Structure detection methods

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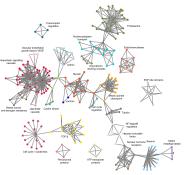
Methods

Hierarchy by shuffling

References



"Community detection in graphs" 🗗 Santo Fortunato, Physics Reports, **486**, 75–174, 2010. [6]



Structure detection

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Hierarchy by shuffling Hierarchies & Missing Links

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Hierarchy by division

Top down:

& Idea: Identify global structure first and recursively uncover more detailed structure.

& Basic objective: find dominant components that have significantly more links within than without, as compared to randomized version.

We'll first work through "Finding and evaluating" community structure in networks" by Newman and Girvan (PRE, 2004). [12]

A See also

1. "Scientific collaboration networks. II. Shortest paths, weighted networks, and centrality" by Newman (PRE, 2001). [10, 11]

2. "Community structure in social and biological networks" by Girvan and Newman (PNAS, 2002). [7]

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Outline

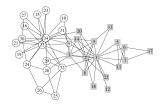
Overview

Methods

Hierarchy by aggregation Hierarchy by division Hierarchy by shuffling Spectral methods Hierarchies & Missing Links Overlapping communities Link-based methods General structure detection

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Structure detection



▲ Zachary's karate club [19, 12]

Possible substructures:

The issue:

how do we elucidate the internal structure of large networks across many scales?

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Hierarchy by aggregation—Bottom up:

- Idea: Extract hierarchical classification scheme for
- Need a measure of distance between all pairs of objects.
- & Example: Ward's method [17]
- Procedure:
 - 1. Order pair-based distances.
 - 2. Sequentially add links between nodes based on closeness.
 - 3. Use additional criteria to determine when clusters are meaningful.

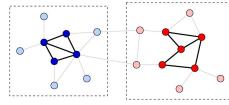
- N objects by an agglomeration process.

- Clusters gradually emerge, likely with clusters inside of clusters.
- Call above property Modularity.
- Works well for data sets where a distance between all objects can be specified (e.g., Aussie Rules [9]).

Hierarchy by aggregation

Bottom up problems:

- Tend to plainly not work on data sets representing networks with known modular structures.
- Good at finding cores of well-connected (or similar) nodes... but fail to cope well with peripheral, in-between nodes.



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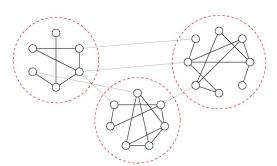
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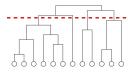


Idea: Edges that connect communities have higher betweenness than edges within communities.

Hierarchy by division

One class of structure-detection algorithms:

- 1. Compute edge betweenness for whole network.
- 2. Remove edge with highest betweenness.
- 3. Recompute edge betweenness
- 4. Repeat steps 2 and 3 until all edges are removed.
- 5 Record when components appear as a function of # edges removed.
- 6 Generate dendogram revealing hierarchical structure.



Red line indicates appearance of four (4) components at a certain level.

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hierarchies, cliques, rings, ... Plus:

All combinations of substructures.

Much focus on hierarchies (pyramids)

Key element for division approach:

- Recomputing betweenness.
- Reason: Possible to have a low betweenness in links that connect large communities if other links carry majority of shortest paths.

When to stop?:

- A How do we know which divisions are meaningful?
- Modularity measure: difference in fraction of within component nodes to that expected for randomized version:

$$Q = \sum_i [e_{i\,i} - a_i^2]$$

where $e_{i,j}$ is the fraction of (undirected) edges travelling between identified communities i and j, and $a_i = \sum_i e_{ij}$ is the fraction of edges with at least one end in community i. \square

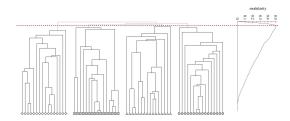
Hierarchy by division

Test case:

- Generate random community-based networks.
- N = 128 with four communities of size 32.
- Add edges randomly within and across communities.
- Example:

$$\langle k \rangle_{\text{in}} = 6 \text{ and } \langle k \rangle_{\text{out}} = 2.$$

Hierarchy by division



- Arr Maximum modularity $Q \simeq 0.5$ obtained when four communities are uncovered.
- Further 'discovery' of internal structure is somewhat meaningless, as any communities arise accidentally.

