



Structural Patterns in Complex Networks

Spectral Analysis

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Complex Systems

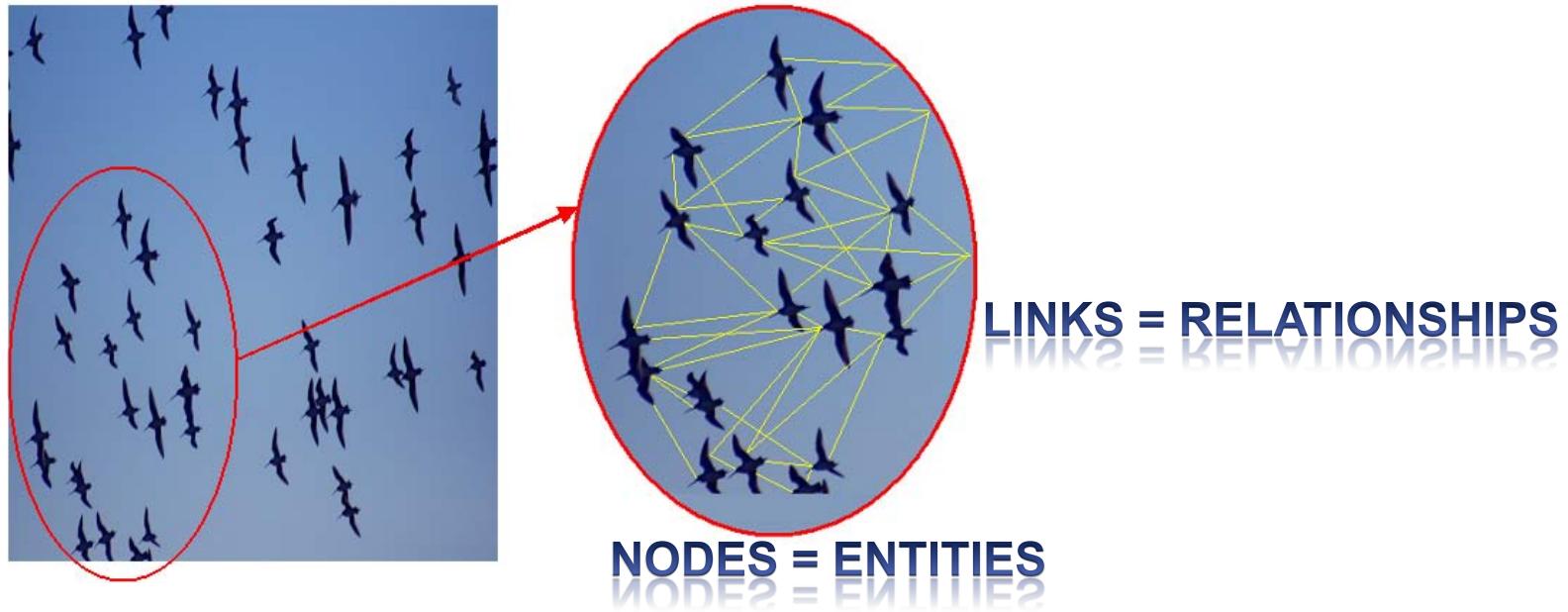
“A complex system is a system composed of interconnected parts that as a whole exhibit one or more properties not obvious from the properties of the individual parts.”



- ✓ Emergence
- ✓ Agent-based
- ✓ Self-organised
- ✓ Short-range interactions
- ✓ Networked

Complex Networks

“Complex networks are the structural skeletons of complex systems”

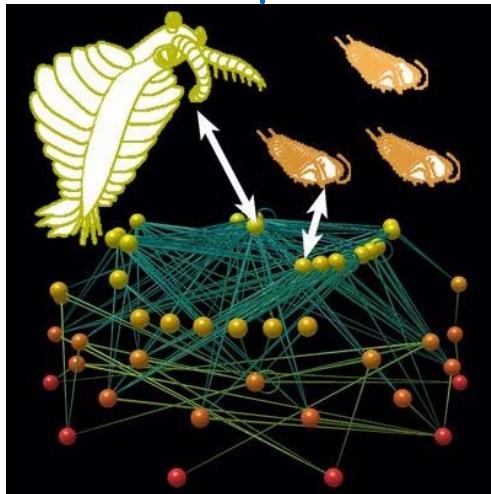


Adjacency Matrix

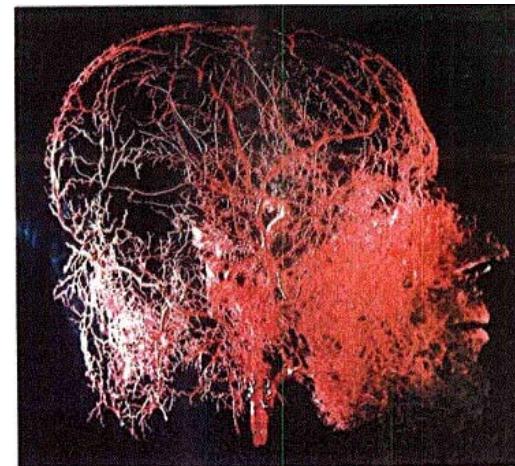
$$(A)_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ have a direct link} \\ 0 & \text{otherwise} \end{cases}$$

Complex Networks in Nature

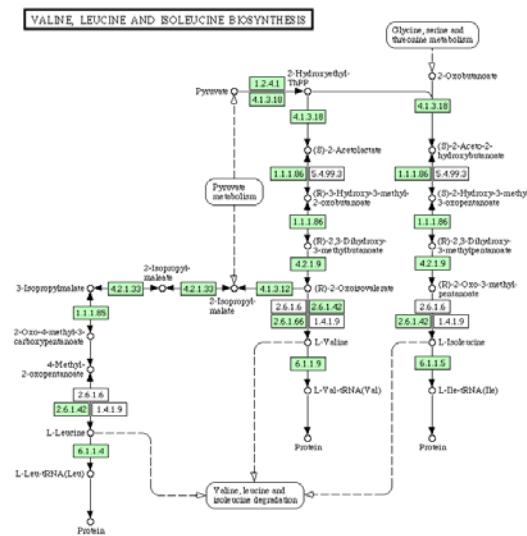
Inter-species



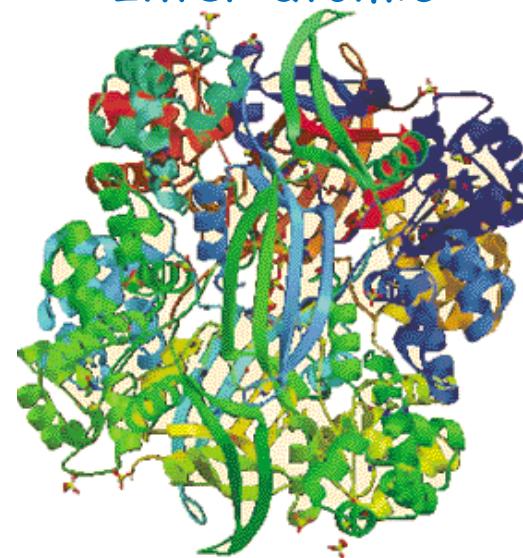
Inter-cellular



Inter-molecular

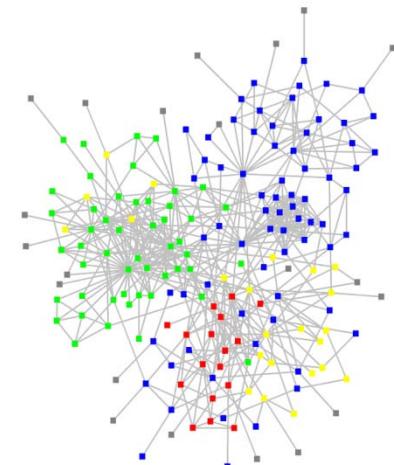
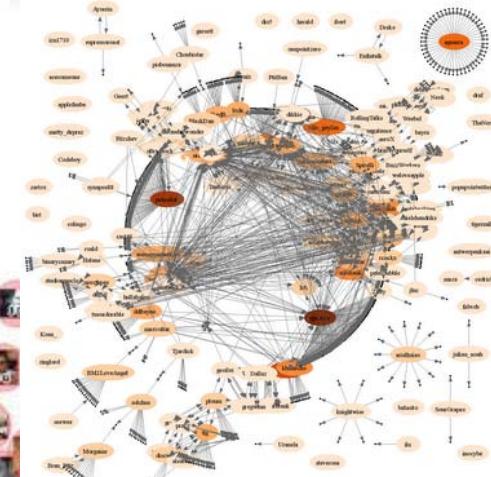
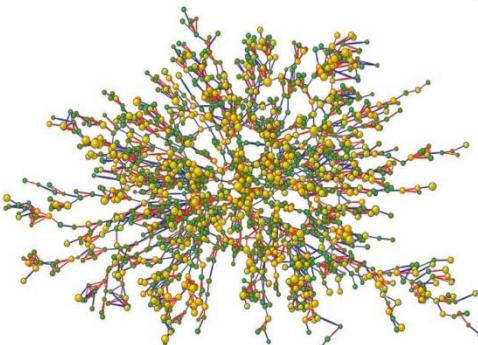
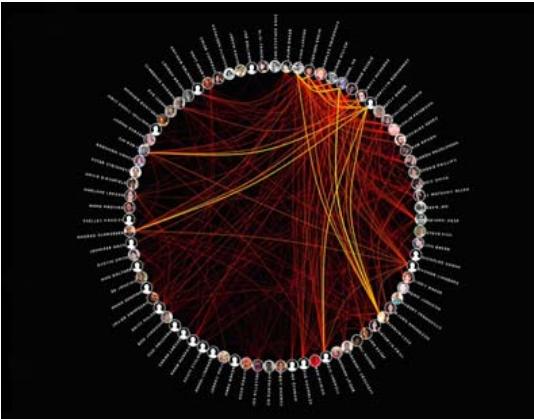


Inter-atomic



Social Networks

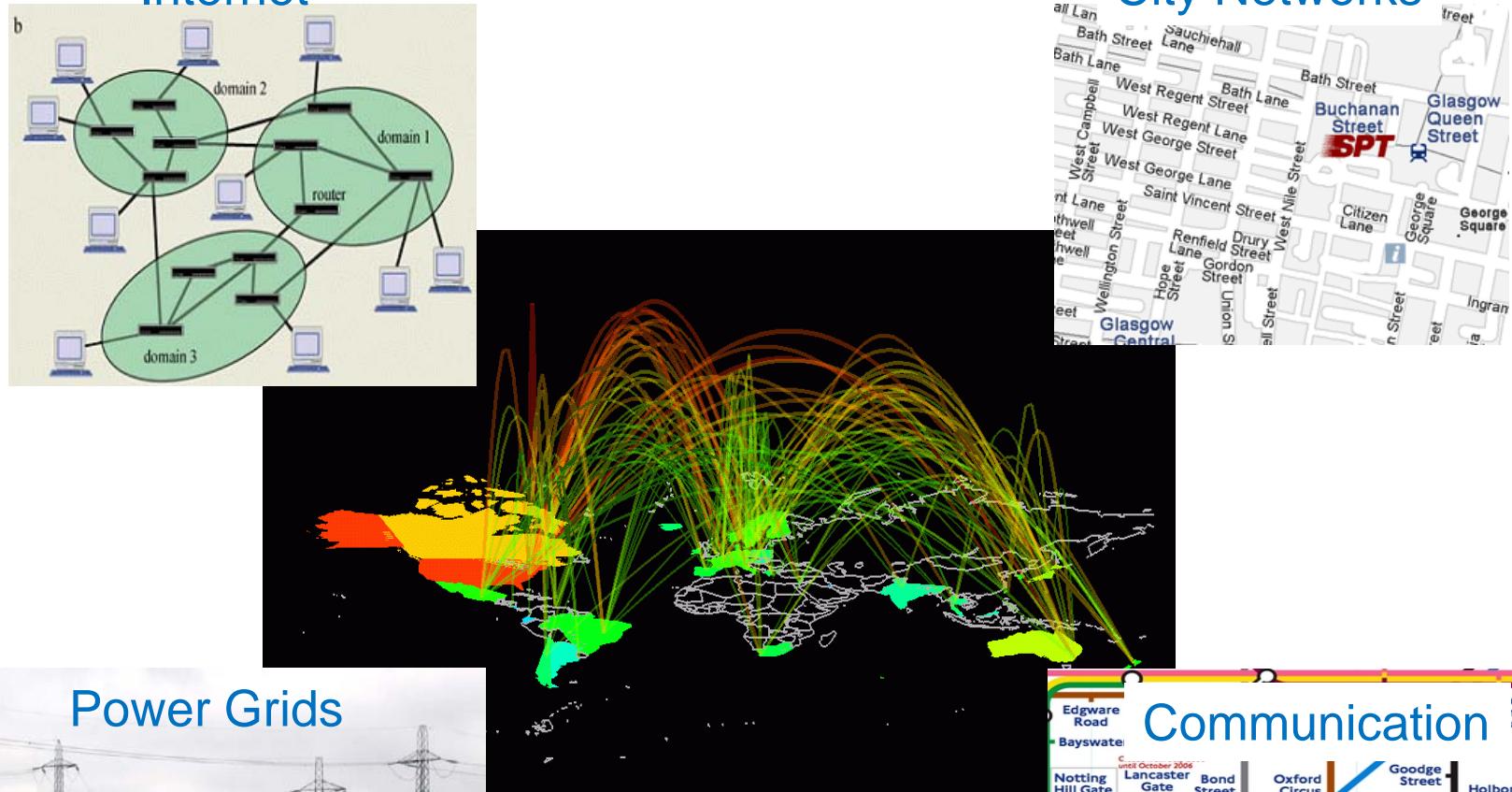
SOCIAL NETWORKS



- ✓ Friendship networks
- ✓ Collaboration networks
- ✓ Sexual networks
- ✓ Buyer-seller networks...

Technological & Infrastructural Networks

Technological & Infrastructural Networks

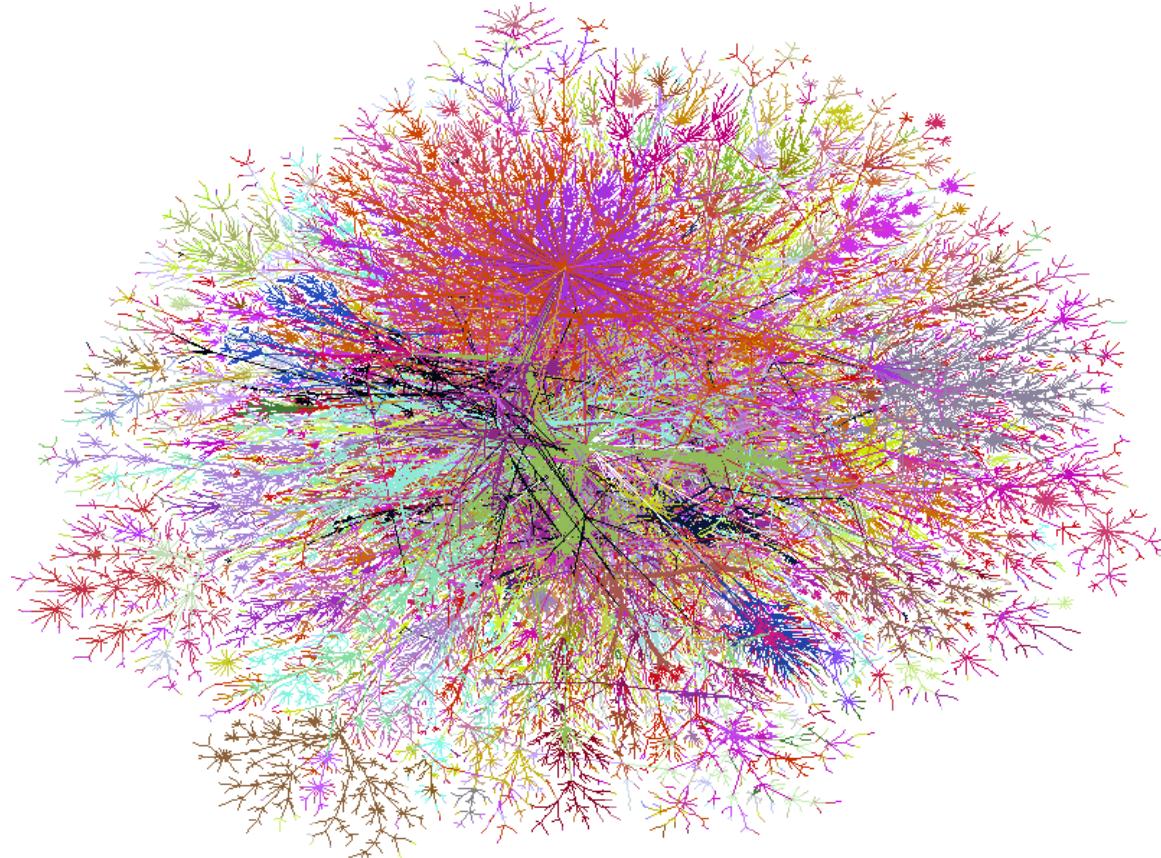


Power Grids



Network Structure: What is She?

