

Optimal supply & Structure detection

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Single Source

Distributed
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Facility location

Size-density law

A reasonable derivation

Global redistribution
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Hierarchy by division

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What's the best way to distribute stuff?

- ▶ Stuff = medical services, energy, nutrients, people, ...
- ▶ Some fundamental network problems:
 1. Distribute stuff from **single source** to **many sinks**
 2. Collect stuff coming from **many sources** at a **single sink**
 3. Distribute stuff from **many sources** to **many sinks**
 4. **Redistribute** stuff between many nodes
- ▶ **Q:** How do optimal solutions scale with system size?

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Single source optimal supply

Basic Q for distribution/supply networks:

- ▶ How does flow behave given cost:

$$C = \sum_j I_j^\gamma Z_j$$

where

I_j = current on link j

and

Z_j = link j 's impedance?

- ▶ Example: $\gamma = 2$ for electrical networks.

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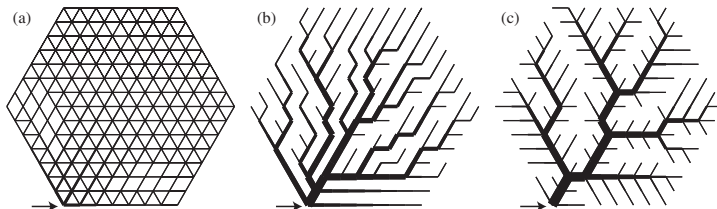
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Single source optimal supply



- (a) $\gamma > 1$: Braided (bulk) flow
- (b) $\gamma < 1$: Local minimum: Branching flow
- (c) $\gamma < 1$: Global minimum: Branching flow

From Bohn and Magnasco^[3]
See also Banavar et al.^[1]

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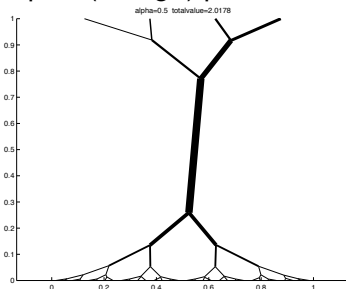
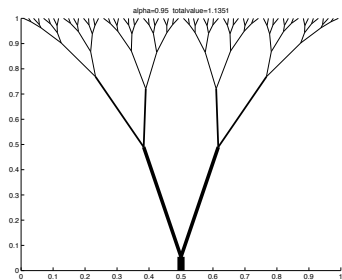
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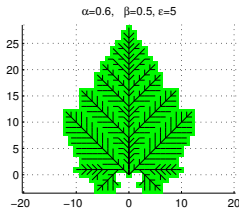
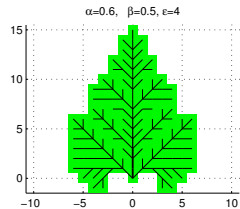
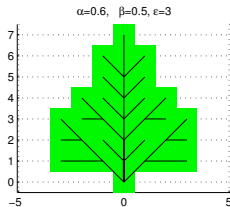
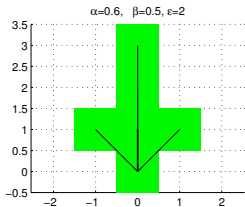
Optimal paths related to transport (Monge) problems:



Xia (2003) [24]

Growing networks:

FIGURE 1. $\alpha = 0.6, \beta = 0.5$



Xia (2007) [23]

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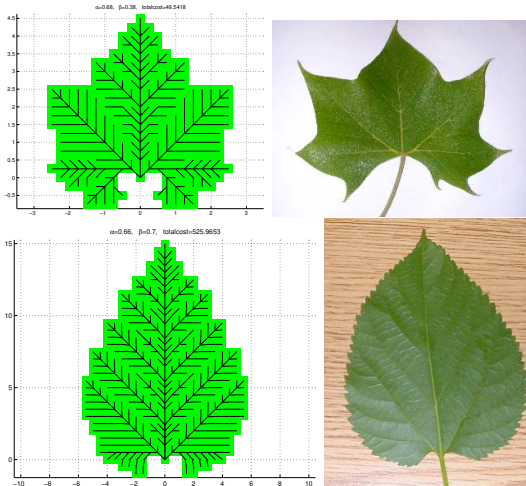
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Growing networks:

FIGURE 3. A maple leaf



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Single source optimal supply

An immensely controversial issue...

- ▶ The form of river networks and blood networks: optimal or not? [22, 2, 7]

Two observations:

- ▶ Self-similar networks appear everywhere in nature for single source supply/single sink collection.
- ▶ Real networks differ in details of scaling but reasonably agree in scaling relations.

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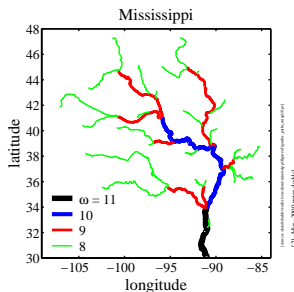
References

Stream Ordering:

- ▶ Label all **source streams** as **order $\omega = 1$** .
- ▶ Follow all labelled streams downstream
- ▶ Whenever two streams of the same order (ω) meet, the resulting stream has order incremented by 1 ($\omega + 1$).
- ▶ If streams of different orders ω_1 and ω_2 meet, then the resultant stream has order equal to the largest of the two.
- ▶ Simple rule:

$$\omega_3 = \max(\omega_1, \omega_2) + \delta_{\omega_1, \omega_2}$$

where δ is the Kronecker delta.



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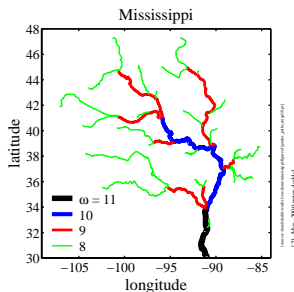
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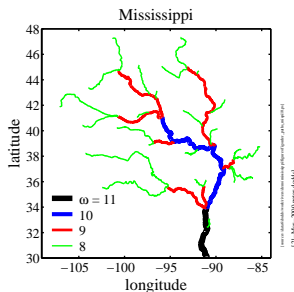
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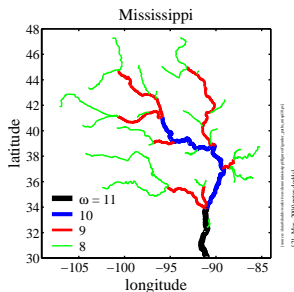


