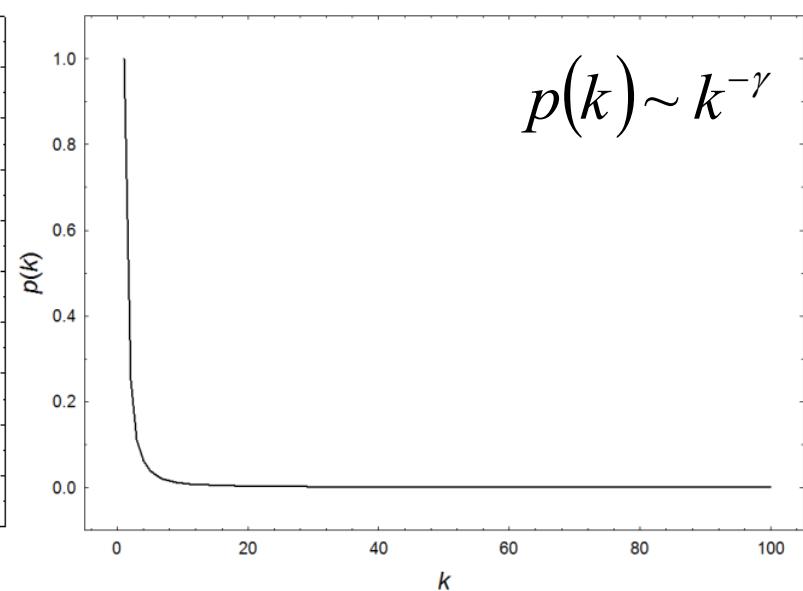
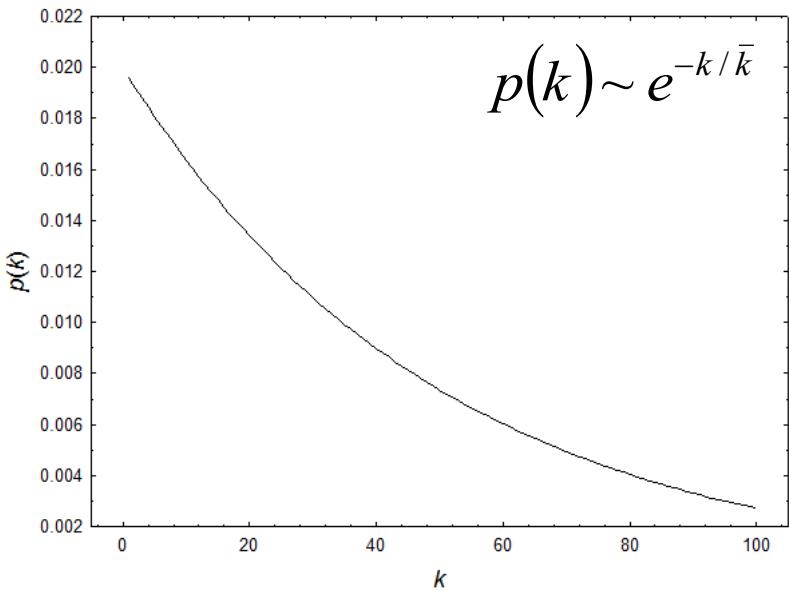
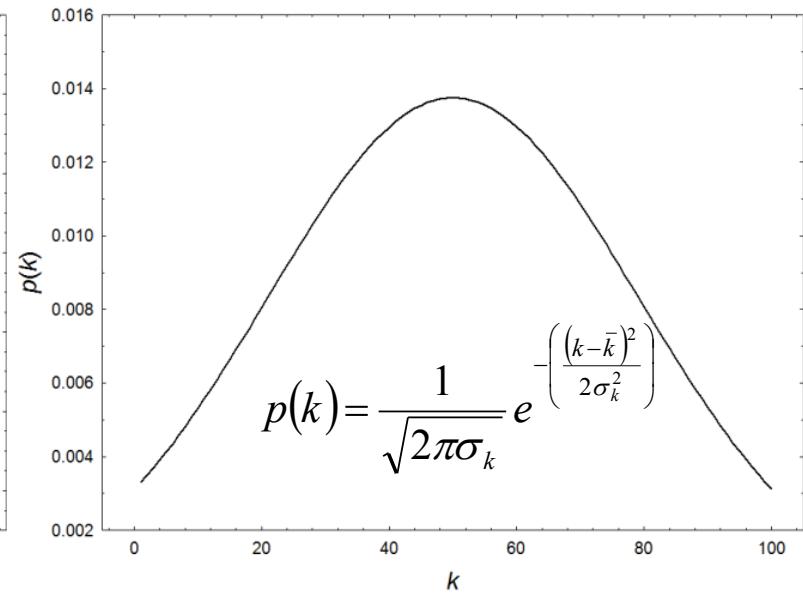
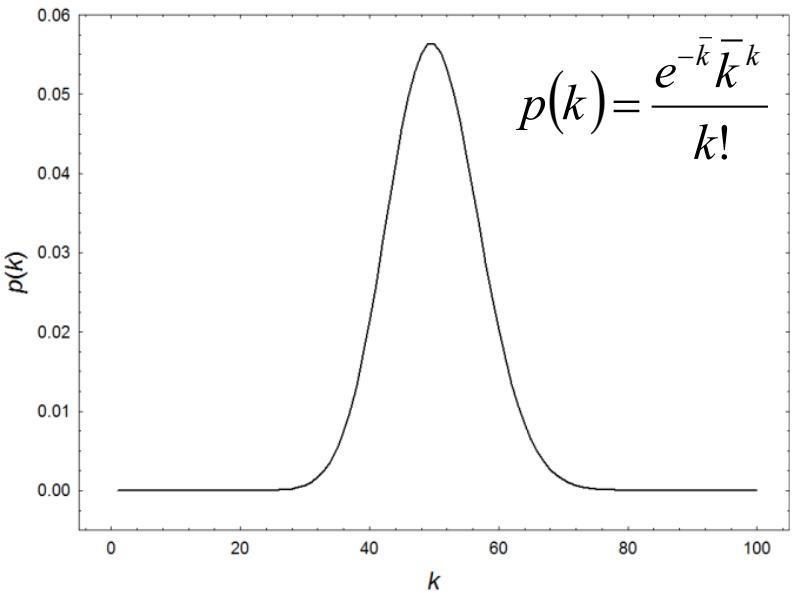




# Degree Irregularity. Distributions vs. Algebraic Approaches

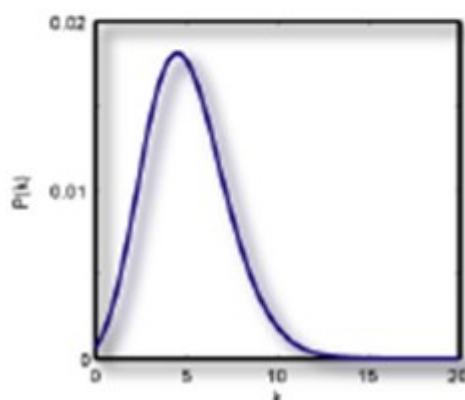
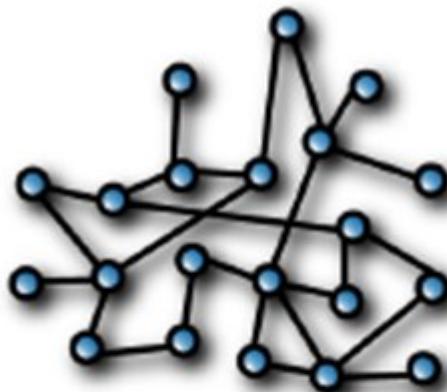
**Professor Ernesto Estrada**  
Department of Mathematics & Statistics  
University of Strathclyde  
Glasgow, UK

# Statistical Distributions



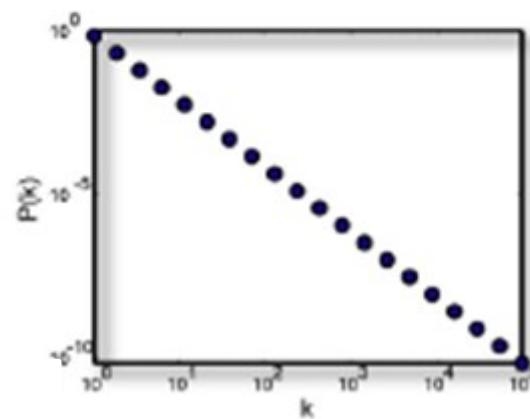
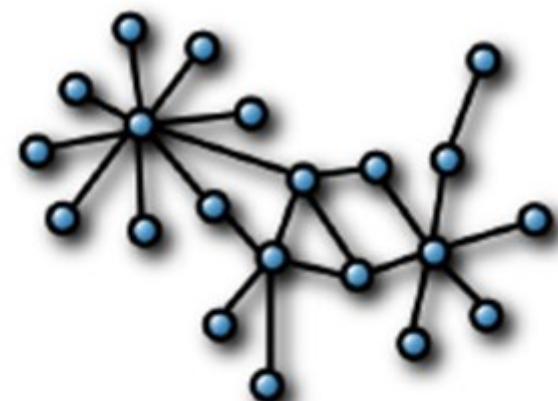
# Degree Distributions

