University of Strathclyde

LECTURE 3: BASED ON CHAPTER 18 & 21

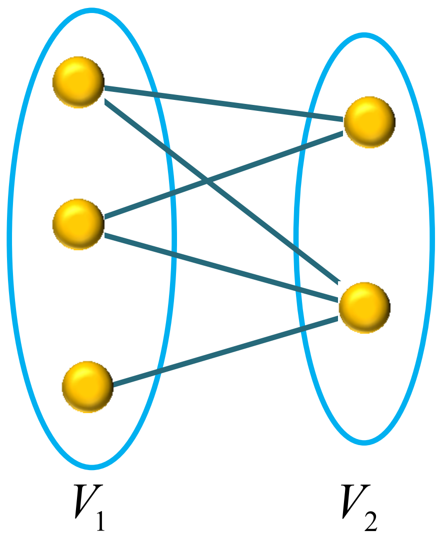
Network Bipartivity. Computational vs. Algebraic Approaches

Professor Ernesto Estrada
Department of Mathematics & Statistics
University of Strathclyde
Glasgow, UK

www.estradalab.org

Network Bipartivity

bipartite graph



$$V = V_1 \cup V_2$$

$$A = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}$$

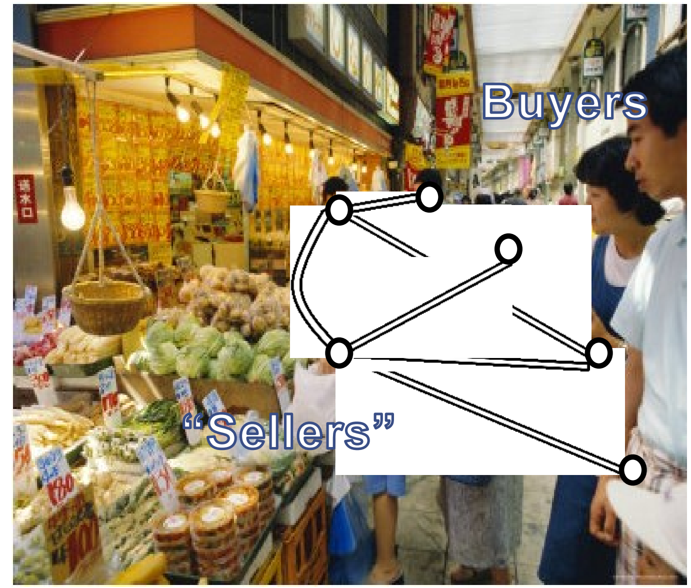
Adjacency matrix

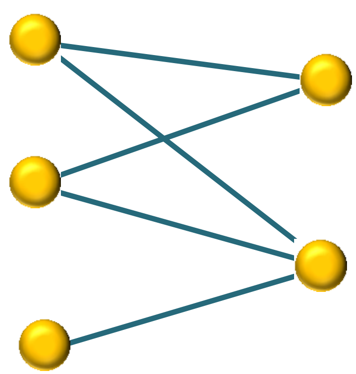
$$\lambda_j = -\lambda_{n-j+1}$$

spectrum

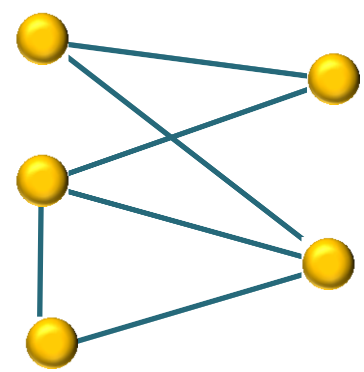
(see Chapters 2 & 5)

Network Bipartivity





Bipartite Network

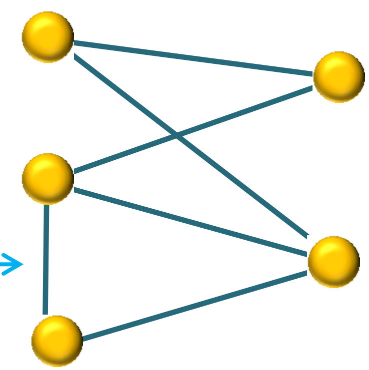


How much bipartite?

Network Bipartivity

Computational approach

$$b = 1 - \frac{m_{fr}}{m}$$



Network Bipartivity

Algebraic approach

$$Bipartivity \Leftrightarrow No\ odd\ \ cycles$$

$$Bipartivity \Leftrightarrow Tr\left(\sinh\left(A\right)\right) = 0$$

Network Bipartivity

Algebraic approach

$$Tr\left(\exp\left(A\right)\right) = Tr\left(\sinh\left(A\right)\right) + Tr\left(\cosh\left(A\right)\right)$$

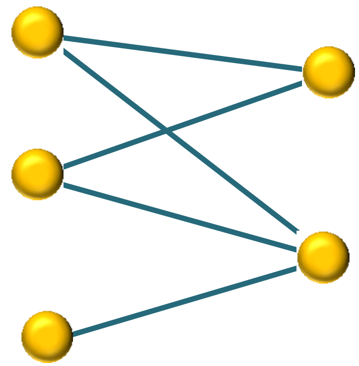
$$Bipartivity \Leftrightarrow Tr\left(\exp\left(A\right)\right) = Tr\left(\cosh\left(A\right)\right)$$

$$b_s = \frac{Tr\left(\cosh\left(A\right)\right)}{Tr\left(\exp\left(A\right)\right)} = \frac{\sum_{j=1}^{n} \cosh\left(\lambda_j\right)}{\sum_{j=1}^{n} \exp\left(\lambda_j\right)} = \frac{EE_{even}}{EE}$$

University of Strathclyde

Network Bipartivity

Algebraic approach

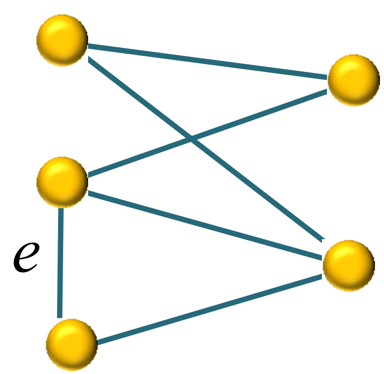


G

a contribution to even CWs

b contribution to odd CWs

$$b \geq a > 0$$



$G + e$

Network Bipartivity

Algebraic approach

$$EE_{even} = \sum_{j=1}^{n} \cosh\left(\lambda_j\right) \geq \sum_{j=1}^{n} \sinh\left(\lambda_j\right) = EE_{odd}$$

$$bEE_{even} \geq aEE_{odd}$$

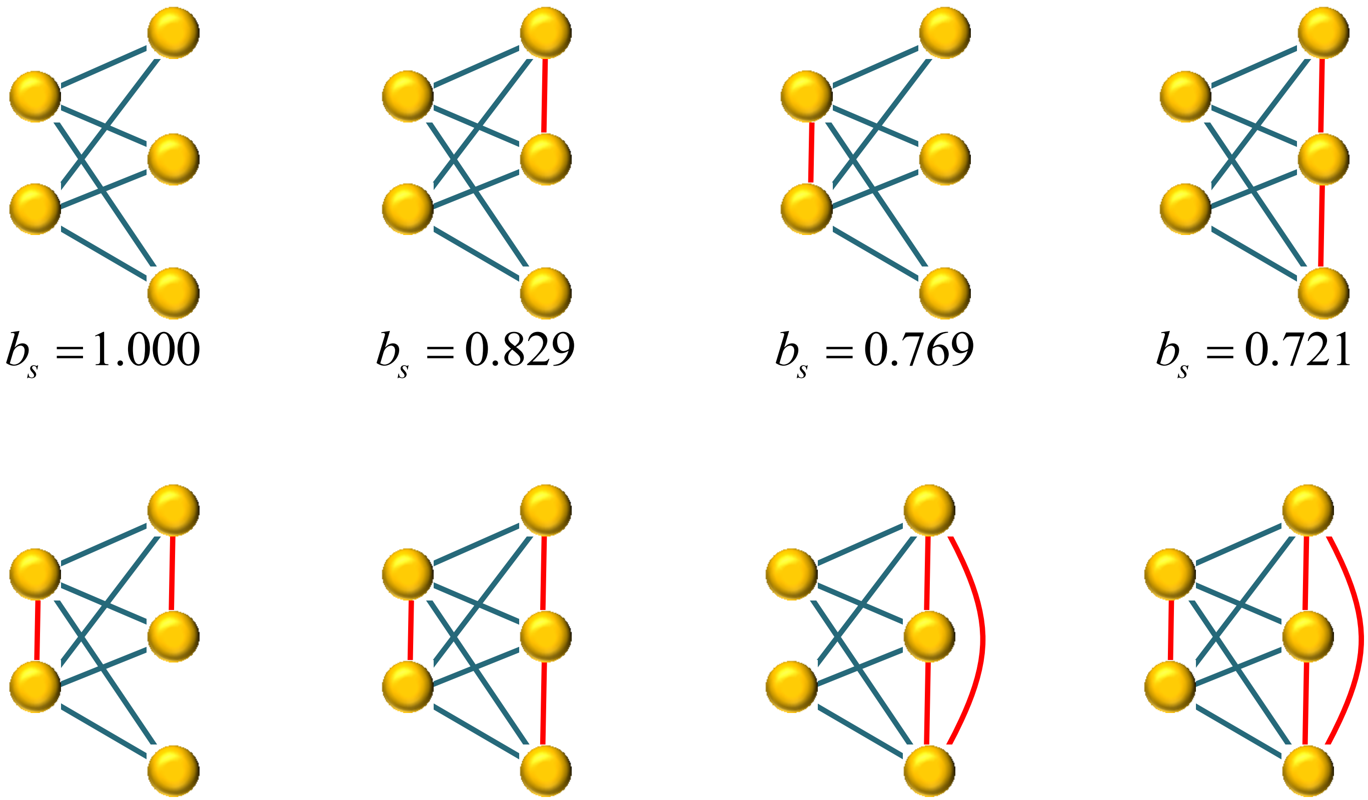
$$aEE_{even} + bEE_{even} \geq aEE_{odd} + aEE_{even}$$
$$\left(a+b\right) EE_{even} \geq aEE.$$

$$\left(a+b\right) EE_{even} + EE \cdot EE_{even} \geq aEE + EE \cdot EE_{even}$$
$$EE_{even}\left(a+b+EE\right) \geq EE\left(EE_{even} + a\right),$$