INFORMATION PLACEMENT ALGORITHMS

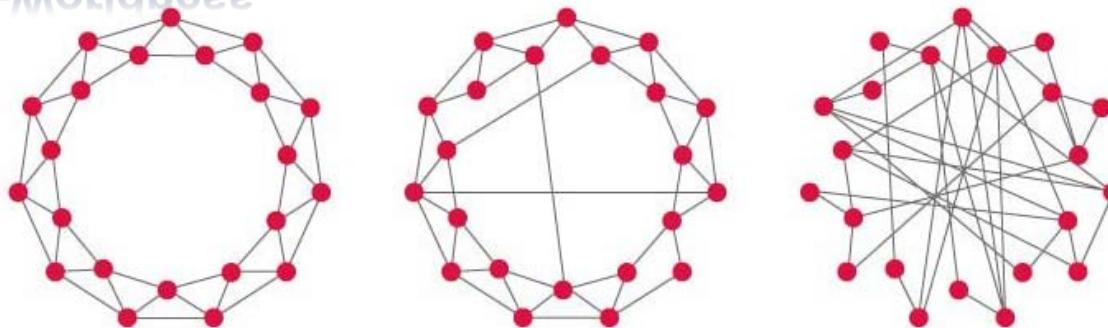


***“What she is not, I can easily perceive –
what she is I fear it is impossible to say.”***

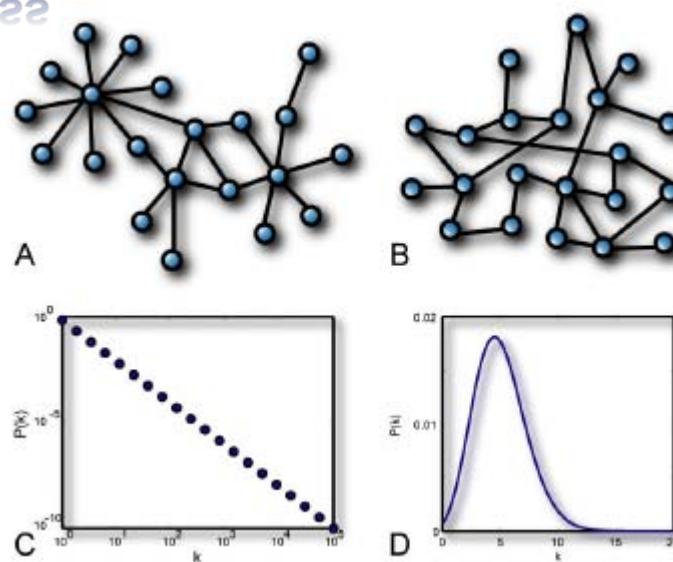
Edgar Allan Poe

Network Structure: Universality

Small-Worldness



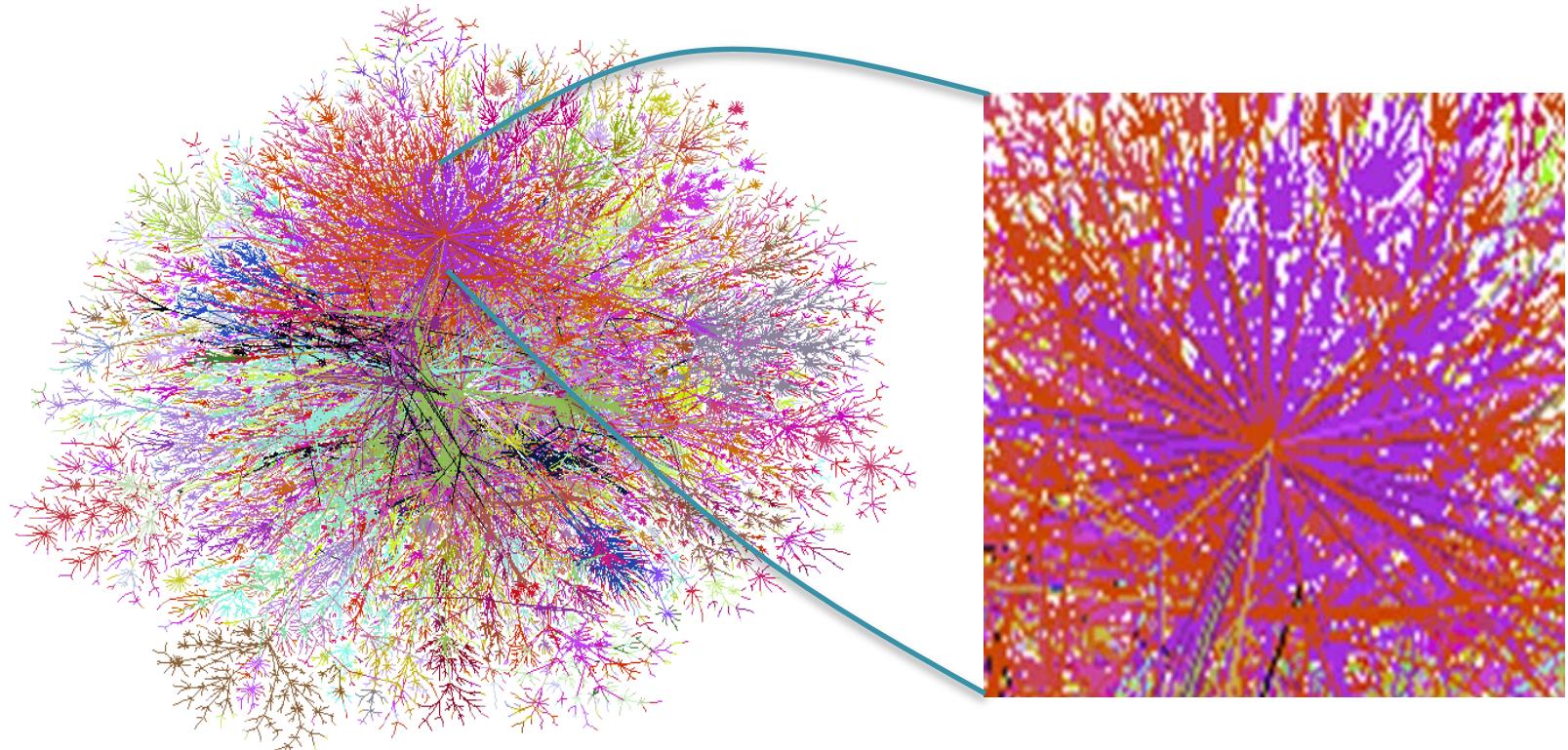
Scale-freeness



S. H. Strogatz, Nature 410, 268 (2001)

Local Network Structure

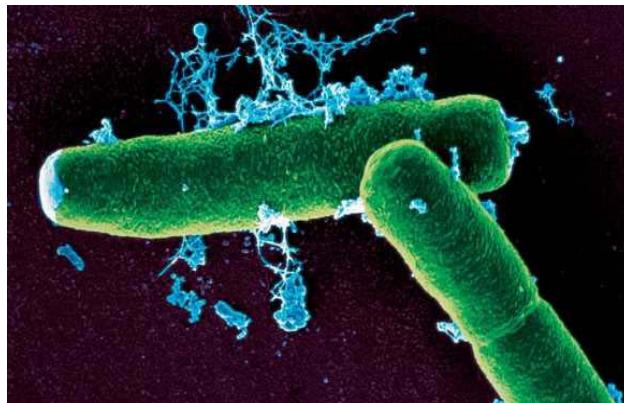
FOCAL NEIGHBORHOOD SCALE



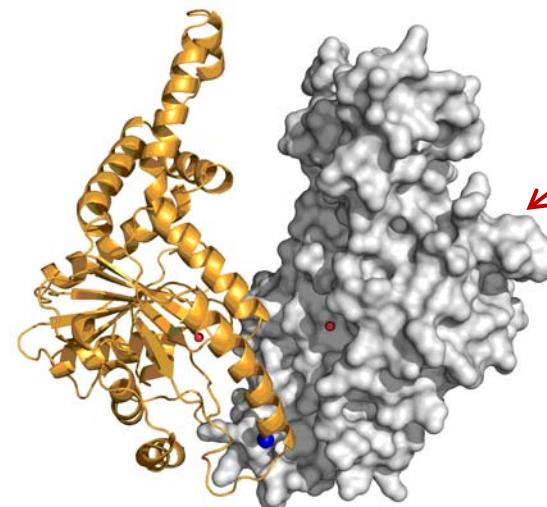
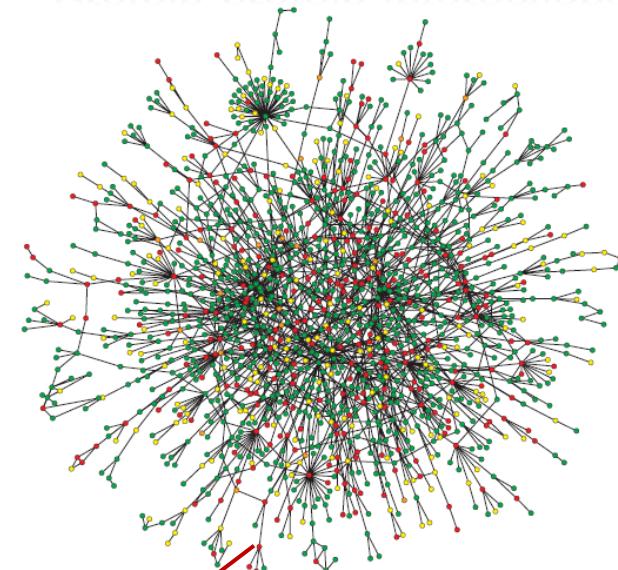
What can we learn by studying the region around a node?

Protein Essentiality

Yeast



Protein-protein Interactions



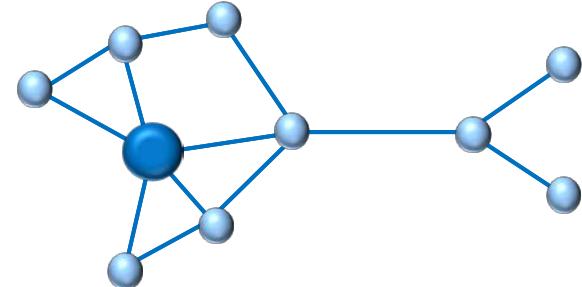
Essential: because if knocked out the cell dies.

Are the most 'central' proteins the essential ones?

Node Centrality

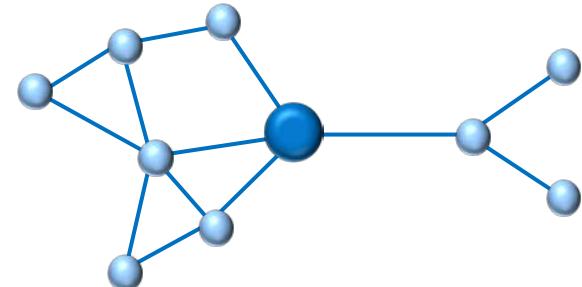
Degree

$$DC(p) = \sum_q A_{pq}$$



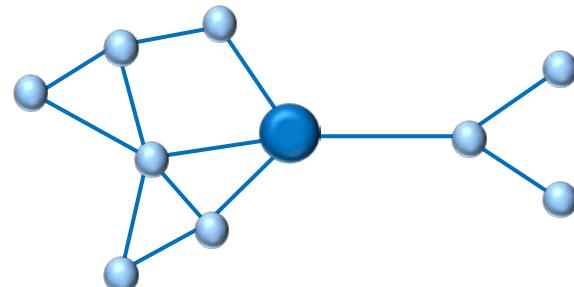
Closeness

$$CC(p) = \frac{n-1}{\sum_q d(p,q)}$$



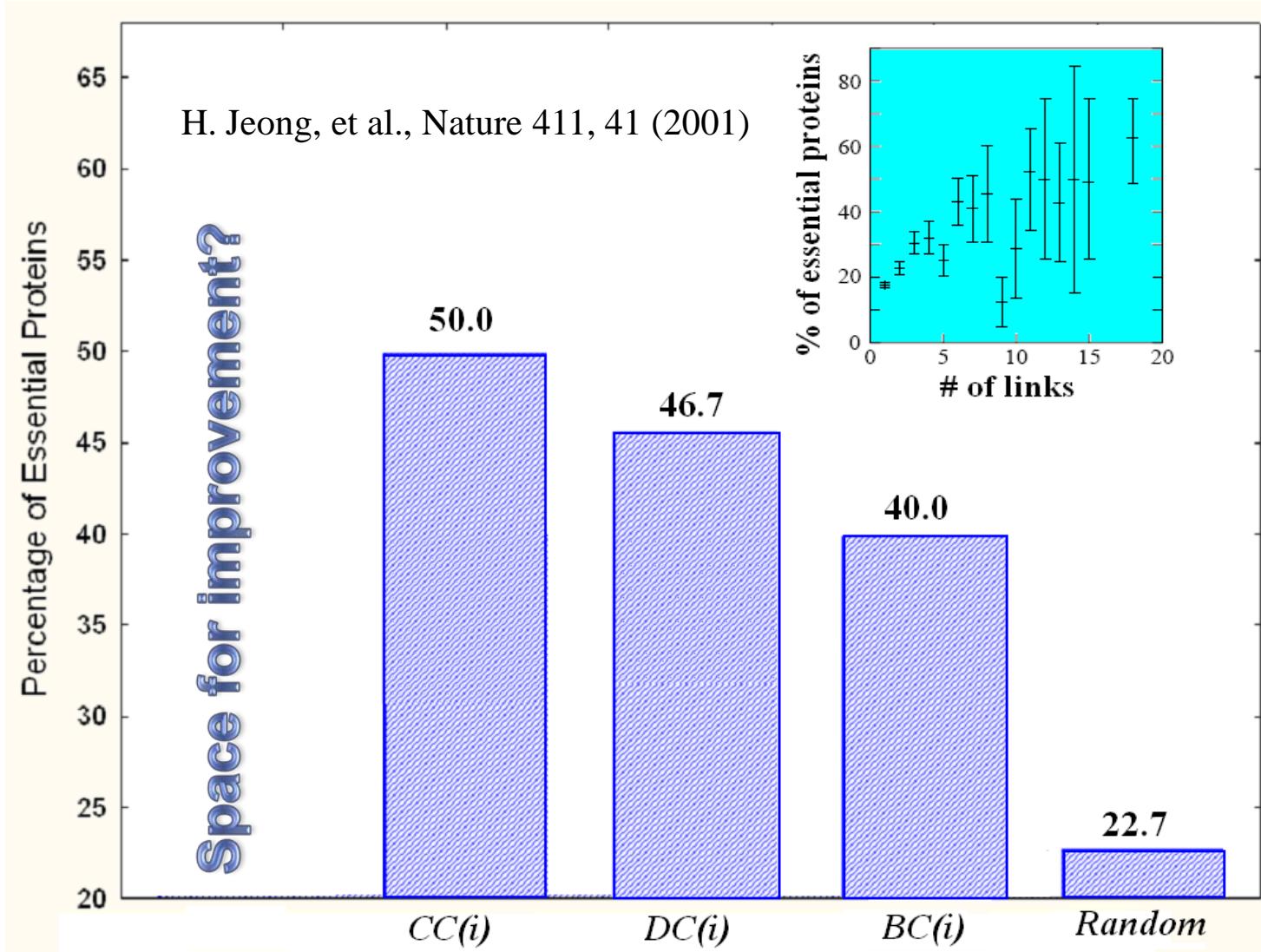
Betweenness

$$BC(p) = \sum_i \sum_j \frac{\rho(i, p, j)}{\rho(i, j)}$$

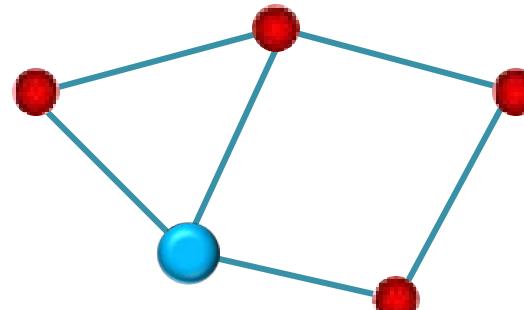


Centrality & Protein Essentiality

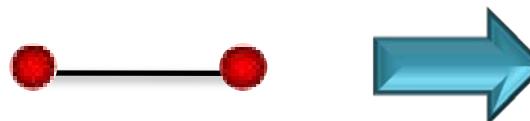
Centrality & Protein Essentiality



Strategy: Use All Possible Routes

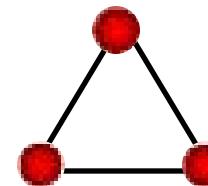


$$CW_2(i) = 3$$



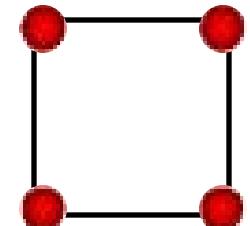
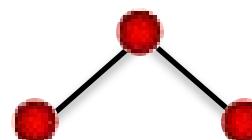
Equal to the degree
of the node

$$CW_3(i) = 2$$



Transitivity

$$CW_4(i) = 15$$



Subgraph Centrality: The Concept

E. Estrada and J.A. Rodríguez-Velázquez: *Phys. Rev. E* 71, 056103 (2005)

$$\begin{aligned} EE_i &= \sum_{k=0}^{\infty} c_k (\text{# of CWs in } k \text{ steps starting at } i) \\ &= \sum_{k=0}^{\infty} c_k (\mathbf{A}^k)_{ii} \end{aligned}$$

$$EE_i = \sum_{k=0}^{\infty} \frac{(\mathbf{A}^k)_{ii}}{k!} = (e^{\mathbf{A}})_{ii}$$

Node centrality

Directed graphs: E. Estrada, *Lin. Algebra Appl.* 430, **2009**, 1886-1896

Spectral Formulae

E. Estrada and J.A. Rodríguez-Velázquez: Phys. Rev. E 71, 056103 (2005)

Eigenvalues of \mathbf{A} : $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_N$

Eigenvector of λ_μ : $\varphi_\mu = (\varphi_\mu(1), \varphi_\mu(2), \dots)$

$$EE_i = \sum_{j=1}^n [\varphi_j(i)]^2 e^{\lambda_j}$$

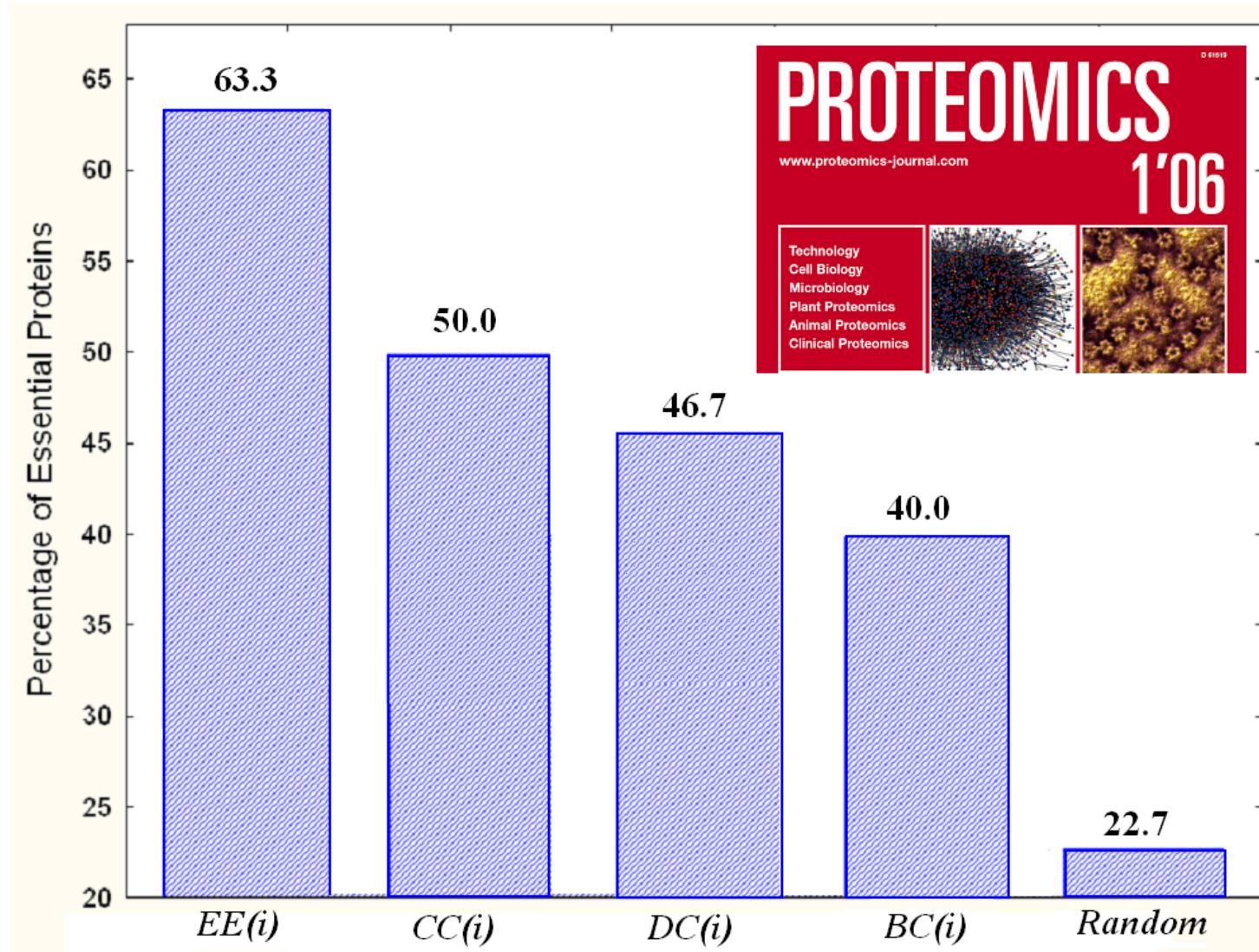
Spectral formula

Bipartivity: Estrada and Rodríguez-Velázquez: Phys. Rev. E 72, **2005**, 046105

$$EE(i) = \sum_{j=1}^N [\gamma_j(i)]^2 \sinh(\lambda_j) + \sum_{j=1}^N [\gamma_j(i)]^2 \cosh(\lambda_j)$$

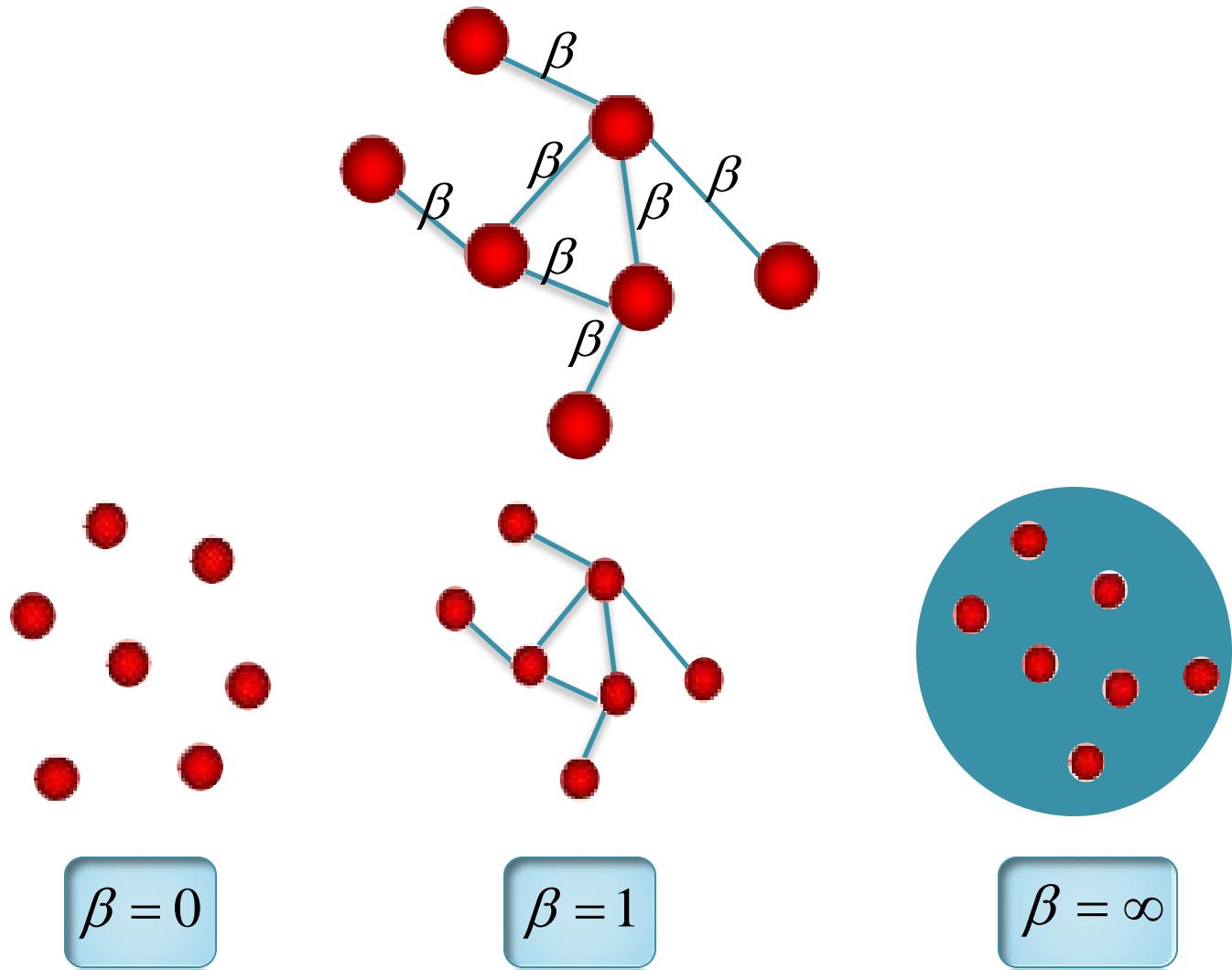
Subgraph Centrality & Protein Essentiality

