Optimal supply & Structure detection

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Principles of Complex Systems, Vols. 1, 2, & 3D CSYS/MATH 6701, 6713, & a pretend number, 2023–2024| @pocsvox

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Outline

Optimal supply networks

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- Q: How do optimal solutions scale with system size?

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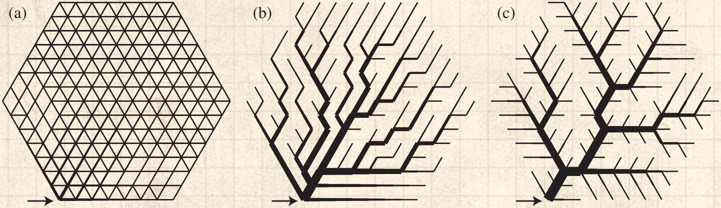
- Example: $\gamma = 2$ for electrical networks.

Single source optimal supply



(a) $\gamma > 1$: Braided (bulk) flow

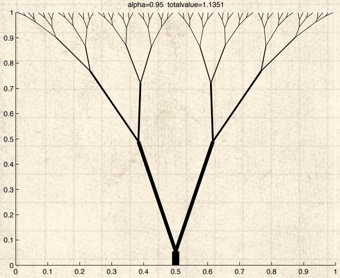
(b) $\gamma < 1$: Local minimum: Branching flow

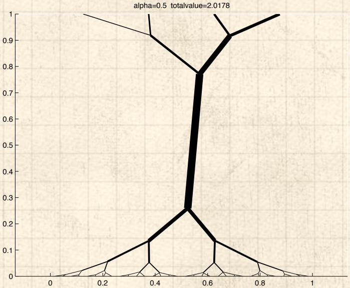
(c) $\gamma < 1$: Global minimum: Branching flow

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

Single source optimal supply

Optimal paths related to transport (Monge) problems:

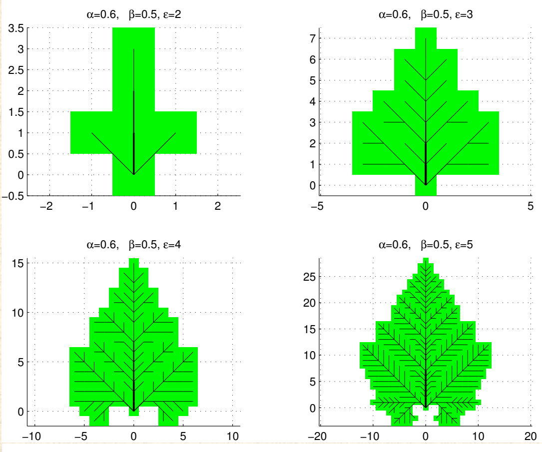




Xia (2003) [24]

Growing networks:

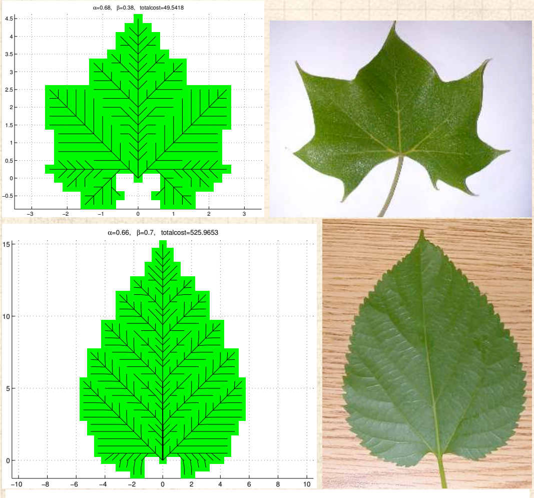
FIGURE 1. $\alpha = 0.6, \beta = 0.5$



Xia (2007) [23]

Growing networks:

FIGURE 3. A maple leaf



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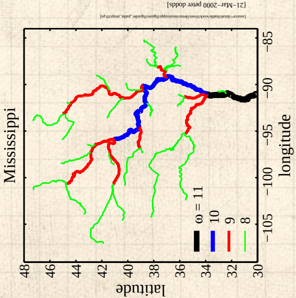
Two observations:

- 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.

Stream Ordering:



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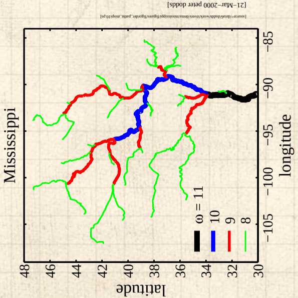

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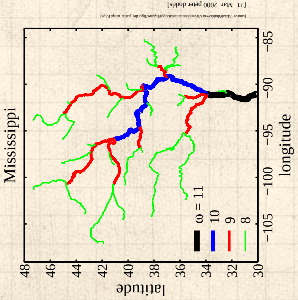

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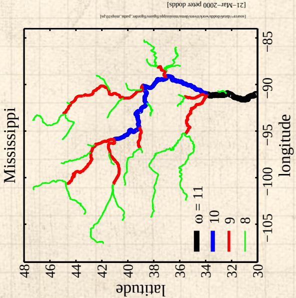

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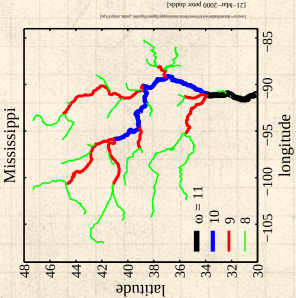

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What's the Story?

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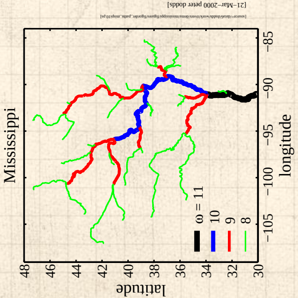
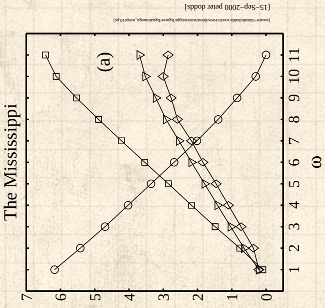
- If streams of different orders ω_1 and ω_2 meet, then the resultant stream has order equal to the largest of the two.
- Simple rule:

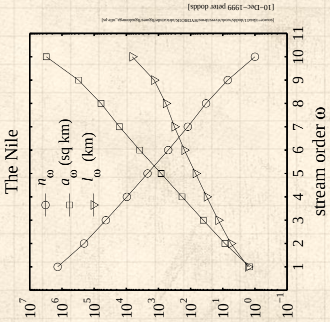
$$\omega_3 = \max(\omega_1, \omega_2) + \delta_{\omega_1, \omega_2}$$

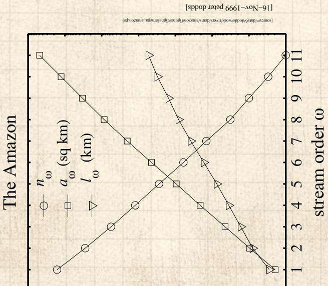
where δ is the Kronecker delta.



