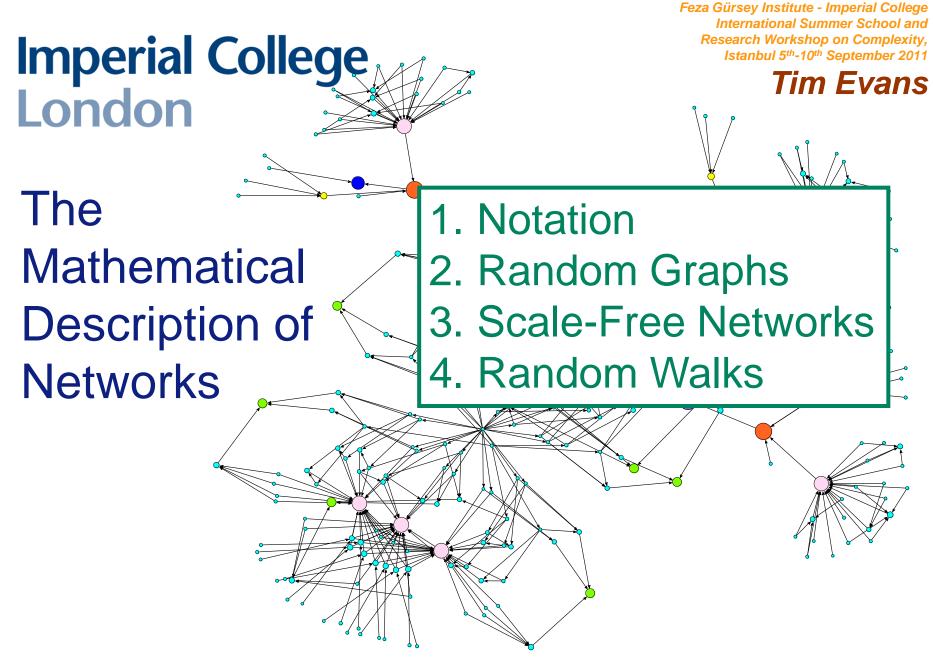
Feza Gürsey Institute - Imperial College International Summer School and Research Workshop on Complexity, Istanbul 5th-10th September 2011

Tim Evans

Imperial College

The Mathematical Description of Networks

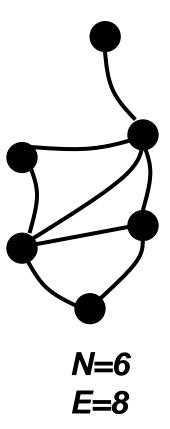


Notation

I will focus on *Simple Graphs* with multiple edges allowed

(no values or directions on edges, no values for vertices)

- **N** = number of vertices in graph
- *E* = number of edges in graph

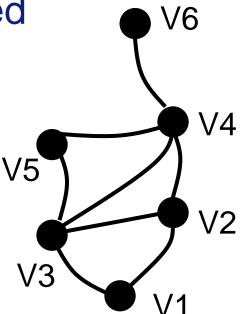


Notation - Adjacency Matrix

The Adjacency Matrix A_{ij} is

- 1 if vertices *i* and *j* are attached
- **0** if vertices *i* and *j* are not attached

vertices	V1	V2	V3	V4	V5	V6
V1	0	1	1	0	0	0
V2	1	0	1	1	0	0
V3	1	1	0	1	1	0
V4	0	1	1	0	1	1
V5	0	0	1	1	0	0
V6	0	0	0	1	0	0



Notation – degree of a vertex

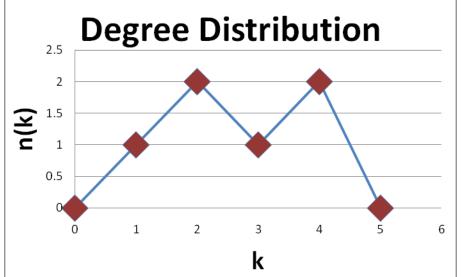
Number of edges connected to a vertex is called the *degree* of a vertex

- **k** = degree of a vertex
- <*k*> = average degree = (2E / N)

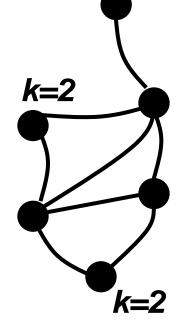
Degree Distribution
 n(k) = number of vertices with degree k
 p(k) = *n(k)/N* = normalised distribution
 = probability a vertex chosen at random (uniformly) has degree k

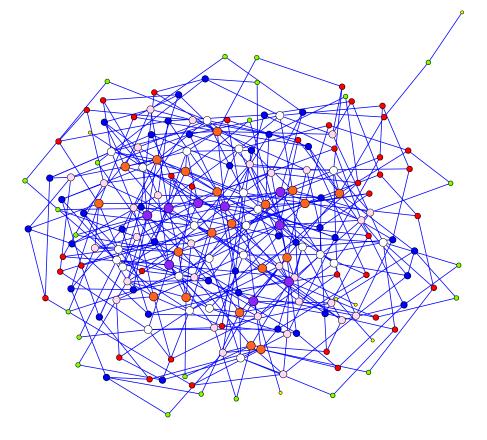
Notation – degree distribution

Degree Distribution is n(k) = number of vertices withdegree k



The normalised degree distribution is p(k) = n(k)/N = probability a vertex chosen at random (uniformly) hasdegree k





How to excite a Mathematician – give them the simplest model

RANDOM GRAPHS

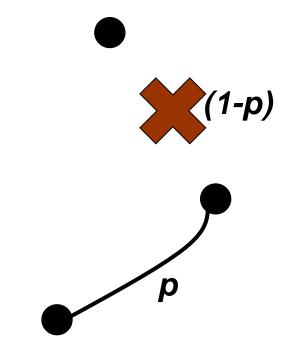


Classical Random Graphs [Solomonoff-Rapoport '51, Erdős-Réyni '59]

For every pair of distinct vertices add a single edge with probability

$$p = \langle k \rangle / (N-1)$$
,

otherwise with probability (1-p) no edge is added



Classical Random Graph

Gives Binomial Degree Distribution

$$p(k) = \binom{\Omega}{k} p^k (1-p)^{\Omega-k}$$

with $\Omega = N(N-1)/2$ number of possible edges and $\langle k \rangle = (N-1)p$

Classical Random Graph

• which is an approximate Normal Distribution

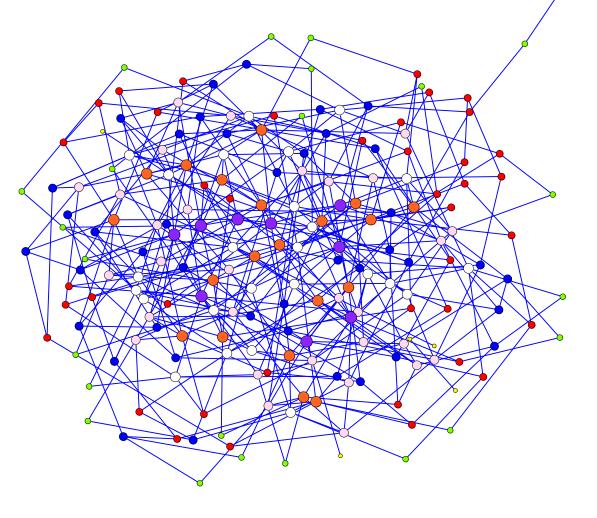
$$p(k) \approx \frac{\exp(\langle k \rangle) \langle k \rangle^k}{k!}$$

with <*k*>=(*N*-1)*p*

Exponential cutoff so no 'hubs'
 e.g. *N=10⁶*, *<k>=4.0*, typically has *k <17*

Example of Classical Random Graph

- N=200 <k>~4.0
- *k* < 11
- In figure
 vertex size
 ∞ k
- Diffuse, no tight cores