Estrada, E., Proteomics 6, 35 (2006)



Networks with Homogeneous Link Weights

E. Estrada and N. Hatano: Chem. Phys. Lett. 439, 247 (2007)



A Physical Analogy

E. Estrada and N. Hatano: Chem. Phys. Lett. 439, 247 (2007)

$$\beta = \frac{1}{k_B T}$$

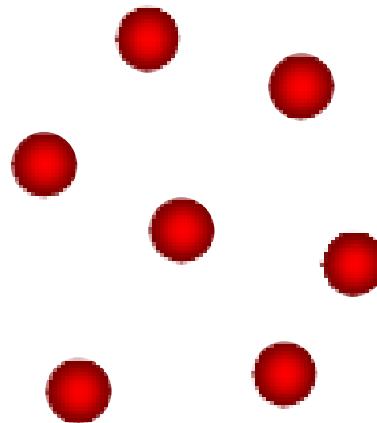
Inverse temperature



A Physical Analogy

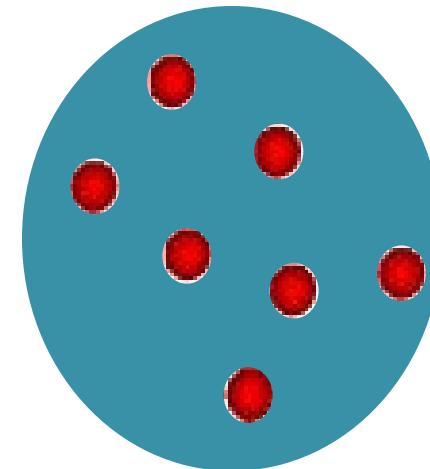
E. Estrada and N. Hatano: Chem. Phys. Lett. 439, 247 (2007)

GAS



$$T \rightarrow \infty$$

SOLID



$$T \rightarrow 0$$

The temperature can be considered as an external “stress”,
e.g., social agitation, physiological stress or an economical situation.

A Statistical-mechanical Approach

E. Estrada and N. Hatano: Chem. Phys. Lett. 439, 247 (2007)

$$EE(G, \beta) = \sum_{j=1}^n e^{\beta \lambda_j}$$

Partition function

$$p_j = \frac{e^{\beta \lambda_j}}{\sum_{j=1}^n e^{\beta \lambda_j}}$$

Probability

$$F(G, \beta) = H - TS = -\beta^{-1} \ln EE$$

Helmholtz Free Energy

$$H(G, \beta) = -\sum_j \lambda_j p_j$$

Total Energy

$$S = -k_B \sum_j [p_j (\beta \lambda_j - \ln EE)]$$

Entropy

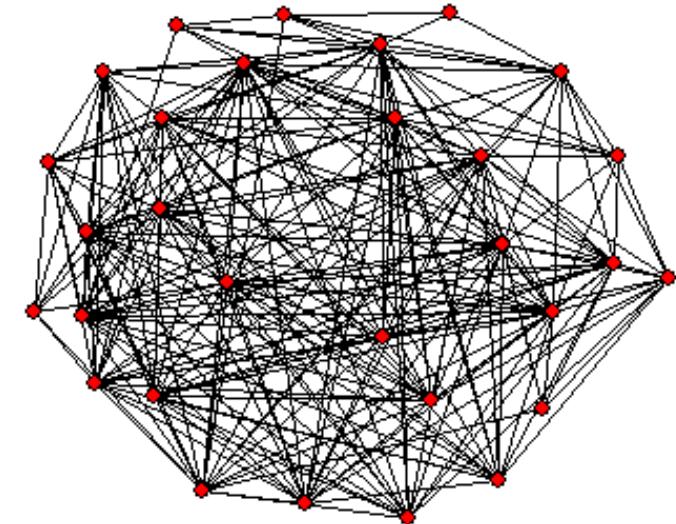
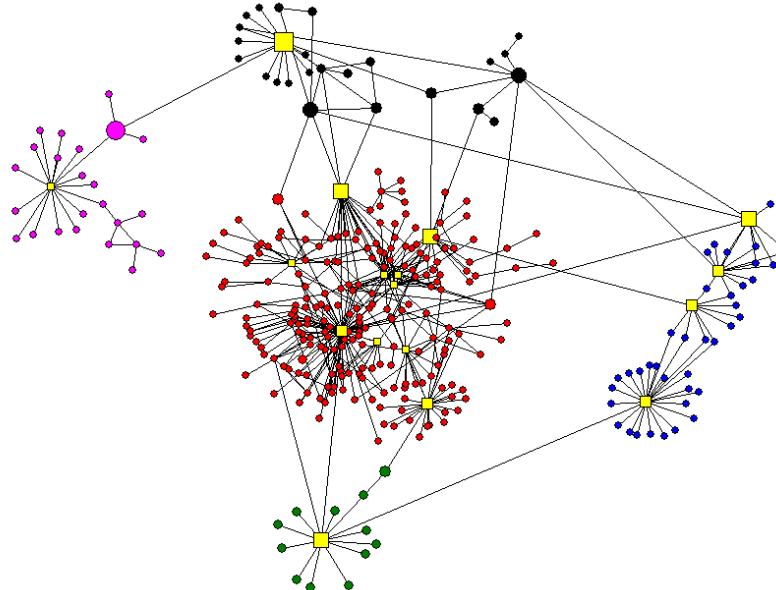
Global Structure of Networks

GLOBAL SCALE OR LOCAL?

MODULAR

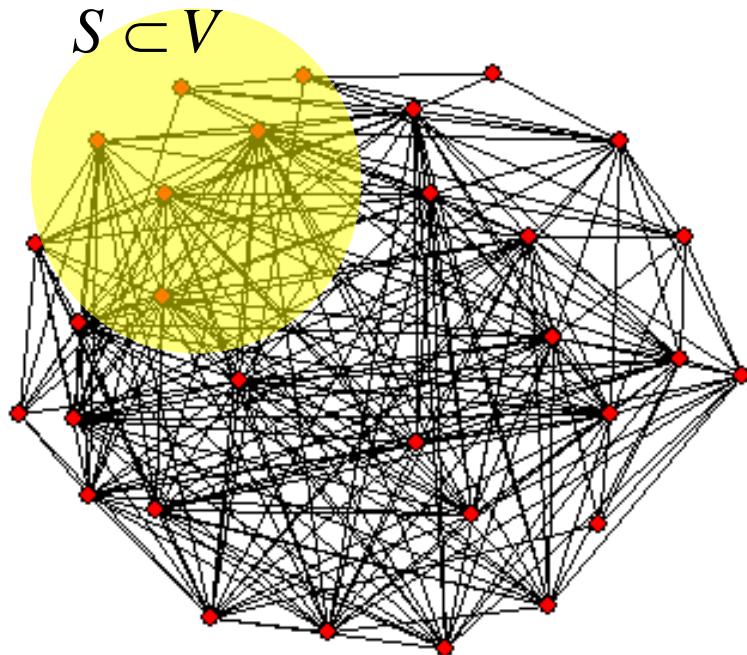
OR
OK

HOMOGENEOUS?



Homogeneous networks

HOMOGENEOUS NETWORKS



Let $|S| \leq 1/2|V|$ and $|\partial(S)|$ represents the number of edges with exactly one endpoint in S .

**Edge Expansion
(Isoperimetric Number)**

$$h(G) = \min_{1 \leq |S| \leq \frac{n}{2}} \frac{|\partial(S)|}{|S|}$$

A good expansion (homogeneous) network is one for which $h(G) = O(1)$. That is, '*what you see locally is what you get globally*'.

Can we identify them?

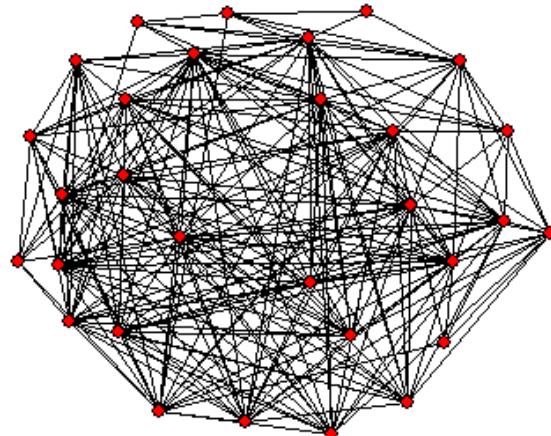
Good Expansion and Graph Spectra

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_N$$

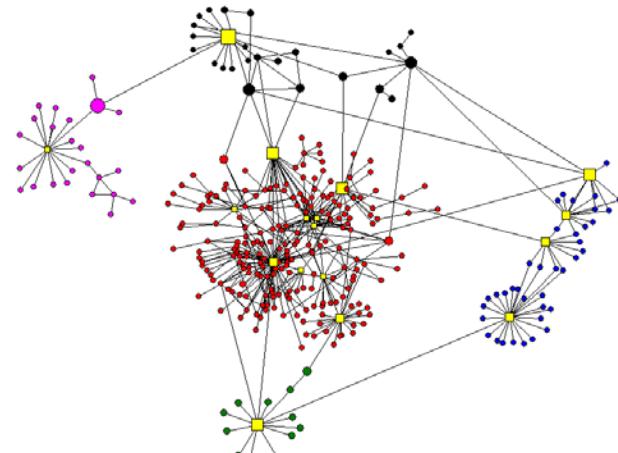
$$\frac{\lambda_1 - \lambda_2}{2} \leq h(G) \leq \sqrt{2\lambda_1(\lambda_1 - \lambda_2)}$$

Alon, Milman, *J. Combin. Theory Ser. B* 1985, 38, 73.

Large spectral gap ($\lambda_1 - \lambda_2$) implies high expansion



$$\lambda_1 - \lambda_2 = 11.147$$



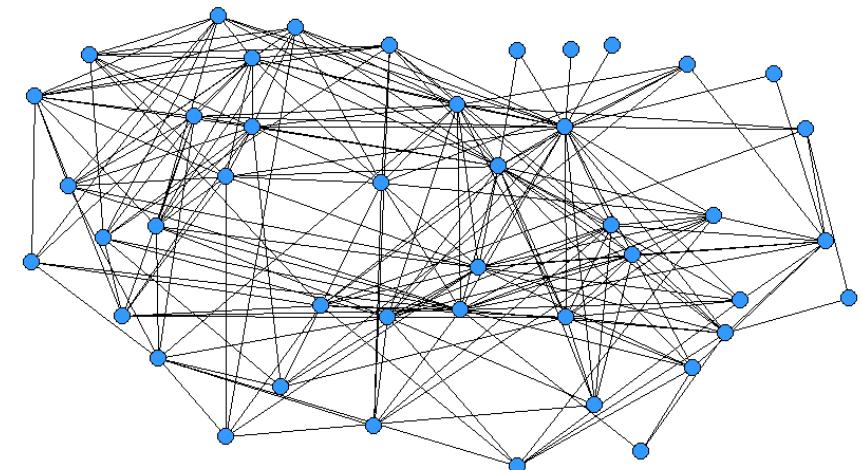
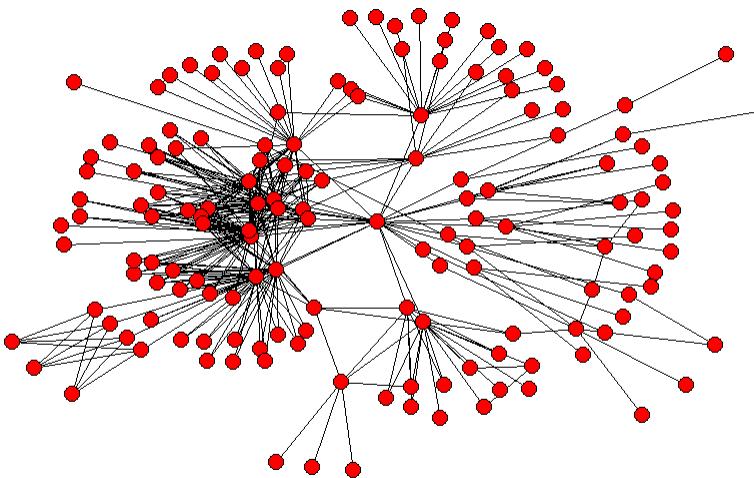
$$\lambda_1 - \lambda_2 = 2.766$$

How large the spectral gap should be?

How large the spectral gap should be?

$$\lambda_1 - \lambda_2 = 8.714$$

$$\lambda_1 - \lambda_2 = 5.559$$



Homogeneous?
Homogeneous?

Modular?
Modular?

Spectral Scaling Method

Let:

$$EE_{odd}(i) = [\gamma_1(i)]^2 \sinh(\lambda_1) + \sum_{j=2}^N [\gamma_j(i)]^2 \sinh(\lambda_j)$$

Homogeneous network: that for which $\lambda_1 - \lambda_2$ is large enough as to consider that:

$$[\gamma_1(i)]^2 \sinh(\lambda_1) \gg \sum_{j=2}^N [\gamma_j(i)]^2 \sinh(\lambda_j)$$

Then:

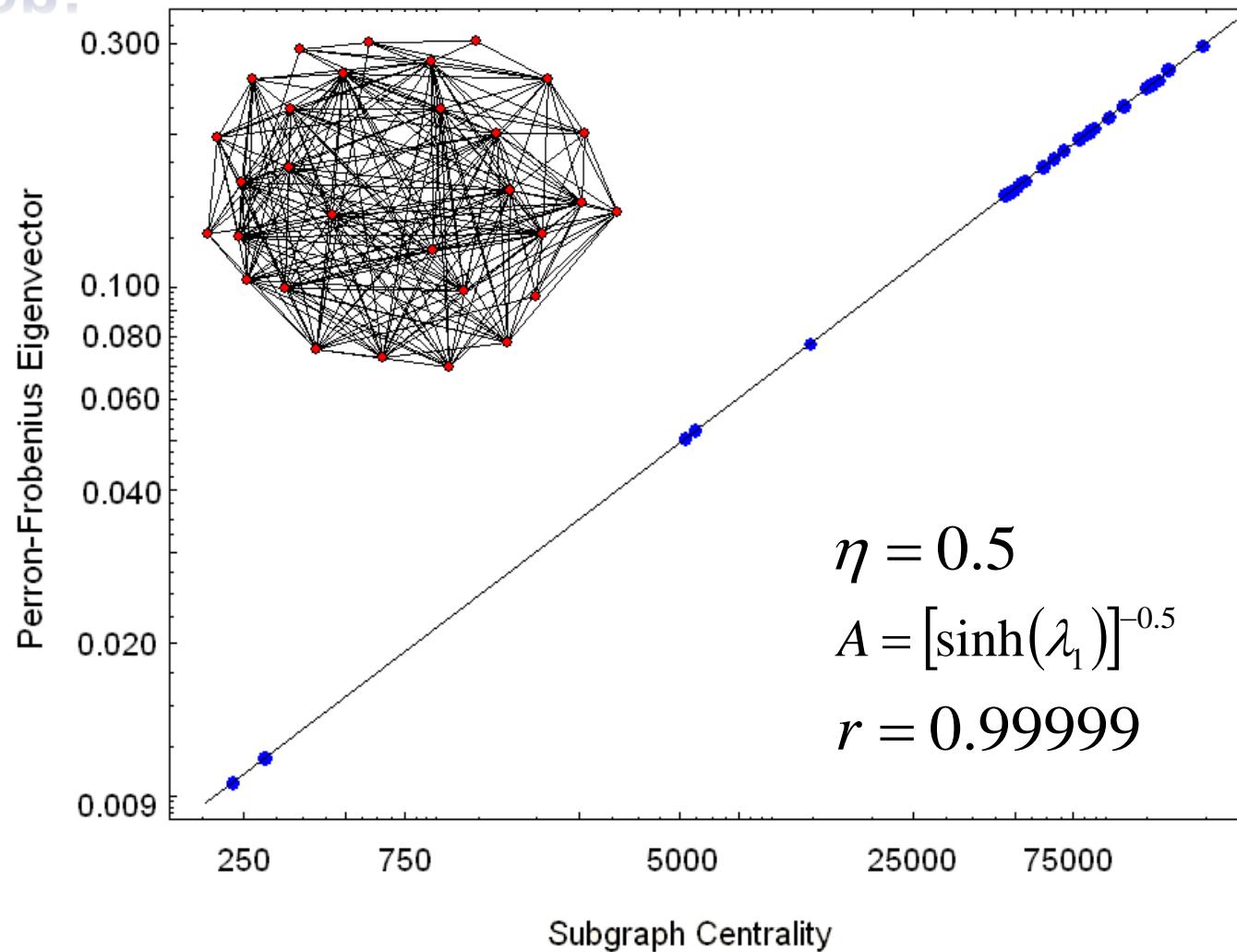
$$EE_{odd}(i) \approx [\gamma_1(i)]^2 \sinh(\lambda_1)$$

Estrada, E. *Europhys. Lett.* 73, 2006, 649
Estrada, E. *Eur. Phys. J. B* 52, 2006, 563

Spectral Scaling Method

Then:
I find:

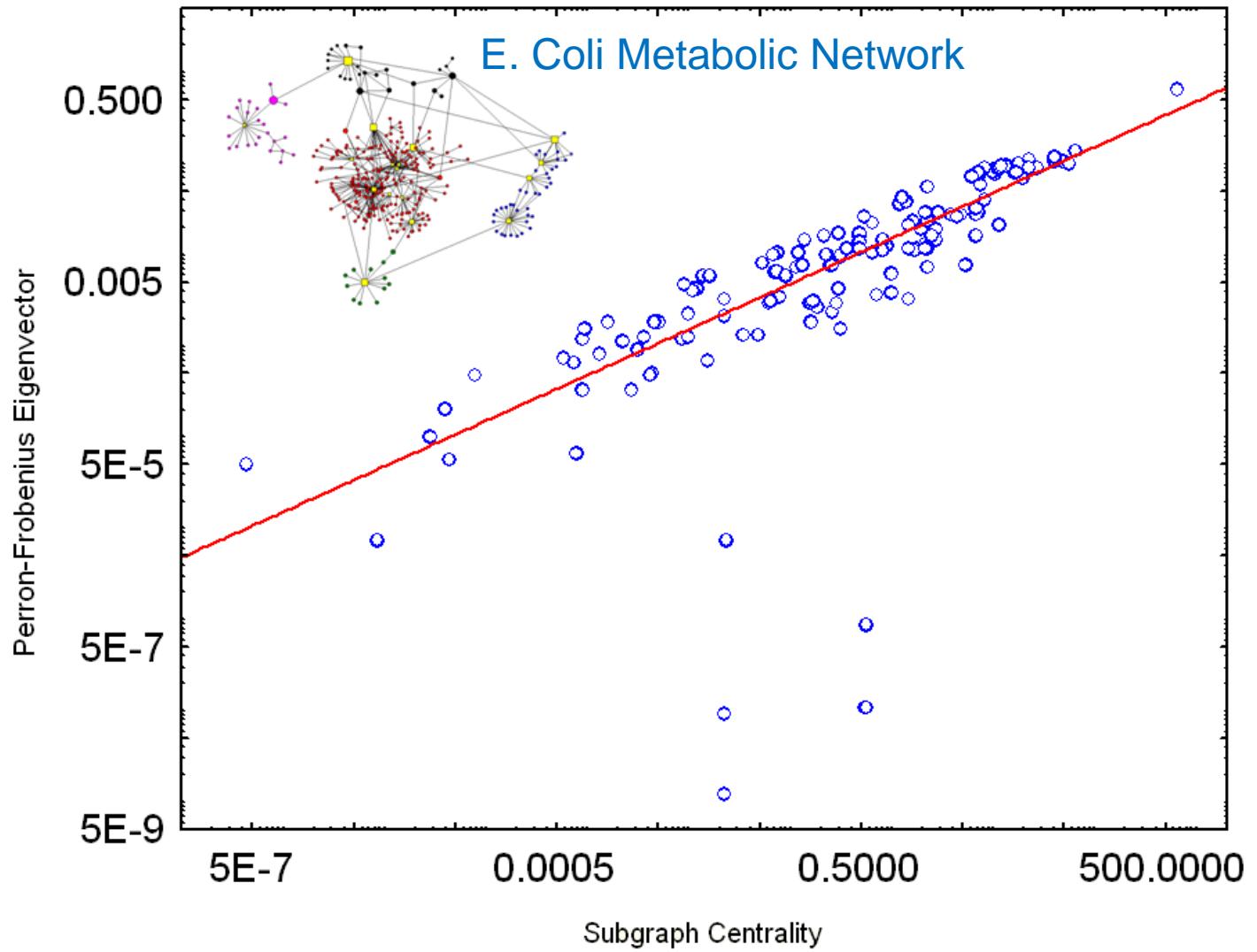
$$\log[\gamma_1(i)] \approx \log A + \eta \log[EE_{odd}(i)]$$



