V} A_{uv}\, x_u$$

where λ is constant and

$$A_{uv} := \begin{cases} 1 & if (u,v) \in E \\ 0 & otherwise \end{cases}$$

I.e. the v^{th} entry of the eigenvector of

$$A\,x = \lambda\,x$$



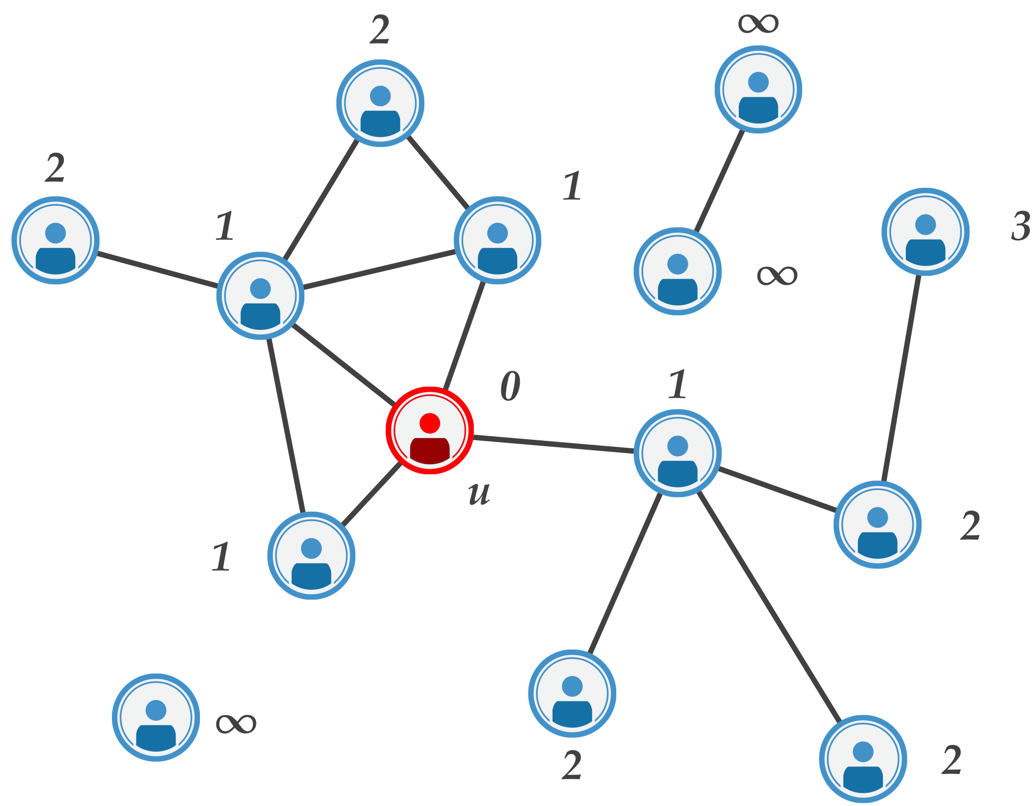
x* > *0 implies λ must be the largest eigenvalue of *A* and ***x*** the corresponding eigenvector

Persistence and Complex Networks

Erdös Distance:

Given two nodes u, v of G = (V, E),

$$E_u(v) := d(u, v)$$



Named after ***Paul Erdös***,

- one of the most prolific mathematicians of the 20th century

Persistence and Complex Networks

Centrality Measures:

A centrality measure for any query!

Degree	***How many individuals can v reach directly?***
Betweenness	***How likely is v to be the most direct route between two individuals?***
Closeness	***How fast can v reach everyone in the network?***
Eigenvector	***How well is v connected to other well-connected individuals?***
Erdös	***How far is v from a specific individual?***

Persistence and Complex Networks

Sociocentric Networks:

- ***Structural Metrics:***
  - *Average of a Centrality Measure*
  - *Diameter*
  - *Density*
  - *Transitivity*
  - ...
- ***Community Decompositions:***
  - *Atomic Communities*
  - *Clustering Techniques*

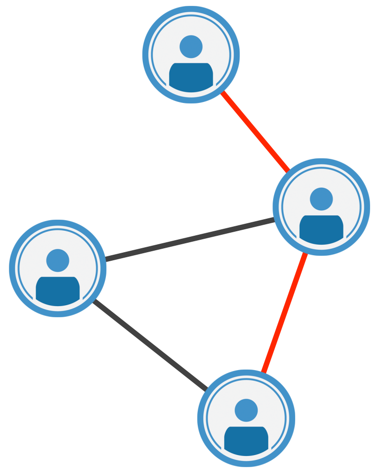
Persistence and Complex Networks

Structural Metrics:

How far are two individuals at most?

Diameter:

The longest shortest path between any two nodes



Diameter(G) = 2

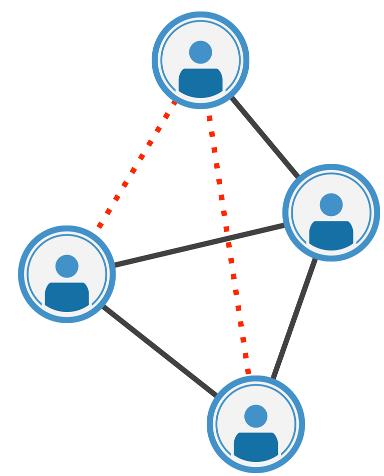
Persistence and Complex Networks

Structural Metrics:

How close is G to being an "everyone knows everyone" network?

Density:

$$\frac{\textit{Number of edges of G}}{\textit{Number of all possible edges}}$$



Density(G) = 4/6 = 0.67

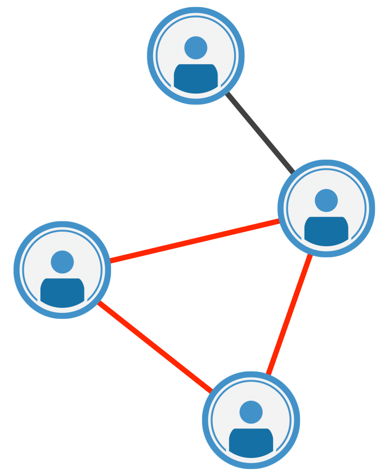
Persistence and Complex Networks

Structural Metrics:

How likely are two individuals connected to an individual v connected to each other?

Transitivity:

$$\frac{\text{Number of closed triplets of nodes}}{\text{Number of connected triplets}}$$



Transitivity(G) = 1/3 = 0.33

Persistence and Complex Networks

Community Decompositions:

- *Atomic Communities:*
  - *Clique*
  - *n-Clique*
  - *n-Clan*
  - *n-Club*
  - *k-Plex*
  - *k-Core*
  - ...

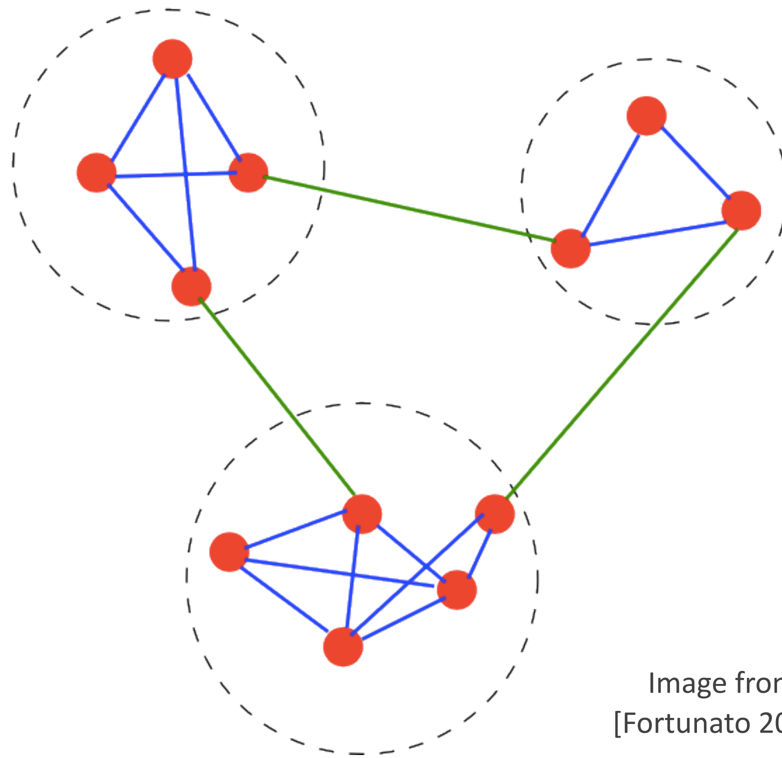


Image from [Fortunato 2009]

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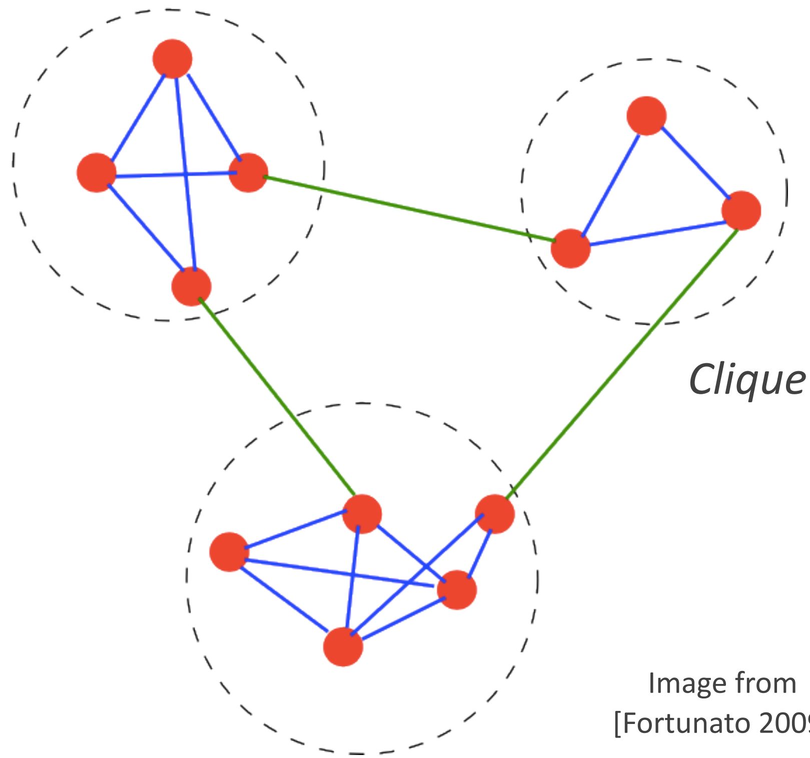

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Clique:

A maximal subgraph whose nodes are all adjacent to each other

Persistence and Complex Networks

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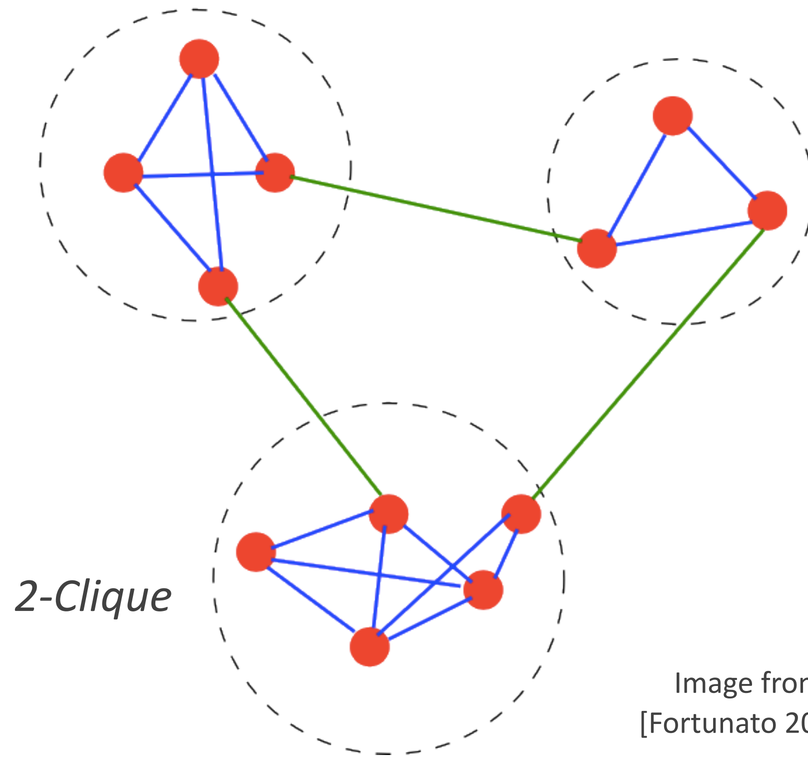

Image from
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n-Clique:

A maximal subgraph such that the distance of each pair of its nodes is not greater than n