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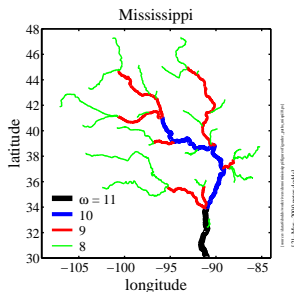
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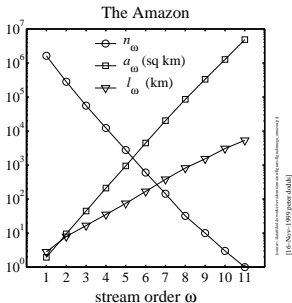
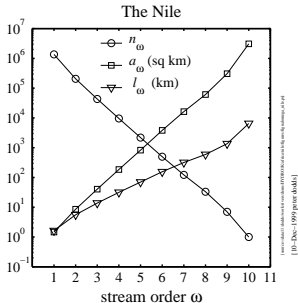
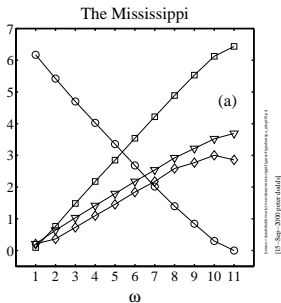
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Horton's laws in the real world:



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Many scaling laws, many connections

relation:	scaling relation/parameter: [6]
$l \sim L^d$	d
$T_k = T_1(R_T)^{k-1}$	$T_1 = R_n - R_s - 2 + 2R_s/R_n$ $R_T = R_s$
$n_\omega/n_{\omega+1} = R_n$	R_n
$\bar{a}_{\omega+1}/\bar{a}_\omega = R_a$	$R_a = R_n$
$\bar{l}_{\omega+1}/\bar{l}_\omega = R_\ell$	$R_\ell = R_s$
$l \sim a^h$	$h = \log R_s / \log R_n$
$a \sim L^D$	$D = d/h$
$L_\perp \sim L^H$	$H = d/h - 1$
$P(a) \sim a^{-\tau}$	$\tau = 2 - h$
$P(l) \sim l^{-\gamma}$	$\gamma = 1/h$
$\Lambda \sim a^\beta$	$\beta = 1 + h$
$\lambda \sim L^\varphi$	$\varphi = d$

Only 3 parameters are independent... [6]

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Reported parameter values: [6]

Parameter:	Real networks:
R_n	3.0–5.0
R_a	3.0–6.0
$R_\ell = R_T$	1.5–3.0
T_1	1.0–1.5
d	1.1 ± 0.01
D	1.8 ± 0.1
h	0.50–0.70
τ	1.43 ± 0.05
γ	1.8 ± 0.1
H	0.75–0.80
β	0.50–0.70
φ	1.05 ± 0.05

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Data from real blood networks

Network	R_n	R_r^{-1}	R_ℓ^{-1}	$-\frac{\ln R_r}{\ln R_n}$	$-\frac{\ln R_\ell}{\ln R_n}$	α
West <i>et al.</i>	–	–	–	0.5	0.33̄	0.75
rat (PAT)	2.76	1.58	1.60	0.45	0.46	0.73
cat (PAT) (Turcotte <i>et al.</i> [21])	3.67	1.71	1.78	0.41	0.44	0.79
dog (PAT)	3.69	1.67	1.52	0.39	0.32	0.90
pig (LCX)	3.57	1.89	2.20	0.50	0.62	0.62
pig (RCA)	3.50	1.81	2.12	0.47	0.60	0.65
pig (LAD)	3.51	1.84	2.02	0.49	0.56	0.65
human (PAT)	3.03	1.60	1.49	0.42	0.36	0.83
human (PAT)	3.36	1.56	1.49	0.37	0.33	0.94

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Fundamental biological and ecological constraint:

$$P = c M^\alpha$$

P = basal metabolic rate

M = organismal body mass



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History

1964: Troon, Scotland:
3rd symposium on energy metabolism.
 $\alpha = 3/4$ made official ...



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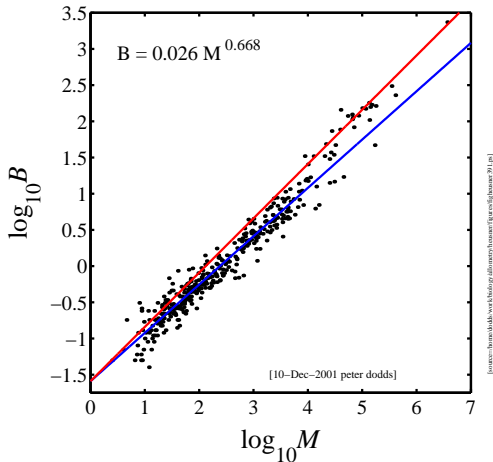
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Some data on metabolic rates



- ▶ Heusner's data (1991)^[11]
- ▶ 391 Mammals
- ▶ blue line: 2/3
- ▶ red line: 3/4.
- ▶ ($B = P$)

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Some regressions from the ground up...

range of M	N	$\hat{\alpha}$
≤ 0.1 kg	167	0.678 ± 0.038
≤ 1 kg	276	0.662 ± 0.032
≤ 10 kg	357	0.668 ± 0.019
≤ 25 kg	366	0.669 ± 0.018
≤ 35 kg	371	0.675 ± 0.018
≤ 350 kg	389	0.706 ± 0.016
≤ 3670 kg	391	0.710 ± 0.021

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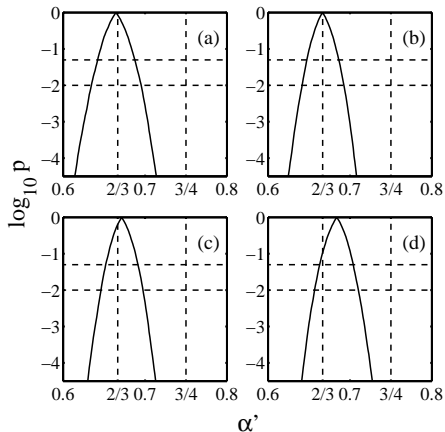
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Analysis of residuals—p-values—mammals:



- ▶ (a) $M < 3.2$ kg
 - ▶ (b) $M < 10$ kg
 - ▶ (c) $M < 32$ kg
 - ▶ (d) all mammals.
- ▶ For a-d,
 $p_{2/3} > 0.05$ and
 $p_{3/4} \ll 10^{-4}$.

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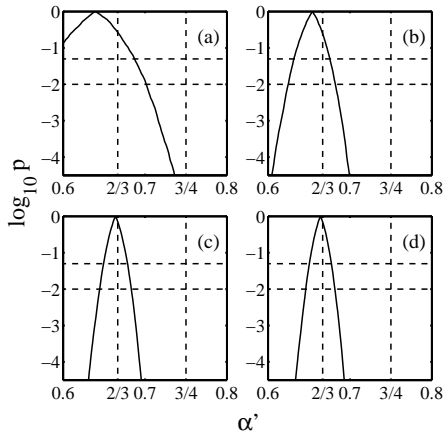
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Analysis of residuals—p-values—birds:



- ▶ (a) $M < 0.1$ kg
 - (b) $M < 1$ kg
 - (c) $M < 10$ kg
 - (d) all birds.
- ▶ For a-d,
 $p_{2/3} > 0.05$ and
 $p_{3/4} \ll 10^{-4}$.