Network Bipartivity

Algebraic approach

$$b_s(G) = \frac{EE_{even}}{EE} \geq \frac{EE_{even} + a}{EE + a + b} = b_s(G + e)$$



$b_s = 1.000$ $b_s = 0.829$ $b_s = 0.769$ $b_s = 0.721$

$b_s = 0.692$ $b_s = 0.645$ $b_s = 0.645$ $b_s = 0.597$

Network Bipartivity

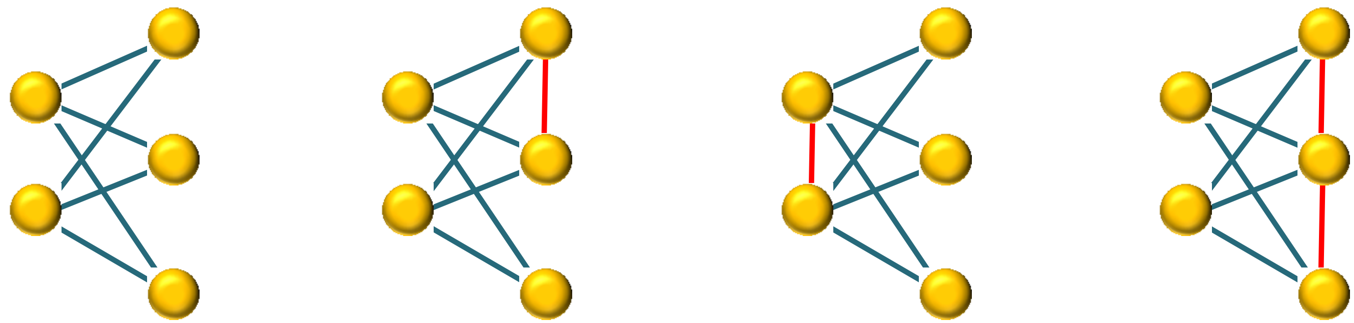
(Another) algebraic approach

$$b_e = \frac{\sum_{j=1}^{n} \cosh(\lambda_j) - \sum_{j=1}^{n} \sinh(\lambda_j)}{\sum_{j=1}^{n} \cosh(\lambda_j) + \sum_{j=1}^{n} \sinh(\lambda_j)}$$

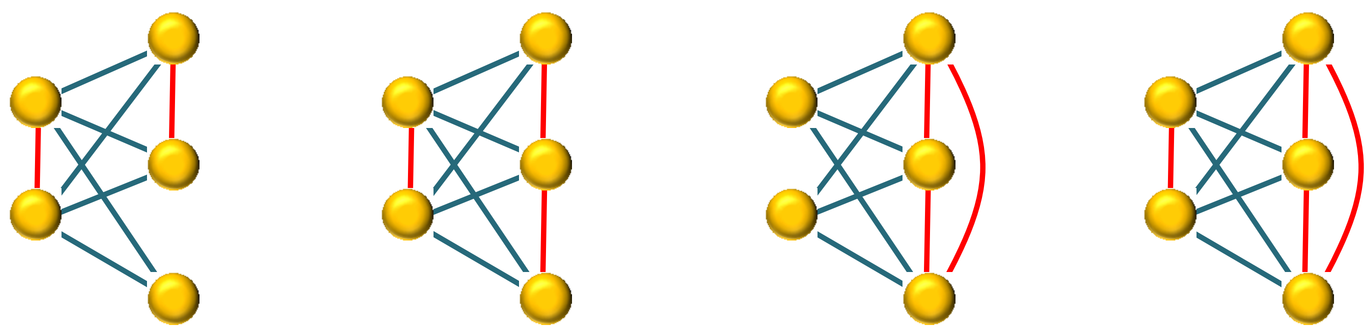
$$b_e = \frac{Tr(\exp(-A))}{Tr(\exp(A))} = \frac{\sum_{j=1}^{n} \exp(-\lambda_j)}{\sum_{j=1}^{n} \exp(\lambda_j)}$$