Persistence and Complex Networks

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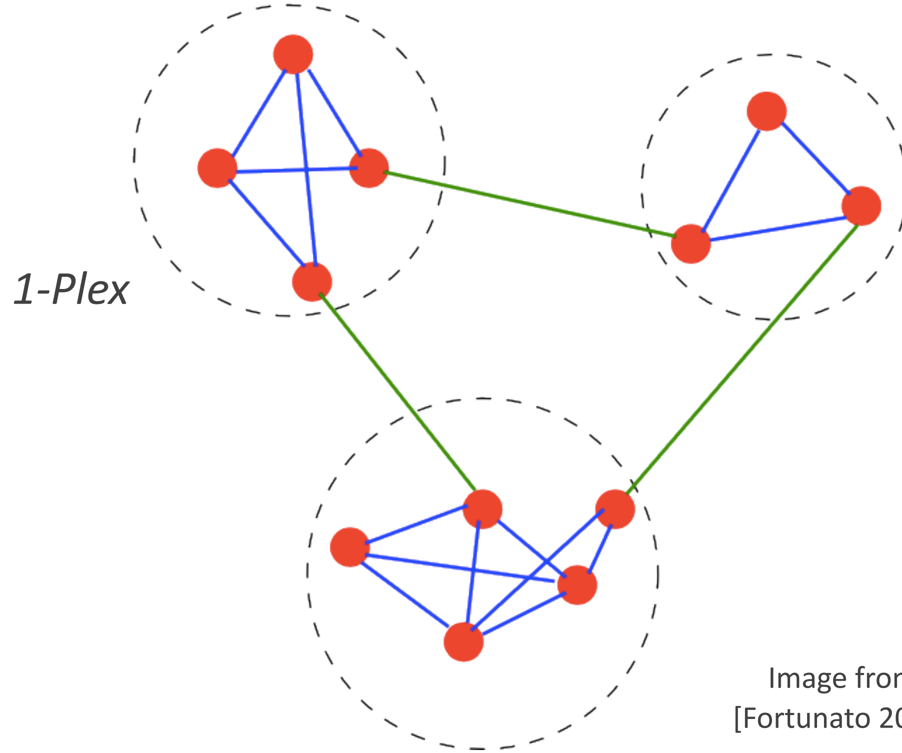

Image from [Fortunato 2009]

k-Plex:

A maximal subgraph in which each node is adjacent to all other nodes of the subgraph except at most k of them

Persistence and Complex Networks

Clustering Techniques:

Agglomerative (bottom-up)

Divisive (top-down)

approach based on

Centrality Measures

Atomic Communities

Quality Functions

Persistence and Complex Networks

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Agglomerative (bottom-up)

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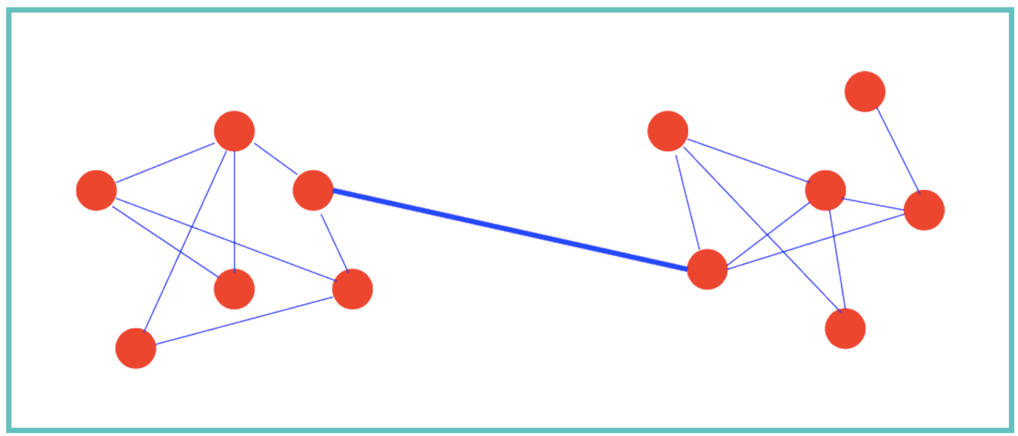
Girvan-Newman Algorithm:

Iterated removal of the edge with largest ***betweenness centrality***



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Persistence and Complex Networks

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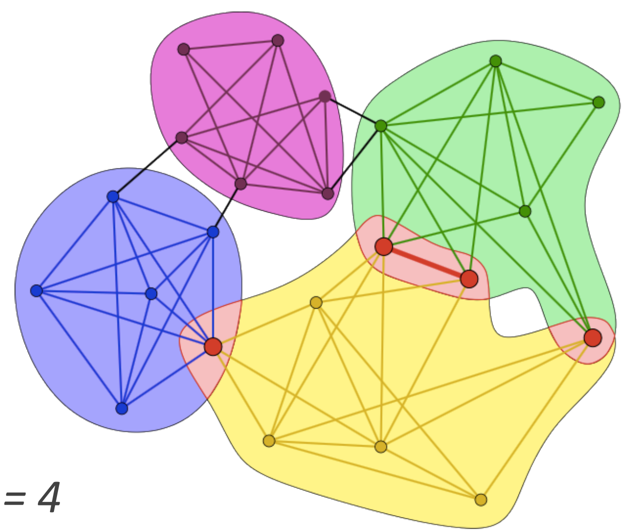
Clique Percolation:

k-adjacency: two cliques of size *k* are *k*-adjacent if they share *k-1* nodes

k-clique community: maximal union of cliques of size *k* pairwise connected by a sequence of *k*-adjacent cliques

Decomposition in *k*-clique communities



k = 4

Image from [Palla et al. 2005]

Persistence and Complex Networks

Clustering Techniques:

Agglomerative (bottom-up)

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Atomic Communities

Quality Functions

Modularity-based Algorithm:

Modularity: measure for clustering quality

Iterated aggregation of communities of nodes whose merging ***increases modularity***

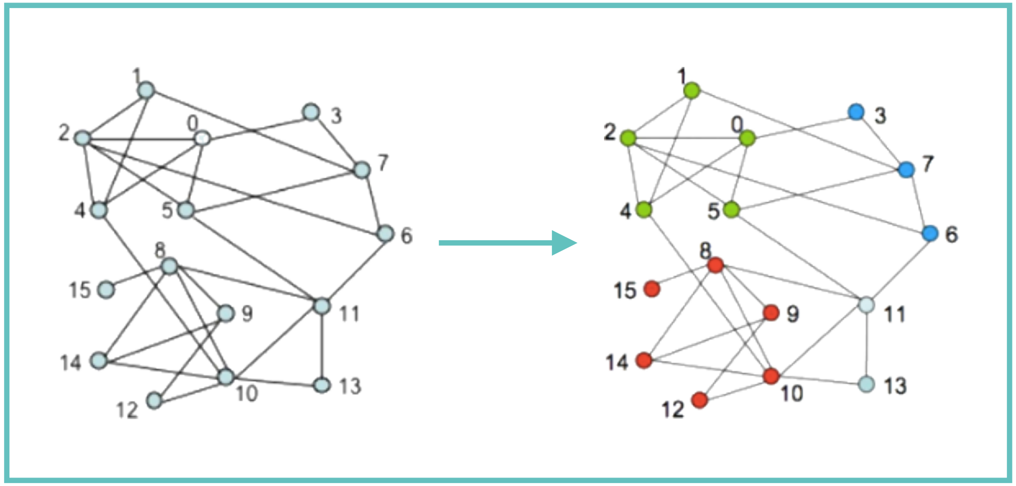


Image from [Blondel et al. 2008]

Persistence and Complex Networks

Several Application based on Persistent Homology:

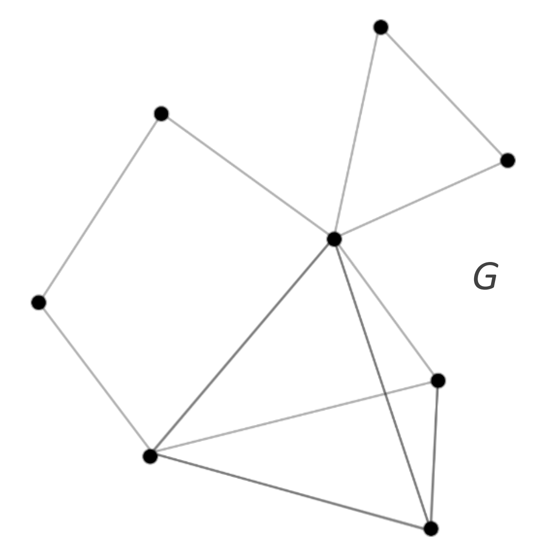
- ***Sensor*** Networks [De Silva 2013]
- ***Brain*** Networks [Lee et al. 2012]
- ***Collaborative/Co-occurence*** Networks [Carstens et al. 2013; Rieck et al. 2016]
- ***Geolocalized*** Networks [Fellegara et al. 2016]
- ...

Simplicial Complex Representation:

A network is represented through:

- Simplicial complex ***Flag(G)*** induced by *G*

Simplices of Flag(G) ⟷ *Cliques of G*



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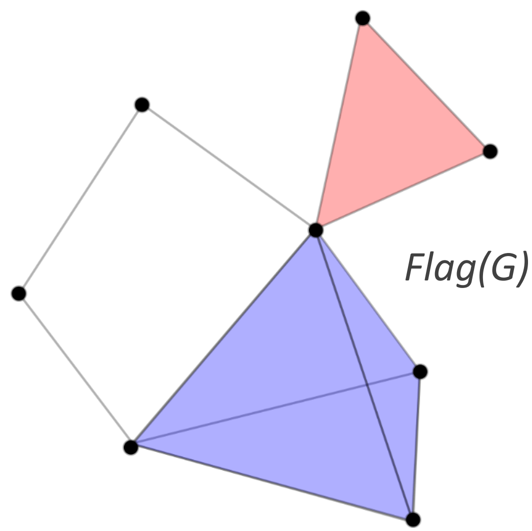
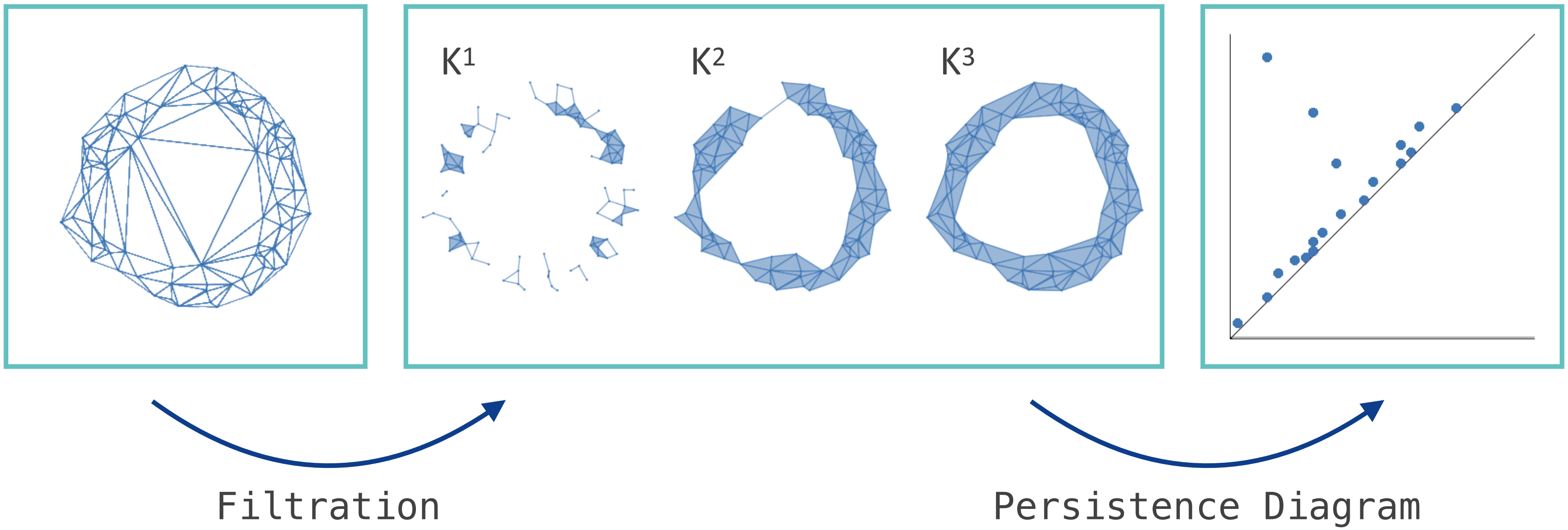
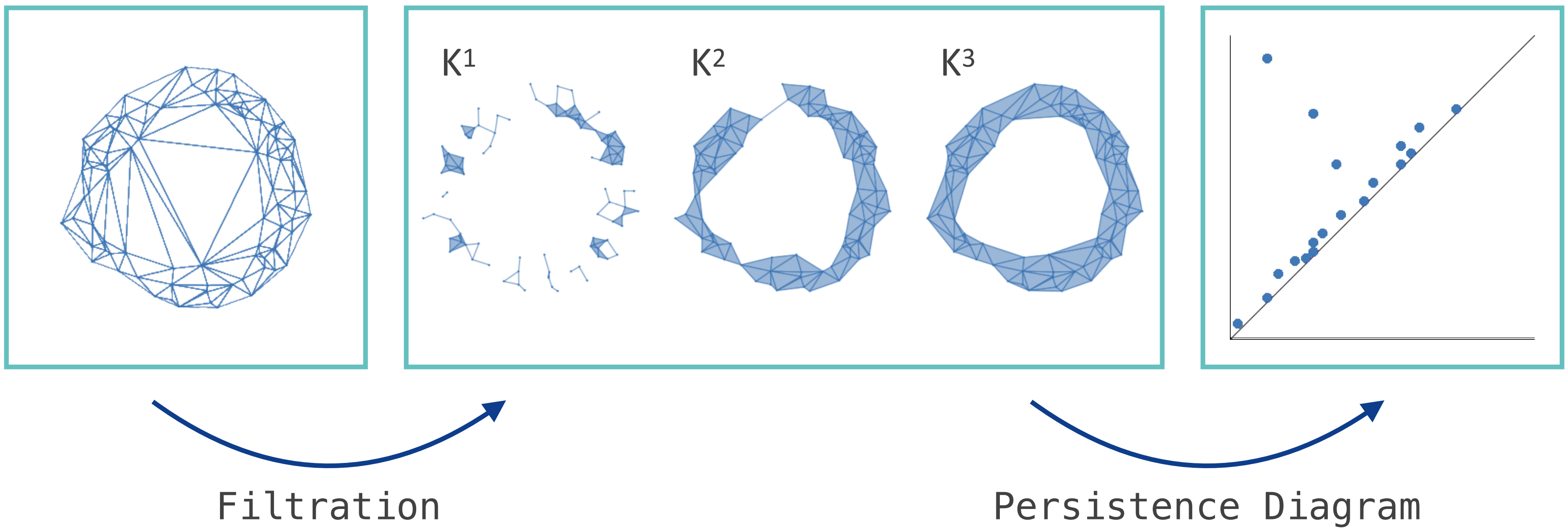


