Network Construction, Inference, and Deconvolution

CS224W: Analysis of Networks
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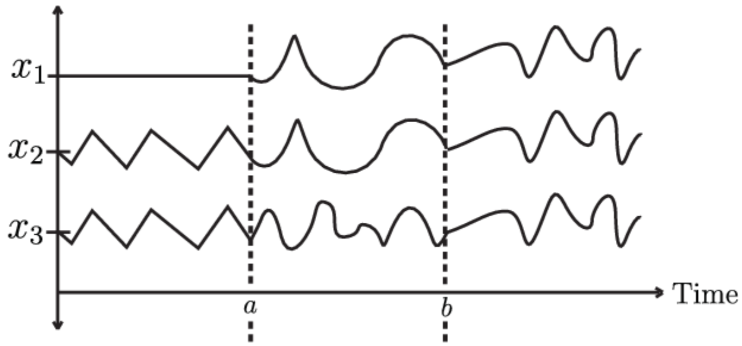
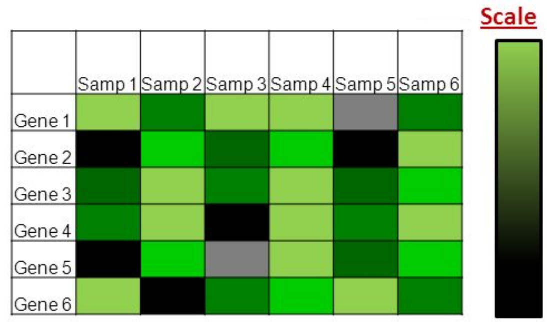
http://cs224w.stanford.edu

Raw Data are often not Networks






[–] Affable_Nitwit 559 points 15 hours ago
NOW That's What I Call Music. We're on 53, everybody. I checked. Online.
permalink save report give gold reply

[–] AggressiveToothbrush 165 points 15 hours ago
For the record, as of May 4th, we're on 54.
http://en.wikipedia.org/wiki/Now_That%27s_What_I_Call_Music!_54_%28U.S._series%2
permalink save parent report give gold reply

[–] summitorother 224 points 15 hours ago
Speak for yourselves, the UK is on 90.
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[–] anideaguy 206 points 10 hours ago
TIL 54 is 90 in metric.
permalink save parent report give gold reply

[–] LumberCockSucker 11 points 3 hours ago
The Uk uses imperial measurements
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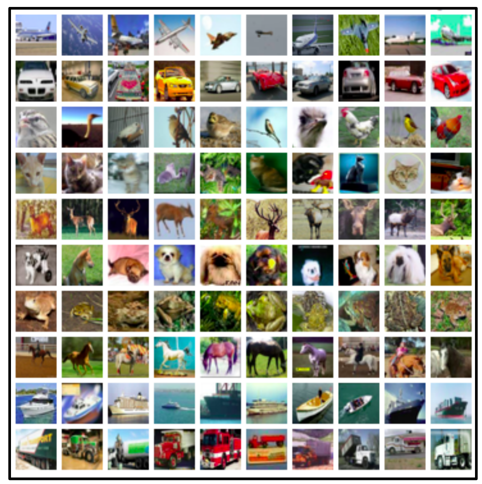
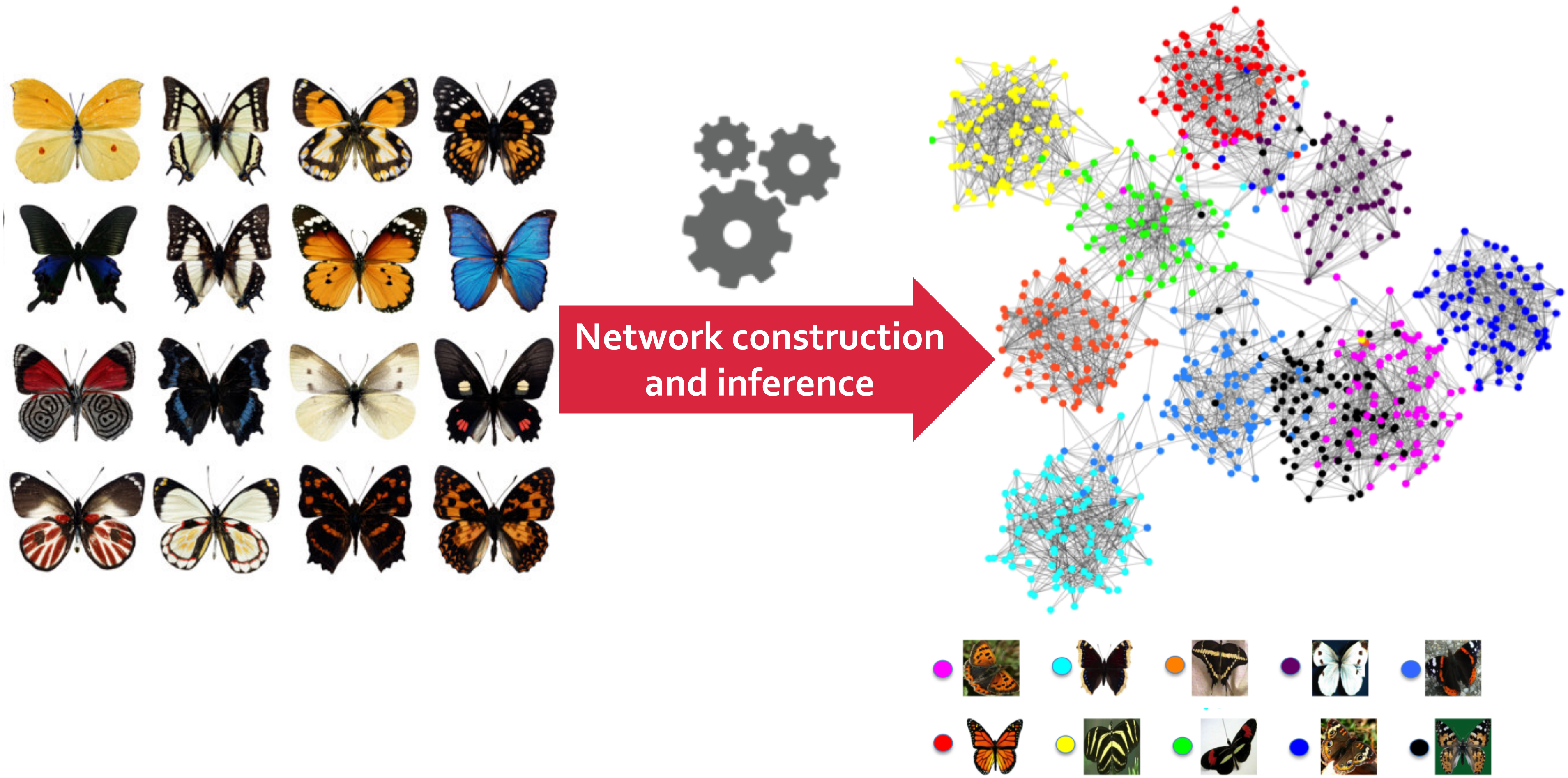


	1	2	3	4	5	6	7	8	9
man	1	0	0	0	0	0	0	0	0
woman	0	1	0	0	0	0	0	0	0
boy	0	0	1	0	0	0	0	0	0
girl	0	0	0	1	0	0	0	0	0
prince	0	0	0	0	1	0	0	0	0
princess	0	0	0	0	0	1	0	0	0
queen	0	0	0	0	0	0	1	0	0
king	0	0	0	0	0	0	0	1	0
monarch	0	0	0	0	0	0	0	0	1

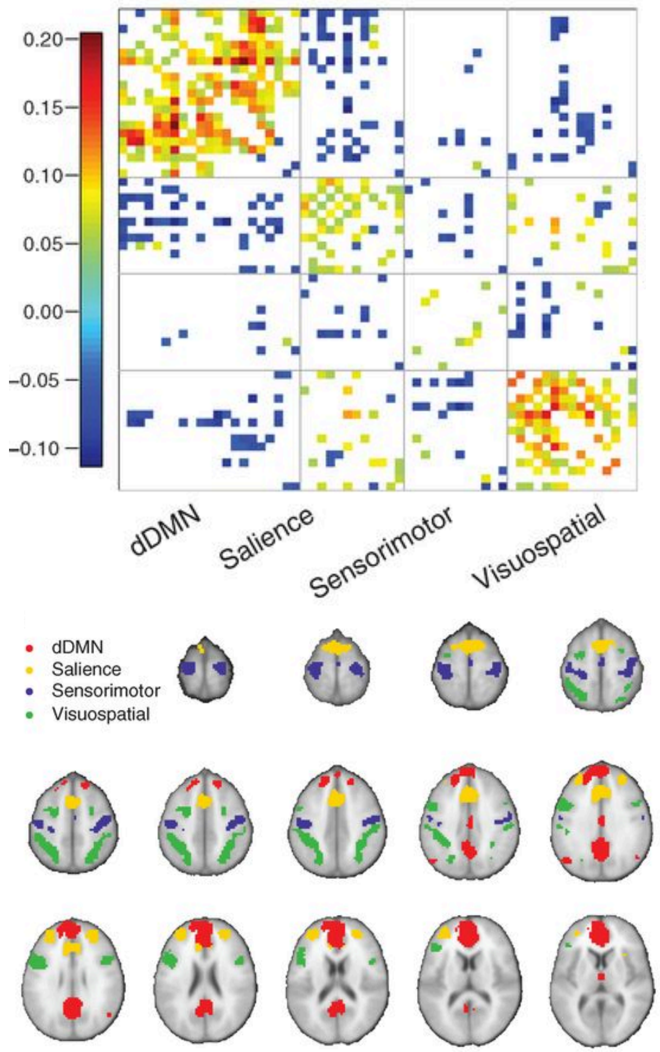
Feature matrices, relationship tables, time series, document corpora, image datasets, etc.

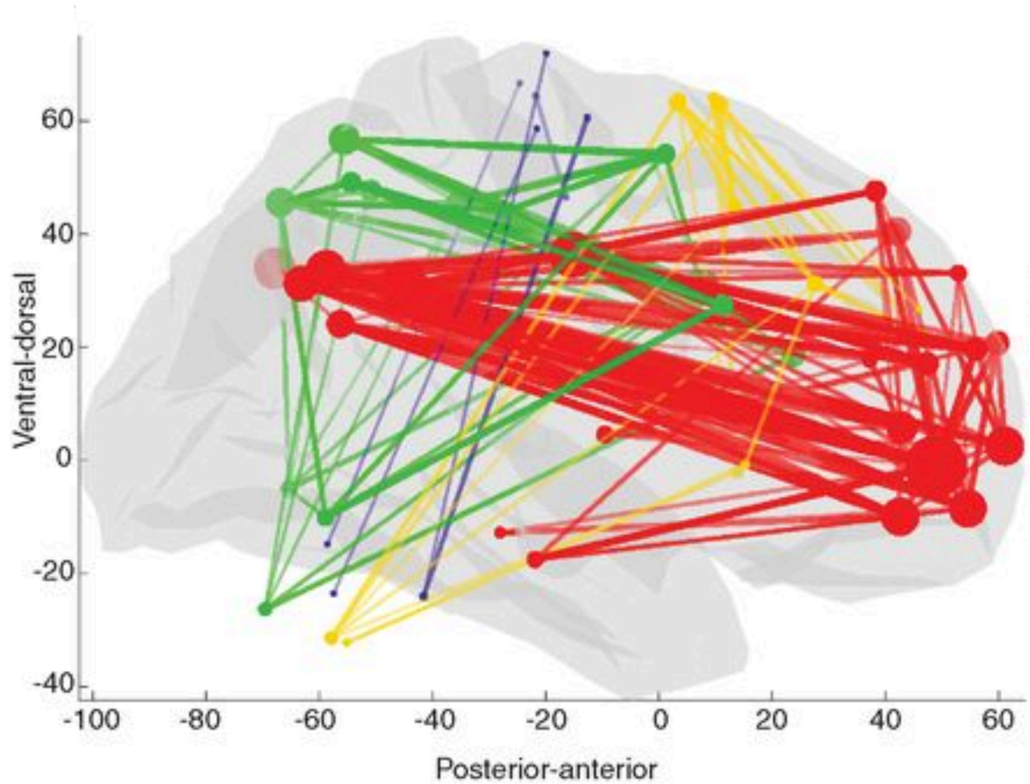
How to Construct Networks?



Today: **How to construct and infer networks from raw data?**

Why? -- Networks are Useful





Jonas Richiardi *et al.*, Correlated gene expression supports synchronous activity in brain networks. *Science* 348:6240, 2015.

Plan for Today

1) Multimode Network Transformations:

- K-partite and bipartite graphs
- One-mode network projections/folding
- Graph contractions

2) K-Nearest Neighbor Graph Construction

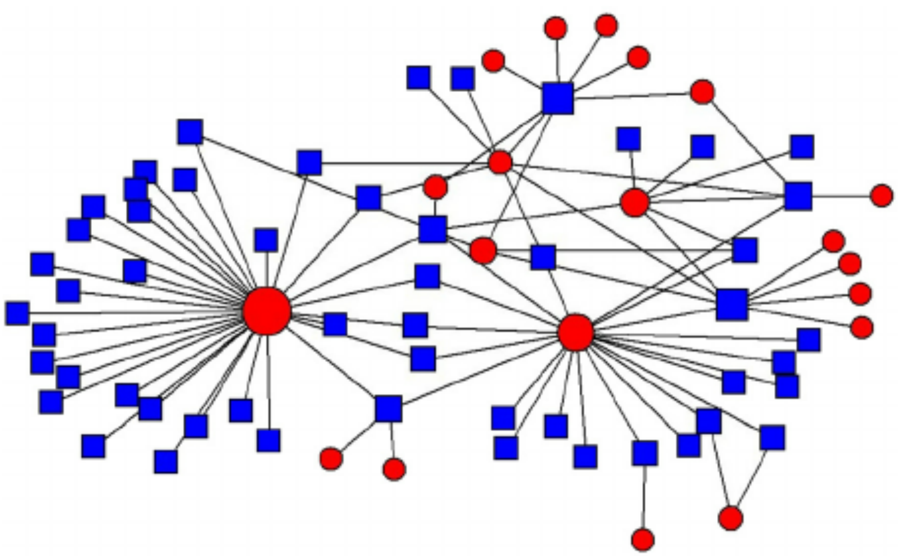
3) Network Deconvolution:

- Direct and and indirect effects in a network
- Inferring networks by network deconvolution

Multimode Network Transformations

Bipartite and K-partite Networks

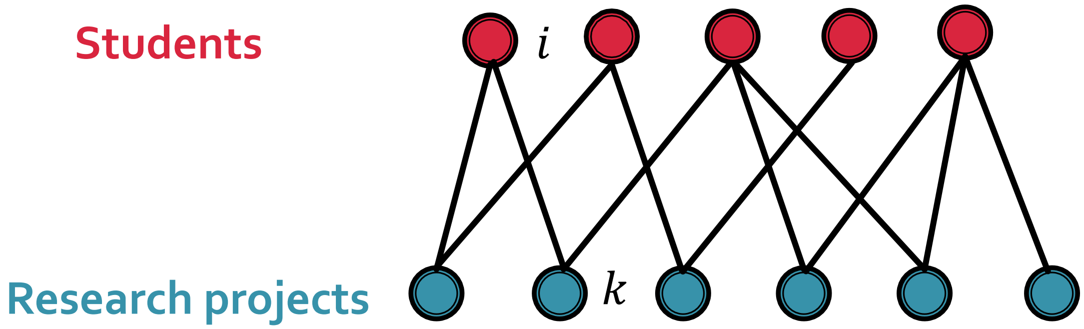
- Most of the time, when we create a network, all nodes represent **objects of the same type:**
  - People in social nets, bus stops in route nets, genes in gene nets
- **Multi-partite networks** have **multiple types of nodes**, where edges exclusively go from one type to the other:
  - **2-partite student net:** Students <-> Research projects
  - **3-partite movie net:** Actors <-> Movies <-> Movie Companies



Network on the left is a social bipartite network. **Blue squares** stand for people and **red circles** represent organizations

One-mode Projections: Example

- **Example:** Bipartite student-project network:
  - **Edge:** Student i works on research project k

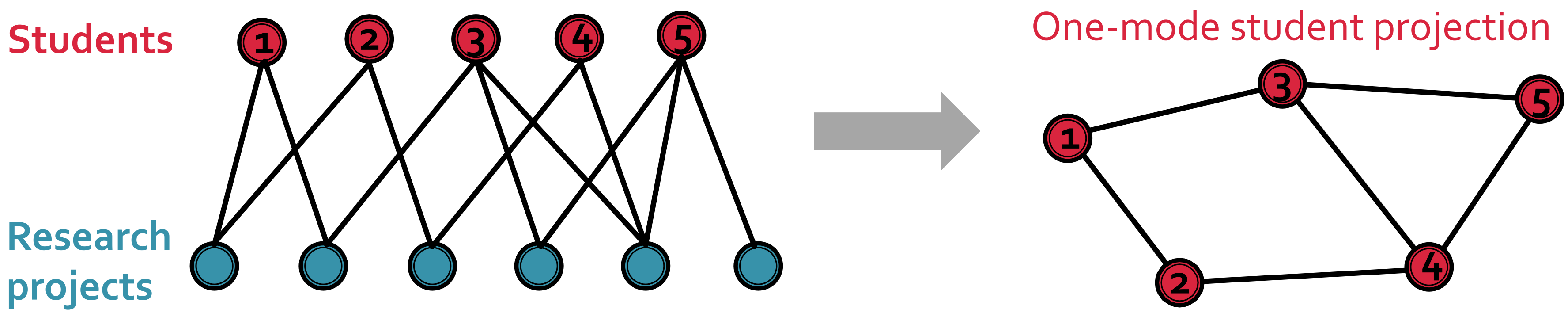


- **Two network projections of student-project network:**
  - **Student network:** Students are linked if they work together in **one or more projects**
  - **Project network:** Research projects are linked if **one or more students** work on both projects

- **In general:** K-partite network has K one-mode network projections

One-mode Projections: Example

- **Example:** Projection of **bipartite student-project network** onto the **student mode**:



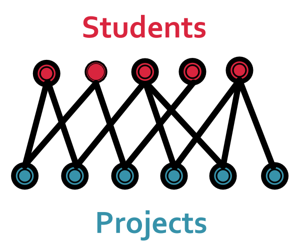
- **Consider students 3, 4, and 5 connected in a triangle:**
  - Triangle can be a result of:
    - **Scenario #1:** Each pair of students work on a different project
    - **Scenario #2:** Three students work on the same project
  - One-mode network projections **discard some information:**
    - Cannot distinguish between #1 and #2 just by looking at the projection

(1) Constructing One-mode Projections

- **One-mode projection** onto **student mode**:
  - #(projects) that students i and j work together on is equivalent to the number of **paths of length 2** connecting i and j in the bipartite network

- Let C be **incidence matrix** of student-project net:

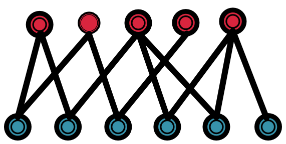
$$C_{ik} = \begin{cases} 1 \text{ if } i \text{ works on project } k \\ 0 \text{ otherwise} \end{cases}$$



- C is an $n \times m$ **binary non-symmetric matrix**:
  - n is #(students), m is #(projects)

(2) Constructing One-mode Projections

- **Idea:** Use C to construct various one-mode network projections
- **Weighted student network**:



$$B_{ij} = \begin{cases} w_{ij}, \#(\text{projects}) \text{ that } i \text{ and } j \text{ collaborate on} \\ 0 \quad \text{otherwise} \end{cases}$$

  - $B_{ij} = \sum_{k=1}^{m} C_{ik} C_{jk}$, *i.e.*, the number of **paths of length 2** connecting students i and j in the bipartite network
  - $\boldsymbol{B} = \boldsymbol{C}\boldsymbol{C}^{\boldsymbol{T}}$ and B_{ii} represents #(projects) that student i works on

- **Similarly, weighted project network**:

$$D_{kl} = \begin{cases} w_{kl}, \#(\text{students}) \text{ that work on } k \text{ and } l \\ 0 \quad \text{otherwise} \end{cases}$$

  - $D_{kl} = \sum_{i=1}^{n} C_{ik} C_{il}$, *i.e.*, the number of **paths of length 2** connecting projects k and l in the bipartite network
  - $\boldsymbol{D} = \boldsymbol{C}^{\boldsymbol{T}}\boldsymbol{C}$ and D_{kk} represents #(students) that work on project k

- **Next:** Use $\boldsymbol{B}$ and $\boldsymbol{D}$ to obtain different network projections