Horton's laws in the real world:







Many scaling laws, many connections

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

Only 3 parameters are independent... [6]

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

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 *et al.*	–	–	–	0.5	$0.3\bar{3}$	0.75
rat (PAT)	2.76	1.58	1.60	0.45	0.46	0.73
cat (PAT)	3.67	1.71	1.78	0.41	0.44	0.79
(Turcotte *et al.* [21])						
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

Animal power

Fundamental biological and ecological constraint:

$$\boxed{P = c\,M^{\alpha}}$$

$P =$ basal metabolic rate

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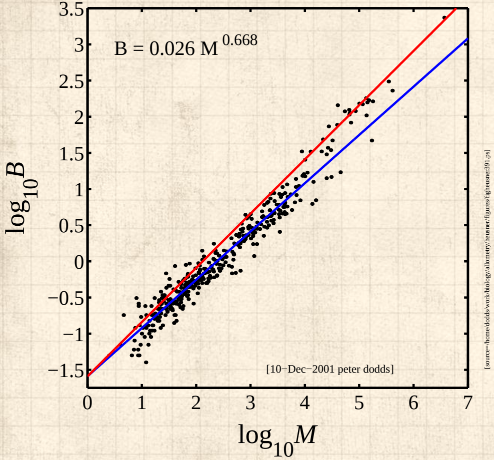
Some data on metabolic rates

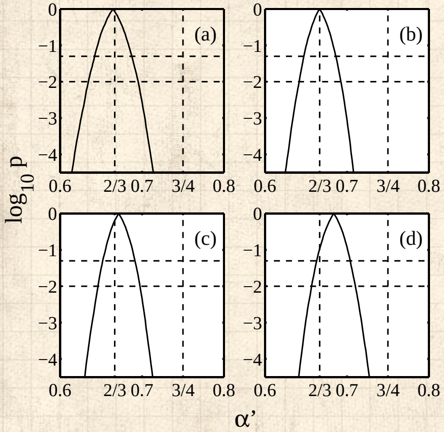


- Heusner's data (1991)[11]
- 391 Mammals
- blue line: 2/3
- red line: 3/4.
- $(B = P)$

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

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
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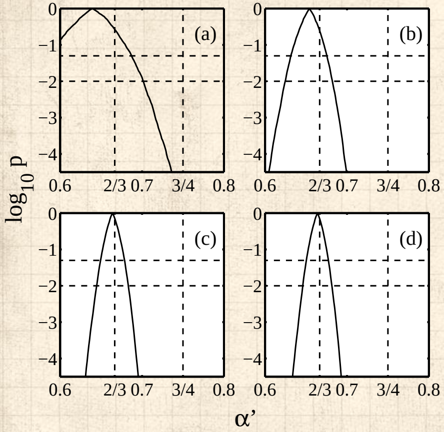
Analysis of residuals—p-values—birds:



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- Q2: Given population density is uneven, what do we do?

Optimal source allocation

Solidifying the basic problem

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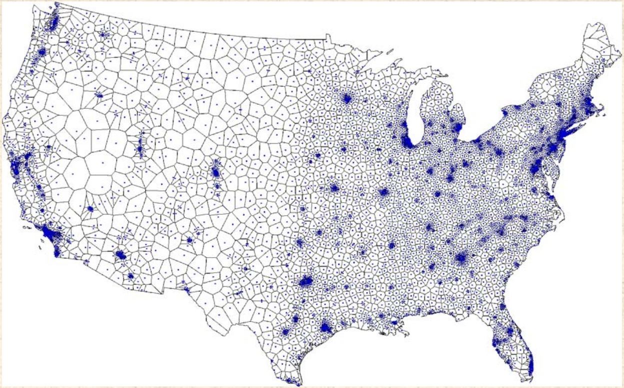
- See work by Stephan [19, 20] and by Gastner and Newman (2006) [8] and work cited by them.

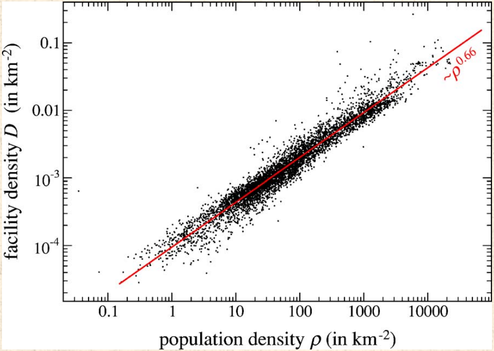
Optimal source allocation



From Gastner and Newman (2006) [8]

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

Optimal source allocation



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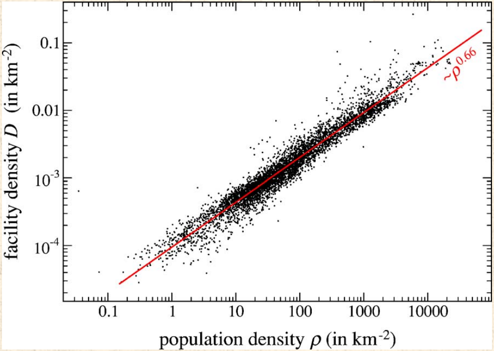

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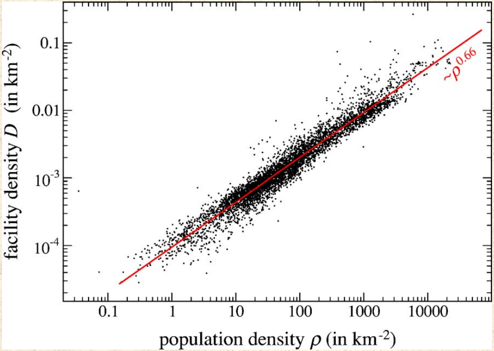

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- Looking good for a 2/3 power...