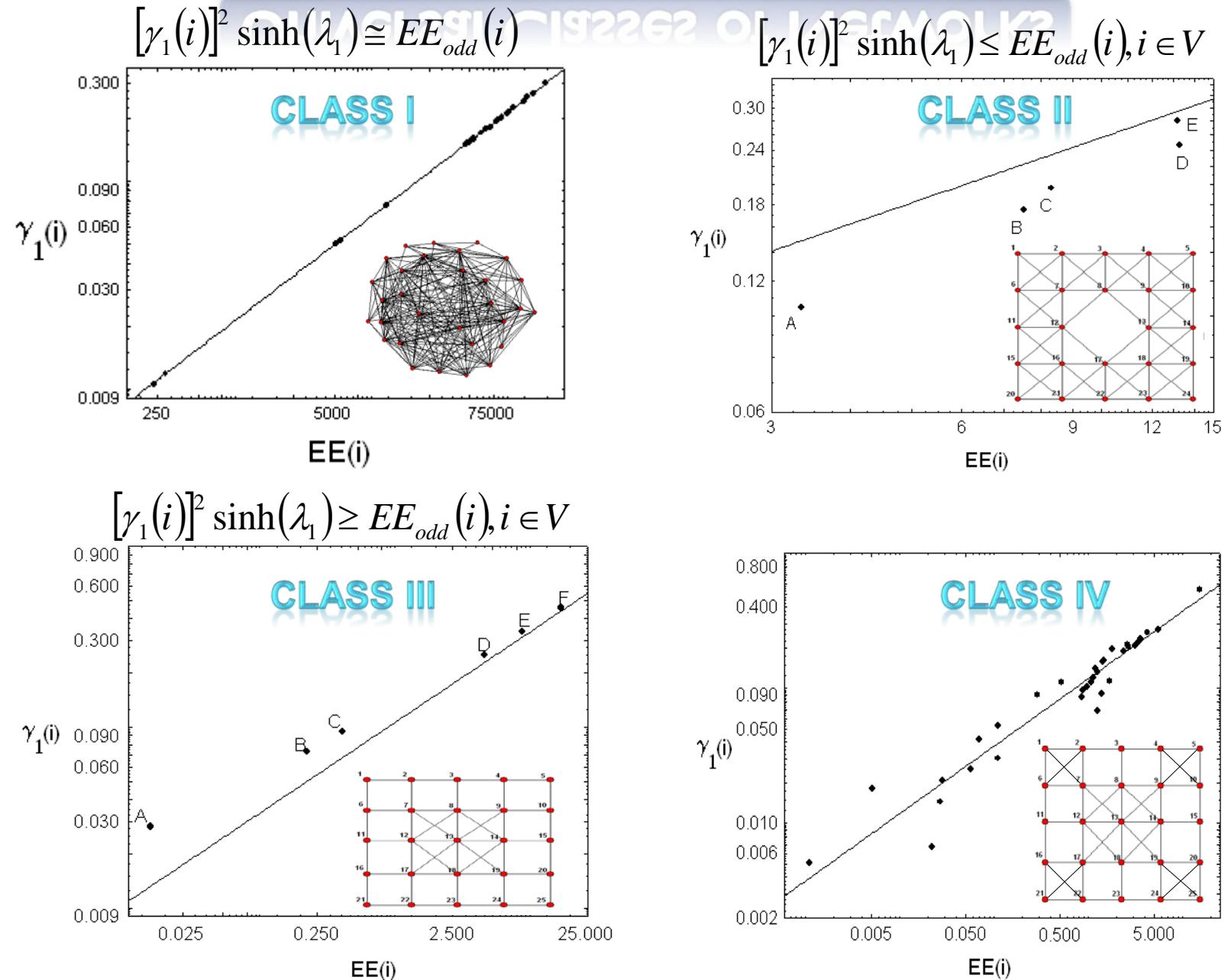
Estrada, E. *Europhys. Lett.* 73, 2006, 649

Estrada, E. *Eur. Phys. J. B* 52, 2006, 563

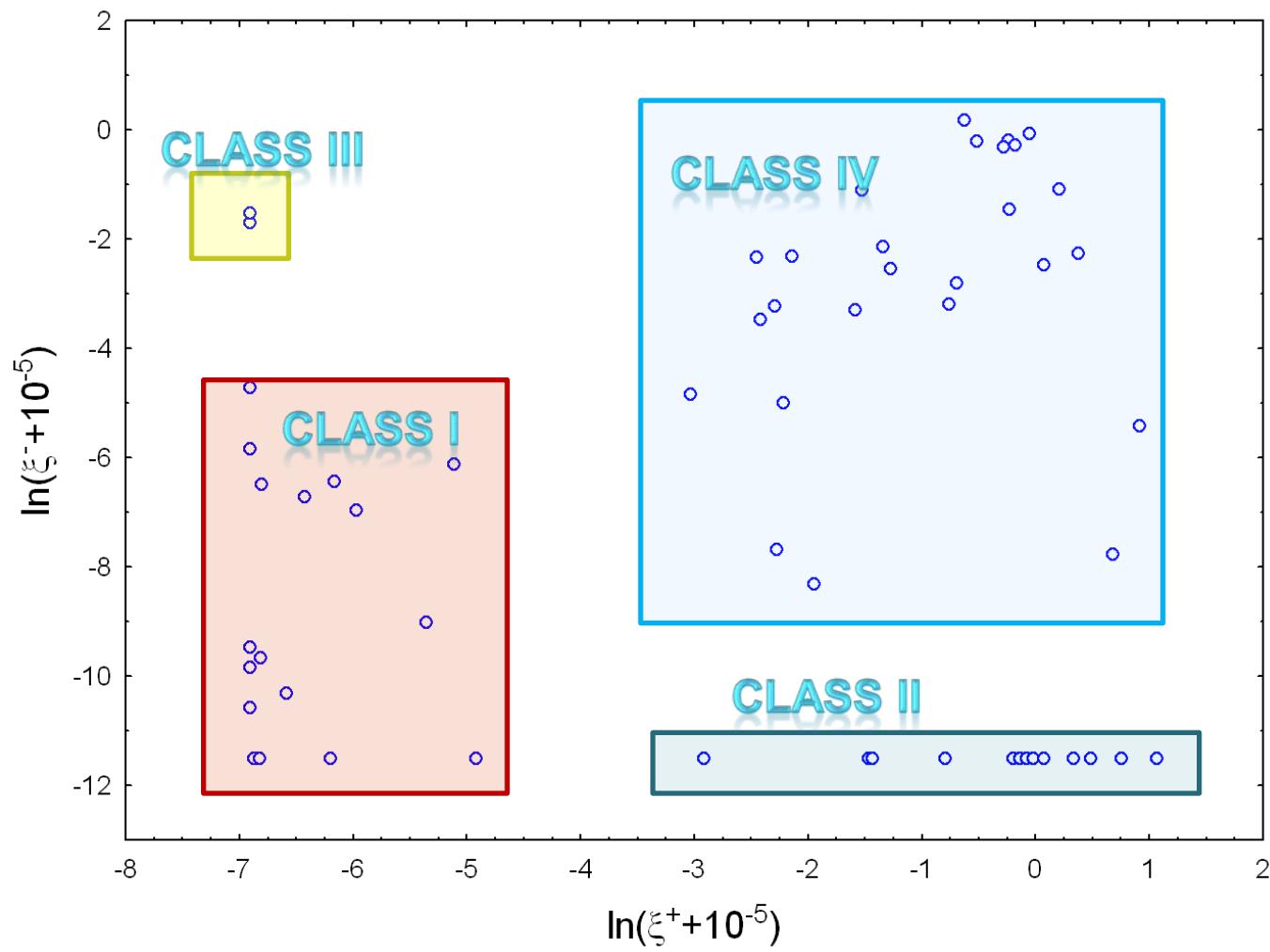
Good Expansion and Modularity



Universal Classes of Networks

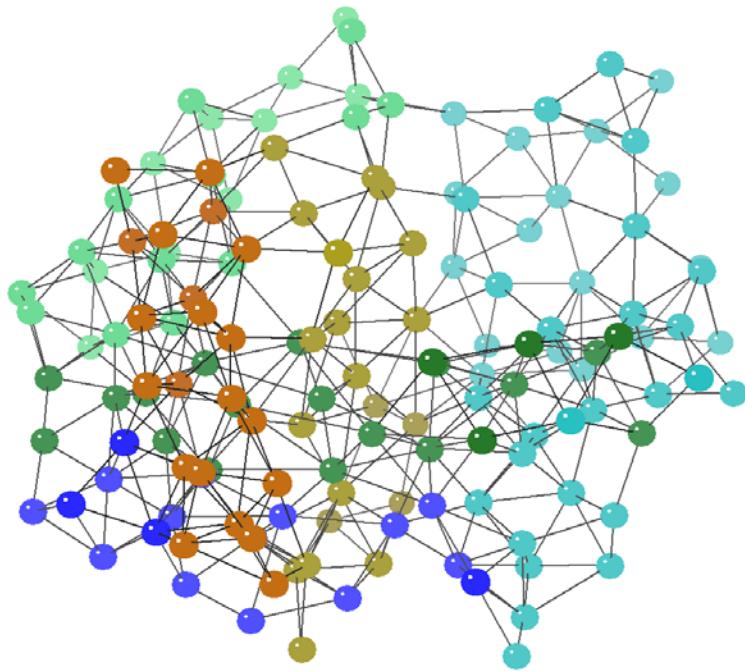


Universal Classes of Real-World Networks

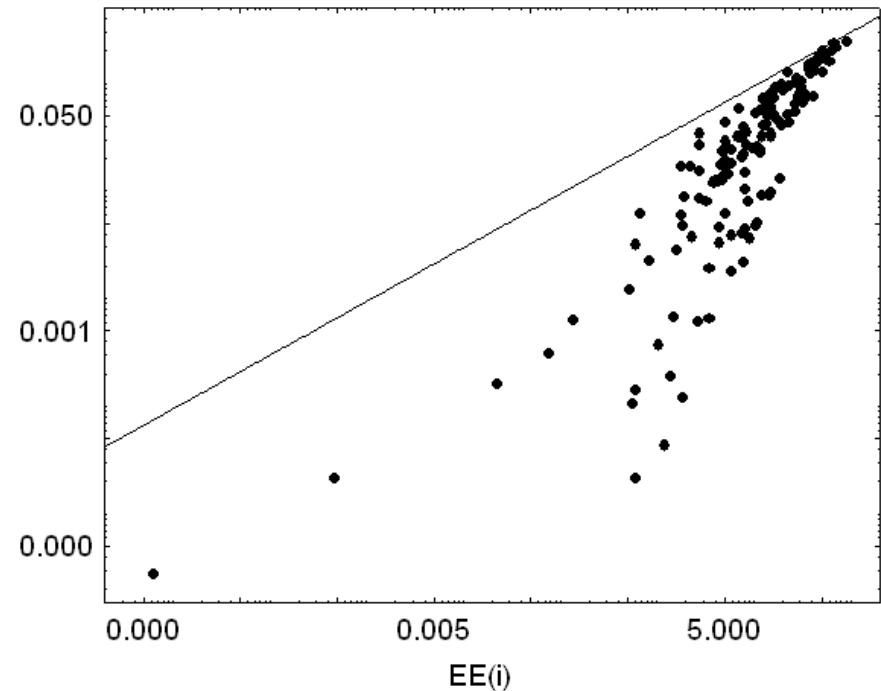


Example: Protein Residue Networks

Example: Bacteriophage MCMV L2

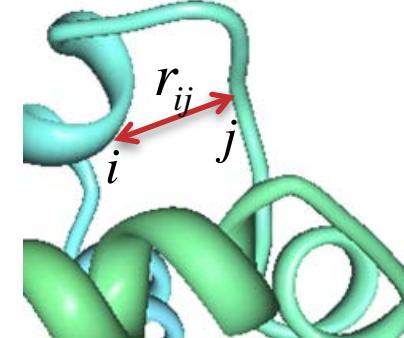
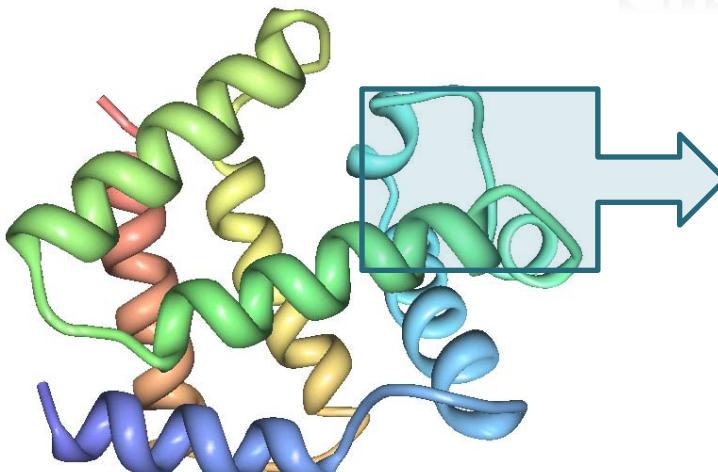


PROTEIN NETWORK



SPECTRAL SCALING

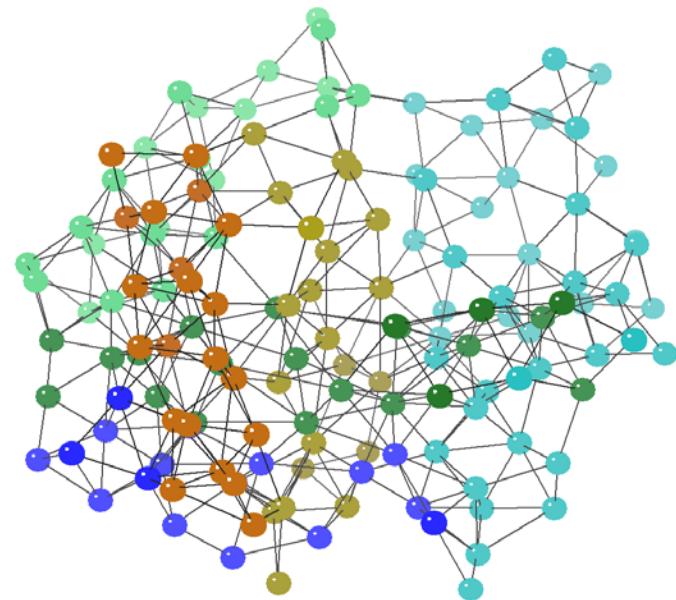
How Protein Residue Networks are Built?



$$A_{ij} = \begin{cases} H(r_c - r_{ij}) & i \neq j \\ 0 & i = j \end{cases}$$

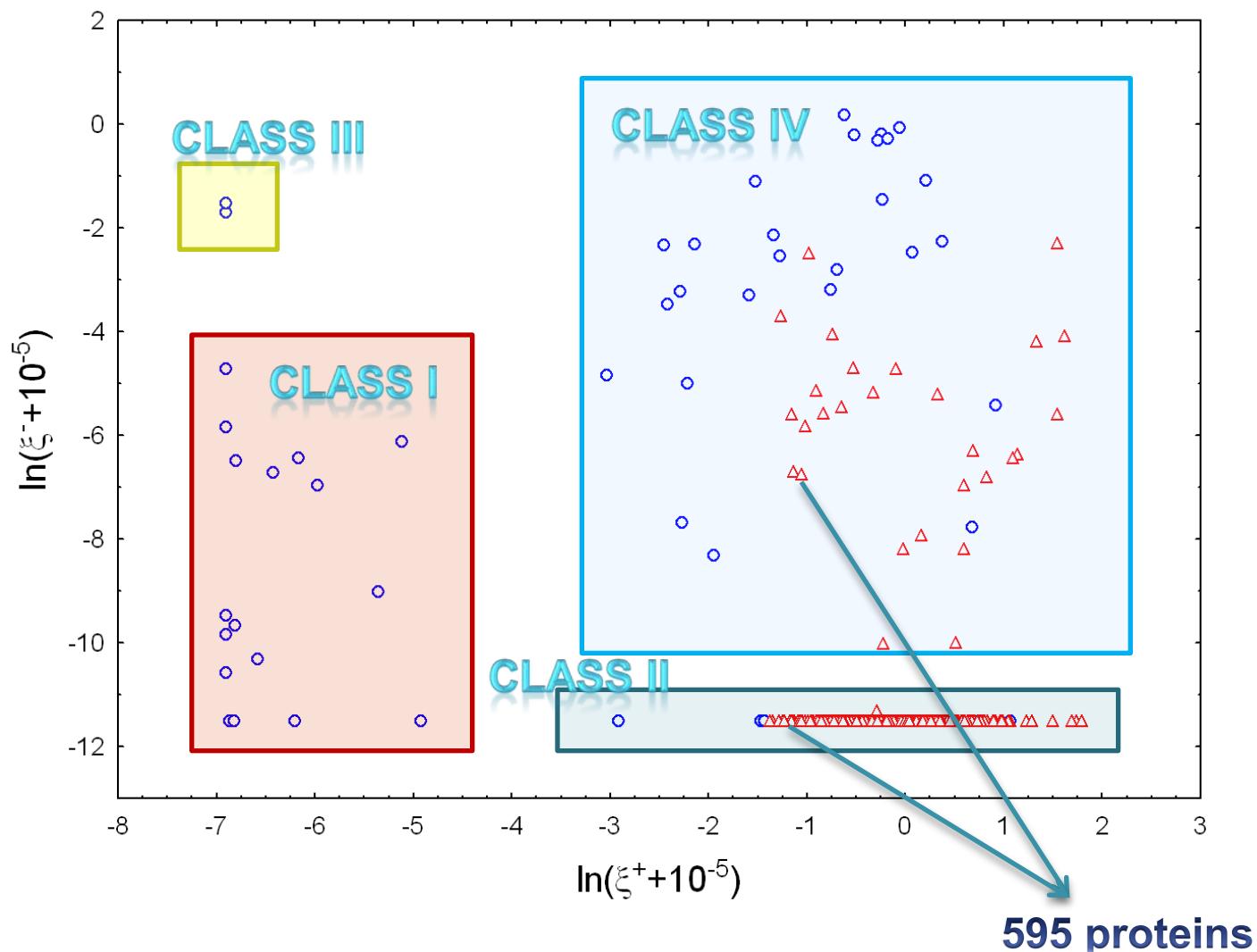
$$H(x > 0) = 1$$

$$H(x \leq 0) = 0$$

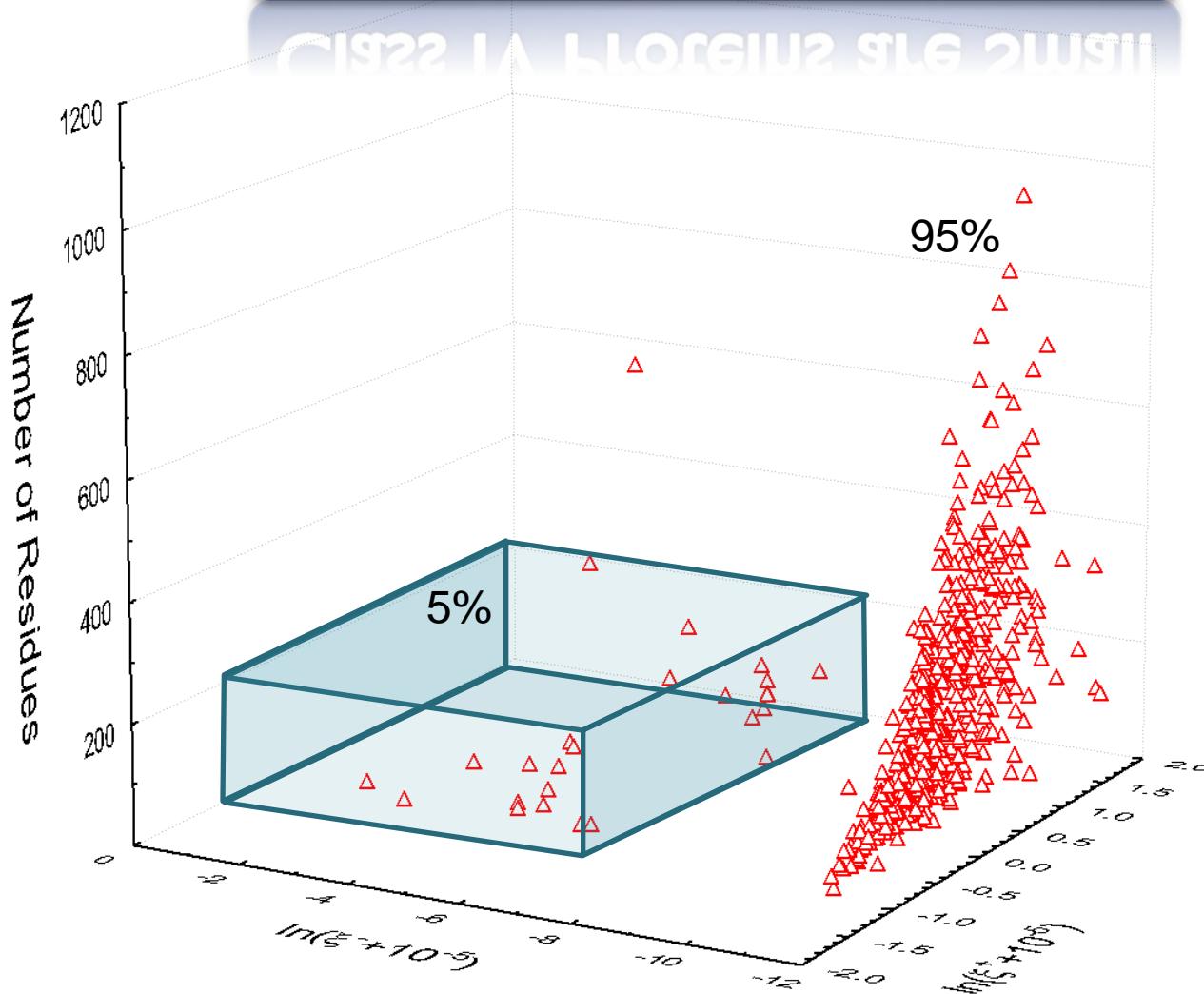


PROTEIN RESIDUE NETWORK
PROTEIN RESIDUE NETWORK

A Universal Class for Protein Networks?