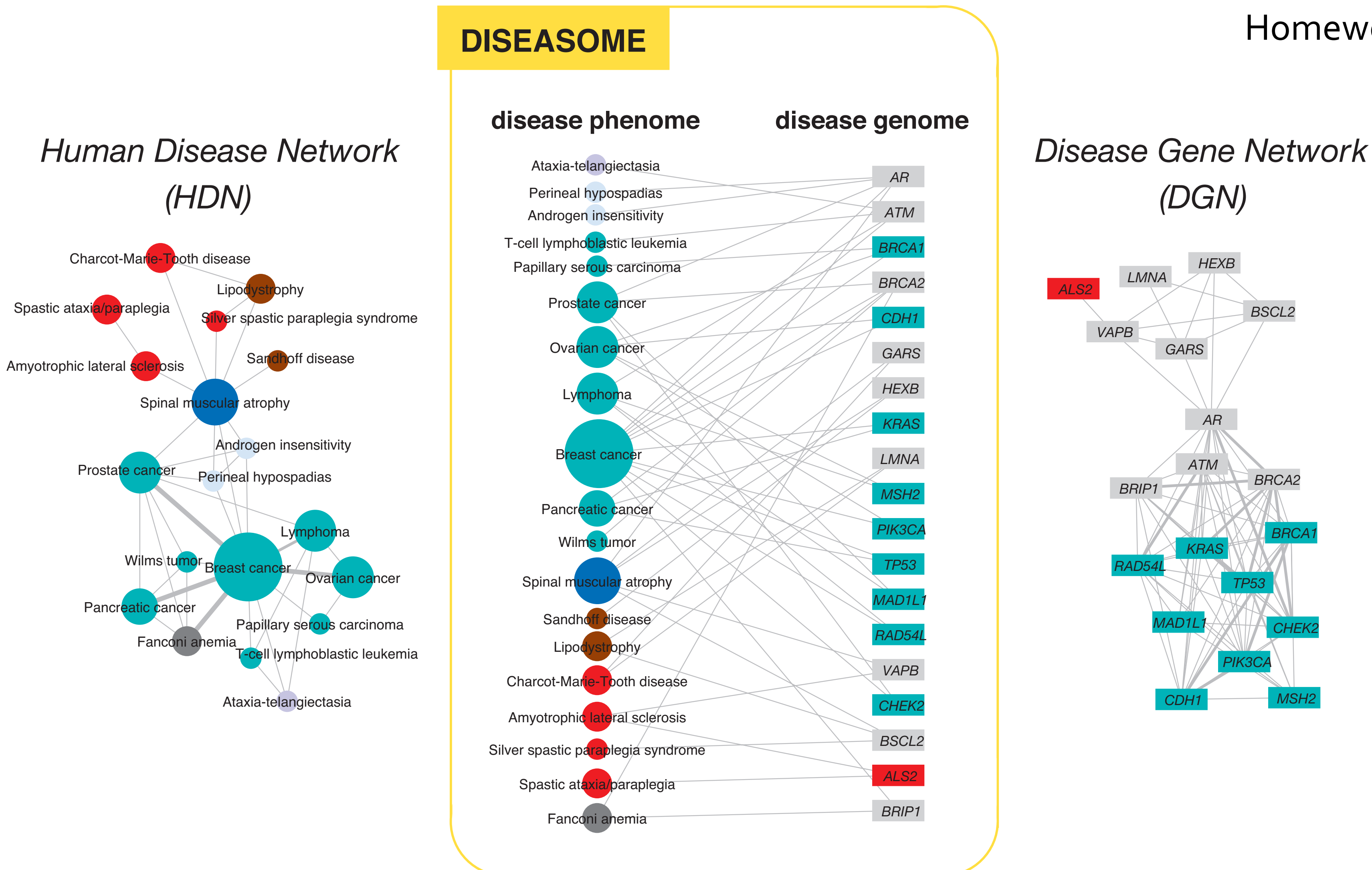
(3) Construct One-mode Projections

- Construct network projections by applying **a node similarity measure** to $\boldsymbol{B}$ and $\boldsymbol{D}$

- **Two node similarity measures:**
  - **Common neighbors:** #(shared neighbors of nodes)
    - **Student network:** i and j are linked if they work together in **r or more projects, *i.e.*,** if $B_{ij} \geq r$
    - **Project network:** k and l are linked if **r or more students** work on both projects, *i.e.*, if $D_{kl} \geq r$
  - **Jaccard index:**
    - Common neighbors with a penalization for each non-shared neighbor:
      - Ratio of shared neighbors in the complete set of neighbors for 2 nodes
    - **Student network:** i and j are linked if they work together in **at least p fraction of their projects, *i.e.*,** if $B_{ij}/(B_{ii} + B_{jj} - B_{ij}) \geq p$
    - **Project network:** k and l are linked if **at least p fraction of their students** work on both projects, *i.e.*, if $D_{kl}/(D_{kk} + D_{ll} - D_{kl}) \geq p$

Example: The Human Disease Net

Homework 1

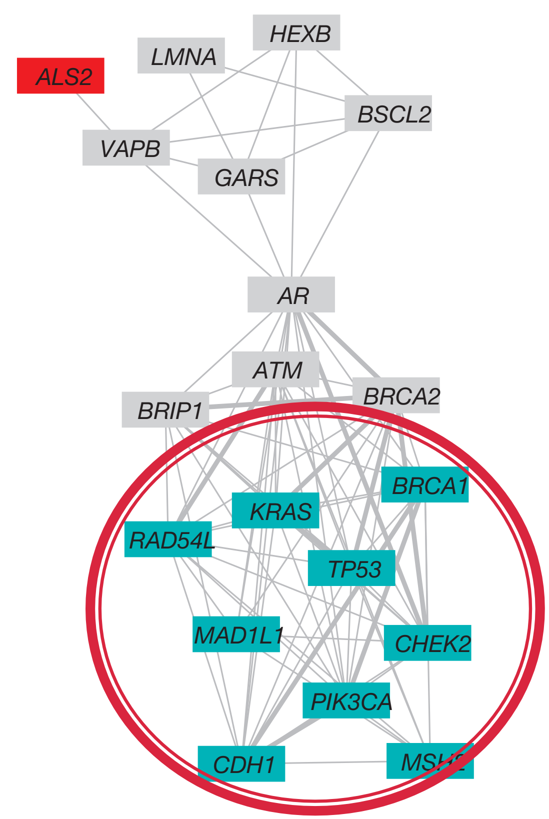


Kwang-Il Goh *et al.*, The human disease network. *PNAS,* 104:21, 2007.

Example: The Human Disease Net

- **Issue:** Folded gene network contains many **cliques:**
  - Why do cliques arise in the folded gene network?
    - **Homework 1**
- **Cliques make the network difficult to analyze:**
  - Computational complexity of many algorithms depends on the **size** and **number of large cliques**
- **Solution:** Use **graph contraction** to eliminate cliques

Disease Gene Network (DGN)



A clique of 9 gene nodes

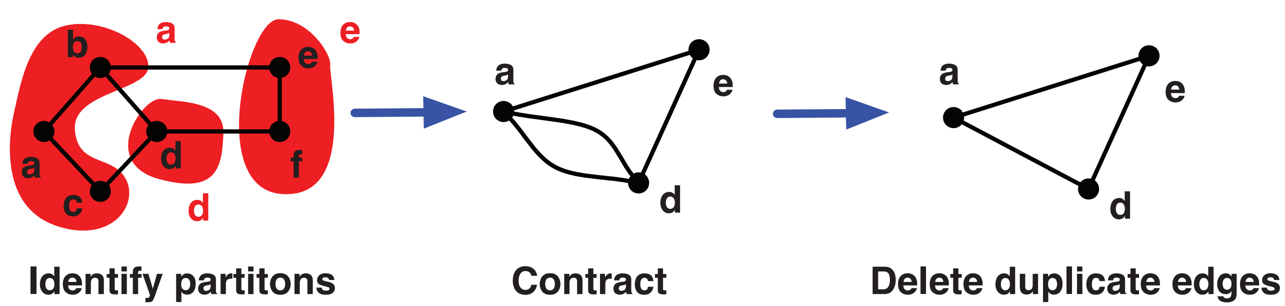
Graph Contraction

- **Graph contraction:** Technique for computing properties of networks in parallel:
  - **Divide-and-conquer principle**
- **Idea:**
  - **Contract the graph** into a smaller graph, ideally a constant fraction smaller
  - Recurse on the smaller graph
  - Use the result from the recursion along with the initial graph to calculate the desired result
- **Next:** How to contract ("shrink") a graph?

Graph Contraction: Algorithm

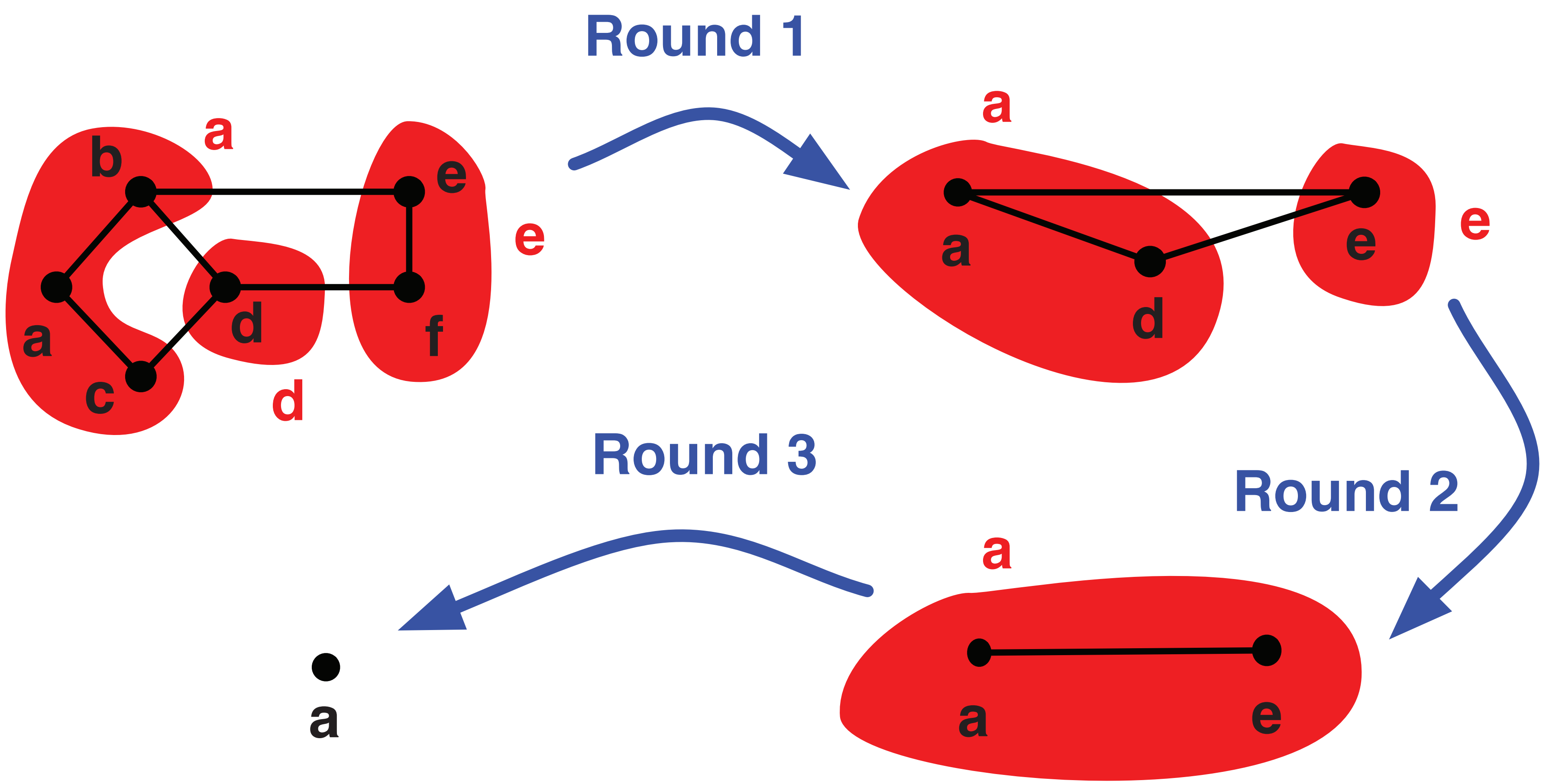
- Start with the input graph G:
  1. Select a **node-partitioning** of G to guide the contraction:
     - Partitions are disjoint and they include all nodes in G
  2. Contract each partition into a single node, a **supernode**
  3. Drop edges internal to a partition
  4. Reroute cross edges to corresponding **supernodes**
  5. Set G to be the smaller graph; Repeat
- Example: one round of graph contraction:

3 partitions: a, d, e



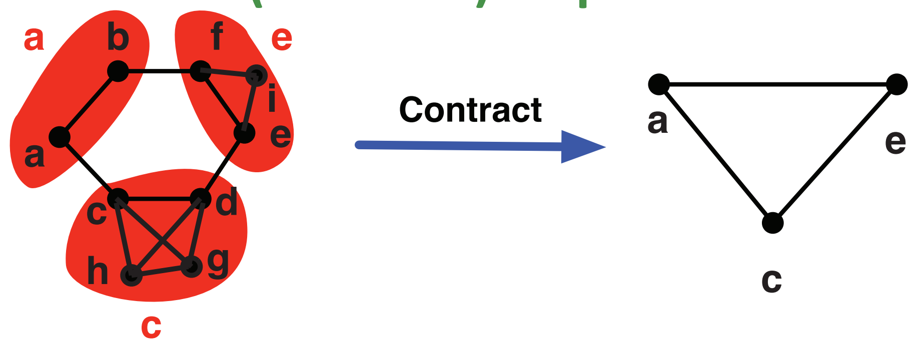
Graph Contraction: Example

Contracting a graph down to a single node in three rounds:

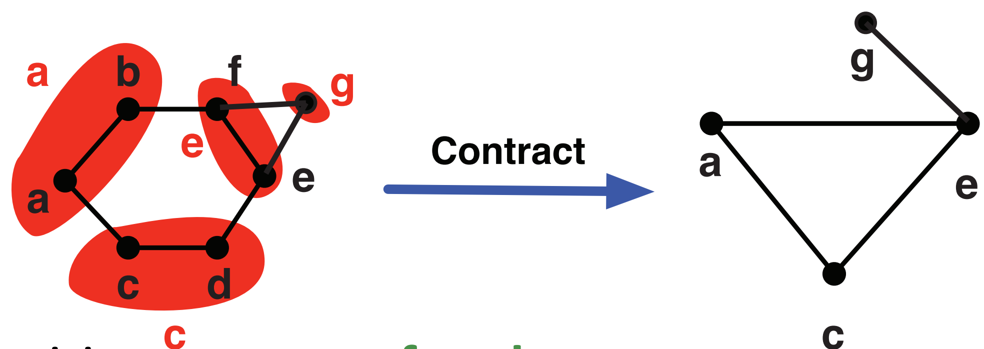


Different Types of Node-partitioning

- Partitions should be **disjoint** and **include all nodes** in G
- Three types of node-partitioning:
  - Each partition is a (maximal) clique of nodes:



  - Each partition is a single node or two connected nodes:



  - Each partition is a star of nodes, etc.

Plan for Today

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2) K-Nearest Neighbor Graph Construction

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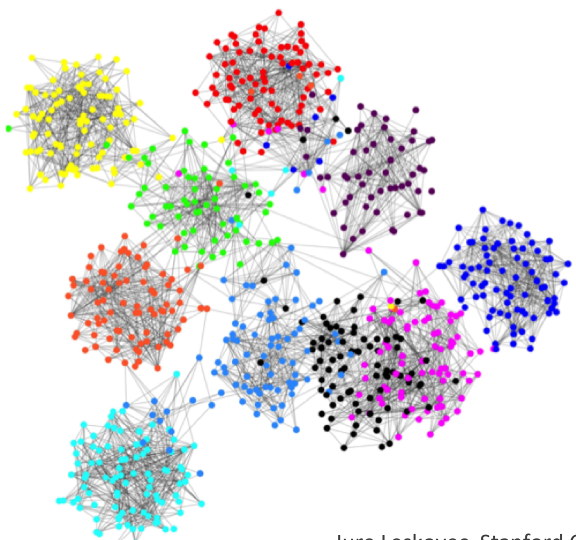
Efficient Construction of K-Nearest Neighbor Graph

K-Nearest Neighbor Graph

- **K-nearest neighbor graph (K-NNG)** for a set of objects V is a directed graph with vertex set V:
  - Edges from each $v \in V$ to its K most similar objects in V under a given similarity measure:
    - *e.g.,* Cosine similarity for text
    - *e.g.,* l_2 distance of CNN-derived features for images



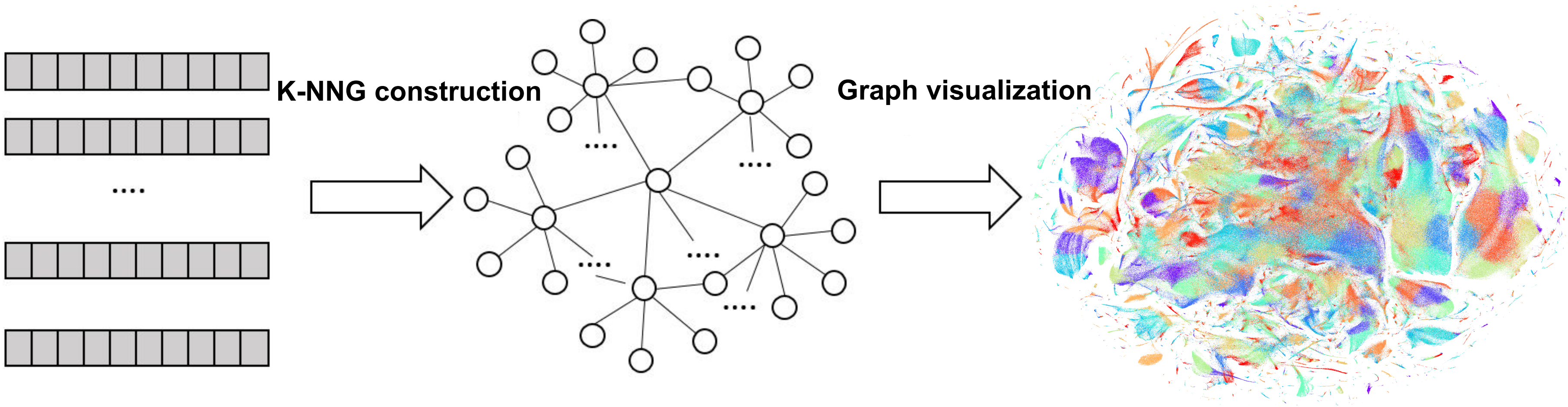
Why Constructing K-NNGs?

- K-NNG construction is an **important operation:**
  - **Recommender systems:** connect users with similar product rating patterns, then make recommendations based on the user's graph neighbors
  - **Document retrieval systems:** connect documents with similar content, quickly answer input queries
  - Other problems in **clustering**, **visualization**, **information retrieval**, **data mining**, **manifold learning**

- K-NNGs allow us to use network methods on datasets with no **explicit graph structure**

Example: K-NNG in Visualization

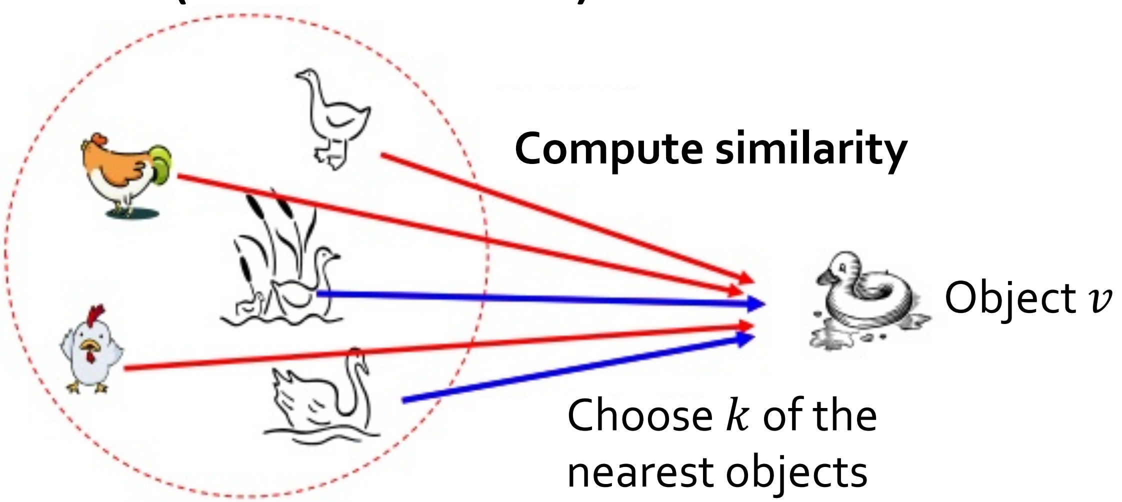
- **Problem:** Visualize large high-dim data in 2D space
- **Traditional approach:**
  - Compute similarities between objects
  - Project objects into a 2D space by preserving the similarities
  - **Does not scale** to millions of objects and hundreds of dimensions
- K-NNG can substantially reduce computational costs



(a) High-dimensional feature vectors (b) K-nearest neighbor graph (K-NNG) (c) 2-dimensional layout WikiDoc data (t-SNE)

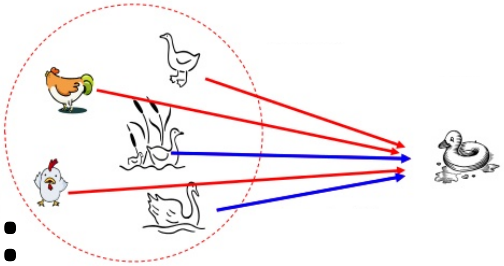
K-NNG: A Brute-force Approach

- Let's construct a K-NNG by **brute-force:**
  - Given n objects V and a distance metric $\sigma: V \times V \rightarrow [0, \infty)$
  - For each possible pair of (u, v), compute $\sigma(u, v)$
  - For each v, let $\boldsymbol{B_K(v)}$ be v's K-NN, *i.e.*, the K objects in V (other than v) most similar to v