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Many sources, many sinks

How do we distribute sources?

- ▶ Focus on 2-d (results generalize to higher dimensions)
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- ▶ **Key problem:** How do we cope with uneven population densities?
- ▶ Obvious: if density is uniform then sources are best distributed **uniformly**.
- ▶ Which lattice is optimal? The **hexagonal lattice**
Q1: How big should the hexagons be?
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Solidifying the basic problem

- ▶ Given a region with some population distribution ρ , most likely uneven.
- ▶ Given resources to build and maintain N facilities.
- ▶ **Q:** How do we locate these N facilities so as to minimize the average distance between an individual's residence and the nearest facility?
- ▶ Problem of interested and studied by geographers, sociologists, computer scientists, mathematicians, ...
- ▶ See work by Stephan ^[19, 20] and by Gastner and Newman (2006) ^[8] and work cited by them.

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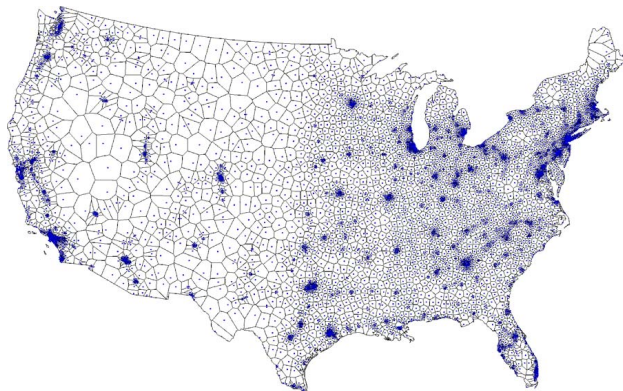
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Optimal source allocation



Gastner and Newman (2006) [8]

- ▶ Approximately optimal location of 5000 facilities.
- ▶ Based on 2000 Census data.
- ▶ Simulated annealing + Voronoi tessellation.

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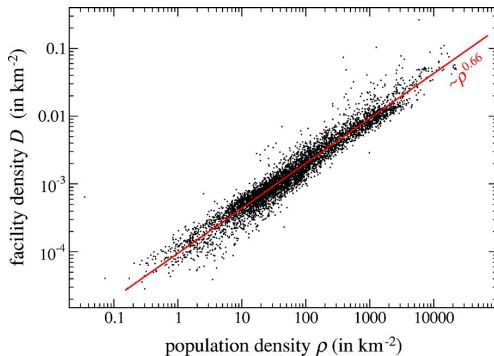
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Optimal source allocation



From Gastner and Newman (2006) [8]

- ▶ Optimal facility density D vs. population density ρ .
- ▶ Fit is $D \propto \rho^{0.66}$ with $r^2 = 0.94$.
- ▶ Looking good for a 2/3 power...

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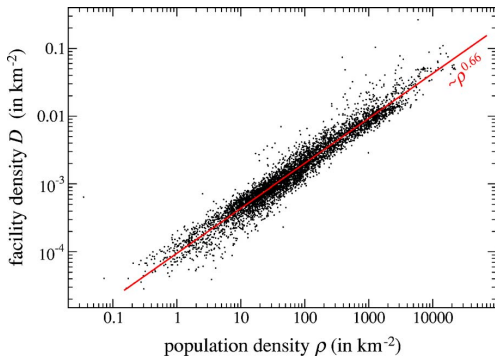
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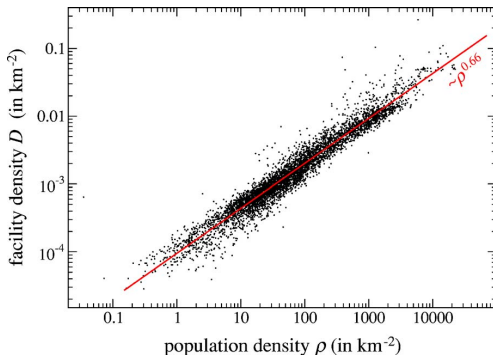
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Size-density law:



$$D \propto \rho^{2/3}$$

- ▶ In d dimensions:

$$D \propto \rho^{d/(d+1)}$$

- ▶ Why?
- ▶ Very different story to branching networks where there is either one source or one sink.
- ▶ Now sources & sinks are distributed throughout region...

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“Territorial Division: The Least-Time Constraint Behind the Formation of Subnational Boundaries” (Science, 1977)
- ▶ Zipf-like approach: invokes principle of minimal effort.
- ▶ Also known as the Homer principle.

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Deriving the optimal source distribution:

- ▶ Stronger result obtained by Gusein-Zade (1982).^[10]
- ▶ **Basic idea:** Minimize the average distance from a random individual to the nearest facility.
- ▶ Assume given a fixed population density ρ defined on a spatial region Ω .
- ▶ Formally, we want to find the locations of **n sources** $\{\vec{x}_1, \dots, \vec{x}_n\}$ that minimizes the **cost function**

$$F(\{\vec{x}_1, \dots, \vec{x}_n\}) = \int_{\Omega} \rho(\vec{x}) \min_i \|\vec{x} - \vec{x}_i\| d\vec{x}.$$

- ▶ Also known as the p-median problem.
- ▶ Not easy... in fact this one is an NP-hard problem.^[8]

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Can (roughly) turn into a Lagrange multiplier story:

- ▶ By varying $\{\vec{x}_1, \dots, \vec{x}_n\}$, minimize

$$G(A) = c \int_{\Omega} \rho(\vec{x}) A(\vec{x})^{1/2} d\vec{x} - \lambda \left(n - \int_{\Omega} [A(\vec{x})]^{-1} d\vec{x} \right)$$

- ▶ Involves estimating typical distance from \vec{x} to the nearest source (say i) as $c_i A(\vec{x})^{1/2}$ where c_i is a shape factor for the i th Voronoi cell.
- ▶ **Sneakiness**: set $c_i = c$.
- ▶ Compute $\delta G / \delta A$, the functional derivative (⊕).
- ▶ Solve and substitute $D = 1/A$, we find

$$D(\vec{x}) = \left(\frac{c}{2\lambda} \rho \right)^{2/3}.$$

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Can (roughly) turn into a Lagrange multiplier story:

- ▶ By varying $\{\vec{x}_1, \dots, \vec{x}_n\}$, minimize

$$G(A) = c \int_{\Omega} \rho(\vec{x}) A(\vec{x})^{1/2} d\vec{x} - \lambda \left(n - \int_{\Omega} [A(\vec{x})]^{-1} d\vec{x} \right)$$

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One more thing:

- ▶ How do we supply these facilities?
- ▶ How do we best redistribute mail? People?
- ▶ How do we get beer to the pubs?
- ▶ Gaster and Newman model: cost is a function of basic maintenance and travel time:

$$C_{\text{maint}} + \gamma C_{\text{travel}}.$$

- ▶ Travel time is more complicated: Take 'distance' between nodes to be a composite of shortest path distance ℓ_{ij} and number of legs to journey:

$$(1 - \delta)\ell_{ij} + \delta(\#\text{hops}).$$

- ▶ When $\delta = 1$, only number of hops matters.