Persistence and Complex Networks



Topological summaries have proven to be particularly effective to ***distinguish networks***

Persistence and Complex Networks

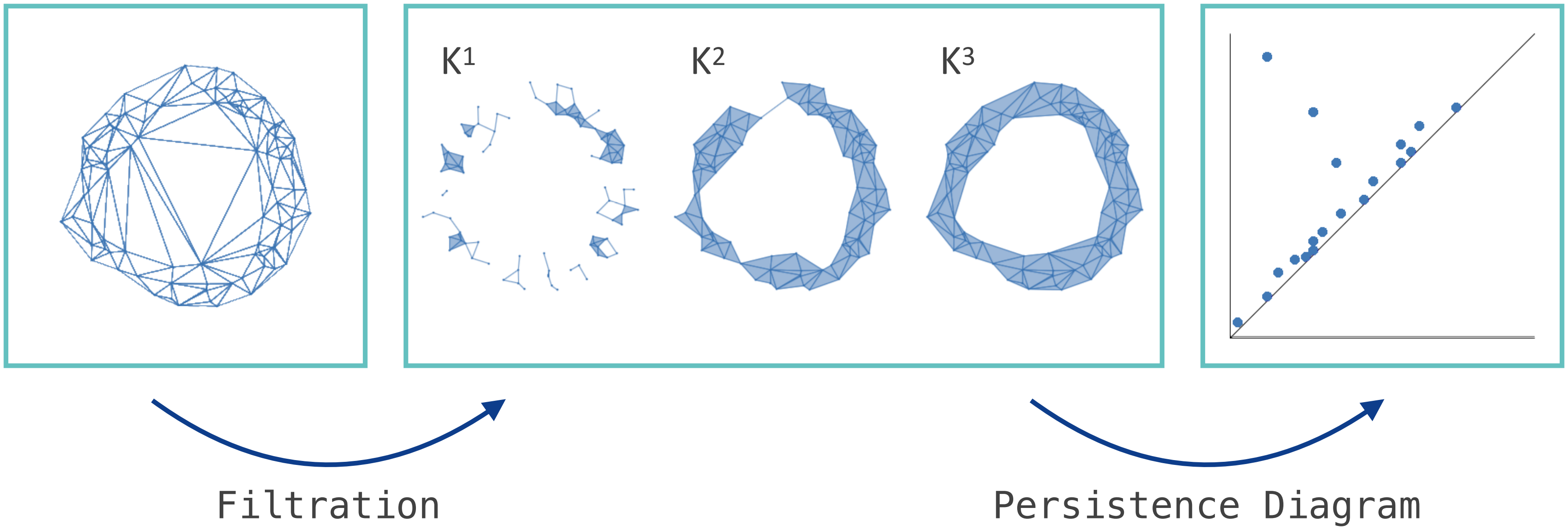


Topological summaries have proven to be particularly effective to ***distinguish networks***

but

It is hard to obtain a ***meaningful interpretation*** for homological cycles

Persistence and Complex Networks



Can we …

- visualize/localize the homological information through a graph?
- study the persistence of something different than homological cycles?

Persistence and Complex Networks

- *A Primer on Complex Networks*
- ***Homological Scaffolds***
- *Clique Community Persistence*

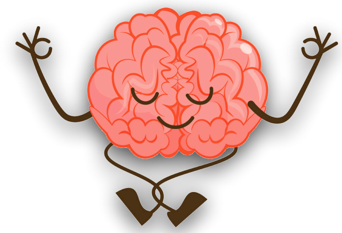
Persistence and Complex Networks

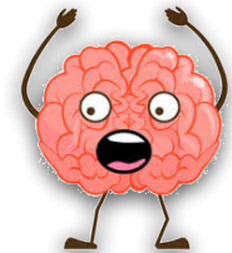
Dataset:

A collection of ***30 weighted graphs*** derived from ***fMRI*** (functional magnetic resonance imaging) obtained by scanning 15 different subjects

For each graph,

Nodes	$\Leftrightarrow$	***169** (Sub)Cortical **Brain Regions***
Arcs Weights	$\Leftrightarrow$	*(Inverse of) **Partial Correlations***





For each subject, 2 graphs obtained on 2 separate occasions, 14 days apart:

- ***Placebo*** (10 ml saline, intravenous injection) in one case
- ***Psilocybin*** (2 mg dissolved in 10 ml saline) in the other one

Goal:

Spot the differences between the two situations

Persistence and Complex Networks

Results: Applying the presented TDA pipeline, one obtains:

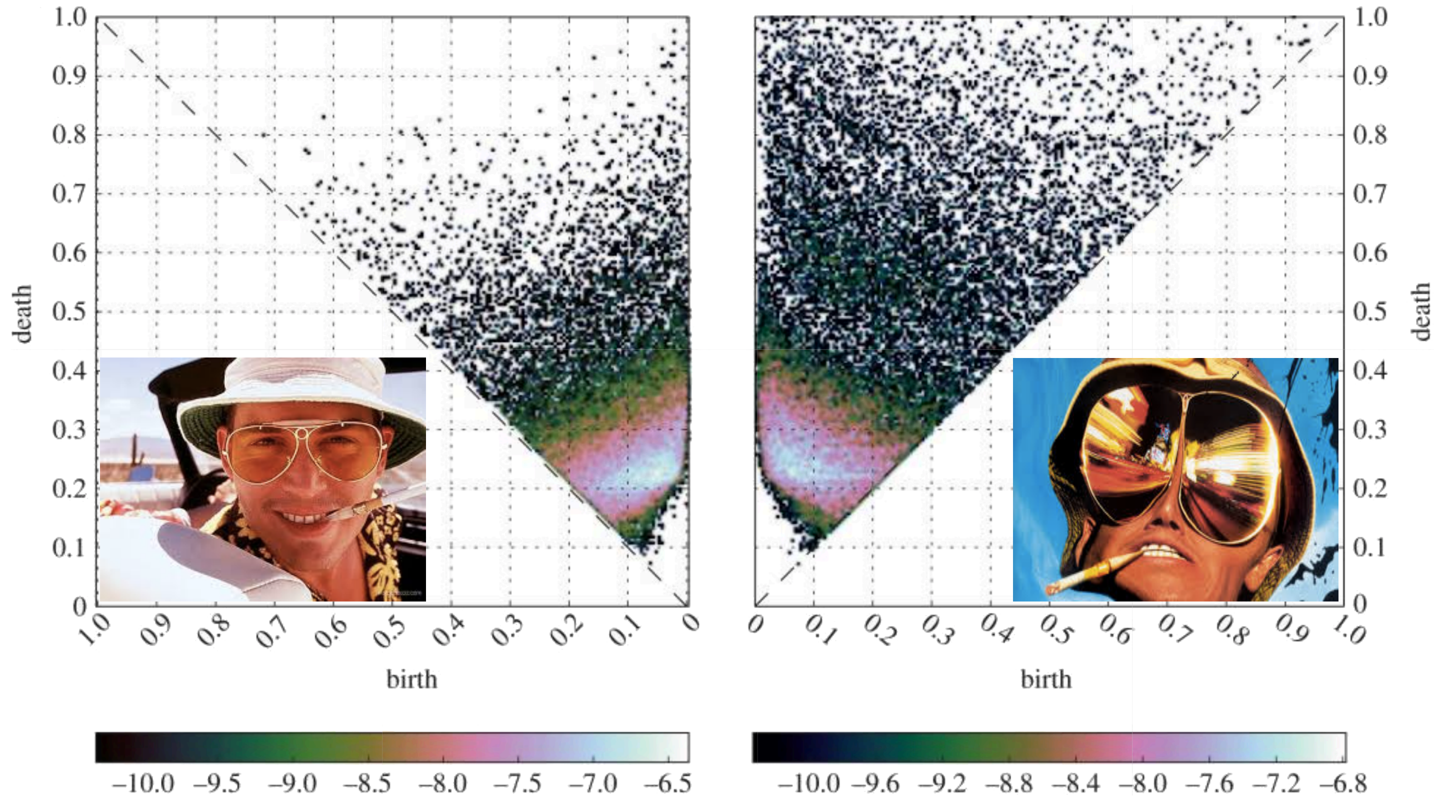


Image from [Petri et al. 2014]

(log-)Probability densities of H_1 for the placebo (left) and the psilocybin (right) groups

Persistence and Complex Networks

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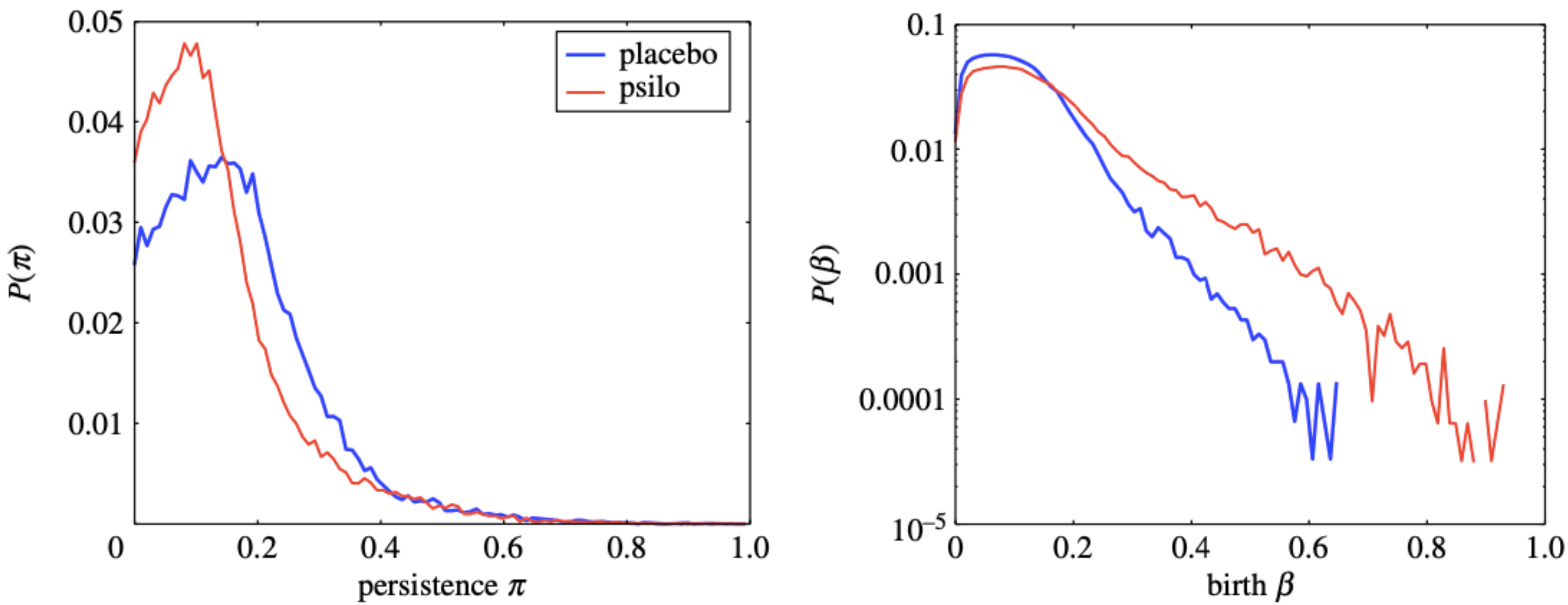