Generalised Random Graphs – The **Molloy-Reed** Construction [1995,1998]

- i. Fix **N** vertices
- ii. Attach k stubs to each vertex, where k is drawn from given distribution p(k)
- iii. Connect pairs of stubs chosen at random

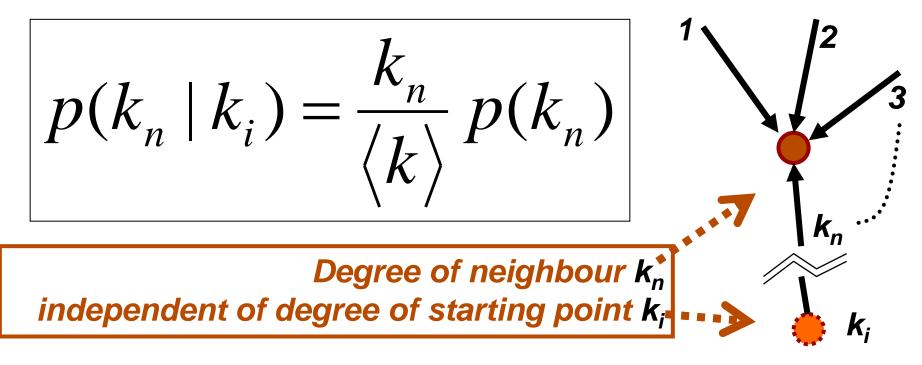
No Vertex-Vertex Correlations

Generalised Random Graphs have given *p(k)* but otherwise completely random in particular -

Properties of all vertices are the same

For any given source vertex, the properties of neighbouring vertices independent of properties of the source vertex Random Walks on Random Graphs The degree distribution of a neighbour is not simply *p(k)*

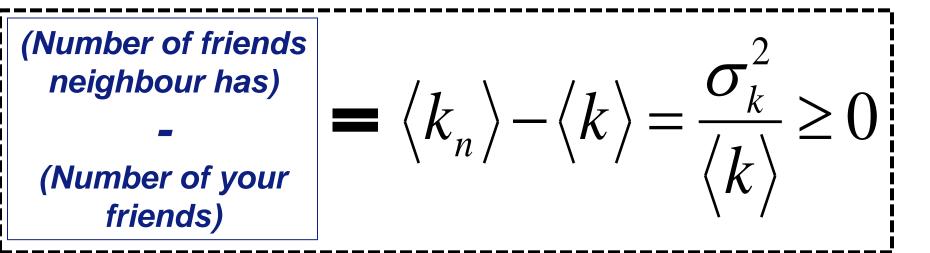
You are more likely to arrive at a high degree vertex than a low degree one





A random friend is more popular than you

$$\langle k_n \rangle = \sum_{k_n} p(k_n \mid k_i) = \frac{\langle k^2 \rangle}{\langle k \rangle}$$

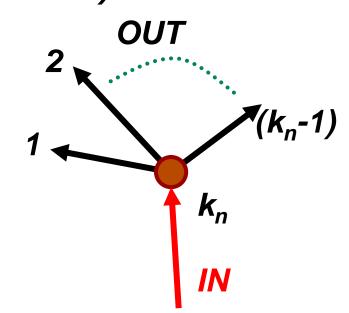


Give a random friend that life saving vaccine (if social networks are random and uncorrelated) Length of Random Walks on Random Graphs Suppose we follow a random walk where we never go back along the edge we just arrived on, then for infinite graphs $(N \rightarrow \infty)$

 \Rightarrow Walks always end if $\langle \mathbf{k}_n \rangle < 2 \Leftrightarrow \text{No GCC}$

 $\Rightarrow \text{Walks never end if} \\ \langle \mathbf{k}_n \rangle > 2 \Leftrightarrow \text{GCC}$

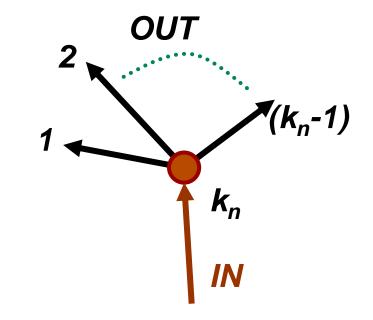
(GCC= Giant Connected Component)



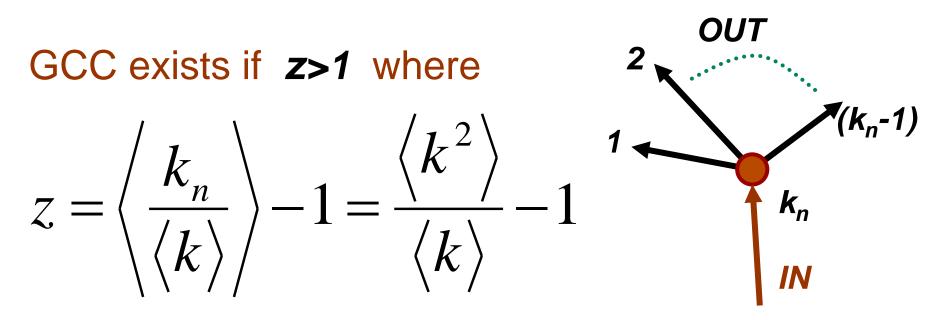
Length of Random Walks on Random Graphs PROVIDED there are no loops. True for sparse random graphs in limit of infinite size $(N \rightarrow \infty)$

- \Rightarrow Walks always end if $\langle \mathbf{k}_n \rangle < 2 \Leftrightarrow \text{No GCC}$
- $\Rightarrow \text{Walks never end if} \\ \langle \mathbf{k}_n \rangle > 2 \Leftrightarrow \text{GCC}$





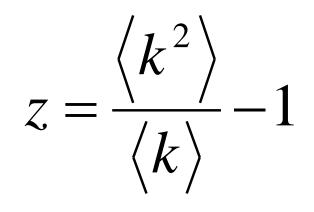
GCC (Giant Connected Component) transition GCC= Giant Connected Component, where a finite fraction of vertices in infinite graph are connected



= Fractional measure of how much more popular your friends are

Other properties of General Random Graphs

All global properties depend on same



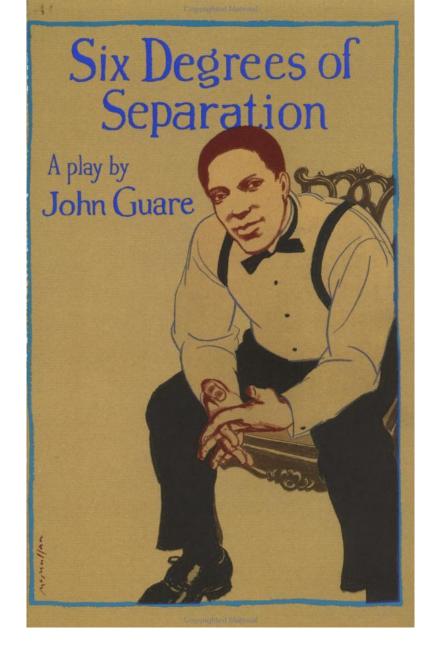
e.g. GCC size, component distribution, average path lengths Average Path Length in MR Random Graph

 For *any* random graph has an average shortest length which scales as

$$\langle d \rangle \approx \frac{\ln(N)}{\ln(z)} + c$$

Six Degrees of Separation [John Guare 1990]