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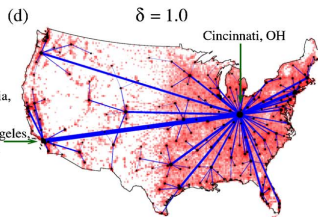
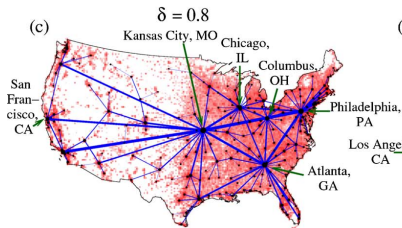
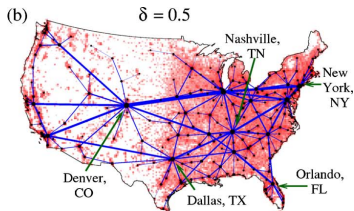
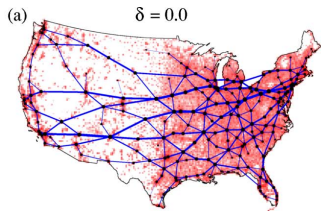
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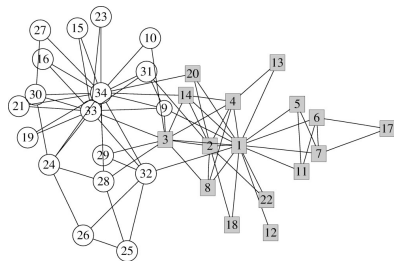
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From Gastner and Newman (2006) [8]

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▲ Zachary's karate club [25, 16]

- ▶ **The issue:**
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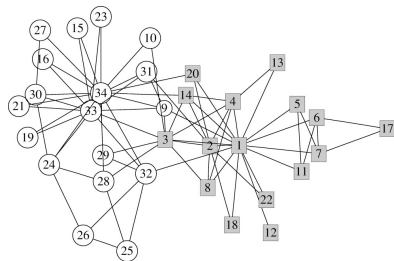
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- ▶ **Possible substructures:**
hierarchies, cliques, rings, ...
- ▶ **Plus:**
All combinations of substructures.
- ▶ Much focus on hierarchies...

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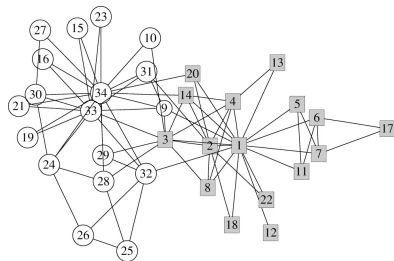
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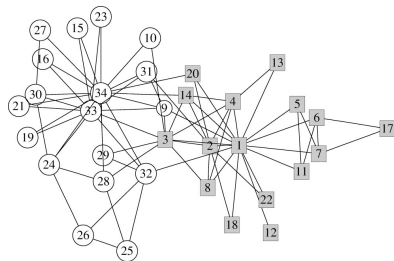
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Hierarchy by division

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- ▶ **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.
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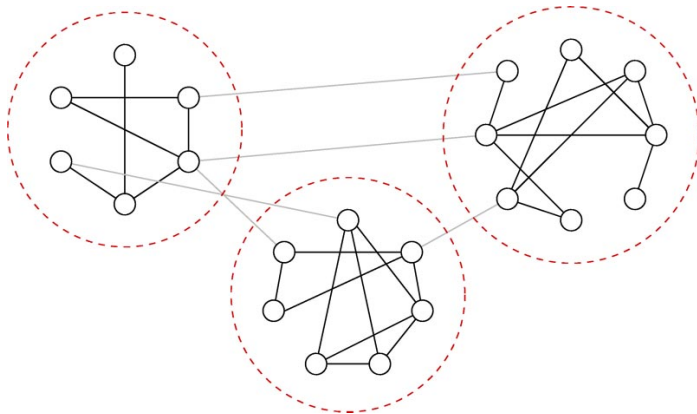
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Hierarchy by division



- ▶ *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.

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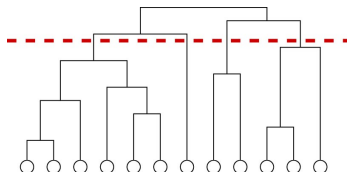
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Red line indicates appearance of four (4) components at a certain level.

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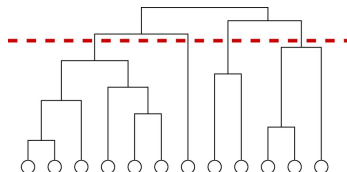
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Key element:

- ▶ **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?:

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

$$Q = \frac{1}{2m} \sum_{i,j} \left(A_{ij} - \frac{k_i k_j}{2m} \right) \delta_{ij} \delta_{i,c_i} \delta_{j,c_j}$$

where δ_{ij} is the fraction of edges between community c_i and c_j .

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Hierarchy by division

Key element:

- ▶ 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?:

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

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

where e_{ij} is the fraction of edges between identified communities i and j .

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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:

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

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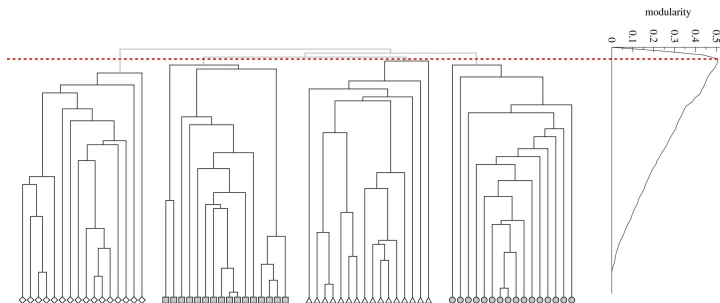
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Hierarchy by division