K-NNG: A Brute-force Approach

- Computational cost of brute-force: $O(n^2)$



- **Issues with brute-force approach:**
  - **Not scalable:** Practical for only small datasets
  - **Not general:** Many custom heuristics designed to speed up computations:
    - Many heuristics are specific to a similarity measure
  - **Not efficient:** Compute all neighbors for every v
    - We only need k nearest neighbors for every v

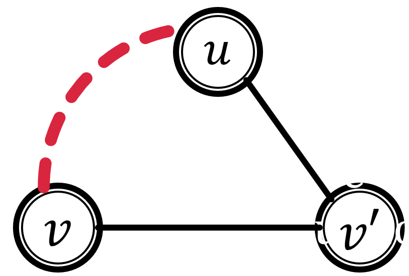
Today: NN-Descent Approach

- **Can we do better than brute-force?**
- **Yes, and we will learn about it today!**

- **NN-Descent** [Dong et al., WWW 2011]:
  - Efficient algorithm to **approximate K-NNG construction** with **arbitrary similarity measure**
- Other published methods (not covered today):
  - **Locality Sensitive Hashing (LSH):** A new hash function needs to be designed for a new similarity measure
  - **Recursive Lanczos bisection:** Recursively divide the dataset, so objects in different partitions are not compared
  - **K-NN search problem:** If K-NN problem is solved, K-NNG can be constructed by running a K-NN query for each $v \in V$

NN-Descent: Key Principle

- **Key principle:** A neighbor of a neighbor is also likely to be a neighbor



- **Use this principle in a NN-Descent method:**
  - Start with an approximation of the K-NNG, B
  - Improve B by **exploring each point's neighbors' neighbors** as defined by the current approximation
  - Stop when no improvement can be made

NN-Descent: Notation

- **Let:**
  - V be a metric space with distance metric $d: V \times V \rightarrow [0, \infty), \sigma = -d$ is the similarity measure
  - $B_K(v)$ be **v's K-NN**
  - $R_K(v) = \{u \in V; v \in B_K(u)\}$ be **v's reverse K-NN**
  - $B[v]$ be **current approximation** of $B_K(v)$
  - $B'[v] = \cup_{v' \in B[v]} B[v']$ be **neighbors of v's neighbors**
  - For any $r > 0$, let **r-ball around v** be:

$$B_r(v) = \{u \in V; d(u, v) \leq r\}$$

(1) NN-Descent: Overview

Details

- **Def:** Metric space V is **growth-restricted** if there exists a constant c, such that:
$$|B_{2r}(v)| \leq c|B_r(v)|, \quad \forall v \in V$$
- The smallest such c is **growing constant** of V
- **Approach:**
  - Start with an approximation of the K-NNG, B
  - Use the **growing constant of V** to show that B can be improved **by comparing each object v against its current neighbors' neighbors $B'[v]$**
- **Next:** Use the **growing-constant argument** on B

(2) NN-Descent: Proof Outline

Details

- **Two assumptions:**
  - Let c be the growing constant of V and let $K = c^3$
  - Have an approximate K-NNG B **that is reasonably good:**
    - For a fixed radius r, for all v, $B[v]$ contains K neighbors that are uniformly distributed in $B_r(v)$
- **Lemma:** $B'[v]$ is likely to contain K nearest neighbors in $B_{r/2}(v)$
- **Corollary:** We expect to **halve the maximal distance** to the set of approximate K nearest neighbors by exploring $B'[v]$ for every v
- **Next:** Let's prove the lemma

(3) NN-Descent: Proof

Details

- **Lemma:** $B'[v]$ is likely to contain K nearest neighbors in $B_{r/2}(v)$

Proof:

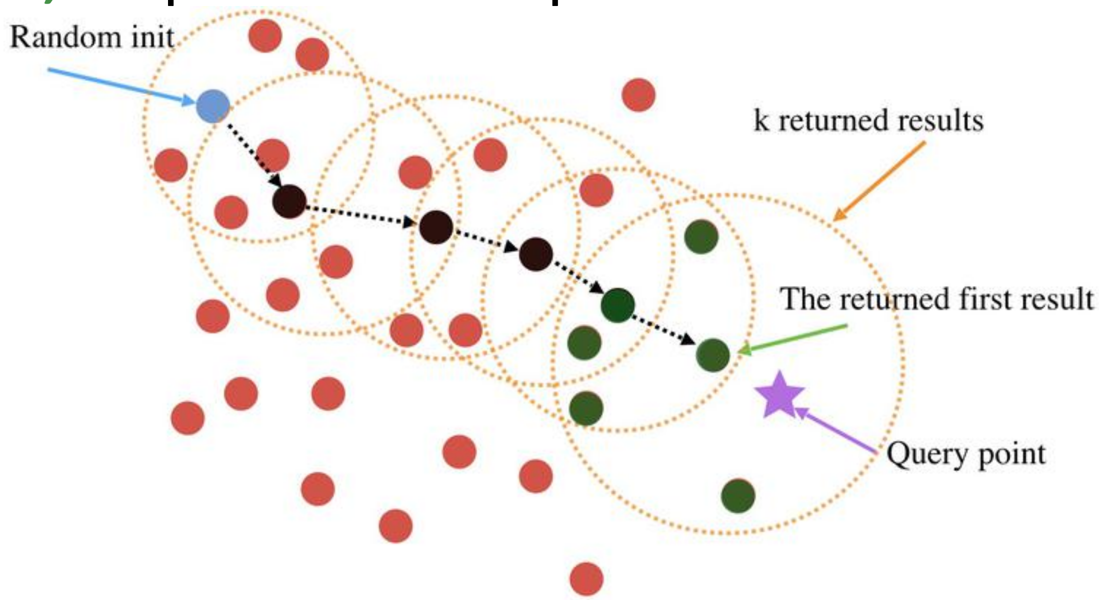
- For any $u \in B_{r/2}(v)$ to be found in $B'[v]$, we need to have at least one v' such that:
$$v' \in B[v] \wedge u \in B[v']$$
- Any $v' \in B_{r/2}(v)$ is likely to satisfy this requirement, as we have:
  1. v' is also in $B_r(v)$, so $\Pr\{v' \in B[v]\} \geq K/|B_r(v)|$
  2. $d(u, v') \leq d(u, v) + d(v, v') \leq r$, so $\Pr\{u \in B[v']\} \geq K/|B_r(v')|$
  3. $|B_r(v)| \leq c|B_{r/2}(v)|$, and $|B_r(v')| \leq c|B_{r/2}(v')| \leq c|B_r(v)| \leq c^2|B_{r/2}(v)|$
- Combining 1-3 and assuming independence, we get:
$$\Pr\{v' \in B[v] \wedge u \in B[v']\} \geq K/\left|B_{r/2}(v)\right|^2$$
- In total, we have $|B_{r/2}(v)|$ candidates for such v', so that: $\Pr\{u \in B'[v]\} \geq 1 - (1 - K/\left|B_{r/2}(v)\right|^2)^{|B_{r/2}(v)|} \approx K/|B_{r/2}(v)|$

QED

NN-Descent: Recap

Details

- **Lemma** suggests the following algorithm:
  - Pick a large enough K (depending on **growing constant c**)
  - Start from a random K-NNG approximation
  - For each v, find K nearest objects by exploring v's neighbors' neighbors, B'
  - **Repeat;** stop when no improvement can be made



NN-Descent: Algorithm

Details

Algorithm 1: NNDESCENT

Data: dataset V, similarity oracle σ, K
Result: K-NN list B
begin
  $B[v] \longleftarrow \textsc{Sample}(V, K) \times \{\infty\}, \quad \forall v \in V$
  loop
    $R \longleftarrow \textsc{Reverse}(B)$
    $\overline{B}[v] \longleftarrow B[v] \cup R[v], \quad \forall v \in V;$
    $c \longleftarrow 0$ //update counter
    for $v \in V$ **do**
      for $u_1 \in \overline{B}[v], u_2 \in \overline{B}[u_1]$ **do**
        $l \longleftarrow \sigma(v, u_2)$
        $c \longleftarrow c + \textsc{UpdateNN}(B[v], \langle u_2, l\rangle)$
    return B **if** $c = 0$

function $\textsc{Sample}(S,\ n)$
return Sample n items from set S

function $\textsc{Reverse}(B)$
begin
  $R[v] \longleftarrow \{u \mid \langle v, \cdots\rangle \in B[u]\} \quad \forall v \in V$
  return R

function $\textsc{UpdateNN}(H,\ \langle u, l, \ldots\rangle)$
Update K-NN heap H; return 1 if changed, or 0 if not.

A. Start by picking a random approximation of K-NN for each object

B. Improve the approximation by comparing each object against its current neighbors' neighbors, including K-NN and reverse K-NN

C. Stop when no improvement can be made

Experimental Setup: Data

- Datasets:
  - **Corel:** Each **image** is segmented into 14 regions, a feature is extracted from each region
  - **Audio:** Each **sentence** is described by 192 features
  - **Shape:** Each **shape** is described by 544-dim feature vector
  - **DBLP:** Each **record** includes authors' names and pub. title
  - **Flickr:** Each **image** is segmented into regions, a pixel-based feature is extracted from each region
- Similarity measures: L1, L2, Cosine, Jaccard, EMD

Dataset	# Objects	Dimension	Similarity Measures
Corel	662,317	14	l_1, l_2
Audio	54,387	192	l_1, l_2
Shape	28,775	544	l_1, l_2
DBLP	857,820	N/A	Cosine, Jaccard
Flickr	100,000	N/A	EMD

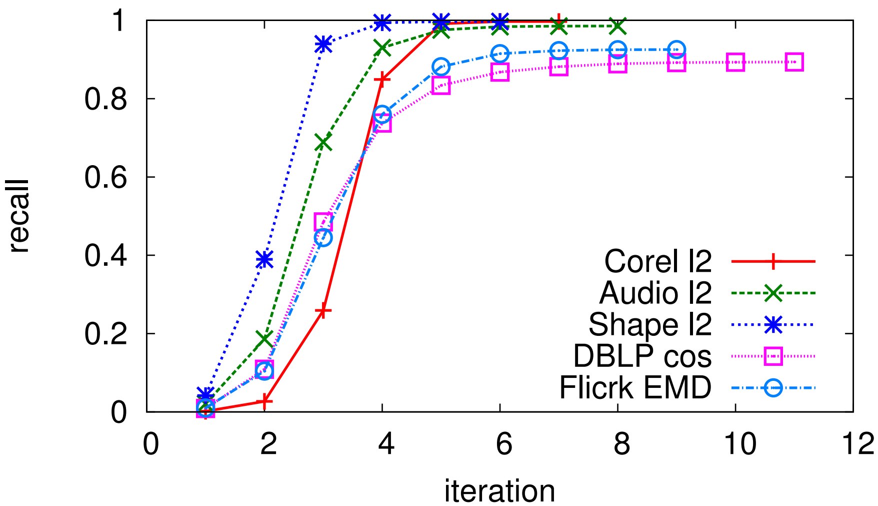
(EMD: earth mover's distance)

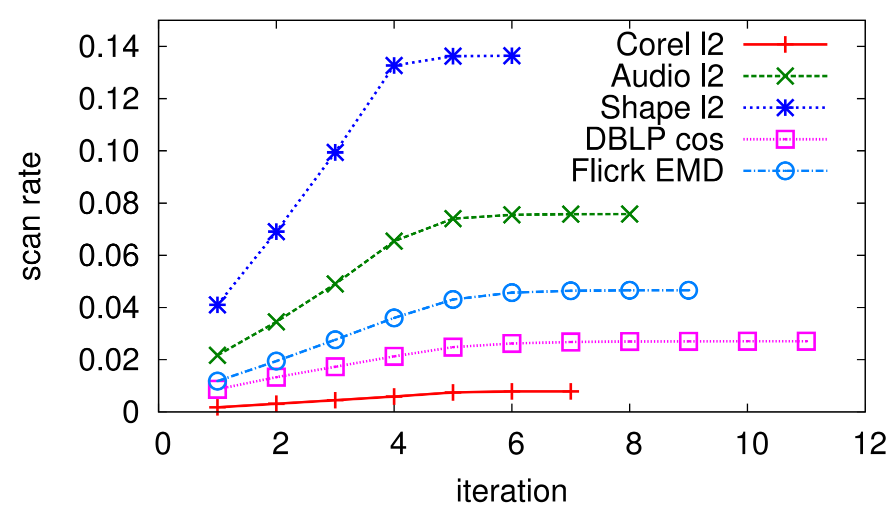
Experimental Setup: Measures

- Use recall as an **accuracy measure:**
  - **Ground-truth:** true K-NNs obtained by scanning the datasets in brute force
  - **Recall of one object** is the number of its true K-NN members found divided by K
  - **Recall of an approximate K-NNG** is the average recall of all objects
- Use #(sim. evaluations) as a **measure of computational cost:**

$$\text{scan rate} = \frac{\#(\text{similarity evaluations})}{n(n-1)/2}$$

(1) Exp.: Overall Performance



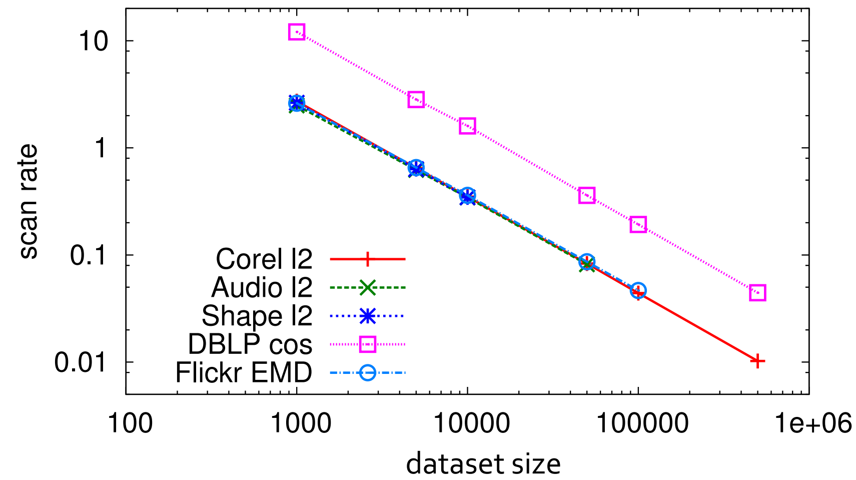


- Similar performance trends on different datasets
- Fast convergence across all datasets:
  - Curves are close to their final recall after 5 iterations
  - All curves converge within 12 iterations

(2) Exp.: Performance as Data Scales

Size	Corel l_2	Audio l_2	Shape l_2	DBLP cos	Flickr EMD
1K	1.000	0.999	1.000	0.959	0.999
5K	1.000	0.996	0.992	0.970	0.991
10K	1.000	0.993	0.998	0.970	0.983
50K	0.999	0.988	-	0.951	0.953
100K	0.999	-	-	0.940	0.925
500K	0.997	-	-	0.907	-

(recall values)



- Run experiments on samples of the full datasets and observe changes in recall and scan rate as sample size grows
- **Results:**
  - As dataset grows, there is only a minor decline in recall
  - All curves form parallel straight lines in the scan rate vs. dataset size:
    - NN-descent has a polynomial time complexity
    - Fit the scan rate curves to obtain empirical complexity of NN-Descent:
      - $O(n^{1.14}) \ll O(n^2)$ (=brute-force)

Plan for Today

1) **Multimode Network Transformations:**
   - K-partite and bipartite graphs
   - One-mode network projections/folding
   - Graph contractions

✓

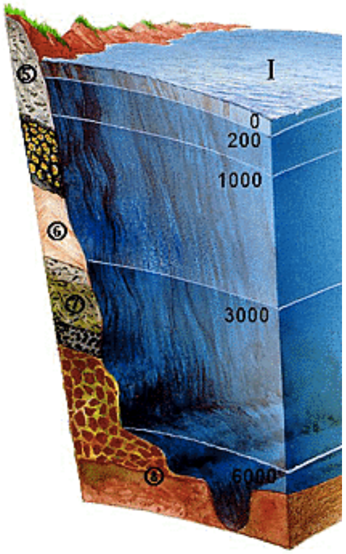
2) **K-Nearest Neighbor Graph Construction** ✓

3) **Network Deconvolution:**
   - Direct and and indirect effects in a network
   - Inferring networks by network deconvolution

Network Deconvolution and Inference

Motivation

- Networks represent **dependencies among objects:**
  - Co-authorships between scientists
  - Friendships between people
  - Who-eats-whom in food webs
  - Bonds between molecular residues
  - Regulatory relationships between genes

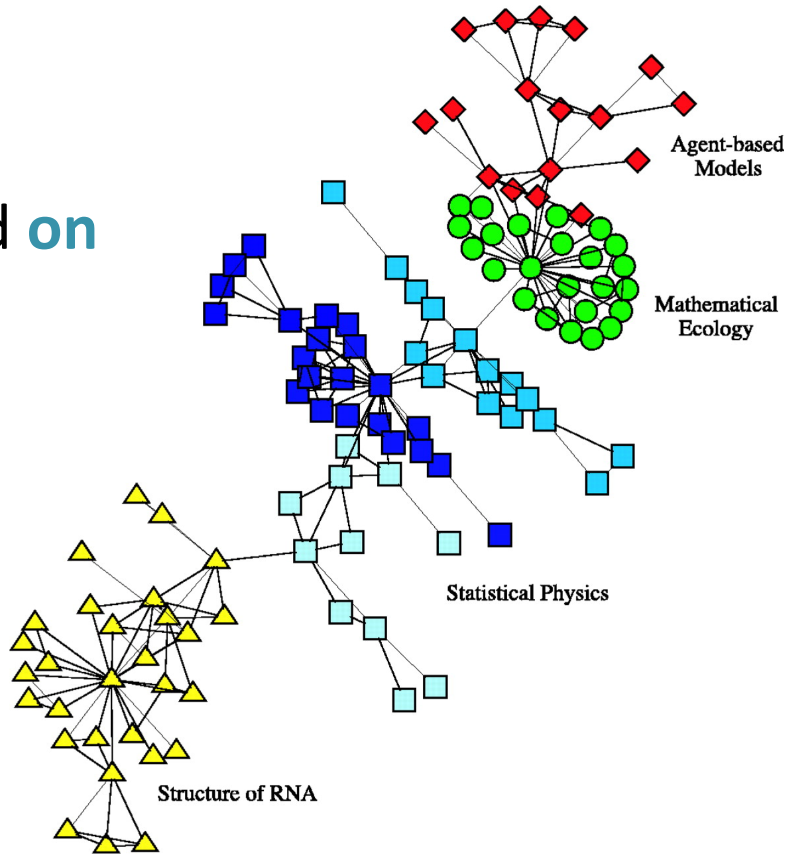


- **Indirect dependencies** occur because of **transitive effects of correlation**

- **Problem: How to separate direct dependencies from indirect ones?**

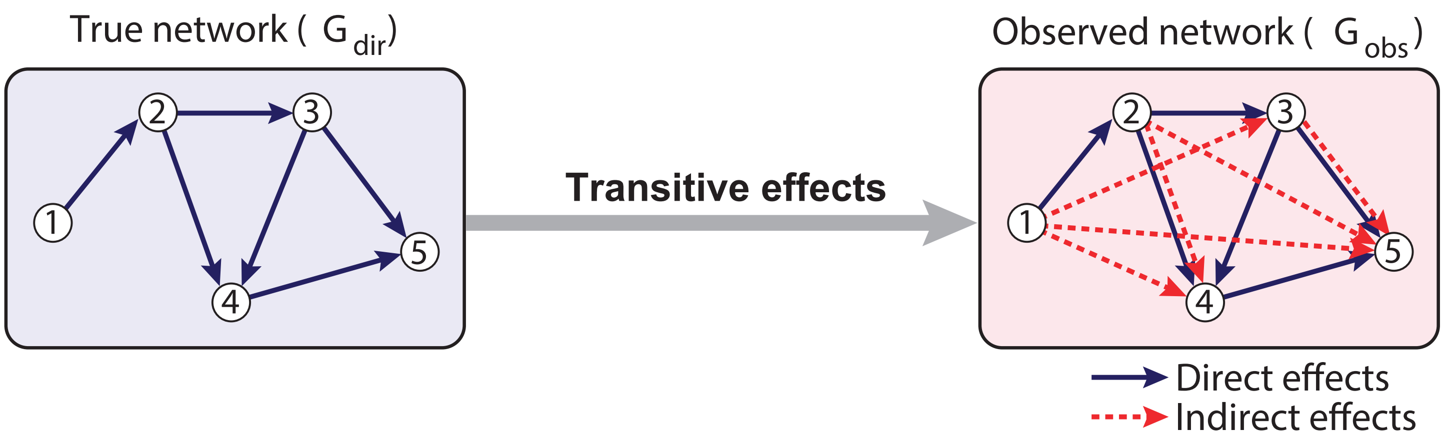
Application: Co-authorship Net

- **Goal:** Distinguish **strong** and **weak** collaborations between scientists
- Collaboration tie strengths depend **on publication details**, such as:
  - #(papers) each pair of scientists has collaborated on
  - #(co-authors) on each of the papers
- Strength of ties are important for:
  - **Recommending friends** and colleagues
  - Recognizing **conflicts of interest**
  - Evaluating authors' **contribution to teams**