Network Bipartivity

(Another) algebraic approach



$b_s = 1.000$ $b_s = 0.658$ $b_s = 0.538$ $b_s = 0.462$

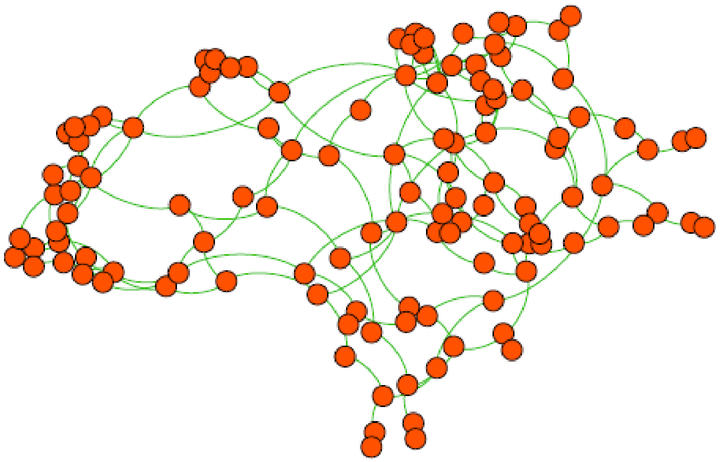


$b_s = 0.383$ $b_s = 0.289$ $b_s = 0.289$ $b_s = 0.194$

Network Bipartivity

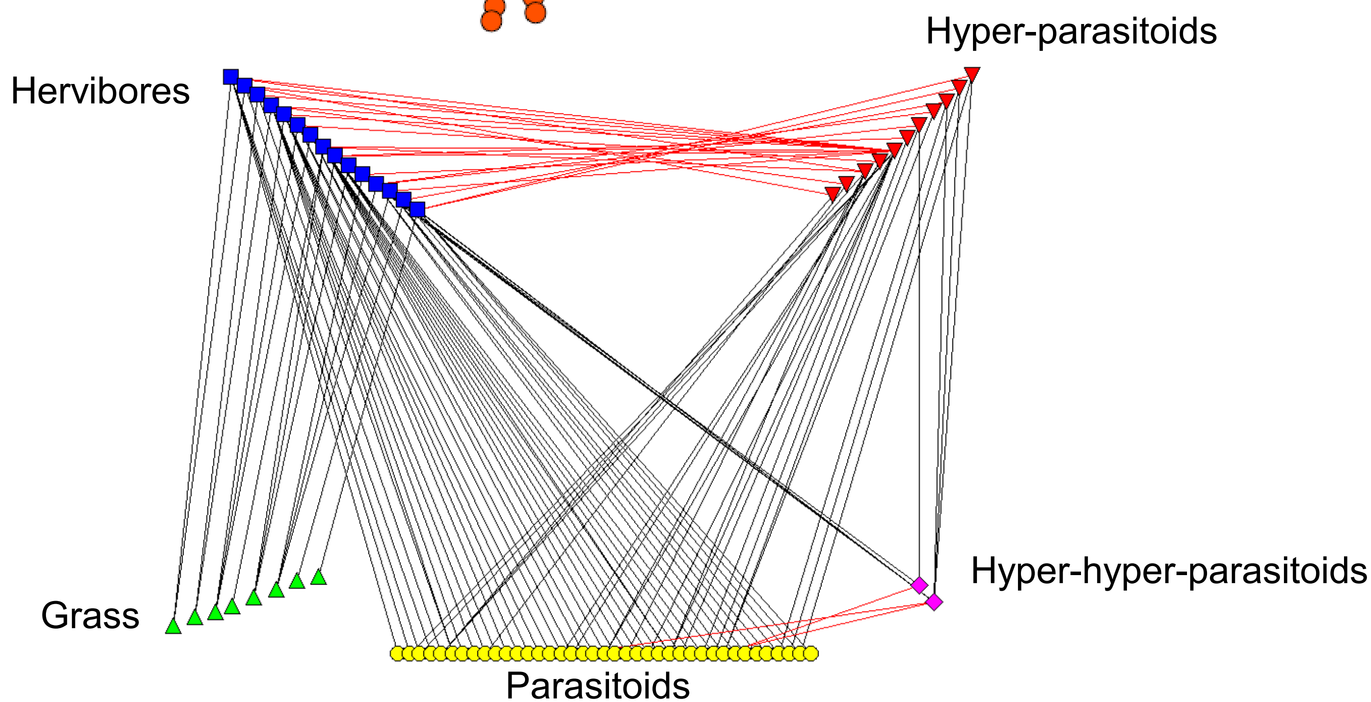
Example

A grassland food wen in England

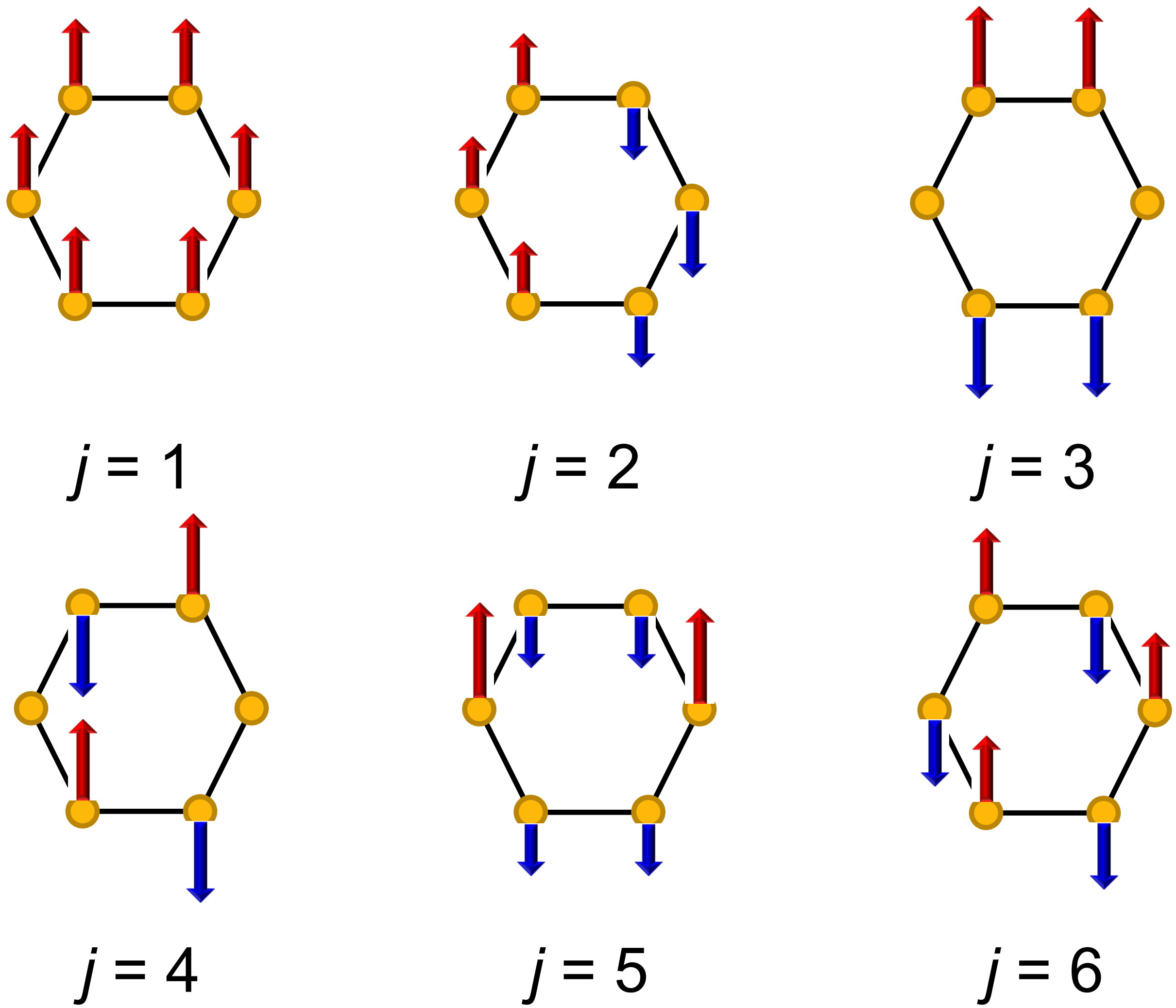


$$b_s = 0.766$$

$$b_e = 0.532$$



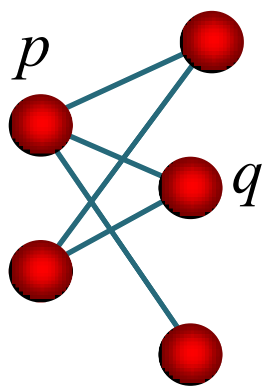
Finding Bipartitions

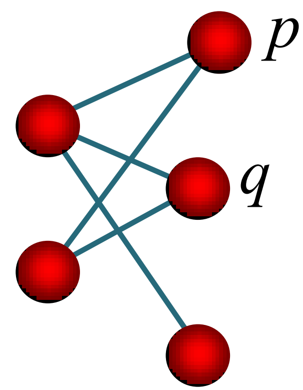


(see Chapter 21)

Finding Bipartitions

$$\hat{G}_{pq} = \left[\exp(-A)\right]_{pq} = \left[\cosh(A) - \sinh(A)\right]_{pq}$$



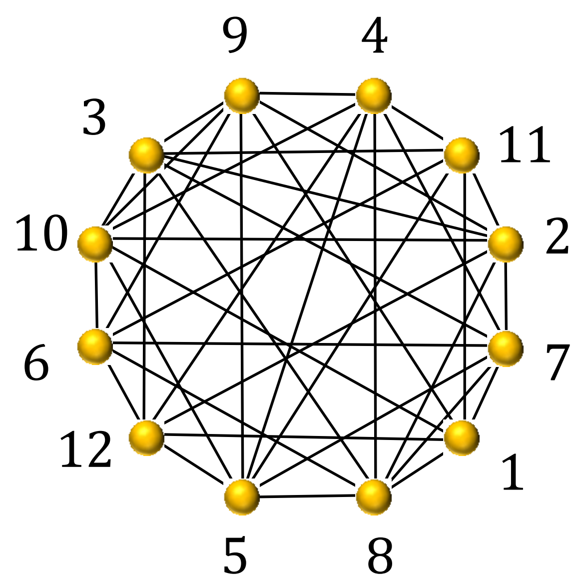


$$\hat{G}_{pq} = \left[-\sinh(A)\right]_{pq} < 0$$

$$\hat{G}_{pq} = \left[\cosh(A)\right]_{pq} > 0$$

$$\hat{G}_{pq} \begin{cases} < 0 & p \text{ and } q \text{ in different partitions} \\ > 0 & p \text{ and } q \text{ in the same partitions} \end{cases}$$

Finding Bipartitions



Finding Bipartitions

1) Build the G(-1) matrix

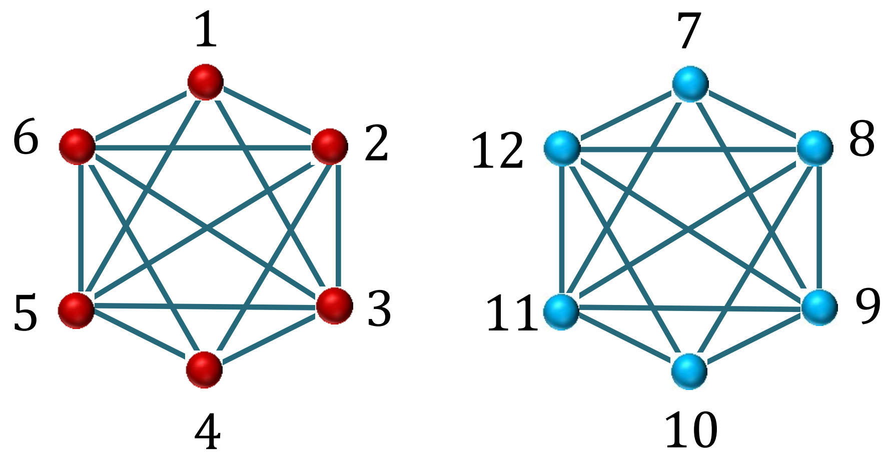
$$\hat{G} = \begin{pmatrix}
10.1 & 6.83 & 7.09 & 7.11 & 6.66 & 8.19 & -5.62 & -7.98 & -7.29 & -7.28 & -9.02 & -8.73 \\
6.83 & 8.03 & 4.17 & 5.87 & 5.43 & 6.72 & -6.31 & -4.32 & -6.56 & -5.65 & -7.28 & -7.04 \\
7.09 & 4.17 & 8.05 & 5.62 & 5.50 & 6.73 & -5.42 & -6.62 & -4.30 & -6.56 & -7.29 & -7.05 \\
7.11 & 5.87 & 5.62 & 8.17 & 3.93 & 6.80 & -5.68 & -5.96 & -6.62 & -4.32 & -7.98 & -7.10 \\
6.66 & 5{,}43 & 5.50 & 3.93 & 7.37 & 6.36 & -5.39 & -5.68 & -5.42 & -6.31 & -5.62 & -6.77 \\
8.19 & 6.72 & 6.73 & 6.80 & 6.36 & 9.38 & -6.77 & -7.10 & -7.05 & -7.04 & -8.73 & -7.28 \\
-5.62 & -6.31 & -5.42 & -5.68 & -5.39 & -6.77 & 7.37 & 3.93 & 5.50 & 5.43 & 6.66 & 6.36 \\
-7.98 & -4.32 & -6.62 & -5.96 & -5.68 & -7.10 & 3.93 & 8.17 & 5.62 & 5.87 & 7.11 & 6.80 \\
-7.29 & -6.56 & -4.30 & -6.62 & -5.42 & -7.05 & 5.50 & 5.62 & 8.05 & 4.17 & 7.09 & 6.73 \\
-7.28 & -5.65 & -6.56 & -4.32 & -6.31 & -7.04 & 5.43 & 5.87 & 4.17 & 8.03 & 6.83 & 6.72 \\
-9.02 & -7.28 & -7.29 & -7.98 & -5.62 & -8.73 & 6.66 & 7.11 & 7.09 & 6.83 & 10.1 & 8.19 \\
-8.73 & -7.04 & -7.05 & -7.10 & -6.77 & -7.28 & 6.36 & 6.80 & 6.73 & 6.72 & 8.19 & 9.38
\end{pmatrix}$$

Finding Bipartitions

2) Dichotomise G(-1). Take the diagonal as zeros

$$\tilde{G} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

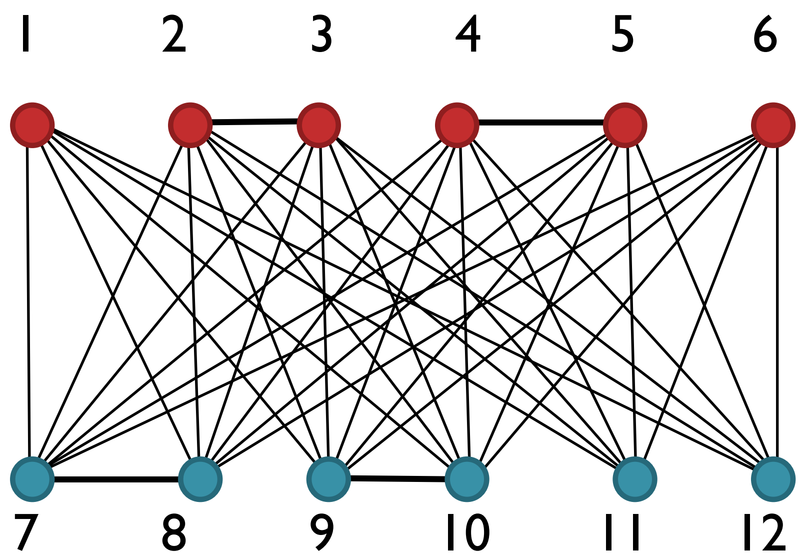
3) Construct the anti-communicability graph