- ▶ 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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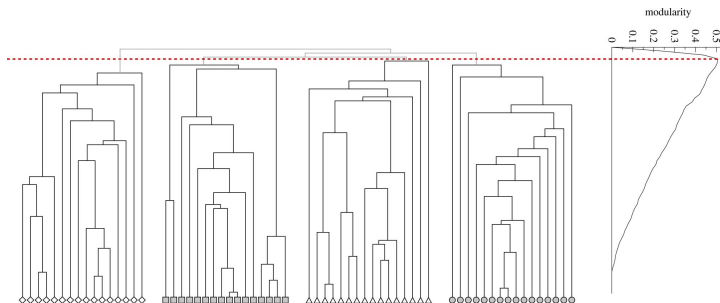
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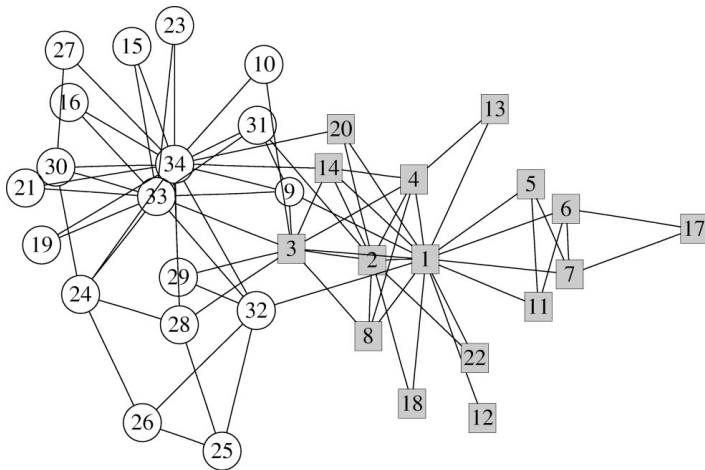
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- **Factions in Zachary's karate club network.** [25]

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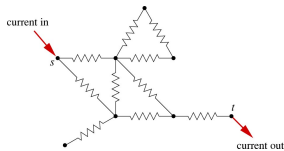
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Betweenness for electrons:



- ▶ 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 , $|I_{\ell, st}|$.

- ▶ Sum $|I_{\ell, st}|$ over all pairs of nodes to obtain **electronic betweenness** for edge ℓ .
- ▶ (Equivalent to **random walk betweenness**.)
- ▶ Electronic betweenness for edge between nodes i and j :

$$B_{ij}^{\text{elec}} = a_{ij} |V_i - V_j|.$$

- ▶ **Upshot**: specific measure of betweenness not too important.

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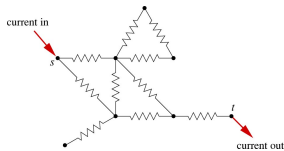
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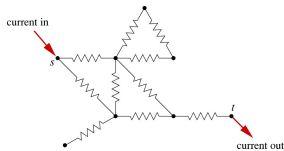
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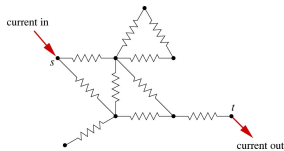
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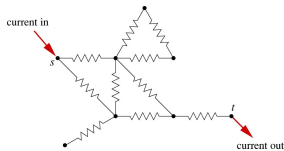
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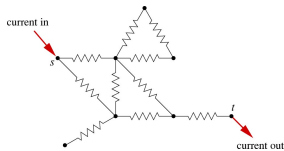
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Frame 44/78

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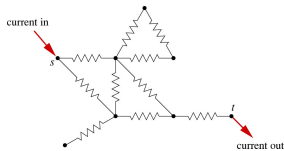
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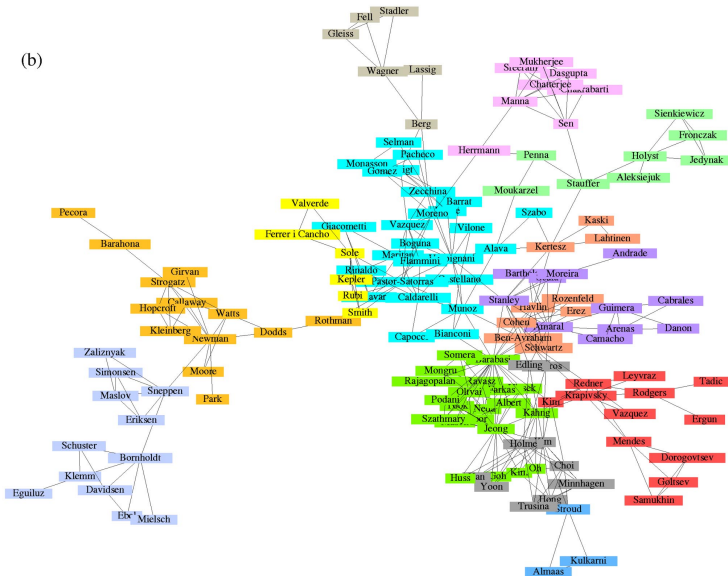
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Scientists working on networks

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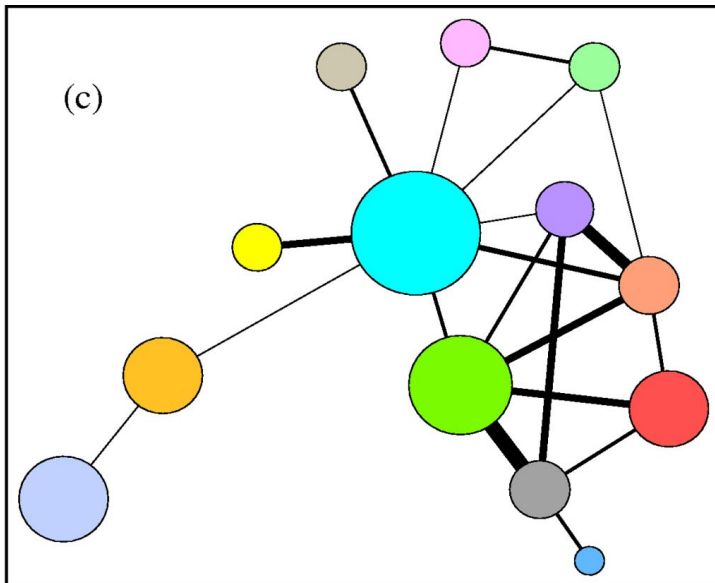
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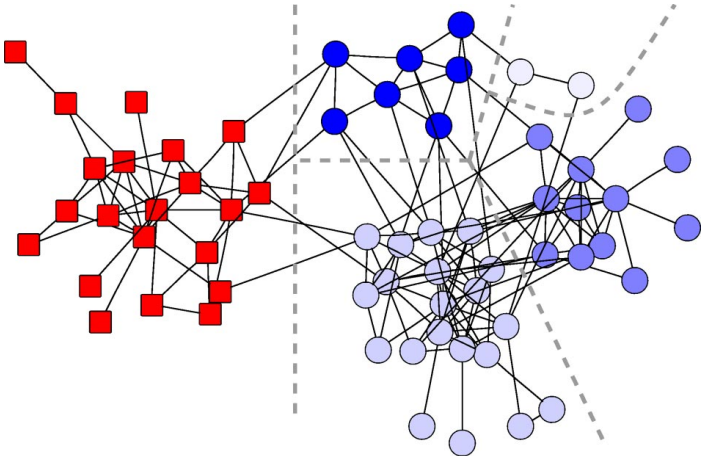
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Dolphins!