Observed Network

- **Observed network:** Combined direct and indirect effects:

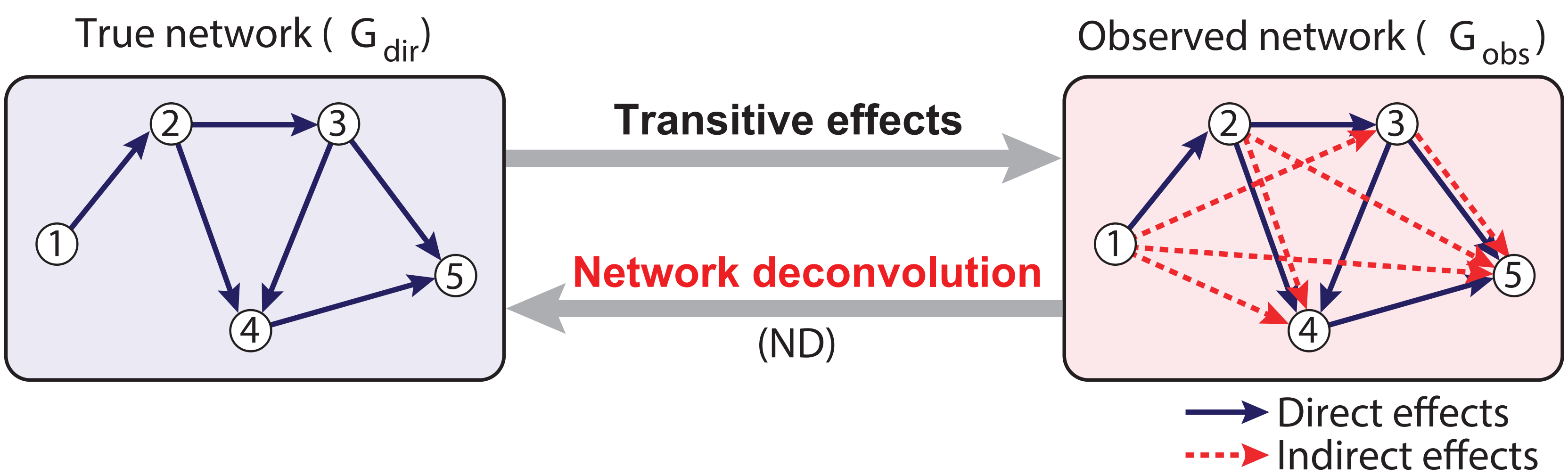


- **Indirect edges** might be due to higher-order interactions (*e.g.*, 1→4)

- Each edge might contain **both direct and indirect components** (*e.g.*, 2→4)

Network Deconvolution

- **Goal:** Reverse the effect of transitive information flow across all indirect paths:
  - Recover **true direct network (blue edges, G_{dir})** based on **observed network (combined blue and red edges, G_{obs})**

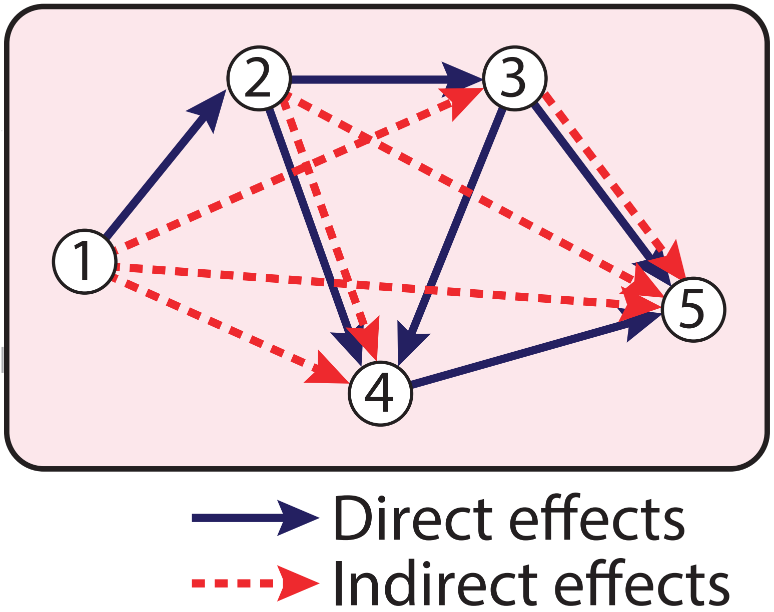


Feizi *et al.*, *Nature Biotechnology*, 31:8, 2013.

Network Deconvolution: Challenge

- Direct edges in a network can lead to indirect relationships:
  - Transitive information flow
- **Indirect effects** can be of **length**:
  - **2** (*e.g.*, 1→2→3)
  - **3** (*e.g.*, 1→2→3→5)
  - **higher-order**
- Indirect effects can combine:
  - **Both direct and indirect** effects (*e.g.*, 2→4)
  - Multiple indirect effects along **varying paths** (*e.g.*, 2→3→5, 2→4→5)

Observed network (G_{obs})



Network Deconvolution: Formally

- **Transitive effects in G_{obs}** can be expressed as an infinite sum of G_{dir} and all indirect effects:

  $$G_{\mathrm{obs}} = \mathrm{G}_{\mathrm{dir}} + \boldsymbol{G}_{\mathbf{indir}}$$

- Indirect effects can be of **increasing lengths:**

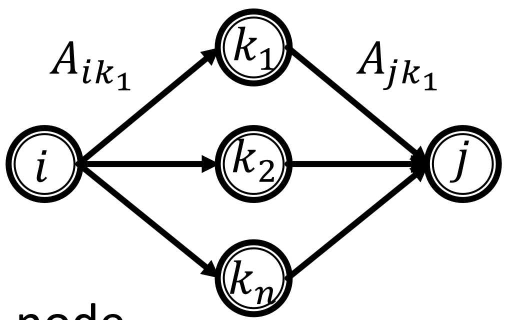
  $$G_{\mathrm{indir}} = \underbrace{\mathrm{G}_{\mathrm{dir}}^{2}}_{2^{nd}\text{ order}} + \underbrace{\mathrm{G}_{\mathrm{dir}}^{3}}_{3^{rd}\text{ order}} + \underbrace{G_{\mathrm{dir}}^{4}}_{4^{th}\text{ order}} + \cdots$$

- **2nd order effects:** $G_{\mathrm{dir}}^{2} = \mathrm{A}_{\mathrm{dir}}^{2}$
  - **The number of edges in G_{obs} of indirect paths of length 2**
- **3rd order effects:** $G_{\mathrm{dir}}^{3} = \mathrm{A}_{\mathrm{dir}}^{3}$
  - **The number of edges in G_{obs} of indirect paths of length 3**

Powers of Adjacency Matrices

- Let's raise adjacency matrix A_{dir} **to the second power:**
  - The (i,j)-th entry of A^2_{dir} is:

$$A^2_{\text{dir}}(i,j) = \sum_{k=1}^{n} A_{\text{dir}}(i,k)\, A_{\text{dir}}(k,j)$$



    - This sum is only greater than zero if there exists a node k for which $A_{\text{dir}}(i,k)$ and $A_{\text{dir}}(k,j)$ are both nonzero:
      - There exists a node **k that is connected to both nodes i and j**
      - The sum counts the number of neighbors that nodes i and j share
      - The sum counts **the paths of length 2 between nodes i and j**

- This reasoning is valid for higher powers of A_{dir}:
  - $A^3_{\text{dir}}(i,j)$ counts the **paths of length 3** between i and j
  - $A^4_{\text{dir}}(i,j)$ counts the **paths of length 4** between i and j

Network Deconvolution: Formally

- **Idea:** Model indirect flow as **power series** of direct flow:

$$\underbrace{G_{\text{obs}}}_{\text{Converges with correct scaling}} = \underbrace{\mathrm{G}_{\text{dir}} + \underbrace{\mathrm{G}_{\text{dir}}^{2} + \mathrm{G}_{\text{dir}}^{3} + G_{\text{dir}}^{4} + \cdots}_{\text{Indirect effects}}}_{\text{Transitive closure of } G_{\text{dir}}}$$

- **Note:** Linear scaling of G_{obs} so that max absolute eigenvalue of $\mathrm{G}_{\text{dir}} < 1$:
  - Indirect effects decay exponentially with path length
  - Infinite series converges

Network Deconvolution: Formally

- **Transitive closure of G_{dir}** can be expressed as an infinite sum of:
  - True direct network, G_{dir}
  - All indirect effects along paths of increasing lengths, G_{dir}^2, G_{dir}^3, G_{dir}^4 , …

- **Idea:** Can be written in a closed form as an infinite-series sum using **Taylor series expansions**:

$$G_{\text{obs}} = \mathrm{G}_{\text{dir}} + \mathrm{G}_{\text{dir}}^2 + \mathrm{G}_{\text{dir}}^3 + G_{\text{dir}}^4 + \cdots =$$
$$G_{\text{dir}}\left(\mathrm{I} + \mathrm{G}_{\text{dir}} + G_{\text{dir}}^2 + \mathrm{G}_{\text{dir}}^3 + \cdots\right) = G_{\text{dir}}(\mathrm{I} \; - \mathrm{G}_{\text{dir}})^{-1}$$

Note: Let X be any square matrix with max absolute eigenvalue < 1. Then the following series converges: $\mathrm{I} + X + X^2 + \mathrm{X}^3 + \cdots$
The series converges to: $\sum_{k=0}^{\infty} X^k = (1 - X)^{-1}$

Network Deconvolution: Solution

- Using **Taylor series expansions** we get a **closed-form expression for $G_{\mathbf{obs}}$**:

$$G_{\text{obs}} = G_{\text{dir}}(\mathrm{I} - \mathrm{G}_{\text{dir}})^{-1}$$

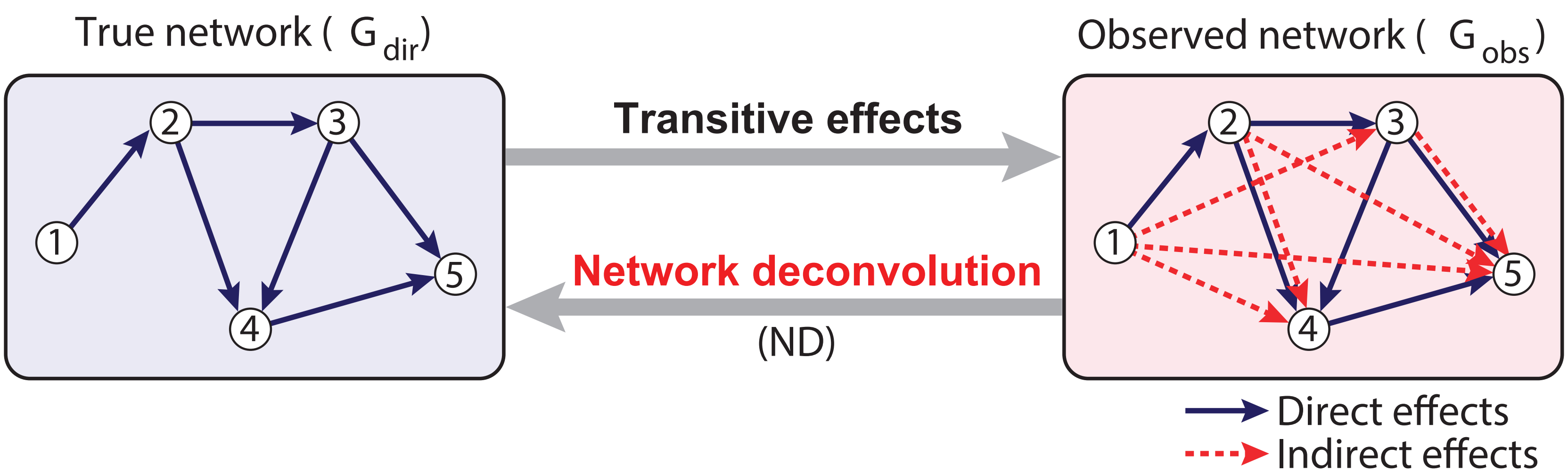
- **In network deconvolution:**
  - **Observed network $G_{\mathbf{obs}}$** is known
  - **True direct network $G_{\mathbf{dir}}$** needs to be **recovered**

- Finally, we get **a closed-form solution for $G_{\mathbf{dir}}$**:

$$G_{\text{dir}} = G_{\text{obs}}(\mathrm{I} + \mathrm{G}_{\text{obs}})^{-1}$$

Network Deconvolution: Recap

- Use **closed-form expression for G_{obs}** to **recover** true direct network G_{dir}



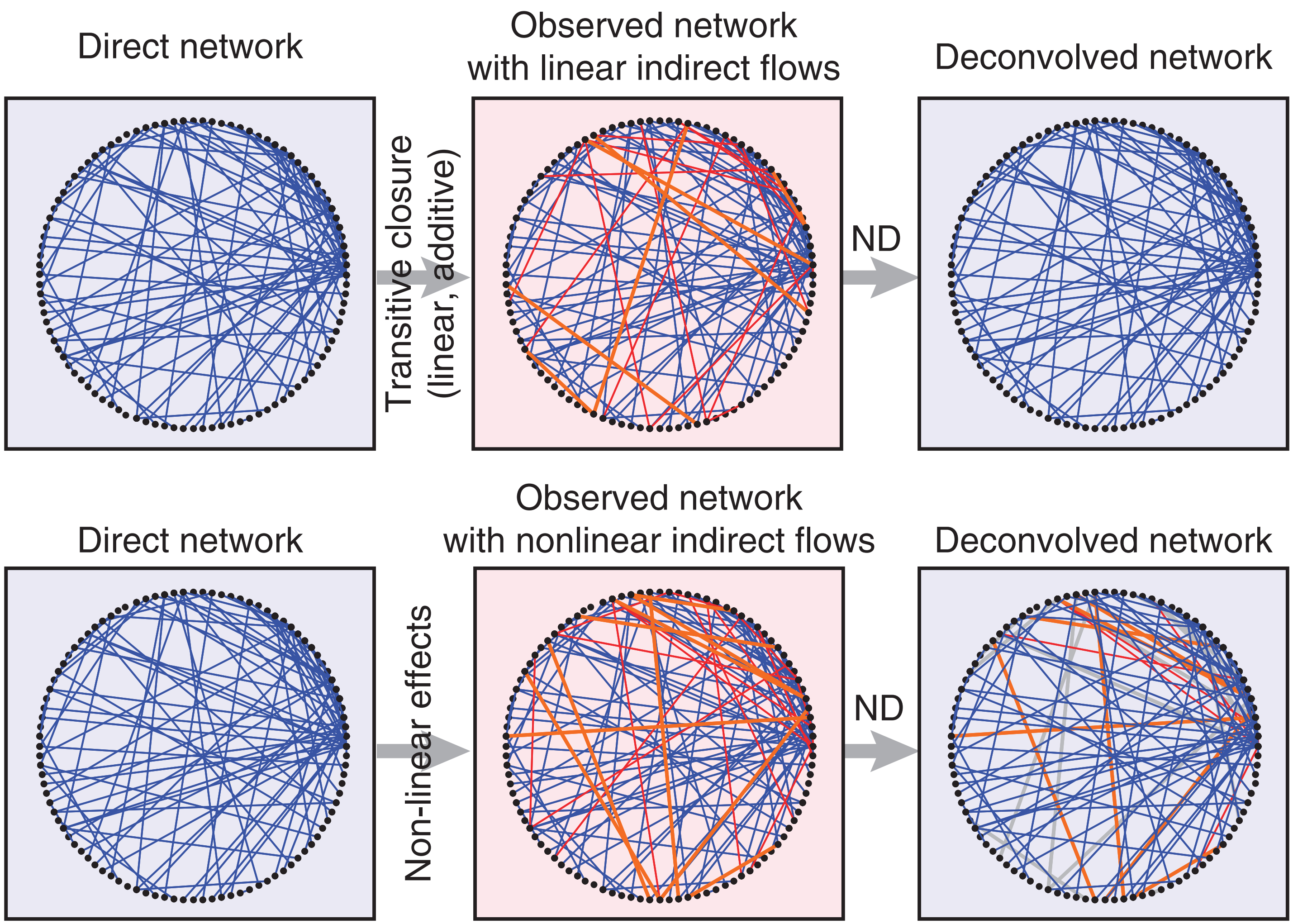
$$\text{Transitive closure:} \quad G_{obs} = G_{dir} + \underbrace{G_{dir}^2 + G_{dir}^3 + \ldots}_{\text{Indirect effects}} = \underbrace{G_{dir}(I - G_{dir})^{-1}}_{\text{Series closed form}}$$

$$\text{Network deconvolution:} \quad G_{dir} = G_{obs}(I + G_{obs})^{-1}$$

How to compute $G_{\mathrm{obs}}(\mathrm{I} + \mathrm{G}_{\mathrm{obs}})^{-1}$

- The solution for G_{dir} is: $G_{\mathrm{dir}} = G_{\mathrm{obs}}(I + G_{\mathrm{obs}})^{-1}$
- How to **efficiently** calculate G_{dir}:
  - Without calculating matrix inverse $(I + G_{\mathrm{obs}})^{-1}$
- **Approach:**
  - Use the **eigen-decomposition principle:**
    1. Express G_{obs} by decomposition into eigenvectors U and eigenvalues Σ_{obs}: $G_{\mathrm{obs}} = U\Sigma_{\mathrm{obs}}\mathrm{U}^{-1}$
    2. Express **each eigenvalue $\boldsymbol{\lambda_i^{\mathrm{dir}}}$** as a nonlinear function of a single corresponding eigenvalue λ_i^{obs}:
    $$\lambda_i^{\mathrm{dir}} = \lambda_i^{\mathrm{obs}}\left(1 + \lambda_i^{\mathrm{obs}}\right)^{-1}$$
    3. Form a diagonal matrix Σ_{dir} such that $\Sigma_{\mathrm{dir}}(i, i) = \lambda_i^{\mathrm{dir}}$
    4. **Recover true direct network as: $\boldsymbol{G_{\mathrm{dir}} = \mathrm{U}\Sigma_{\mathrm{dir}}\mathrm{U}^{-1}}$**

Network Deconvolution: Overview



Ground-truth/True net **Input** **Output**

Length $n > 2$ indirect interactions (false positives)

True interactions removed by ND (false negatives)

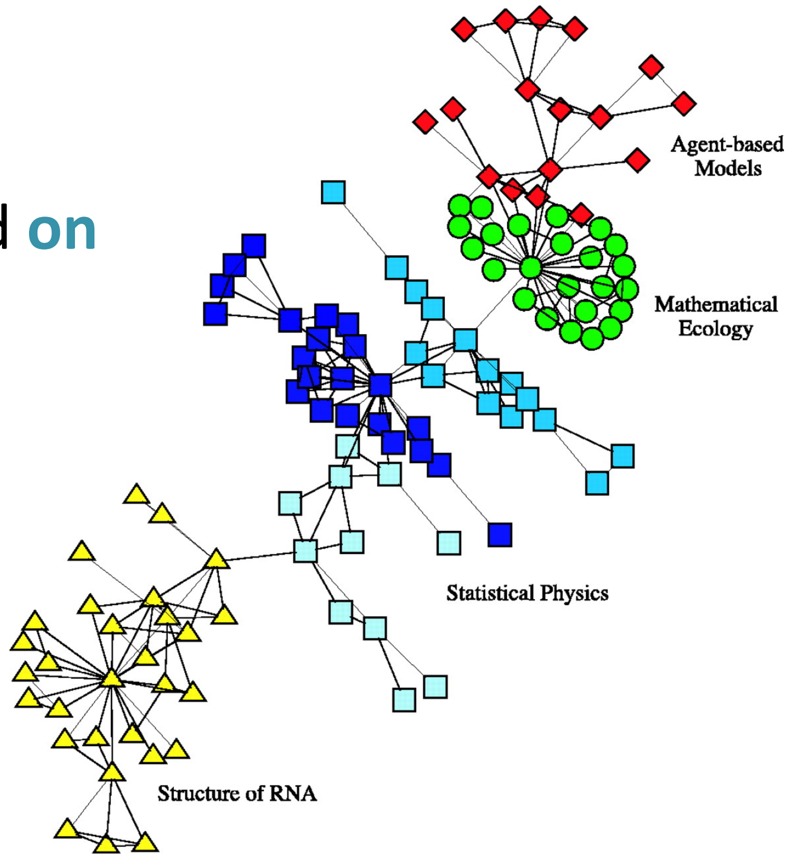
Direct interactions, correctly recovered (true positives)

Length-2 indirect interactions (false positives)

Application: Co-authorship Net

- **Goal:** Distinguish **strong** and **weak** collaborations between scientists

- Collaboration tie strengths depend **on publication details**, such as:
  - #(papers) each pair of scientists has collaborated on
  - #(co-authors) on each of the papers