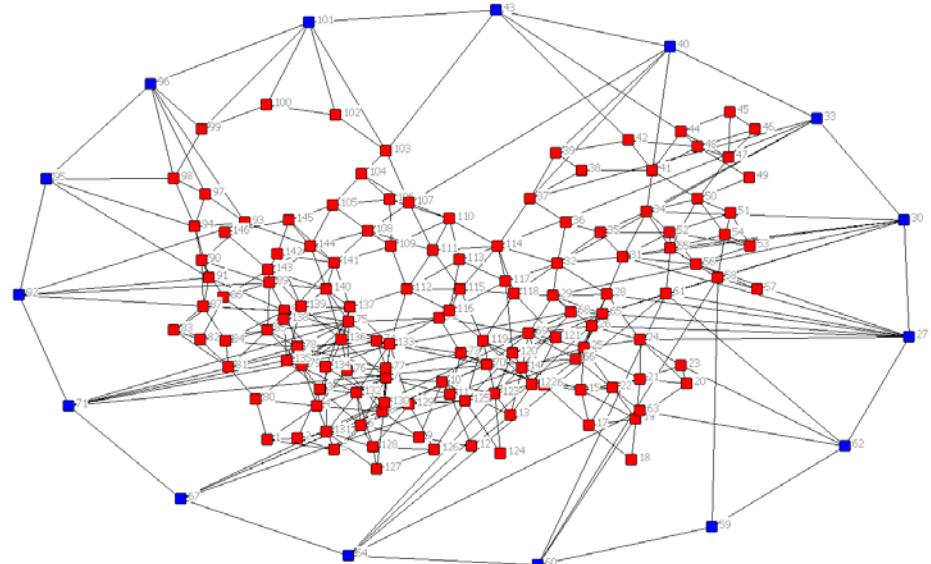


Class IV Proteins are Small

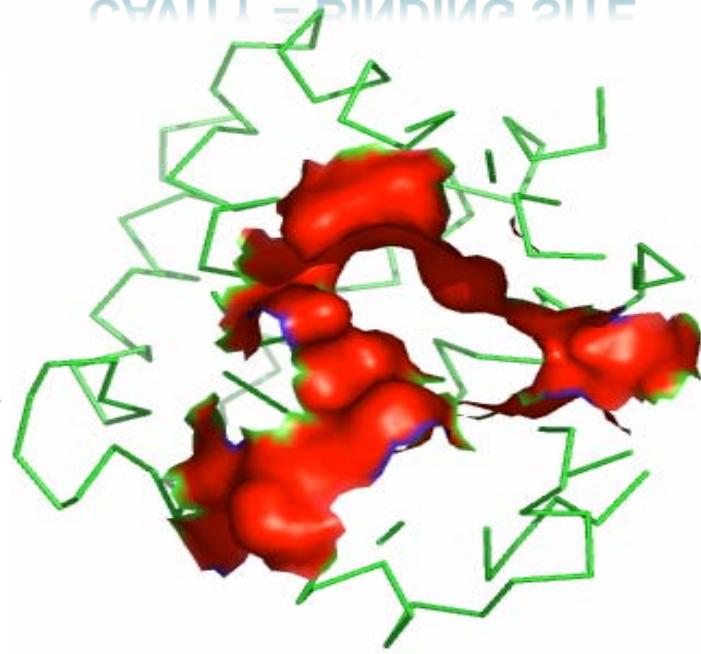


Holes in Proteins

CHORDLESS 15-CYCLE



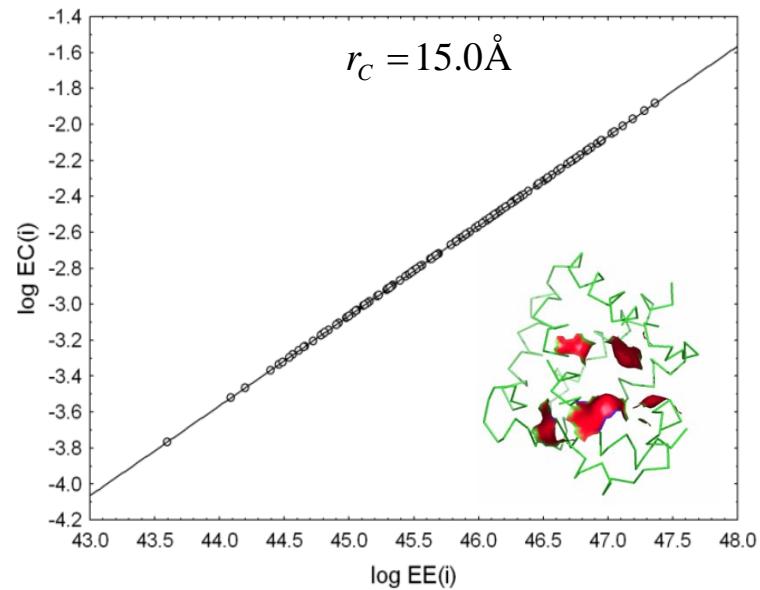
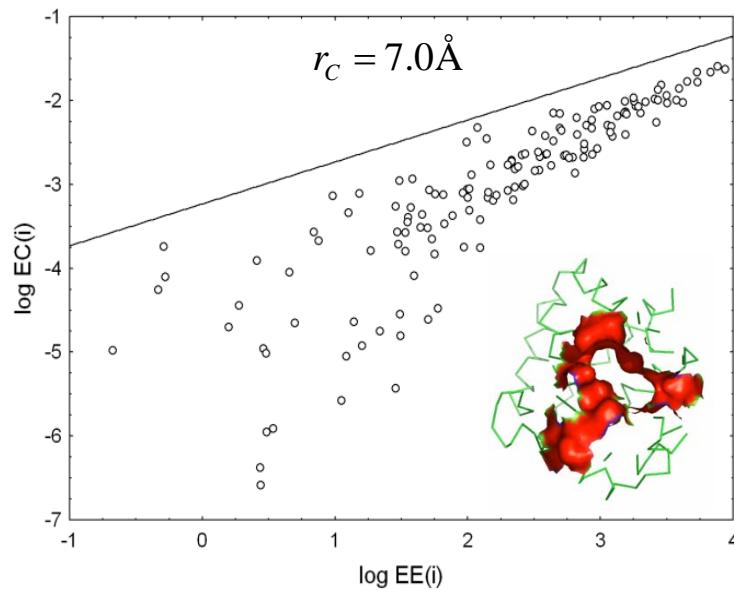
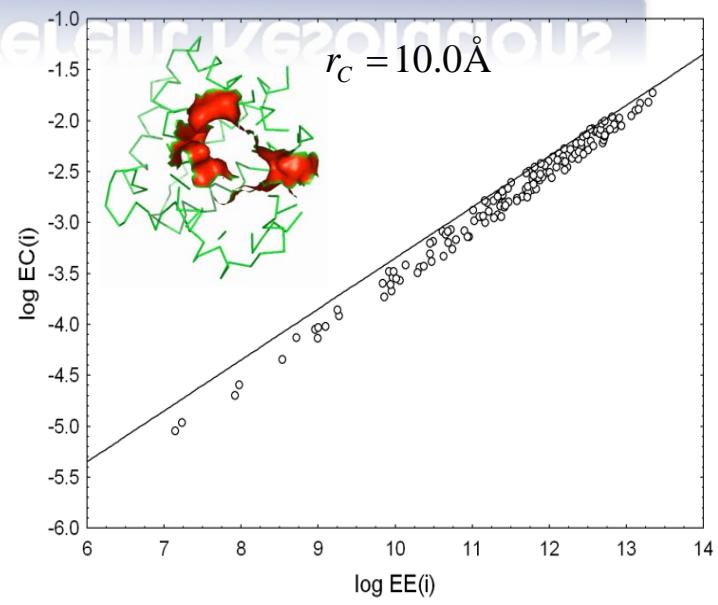
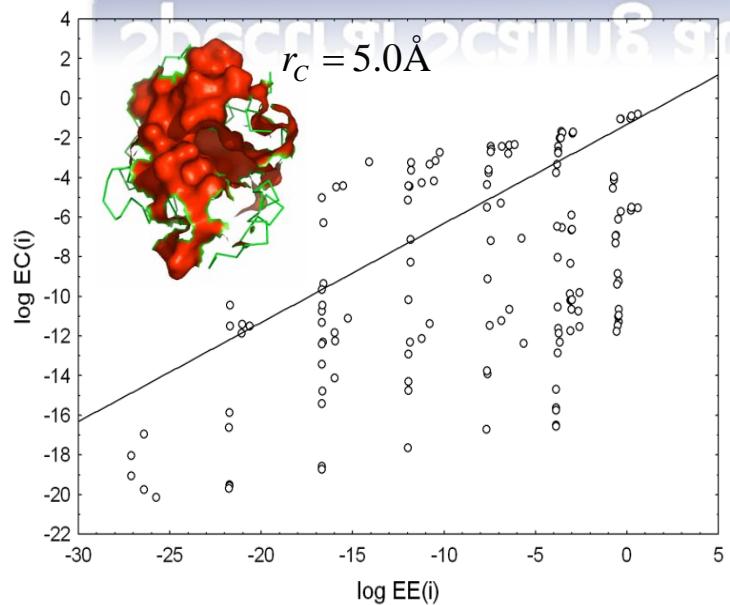
CAVITY = BINDING SITE



NODE VS. AMINO ACIDS IN BINDING SITES

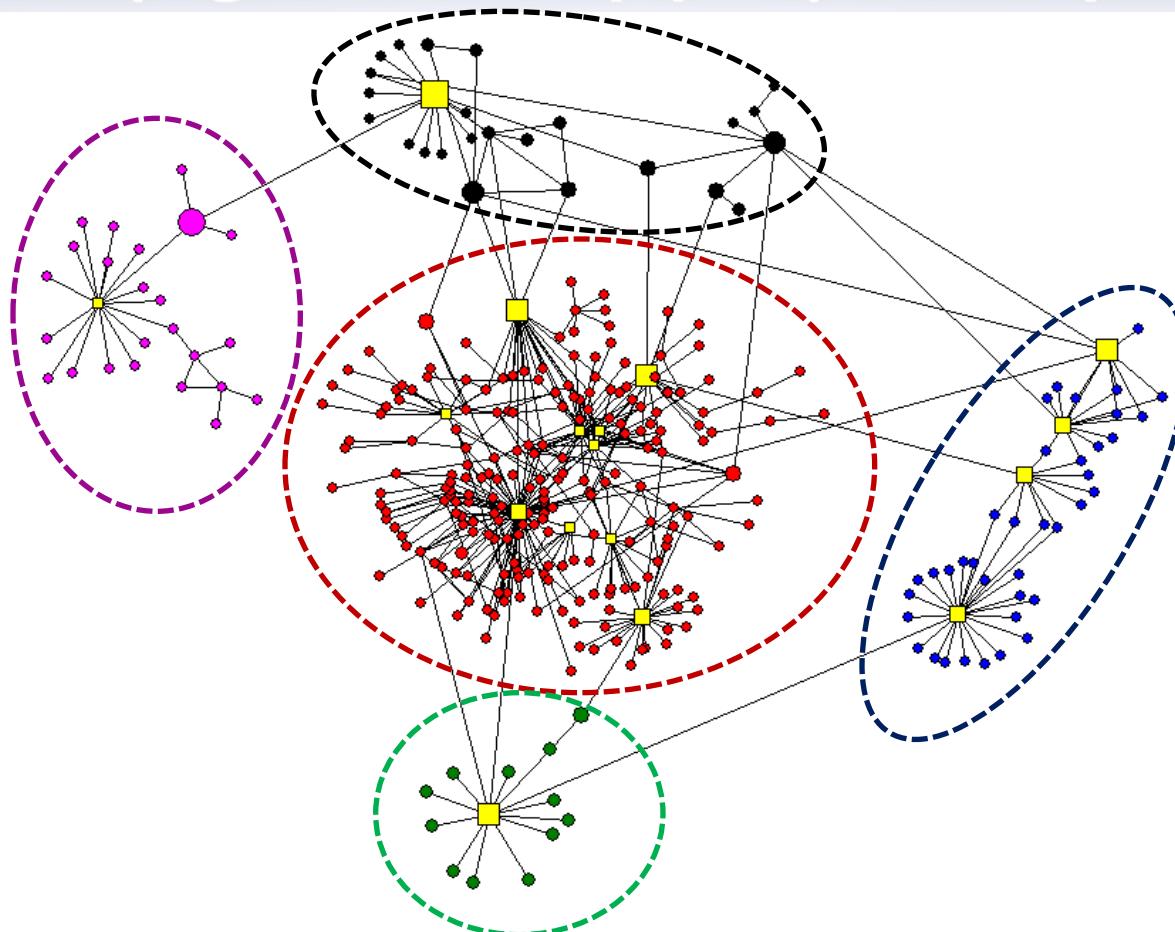
| | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|
| 30 | 33 | 40 | 43 | 44 | 60 | 64 | 67 | 68 | 71 | 95 | 96 | 101 | 103 | 108 | 140 |
| 27 | 30 | 33 | 40 | 43 | 59 | 60 | 62 | 64 | 67 | 71 | 92 | 95 | 96 | 101 | |

Spectral Scaling at Different Resolutions



Can we Identify Network Communities? A Communicability Approach

A Communicability Approach



Communicability: Definition

E. Estrada and N. Hatano: Phys. Rev. E 77, 036111 (2008)

$$G_{pq} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} (\# \text{ of walks in } n \text{ steps})$$

$$= \sum_{n=0}^{\infty} \frac{(\mathbf{A}^n)_{pq}}{n!} = (e^{\mathbf{A}})_{pq}$$

$$G_{pq} = (e^{\mathbf{A}})_{pq} = \sum_{\mu=1}^N e^{\lambda_\mu} \varphi_\mu(p) \varphi_\mu(q)$$

Eigenvector Expansion

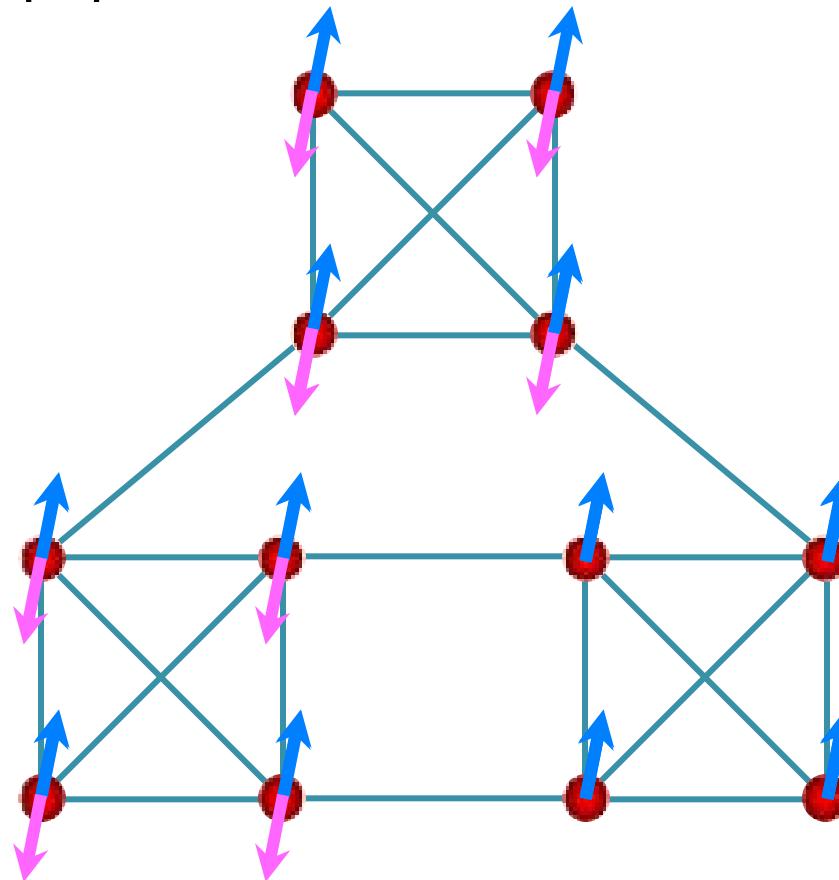
E. Estrada and N. Hatano: Phys. Rev. E 77, 036111 (2008)

$$G_{pq} = \left(e^{\mathbf{A}} \right)_{pq} = \sum_{\mu=1}^N e^{\lambda_\mu} \phi_\mu(p) \phi_\mu(q)$$

$$\begin{aligned} G_{pq} = & \phi_1(p) \phi_1(q) e^{\lambda_1} + \sum_{j \geq 2}^{++} \phi_j(p) \phi_j(q) e^{\lambda_j} + \sum_{j \geq 2}^{--} \phi_j(p) \phi_j(q) e^{\lambda_j} \\ & + \sum_{j \geq 2}^{+-} \phi_j(p) \phi_j(q) e^{\lambda_j} + \sum_{j \geq 2}^{-+} \phi_j(p) \phi_j(q) e^{\lambda_j} \end{aligned}$$

Eigenvector Expansion

$\phi_3(p)$ for $\lambda_B = 2.054093 \square$



Eigenvector Expansion

$$G_{pq} = \overbrace{\phi_1(p)\phi_1(q)e^{\lambda_1}}^A + \underbrace{\sum_{j \geq 2}^{++} \phi_j(p)\phi_j(q)e^{\lambda_j}}_B + \overbrace{\sum_{j \geq 2}^{--} \phi_j(p)\phi_j(q)e^{\lambda_j}}_C + \underbrace{\sum_{j \geq 2}^{+-} \phi_j(p)\phi_j(q)e^{\lambda_j}}_C + \underbrace{\sum_{j \geq 2}^{-+} \phi_j(p)\phi_j(q)e^{\lambda_j}}_C$$

- A. Translational motion
- B. Intra-cluster communicability
- C. Inter-cluster communicability