Image from [Petri et al. 2014]

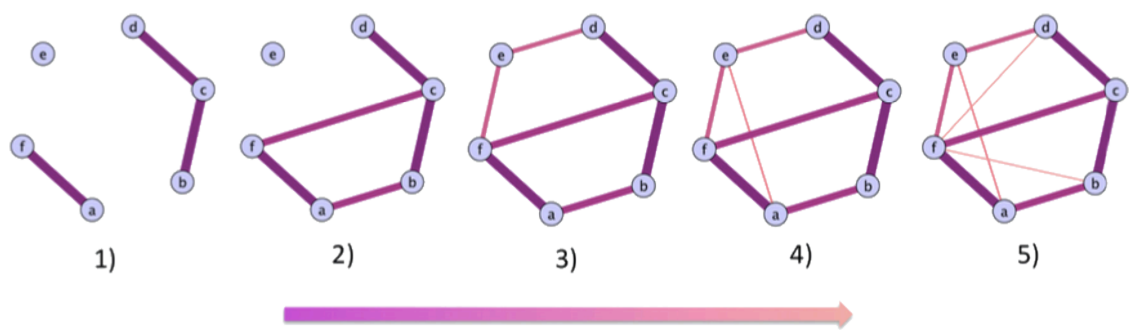
Persistence and birth distributions of H_1 for the placebo (blue) and the psilocybin (red) groups

Persistence and Complex Networks

Homological Scaffolds: *How to visualize/localize the homological information?*

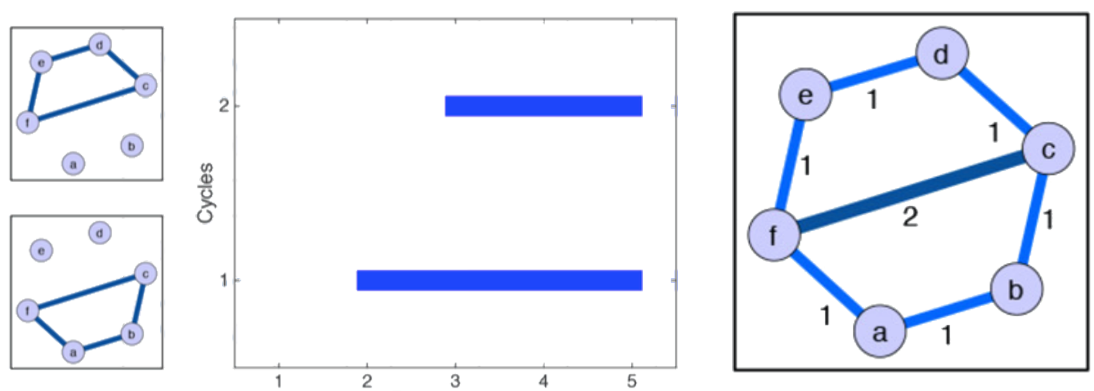
Let $g_1, g_2, \ldots, g_m$ be the representative cycles of H_1 occurring along the filtration of a weighted graph $G = (V, E, w: E \longrightarrow \mathbb{R})$, the ***frequency homological scaffold*** is the graph

$$H^f_G = (V, E, w^f: E \longrightarrow \mathbb{R})$$



defined by

$$w^f(e) = \#\{i \,|\, e \in g_i\}$$



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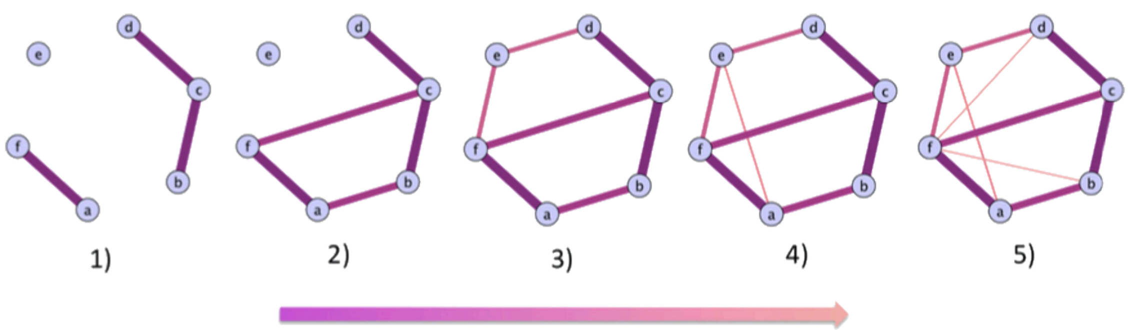
$$H^p{}_G = (V, E, w^p: E \longrightarrow \mathbb{R})$$



defined by

$$w^p(e) = \sum_{i \,|\, e \in g_i} \pi_{g_i}$$

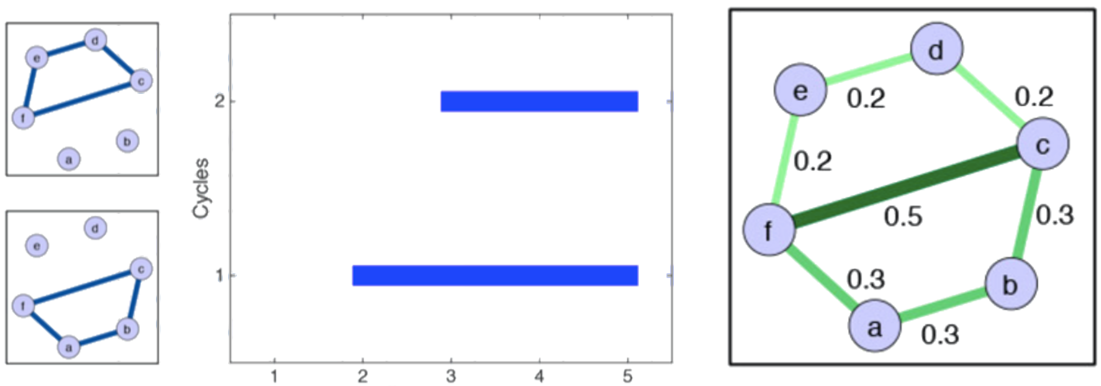


Image from [Lord et al. 2016]

Persistence and Complex Networks

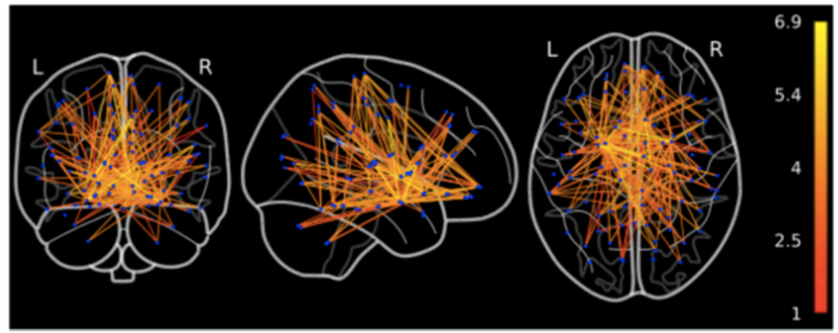
Homological Scaffolds:

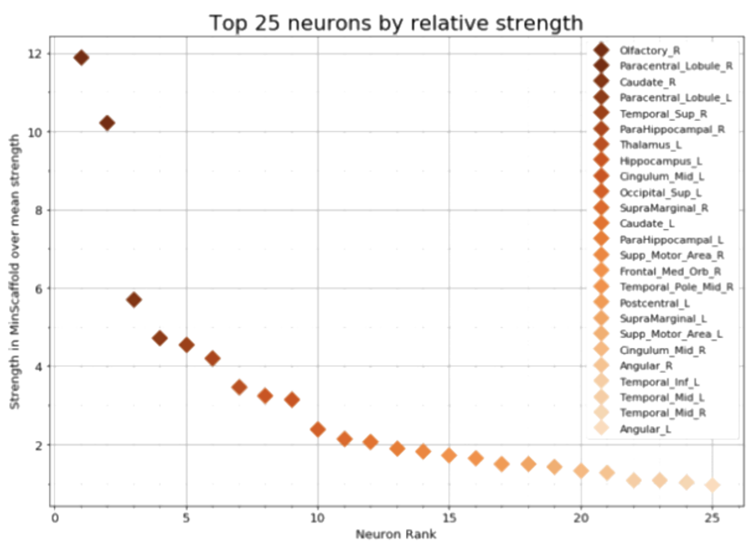
Image from [Petri et al. 2014]

Persistence homological scaffolds for the placebo (left) and the psilocybin (right) groups

Persistence and Complex Networks

Homological Scaffolds:





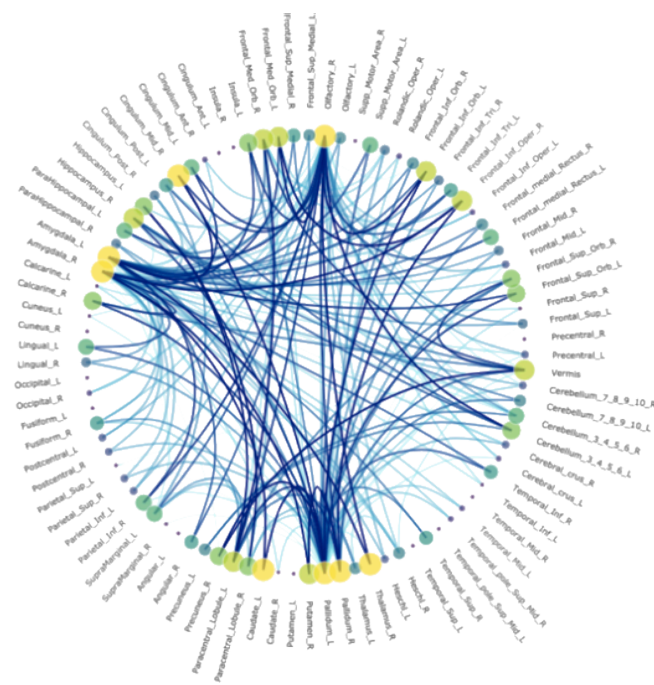


Image from [Guerra et al. 2021]

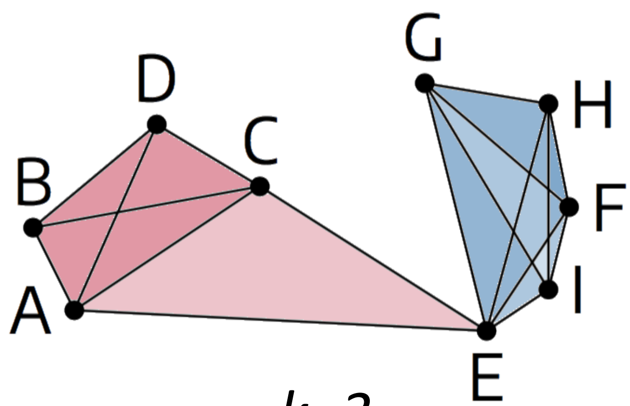
Persistence and Complex Networks

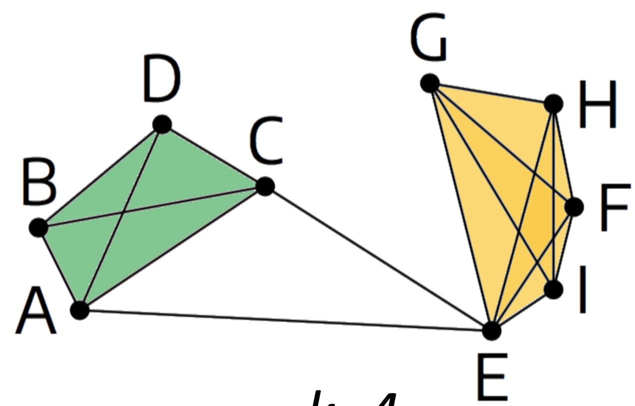
- *A Primer on Complex Networks*
- *Homological Scaffolds*
- ***Clique Community Persistence***

Persistence and Complex Networks

k-Clique Community:

A ***maximal union*** of *k*-cliques ***pairwise connected*** by a ***sequence of k-adjacent cliques***