$$C_1 = \{1, 2, 3, 4, 5, 6\}$$

$$C_2 = \{6, 7, 8, 9, 10, 11, 12\}$$

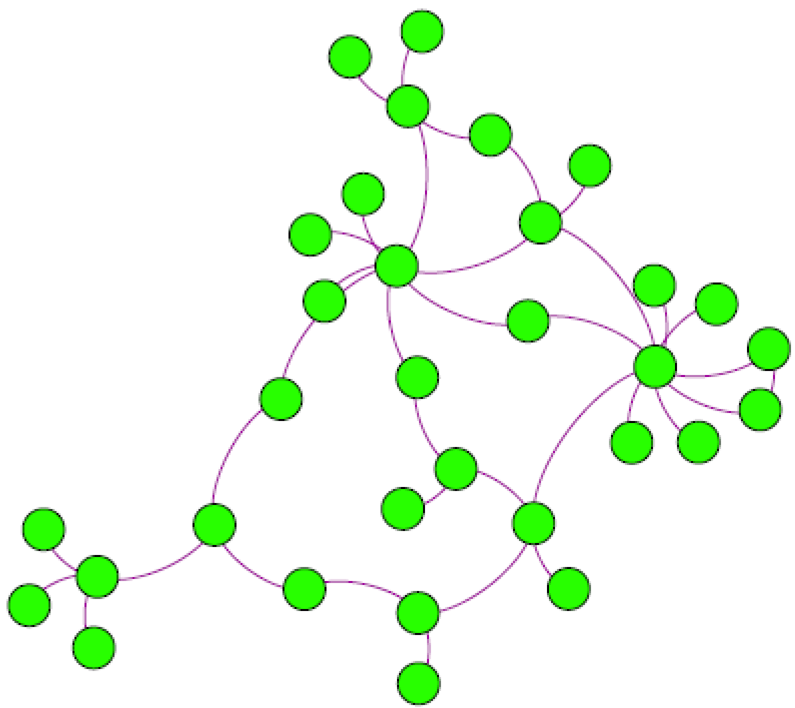
4) Represent the partitions of the network

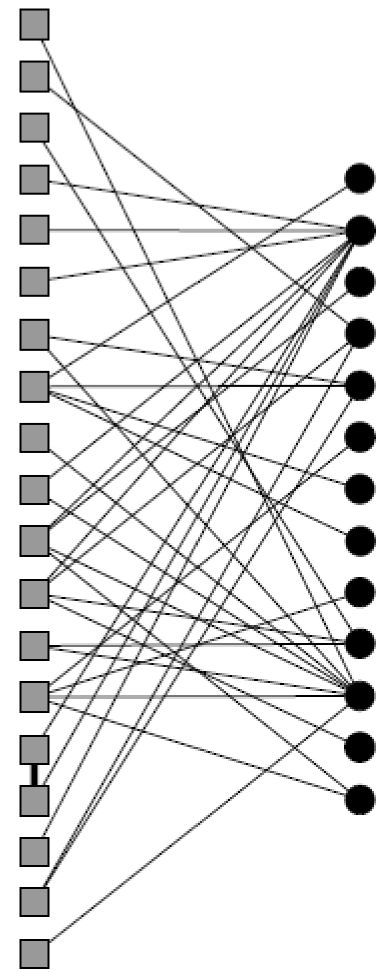


Finding Bipartitions

Example

Protein-protein interaction network of *A. fulgidus*

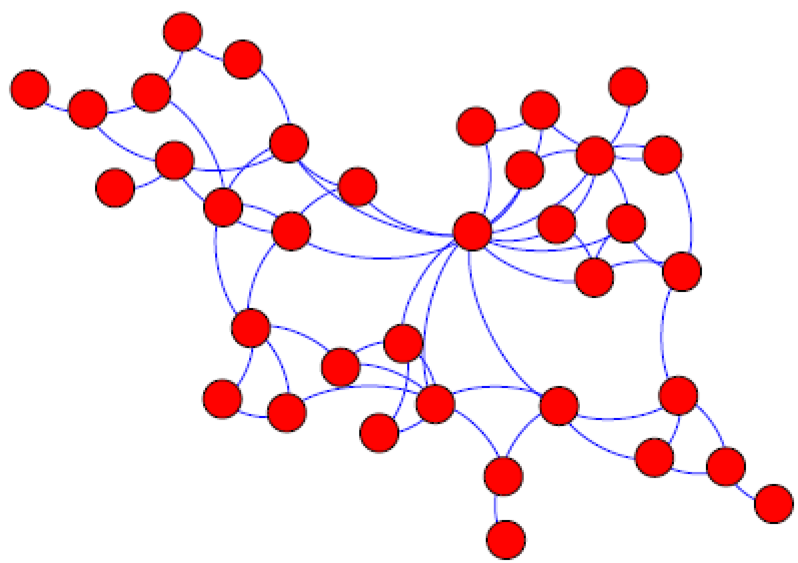


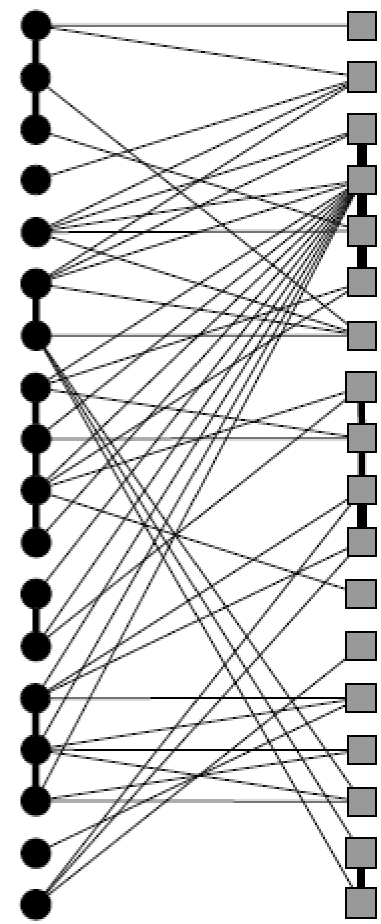


Finding Bipartitions

Example

Social network in a sawmill





LECTURE 4: BASED ON CHAPTER 18

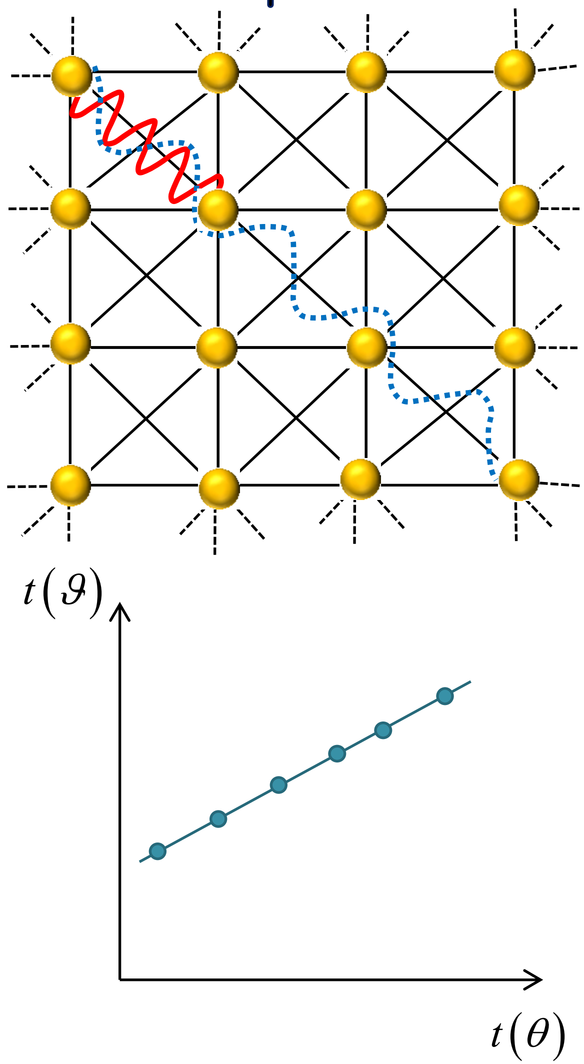
Topological Structural Classes. Graph vs. Network Theory

Professor Ernesto Estrada
Department of Mathematics & Statistics
University of Strathclyde
Glasgow, UK