## Poisson



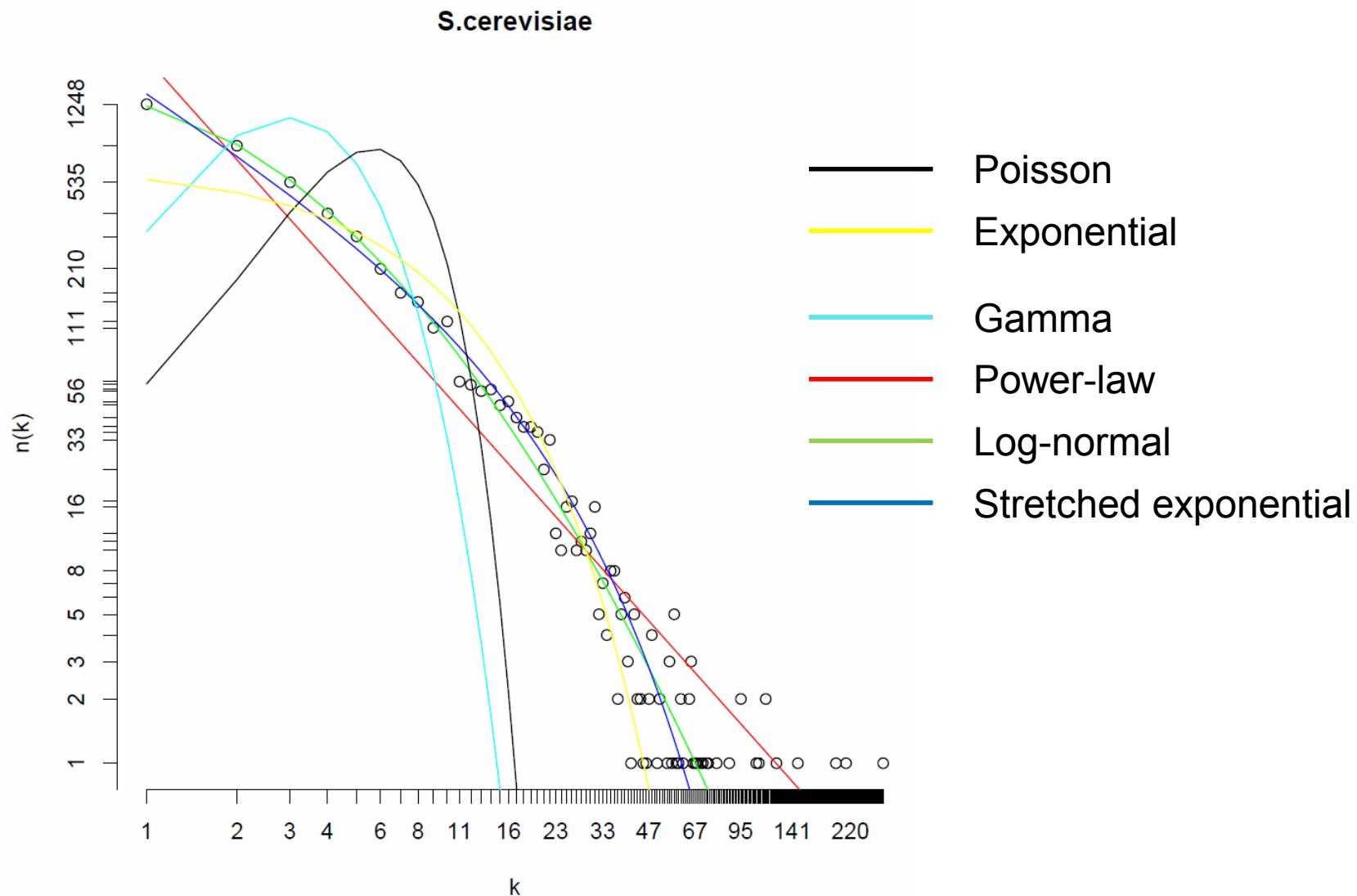
$$p(k) = \frac{e^{-\bar{k}} \bar{k}^k}{k!}$$

## Power-law



$$p(k) \sim k^{-\gamma}$$

# What is the best fit?



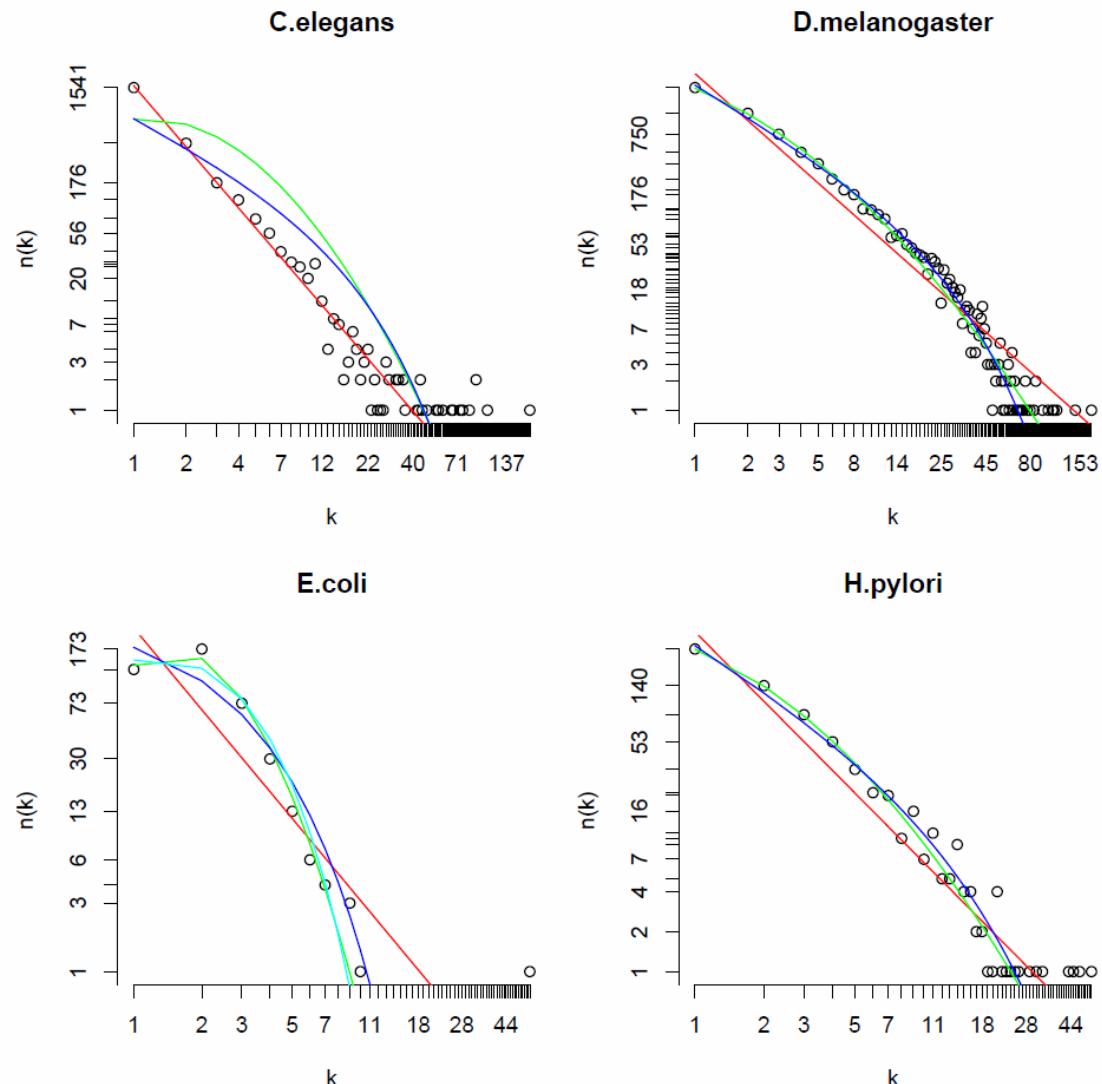
# The Zoo of Distributions

Bernoulli .....			
Beta .....	Generalized Error .....	Kumaraswamy.....	Pareto2 .....
Four-parameter Beta...	Exponential .....	Four-parameter Kumaraswamy..	Pearson Type 5.....
Beta-Binomial.....	Extreme Value Max .....	Laplace.....	Pearson Type 6.....
Beta-Geometric.....	Extreme Value Min.....	Levy .....	PERT.....
Beta-Negative Binomial .....	F.....	Logarithmic (Series).....	Poisson.....
Binomial.....	Fatigue Life.....	LogGamma.....	Pólya .....
Bradford.....	Gamma .....	Logistic.....	Rayleigh .....
Burr.....	Geometric .....	LogLaplace .....	Reciprocal .....
Cauchy .....	Generalized Logistic .....	LogLogistic .....	Relative .....
Chi.....	Histogram .....	Lognormal.....	Slash .....
Chi-Square(d) .....	Hyperbolic Secant .....	LognormalB.....	Split Triangle .....
Cumulative Ascending .....	Hypergeometric .....	LognormalE .....	Step Uniform.....
Cumulative Descending .....	Inverse Gaussian .....	Modified PERT.....	Student .....
Dagum .....	Inverse Hypergeometric .....	Negative Binomial .....	Triangle .....
Delaporte .....	Johnson Bounded.....	Normal.....	Uniform.....
Discrete.....	Johnson Unbounded .....	Ogive.....	Weibull.....
Discrete Uniform .....		Pareto .....	
Error Function .....			
m-Erlang.....			

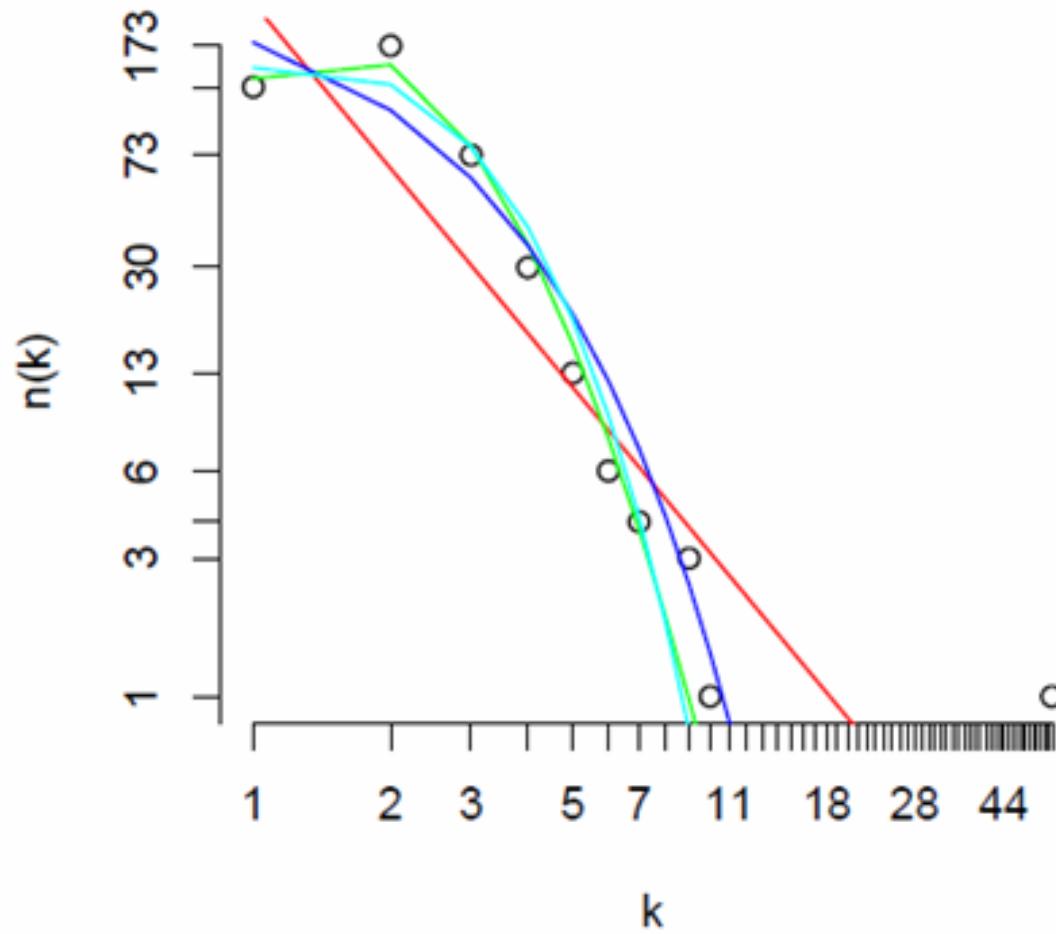
# How to Compare?