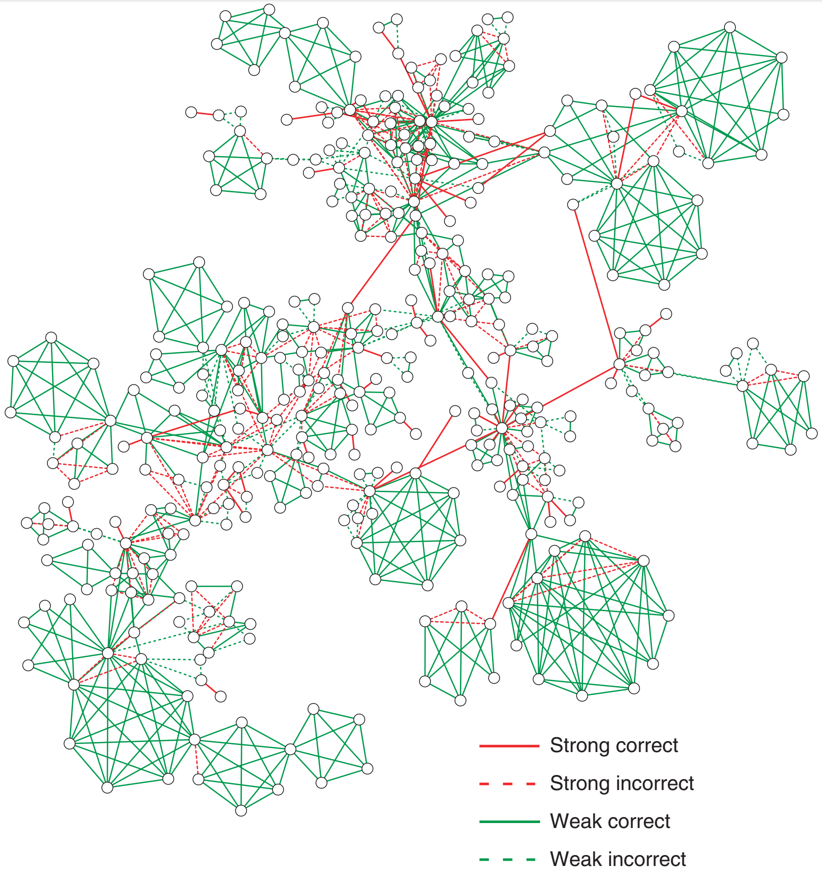


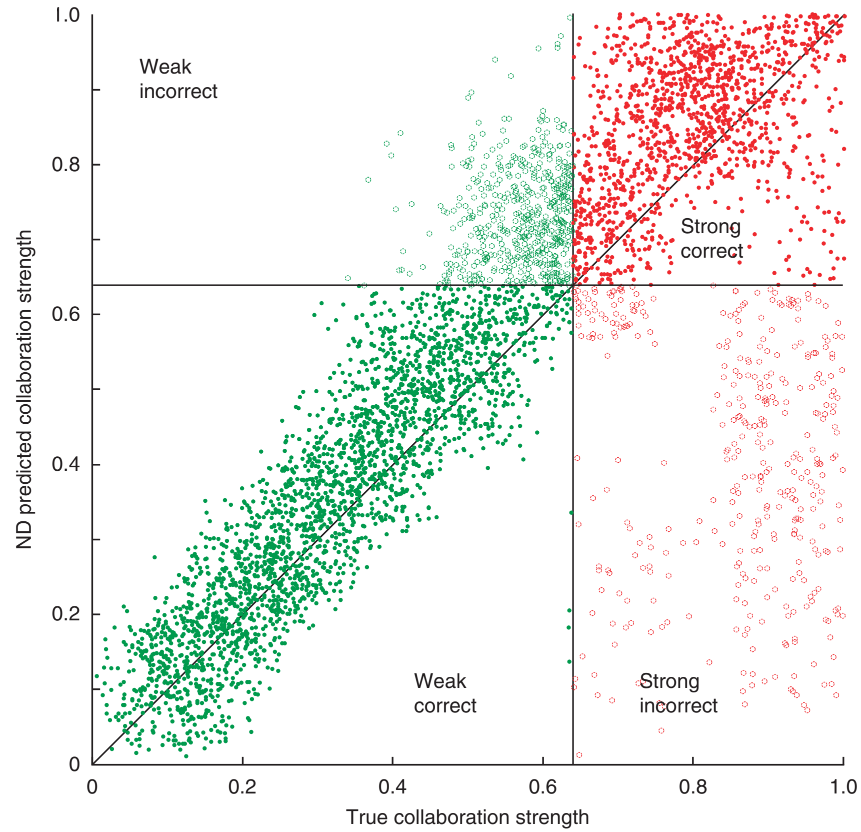
- Strength of ties are important for:
  - **Recommending friends** and colleagues
  - Recognizing **conflicts of interest**
  - Evaluating authors' **contribution to teams**

Application: Co-authorship Net

- **Data:** Unweighted network of **scientists** working in the field of network science:
  - Two authors are linked if they co-authored at least one paper
- **Setup:** Apply ND on the co-authorship network:
  - ND returns a weighted network whose:
    - Transitive closure most closely captures the input network
    - Weights represent the inferred strength of direct interactions
  - **Output:** Rank co-authorship edges by **the ND-assigned weights**
- **Ground-truth data:**
  - **True collaboration strengths** are computed by summing the number of co-authored papers and down-weighting each paper by the number of additional co-authors
  - Compute **correlation** between **ND-assigned weights** and **true collaboration strengths**

Co-authorship Network: Results



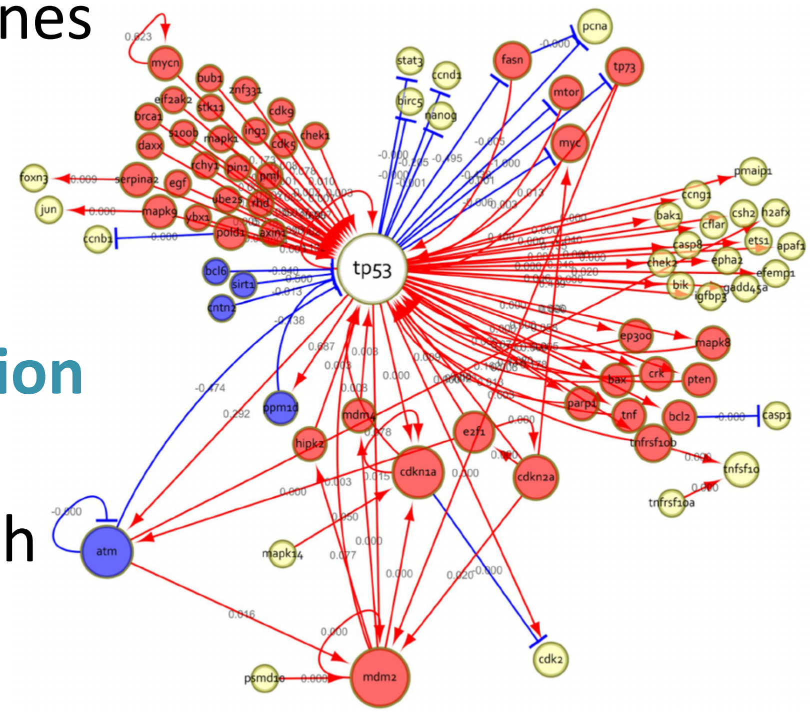


- Agreement between the rank obtained by the true collaboration strength and the rank provided by the ND weight, $R^2 = 0.76$
- **Conclusion:** ND predict collaboration tie strengths **solely by using network topology** (*i.e.*, not using other publication details)

Application: Gene Network Inference

- **Goal:** Infer a **gene regulatory network** from gene feature vectors describing gene activity:
  - **Nodes** represent genes
  - **Edges** represent regulatory relationships between regulators and their target genes

- Well-studied **problem in bioinformatics:**
  - A dataset is a **gene-by-condition expression matrix**
  - Expression matrix is **noisy** with many **indirect** measurements



Application: Gene Network Inference

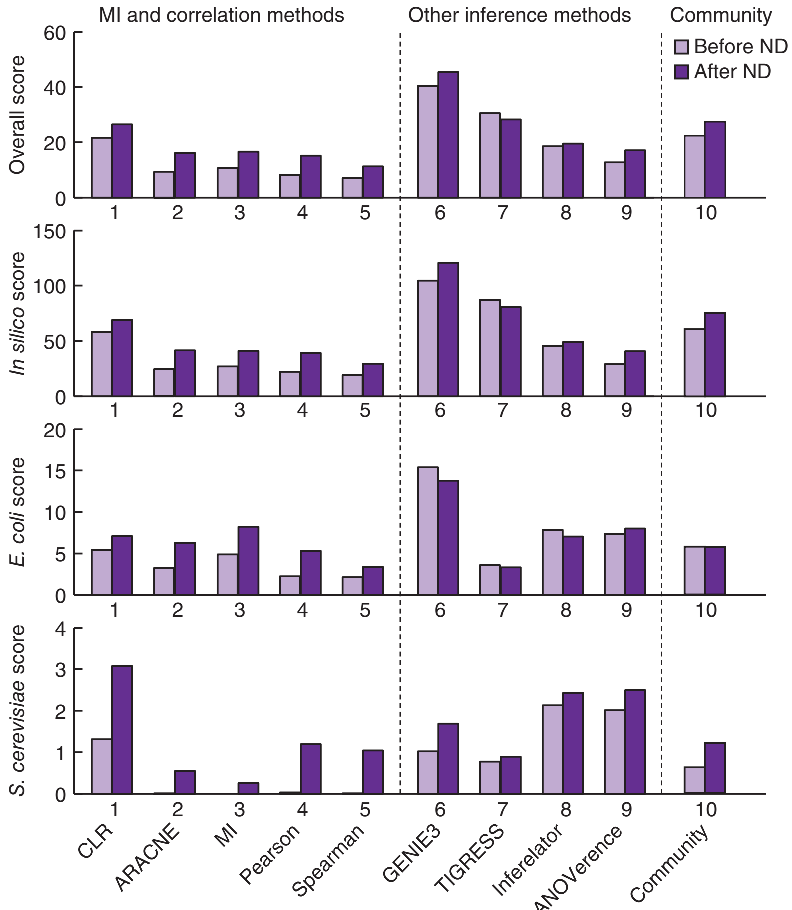
- **3 datasets:** Gene expression datasets from: bacterium *E. coli,* yeast *S. cerevisiae,* and a simulated env (*in silico)*

- **Setup:** Use ND to improve network inference methods by eliminating indirect edges in the inferred networks:
  1. Infer a gene regulatory network using a particular network inference method
  2. Apply ND to the inferred network to deconvolve the network
  3. Evaluate deconvolved network against ground-truth data

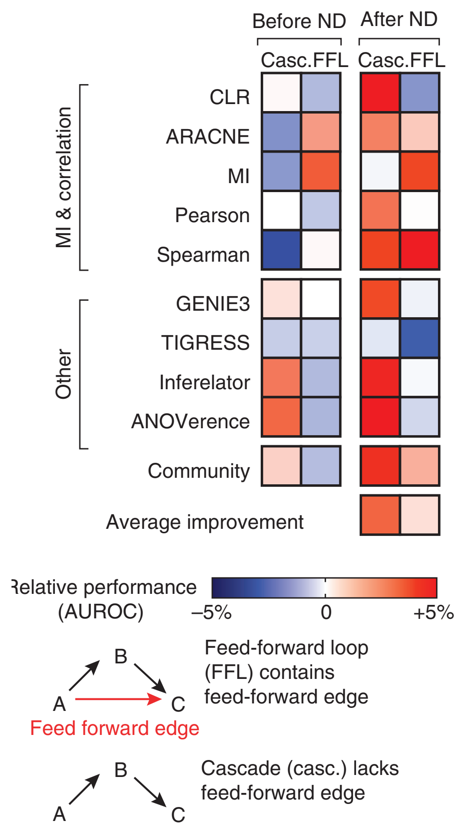
- **Ground-truth data:**
  - True positive regulatory relationships (*i.e.,* edges) are defined as a set of interactions experimentally validation in a laboratory

Gene Network Inference: Results

Datasets



Network inference methods



Relative performance of inference methods for cascades **(casc.)** and feed-forward loops **(FFL)** before and after network deconvolution

ND improves the performance of top-performing network inference methods

Network Deconvolution: Recap

- General approach to **identify direct dependencies between objects in a network:**
  - Remove **spurious edges** that are due to indirect effects
  - Decrease **over-estimated edge weights**
  - **Rescale edge weights** so that they correspond to direct dependencies between objects
- Other published methods (not covered today):
  - Partial correlations and random matrix theory
  - Graphical models, *e.g.*, Graphical lasso, Bayesian nets, Markov random fields
  - Causal inference models

Plan for Today

1) **Multimode Network Transformations:**
   - K-partite and bipartite graphs ✓
   - One-mode network projections/folding
   - Graph contractions

2) **K-Nearest Neighbor Graph Construction** ✓

3) **Network Deconvolution:**
   - Direct and and indirect effects in a network ✓
   - Inferring networks by network deconvolution

Time Series meets Network Science

Lucas Lacasa

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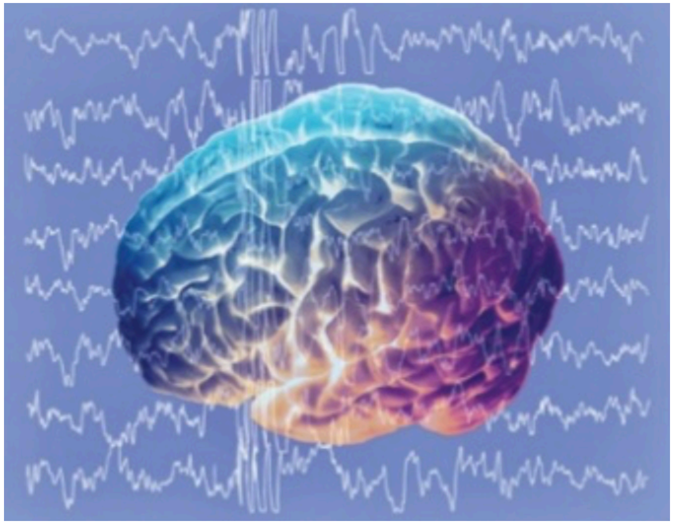
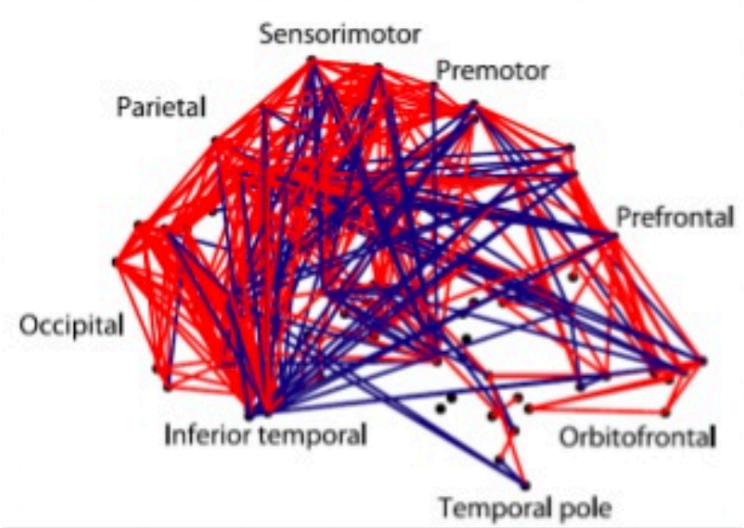
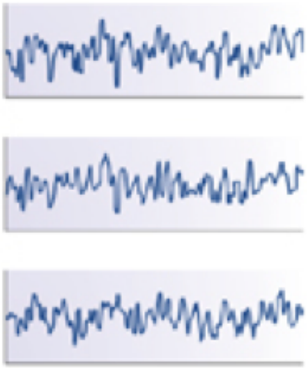
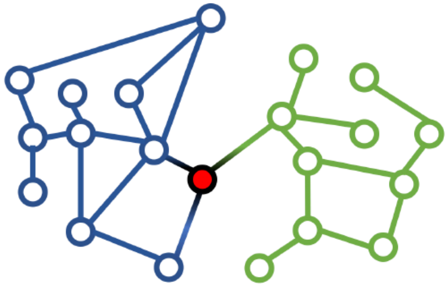
Porto, 17 December 2018

Porto
Winter School on
Network Science

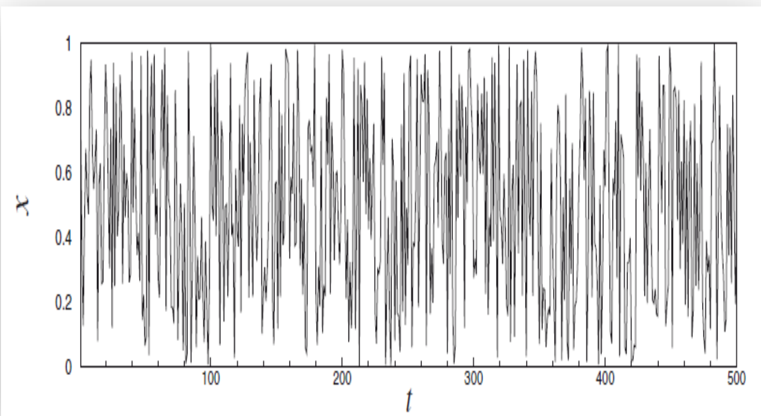



Sensorimotor
Premotor
Parietal
Prefrontal
Occipital
Inferior temporal
Orbitofrontal
Temporal pole

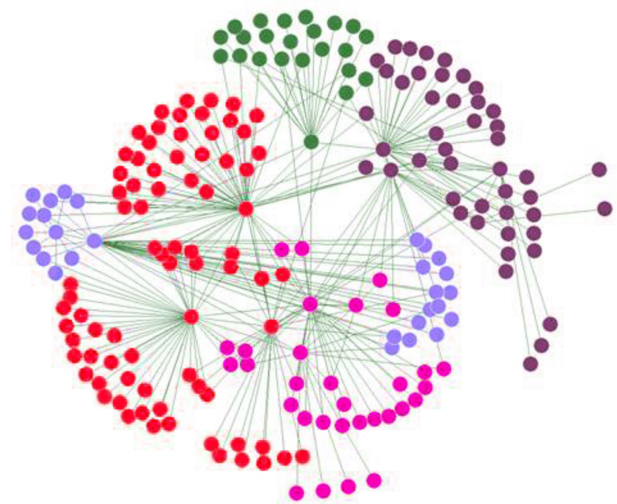




Leveraging the interface between signal processing and network science



SIGNAL PROCESSING



NETWORK SCIENCE

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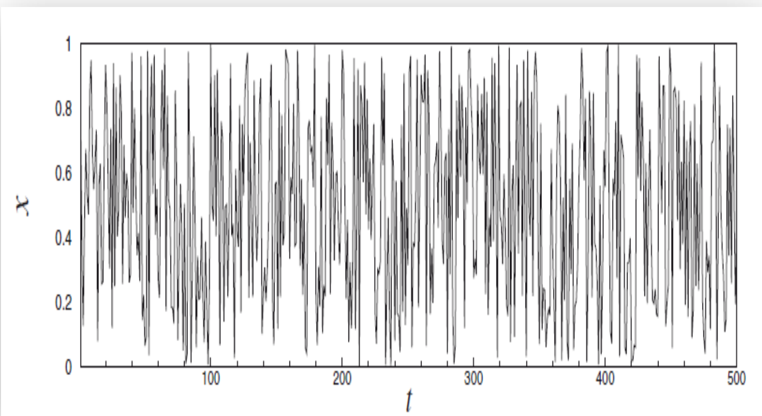
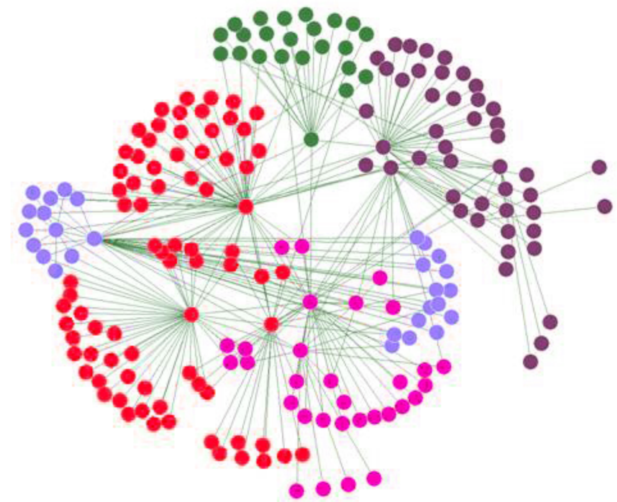
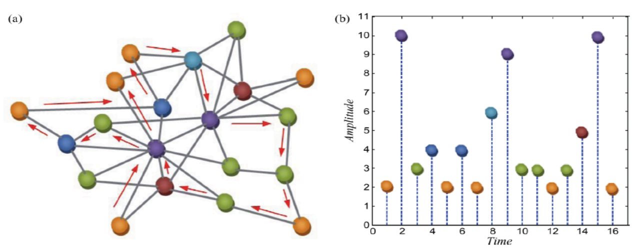