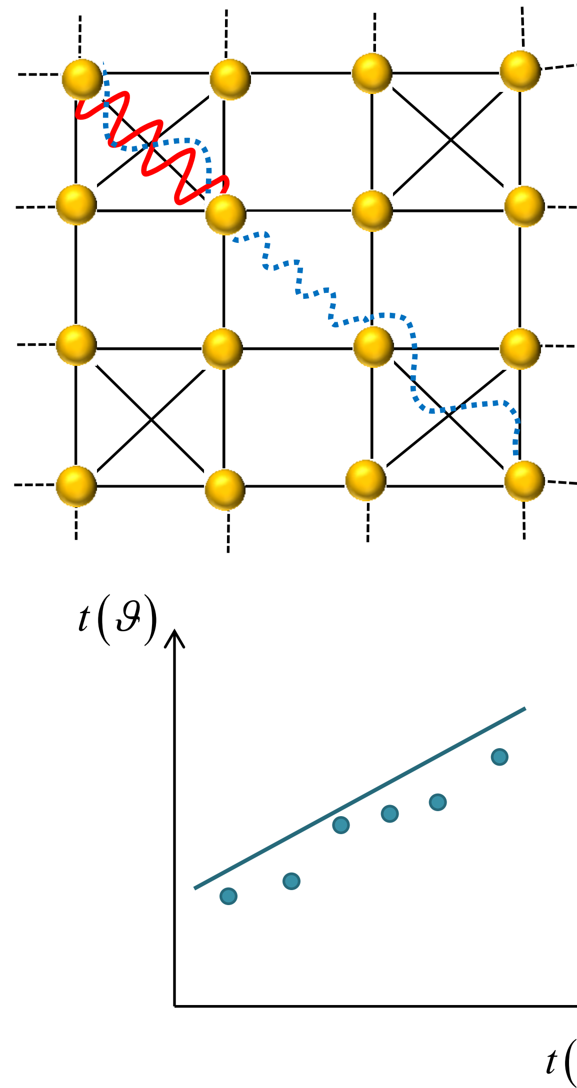
www.estradalab.org

Global Topological Structures

local exploration



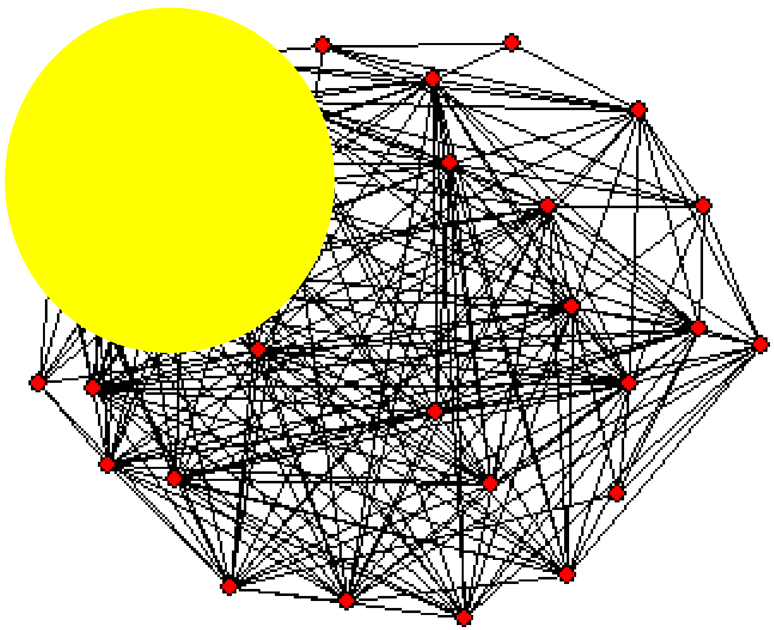
global exploration



Graph Theory

Graph expansion

$S \subset V$



Let $|S| \leq 1/2|V|$ and

$|\partial(S)|$ represents the number of edges with exactly one endpoint in S.

Edge Expansion (Isoperimetric Number)

$$\phi(G) = \min_{1 \leq |S| \leq \frac{n}{2}} \frac{|\partial(S)|}{|S|}, S \subseteq V, 0 < |S| \leq \frac{|V|}{2} < +\infty$$

University of Strathclyde

Graph Theory

Graph expansion

Theorem (Alon-Milman): Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_N$

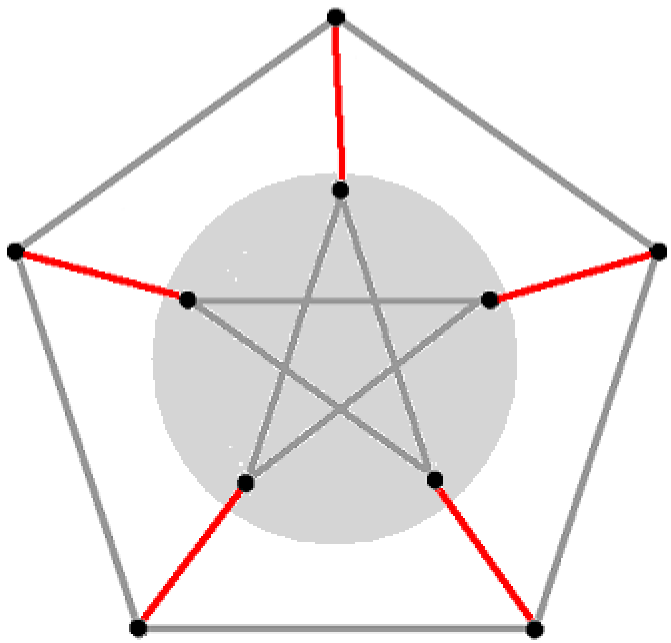
$$\frac{\lambda_1 - \lambda_2}{2} \leq \phi(G) \leq \sqrt{2\lambda_1(\lambda_1 - \lambda_2)}$$

$\lambda_1 - \lambda_2$ ⇨ **SPECTRAL GAP**

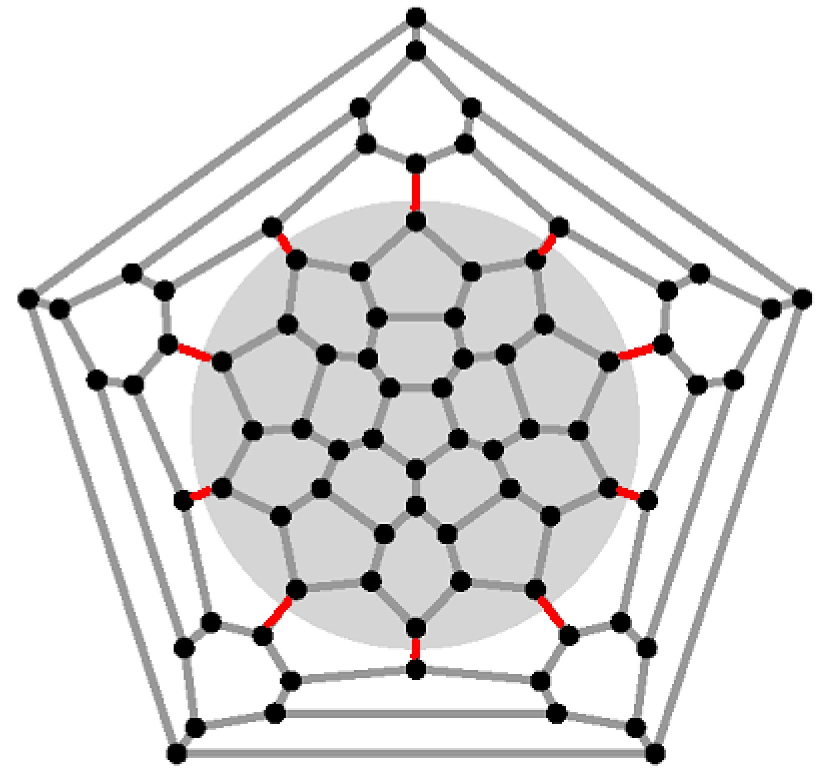
implies .

Graph Theory

Graph expansion



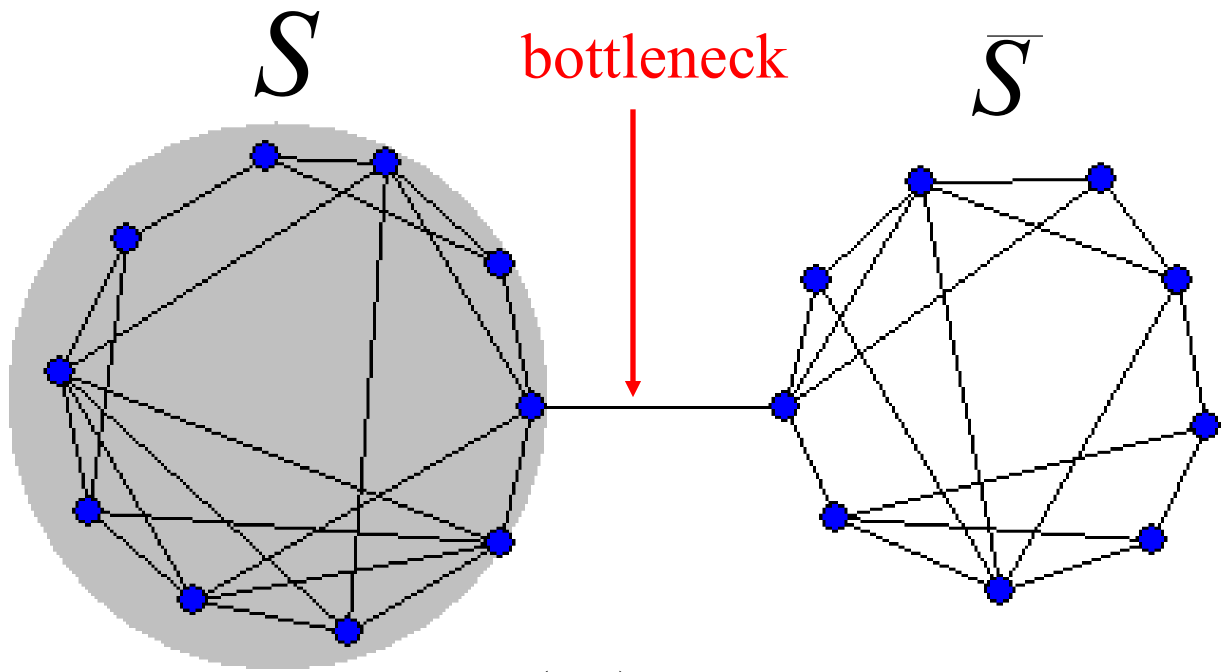
The Petersen graph
$n = 10,\ \phi = 1$



A Ramanujan graph
$n = 80,\ \phi = 1/4$

Graph Theory

Graph expansion



$$|\partial(S)| << |S|$$

Network Theory Approach

Spectral scaling

$$G_{ii} = \psi_{1,i}^2 \exp(\lambda_1) + \sum_{j=2}^{n} \psi_{j,i}^2 \exp(\lambda_j)$$