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- Now sources & sinks are distributed throughout region...

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- Also known as the Homer principle.

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- Formally, we want to find the locations of n sources $\{\vec{x}_1, \dots, \vec{x}_n\}$ that minimizes the cost function

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

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- Not easy... in fact this one is an NP-hard problem. [8]

Size-density law

Can (roughly) turn into a Lagrange multiplier story:

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

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

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- 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 ith Voronoi cell.

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- Solve and substitute $D = 1/A$, we find

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

Outline

Global redistribution networks

One more thing:

- How do we supply these facilities?

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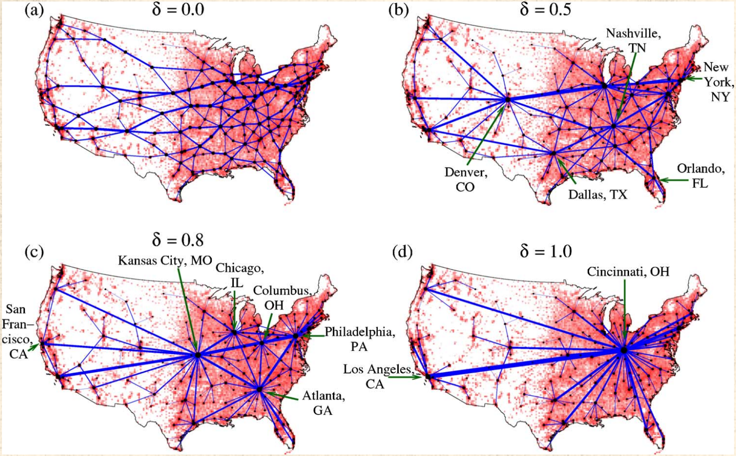
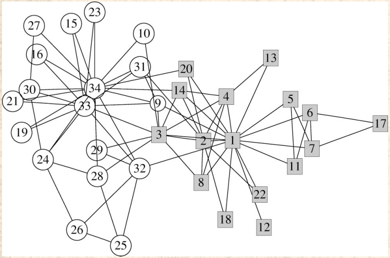
- When $\delta = 1$, only number of hops matters.

Global redistribution networks



From Gastner and Newman (2006) [8]

Structure detection



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

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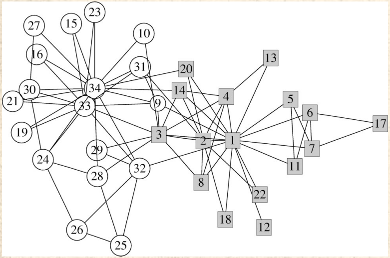

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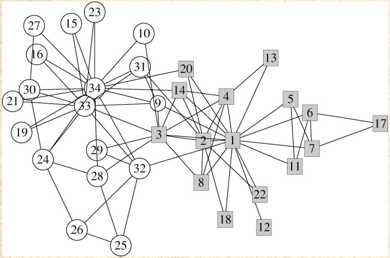

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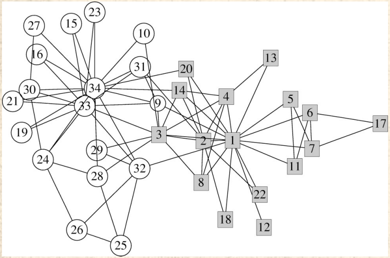

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- Much focus on hierarchies...

Outline

Single Source

Distributed Sources
Facility location
Size-density law
A reasonable derivation
Global redistribution networks

Structure Detection
Hierarchy by division
Hierarchy by shuffling
Spectral methods
Hierarchies & Missing Links
General structure detection

Final words

References

Hierarchy by division

Top down:

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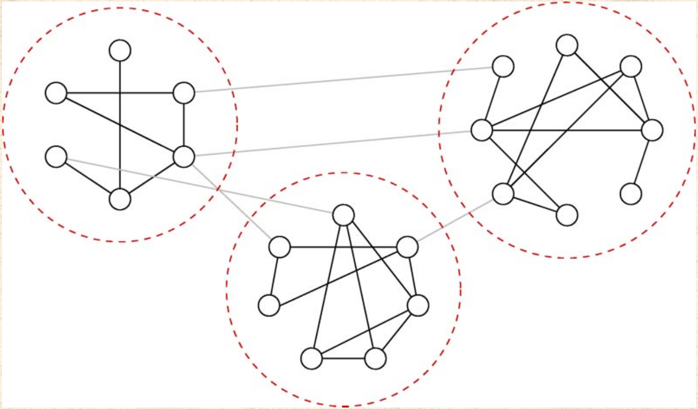

Idea:
Edges that connect communities have higher betweenness than edges within communities.

Hierarchy by division

One class of structure-detection algorithms:

1. Compute edge betweenness for whole network.

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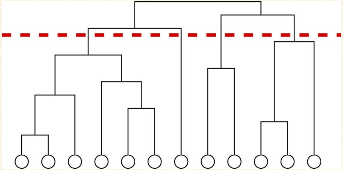

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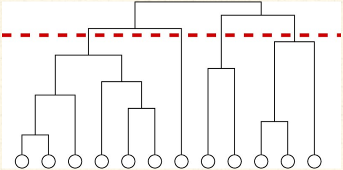

Red line indicates appearance of four (4) components at a certain level.

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

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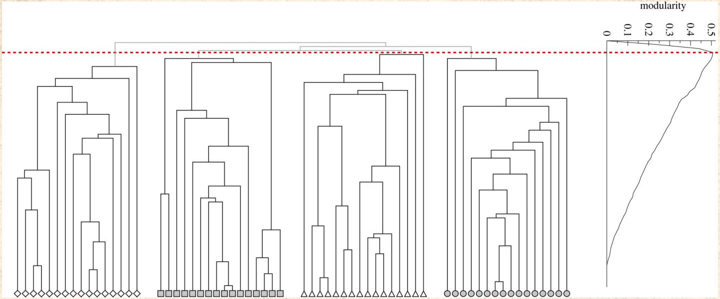
- Example:

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

Hierarchy by division



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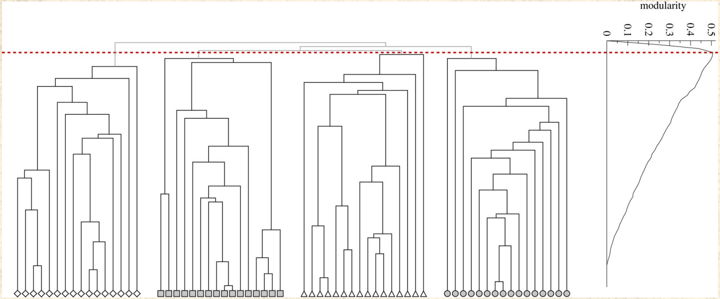

- Maximum modularity $Q \simeq 0.5$ obtained when four communities are uncovered.
- Further 'discovery' of internal structure is somewhat meaningless, as any communities arise accidentally.