SIGNAL PROCESSING

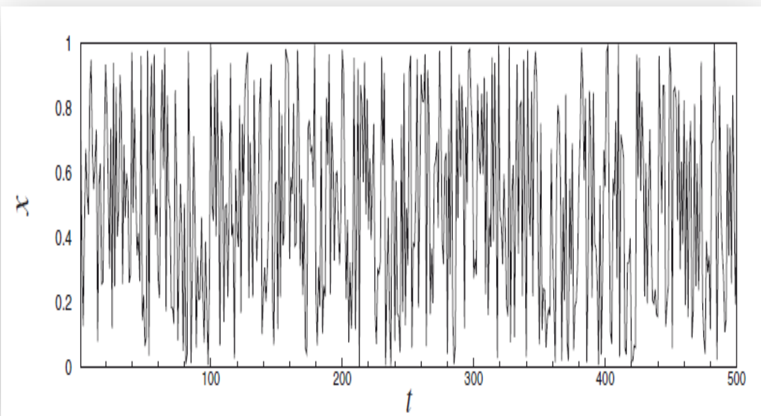


NETWORK SCIENCE

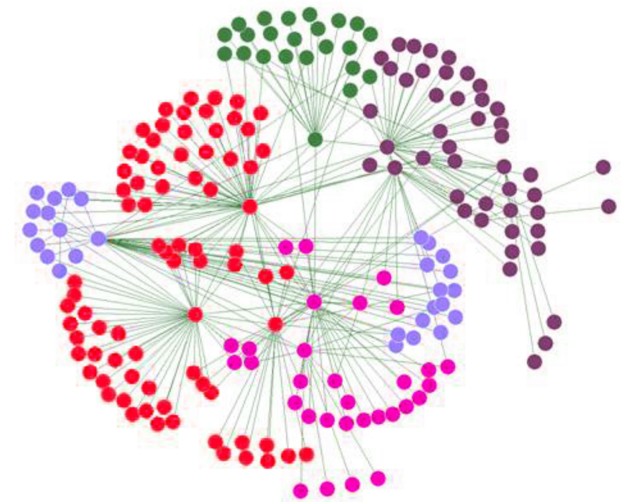


Signal processing of graphs

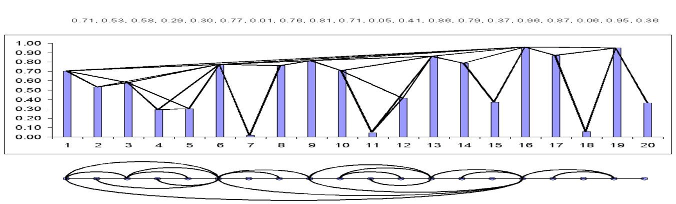
Leveraging the interface between signal processing and network science



SIGNAL PROCESSING

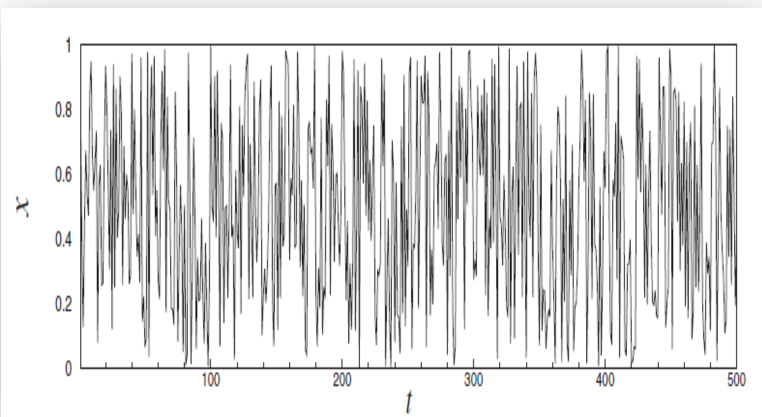


NETWORK SCIENCE

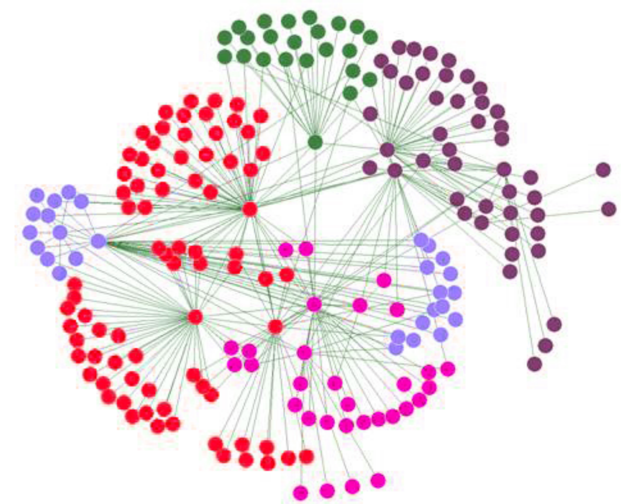


Graph-theoretical time series analysis

2. Time series meets Networks
   - Functional networks
   - Probing networks using random walks
   - Visibility graphs

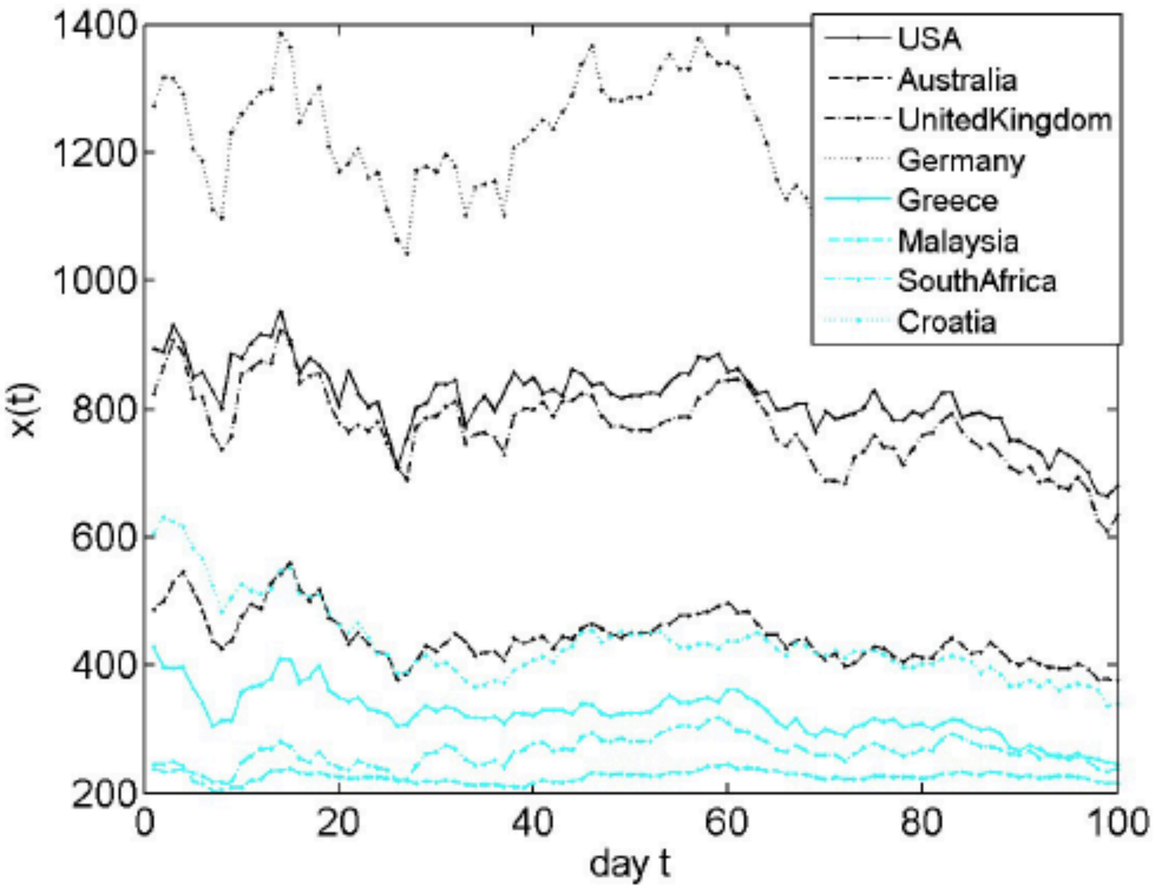


SIGNAL PROCESSING



NETWORK SCIENCE

$N = 8$ world stock markets, daily indices, $n = 100$ days.

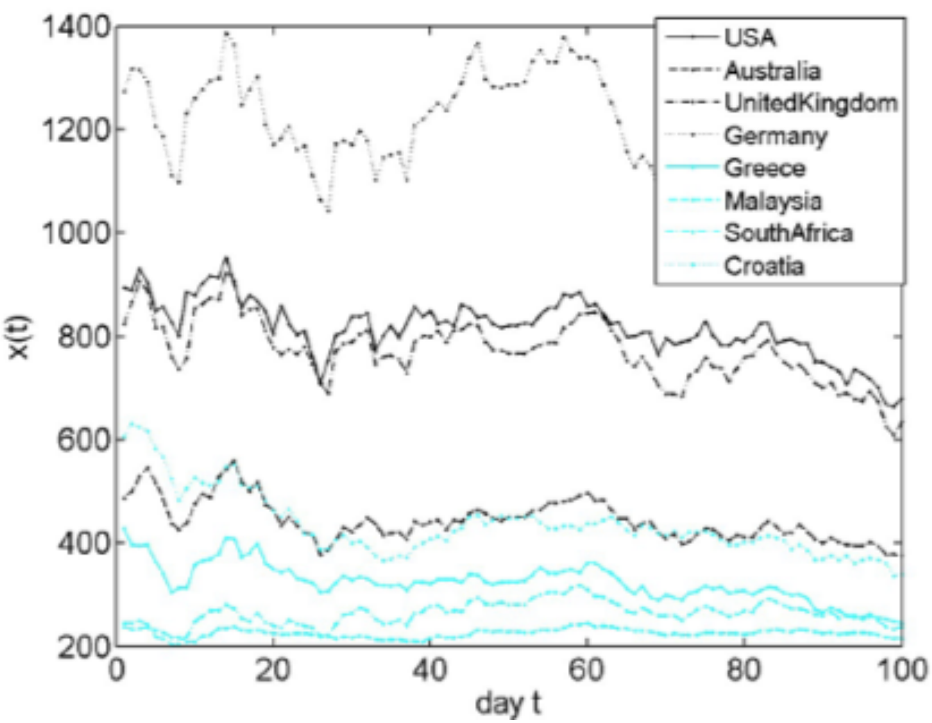


Similar indices, links among world stock markets?

A similarity measure sim(i, j) quantifies the level of

- correlation or coupling between X_i and X_j (undirected link)
- causality from X_i and X_j, and vice versa (directed link).

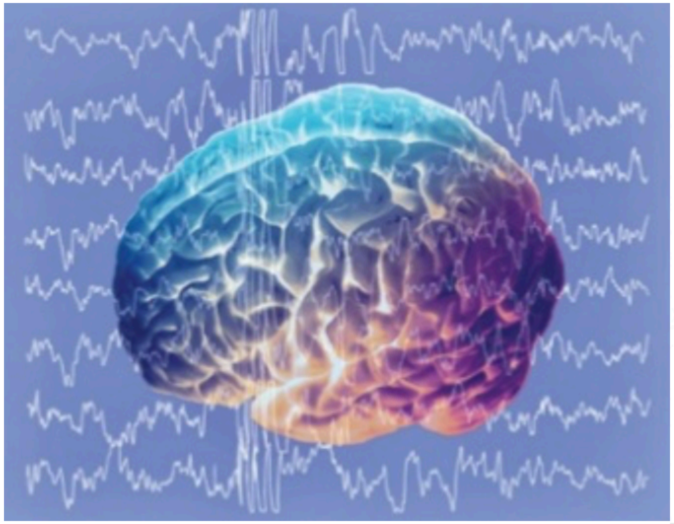
A standard similarity measure is again $\mathrm{Corr}(X_i, X_j) = r_{X_i, Y_j}$.

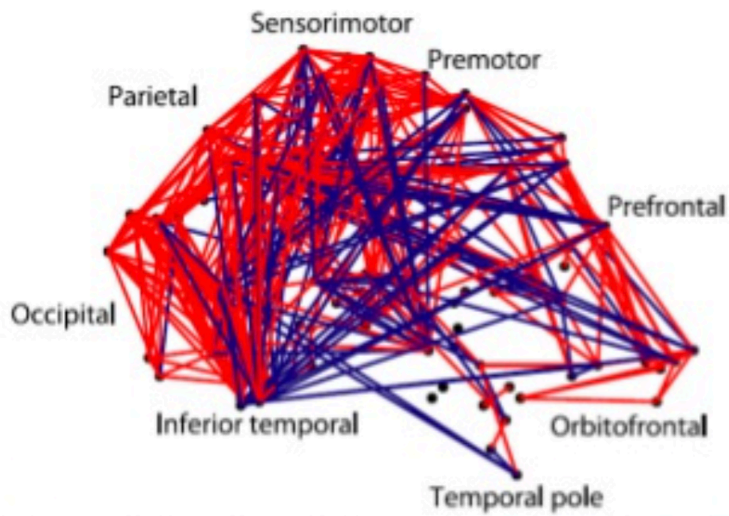


One can interpret this matrix as a weighted adjacency matrix!

Correlation network

Correlation & functional networks



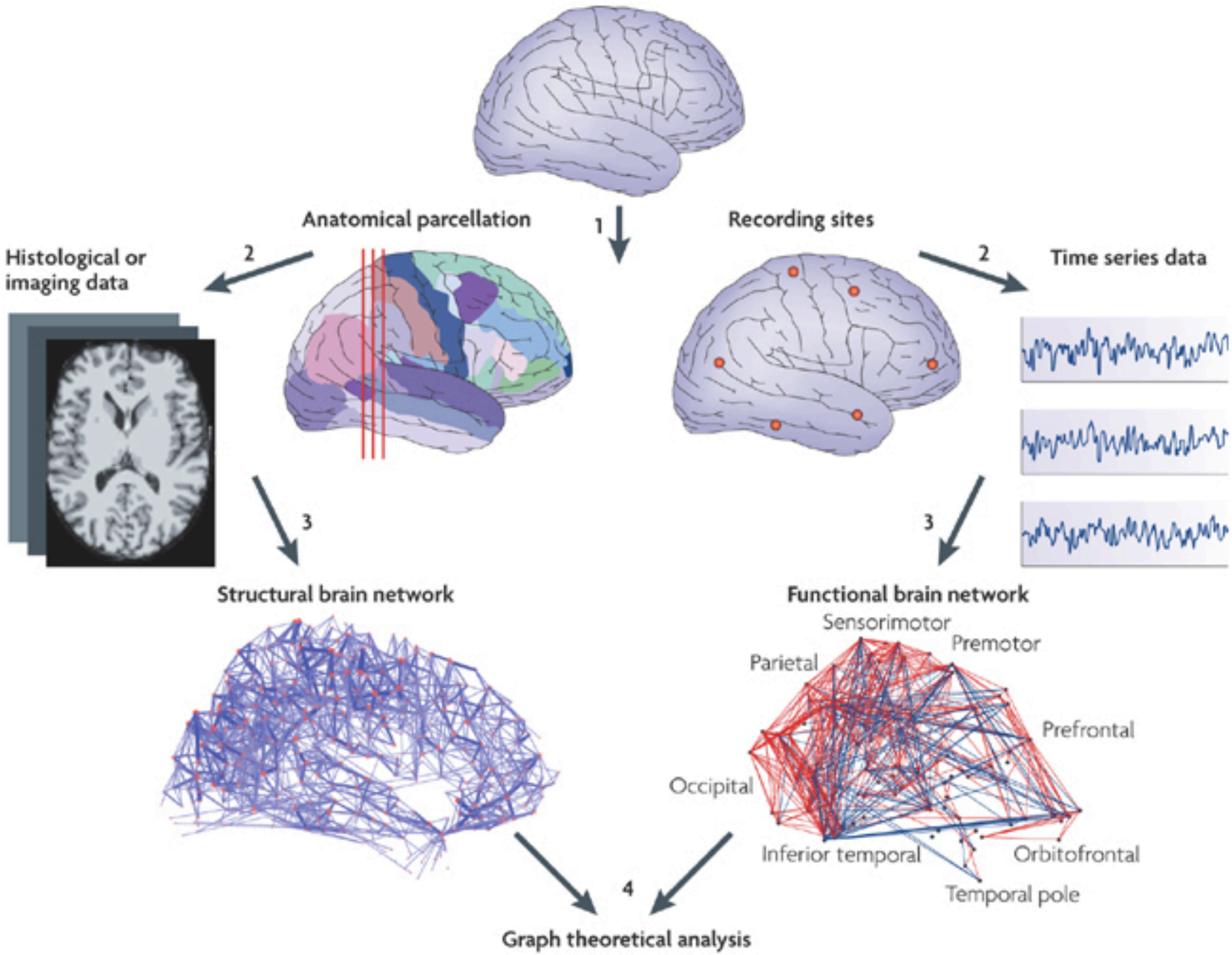


Functional networks

One can measure signals from the brain (EEG, fmri) at different regions and extract a correlation network from the multivariate time series.

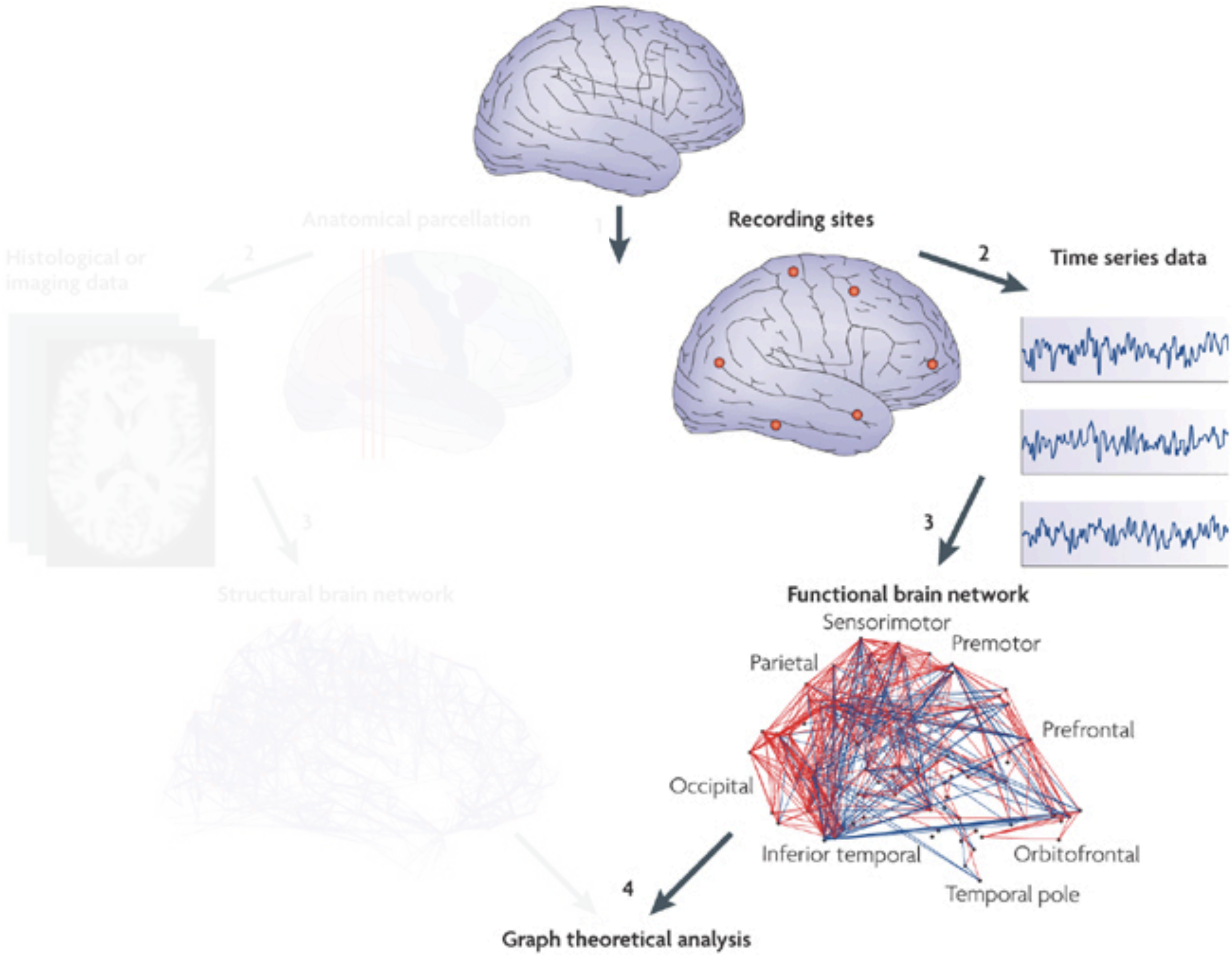
This network describes correlations between the activity of different regions of the brain, and it's called a **functional network**.