$$\lambda_1 >> \lambda_2$$

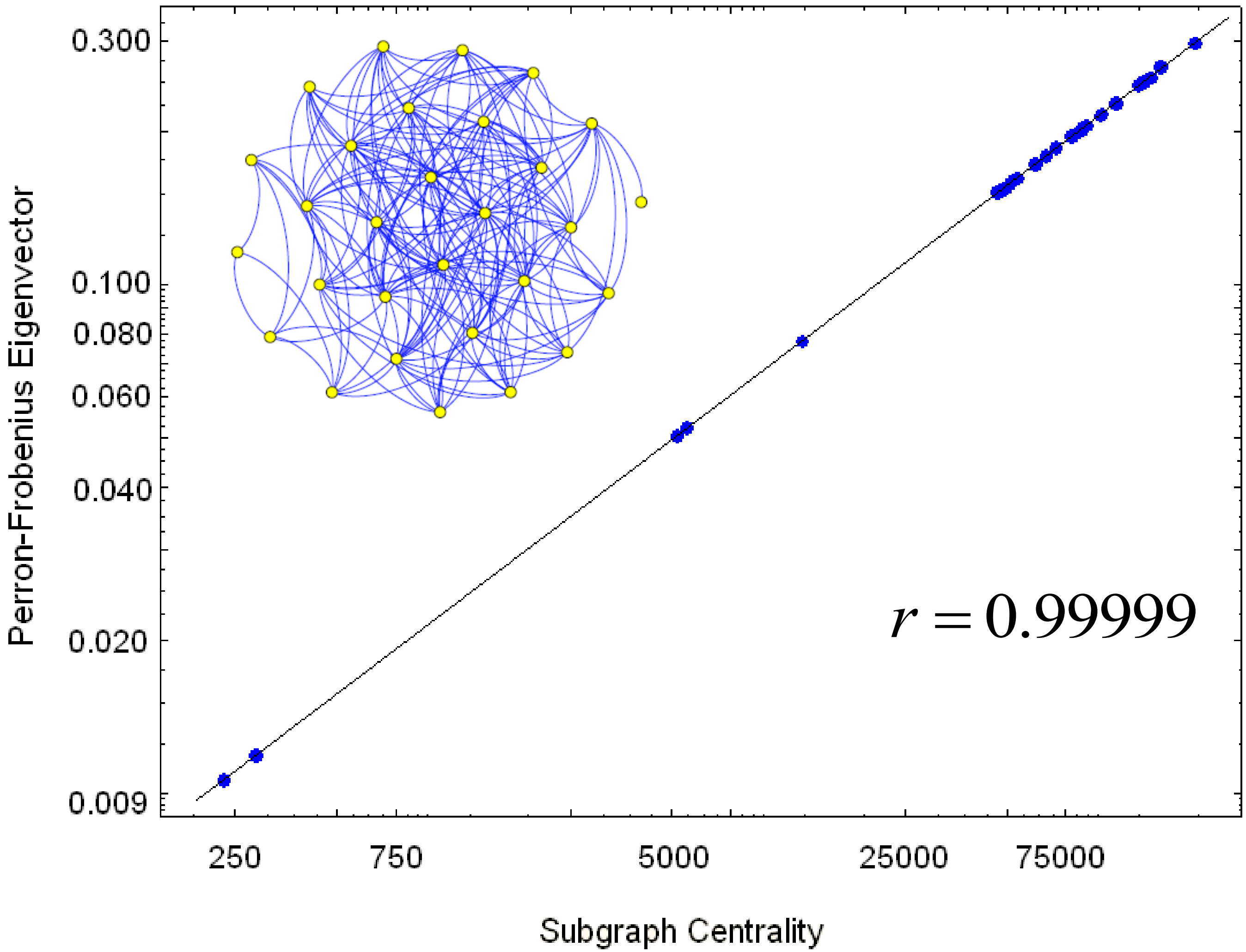
$$G_{ii} \cong \psi_{1,i}^2 \exp(\lambda_1)$$

$$\ln \psi_{1,i} \cong \frac{1}{2} \ln G_{ii} - \frac{\lambda_1}{2}$$

Network Theory Approach

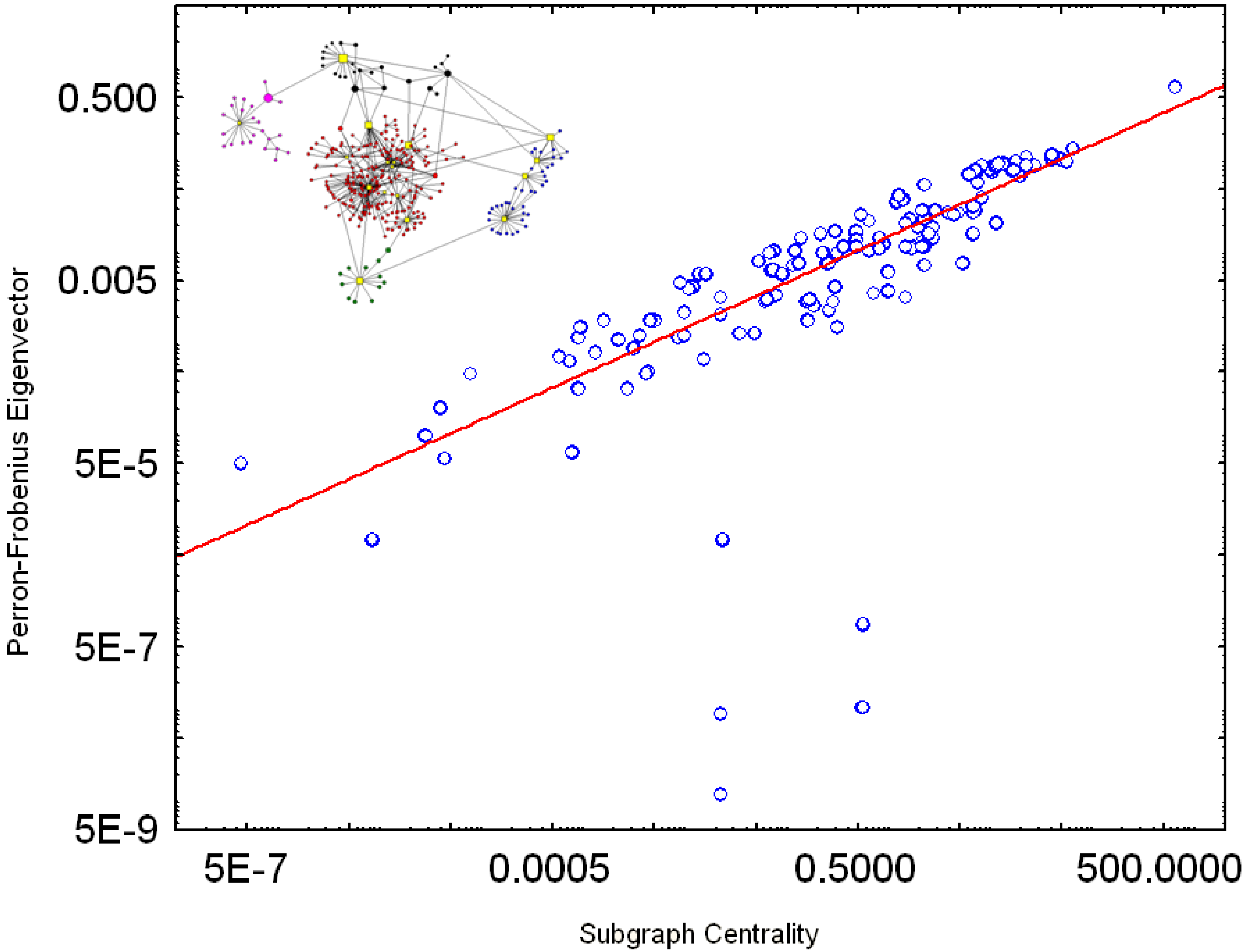
Spectral scaling

$$\ln \psi_{1,i} \cong 0.5 \ln G_{ii} - b$$



Network Theory Approach

Spectral scaling



Network Theory Approach

Does the eigenvector centrality a global exploration of the network?

Let G a non-bipartite network and let

$N_k(i)$ number of walks of length *k* starting at *i*

$$s_k(i) = N_k(i) \cdot \left(\sum_{j=1}^{n} N_k(j) \right)^{-1}$$

Network Theory Approach

$$N_k(i) = \sum_{p=1}^{n} \sum_{j=1}^{n} \varphi_{j,i} \varphi_{j,p} \lambda_j^k$$

$$\sum_{p=1}^{n} N_k(p) = \sum_{p=1}^{n} \sum_{q=1}^{n} \sum_{j=1}^{n} \varphi_{j,p} \varphi_{j,q} \lambda_j^k$$

$$s_k(i) = \frac{\sum_{p=1}^{n} \sum_{j=1}^{n} \varphi_{j,i} \varphi_{j,p} \lambda_j^k}{\sum_{p=1}^{n} \sum_{q=1}^{n} \sum_{j=1}^{n} \varphi_{j,p} \varphi_{j,q} \lambda_j^k}$$

Network Theory Approach

University of Strathclyde

$$k \to \infty$$

$$s_k(i) = \frac{\sum_{p=1}^{n} \varphi_{1,i}\varphi_{1,p}\lambda_1^k}{\sum_{p=1}^{n}\sum_{q=1}^{n} \varphi_{1,p}\varphi_{1,q}\lambda_1^k} = \frac{\varphi_{1,i}\sum_{p=1}^{n} \varphi_{1,p}}{\sum_{p=1}^{n}\sum_{q=1}^{n} \varphi_{1,p}\varphi_{1,q}}.$$

$$\sum_{p=1}^{n}\sum_{q=1}^{n} \varphi_{1,p}\varphi_{1,q} = \left(\sum_{j=1}^{n} \varphi_{1,p}\right)^2$$

$$s_k(i) \to \frac{\varphi_{1,i}}{\sum_{p=1}^{n} \varphi_{1,p}} = \alpha \cdot \varphi_{1,i}$$

Network Theory Approach

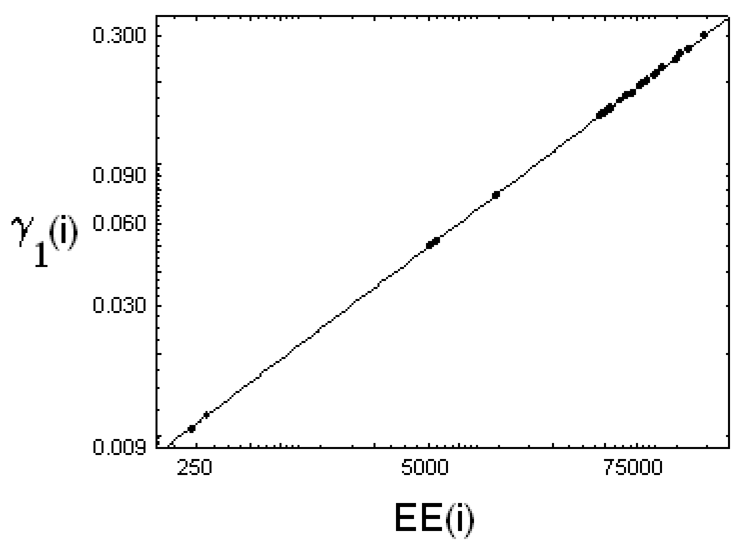
Spectral scaling (standard deviation of the scaling)