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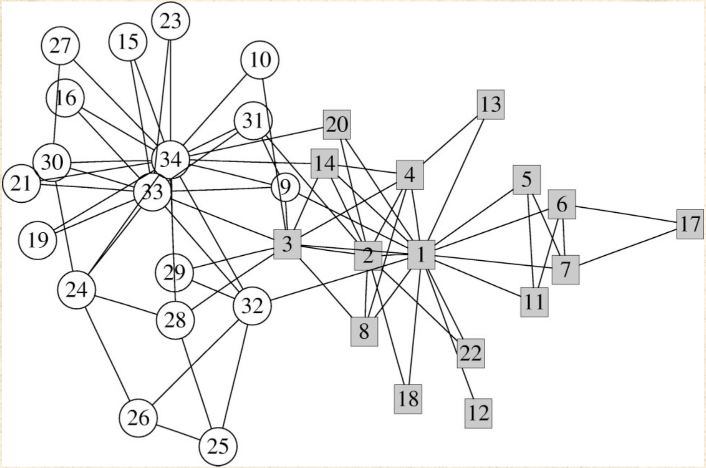

- Factions in Zachary's karate club network. [25]

Betweenness for electrons:

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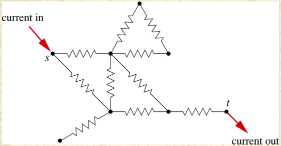

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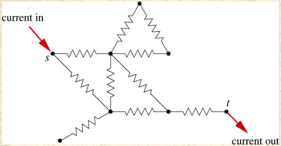

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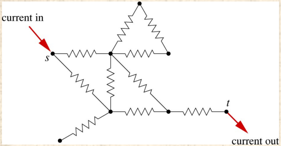

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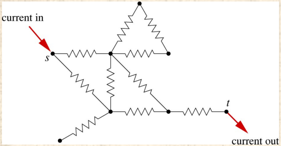

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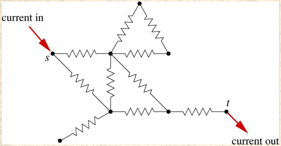

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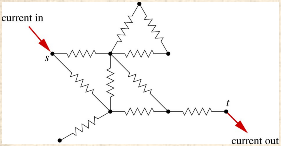

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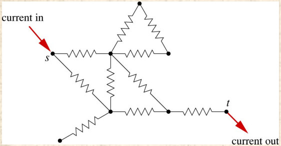

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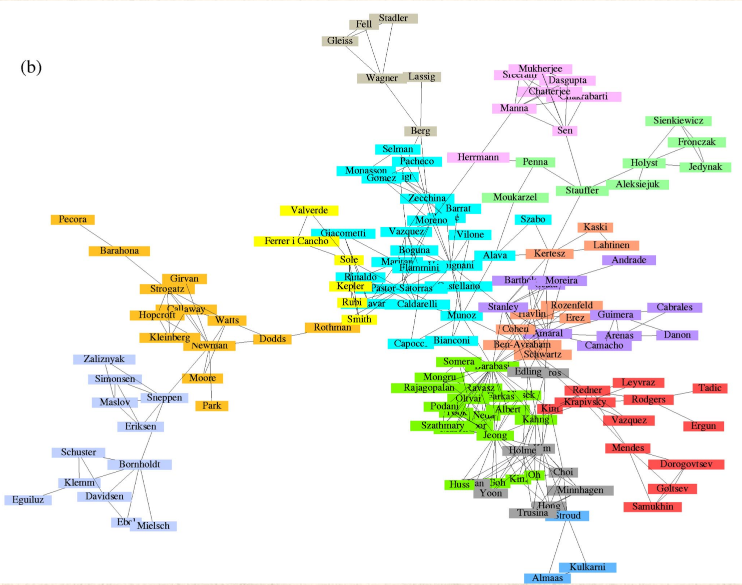
- Upshot: specific measure of betweenness not too important.

Scientists working on networks



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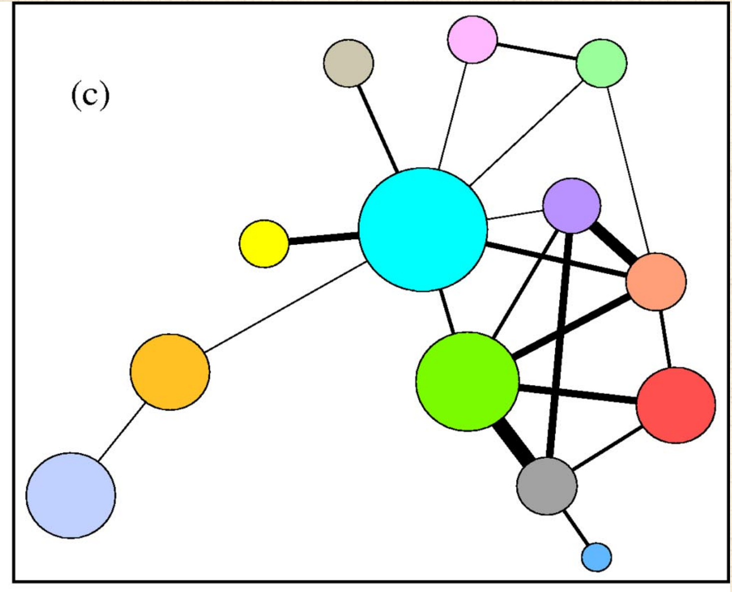
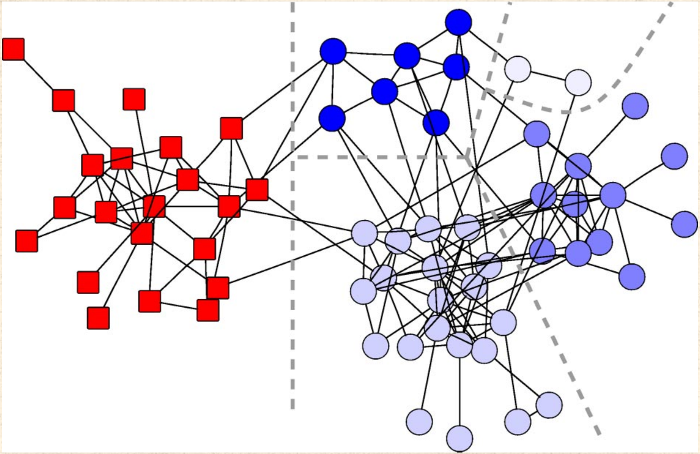
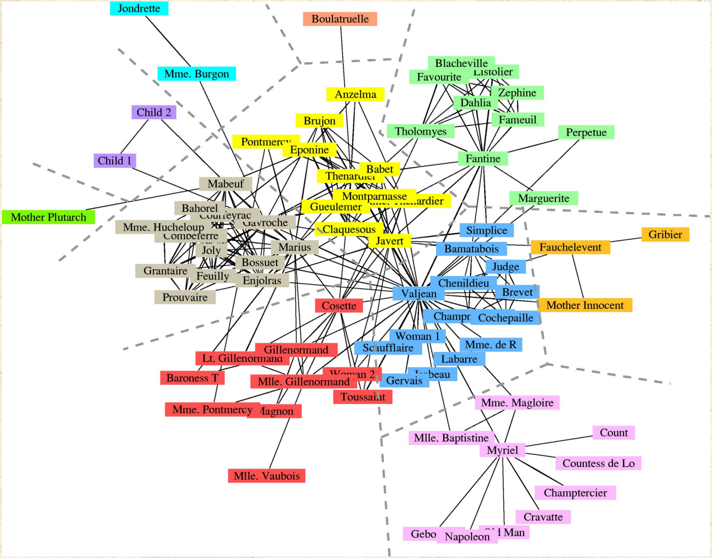