Communities

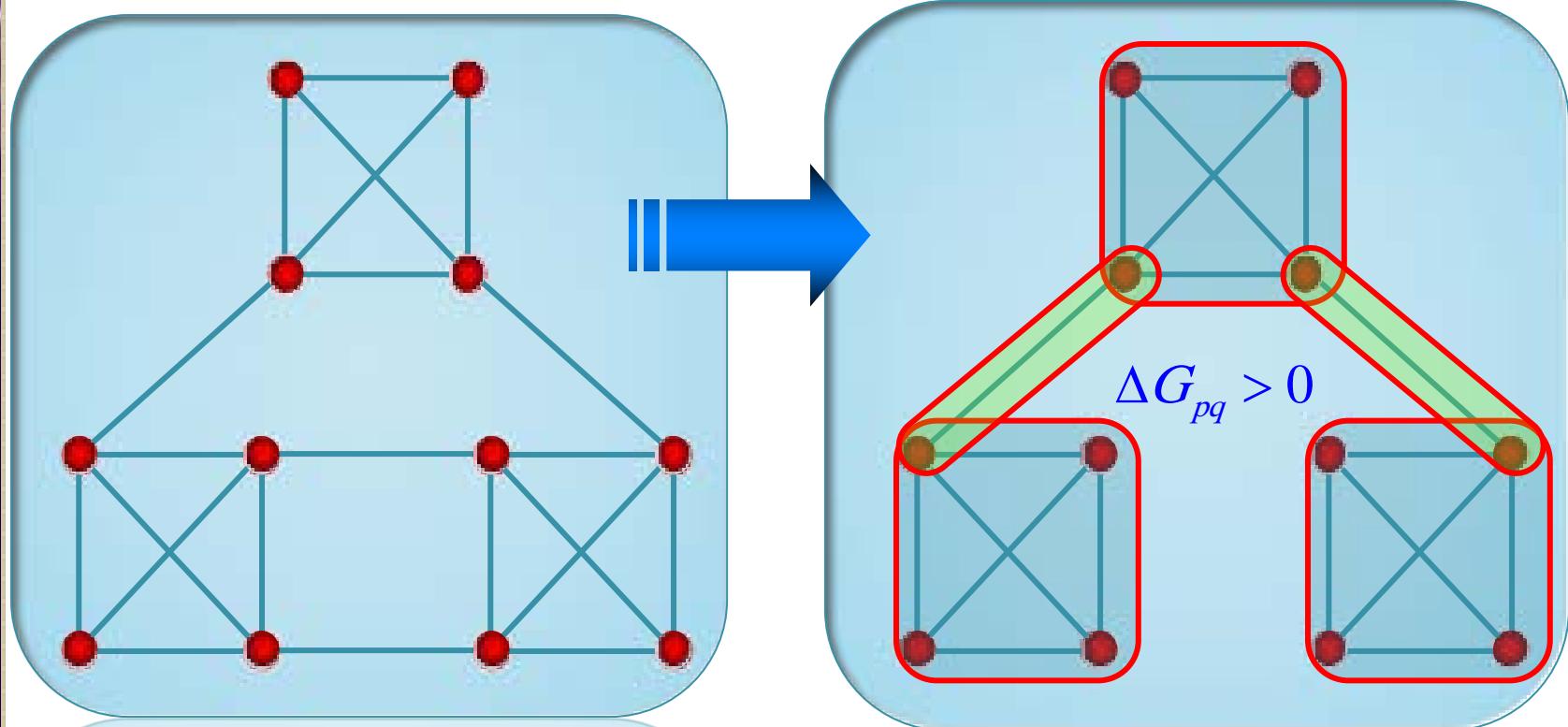
COMMUNICABILITY

$$\Delta G_{pq} = \sum_{j \geq 2}^{\text{intra-cluster}} \varphi_j(p) \varphi_j(q) e^{\lambda_j} + \sum_{j \geq 2}^{\text{inter-cluster}} \varphi_j(p) \varphi_j(q) e^{\lambda_j}$$

Community: group of nodes for which the *intracluster* communicability is larger than the *intercluster* one.

Communicability Graph

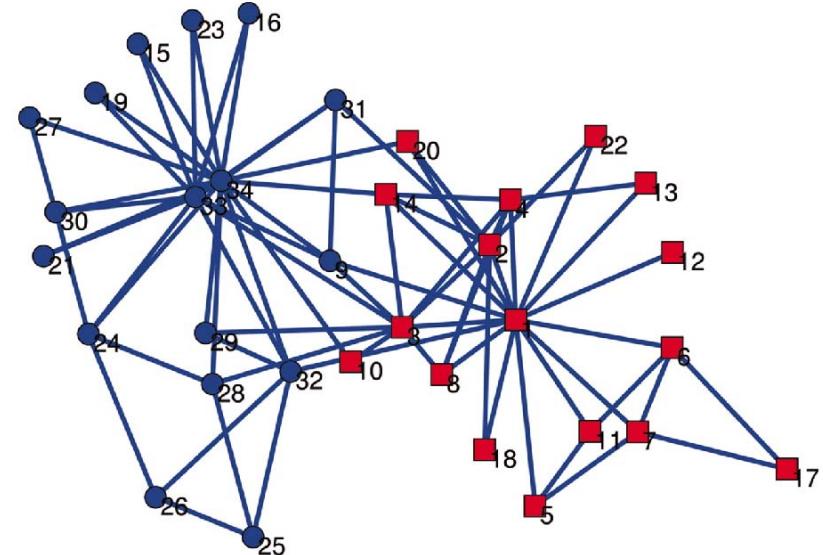
E. Estrada and N. Hatano: Appl. Math. Comp. 214, 2009, 500-511.