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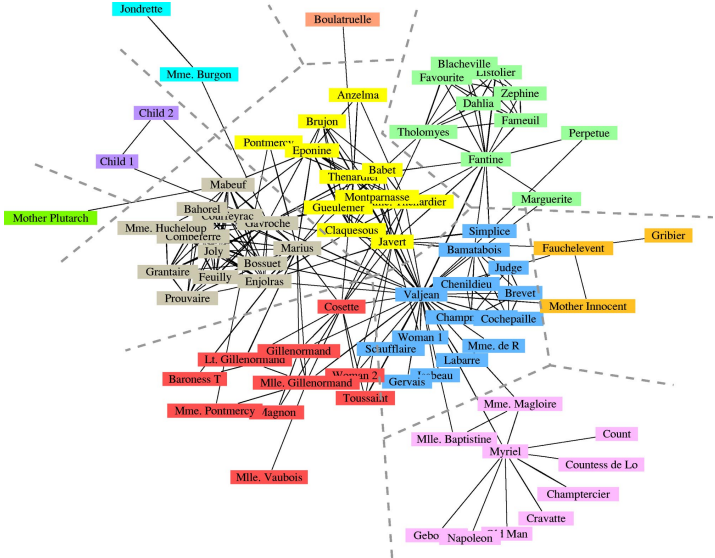
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- ▶ “Extracting the hierarchical organization of complex systems”

Sales-Pardo *et al.*, PNAS (2007) [17, 18]

- ▶ Consider all partitions of networks into m groups
- ▶ As for Newman and Girvan approach, aim is to find partitions with maximum modularity:

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- ▶ 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 A_{ij} .
- ▶ $A_{ij} = \mathbf{Pr}$ 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 .

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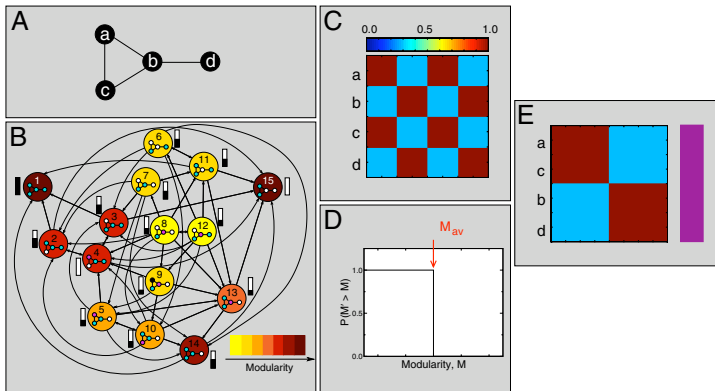
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Shuffling for structure



- ▶ **A:** Base network; **B:** Partition network; **C:** Coclassification matrix; **D:** Comparison to random networks (all the same!); **E:** Ordered coclassification matrix;

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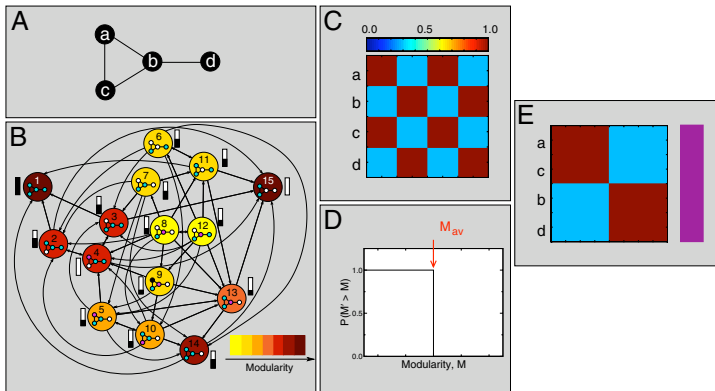
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- ▶ **A:** Base network; **B:** Partition network; **C:** Coclassification matrix; **D:** Comparison to random networks (all the same!); **E:** Ordered coclassification matrix; Conclusion: no structure...

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Shuffling for structure

- ▶ 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

$$C = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N A_{ij} |i - j|.$$

- ▶ Use simulated annealing (slow).

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Shuffling for structure

- ▶ Method obtains a distribution of classification hierarchies.
- ▶ Note: the hierarchy with the highest modularity score isn't chosen.
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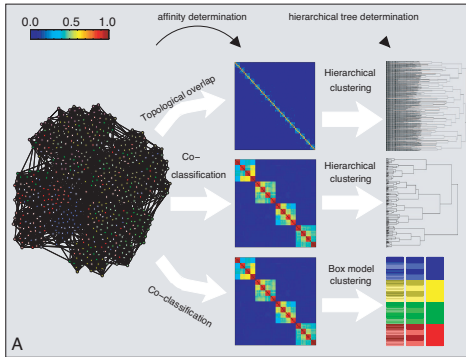
Hierarchies & Missing Links

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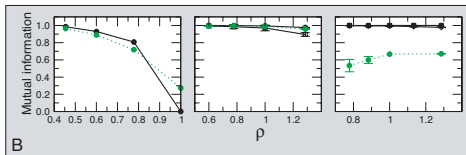
Final words

References

Shuffling for structure



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



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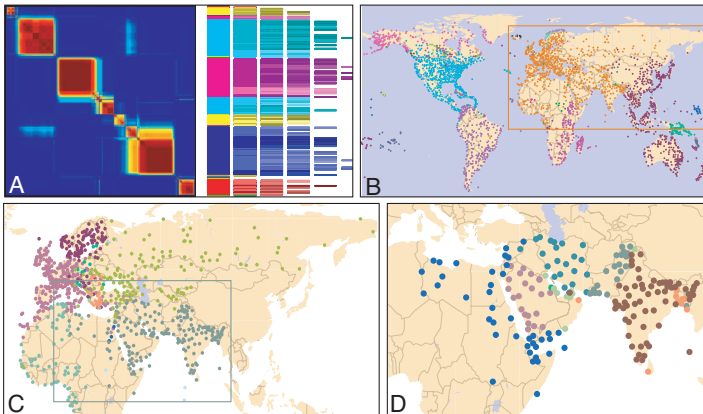
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Air transportation:



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- Modules found match up with geopolitical units.