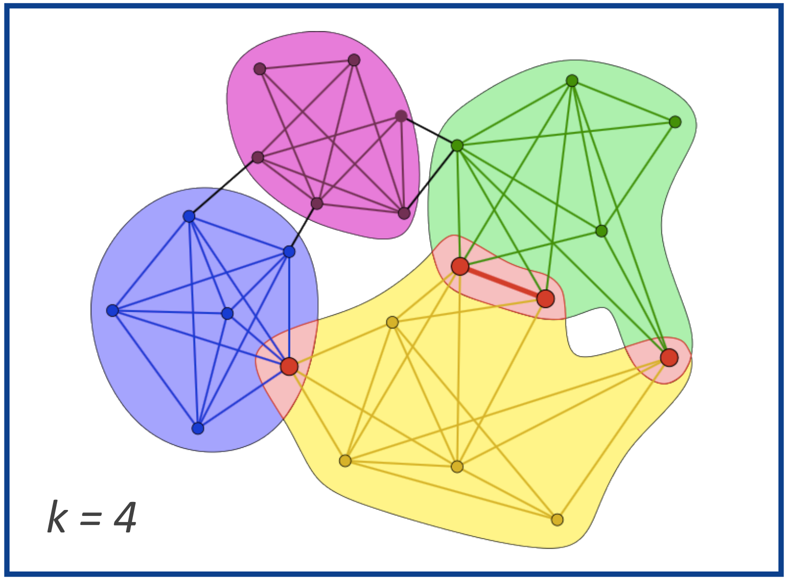


k-Adjacency:

Two *k*-cliques are ***k-adjacent*** if they ***share k-1 nodes***

Persistence and Complex Networks

k-Clique Community Decomposition:

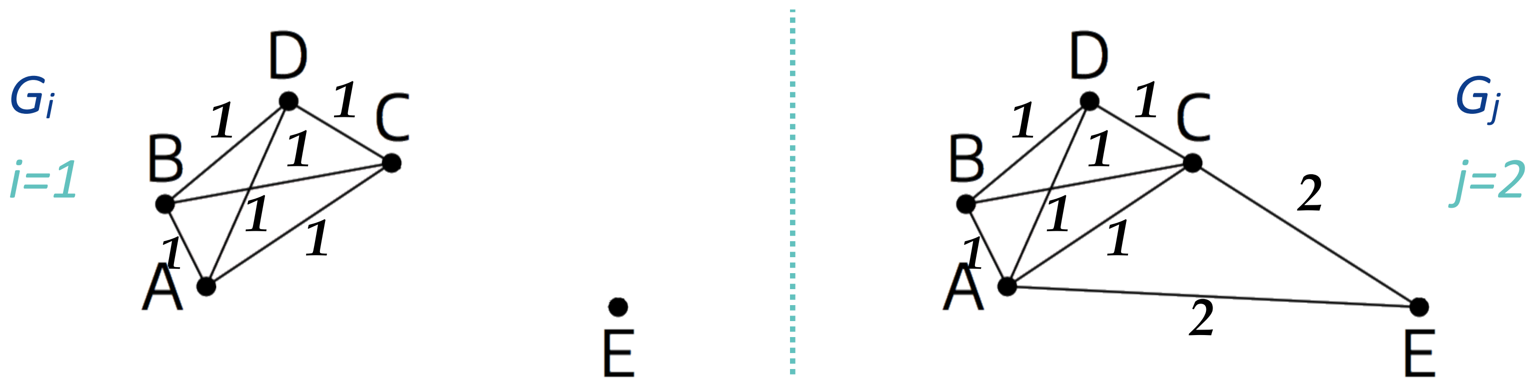


- Reveal ***highly connected*** communities
- Allow ***overlaps***
- Have a ***hierarchical structure***

Persistence and Complex Networks

Clique Communities and Weighted Networks:

Given a weighted network ***G*** and two threshold values ***i*** < ***j***,

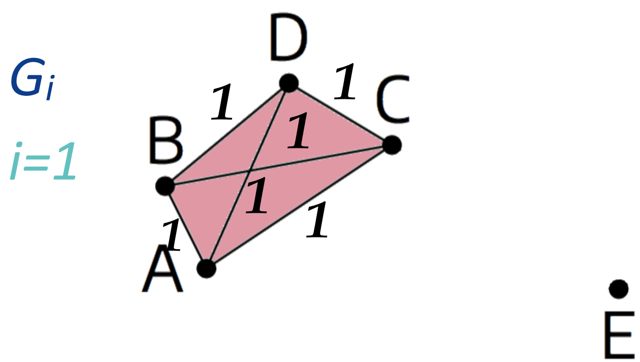


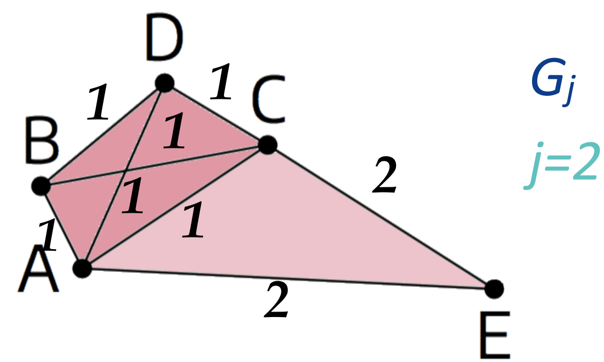
G_i is contained in G_j

Persistence and Complex Networks

Clique Communities and Weighted Networks:

Given a weighted network ***G*** and two threshold values ***i < j***,





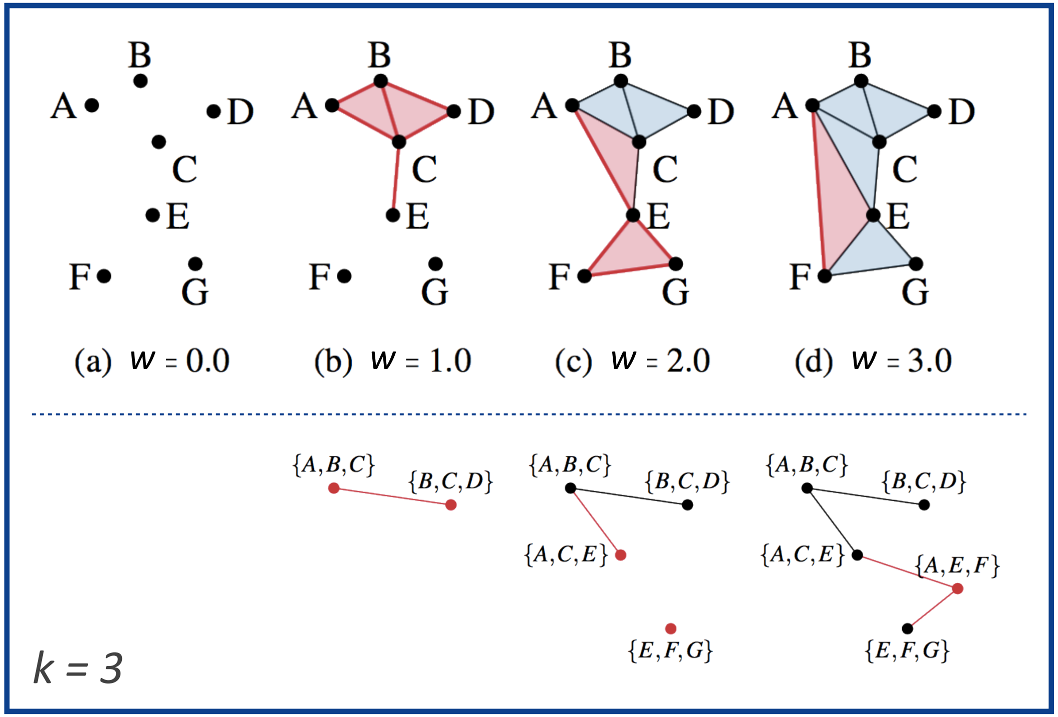
Each k-clique community of G_i is ***contained*** in ***exactly one*** k-clique community of G_j

Persistence and Complex Networks

Clique Community Persistence:

Fixing a value for k and varying the edge-weight threshold, the **persistence** of **k-clique communities** of G can be tracked by:

- Building a sequence of *k*-dual graphs:
  - ***vertices ⟷ k-cliques***
  - ***edges ⟷ adjacent k-cliques***
- Tracking the ***connected components*** of the sequence of *k*-dual graphs



Persistence and Complex Networks

Clique Community Persistence:

The presented approach allows for designing tools for:

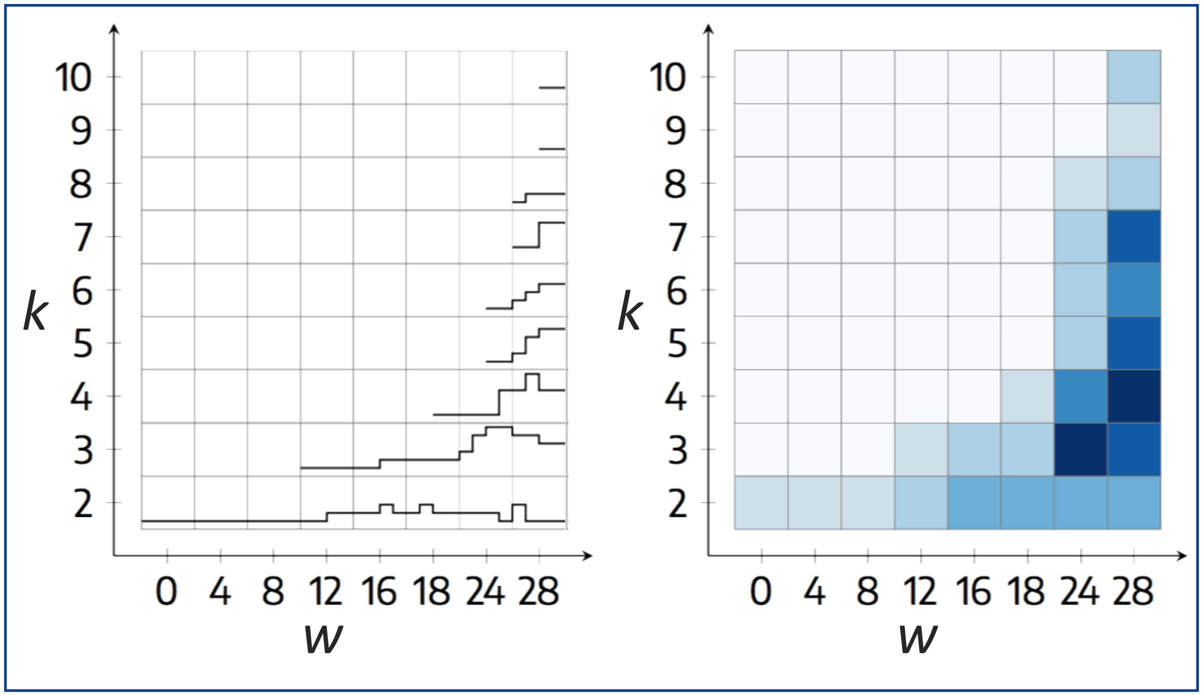
- ***Network Comparison***
  - ***Comparison Measures***
    - ***Persistence Indicator Function (PIF)***
    - ***PIF-based distance***
  - Clique Community ***Centrality Measure***
- ***Single Network Analysis***
  - ***Interactive Visualization Tool*** based on Nested Graphs

Persistence and Complex Networks

Persistence Indicator Function: Defined as the function $f_k : \mathbb{R} \longrightarrow \mathbb{N}$

assigning:

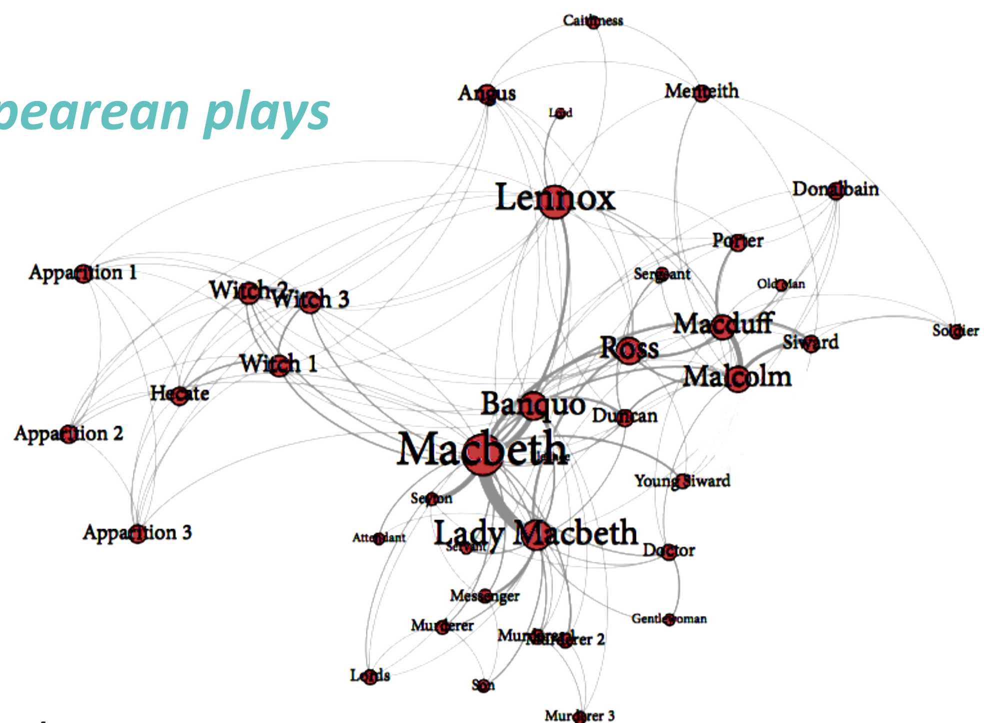
w $\longmapsto$ ***# k-cliques communities "alive" at threshold w***