$$p(k) \sim e^{-\alpha k/\bar{k}} k^{-\gamma}$$

$$p(k) \sim \frac{e^{-\ln((k-\theta)/m)^2/(2\sigma^2)}}{(k-\theta)\sigma\sqrt{2\pi}}$$

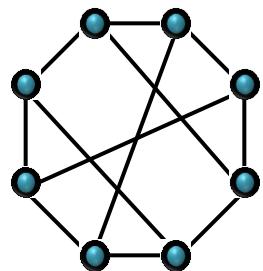


# How to Manage Scarce Data?

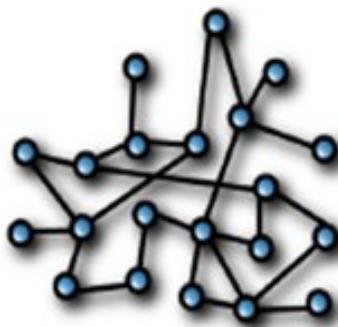


# Is There an Order?

Regular



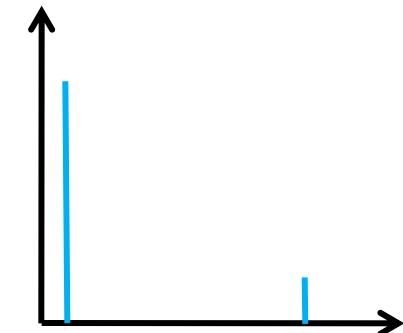
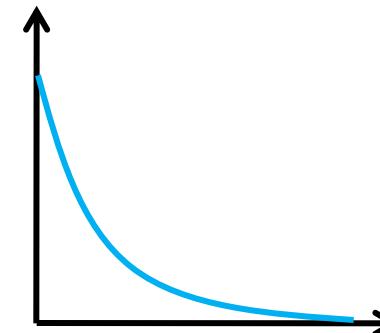
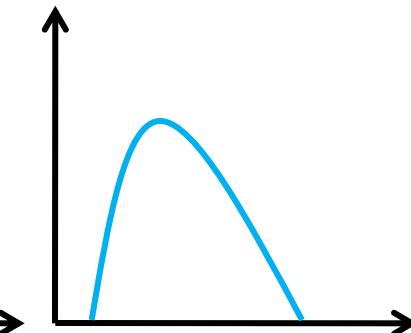
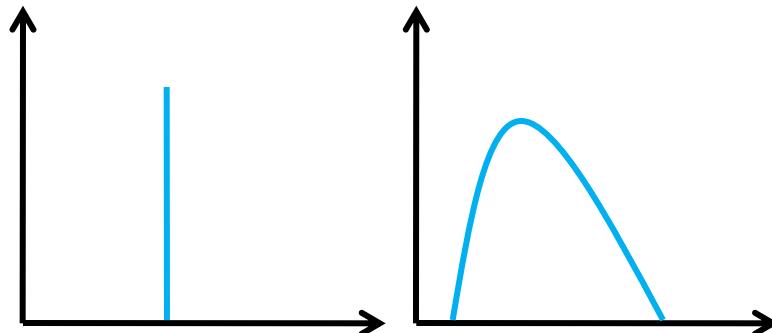
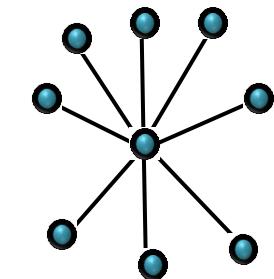
Poisson



Fat-tail



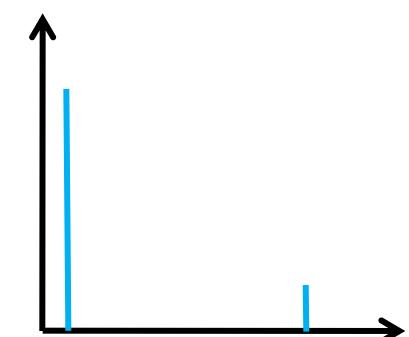
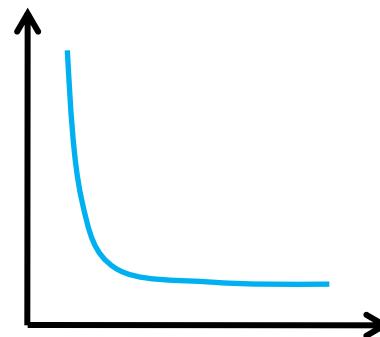
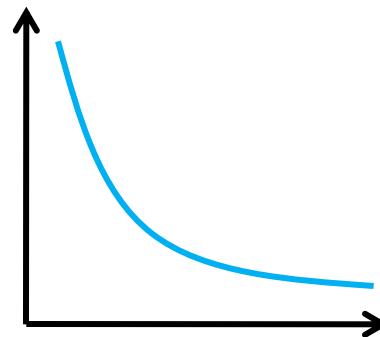
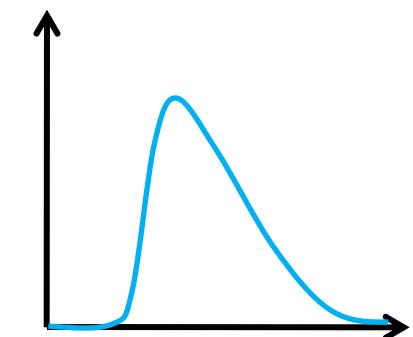
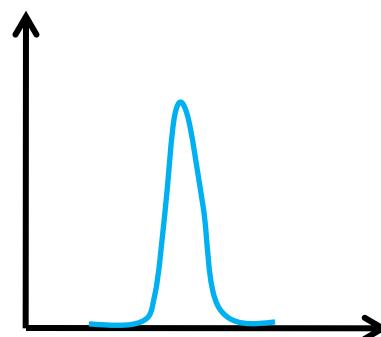
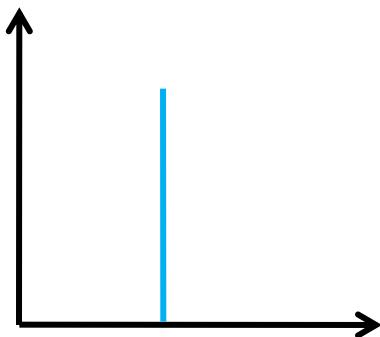
Star



DEGREE HETEROGENEITY



# Is There an Order?



# Graph Theory Approach

Degree irregularity indices

- Collatz-Sinogowitz Index (1957)

$$CS(G) = \lambda_1 - \langle k \rangle$$

- Bell Index (1992)

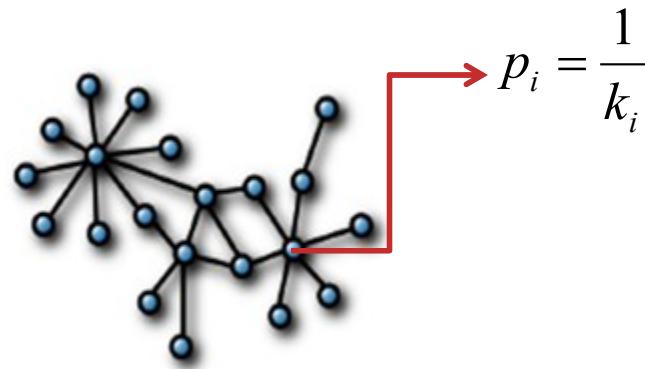
$$Var(G) = \frac{1}{n} \sum_i k_i^2 - \left( \frac{1}{n} \sum_i k_i \right)^2$$

- Albertson Index (1997)

$$irr(G) = \sum_{(i,j) \in E} |k_i - k_j|$$

# A New Index: Degree Skewness

probability of picking at random an incident edge



Non-standardised skewness:  $\rho_{ij} = \langle p_{ij} \rangle - \hat{p}_{ij}$

Arithmetic mean

$$\langle p_{ij} \rangle = \frac{1}{2} \left( \frac{1}{k_i} + \frac{1}{k_j} \right)$$

geometric mean

$$\hat{p}_{ij} = \sqrt{\frac{1}{k_i k_j}}$$

# Degree Skewness

$$2\rho_{ij} = \left( \frac{1}{k_i} + \frac{1}{k_j} \right) - \frac{2}{\sqrt{k_i k_j}}$$
$$= \left( \frac{1}{\sqrt{k_i}} - \frac{1}{\sqrt{k_j}} \right)^2$$

Network degree skewness

$$\rho(G) = 2 \sum_{(ij) \in E} \rho_{ij} = \sum_{(ij) \in E} \left( \frac{1}{\sqrt{k_i}} - \frac{1}{\sqrt{k_j}} \right)^2$$

# The Laplacian Encounter

Graph Laplacian

$$L = K - A$$

$$L_{ij} = \begin{cases} k_i & \text{for } i = j, \\ -1 & \text{for } i \sim j, \\ 0 & \text{otherwise,} \end{cases}$$

Normalised Graph Laplacian

$$\begin{aligned} \mathcal{L} &= K^{-1/2} \cdot L \cdot K^{-1/2} \\ &= I - K^{-1/2} \cdot A \cdot K^{-1/2} \end{aligned}$$

$$\mathcal{L}_{ij} = \begin{cases} 1 & \text{for } i = j, \\ -\frac{1}{\sqrt{k_i k_j}} & \text{for } i \sim j, \\ 0 & \text{otherwise,} \end{cases}$$

# The Laplacian Encounter

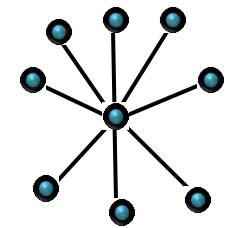
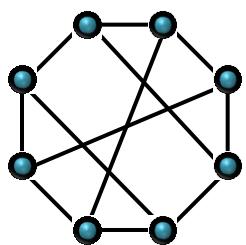
Network degree skewness

$$\begin{aligned}\rho(G) &= \vec{1} \cdot \mathcal{L} \cdot \vec{1}^T \\ &= n - 2 \sum_{(i,j) \in E} (k_i k_j)^{-1/2} \\ &= n - 2 \chi(G).\end{aligned}$$