Dolphins!



Les Miserables



Outline

Shuffling for structure

- "Extracting the hierarchical organization of complex systems"
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- Consider all partitions of networks into m groups
- As for Newman and Girvan approach, aim is to find partitions with maximum modularity:

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

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- 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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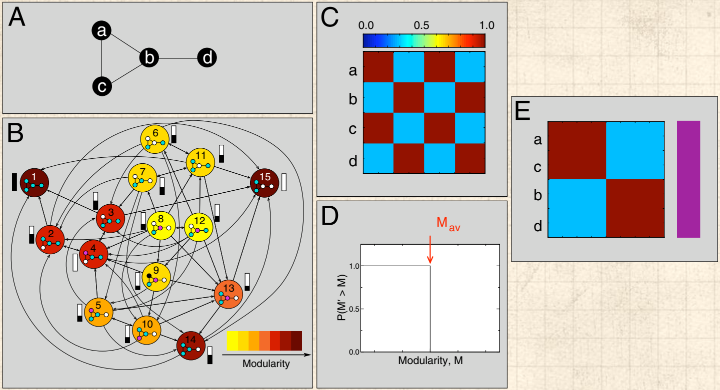

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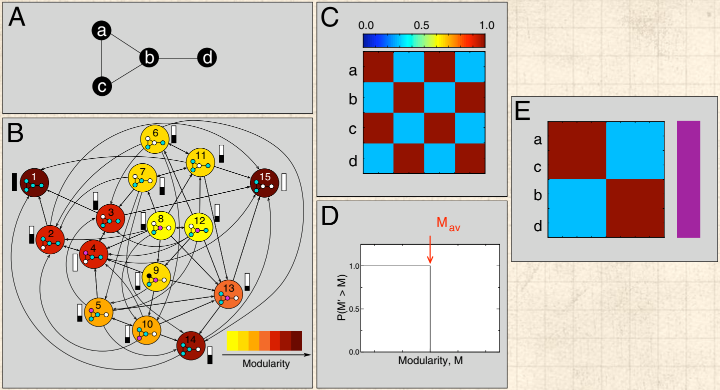

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- Use simulated annealing (slow).

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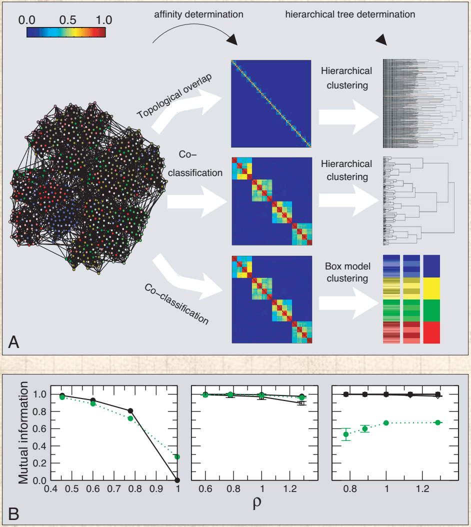
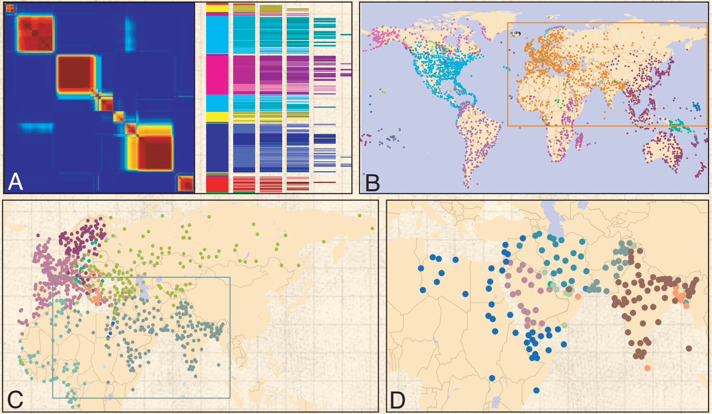


- $N = 640$,
- $\langle k \rangle = 16$,
- 3 tiered hierarchy.

Air transportation:



- Modules found match up with geopolitical units.