Persistence and Complex Networks

Persistence Indicator Function:

- ***Co-occurrence networks*** of ***Shakespearean plays***
  - *37 plays considered*

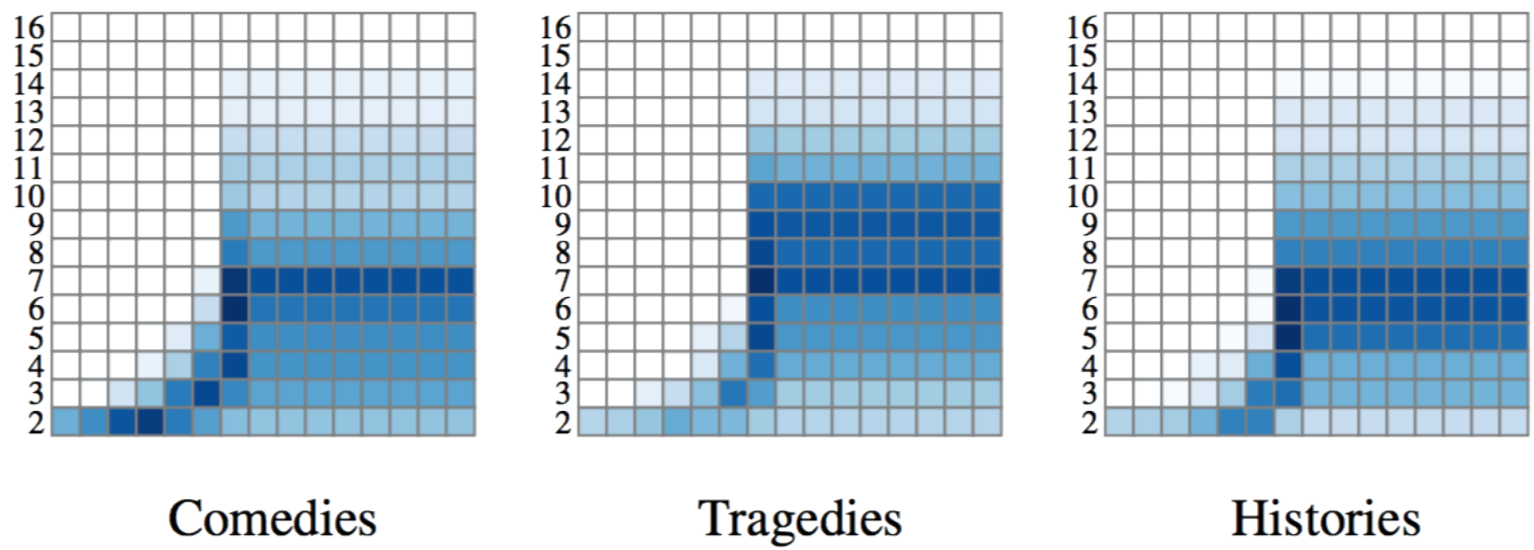


- In each network:
  - ***nodes*** ⟷ ***characters*** *of the play*
  - ***edges*** ⟷ *characters appearing in the* ***same scene***
  - ***edge weight*** ⟷ *inverse of the* ***number of interactions***

Persistence and Complex Networks

Persistence Indicator Function:

PIF enables a comparison of structural differences between groups of plays



Persistence and Complex Networks

PIF-Based Distance:

Given two persistence indicator functions f and g,

PIF-based distance *is defined to be the L^p distance between f and g:*

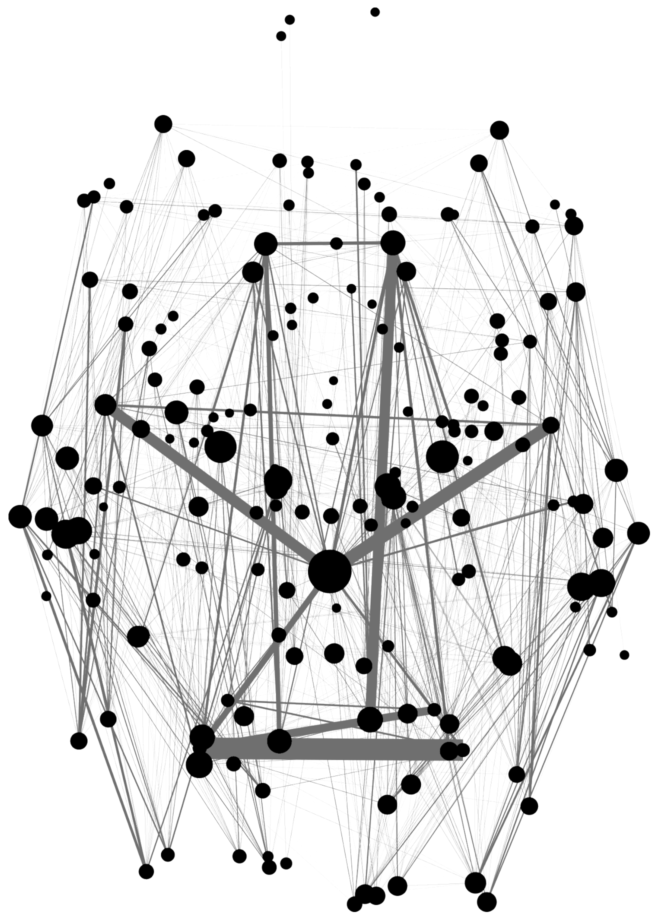
$$dist(f,g) = \left(\int_{\mathbb{R}} |f(x) - g(x)|^p \, dx \right)^{\frac{1}{p}}$$

- Quantifies dissimilarities between PIFs
- Easier to be computed than Wasserstein and bottleneck distances
- Highly correlated to Wasserstein distance

Persistence and Complex Networks

PIF-Based Distance:

- ***Biological networks*** representing variants of ***human brain connectivity***
  - *9 instances considered*

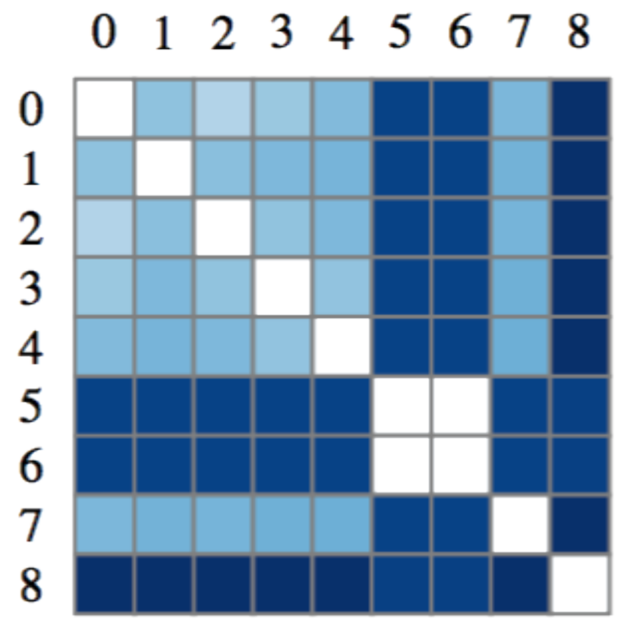


- In each network:
  - ***nodes*** $\leftrightarrow$ ***brain areas***
  - ***edges*** $\leftrightarrow$ ***fibers connecting different areas***

Persistence and Complex Networks

PIF-Based Distance:

Variant	Density	Diam. (weighted)	Avg. degree (weighted)
0	0.125	4 (60.0)	21.21 (2300.3)
1	0.124	4 (60.0)	21.06 (2296.0)
2	0.124	4 (60.0)	21.13 (2295.2)
3	0.124	4 (60.0)	21.16 (2282.0)
4	0.124	4 (60.0)	21.15 (2279.3)
5	0.125	4 (60.0)	21.19 (2264.0)
6	0.125	4 (60.0)	21.19 (2264.0)
7	0.124	4 (60.0)	21.16 (2279.6)
8	0.125	4 (60.0)	21.20 (2257.5)



PIF-based distance reveals differences between networks that common graph measures are incapable of detecting

Persistence and Complex Networks

Clique Community Centrality:

Clique community centrality of a node *v* is defined as

$$centrality(v) = \sum_{C \ni v} pers(C)$$

where:

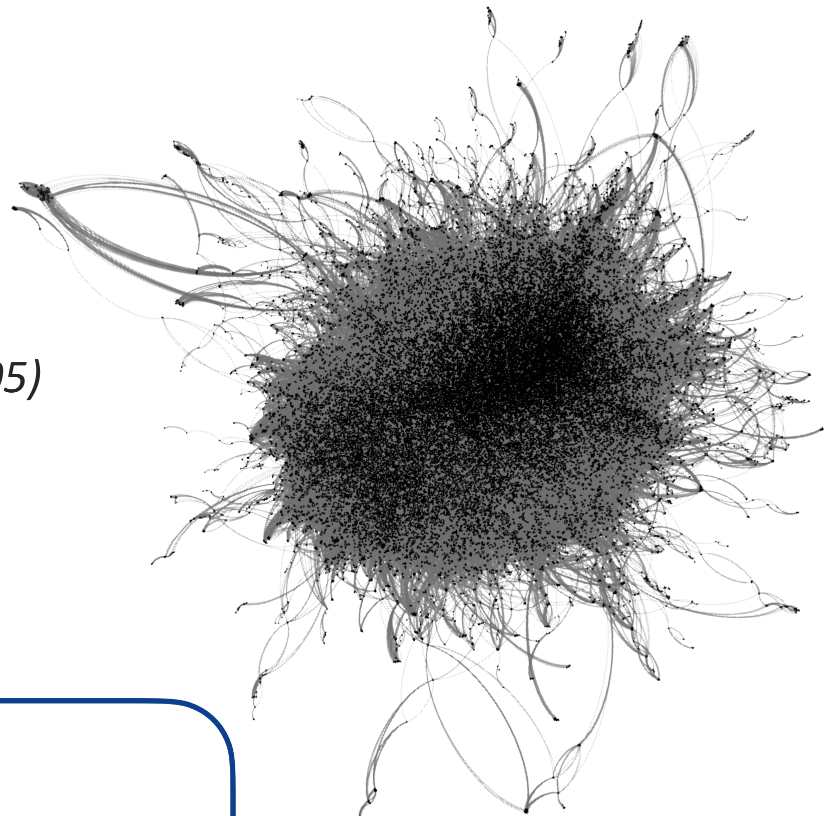
- C is any clique community containing *v*
- ***pers(C)*** is the “lifespan” of C

*Nodes belonging to high-persistence communities are identified as **relevant***

Persistence and Complex Networks

Clique Community Centrality:

- ***Collaborative networks*** describing ***scientist co-authorship of the "Condensed Matter"*** arXiv category
  - *3 snapshots in time considered (1999, 2003, 2005)*
- Network sizes:
  - ***16K - 40K*** *nodes*
  - ***47K - 175K*** *edges*