Randic index

# A Nice Normalisation

$$\sqrt{n-1} \leq \chi(G) \leq \frac{n}{2}$$



Normalised network degree skewness

$$\tilde{\rho}(G) = \frac{n - 2\chi(G)}{n - 2\sqrt{n-1}}$$

$$0 \leq \tilde{\rho}(G) \leq 1$$

# Back to the Normalised Laplacian

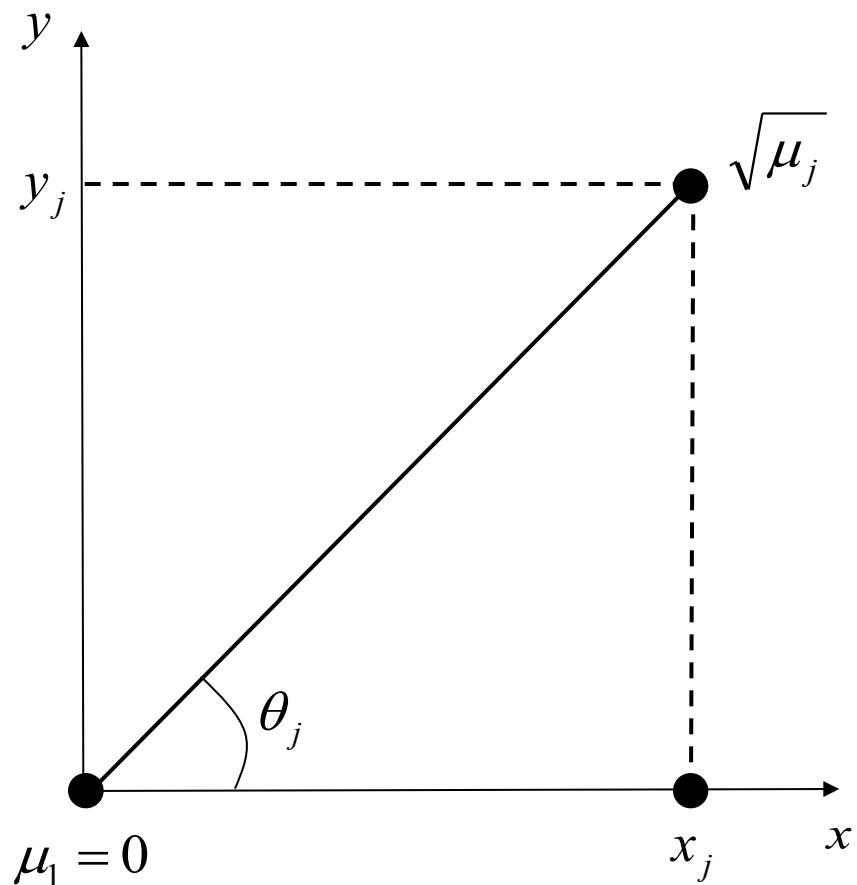
$$\rho(G) = \vec{1}^T \cdot \mathcal{L} \cdot \vec{1} = n \sum_j \mu_j \cos^2 \theta_j$$

$$0 = \mu_1 < \mu_2 \leq \dots \leq \mu_n$$

$$\cos \theta_j = \frac{\vec{1}^T \cdot \vec{\varphi}_j}{\|\vec{1}\| \|\vec{\varphi}_j\|} = \frac{1}{\sqrt{n}} \sum_{i=1}^n \varphi_j(i)$$

$$\rho(G) = \vec{1}^T \cdot \mathcal{L} \cdot \vec{1} = \sum_j \mu_j \left( \sum_i \varphi_j(i) \right)^2$$

# Spectral Representation



$$x_j = \sqrt{\mu_{j>1}} \cos \theta_j$$

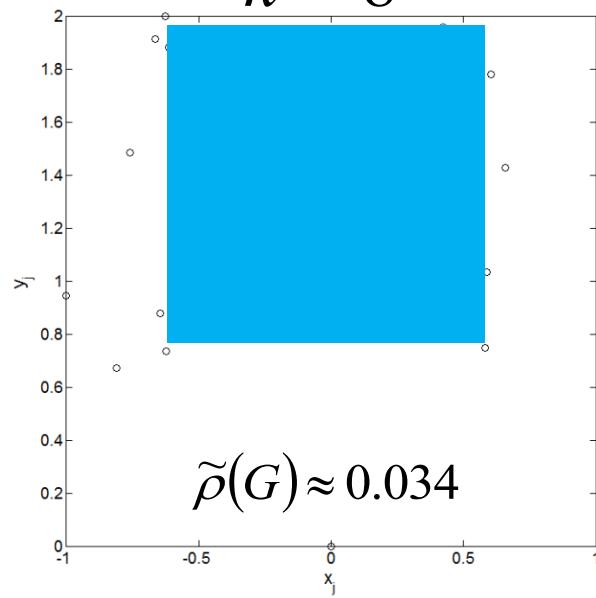
$$y_j = \sqrt{\mu_{j>1}} \sin \theta_j$$

$$\tilde{\rho}(G) = \frac{n}{n - 2\sqrt{n-1}} \sum_{j=1}^n x_j^2$$

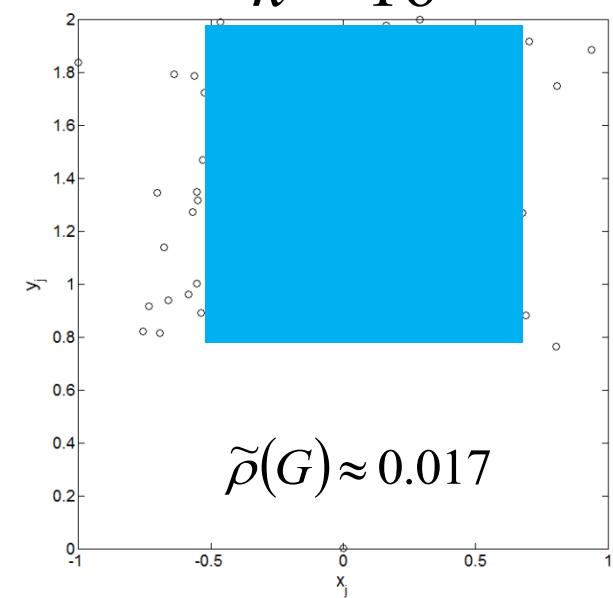
# Results

Erdős-Rényi Random Graphs  $G_{n,p}$

$$\bar{k} = 8$$



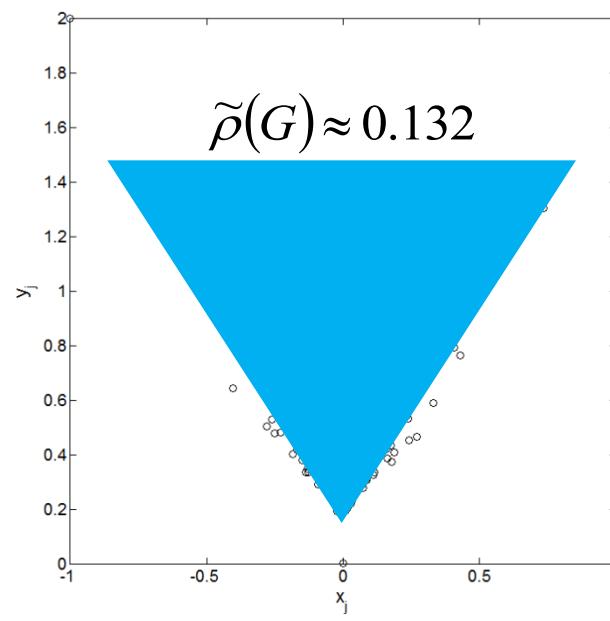
$$\bar{k} = 16$$



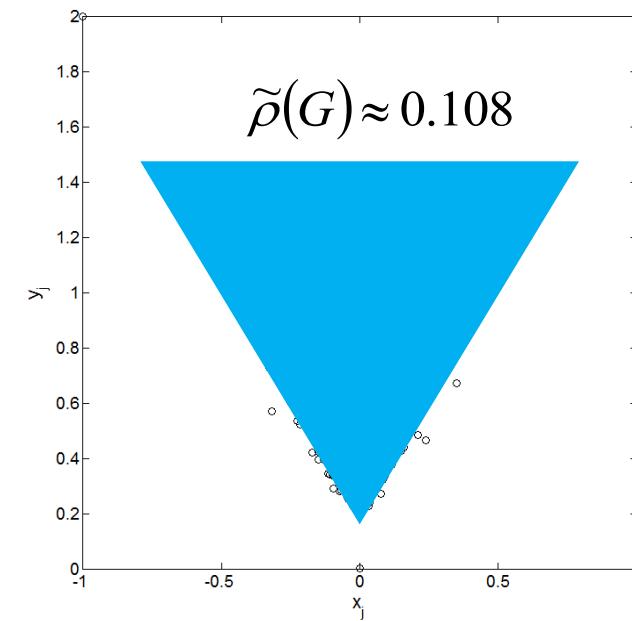
# Barabási-Albert Random Graphs

$$\rho(BA) \approx \left( \frac{0.27 + \langle k \rangle^{-1.18}}{2.27 + \langle k \rangle^{-1.18}} \right) \left( \frac{n}{n - 2\sqrt{n-1}} \right)$$