Correlation & functional networks



Bullmore, Sporns, **Nature Reviews Neuroscience** 10 (2009)

Correlation & functional networks



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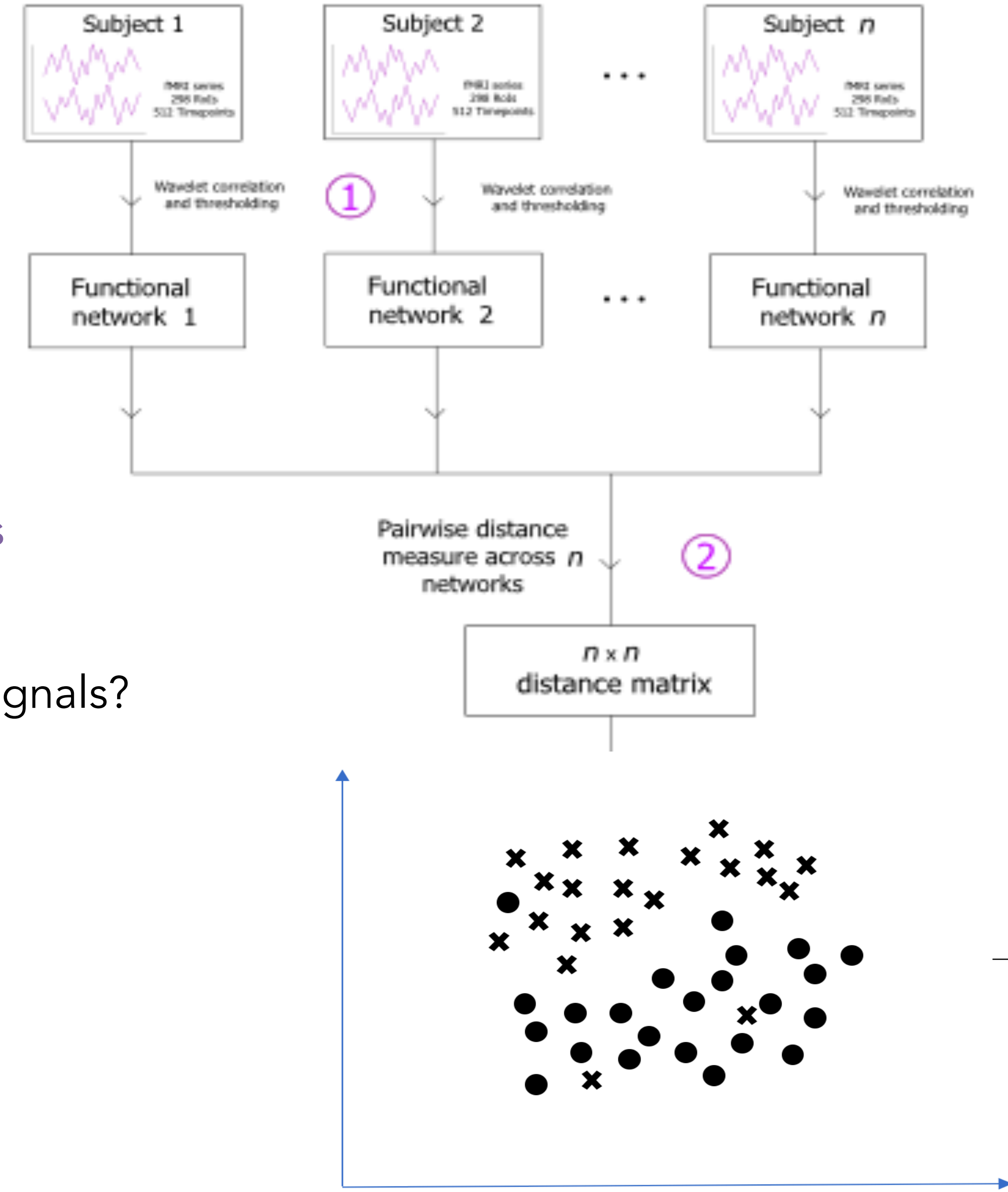
Correlation & functional networks

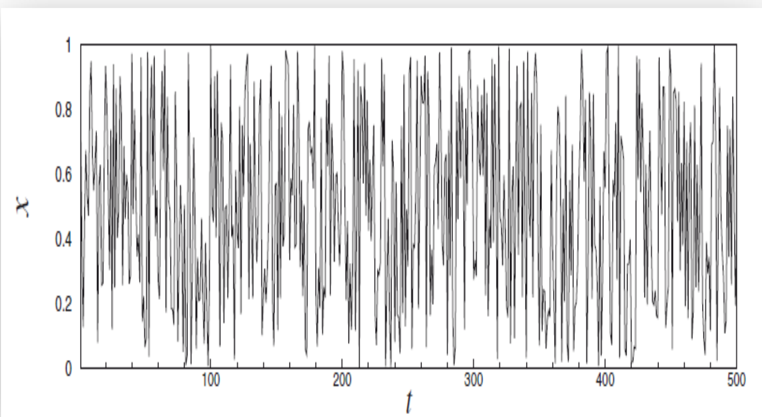


Typical study:
unsupervised clustering of diseases

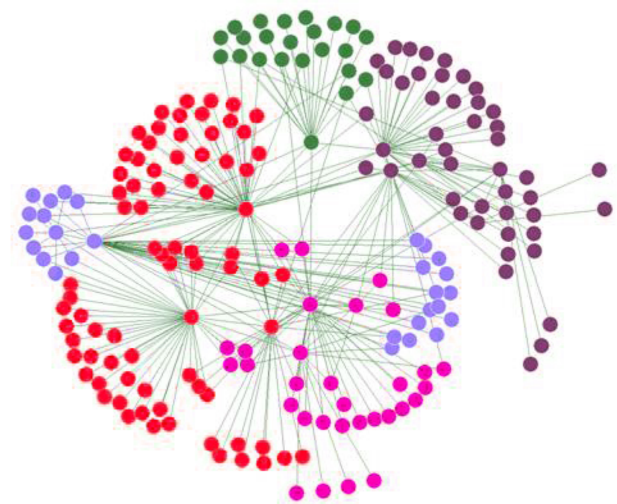
Can we predict which subject have schizophrenia by looking at brain signals?

2 Time series meets Networks

- Functional networks
- Probing networks using random walks
- Visibility graphs



SIGNAL PROCESSING



NETWORK SCIENCE

Visibility graphs were defined in computational geometry/computer science as the backbone graph capturing visibility paths (intervisible locations) in landscapes

- Each node represents a location
- Two locations are connected by a link if they are visible

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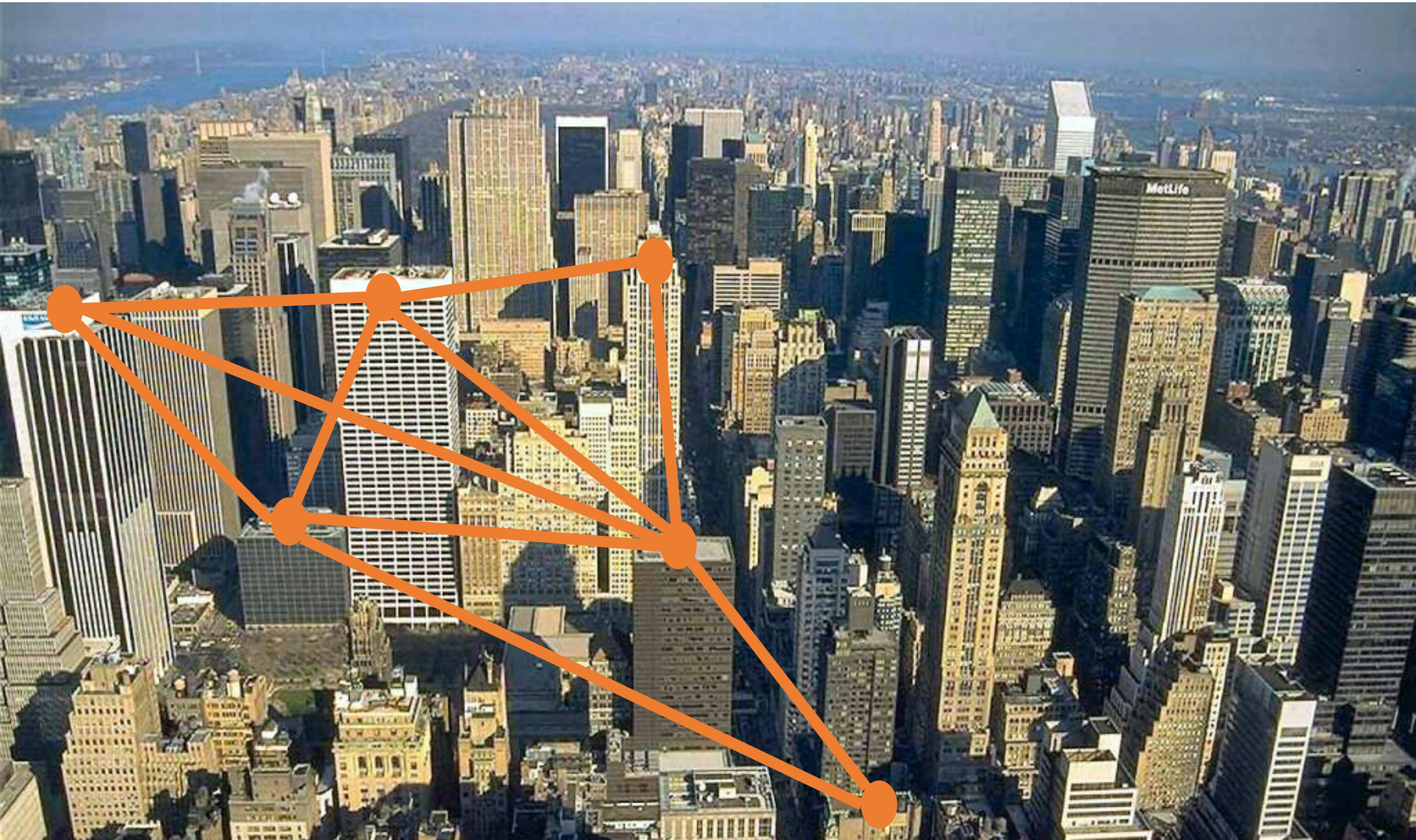

1D LANDSCAPES CAN BE CONSIDERED AS TIME SERIES

1D LANDSCAPES CAN BE CONSIDERED AS TIME SERIES

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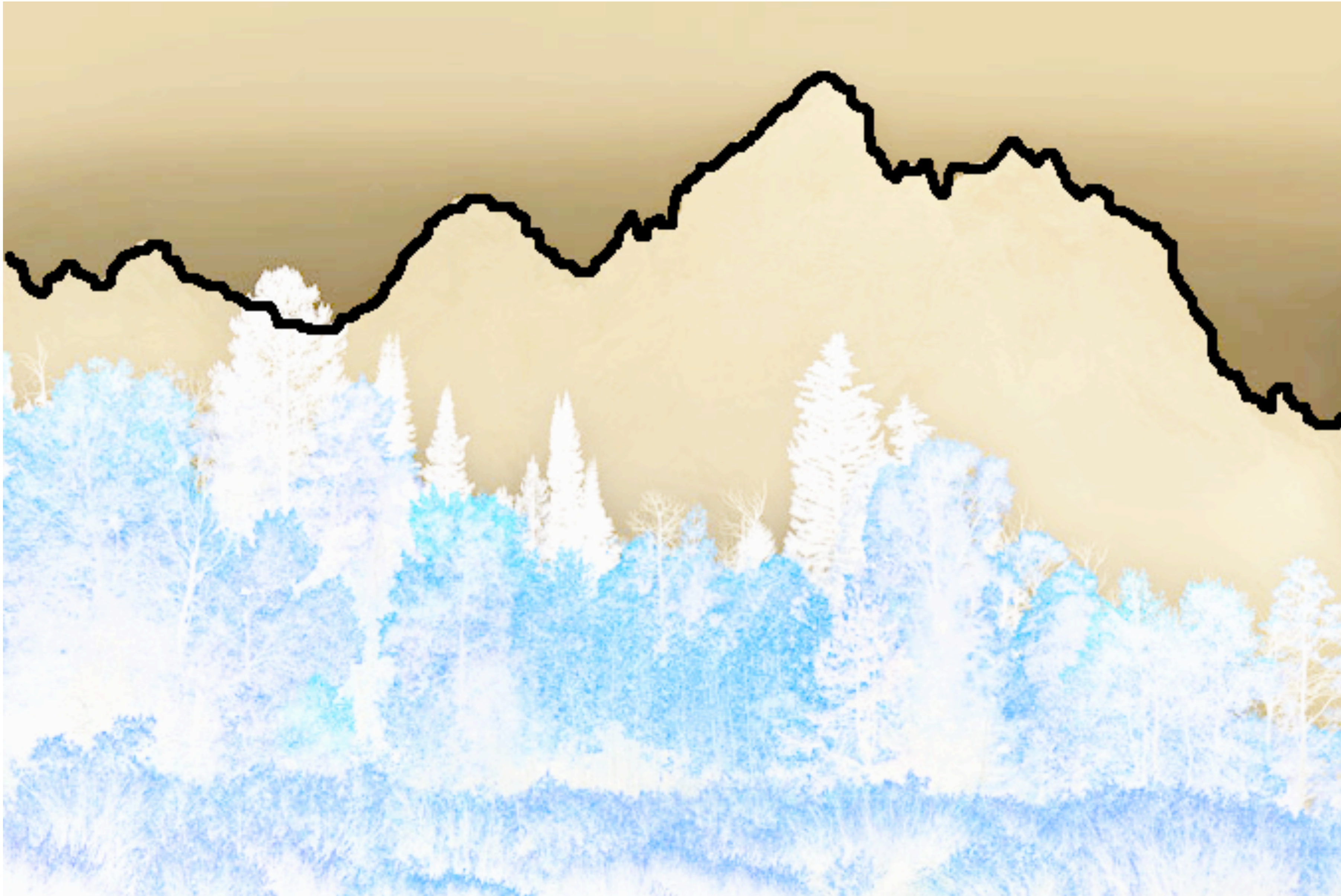
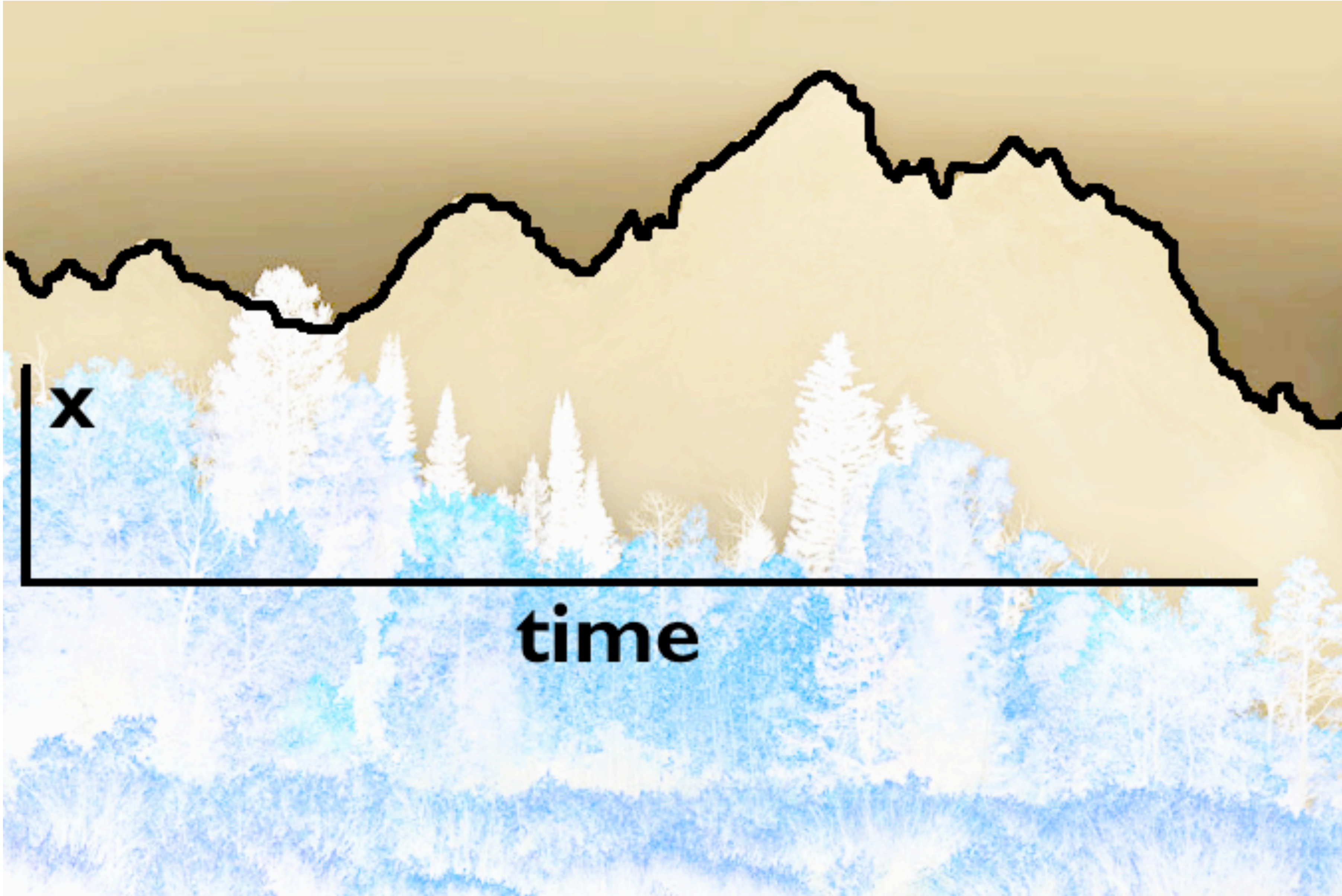
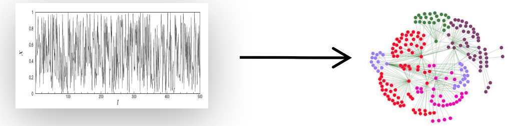


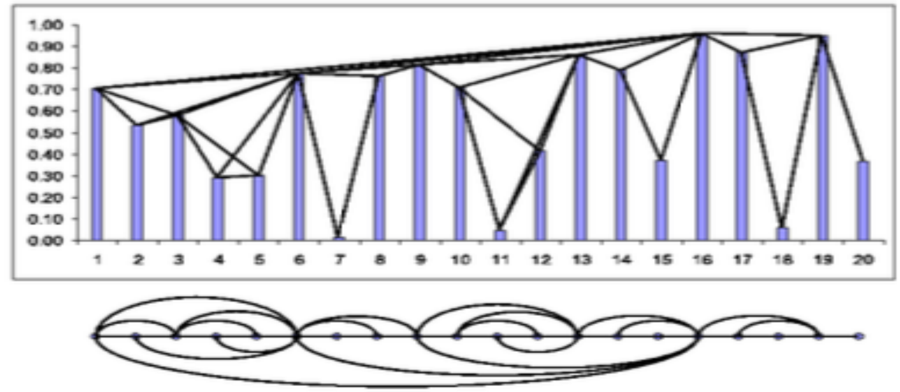
1D LANDSCAPES CAN BE CONSIDERED AS TIME SERIES



Visibility graphs: A combinatoric encription of time series
(univariate & multivariate)

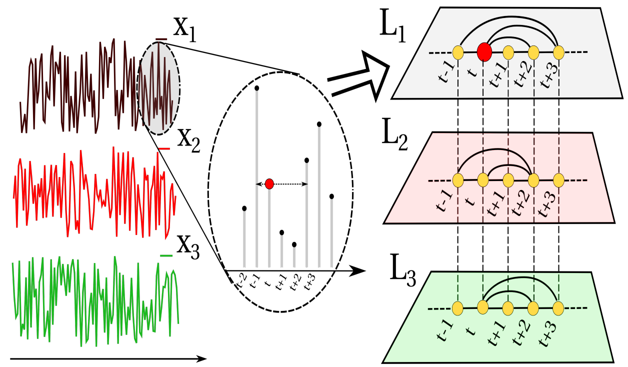


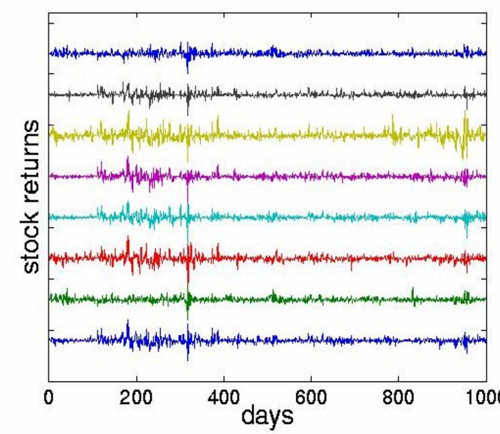
Univariate



*L. Lacasa, B. Luque, F. Ballesteros, J. Luque, JC Nuño , **PNAS** 105 (2008)*

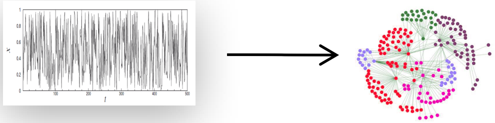
Multivariate



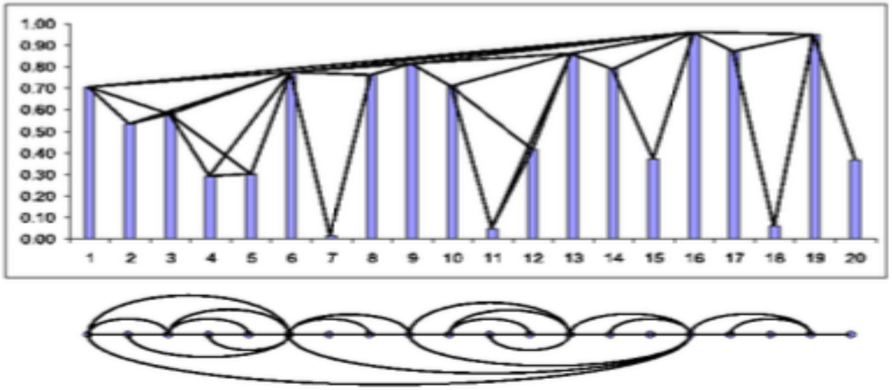


*L. Lacasa, E. Nicosia, V. Latora , **Sci. Rep.** 5 (2015)*

Visibility graphs: A combinatoric encription of time series (univariate & multivariate) and beyond