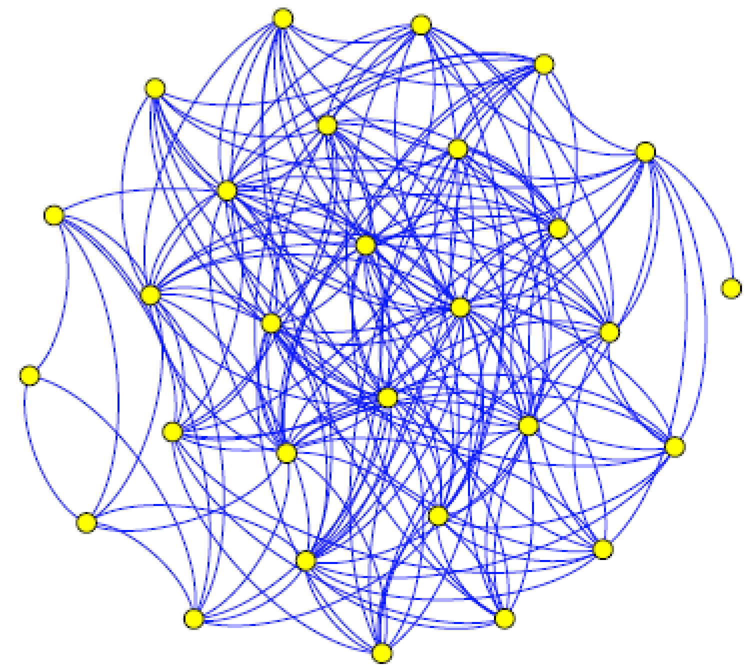
$$\Delta \ln \varphi_{1,i} = \ln\left[\frac{\varphi_{1,i}^{2}\exp\left(\lambda_1\right)}{G_{ii}}\right]^{0.5}$$

Universal Structural Classes

Class I

$$\Delta \ln \varphi_{1,i} \cong 0, \forall i \in V \Rightarrow \varphi_{1,i}^{2} \exp(\lambda_1) \cong G_{ii}$$

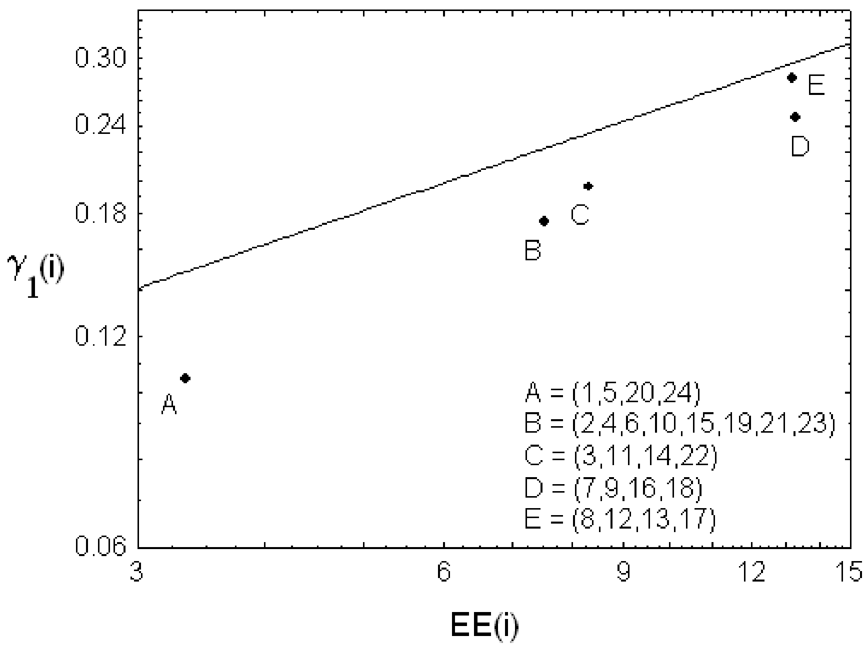


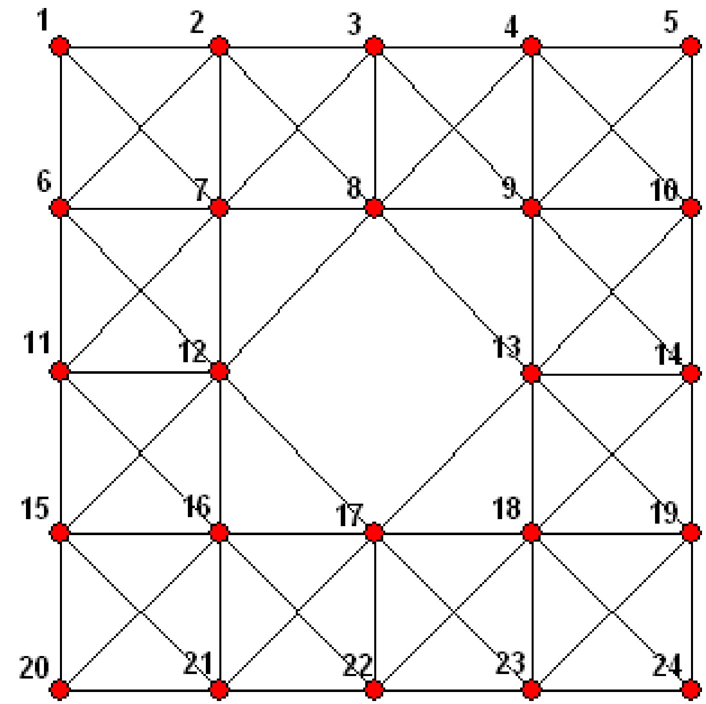


Universal Structural Classes

Class II

$$\Delta \ln \varphi_{1,i} \le 0, \forall i \in V \Rightarrow \varphi_{1,i}^2 \exp(\lambda_1) \le G_{ii}$$

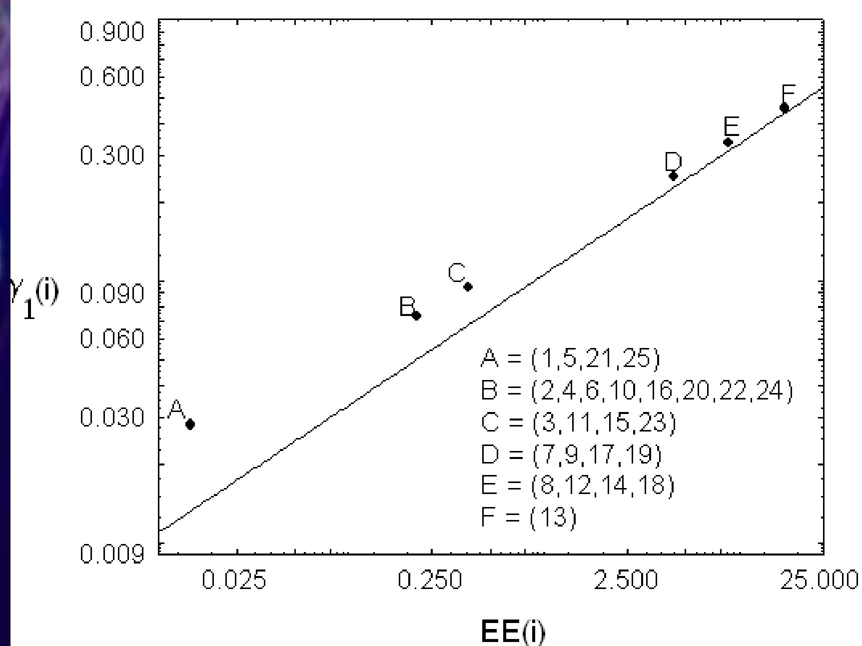


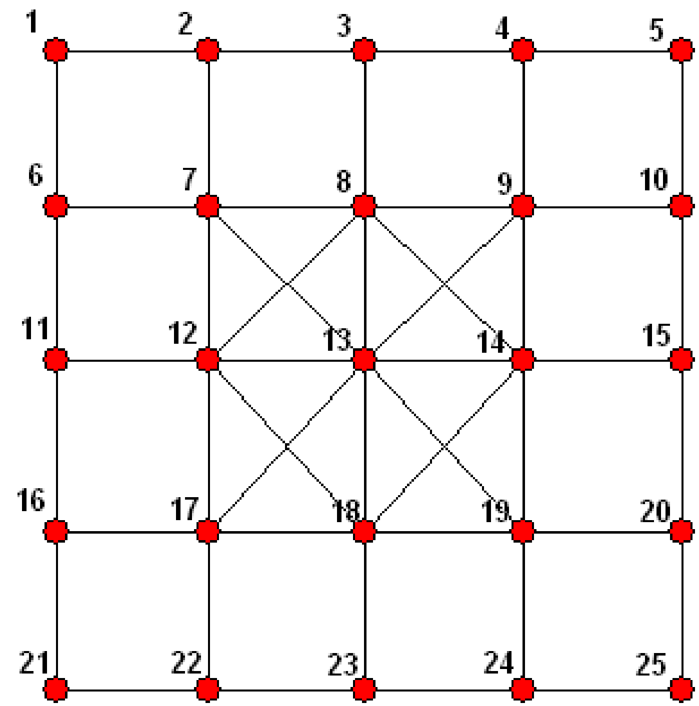


Universal Structural Classes

Class III

$$\Delta \ln \varphi_{1,i} \geq 0, \forall i \in V \Rightarrow \varphi_{1,i}^{2} \exp(\lambda_1) \geq G_{ii}$$