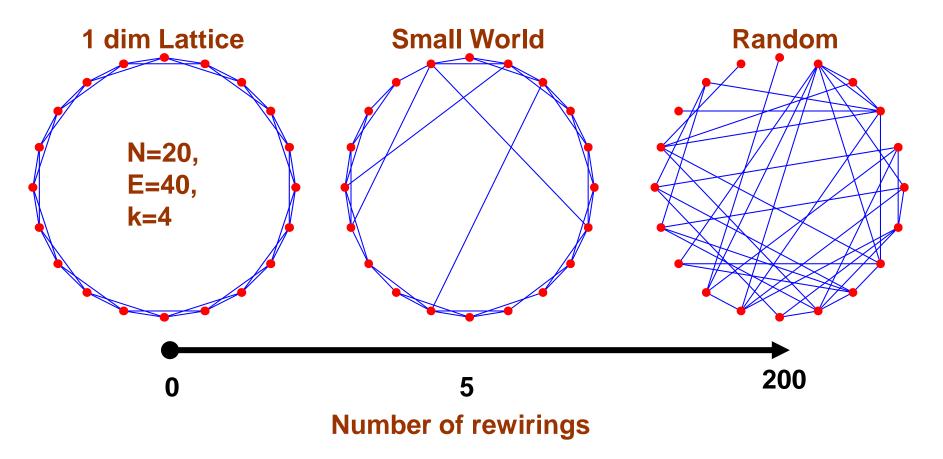
"I read somewhere that everybody on this planet is separated by only six other people. Six degrees of separation."



Small World

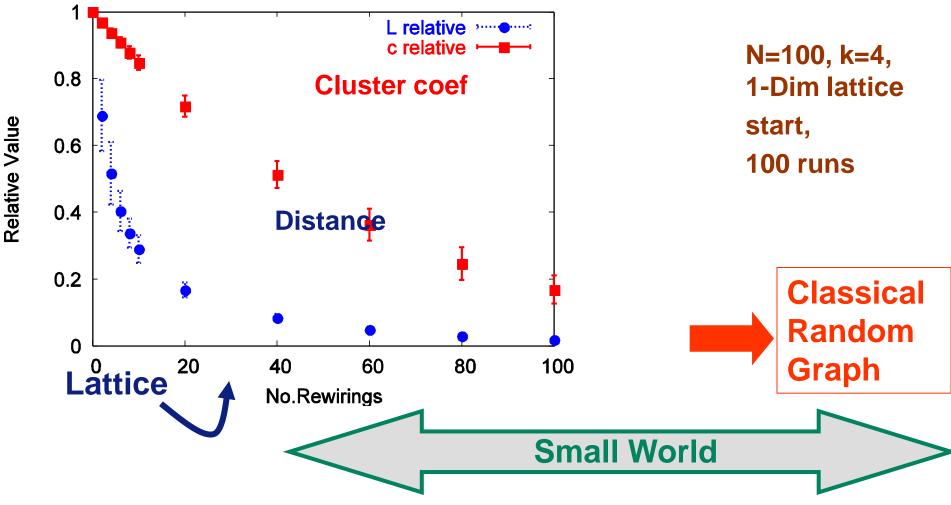
- A Small World network is one where the average shortest distance is <d> ~ O(In(N))
- All random graphs are small world
- In fact most complex networks are small world
- c.f. a regular lattice in d-dimensions where the distance scales as $\langle d \rangle \sim O(N^{1/d})$

Watts and Strogatz's Small World Model (1998) Start with lattice, pick random edge and rewire – move it to two link two new vertices chosen at random.



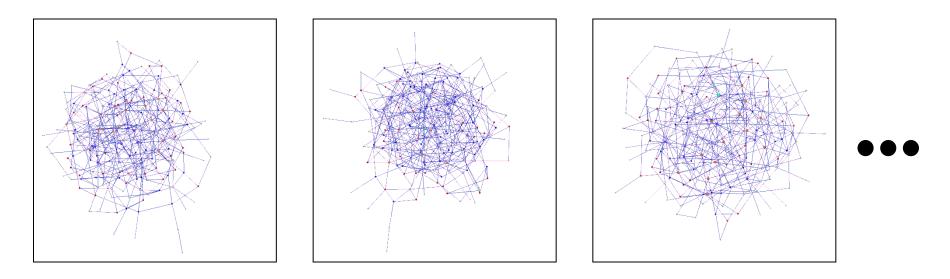
Clustering and Length Scale in WS network

- Average distance drops very quickly,
- Loss of local lattice structure much slower

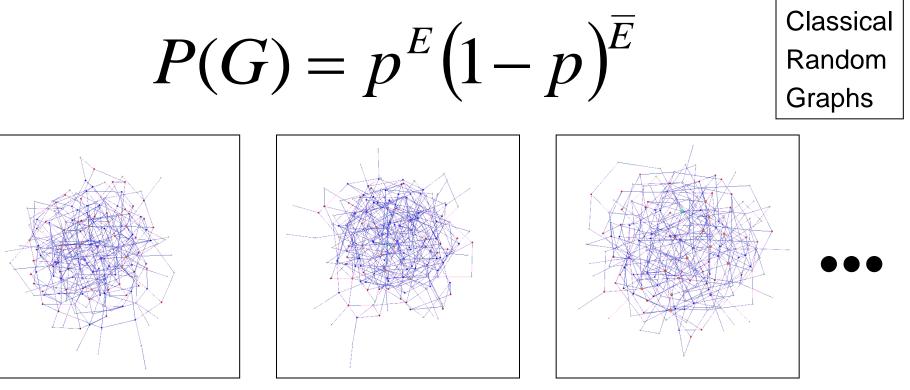


Ensembles of Graphs

Mathematically we *do not* consider a single instance of a random graph but an *ensemble* of random graphs



Ensembles of Graphs e.g. The probability of creating a particular simple graph with E edges and \overline{E} empty edges is



Ensemble Averages

Averages of quantities are strictly over both a) different graphs and b) over some element of a graph e.g. vertices

 $=\sum P$

Exponential Random Graphs (p* models)

General ensemble of graphs, those with highest probability obey any given constraints

$$\langle f \rangle = \sum_{G} P(G) f(G)$$

 $P(G) = \frac{1}{Z} e^{H(G)}$

H(*G*) chosen so that graphs with preferred properties are most likely

Example Graph Hamiltonians H(G)