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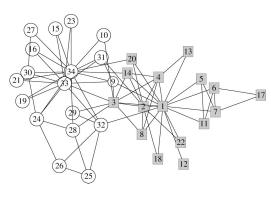
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Hierarchy by division



Factions in Zachary's karate club network. [19]

Betweenness for electrons:

- Unit resistors on each edge.
- For every pair of nodes s (source) and t (sink), set up unit currents in at s and out at t.
- Measure absolute current along each edge ℓ , $|I_{\ell,st}|$.
- \Re Sum $|I_{\ell,st}|$ over all pairs of nodes to obtain electronic betweenness for edge ℓ .
- (Equivalent to random walk betweenness.)
- Contributing electronic betweenness for edge between nodes *i* and *i*:

$$B_{ij,st}^{\,\mathrm{elec}} = a_{ij} |V_{i,st} - V_{j,st}|. \label{eq:Belecher}$$

Electronic betweenness

- Define some arbitrary voltage reference.
- & Kirchhoff's laws: current flowing out of node i must balance:

$$\sum_{j=1}^N \frac{1}{R_{ij}}(V_j-V_i) = \delta_{is} - \delta_{it}.$$

- \Re Between connected nodes, $R_{ij} = 1 = a_{ij} = 1/a_{ij}$.
- \Re Between unconnected nodes, $R_{ij} = \infty = 1/a_{ij}$.
- We can therefore write:

$$\sum_{i=1}^N a_{ij}(V_i-V_j) = \delta_{is} - \delta_{it}.$$

Some gentle jiggery-pokery on the left hand side: $\sum_{j} a_{ij} (V_i - V_j) = \frac{V_i}{\sum_{j} a_{ij}} - \sum_{j} a_{ij} V_j$ $= V_i \mathbf{k_i} - \sum_i a_{ij} V_j = \sum_j \left[\mathbf{k_i} \delta_{ij} V_j - a_{ij} V_j \right]$ $=[(\mathbf{K}-\mathbf{A})\vec{V}]_{i}$

Electronic betweenness

- & Write right hand side as $[I^{\text{ext}}]_{i,st} = \delta_{is} \delta_{it}$, where I_{ext}^{ext} holds external source and sink currents.
- Matrixingly then:

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$$(\mathbf{K} - \mathbf{A})\vec{V} = I_{st}^{\mathsf{ext}}.$$

- & **L** = **K A** is a beast of some utility—known as the Laplacian.
- Solve for voltage vector \vec{V} by **LU** decomposition (Gaussian elimination).
- Do not compute an inverse!
- Note: voltage offset is arbitrary so no unique
- Presuming network has one component, null space of $\mathbf{K} - \mathbf{A}$ is one dimensional.
- \Re In fact, $\mathcal{N}(\mathbf{K} \mathbf{A}) = \{c\vec{1}, c \in R\}$ since $(\mathbf{K} \mathbf{A})\vec{1} = \vec{0}$.

Alternate betweenness measures:

Random walk betweenness:

- Asking too much: Need full knowledge of network to travel along shortest paths.
- One of many alternatives: consider all random walks between pairs of nodes i and j.
- Walks starts at node *i*, traverses the network randomly, ending as soon as it reaches j.
- Record the number of times an edge is followed by a walk.
- Consider all pairs of nodes.
- Random walk betweenness of an edge = absolute difference in probability a random walk travels one way versus the other along the edge.
- Equivalent to electronic betweenness (see also diffusion).