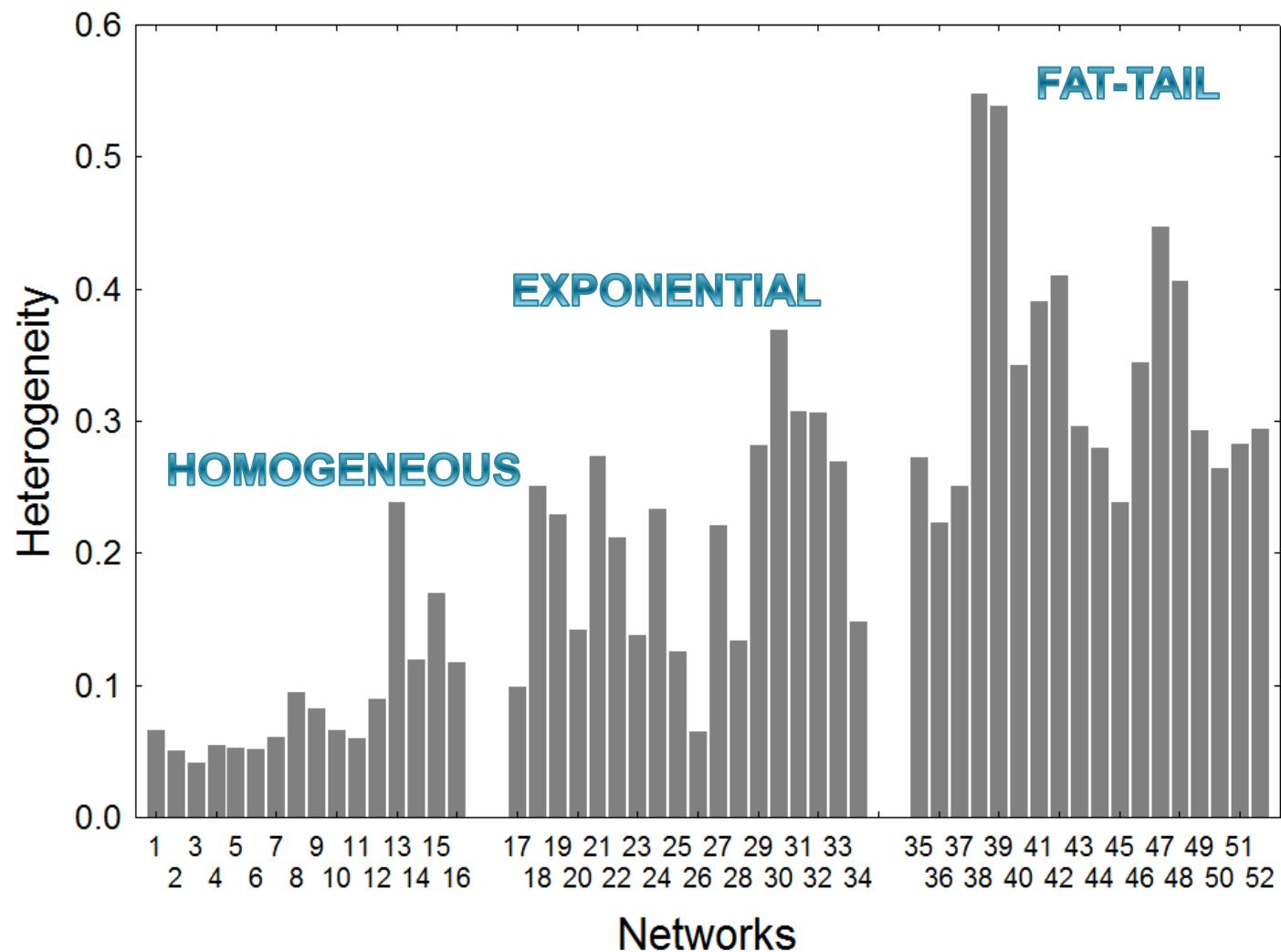
$$\bar{k} = 8$$



$$\bar{k} = 16$$

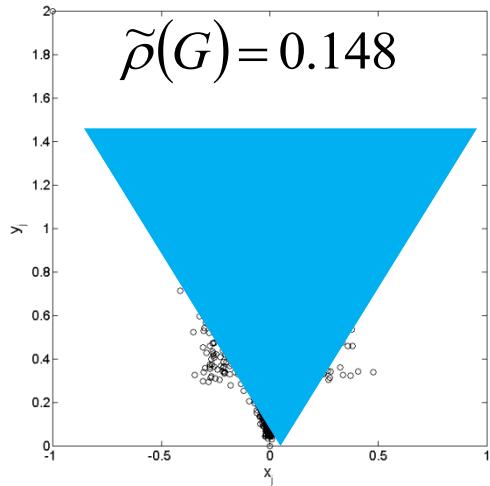


# Real-World Networks

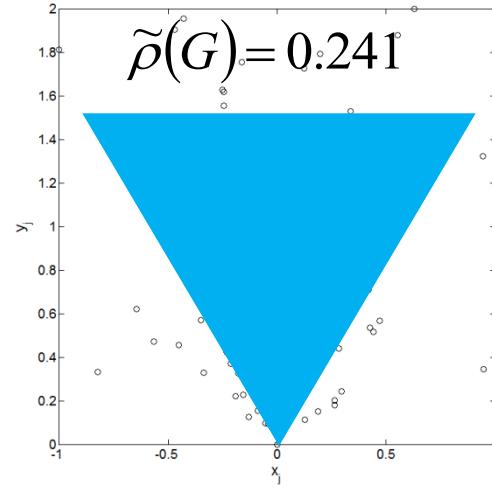


# Real-World Networks

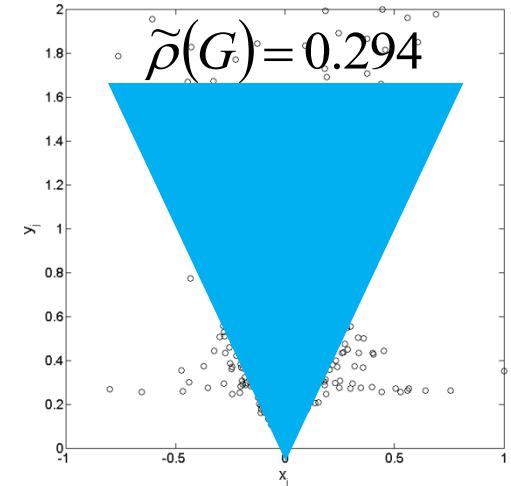
*D. melanogaster*



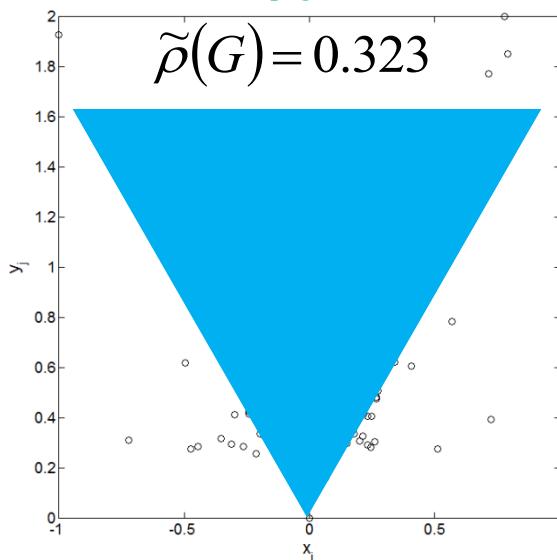
*E. coli*



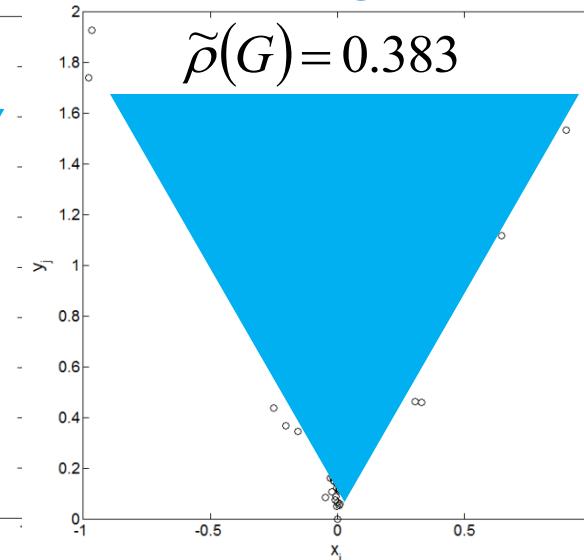
*S. cereviciae*



*H. pylori*



*C. elegans*

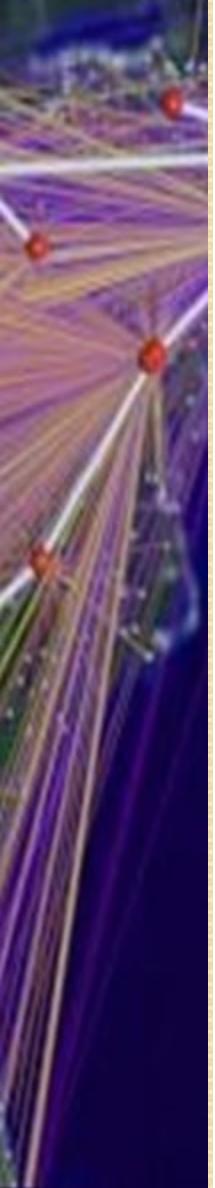


**Stretched exponential**

$$p(k) \sim e^{-\alpha k / \bar{k}} k^{-\gamma}$$

**Log-normal**

$$p(k) \sim \frac{e^{-\ln((k-\theta)/m)^2/(2\sigma^2)}}{(k-\theta)\sigma\sqrt{2\pi}}$$



# Degree Assortativity. Statistical vs. Combinatorial Approaches

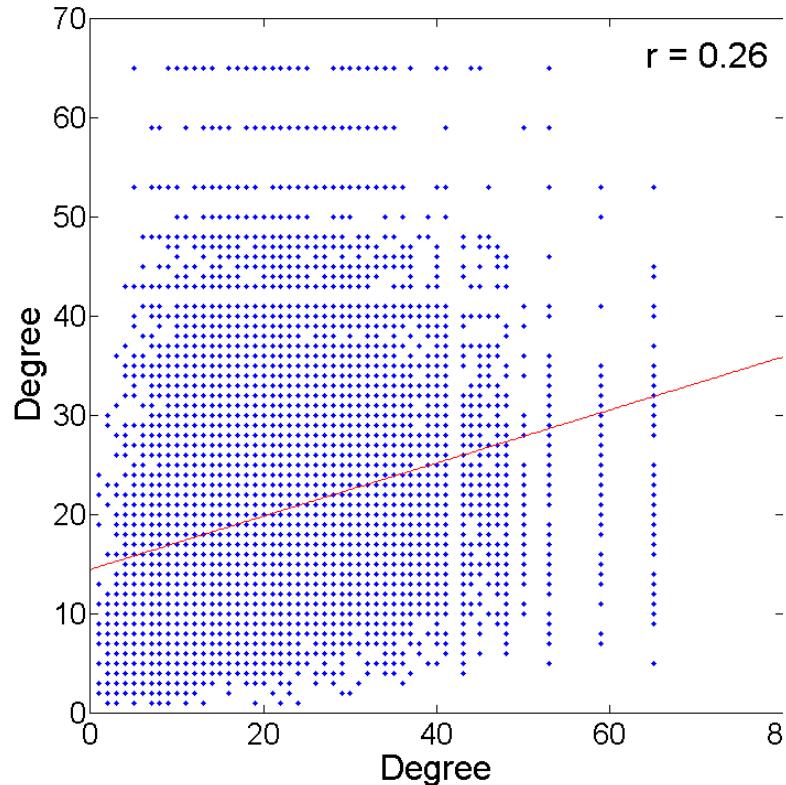
**Professor Ernesto Estrada**  
Department of Mathematics & Statistics  
University of Strathclyde  
Glasgow, UK

[www.estradalab.org](http://www.estradalab.org)