• $H(G) = \beta E$ Classical random graph with *p***=2E/(N(N-1))**

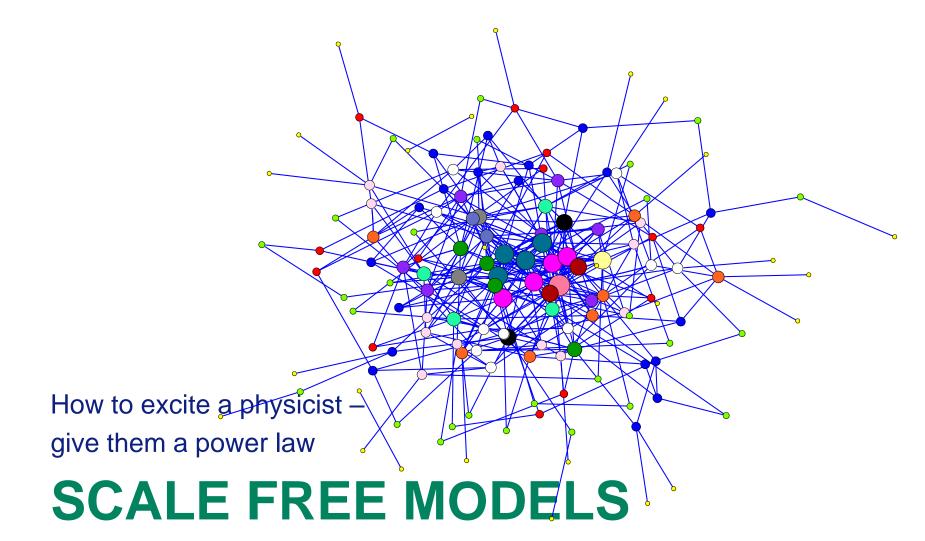
•
$$H(G) = \sum_{v \in V} \beta_v k_v$$

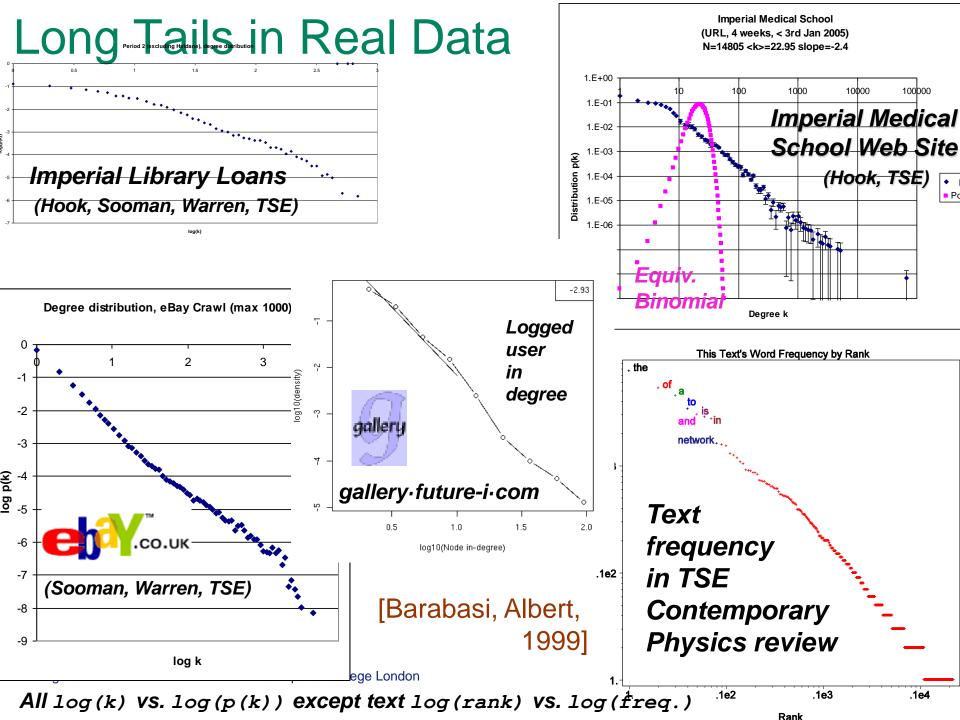
Random Graph with given degree distribution.

In both cases Lagrange multipliers β , β_v fixed by specifying desired values of $\langle E \rangle$ and $\langle k_v \rangle$

Summary of Random Graphs

- Calculations work because
 - lack of correlations between vertices
 - few loops for large sparse graphs, graphs are basically trees
- Accessible analytically so can suggest typical behaviour even if very weak e.g. diameter vs N
- These can be reasonable approximations for many theoretical models
- Probably not for real world so then use these as a *null model*.





Growth with Preferential Attachment

11(K

2/(2E)

5/(2E)

4/(2E)

2/(2E)

Result:

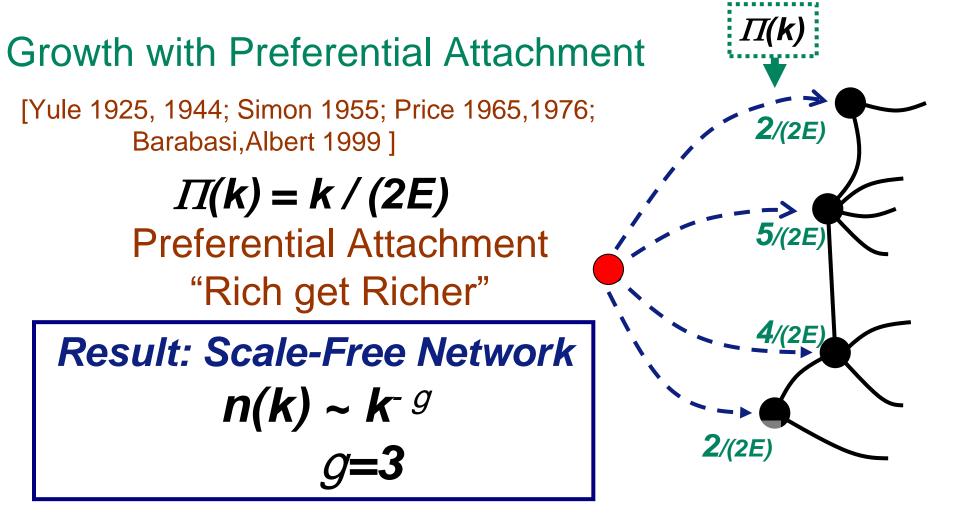
Scale-Free

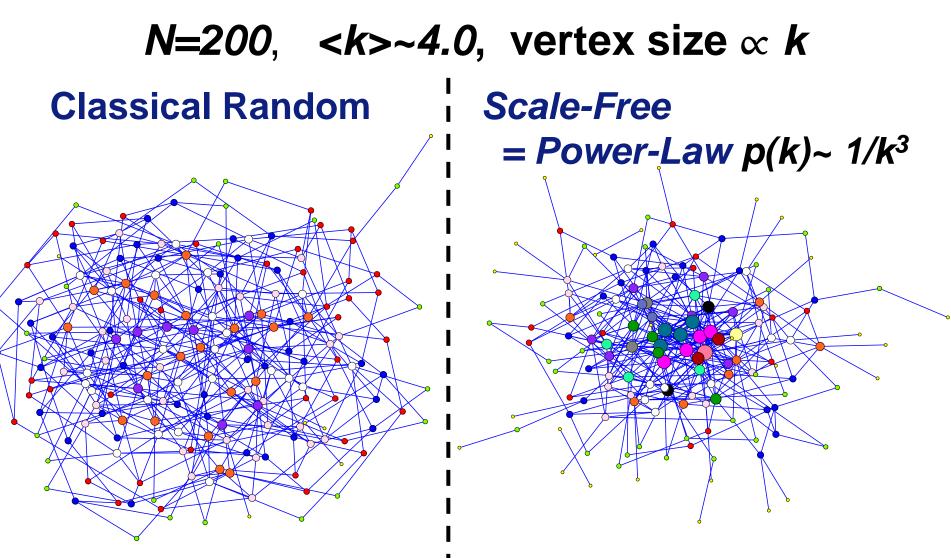
n(k) ~ **k**^{-g}

[Yule 1925, 1944; Simon 1955; Price 1965,1976; Barabasi,Albert 1999]

- Add new vertex attached to one end of *m=¹/₂<k>* new edges
- 2. Attach other ends to existing vertices chosen with by picking random end of an existing edge chosen randomly, so probability is

Π(k) = k / (2E) Preferential Attachment "Rich get Richer"





Tight core of large hubs

 $k_{max} = O(N^{1/2})$

Diffuse, small degree vertices k_{max}=O(ln(N)) **Master Equation Approach**

- Let *n(k,t)* represent the *average* number of vertices at time *t*. (I should really use <*n(k,t)*>)
- Again average means we look at an ensemble of such networks.