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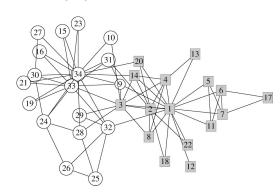
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Factions in Zachary's karate club network. [19]

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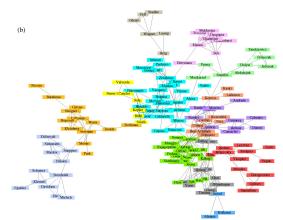
Hierarchy by division

recompute betweenness after each edge removal.

Hierarchy by division

Structure detection

Scientists working on networks (2004)



Shuffling for structure

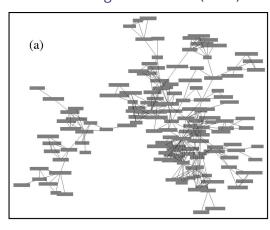
- "Extracting the hierarchical organization of complex systems" Sales-Pardo et al., PNAS (2007) [14, 15]
- & Consider all partitions of networks into m groups
- As for Newman and Girvan approach, aim is to find partitions with maximum modularity:

$$Q = \sum_i [e_{ii} - (\sum_j e_{ij})^2] = {\rm Tr} {\bf E} - ||{\bf E}^2||_1.$$

Structure

Third column shows what happens if we don't

Scientists working on networks (2004)



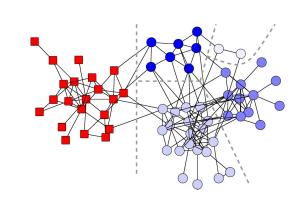
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Dolphins!



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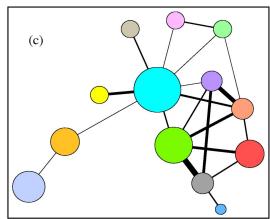
Shuffling for structure

- & Consider partition network, i.e., the network of all possible partitions.
- & Defn: Two partitions are connected if they differ only by the reassignment of a single node.
- & Look for local maxima in partition network.
- & Construct an affinity matrix with entries M_{ij}^{aff} .
- $\Re M_{i,i}^{\text{aff}} = \mathbf{Pr}$ random walker on modularity network ends up at a partition with i and j in the same group.
- C.f. topological overlap between i and j = # matching neighbors for i and j divided by maximum of k_i and k_j .

Structure detection

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Scientists working on networks (2004)



Structure detection Overview

Hierarchy by divisio

Les Miserables

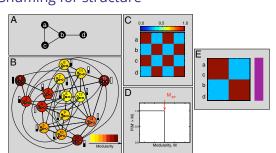
More network analyses for Les Miserables here and here .

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Shuffling for structure



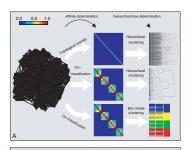
A: Base network; B: Partition network; C: Coclassification matrix; **D:** Comparison to random networks (all the same!); E: Ordered coclassification matrix; Conclusion: no structure... Structure detection 32 of 76 Overview

- Method obtains a distribution of classification hierarchies.
- Note: the hierarchy with the highest modularity score isn't chosen.
- Idea is to weight possible hierarchies according to their basin of attraction's size in the partition network.
- Next step: Given affinities, now need to sort nodes into modules, submodules, and so on.
- & Idea: permute nodes to minimize following cost

$$C = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N M_{ij}^{\mathrm{aff}} |i-j|. \label{eq:constraint}$$

- Use simulated annealing (slow).
- where f is a strictly monotonically increasing function of 0, 1, 2, ...

Shuffling for structure



- N = 640,
- $\langle k \rangle = 16$,
- 3 tiered hierarchy.