# Degree-degree Correlation

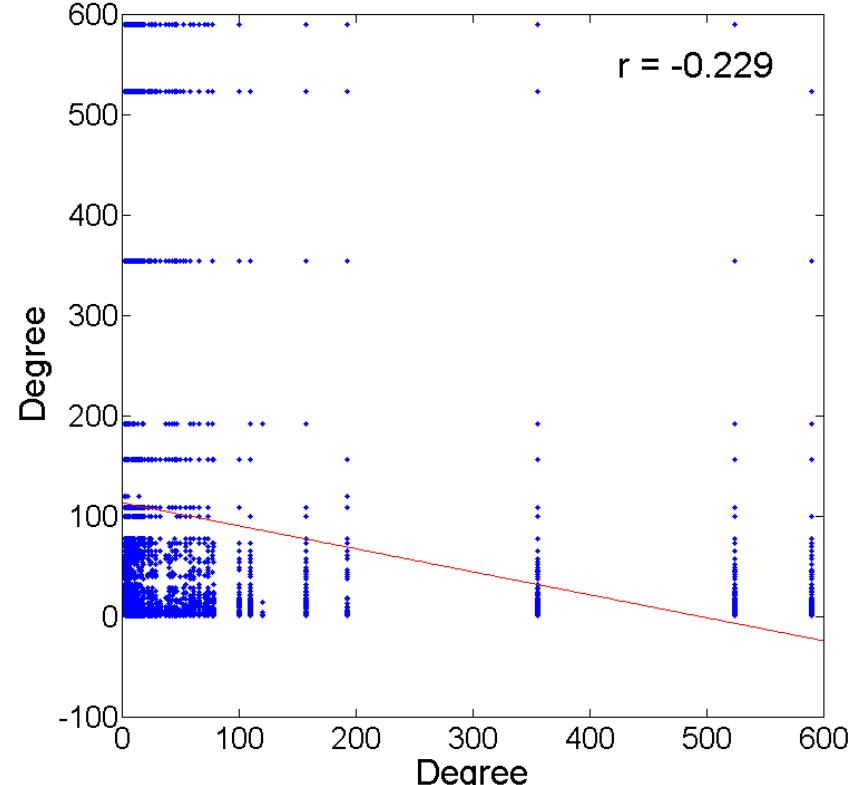
*Statistical approach*

**SOCIAL NETWORK**



*Assortative*

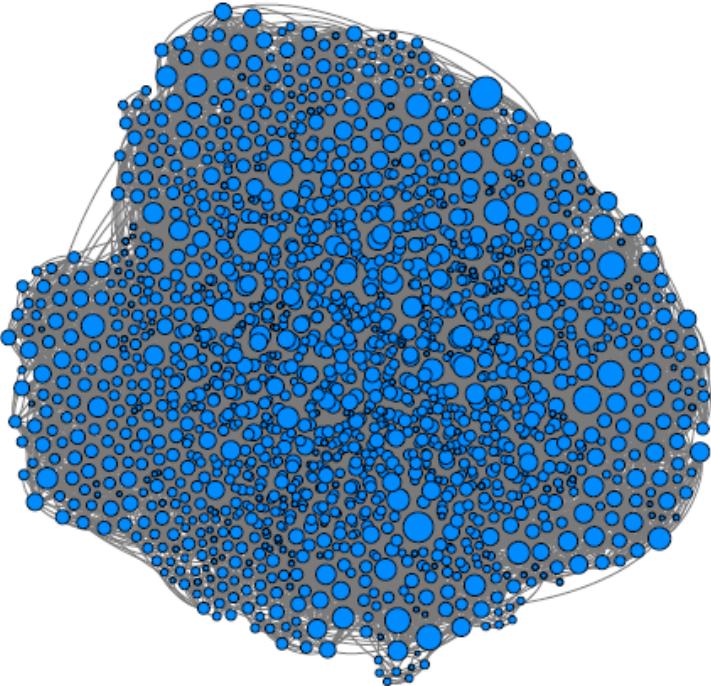
**INTERNET**



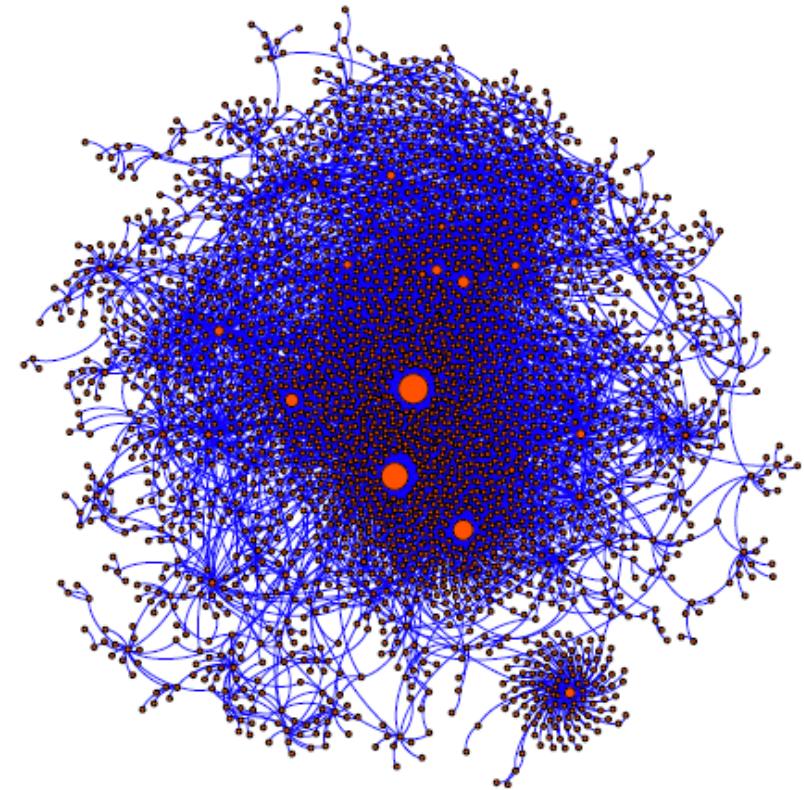
*Disassortative*

# Degree-degree Correlation

*Example*

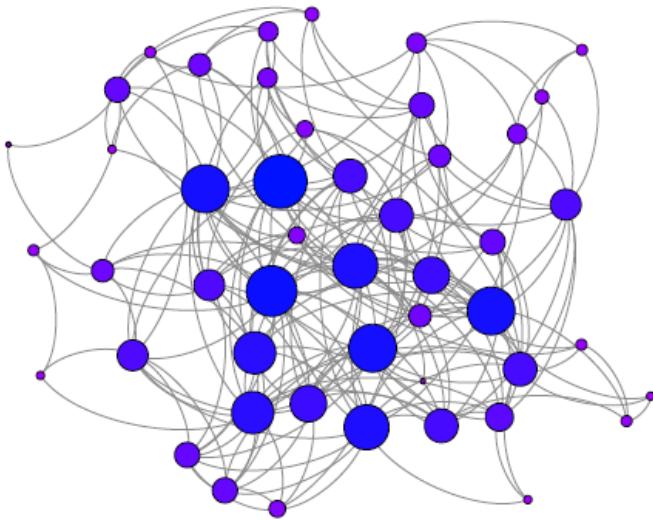


Assortative

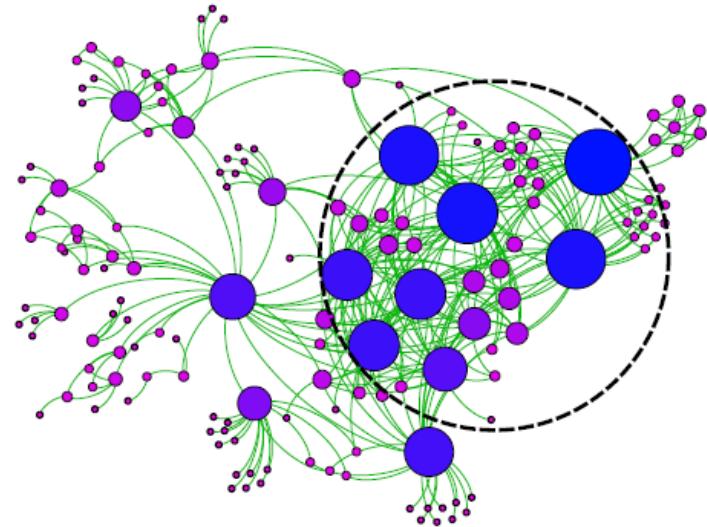


Disassortative

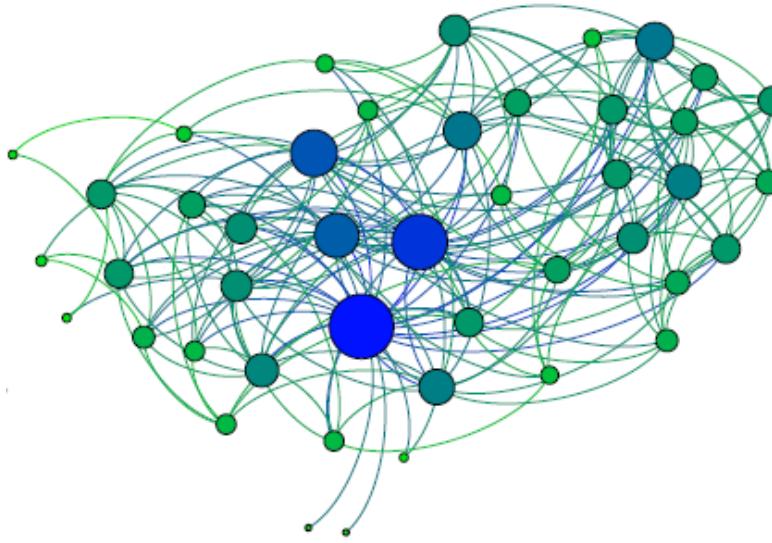
# Degree-degree Correlation



$$r = 0.118$$



$$r = -0.304$$



$$r = -0.153$$

# Degree-degree Correlation

*Statistical approach*

$$r = \frac{\frac{1}{m} \sum_{(i,j) \in E} k_i k_j - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}{\frac{1}{2m} \sum_{(i,j) \in E} (k_i^2 + k_j^2) - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}$$