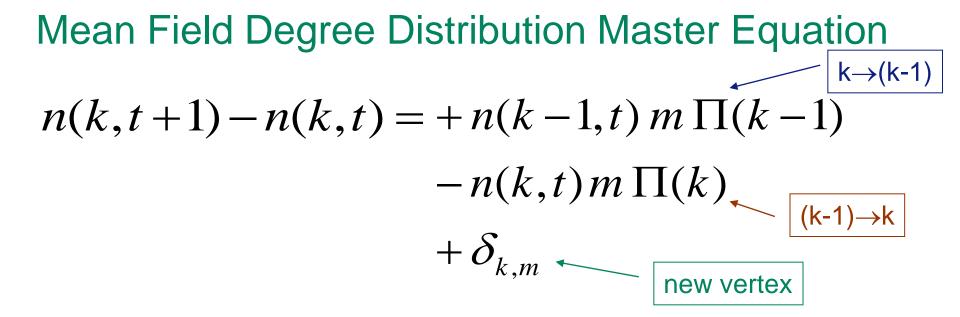
The master equation the equation for evolution of the degree distribution averaged over different instances of network in the ensemble *n(k,t)* to *n(k,t+1)*

Master Equation Processes

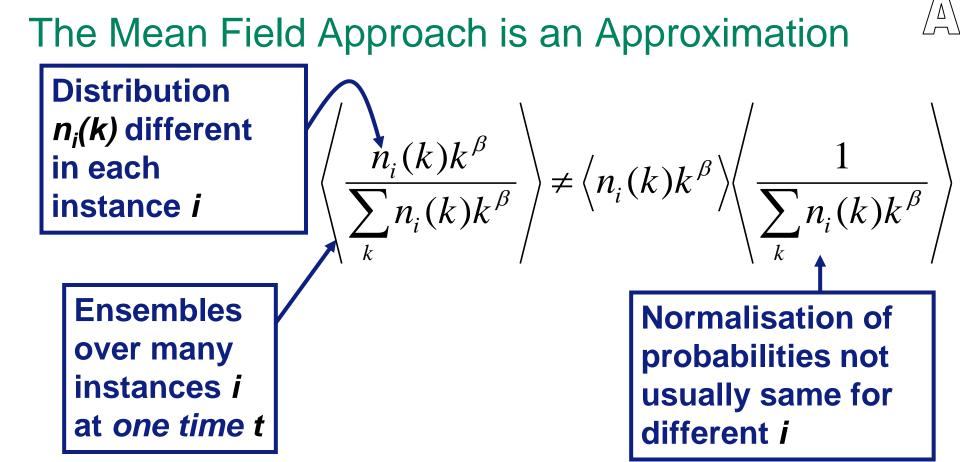
n(k,t) changes in one of three ways:-

- Increases as we add an edge to existing $k \rightarrow (k-1)$.
- Decreases as we add an edge to existing (k-1)
 vertex of degree k.
- Number of vertices of degree k=m= ½<k> always increase by 1 as add new vertex.





$\Pi(\mathbf{k}) = \text{Probability of attaching to a vertex of} \\ \text{degree } \mathbf{k} \\ \infty \mathbf{k} \text{ in simplest preferential attachment} \\ \text{models} \end{aligned}$



If $\Pi(\mathbf{k})$ is a function of degree k then normalisation of this probability is different in each instance of a network in the ensemble at a single time t.

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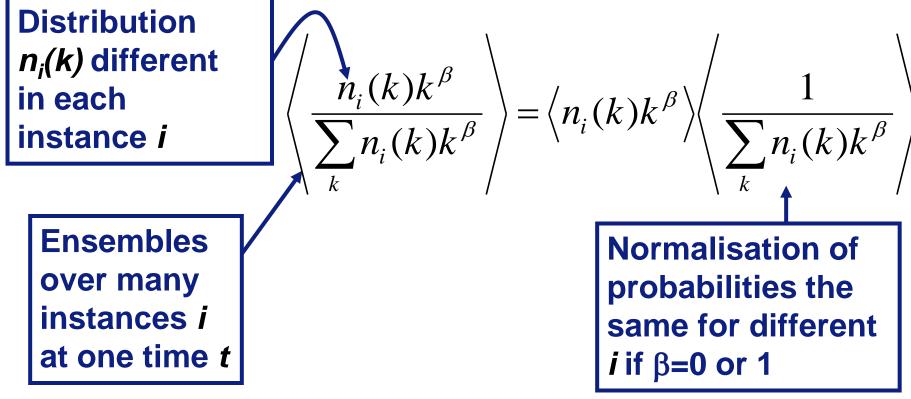
Ensemble Invariants $n(k,t+1) - n(k,t) = +n(k-1,t)\Pi(k-1)$ $-n(k,t)\Pi(k)$ $+\delta_{k,m}$

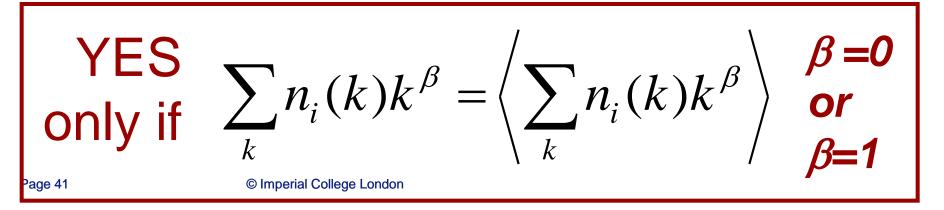
Adding one vertex and $m = \frac{1}{2} < k >$ edges at each time means that the

- number of edges E(t) = mt + E(0)
- number of vertices N(t) = t + N(0)
 are the same for all instances of network in the ensemble at any one time t.

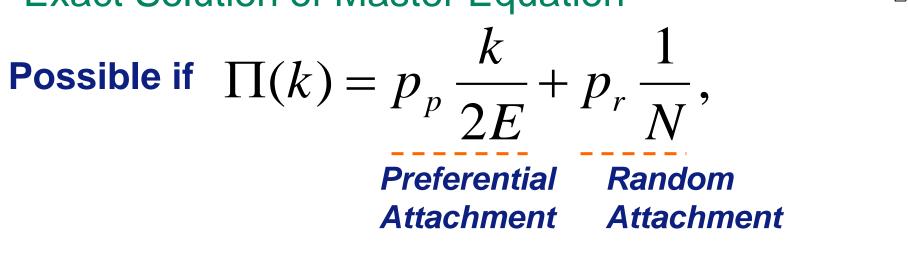


The Mean Field Approach Can Be Exact









- Note probability so $0 \le \Pi(k) \le 1$ & $p_p + p_r = 1$
- Lowest degree is $1 \le k_{\min} \le m = \langle k \rangle / 2$
- Thus $0 \le p_p \le \frac{\langle k \rangle}{\langle k \rangle k_{\min}} \le 1$