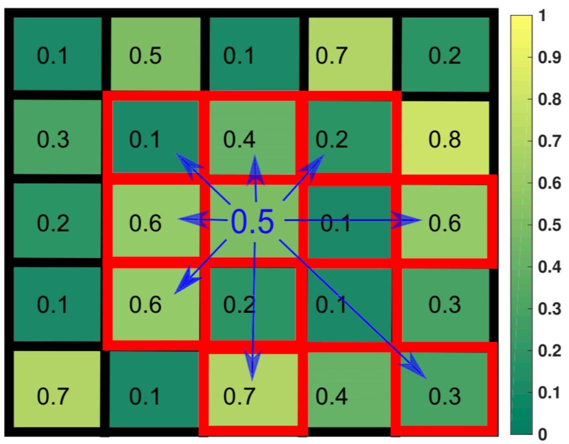


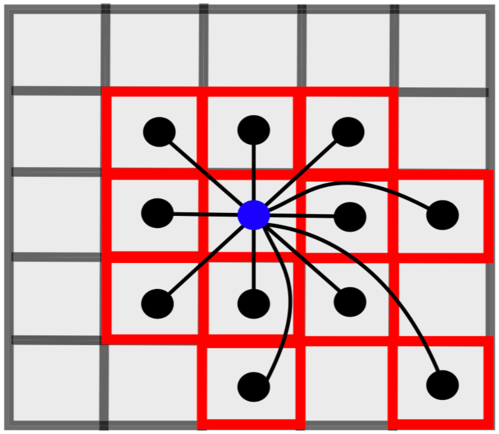
Univariate



L. Lacasa, B. Luque, F. Ballesteros, J. Luque, JC Nuño , **PNAS** 105 (2008)

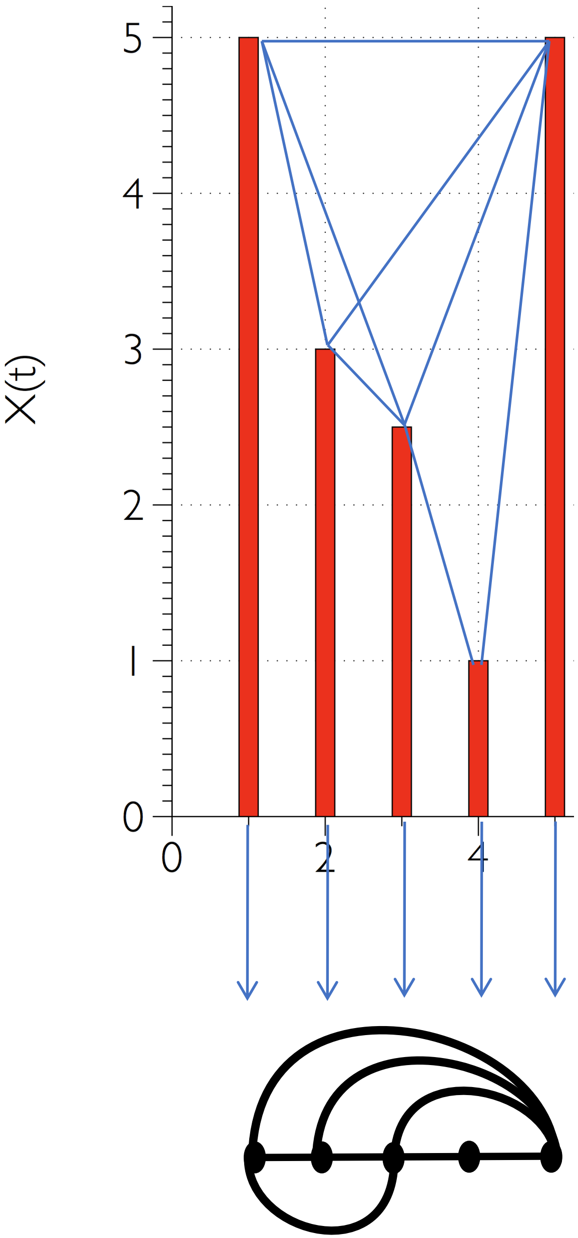
Spatial





L. Lacasa, J. Iacovacci, **Phys. Rev. E** 96 (2017)

Natural Visibility Algorithm



For a time series of N data:

* each datum is mapped into a node
* two nodes are linked if a visibility criterion holds in the series

The resulting visibility graph:

* has N ordered nodes
* is connected by a Hamiltonian path
* is invariant under certain transformations in the series

Lacasa, Luque, Ballesteros, Luque, Nuño, **PNAS** *105 (2008)*

(Vanessa Silva Msc Thesis)

Example Application: Clustering of Time Series

- Alternative approach to statistical time series analysis;
- Representing time series as complex networks:
  - Mapping concepts;
  - Topological measures.

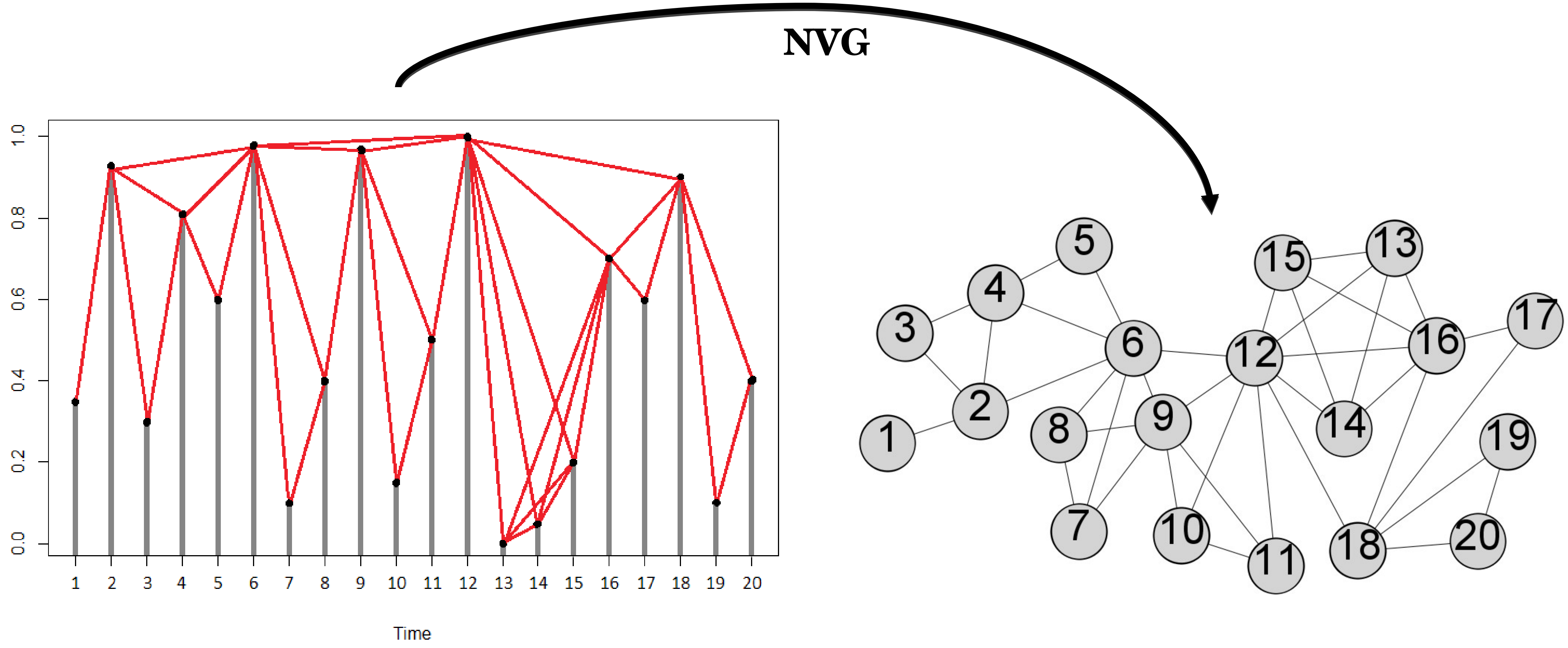
Key question:

- Can simple topological measures of different networks distinguish different processes of time series?

From Time Series to Complex Networks

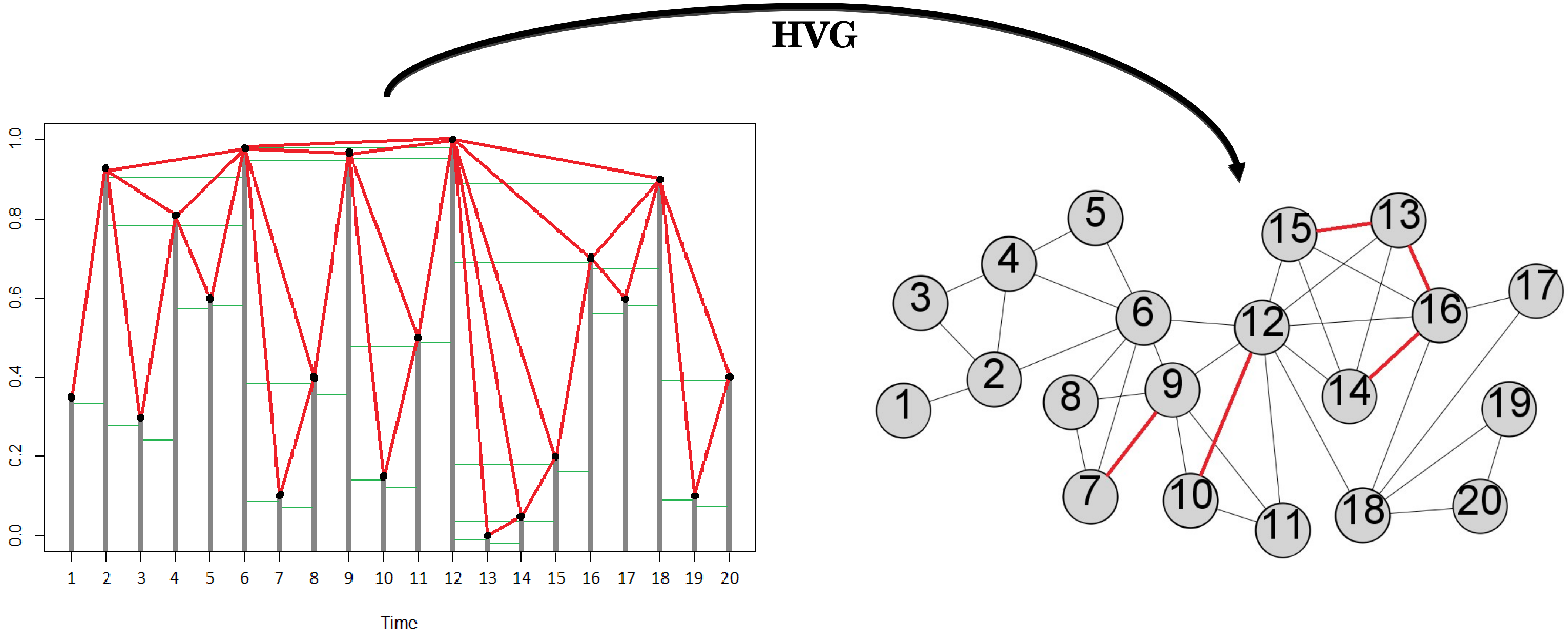
$$y_c = y_b + (y_a - y_b)\frac{(t_b - t_c)}{t_b - t_a}, \qquad t_a < t_c < t_b$$

Natural Visibility Graph

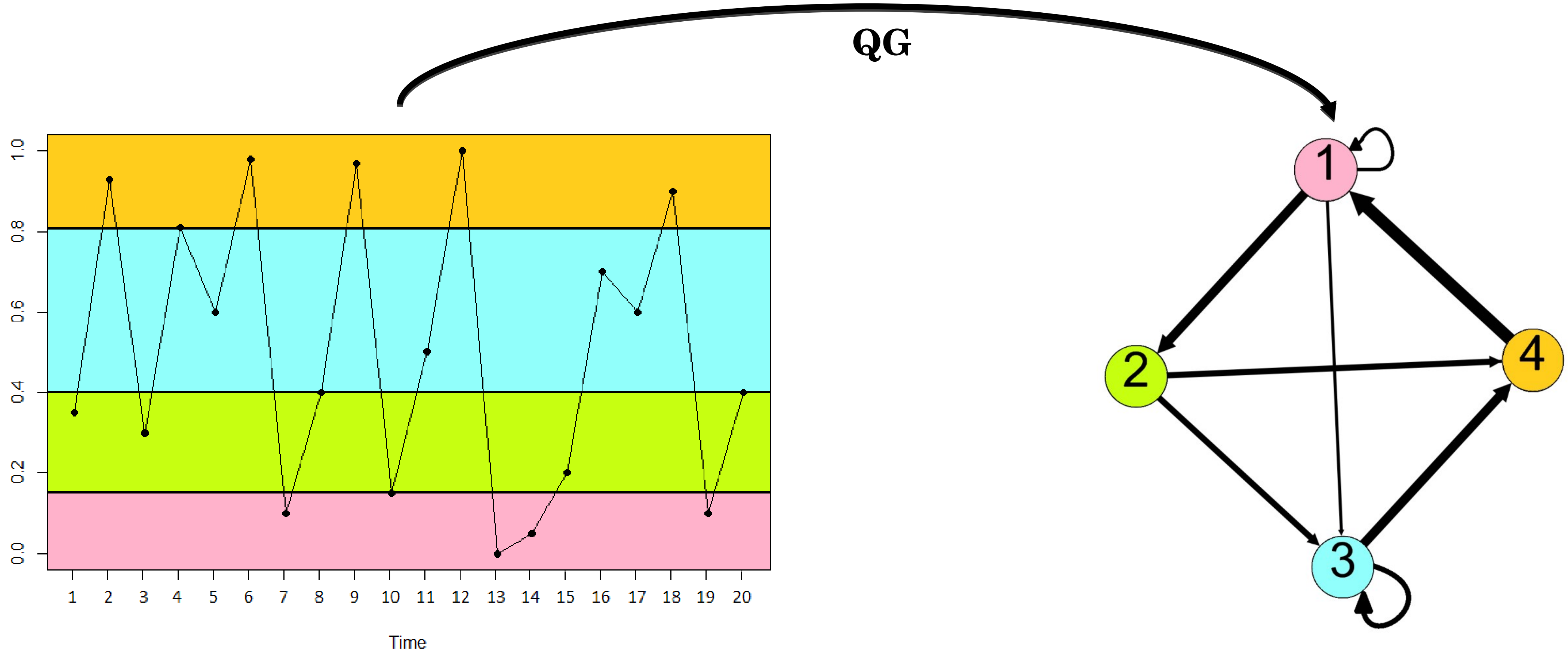


$y_a, y_b > y_c, \qquad t_a < t_c < t_b$

Horizontal Visibility Graph

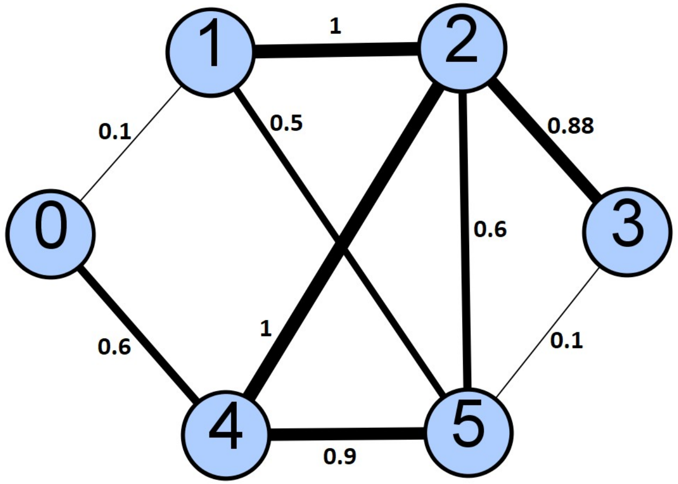


Quantile Graph



Topological Metrics

- There is a vast set of topological metrics of graphs to study the particular characteristics of the system.
  - **Average Degree** ($\bar{k}$)
  - **Average Path Length** ($\bar{d}$)
  - **Global Clustering Coefficient** (C)
  - **Number of Communities** (S)
  - **Modularity** (Q)



$$\bar{k} = 1{,}89$$
$$\bar{d} = 1{,}47$$
$$C = 0{,}45$$
$$S = 2{,}00$$
$$Q = 0{,}05$$

Time Series Clustering

- Distance-based methods
  - Similarity between observations
    - e.g. Dynamic Time Warping
- Characteristics-based methods
  - Similarity between global characteristics
    - e.g. trend, frequency, autocorrelation, Hurst
- **Network-based methods**
  - Similarity between topological measures
    - e.g. average degree, number of communities, clustering coefficient

Method

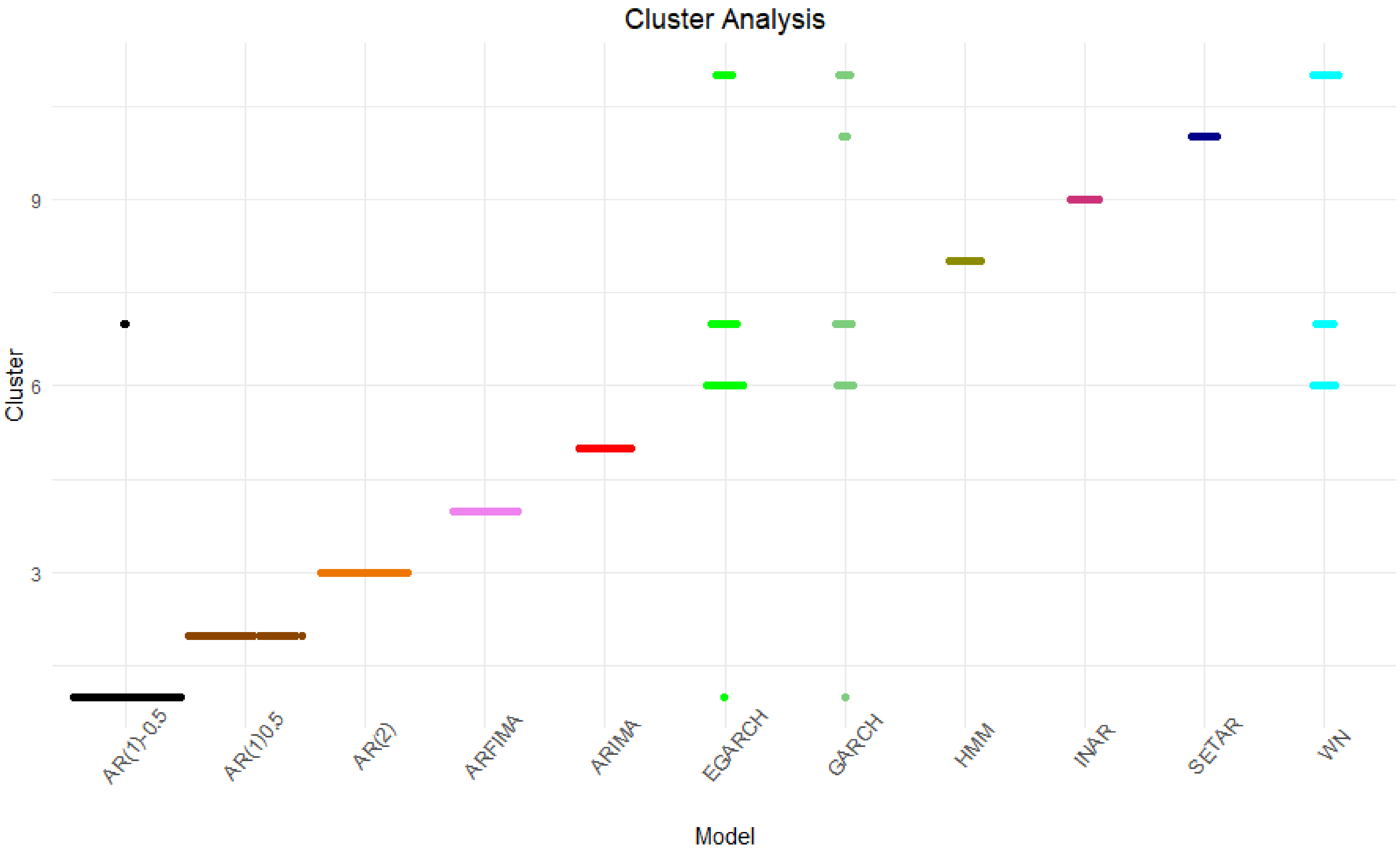
1. **Generate Complex Networks**
   a. NVG, HVG, and QGs
2. **Calculate Metrics and Normalize**
   a. $\bar{k}$, $\bar{d}$, C, S and Q
   b. Min-Max normalization
3. **Dimensionality Reduction**
   a. PCA and t-SNE
4. **Clustering Analysis**
   1. k-means

Time Series Models

- White Noise (i.i.d)

- Linear models
  - AR(1) | Smoother
  - AR(2) | Pseudo-Periodic
  - ARIMA | Stochastic Trend
  - ARFIMA | Long Memory

- Nonlinear models
  - SETAR | Regimes
  - HMM | States
  - INAR | Integer Valued Data
  - GARCH
  - EGARCH | Conditional Heterocesdaticity and Asymmetry


Cluster Analysis
Cluster
9
6
3
Model
AR(1)-0.5
AR(1)0.5
AR(2)
ARFIMA
ARIMA
EGARCH
GARCH
HMM
INAR
SETAR
WN