$$r > 0$$

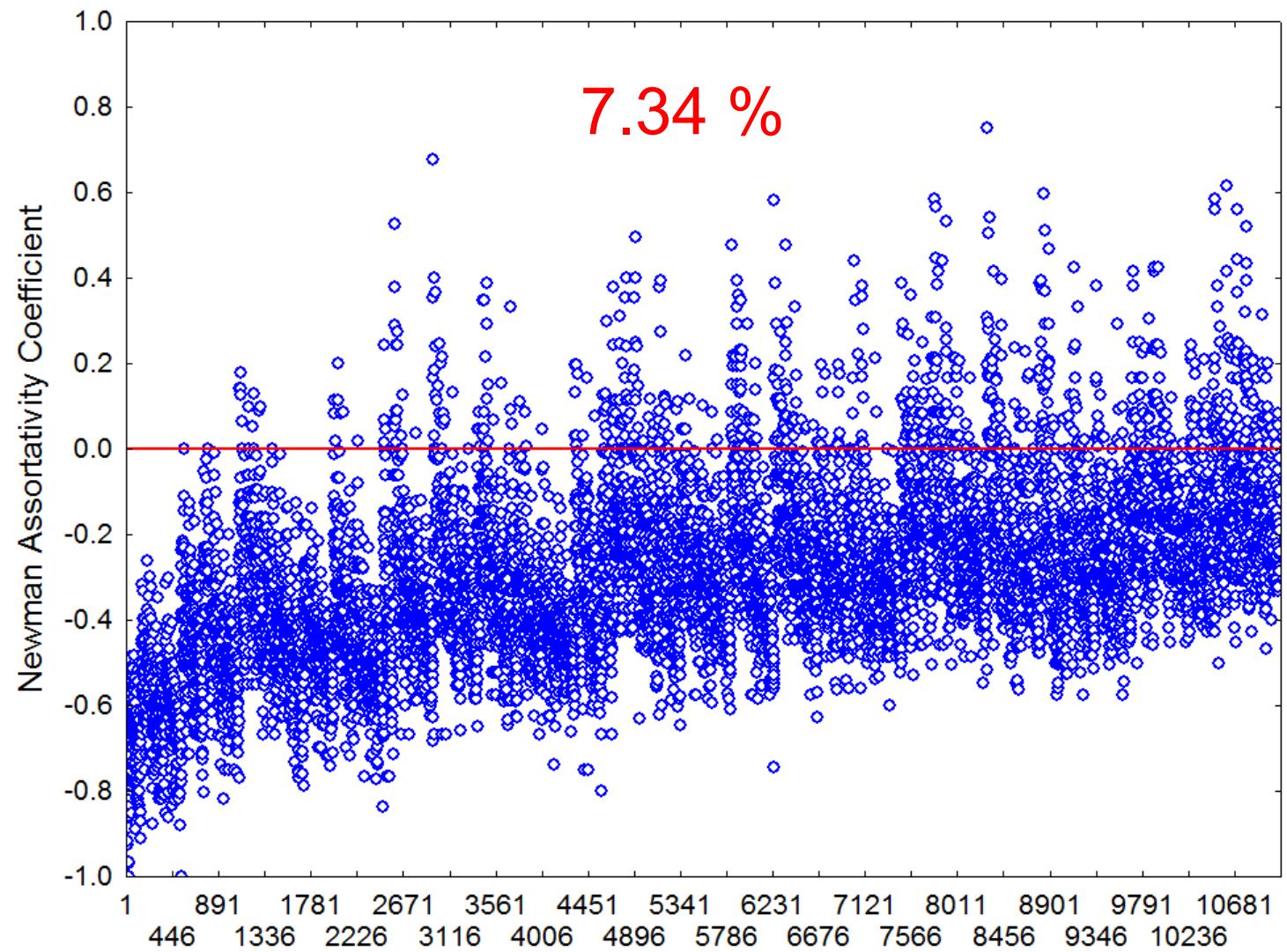
**Assortative**

$$r < 0$$

**Disassortative**

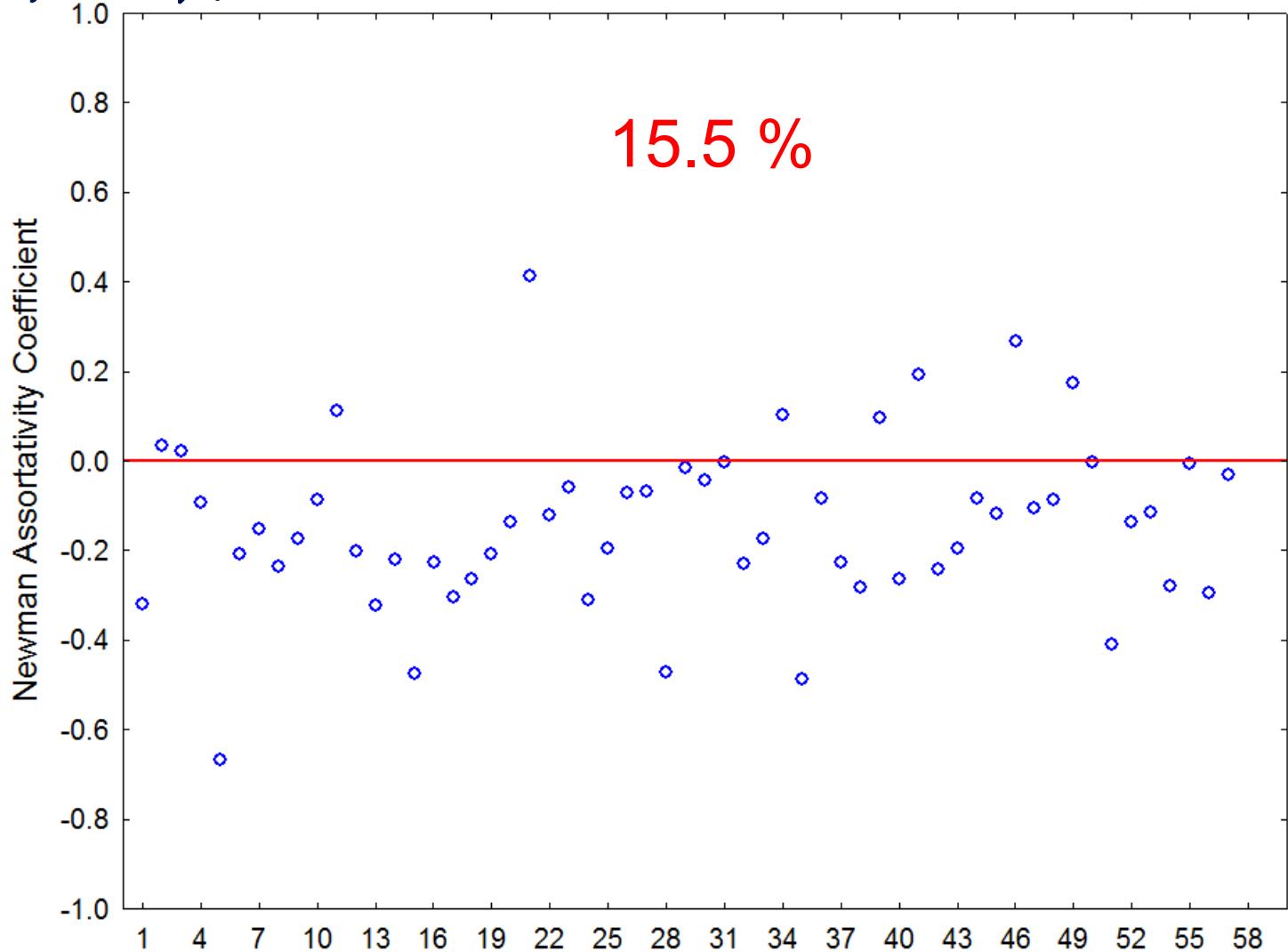
# Degree-degree Correlation

*Small graphs*



# Degree-degree Correlation

*Real-world networks*



# Degree-degree Correlation

*Statistical approach*

$$r = \frac{\frac{1}{m} \sum_{(i,j) \in E} k_i k_j - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}{\frac{1}{2m} \sum_{(i,j) \in E} (k_i^2 + k_j^2) - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}$$

$\sum_{(i,j) \in E} (k_i^2 + k_j^2) = \sum_t k_t^3$ 
↓
 $\left( \sum_{(i,j) \in E} (k_i + k_j) \right)^2 = \left( \sum_t k_t^2 \right)^2$

$\frac{1}{2m} \left[ \sum_t k_t^3 - \frac{1}{2m} \left( \sum_t k_t^2 \right)^2 \right]$ 
↓
 $\frac{1}{4m^2} \left[ \left( \sum_t k_t \right) \left( \sum_t k_t^3 \right) - \left( \sum_t k_t^2 \right)^2 \right]$

# Degree-degree Correlation

*Statistical approach*

$$\frac{1}{4m^2} \left[ \left( \sum_t k_t \right) \left( \sum_t k_t^3 \right) - \left( \sum_t k_t^2 \right)^2 \right]$$

$$\left( \sum_i k_i \right) \left( \sum_i k_i^3 \right) - \left( \sum_i k_i^2 \right)^2 ? \geq 0$$

$$\sum_{i,j} k_i k_j \left( k_i^2 + k_j^2 \right) - 2 \sum_{i,j} \left( k_i k_j \right)^2 ? \geq 0$$

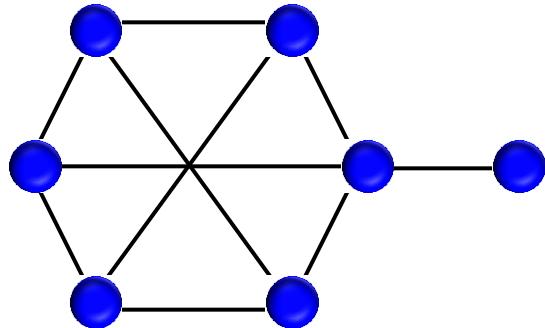
$$\sum_{i,j} k_i k_j \left( k_i^2 + k_j^2 - 2 k_i k_j \right) ? \geq 0$$

$$\sum_{i,j} k_i k_j \left( k_i - k_j \right)^2 \geq 0.$$

# Degree-degree Correlation

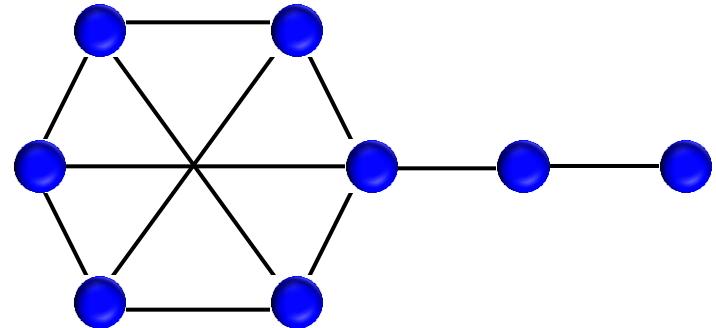
*What is it?*

**Disassortative**



$$r = -0.538$$

**Assortative**



$$r = 0.200$$

# Degree-degree Correlation

*Combinatorial approach*

$$r = \frac{\frac{1}{m} \sum_{(i,j) \in E} k_i k_j - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}{\frac{1}{2m} \sum_{(i,j) \in E} (k_i^2 + k_j^2) - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}$$

$$\begin{aligned} \sum_t k_t^2 &= \sum_t (k_t^2 - k_t + k_t) & \sum_{(i,j) \in E} (k_i + k_j) &= \sum_t k_t^2 \\ &= \sum_t (k_t(k_t - 1)) + \sum_t k_t & \longrightarrow &= 2|P_2| + 2m \\ &= 2|P_2| + 2m; \end{aligned}$$

$$\left( \sum_{(i,j) \in E} (k_i + k_j) \right)^2 = (2|P_2| + 2m)^2$$

# Degree-degree Correlation

*Combinatorial approach*

$$r = \frac{\frac{1}{m} \sum_{(i,j) \in E} k_i k_j - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}{\frac{1}{2m} \sum_{(i,j) \in E} (k_i^2 + k_j^2) - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}$$