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- ▶ “Detecting communities in large networks”
Capocci *et al.* (2005) ^[4]
- ▶ Consider normal matrix $\mathbf{K}^{-1} \mathbf{A}$, random walk matrix $\mathbf{A}^T \mathbf{K}^{-1}$, Laplacian $\mathbf{K} - \mathbf{A}$, and $\mathbf{A} \mathbf{A}^T$.
- ▶ Basic observation is that eigenvectors associated with secondary eigenvalues reveal evidence of structure.
- ▶ Build on Kleinberg’s HITS algorithm. ^[13]

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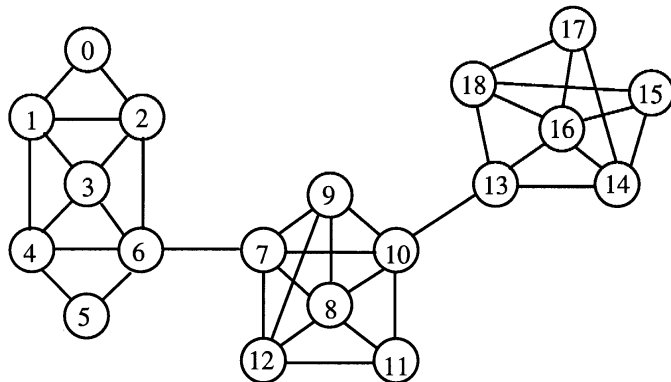
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► Example network:



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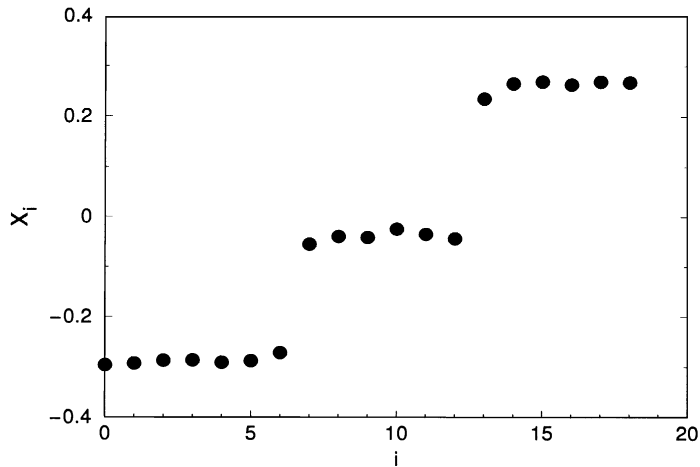
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► Second eigenvector's components:



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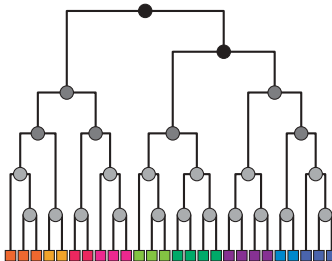
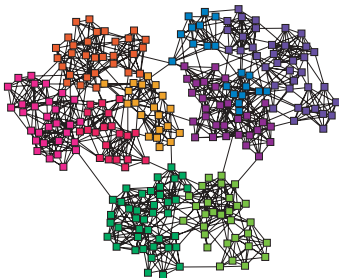
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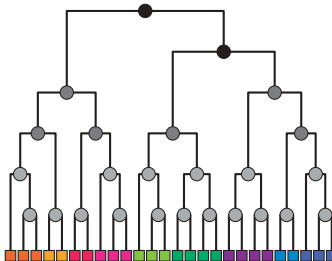
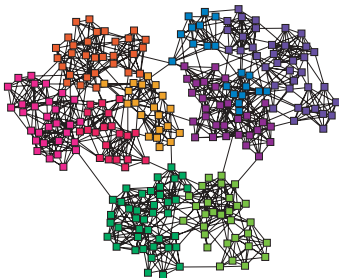
Clauset *et al.*, Nature (2008) [5]



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

Hierarchies and missing links

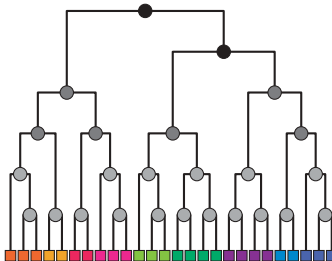
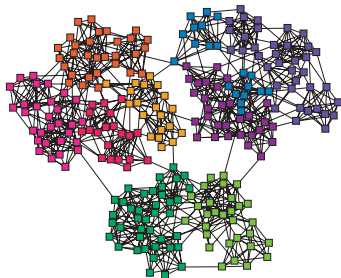
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Hierarchies and missing links

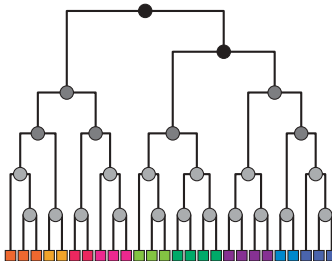
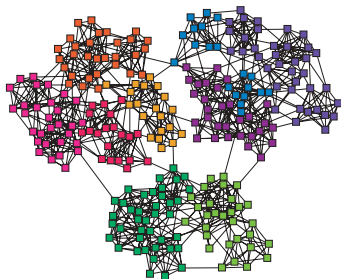
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Clauset *et al.*, Nature (2008) [5]



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- ▶ Handle: **Hierarchical random graph models.**
- ▶ Plan: Infer **consensus dendrogram** for a given real network.
- ▶ Obtain probability that links are missing (big problem...).

- ▶ 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	$\langle k \rangle_{\text{real}}$	$\langle k \rangle_{\text{samp}}$	C_{real}	C_{samp}	d_{real}	d_{samp}
<i>T. pallidum</i>	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.

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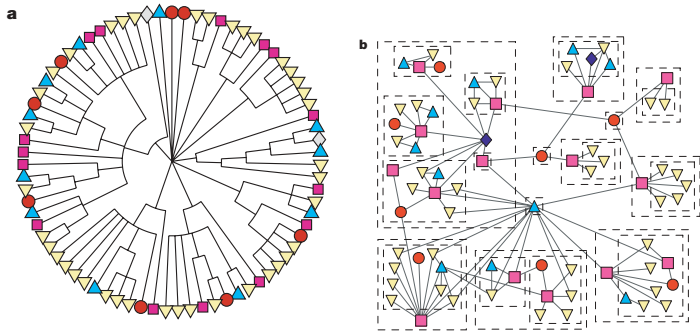
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- ▶ **Consensus dendrogram** for grassland species.
- ▶ Copes with disassortative and assortative communities.