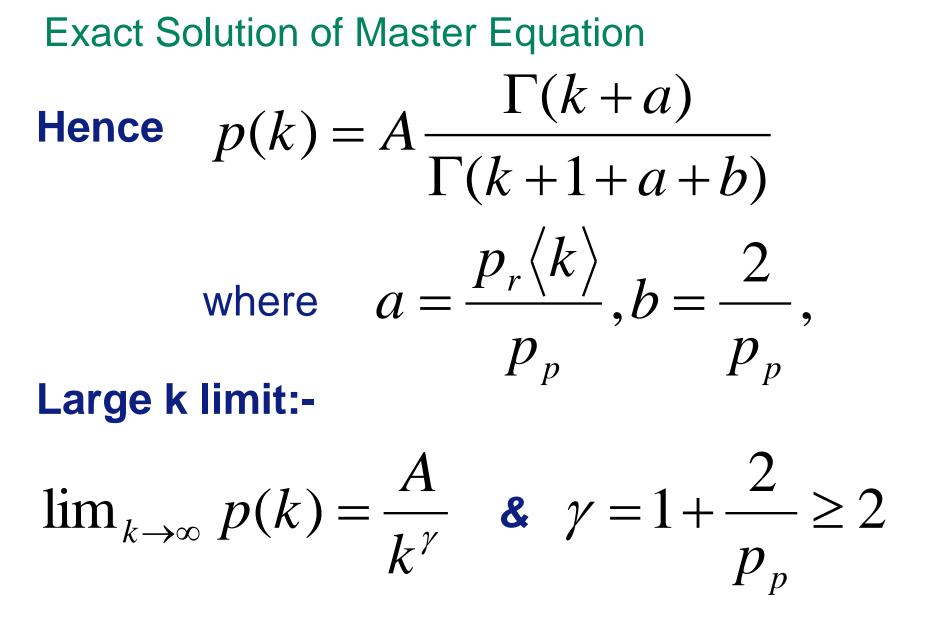
Exact Solution of Master Equation

Look for asymptotic solutions

$$n(k,t) = N(t)p(k)$$

• Find for *k* > *m* = ½<*k*>

$$\frac{p(k)}{p(k-1)} = \frac{N.\Pi(k-1)}{1+N.\Pi(k)} = \frac{(1/2) p_p(k-1) + p_r m}{1+(1/2) p_p k + p_r m}$$



Scale-Free Growing Model comments

- Illustrates use of master equations and their approximations ⇒ statistical physics experience
- Exact solutions for ensemble average asymptotic value of degree distribution p(k) if $\Pi(k) = (1 - p_r) \frac{k}{2E} + p_r \frac{1}{N}$,
- Interpretation of parameters $p_p > 1$ allowed
- Finite Size effects? real networks are mesoscopic [TSE, Saramäki 2004]
- Fluctuations in ensemble?
- Network not essential *k*=frequency of previous choices
- Growth not essential network rewiring $\Rightarrow g \sim 1.0$ [Moran model, see TSE,Plato, 2008]

Scale-Free in the Real World Attachment probability used was

$$\Pi(k) = p_p \frac{k}{2E} + p_r \frac{1}{N},$$

BUT if $\lim_{k\to\infty} P(k) \propto k^a$ for any $a \neq 1$ then a power law degree distribution is not produced!

Preferential Attachment for Real Networks [Saramäki, Kaski 2004; TSE, Saramäki 2004]

- Add a new vertex with ½<k> new edges
- 2. Attach to existing vertices, found by executing a random walk on the network of *L* steps

→Probability of arriving at a vertex
Walk Here
∞ number of ways of arriving at vertex
= k, the degree
→ Preferential Attachment ⇒ g=3
✓ Can also mix in random attachment with probability p,)



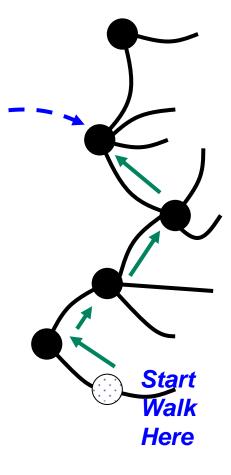


Preferential Attachment for Real Networks

→Probability of arriving at a vertex
 ∞ number of ways of
 arriving at vertex
 = k, the degree

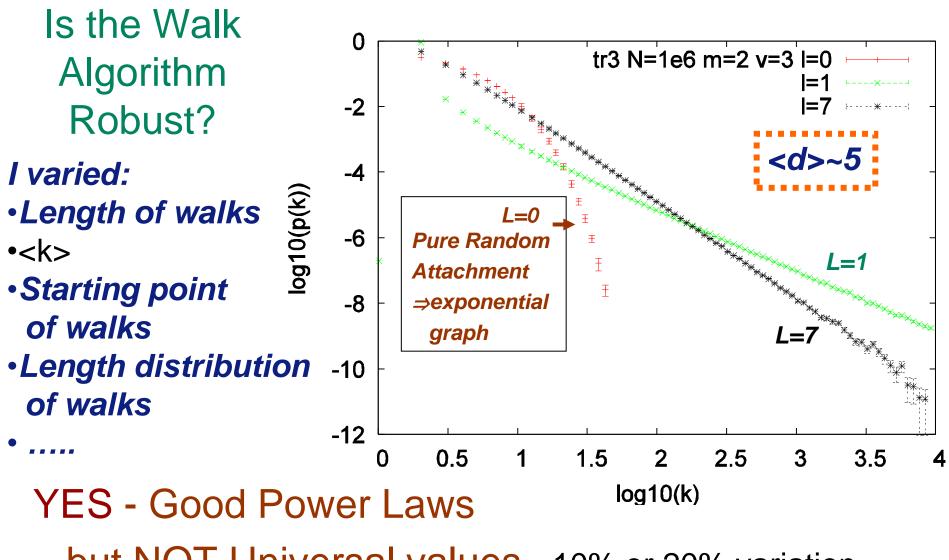
 \Rightarrow Preferential Attachment $\Rightarrow \gamma=3$

Can also mix in random attachment with probability p_r



Naturalness of the Random Walk algorithm

- Gives preferential attachment from any network and hence a *scale-free network*
- Uses only LOCAL information at each vertex
 - Simon/Barabasi-Albert models use global information in their normalisation
- Uses structure of Network to produce the networks
 - a self-organising mechanism
 e.g. informal requests for work on the film actor's social network
 e.g. finding links to other web pages when writing a new one

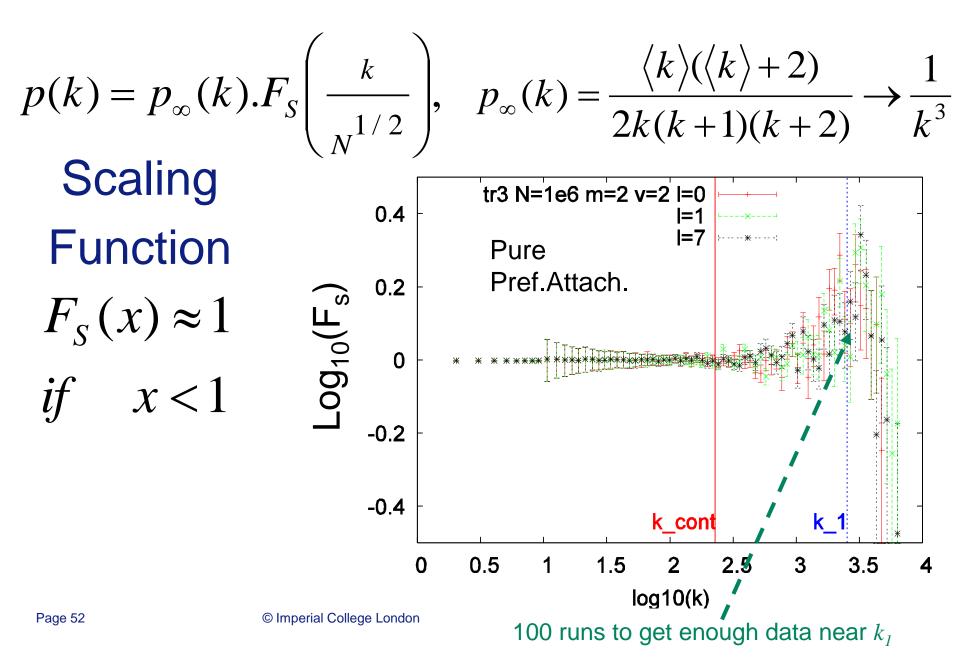


but NOT Universal values - 10% or 20% variation

Finite Size Effects Networks are *mesoscopic* systems

In practice a network of *N* ~ 1 million is still *not large* since many quatitities scale with the logarithm of system size e.g. Diameter scales as *log(N)* ~ 6.