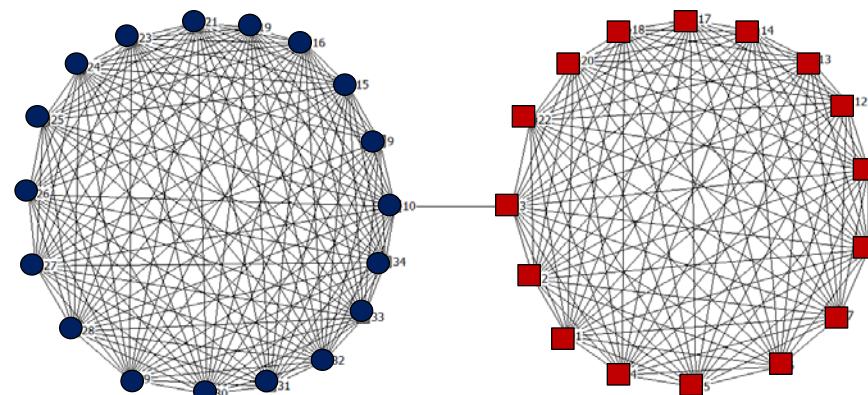
Social Communities

SOCIAL COMMUNITIES

Karate Club

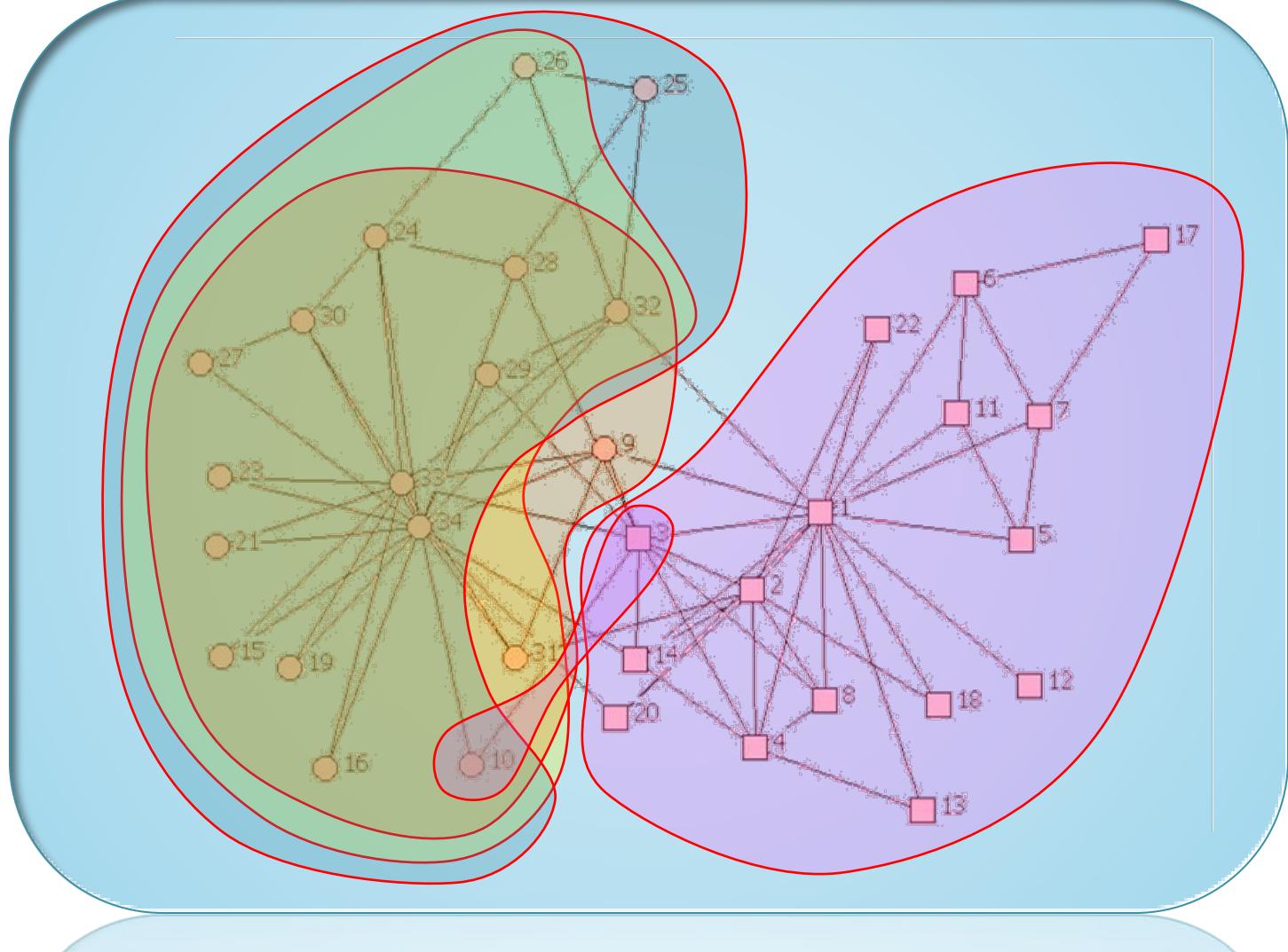


Communicability graph

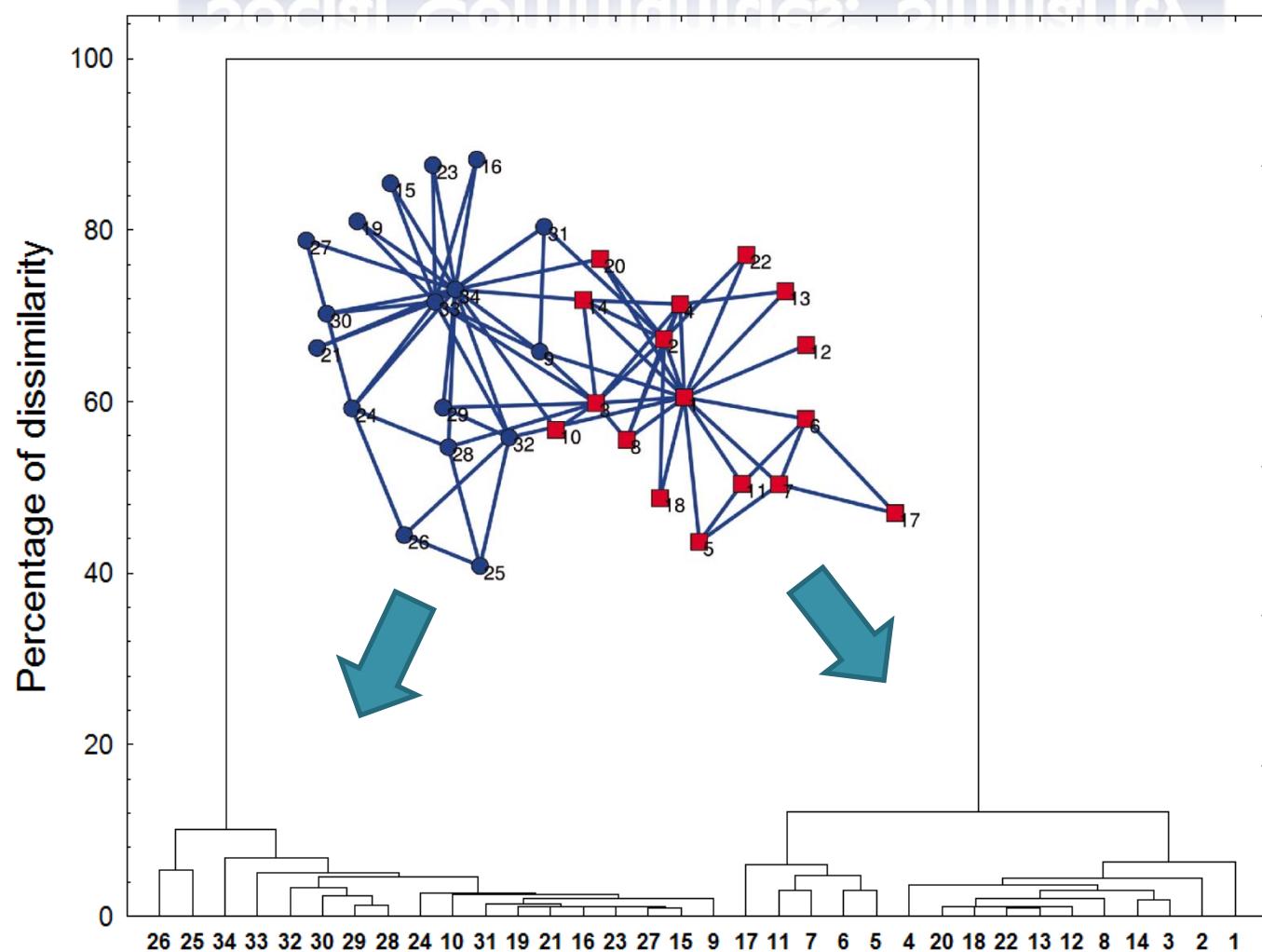


Social Communities: All-cliques

Social Communities: All-cliques



Social Communities: Similarity

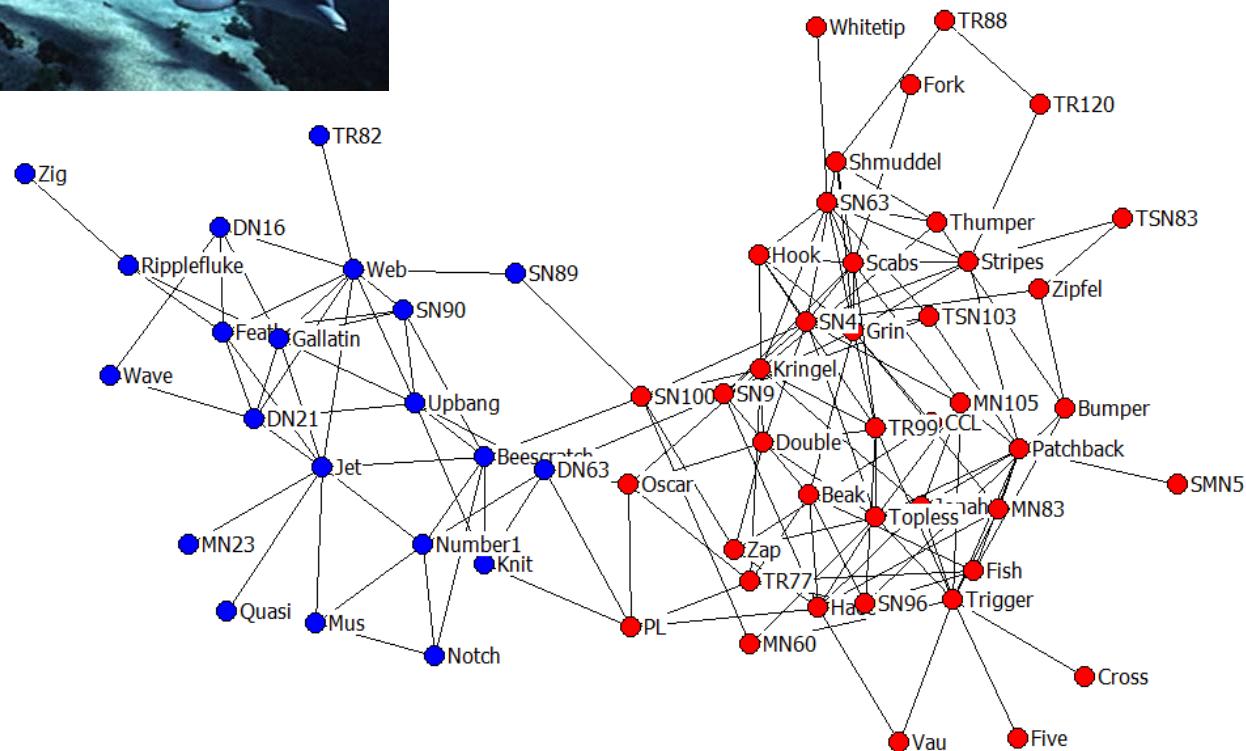


Animal Communities

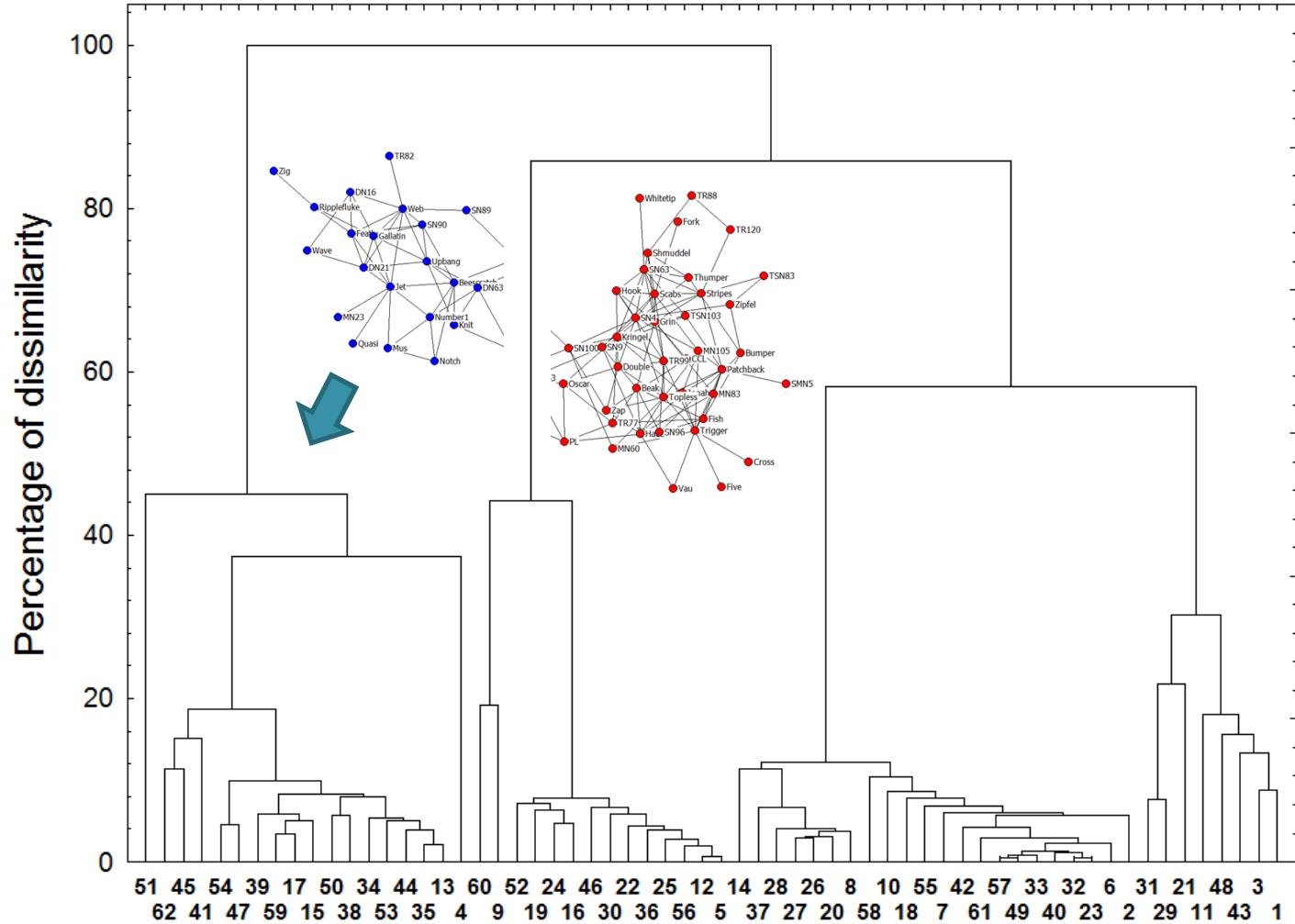
Bottlenose dolphins



Network

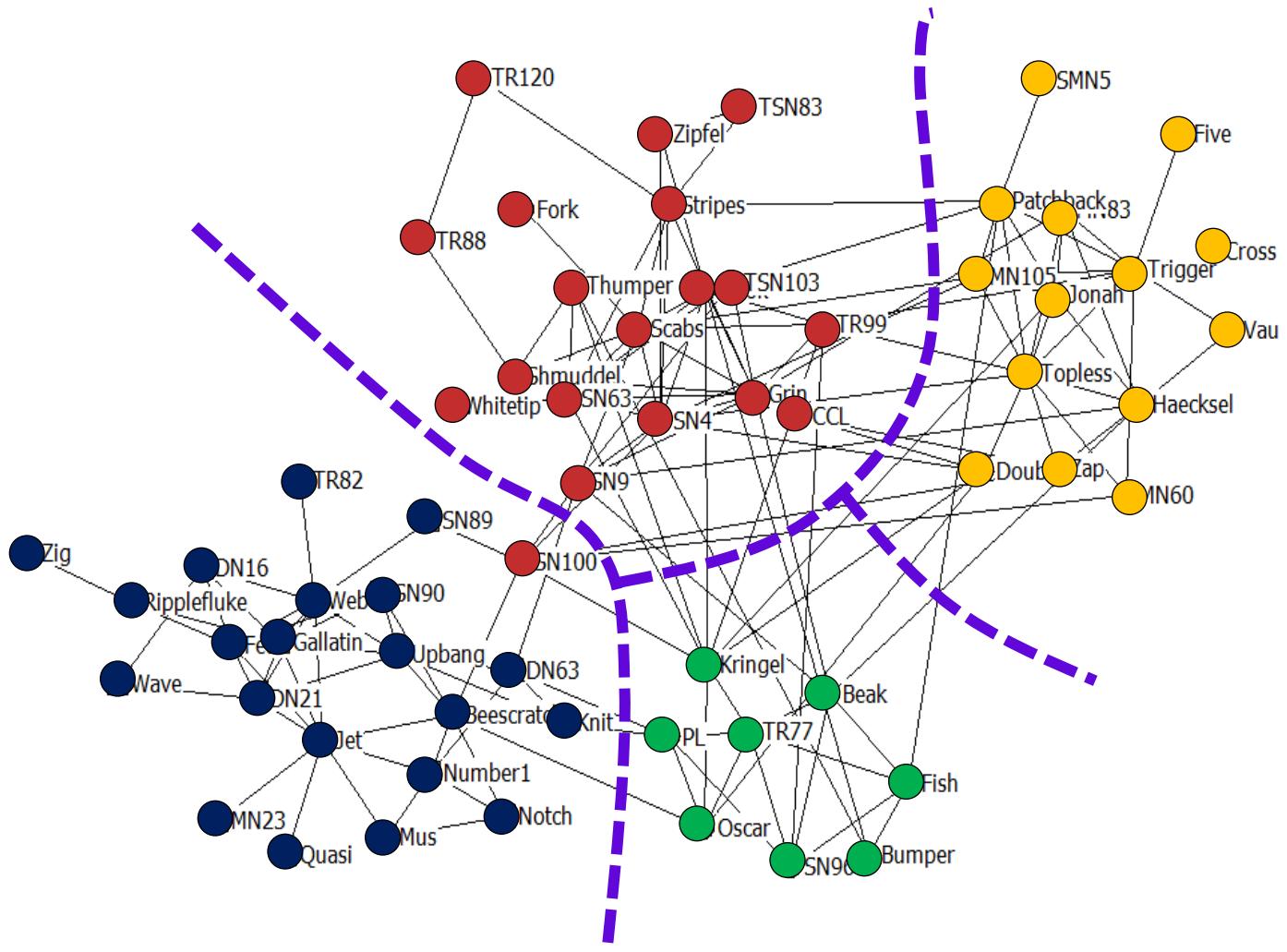


Dolphin Communities



Dolphin Communities

Dolphin Communities



Variable Temperature

Thermal Green's function

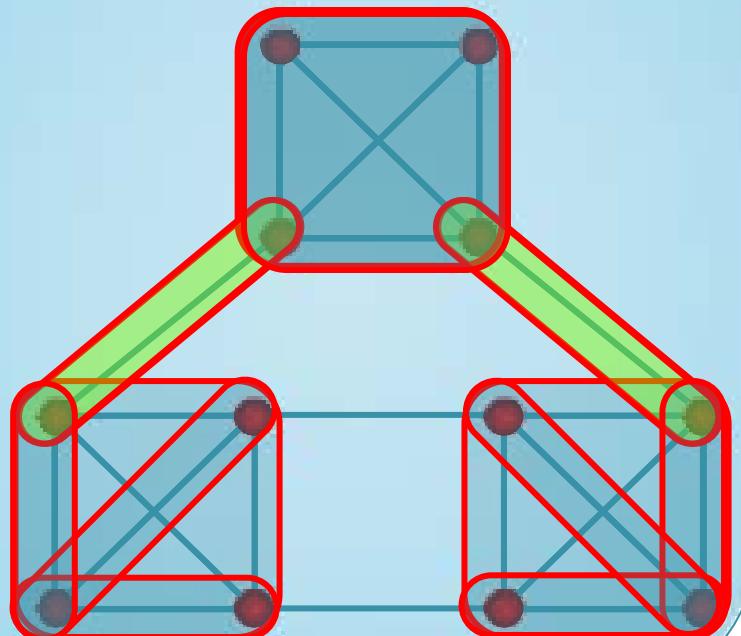
$$G_{pq}(\beta) = \left(e^{\beta A} \right)_{pq} = \sum_{\mu=1}^N e^{\beta \lambda_\mu} \varphi_\mu(p) \varphi_\mu(q)$$

$$\begin{aligned} \Delta G_{pq}(\beta) &= \sum_{\mu=2}^N e^{\beta \lambda_\mu} \varphi_\mu(p) \varphi_\mu(q) \\ &= (\Sigma^{++} + \Sigma^{--} - \Sigma^{+-} - \Sigma^{-+}) e^{\beta \lambda_\mu} |\varphi_\mu(p) \varphi_\mu(q)| \end{aligned}$$