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Shuffling for structure

$$\begin{split} \left(\vec{v}_1\right)_i &= \left(i - \frac{n+1}{2}\right),\\ \left(\vec{v}_2\right)_i &= \left(i - \frac{n+1}{2}\right)^2 + \sqrt{S_{n,4}/n}, \text{ and }\\ \left(\vec{v}_3\right)_i &= \left(i - \frac{n+1}{2}\right)^2 - \sqrt{S_{n,4}/n}. \end{split}$$

Remarkably,

$$T = \lambda_1 \hat{v}_1 \hat{v}_1^\mathsf{T} + \lambda_2 \hat{v}_2 \hat{v}_2^\mathsf{T} + \lambda_3 \hat{v}_3 \hat{v}_3^\mathsf{T}.$$

The next step: figure out how to capitalize on this...

Shuffling for structure

Table 1. Top-level structure of real-world networks

•				
Network	Nodes	Edges	Modules	Main modules
Air transportation	3,618	28,284	57	8
E-mail	1,133	10,902	41	8
Electronic circuit	516	686	18	11
Escherichia coli KEGG	739	1,369	39	13
E. coli UCSD	507	947	28	17

General structure detection

Shuffling for structure

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- "Detecting communities in large networks" Capocci *et al.* (2005) [4]
- & Consider normal matrix $\mathbf{K}^{-1}A$, random walk matrix $A^{\mathsf{T}}\mathbf{K}^{-1}$, Laplacian $\mathbf{K} - \mathbf{A}$, and AA^{T} .
- Basic observation is that eigenvectors associated with secondary eigenvalues reveal evidence of structure.
- Builds on Kleinberg's HITS algorithm.

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Modularity

(UCSD

structure for

network of E. coli

reconstruction).

metabolic

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Shuffling for structure

- \mathfrak{F} Weird observation: if $T_{ij} = (i-j)^2$ then **T** is of rank 3, independent of N.
- Discovered by numerical inspection ...
- The eigenvalues are

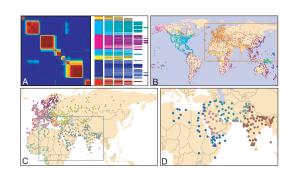
$$\begin{split} \lambda_1 &= -\frac{1}{6} n(n^2 - 1), \\ \lambda_2 &= + \sqrt{nS_{n,4}} + S_{n,2}, \text{ and} \\ \lambda_3 &= - \sqrt{nS_{n,4}} + S_{n,2}. \end{split}$$

where

$$S_{n,2} = \frac{1}{12} n(n^2-1), \text{ and}$$

$$S_{n,4} = \frac{1}{240} n(n^2-1)(3n^2-7).$$

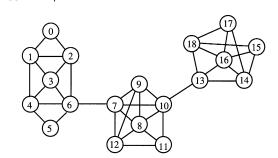
Shuffling for structure



Modules found match up with geopolitical units.

General structure detection

Example network:

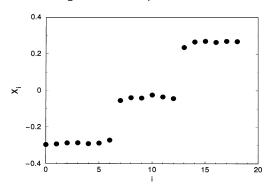


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Spectral methods

General structure detection

Second eigenvector's components:



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Hierarchies and missing links

Model also predicts reasonably well

- 1. average degree,
- 2. clustering,
- 3. and average shortest path length.

Table 1 | Comparison of original and resampled networks

Network	$\langle k \rangle_{\rm real}$	$\langle k \rangle_{\rm samp}$	C_{real}	C_{samp}	$d_{\rm real}$	d_{samp}	
T. pallidum	4.8	3.7(1)	0.0625	0.0444(2)	3.690	3.940(6)	
Terrorists	4.9	5.1(2)	0.361	0.352(1)	2.575	2.794(7)	
Grassland	3.0	2.9(1)	0.174	0.168(1)	3.29	3.69(2)	
							-

Statistics are shown for the three example networks studied and for new networks generated by resampling from our hierarchical model. The generated networks closely match the average degree $\langle k \rangle$, clustering coefficient C and average vertex-vertex distance d in each case, suggesting that they capture much of the structure of the real networks. Parenthetical values indicate standard errors on the final digits.