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- "Detecting communities in large networks" Capocci *et al.* (2005) [4]

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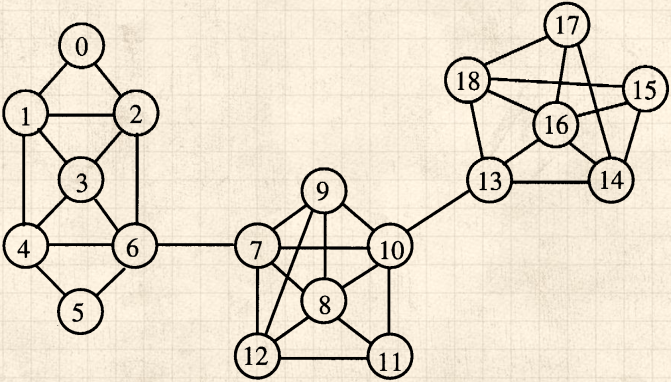
- Build on Kleinberg's HITS algorithm. [13]

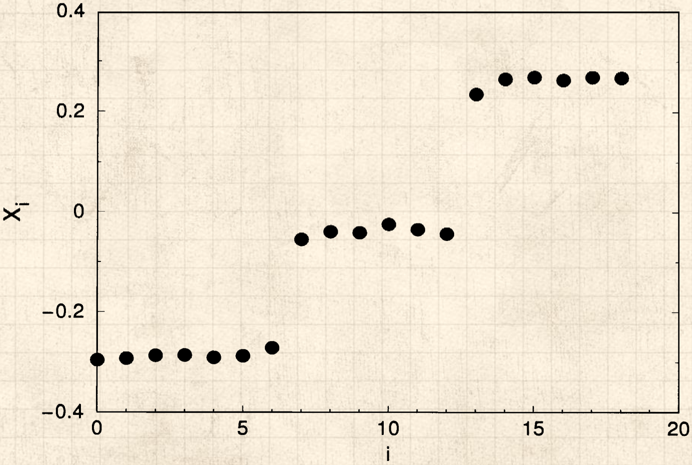
General structure detection

- Example network:



General structure detection

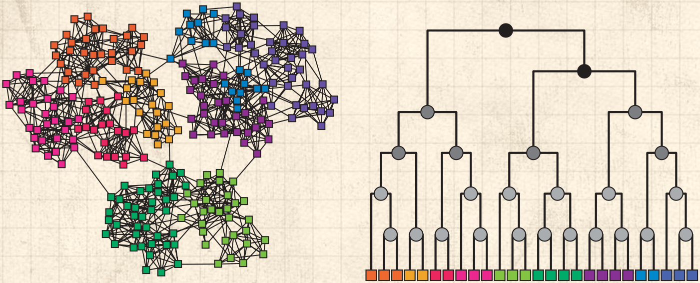
- Second eigenvector's components:



Outline

Hierarchies and missing links

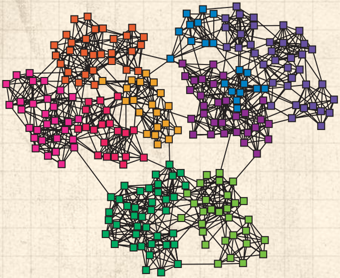
Clauset *et al.*, Nature (2008) [5]

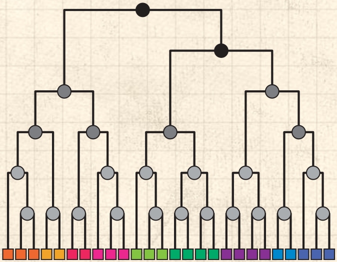


- Idea: Shades indicate probability that nodes in left and right subtrees of dendogram are connected.

Hierarchies and missing links

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

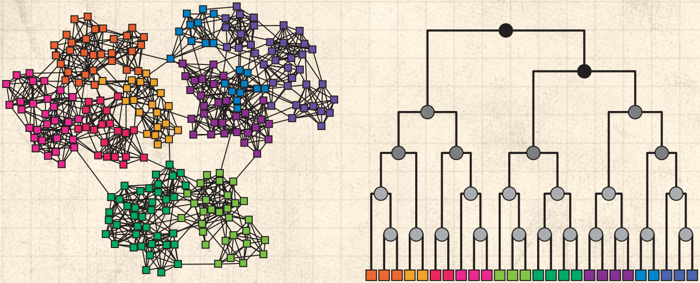




- Idea: Shades indicate probability that nodes in left and right subtrees of dendogram are connected.
- Handle: Hierarchical random graph models.

Hierarchies and missing links

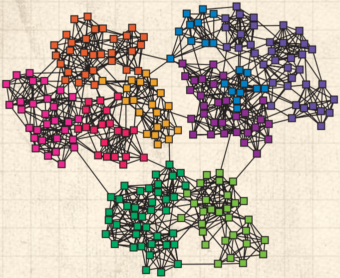
Clauset *et al.*, Nature (2008) [5]

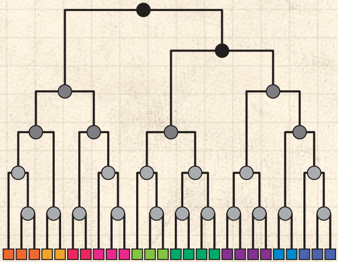


- Idea: Shades indicate probability that nodes in left and right subtrees of dendogram are connected.
- Handle: Hierarchical random graph models.
- Plan: Infer consensus dendogram for a given real network.

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

Hierarchies and missing links

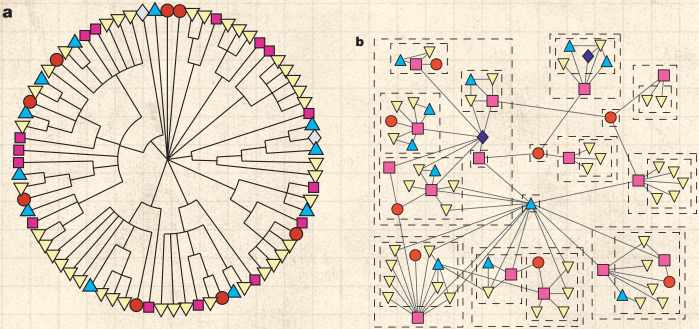
- Model also predicts reasonably well
  1. average degree,
  2. clustering,
  3. and average shortest path length.