$$\begin{aligned} |P_3| &= \sum_{(i,j) \in E} (k_i - 1)(k_j - 1) - 3|C_3| \\ &= \sum_{(i,j) \in E} (k_i k_j) - \sum_{(i,j) \in E} (k_i + k_j) + m - 3|C_3| \end{aligned}$$

$$\sum_{(i,j) \in E} (k_i k_j) = \sum_{(i,j) \in E} (k_i + k_j) - m + 3|C_3| + |P_3|$$

$$= m + 2|P_2| + |P_3| + 3|C_3|$$

# Degree-degree Correlation

*Combinatorial approach*

$$r = \frac{\frac{1}{m} \sum_{(i,j) \in E} k_i k_j - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}{\frac{1}{2m} \sum_{(i,j) \in E} (k_i^2 + k_j^2) - \left( \frac{1}{2m} \sum_{(i,j) \in E} (k_i + k_j) \right)^2}$$

$$\begin{aligned} |S_{1,3}| &= \sum_t \binom{k_t}{3} = \frac{1}{6} \sum_i k_t (k_t - 1)(k_t - 2) \\ &= \frac{1}{6} \sum_t k_t^3 - \frac{1}{2} \sum_t k_t^2 + \frac{1}{3} \sum_t k_t \end{aligned}$$

$$\begin{aligned} \sum_t k_t^3 &= 6|S_{1,3}| + 3 \sum_t k_t^2 - 2 \sum_t k_t \\ &= 6|S_{1,3}| + 6|P_2| + 2m \end{aligned}$$

$$\sum_{(i,j) \in E} (k_i^2 + k_j^2) = 6|S_{1,3}| + 6|P_2| + 2m$$

# Degree-degree Correlation

*Combinatorial approach*

$$r = \frac{\frac{1}{m} (m + 2|P_2| + |P_3| + 3|C_3|) - \frac{1}{4m^2} (2|P_2| + 2m)^2}{\frac{1}{2m} (6|S_{1,3}| + 6|P_2| + 2m) - \frac{1}{4m^2} (2|P_2| + 2m)^2}$$

$$r = \frac{|P_3| + 3|C_3| - \frac{|P_2|^2}{m}}{3|S_{1,3}| + |P_2| - \frac{|P_2|^2}{m}}$$

$$|P_{r/s}| = |P_r| / |P_s|$$

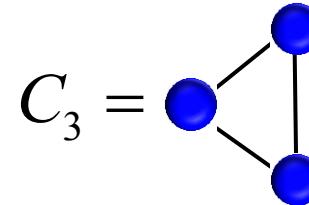
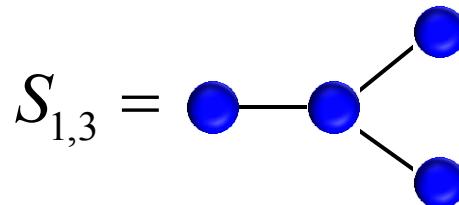
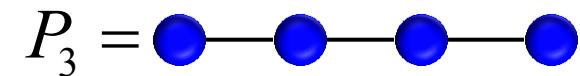
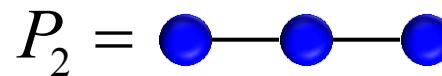

$$r = \frac{|P_2| \left( |P_{3/2}| + \frac{3|C_3|}{|P_2|} - |P_{2/1}| \right)}{3|S_{1,3}| + |P_2| (1 - |P_{2/1}|)}$$

$$r = \frac{|P_2| (|P_{3/2}| + C - |P_{2/1}|)}{3|S_{1,3}| + |P_2| (1 - |P_{2/1}|)}$$

# Degree-degree Correlation

*Combinatorial approach*

$$r = \frac{|P_2|(|P_{3/2}| + C - |P_{2/1}|)}{3|S_{1,3}| + |P_2|(1 - |P_{2/1}|)}$$
$$|P_{r/s}| = |P_r| / |P_s|$$
$$C = 3|C_3| / |P_2|$$



# Degree-degree Correlation

*Combinatorial approach*

**Remark:** Because we have already proved that the denominator of the Pearson correlation coefficient is always nonnegative, the assortativity/disassortativity of a network is determined by the sign of the numerator.

**Assortative**

$$r > 0$$

$$|P_{2/1}| < |P_{3/2}| + C$$

**Disassortative**

$$r < 0$$

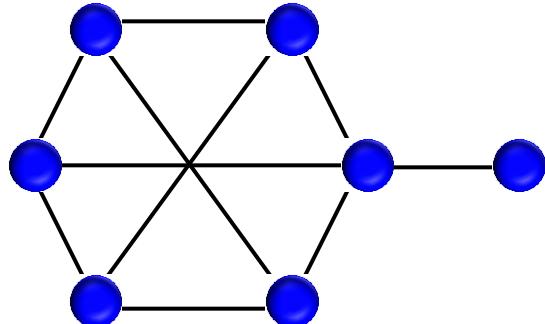
$$|P_{2/1}| > |P_{3/2}| + C$$

# Degree-degree Correlation

*Combinatorial approach*

**DISASSORTATIVE**

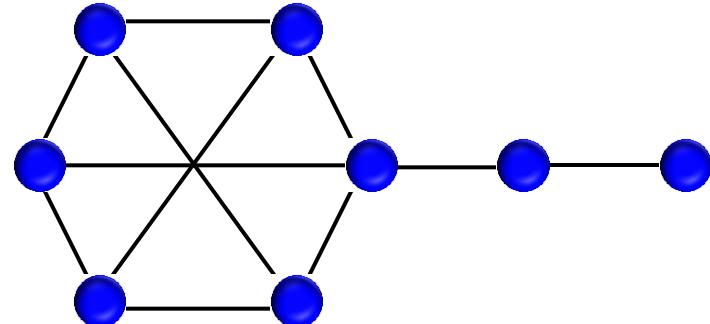
$$|P_{2/1}| > |P_{3/2}| (C = 0)$$



$$r = -0.538$$

**ASSORTATIVE**

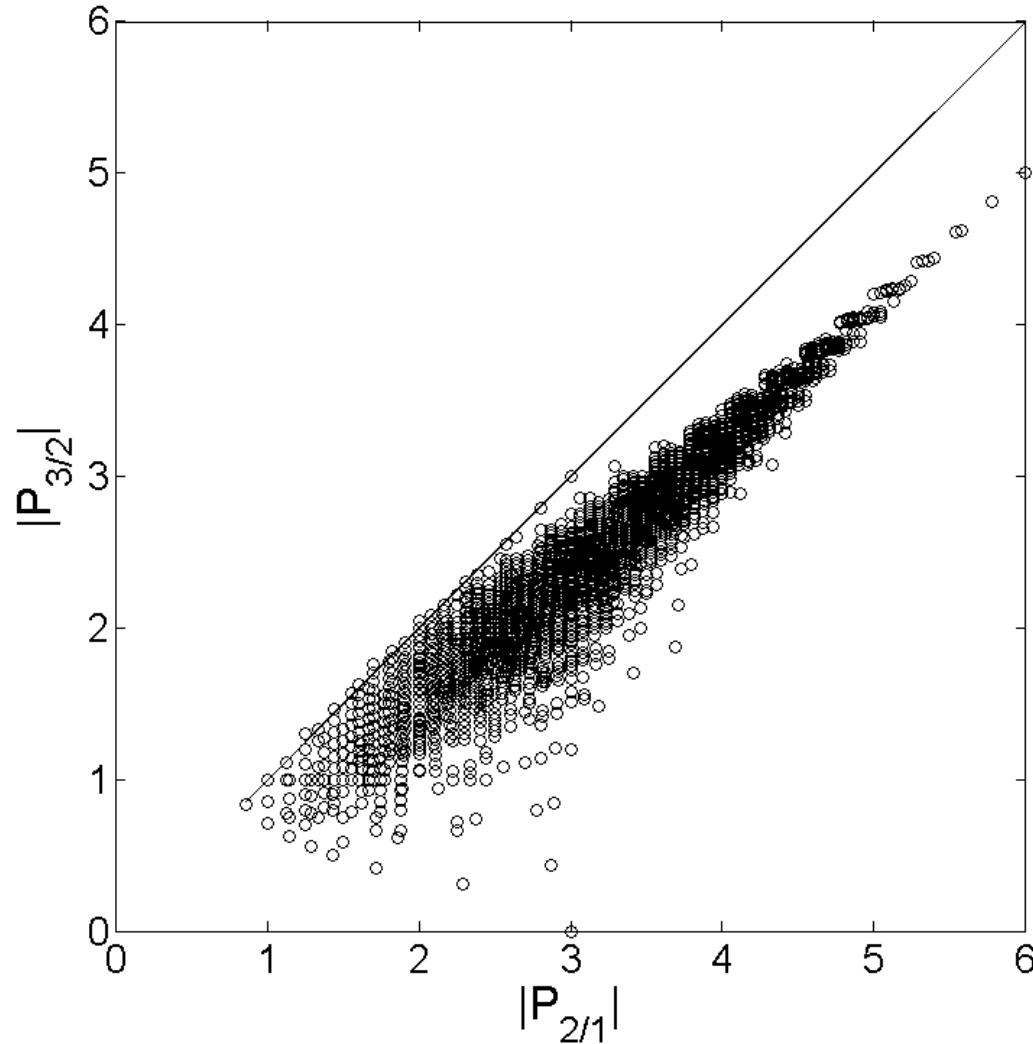
$$|P_{2/1}| < |P_{3/2}| (C = 0)$$



$$r = 0.200$$

# Degree-degree Correlation

*Combinatorial approach*



# Degree-degree Correlation

$$r = \frac{|P_2|(|P_{3/2}| + C - |P_{2/1}|)}{3|S_{1,3}| + |P_2|(1 - |P_{2/1}|)}$$

TABLE I. Relative branching ( $|P_{2/1}|$ ), transitivity ( $C$ ), intermodular connectivity ( $|P_{3/2}|$ ) , and assortativity coefficient for real-world networks.

Network	$ P_{2/1} $	$ P_{3/2} $	$C$	$r$
Prison	4.25	< (4.09	+ 0.288)	
Protein residue	4.41	< (4.45	+ 0.417)	
St. Marks	10.54	< (10.46	+ 0.291)	
Geom	17.42	< (22.09	+ 0.224)	
Corporate	19.42	< (20.60	+ 0.498)	
Roget	9.55	< (10.08	+ 0.134)	
Jazz	127.30	< (144.84	+ 0.771)	
Zachary	6.77	> (4.49	+ 0.256)	
Drugs	14.58	> (12.84	+ 0.368)	
Transcription	12.51	> (3.01	+ 0.016)	
Bridge Brook	22.42	> (17.31	+ 0.191)	
USAir97	43.36	> (36.97	+ 0.396)	
Internet	91.00	> (11.53	+ 0.015)	