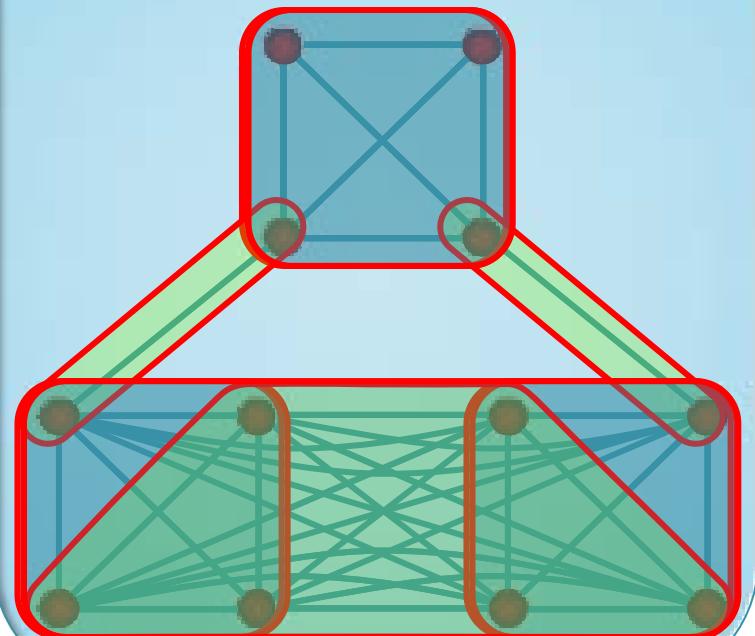
Variable Temperature

AUDIO: Jamboree

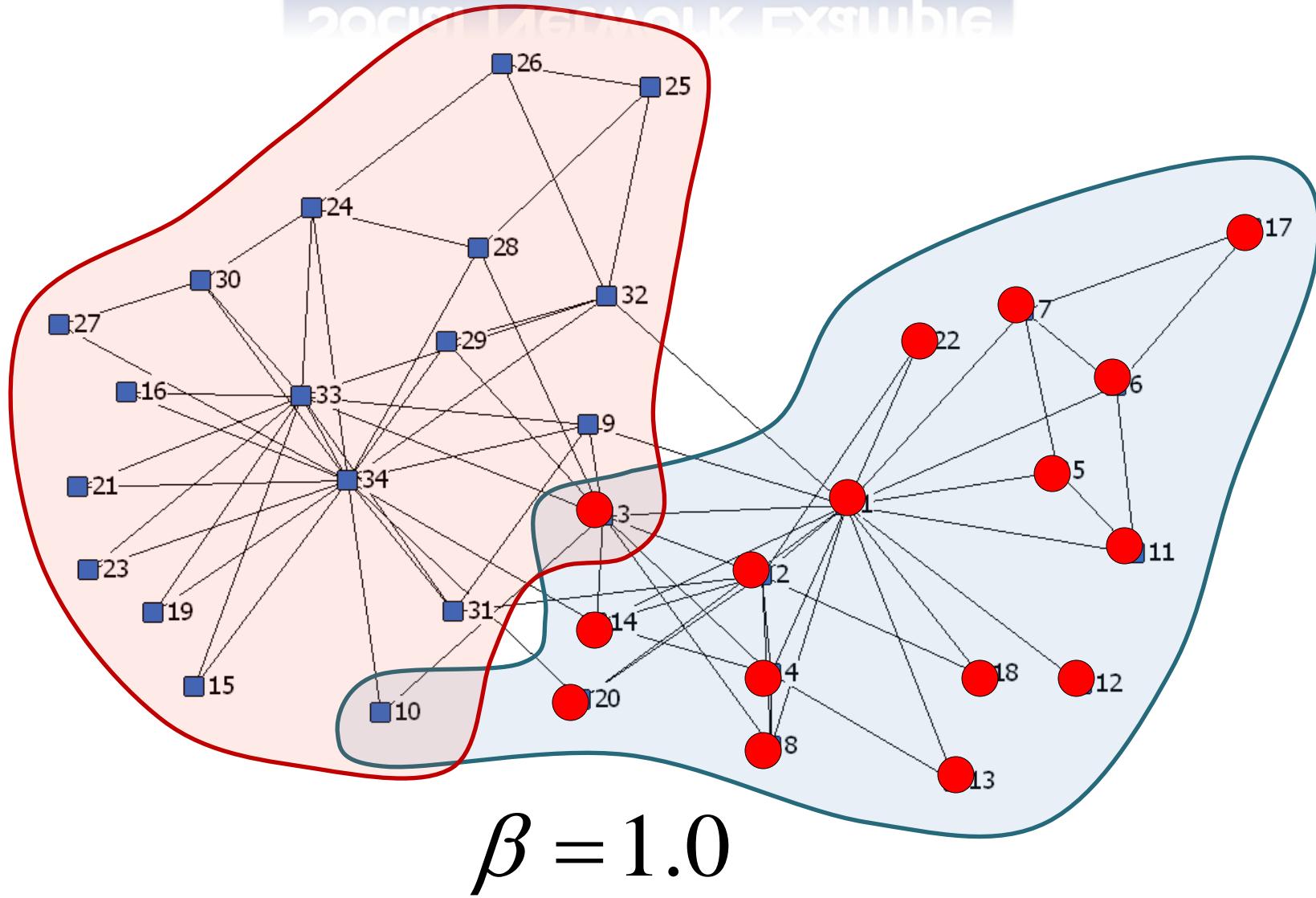
$\beta=0.15$



$\beta=200$

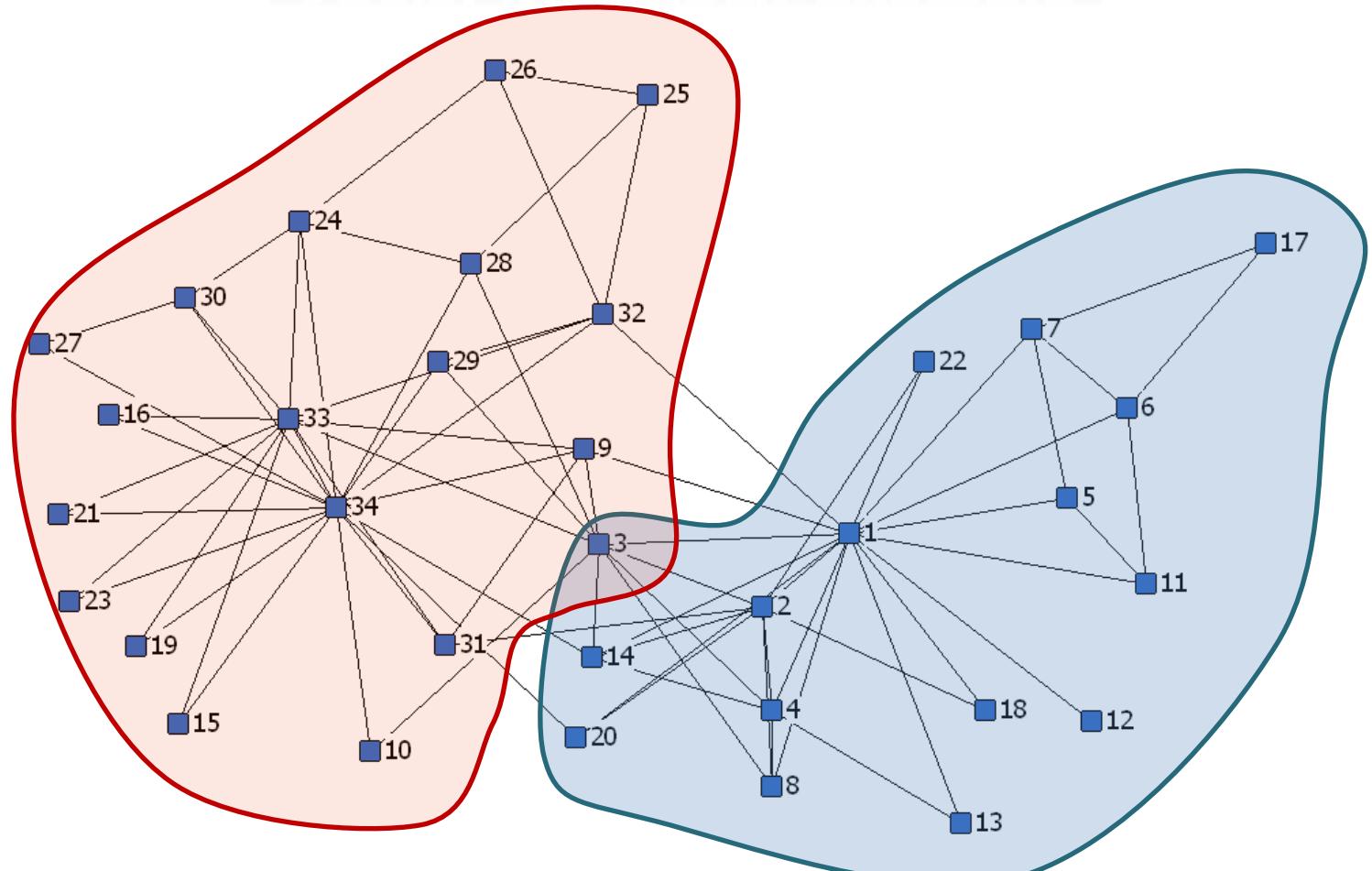


Social Network Example



Social Network Example

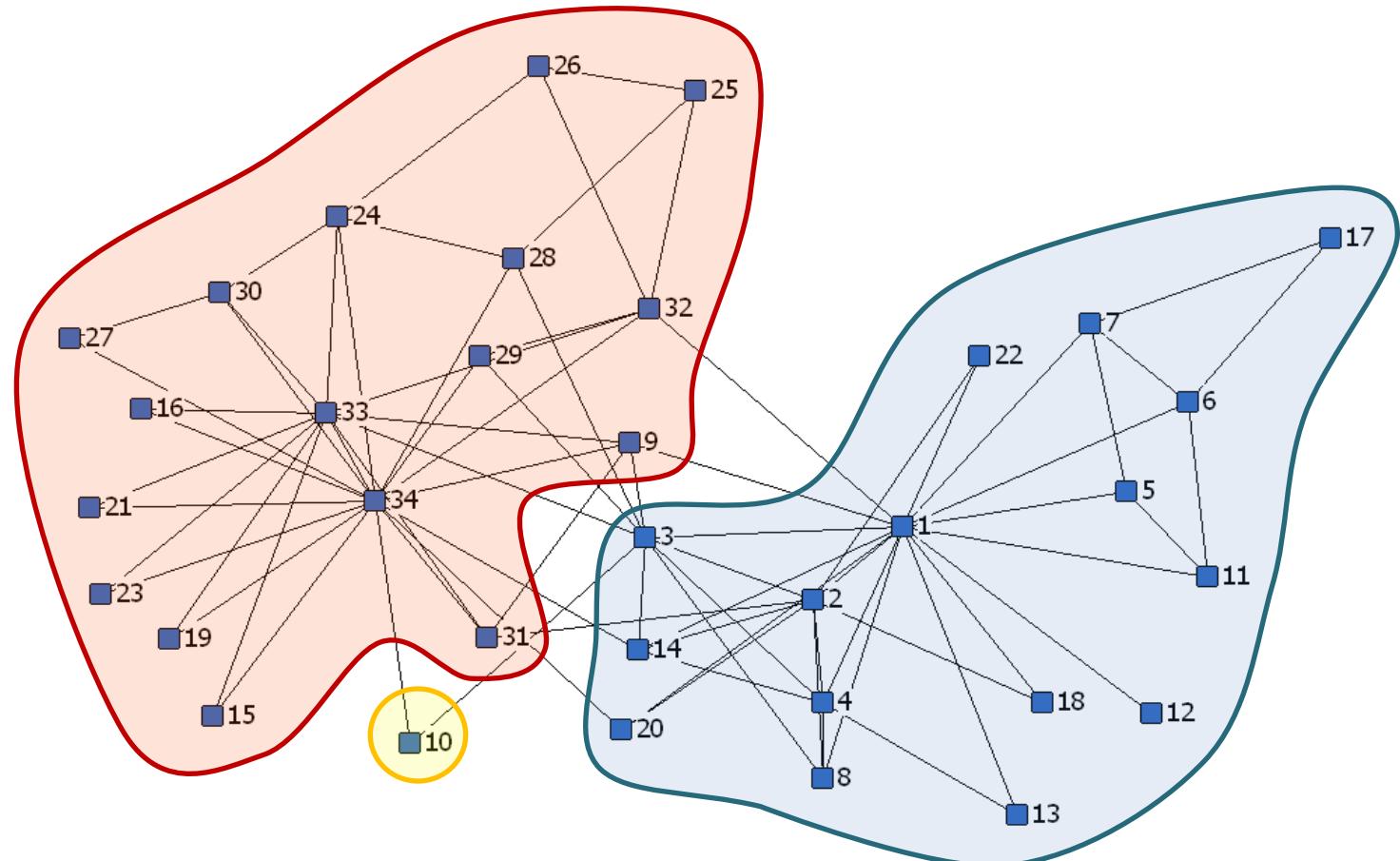
SOCIAL NETWORK EXAMPLE



$$\beta = 0.3$$

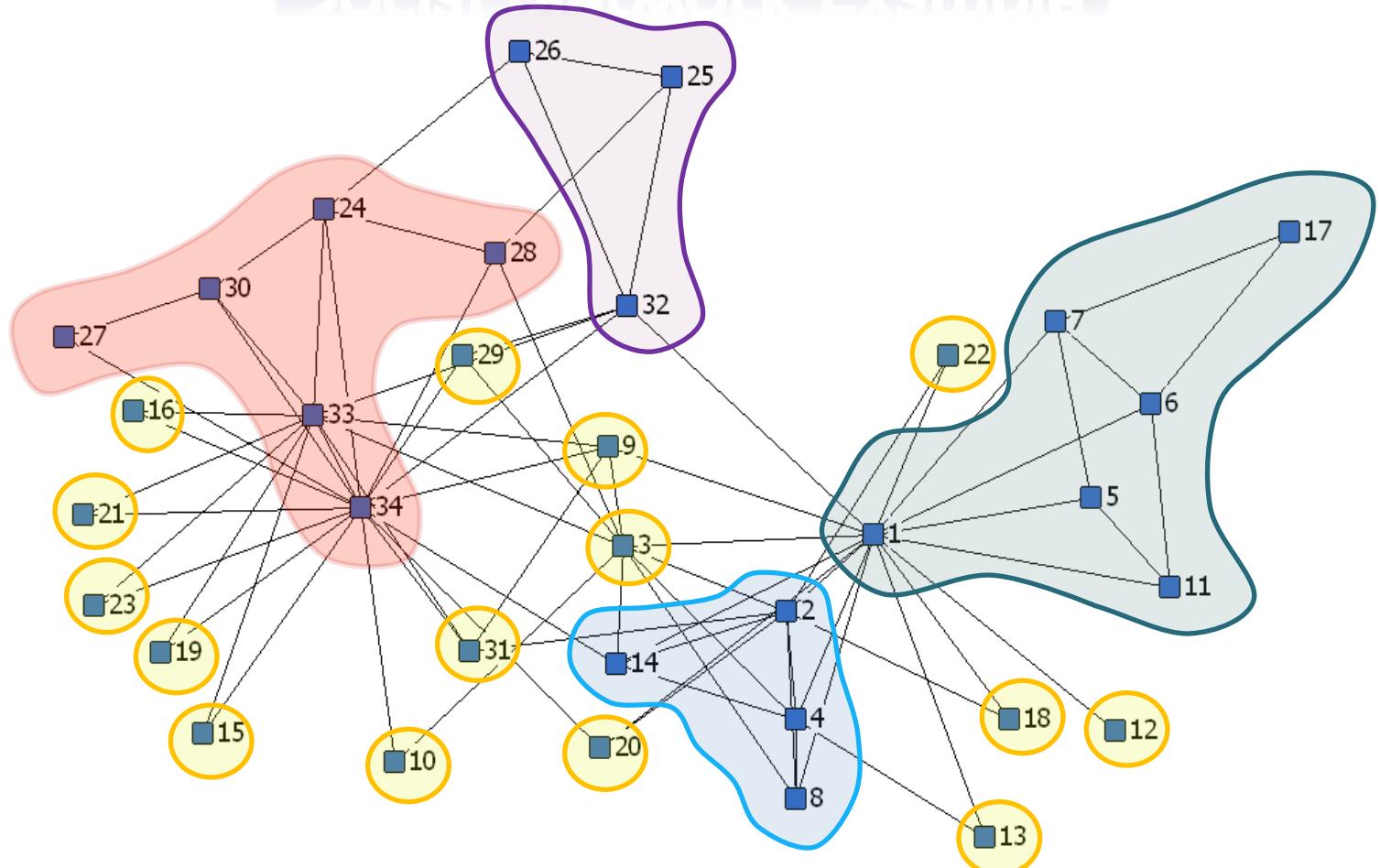
Social Network Example

SOCIAL NETWORK EXAMPLE



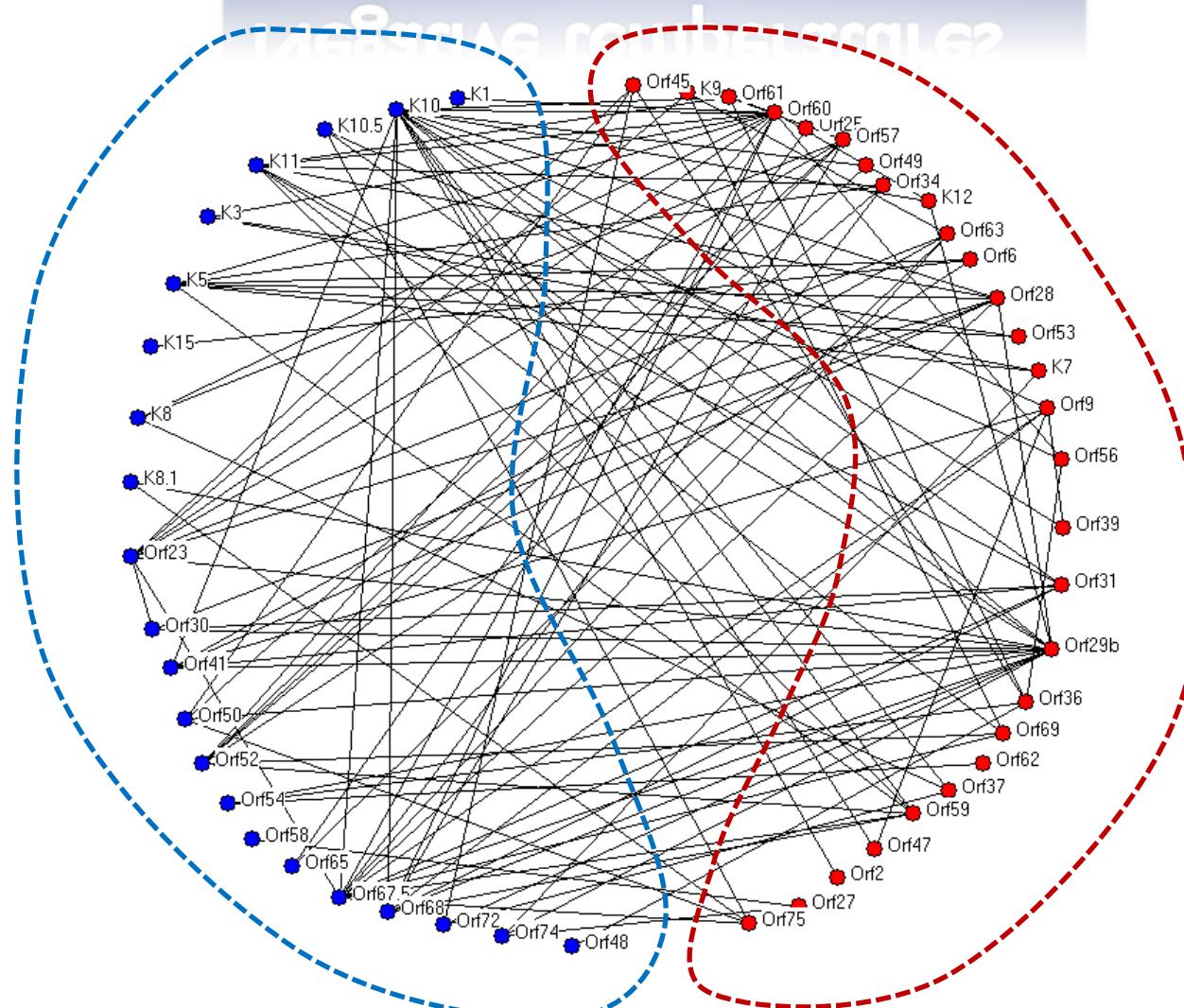
$$\beta = 0.2$$

Social Network Example



$$\beta = 0.1$$

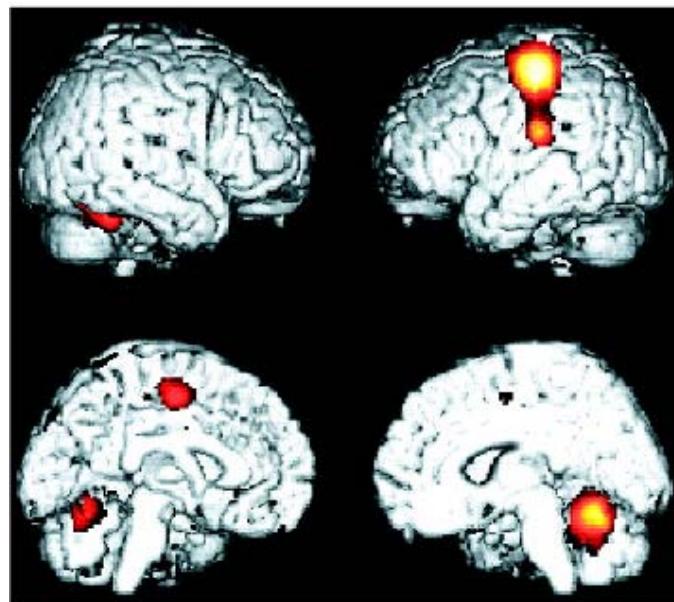
Negative temperatures



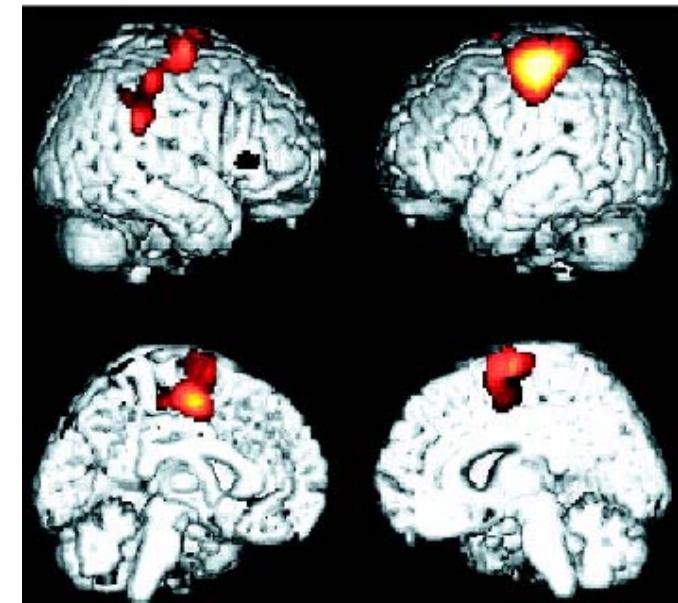
Estrada, Higham and Hatano: Phys. Rev. E 78, 2008, 026102

Communicability as a Classifier

Communicability as a Classifier
Healthy



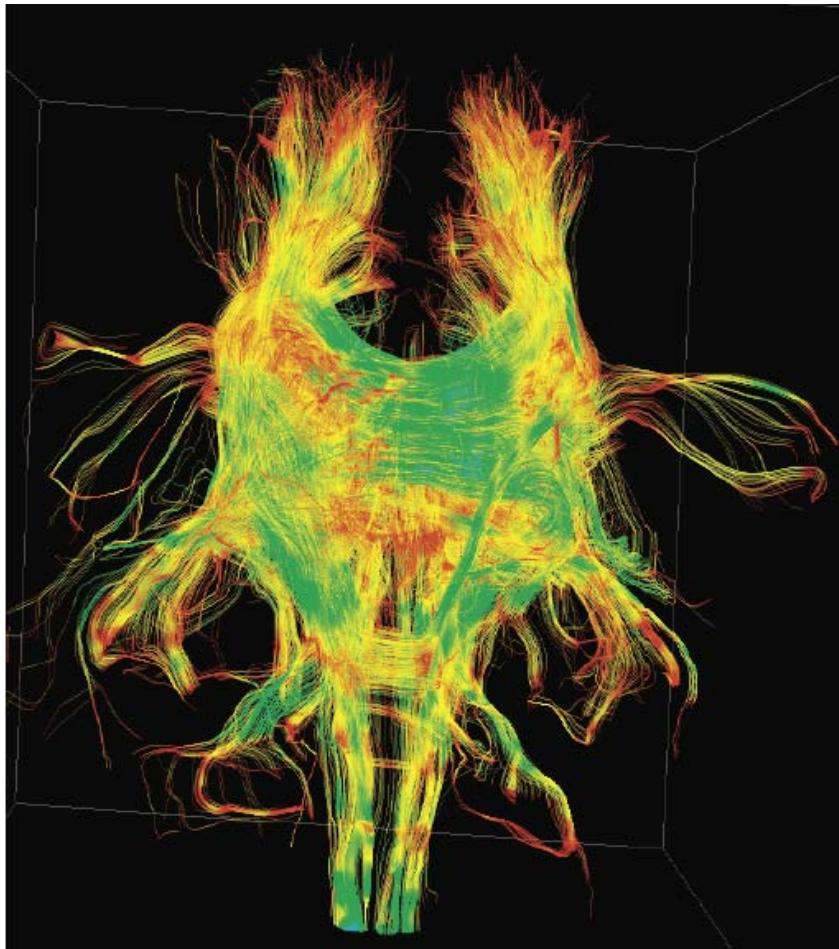
Months after Stroke



Communicability in the Brain

Communicability in the Brain

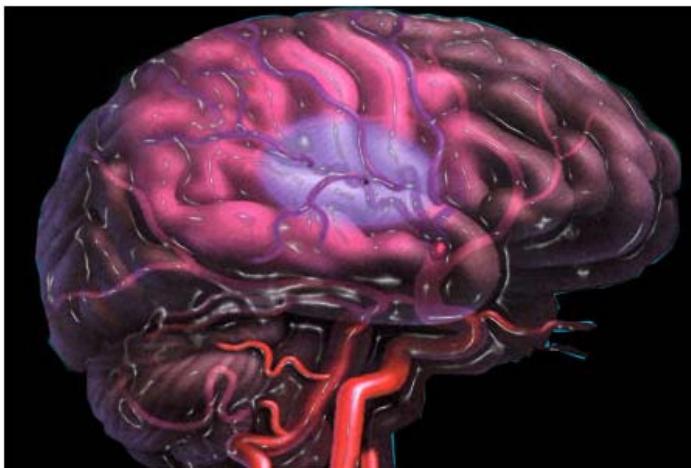
Diffusion Tractography Imaging



DTI exploits the fact that water diffusion in the brain is anisotropic; in particular diffusion along tracts is greater than diffusion across them.

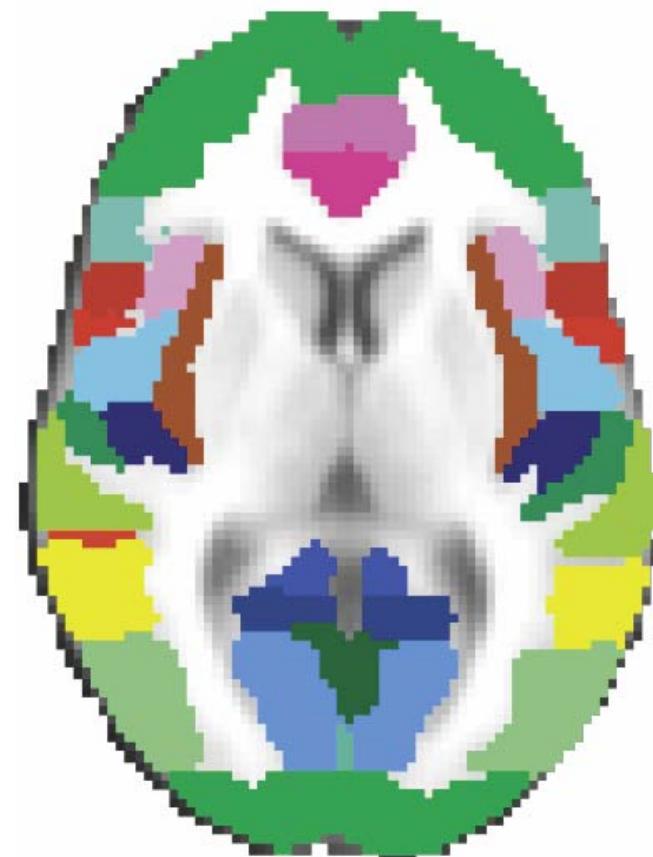
Communicability in stroked brains

- 9 subjects - suffered subcortical strokes;



- 10 controls.

- DTI computes all connections between all voxels.

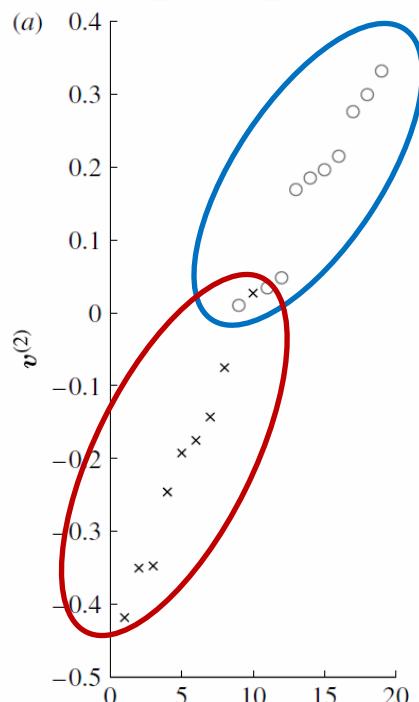


Discrimination Analysis

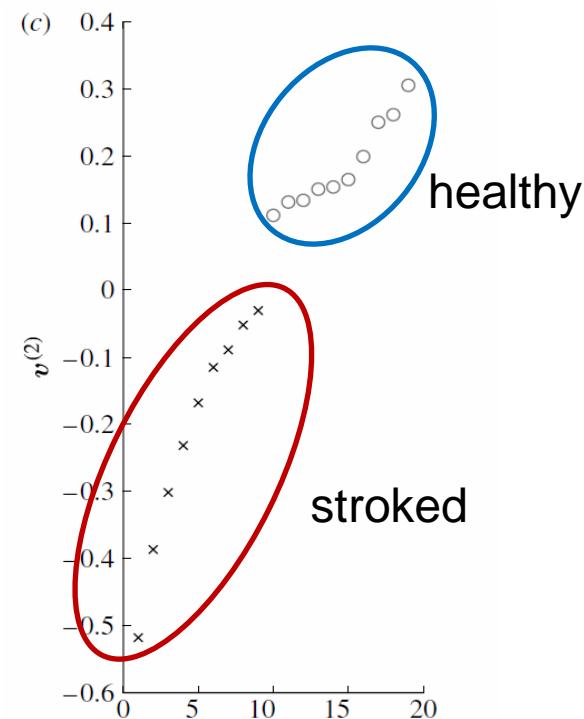
J.J. Crofts and D.H. Higham: J. Roy. Soc., Interface, 2009, 6, 411-414.

$$W = \tilde{A} = D^{-1/2} A D^{-1/2}$$

Raw Data



Communicability

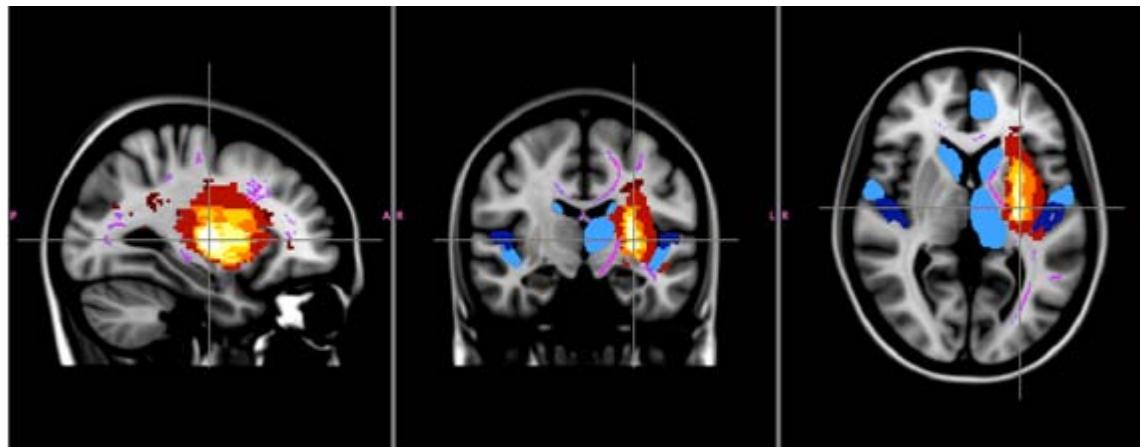


Communicability in damaged brains

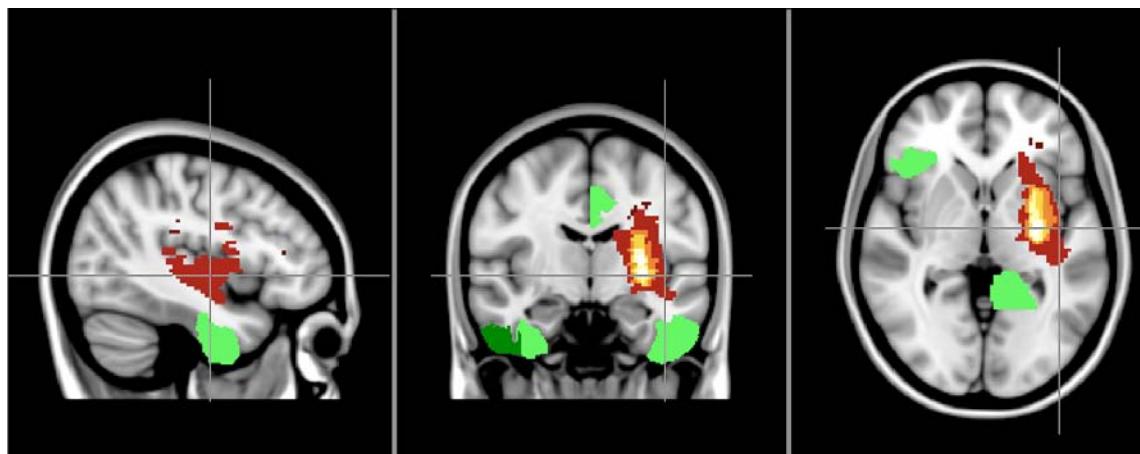
Communicability in stroke brain

J.J. Crofts et al. submitted, 2010

Red: Stroke Blue: Decreased communicability



Red: Stroke Green: Increased communicability



Images courtesy of Dr. Jonathan J. Crofts.

The End



THANK YOU!

More info at:

www.estradalab.org