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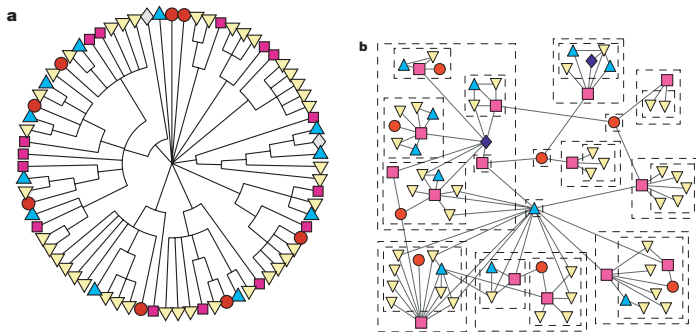
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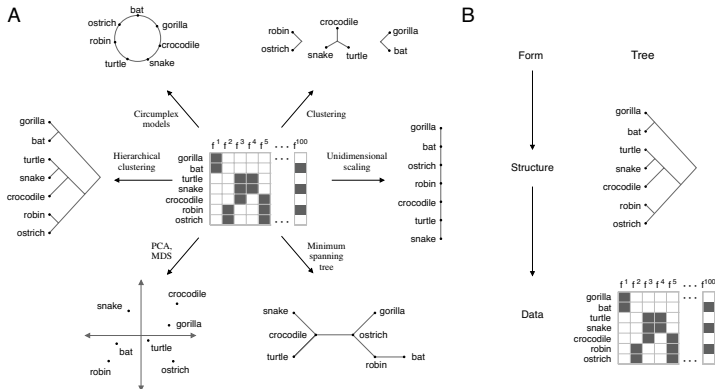
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- ▶ “The discovery of structural form”
Kemp and Tenenbaum, PNAS (2008) ^[12]



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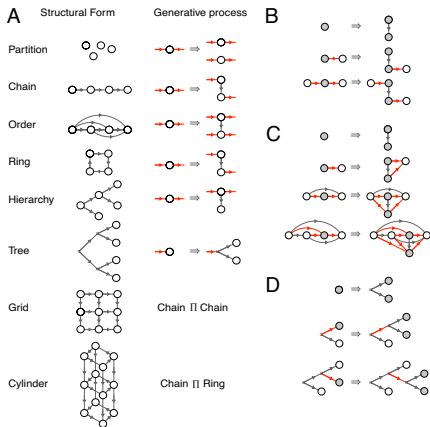
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► Top down description of form.

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

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

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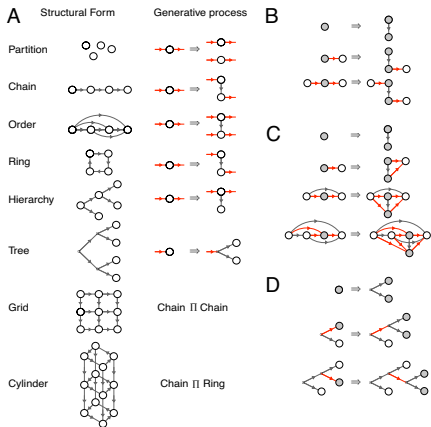
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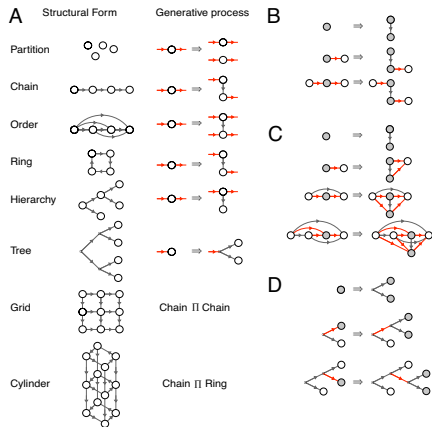
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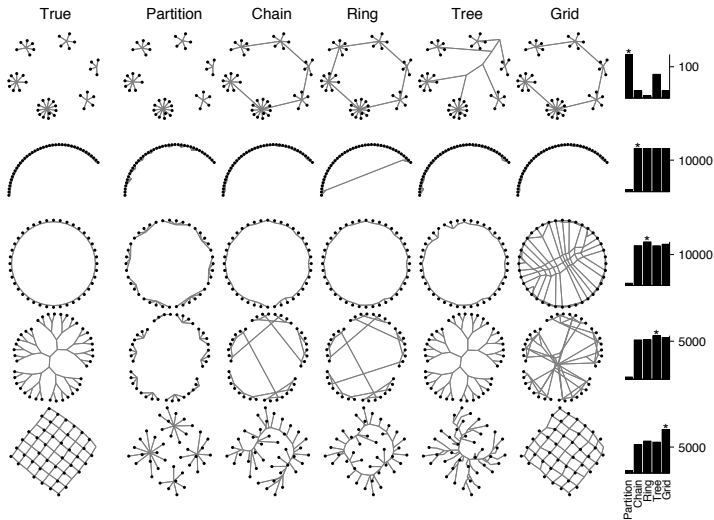
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► Performance for test networks.



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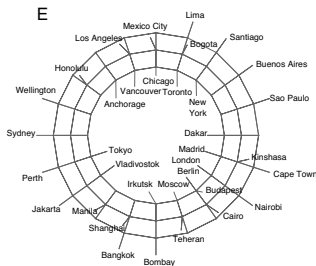
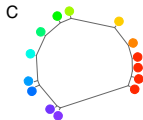
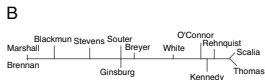
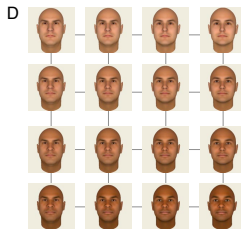
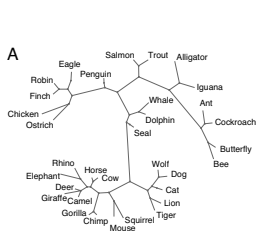
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Example learned structures:



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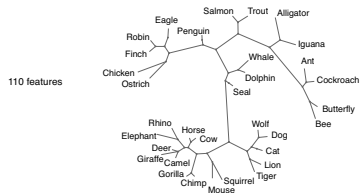
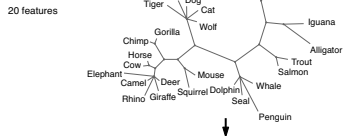
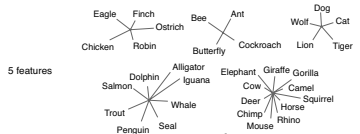
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- Biological features; Supreme Court votes; perceived color differences; face differences; & distances between cities.

General structure detection



► Effect of adding features on detected form.

Straight partition

simple tree

complex tree

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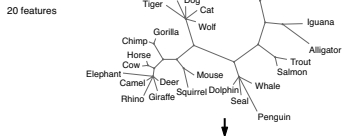
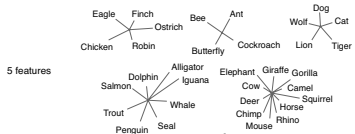
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Final words:

Science in three steps:

1. Find interesting/meaningful/important phenomena involving spectacular amounts of data.
2. Describe what you see.
3. Explain it.

A plea/warning

Beware your assumptions—don't use tools/models because they're there, or because everyone else does...

Final words:

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A plea/warning

Beware your assumptions—don't use tools/models because they're there, or because everyone else does...

More final words:

A real theory of everything:

1. Is not just about the small stuff...
2. It's about the increase of complexity

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More final words:

A real theory of everything:

1. Is not just about the small stuff...
2. It's about the increase of complexity

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