Social distance—Bipartite affiliation networks

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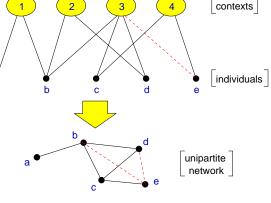
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occupation

kindergarter

teacher

health care

nurse

General structure detection

- Network of word associations for 10616 words.
- Average in-degree of 7.
- Using 2nd to 11th evectors of a modified version of AA^T :

Table 1 Words most correlated to science, literature and piano in the eigenvectors of $Q^{-1}WW^{\mathrm{T}}$

Science	1	Literature	1	Piano	1
Scientific	0.994	Dictionary	0.994	Cello	0.993
Chemistry	0.990	Editorial	0.990	Fiddle	0.992
Physics	0.988	Synopsis	0.988	Viola	0.990
Concentrate	0.973	Words	0.987	Banjo	0.988
Thinking	0.973	Grammar	0.986	Saxophone	0.985
Test	0.973	Adjective	0.983	Director	0.984
Lab	0.969	Chapter	0.982	Violin	0.983
Brain	0.965	Prose	0.979	Clarinet	0.983
Equation	0.963	Topic	0.976	Oboe	0.983
Examine	0.962	English	0.975	Theater	0.982

Values indicate the correlation

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Spectral methods

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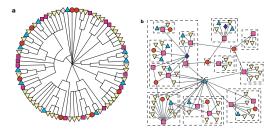
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Hierarchies and missing links



- Consensus dendogram for grassland species.
- Copes with disassortative and assortative communities.

Social distance—Context distance

education

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Hierarchies & Missing Links

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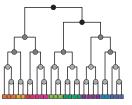
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References

Hierarchies and missing links

Clauset et al., Nature (2008) [5]





- & Idea: Shades indicate probability that nodes in left and right subtrees of dendogram are connected.
- A Handle: Hierarchical random graph models.
- Plan: Infer consensus dendogram for a given real
- Obtain probability that links are missing (big problem...).

From PoCS: Small-worldness and social searchability

Social networks and identity:

Identity is formed from attributes such as:

- Geographic location
- Type of employment
- Religious beliefs
- Recreational activities.

Groups are formed by people with at least one similar attribute.

Attributes ⇔ Contexts ⇔ Interactions ⇔ Networks.

Models

high school

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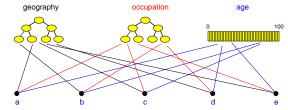
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Generalized affiliation networks



Blau & Schwartz [2], Simmel [16], Breiger [3], Watts et al. [18]; see also Google+ Circles.

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Overlapping communiti

Dealing with community overlap:

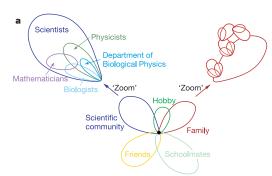
- & Earlier structure detection algorithms, agglomerative or divisive, force communities to be purely distinct.
- & Overlap: Acknowledge nodes can belong to multiple communities.
- Palla et al. [13] detect communities as sets of adjacent k-cliques (must share k-1 nodes).
- \triangle One of several issues: how to choose k?
- Four new quantities:
 - m, number of a communities a node belongs to.
 - $s_{\alpha,\beta}^{ov}$, number of nodes shared between two given communities, α and β .

 - s_{α}^{com} , community α 's size.
- Associated distributions: $P_{>}(m)$, $P_{>}(s_{\alpha,\beta}^{ov})$, $P_{>}(d_{\alpha}^{com})$, and $P_{>}(s_{\alpha}^{com})$.



"Uncovering the overlapping community structure of complex networks in nature and society"

Palla et al.. Nature, **435**, 814–818, 2005. [13]



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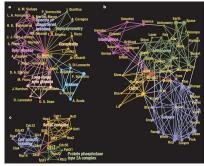
Hierarchies & Missing

Overlapping communities

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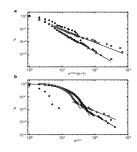
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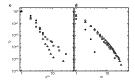
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be associated with his fields of interest. **b**, The communities of the word bright in the South Florida Free Association norms list (for $w^* = 0.025$ represent the different meanings of this word. c, The communities of the protein Zdst in the DIP core list of the protein-protein interactions of S and S are closed with although the protein complexes exceeding the size of the protein-protein interactions of S and S are called the size of S and S are called a size of S and S

& Two tunable parameters: w^* , the link weight threshold, and k, the clique size.