Finite Size Effects for pure preferential attachment

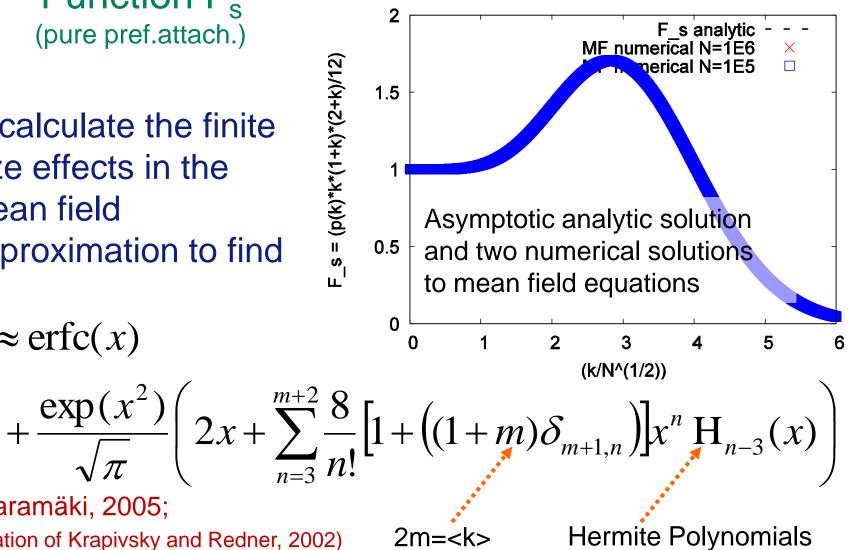


Mean Field Exact Finite Size Scaling Function F_s (pure pref.attach.)

Can calculate the finite size effects in the mean field approximation to find

 $F_{s}(x) \approx \operatorname{erfc}(x)$

(TSE+Saramäki, 2005;



generalisation of Krapivsky and Redner, 2002) © Imperial College London

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What can physicsts and mathematicians do well?

RANDOM WALKS

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© Imperial College London

Properties of irreducible non-negative matrices (1) Will phrase this in terms of *Adjacency Matrix A_{ii}* for a network

- $A_{ij} = A_{ji} = 1$ for edges in **simple graphs**
- A_{ij} is the weight of edge from j to i for weighted network
- A_{ij} ≠ A_{ji} (symmetric matrix) if
 directed network

Definition of irreducible non-negative matrices (1) In terms of an Adjacency Matrix A_{ij} for a network

- A non-negative matrix is A_{ij}≥0
- *Irreducible* if there is a path from each vertex to every other vertex

$$\forall i, j \quad \exists n > 0 \quad s.t. \quad (A^n)_{ij} > 0$$

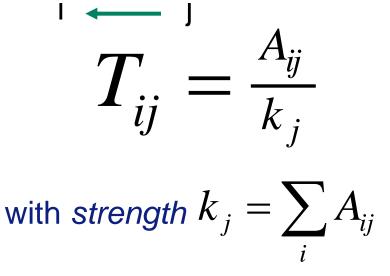
Properties of irreducible non-negative matrices (2)

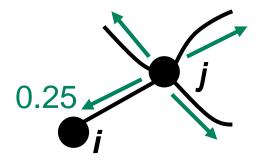
- Largest eigenvalue (λ_1) is real and positive
- Largest eigenvalue is bounded by largest and smallest sums of each row and each column
- Eigenvector of largest eigenvalue has only positive entries
- Entries in all other eigenvectors differ in sign

Random Walk Transition Matrix

The transition matrix for a simple unbiased random walk on a network is *T* where the probability of moving *from* vertex *j*

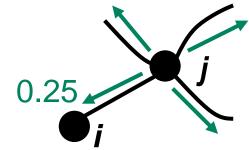
to vertex *i* is

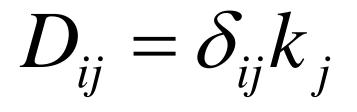




Probability of following an edge from j to any vertex i is 0.25 Random Walk Transition Matrix (2) Another useful form is

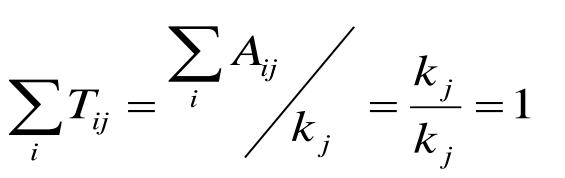
 $T = A.D^{-1}$

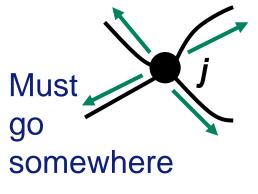




Probability of following an edge from j to any vertex i is 0.25 Transition matrix properties (1)

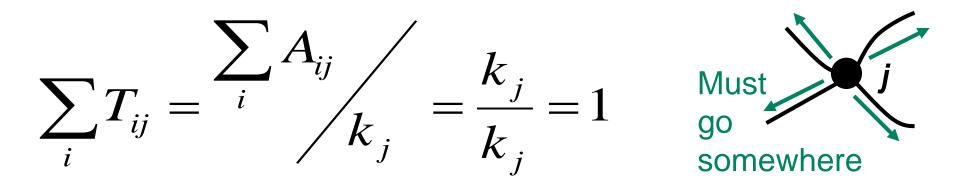
- Adjacency matrices of networks are nonnegative (almost always)
- Irreducible if network fully connected (or add some weak links to make it so)
- Transition matrix is also non-negative and irreducible





Transition matrix properties (2)

Transition matrix columns always sum to 1



 \Rightarrow Transition matrix has unique largest eigenvalue equal to $1 = \lambda_1$

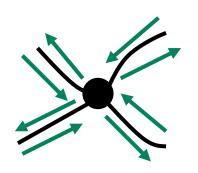
Transition matrix properties (3)

 Eigenvector of largest eigenvalue of transition matrix, v₁, of undirected network is just k_i.

$$(T \vec{v}_1)_i = \sum_j \frac{A_{ij}}{k_j} k_j = \sum_j A_{ij} = k_j = (\vec{v}_1)_i$$

i.e. *Flow in* = *Flow Out* is equilibrium reached if flow along each edge is equal to the weight of the edge Transition matrix properties (4)

 Flow in = Flow Out is equilibrium reached if flow along each edge is equal to the weight of the edge



For simple graph, ONE walker passes along each edge in each direction at each time step

⇒**k** walkers arrive and leave each vertex

*** NOT solution if number of in- and out-edges different

Random walk as linear algebra Let w_i(t) be the number of random walkers at vertex *i* at time t