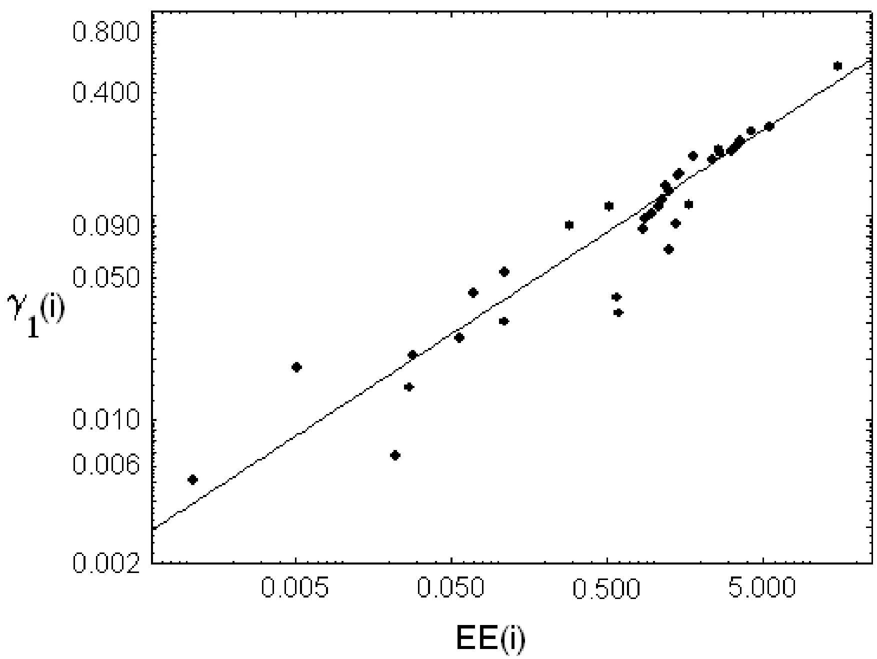


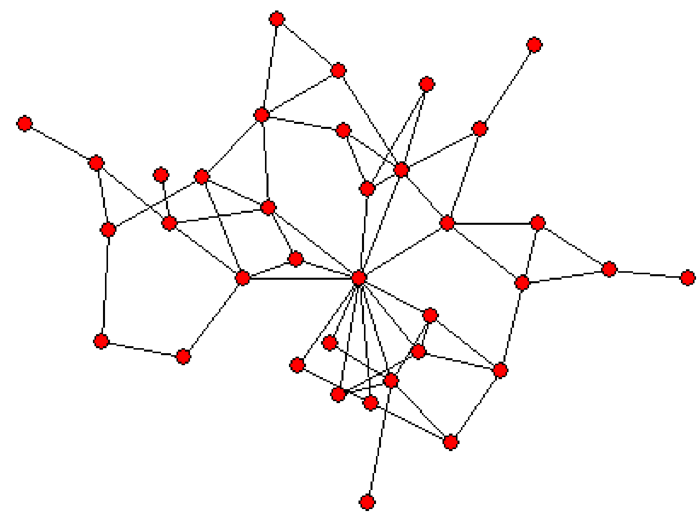


Universal Structural Classes

Class IV

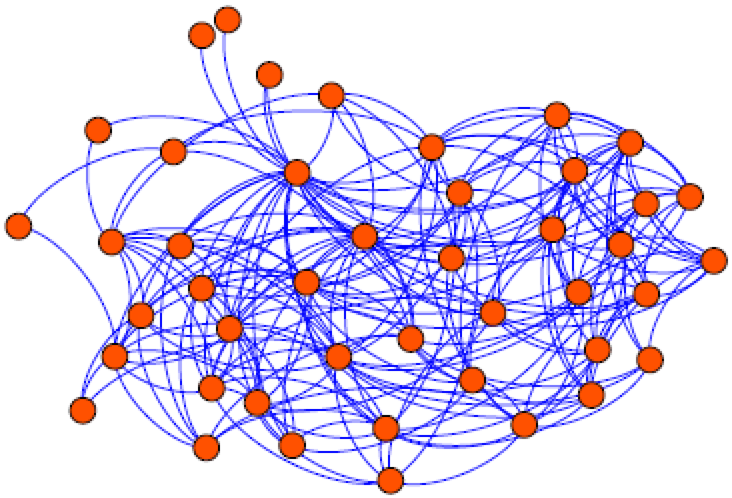
$$\Delta \ln \varphi_{1,p} \leq 0, p \in V \quad \text{and} \quad \Delta \ln \varphi_{1,q} > 0, q \in V$$



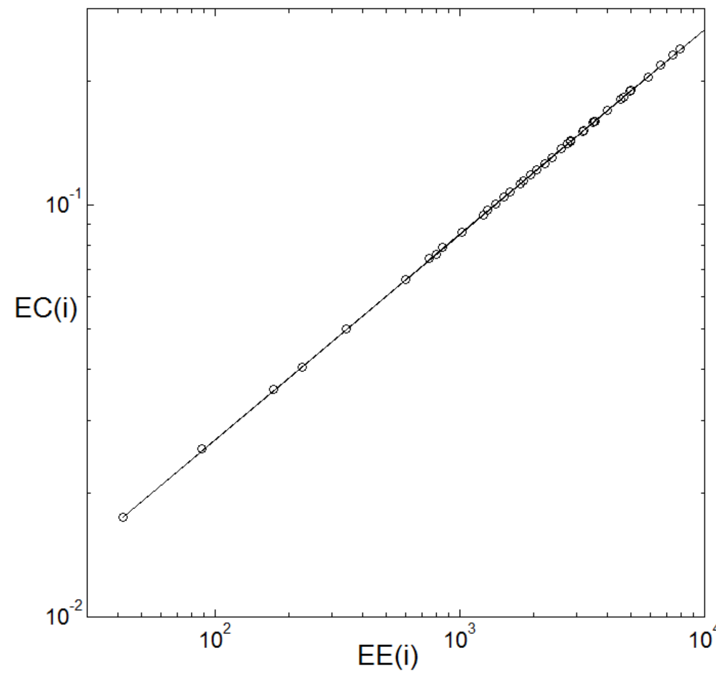


Universal Structural Classes

Example

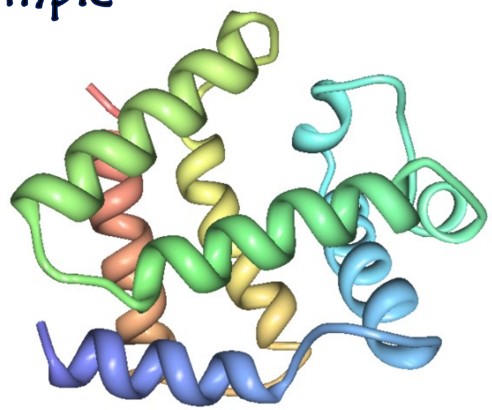


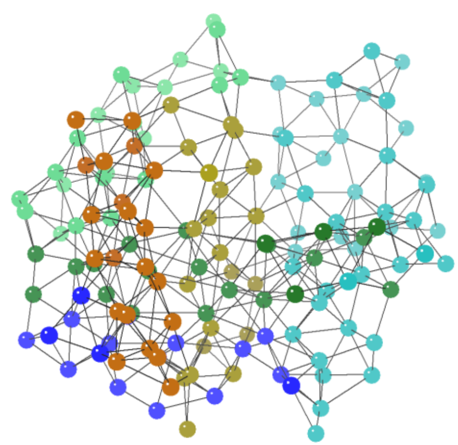
Food web of St. Martin Island

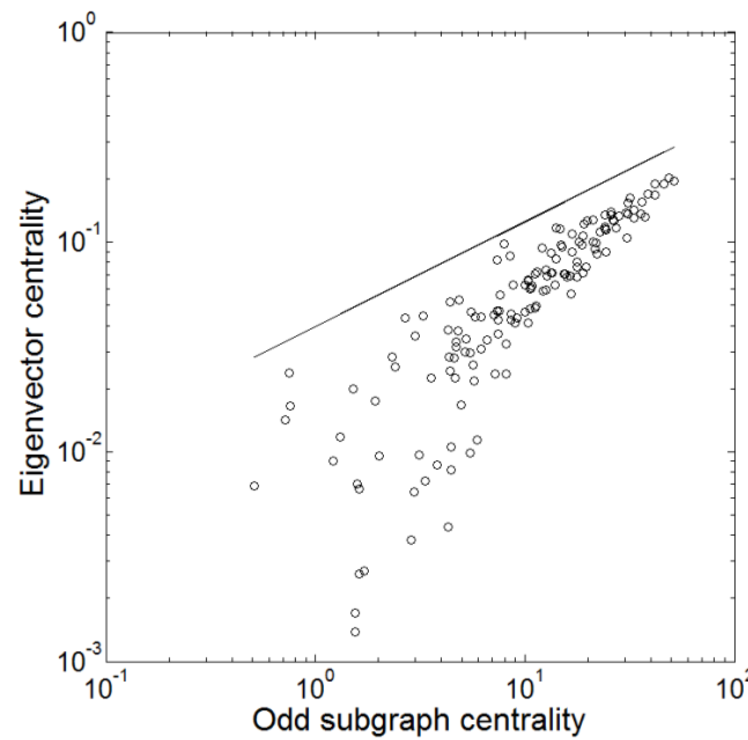


Universal Structural Classes

Example





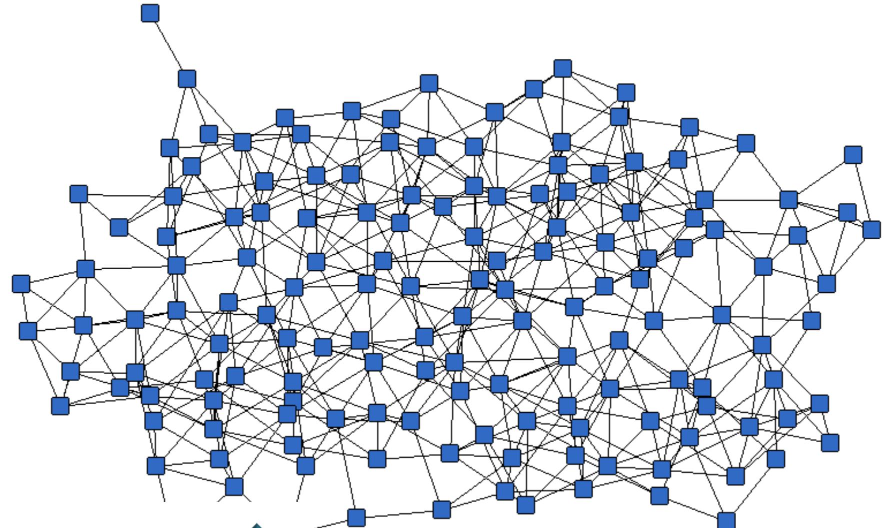


PROTEIN STRUCTURE

SPECTRAL SCALING

Universal Structural Classes

Example



Chordless cycle of length 15