Table 1 | Comparison of original and resampled networks

Network	$\langle k\rangle_{\text{real}}$	$\langle k\rangle_{\text{samp}}$	C_{real}	C_{samp}	d_{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)

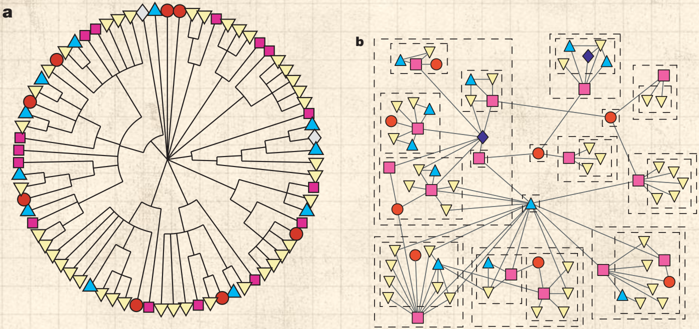
Statistics are shown for the three example networks studied and for new networks generated by resampling from our hierarchical model. The generated networks closely match the average degree $\langle k\rangle$, clustering coefficient C and average vertex–vertex distance d in each case, suggesting that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

Hierarchies and missing links



- Consensus dendogram for grassland species.

Hierarchies and missing links

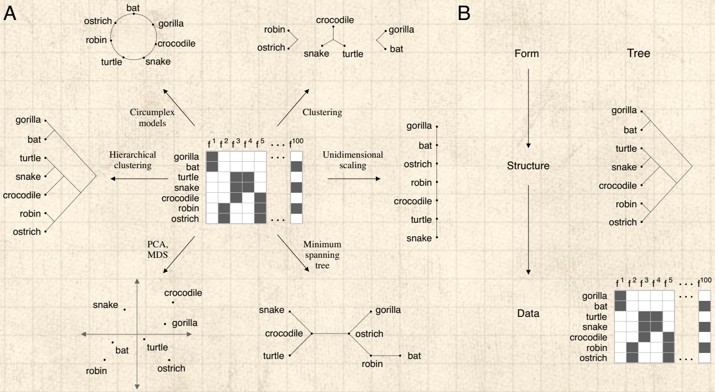


- Consensus dendogram for grassland species.
- Copes with disassortative and assortative communities.

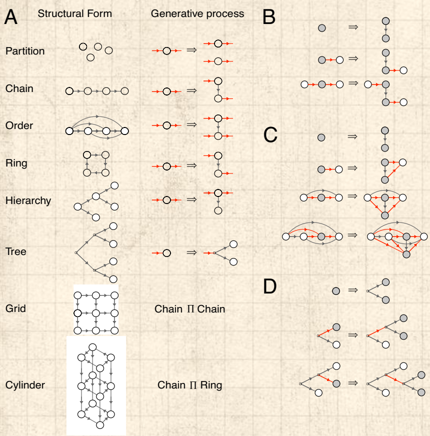
Outline

General structure detection

- "The discovery of structural form"
  Kemp and Tenenbaum, PNAS (2008) [12]

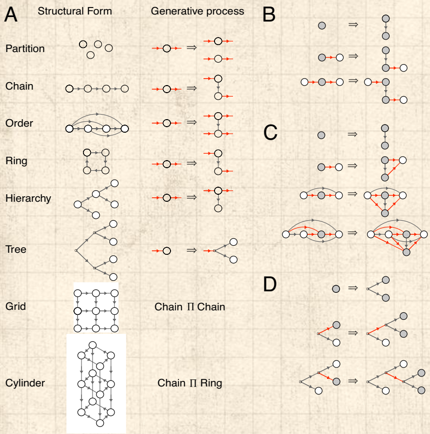


General structure detection



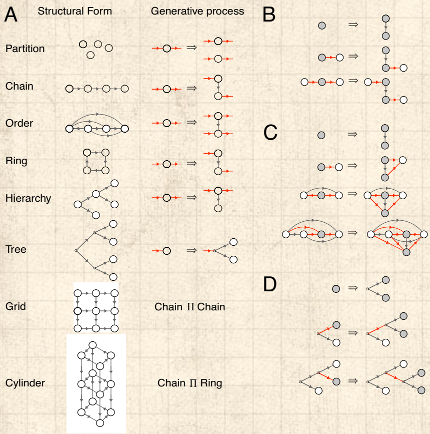
- Top down description of form.

General structure detection



- Top down description of form.
- Node replacement graph grammar: parent node becomes two child nodes.

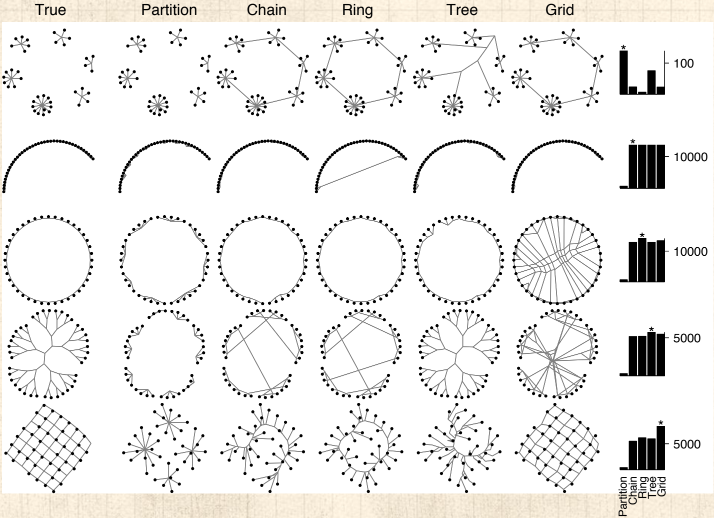
General structure detection



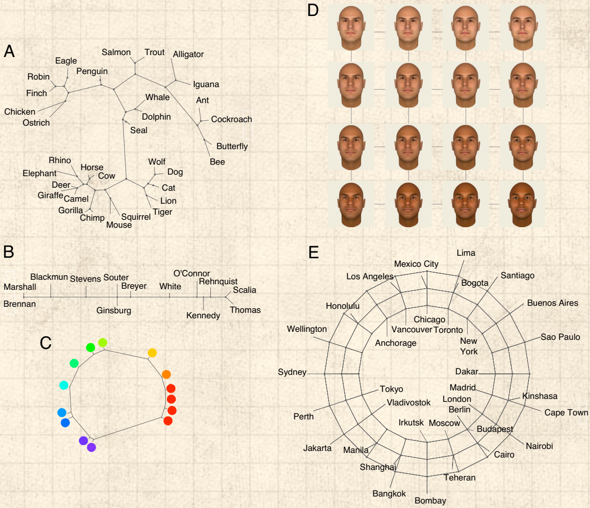
- Top down description of form.
- Node replacement graph grammar: parent node becomes two child nodes.
- B-D: Growing chains, orders, and trees.

General structure detection

Performance for test networks.