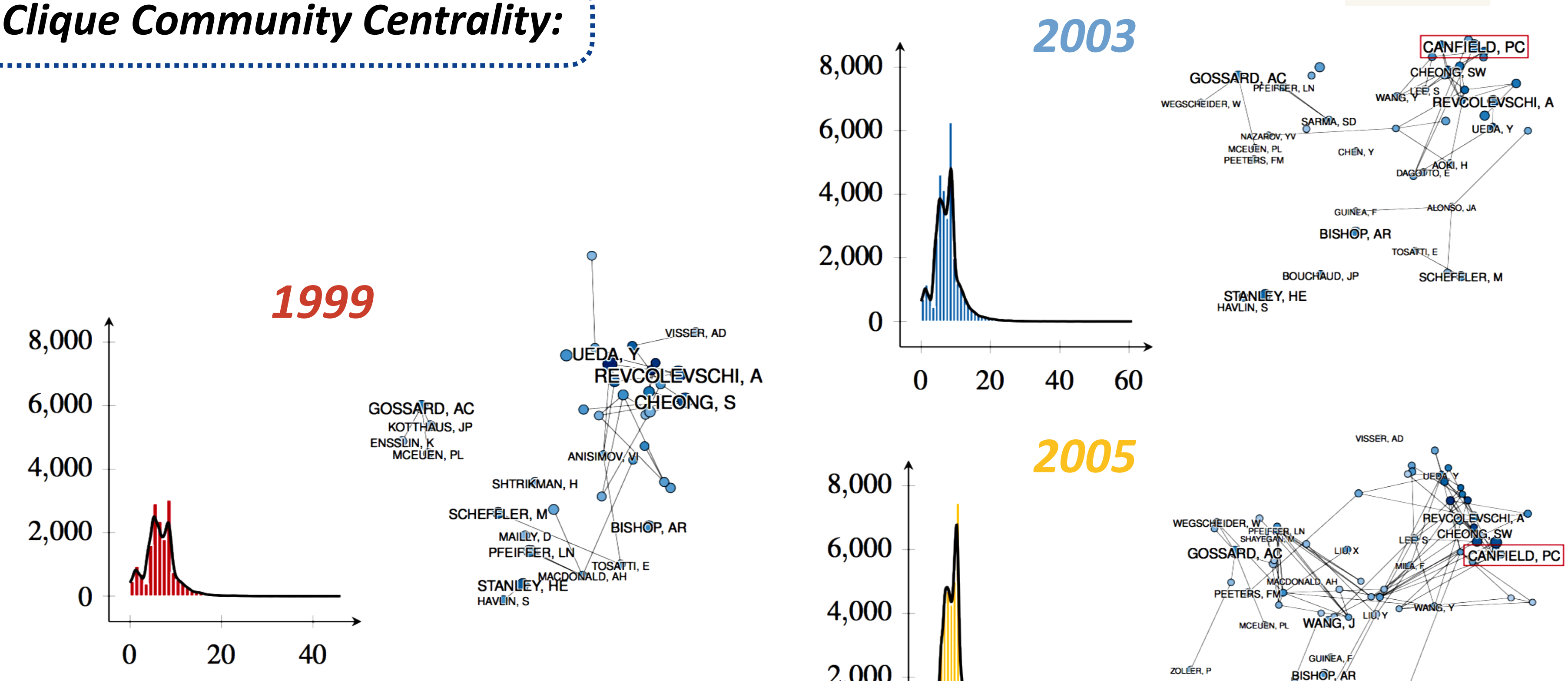


Clique community centrality allows for

- *evaluating the* ***evolution of network connectivity***
- *filtering away the* ***less relevant nodes***

Persistence and Complex Networks

Clique Community Centrality:



Density estimates of the clique community centrality values

Persistence and Complex Networks

Clique Community Persistence:

The presented approach allows for designing tools for:

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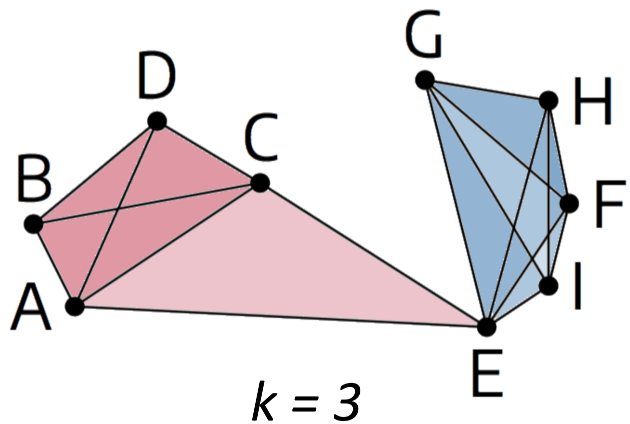
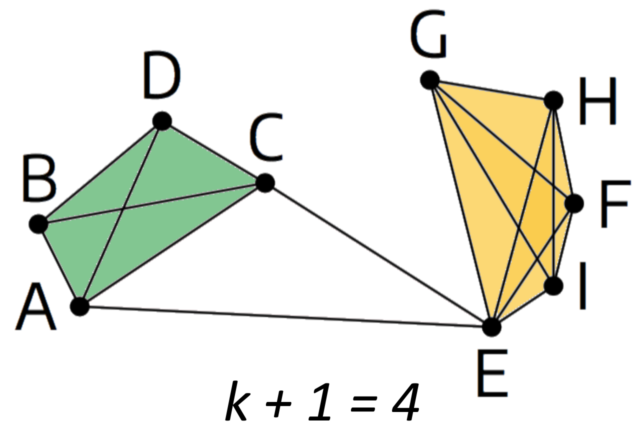
  - Clique Community ***Centrality Measure***
- ***Single Network Analysis***
  - ***Interactive Visualization Tool*** based on Nested Graphs

Persistence and Complex Networks

Clique Communities and Multiple k-Values:

Given a weighted network ***G*** and any threshold value ***i***,



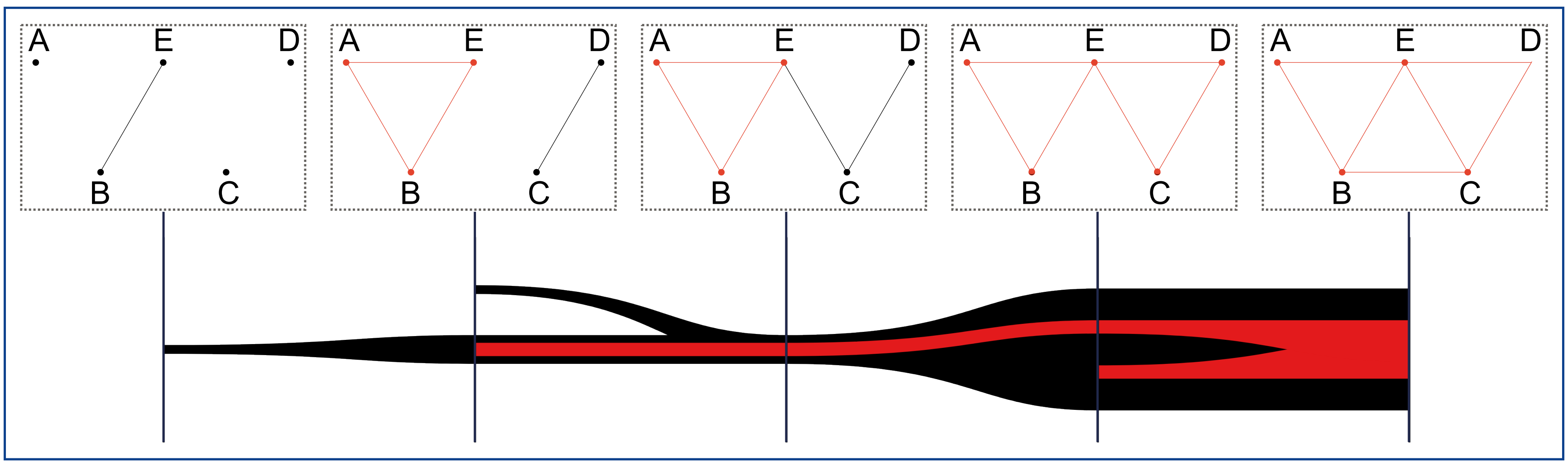


Each *(k+1)*-clique community of G_i is **contained** in ***exactly one*** *k*-clique community of G_i

Persistence and Complex Networks

Nested Graph:

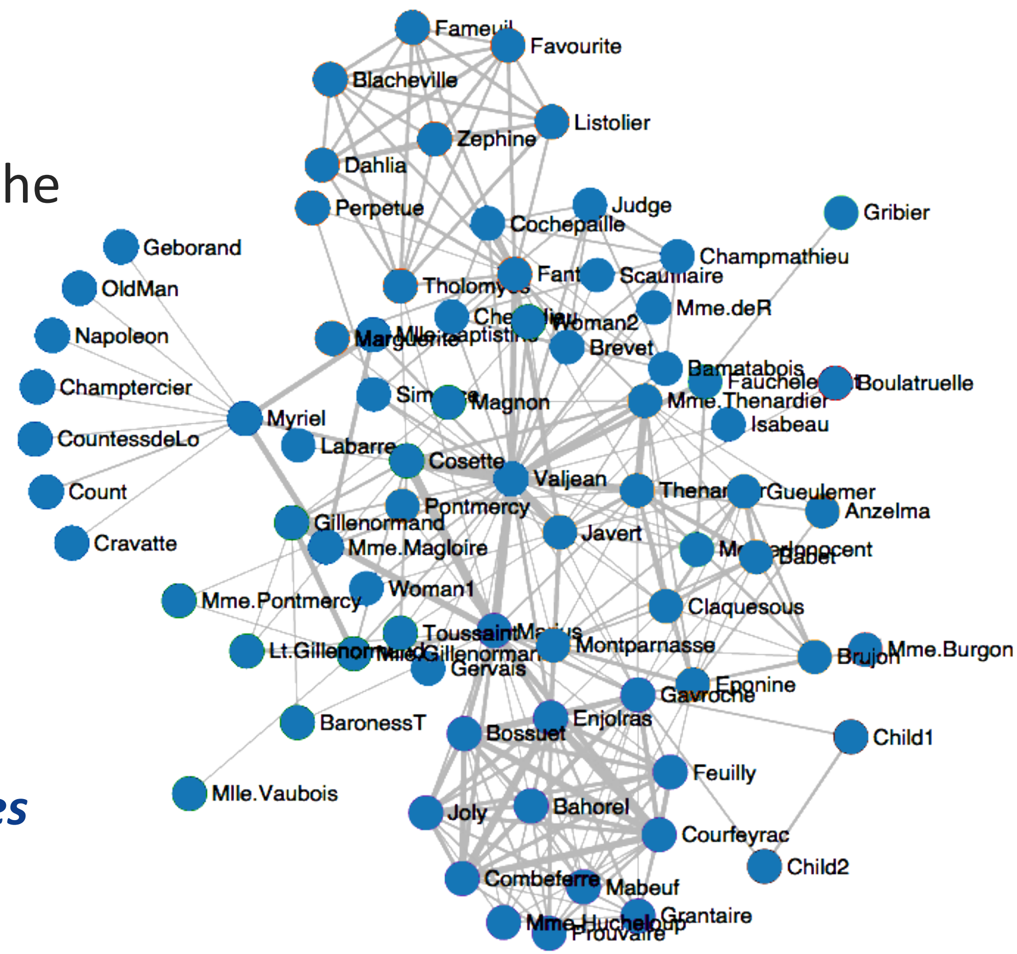
- Originally defined for connected components in scalar fields [Lukasczyk et al. 2017]
- Illustrates ***evolutions across two parameters***



Persistence and Complex Networks

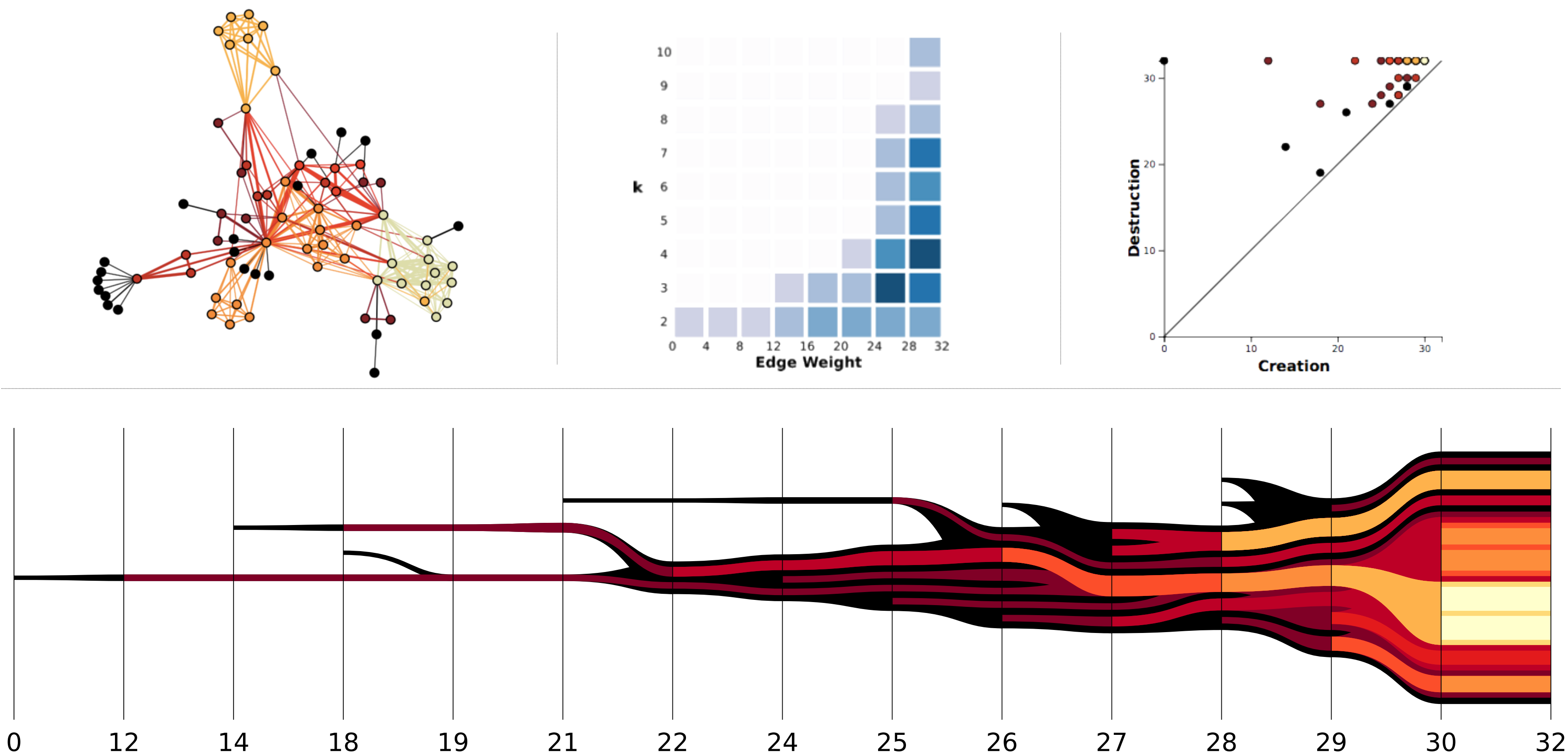
Nested Graph:

- ***Co-occurrence network*** between the characters in **Victor Hugo's novel** ***"Les Misérables"***
  - *77 nodes*
  - *254 edges*



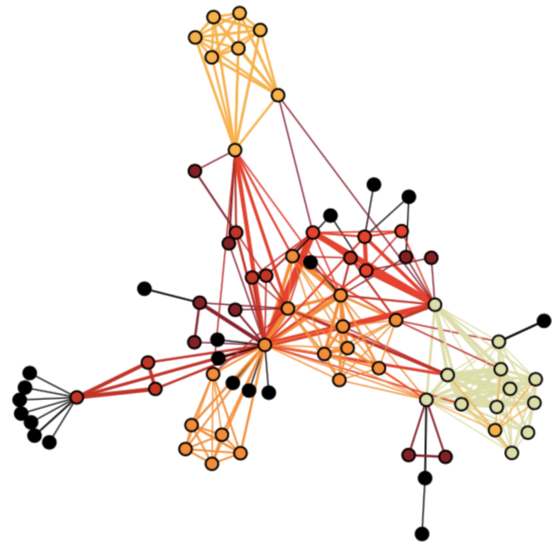
- ***edge weight*** ↔ ***1 / # co-occurrences***

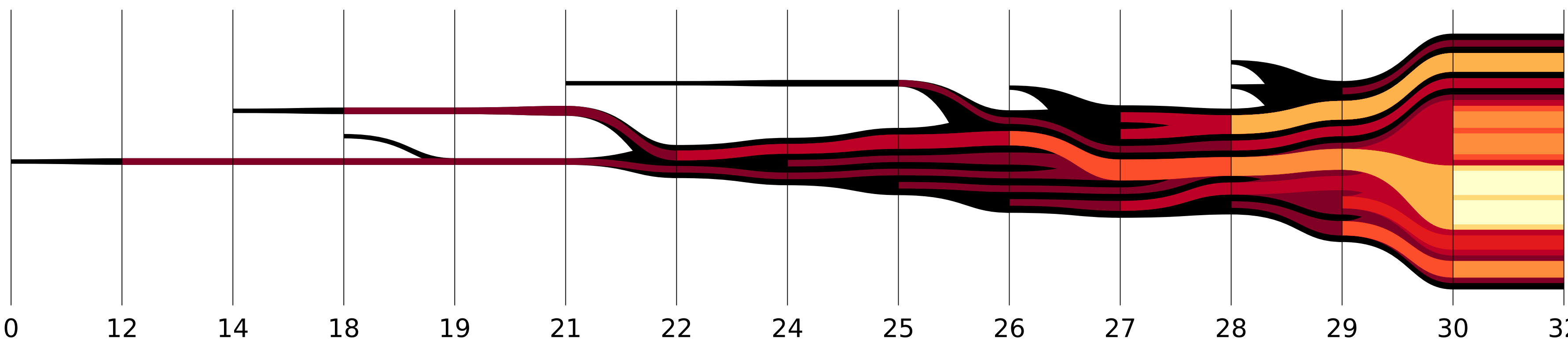
Persistence and Complex Networks



Persistence and Complex Networks

Nested-based visualization tool allows the user for

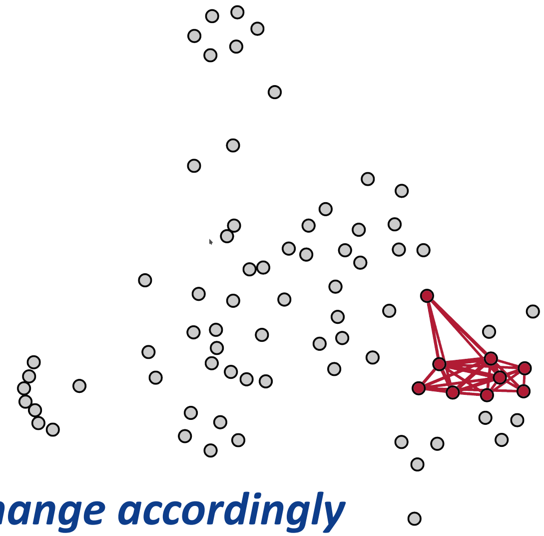




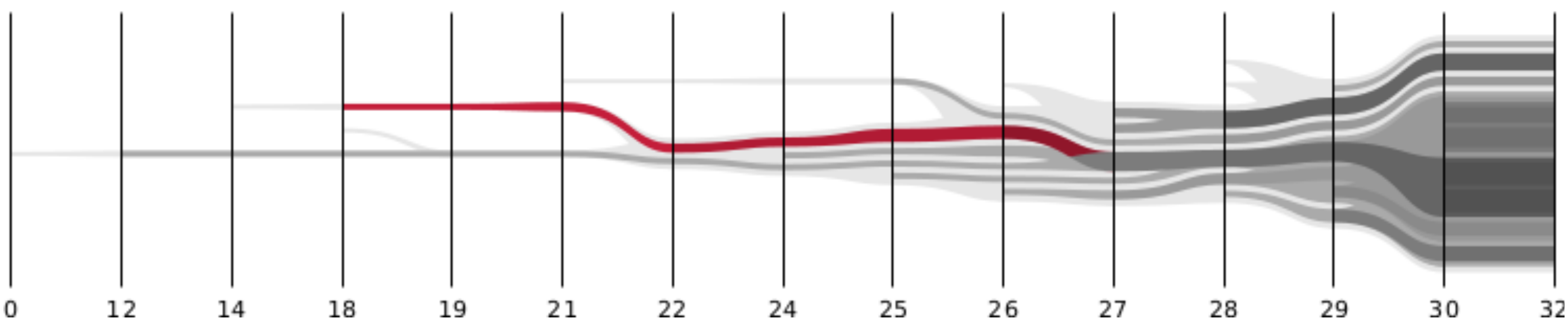
Persistence and Complex Networks

Nested-based visualization tool allows the user for

- ***focusing on*** *the evolution of a* ***specific clique community***
- ***selecting*** *and* ***interactivity exploring different edge weights*** *and* ***clique degrees***



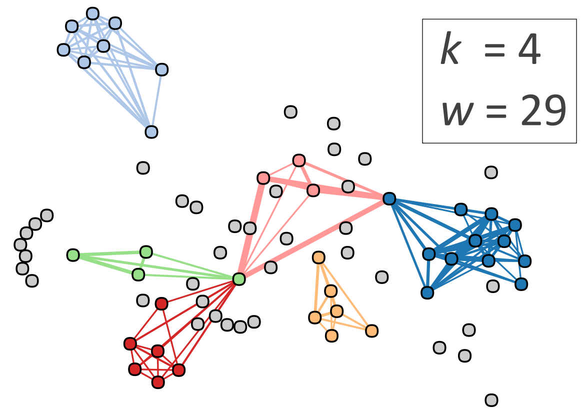
while the force-directed graph layout and the nested graph ***change accordingly***



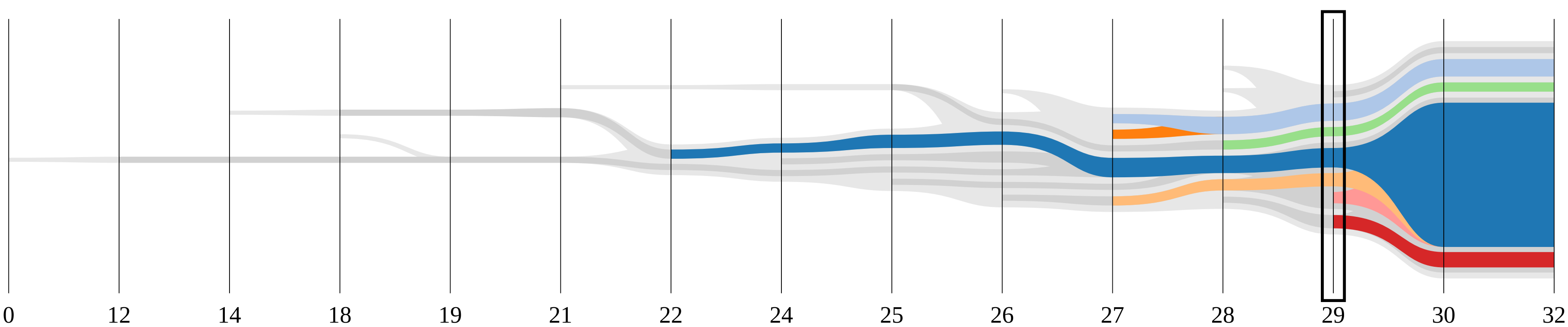
Persistence and Complex Networks

Nested-based visualization tool allows the user for

- *focusing on the evolution of a specific clique community*
- ***selecting** and **interactivity exploring different edge weights** and **clique degrees***



while the force-directed graph layout and the nested graph ***change accordingly***



Persistence and Complex Networks

Nested-based visualization tool allows the user for

- ***focusing on*** *the evolution of a* ***specific clique community***
- ***selecting*** *and* ***interactivity exploring different edge weights*** *and* ***clique degrees***

while the force-directed graph layout and the nested graph ***change accordingly***

Intuitively:

edge-weight *variation*	⟷	*reveal the* ***core part of a community***
clique-degree *variation*	⟷	*analyze* ***community according to different granularities***

Bibliography

General References:

- *Books on TDA:*
  - A. J. Zomorodian. ***Topology for computing.*** Cambridge University Press, 2005.
  - H. Edelsbrunner, J. Harer. ***Computational topology: an introduction***. American Mathematical Society, 2010.
  - R. W. Ghrist. ***Elementary applied topology***. Seattle: Createspace, 2014.
- *Papers on TDA:*
  - G. Carlsson. ***Topology and data***. Bulletin of the American Mathematical Society 46.2, pages 255-308, 2009.

Today's References:

- *Complex Networks:*
  - G.Palla, I.Derényi, I. Farkas, T. Vicsek. ***Uncovering the overlapping community structure of complex networks in nature and society.*** Nature, 435.7043, pages 814-818, 2005.
  - S. Fortunato. ***Community detection in graphs.*** Physics Reports, 486(3-5), pages 75-174, 2010.
  - J. Scott. ***Social network analysis.*** SAGE Publications Ltd, 2017.
  - M. Newman. ***Networks.*** Oxford university press, 2018.

Bibliography

Today's References:

- ***Homological Scaffolds:***
  - G. Petri, P. Expert, F. Turkheimer, R. Carhart-Harris, D. Nutt, P. J. Hellyer, F. Vaccarino. ***Homological scaffolds of brain functional networks.*** Journal of The Royal Society Interface, 11.101, 20140873, 2014.
  - L. D. Lord, et al. ***Insights into brain architectures from the homological scaffolds of functional connectivity networks.*** Frontiers in systems neuroscience, 10.85, 2016.
  - M. Guerra, A. De Gregorio, U. Fugacci, G. Petri, F. Vaccarino. ***Homological scaffold via minimal homology bases.*** Scientific Reports, 11.1, pages 1-17, 2021.
- ***Clique Community Persistence:***
  - B. Rieck, U. Fugacci, J. Lukasczyk, H. Leitte. ***Clique community persistence: a topological visual analysis approach for complex networks.*** IEEE Transactions on Visualization and Computer Graphics, 24.1, pages 822-831, 2018.