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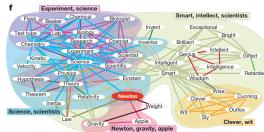
Overlapping commi

References



"Link communities reveal multiscale complexity in networks"

Ahn, Bagrow, and Lehmann, Nature, **466**, 761-764, 2010. [1]



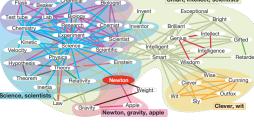
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Link-based methods

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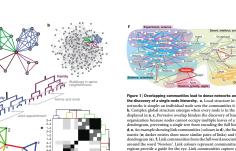


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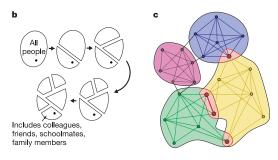
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Note: See details of paper on how to choose link communities well based on partition density D.



in a single node, whereas it shares two nodes and a link with the green or These overlapping regions are emphasized in red. Notice that any k-cliques (complete subgraph of size k) can be reached only from the k-cliques of the same community through a series of adjacent k-cliques. Two k-cliques are adjacent if they share k = 1 nodes.

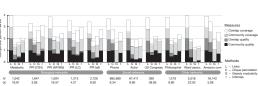
Overview A link-based approach:

- What we know now: Many network analyses profit from focusing on links.
- & Idea: form communities of links rather than communities of nodes.
- & Observation: Links typically of one flavor, while nodes may have many flavors.
- & Link communities induce overlapping and still hierarchically structured communities of nodes.
- (Applause.)

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References



networks were chosen for their varied sizes and topologi the different domains where network analysis is used. Sho number of nodes, N, and the average number of neighb Link clustering finds the most relevant community stru-networks. AP/MS, affinity-purification/mass spectromet

& Comparison of structure detection algorithms using four measures over many networks.

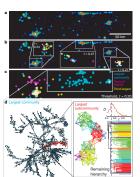
Revealed communities are matched against 'known' communities recorded in network metadata.

Link approach particularly good for dense, overlapful networks.

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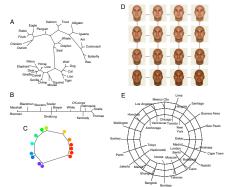
social network within the largest community in e, with its largest subcommunity highlighted. The highlighted subcommunity is sho with its link dendrogram and partition density, D, as a function of the Link colours correspond to dendrogram branches. e. Community

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Example learned structures:



Biological features; Supreme Court votes; perceived color differences; face differences; & distances between cities.

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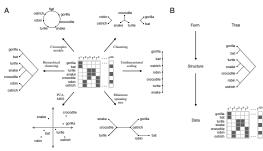
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"The discovery of structural form" Kemp and Tenenbaum, PNAS (2008)[8]



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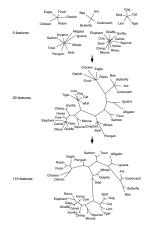
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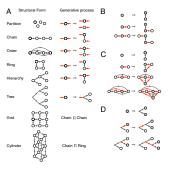
General structure detection



Effect of adding features on detected form.

> Straight partition simple tree complex tree

General structure detection



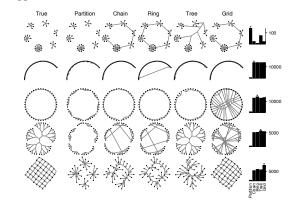
Top down description of form.

Node replacement graph grammar: parent node becomes two child nodes.

B-D: Growing chains, orders, and trees.

General structure detection

Performance for test networks.



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