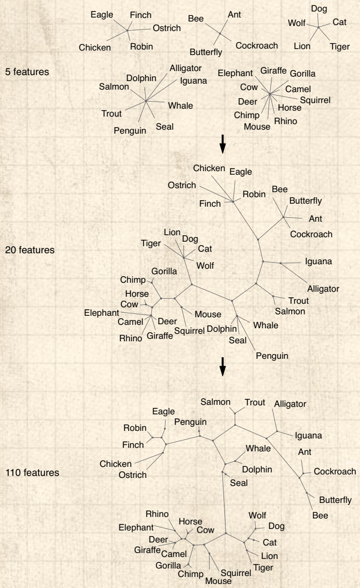


Example learned structures:



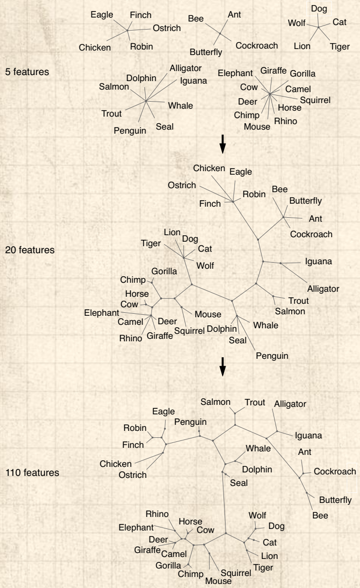
Biological features; Supreme Court votes; perceived color differences; face differences; & distances between cities.

General structure detection



Effect of adding features on detected form.

General structure detection



Effect of adding features on detected form.

Straight partition

⇓

simple tree

⇓

complex tree

Final words:

Science in three steps:

1. Find interesting/meaningful/important phenomena involving spectacular amounts of data.

Final words:

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

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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...

More final words:

A real theory of everything:

More final words:

A real theory of everything:

1. Is not just about the small stuff...

More final words:

A real theory of everything:

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

More final words:

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Symmetry breaking/ Accidents of history	vs.	Universality

More final words:

A real theory of everything:

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

Symmetry breaking/ Accidents of history	vs.	Universality

How probable is a certain level of complexity?

References I

[1] J. R. Banavar, F. Colaiori, A. Flammini, A. Maritan, and A. Rinaldo.
Topology of the fittest transportation network.
Phys. Rev. Lett., 84:4745–4748, 2000. pdf

[2] J. R. Banavar, A. Maritan, and A. Rinaldo.
Size and form in efficient transportation networks.
Nature, 399:130–132, 1999. pdf

[3] S. Bohn and M. O. Magnasco.
Structure, scaling, and phase transition in the optimal transport network.
Phys. Rev. Lett., 98:088702, 2007. pdf

References II

[4] A. Capocci, V. Servedio, G. Caldarelli, and F. Colaiori.
Detecting communities in large networks.
Physica A: Statistical Mechanics and its Applications, 352:669–676, 2005. pdf

[5] A. Clauset, C. Moore, and M. E. J. Newman.
Hierarchical structure and the prediction of missing links in networks.
Nature, 453:98–101, 2008. pdf

[6] P. S. Dodds and D. H. Rothman.
Unified view of scaling laws for river networks.
Physical Review E, 59(5):4865–4877, 1999. pdf

References III

[7] P. S. Dodds and D. H. Rothman.
Geometry of river networks. I. Scaling, fluctuations, and deviations.
Physical Review E, 63(1):016115, 2001. pdf

[8] M. T. Gastner and M. E. J. Newman.
Optimal design of spatial distribution networks.
Phys. Rev. E, 74:016117, 2006. pdf

[9] M. Girvan and M. E. J. Newman.
Community structure in social and biological networks.
Proc. Natl. Acad. Sci., 99:7821–7826, 2002. pdf

[10] S. M. Gusein-Zade.
Bunge's problem in central place theory and its generalizations.
Geogr. Anal., 14:246–252, 1982. pdf

References IV

[11] A. A. Heusner.
Size and power in mammals.
Journal of Experimental Biology, 160:25–54, 1991.
pdf

[12] C. Kemp and J. B. Tenenbaum.
The discovery of structural form.
Proc. Natl. Acad. Sci., 105:10687–10692, 2008.
pdf

[13] J. M. Kleinberg.
Authoritative sources in a hyperlinked environment.
Proc. 9th ACM-SIAM Symposium on Discrete Algorithms, 1998. pdf

References V

[14] M. E. J. Newman.
Scientific collaboration networks. II. Shortest paths, weighted networks, and centrality.
Phys. Rev. E, 64(1):016132, 2001. pdf

[15] M. E. J. Newman.
Erratum: Scientific collaboration networks. II. Shortest paths, weighted networks, and centrality [Phys. Rev. E 64, 016132 (2001)].
Phys. Rev. E, 73:039906(E), 2006. pdf

[16] M. E. J. Newman and M. Girvan.
Finding and evaluating community structure in networks.
Phys. Rev. E, 69(2):026113, 2004. pdf

References VI

[17] M. Sales-Pardo, R. Guimerà, A. A. Moreira, and L. A. N. Amaral.
Extracting the hierarchical organization of complex systems.
Proc. Natl. Acad. Sci., 104:15224–15229, 2007. pdf

[18] M. Sales-Pardo, R. Guimerà, A. A. Moreira, and L. A. N. Amaral.
Extracting the hierarchical organization of complex systems: Correction.
Proc. Natl. Acad. Sci., 104:18874, 2007. pdf

[19] G. E. Stephan.
Territorial division: The least-time constraint behind the formation of subnational boundaries.
Science, 196:523–524, 1977. pdf

References VII

[20] G. E. Stephan.
Territorial subdivision.
Social Forces, 63:145–159, 1984. pdf

[21] D. L. Turcotte, J. D. Pelletier, and W. I. Newman.
Networks with side branching in biology.
Journal of Theoretical Biology, 193:577–592, 1998.
pdf

[22] G. B. West, J. H. Brown, and B. J. Enquist.
A general model for the origin of allometric scaling laws in biology.
Science, 276:122–126, 1997. pdf

[23] Q. Xia.
The formation of a tree leaf.
Submitted. pdf

References VIII

[24] Q. Xia.
Optimal paths related to transport problems.
Communications in Contemporary Mathematics, 5:251–279, 2003. pdf

[25] W. W. Zachary.
An information flow model for conflict and fission in small groups.
J. Anthropol. Res., 33:452–473, 1977.