(or the probability of finding one walker at *i*) then the evolution is simply

$\vec{w}(t+1) = T.\vec{w}(t)$

 $w_i(t+1) = \sum_j T_{ij} w_j(t)$

Random walk as linear algebra

Decompose $w_i(t)$ in terms of eigenvectors v_n as

$$\vec{w}(t=0) = \sum c_n \vec{v}_n$$

then the evolution is simply n

$$\vec{w}(t) = \sum_{n} c_n (\lambda_n)^t \vec{v}_n$$

Equilibrium

Equilibrium reached is eigenvector with largest eigenvalue as $1 = \lambda_1 > |\lambda_n| \quad \forall n > 1$

$$\vec{w}(t \rightarrow \infty) \propto \vec{v}_1$$

So for simple networks we have

$$w(t \rightarrow \infty)_i \propto k_i$$

PageRank

- Google ranks web pages using v₁
- Follows links between web pages like a random walker
- Google makes money because the web is a *directed* graph so largest eigenvector,
 v₁, is not trivial

PageRank for Mathematicians Using MacTutor bibliography of over 200 mathematicians finds [Clarke, TSE, Hopkins, 2010]

Rank	Degree	Closeness	Betweenness	Page Rank
$1 \mathrm{st}$	Newton	Newton	Euclid	Euclid
2nd	Hilbert	Hilbert	Newton	Newton
3rd	Euclid	$\operatorname{Riemann}$	Euler	Laplace
4th	Riemann	Euler	Riemann	Hilbert
5th	Euler	Euclid	Van der Waerden	Lagrange

Centrality Measures

The closer a vertex is to the *"centre"* of a network, the higher its *Centrality Measures*:-

- Degree
- PageRank
- Betweenness

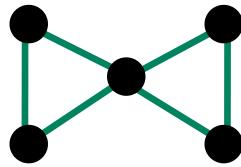
Simple Betweenness = number of shortest paths passing through each vertex

• etc.

Simple Betweenness

Example

- 1. Calculate the shortest paths between all pairs of vertices.
- **2. Betweenness** = number of shortest paths passing through each vertex



BUT ONLY defined for simple graphs

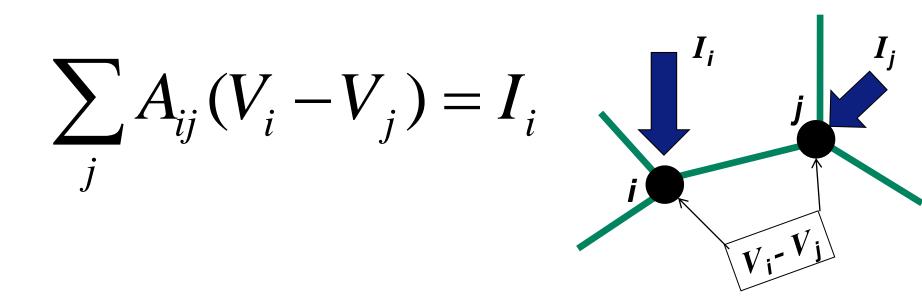
Electric Current Betweenness

[Newman 2005]

$$I = \frac{V}{R}$$
 Ohm's Law

Treat undirected network as resistors, with

- Conductivity of resistor edge weights = A_{ij} = A_{ij}
- Voltage at vertex $i = V_i$
- External current flowing into vertex $i = I_i$



Betweenness and Currents (2)

$$\sum_{j} A_{ij} (V_i - V_j) = I_i$$

$$(D-A)V = I$$

where $D_{ij} = k_i \delta_{ij}$ a diagonal matrix using degree

$$\Rightarrow \vec{V} = (D - A)^{-1} \vec{I}$$

Wait till later to see why inverse is OK Betweenness and Currents (3)

$$\vec{V} = (D - A)^{-1} \vec{I}$$
$$= D^{-1} (1 - AD^{-1})^{-1} \vec{I}$$
$$= D^{-1} (1 - T)^{-1} \vec{I}$$

where **T** = **AD**⁻¹ is the random walker transition matrix

Betweenness and Currents (4)

Define the *net flow* of current through a vertex to be F_i so F_i

$$F_{i} = \frac{1}{2} \sum_{j} |A_{ij}(V_{i} - V_{j})|$$

$$F_i$$
 j
 i V_i V_j

then using $\vec{V} = D^{-1}(1-T)^{-1}\vec{I}$ we find that

$$F_{i} = \frac{1}{2} \sum_{j} \left| T_{ij} \left((1 - T)^{-1} I \right)_{j} - T_{ji} \left((1 - T)^{-1} I \right)_{i} \right|$$

Betweenness and Currents (5) So net flow of current F_i through vertex *i* is

 $= \frac{1}{2} \sum_{j,k} |\Phi_{ijk} I_k - \Phi_{jik} I_k|$ $_{iik} = \sum T_{ii} \left[(1 - T)^{-1} \right]_{ik}$ where is the current flowing from *j* to *i* due to external current put in at k

Betweenness and Currents (6) However in terms of random walkers

$$(1-pT)^{-1} = \sum (pT)^n \qquad \text{if } |p\lambda_1| < 1$$

So Φ_{ijk} counts the number of random walkers starting at *k*, arriving at *j* after *n* steps, followed by a move *to i*

$$\Phi_{ijk} = \sum_{n} T_{ij} \begin{bmatrix} T^n \end{bmatrix}_{jk}$$

Betweenness and Currents (7)

The total current put into the circuit must match the current taken out

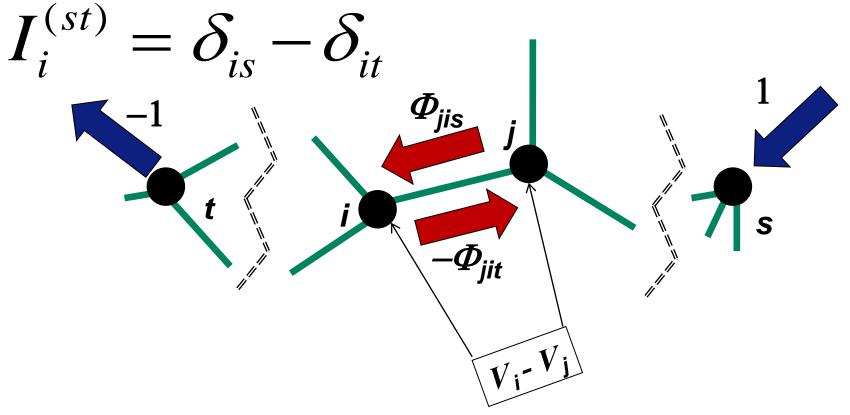
$$\sum_{i} I_{i} = 0$$

In terms of the transition matrix, this means this vector I_i does **not** contain the equilibrium eigenvector with eigenvalue **1**

Thus
$$\Phi_{ijk} = \sum_{n} T_{ij} \begin{bmatrix} T^n \end{bmatrix}_{jk}$$
 is well defined
if **p<1** or if acts on **I**.

Betweenness and Currents (8) Suppose

- we put one unit of current in at **source** vertex **s**
- we take one unit of current out at target vertex t



Betweenness and Currents (9)

1

The net flow in terms of positive (from **s**) and negative (from **t**) random walkers is

$$F_{i}^{(st)} = \frac{1}{2} \sum_{j} \left| \Phi_{ijs} - \Phi_{ijt} - \Phi_{jis} + \Phi_{jit} \right|$$
neg
t
s

Betweenness and Currents (10) Newman suggests a centrality measure of summing over all possible source and sink currents

$$F_i = \sum_{s,t} F_i^{(st)}$$

with
$$F_i^{(st)} = \frac{1}{2} \sum_{j} \left| \Phi_{ijs} - \Phi_{ijt} - \Phi_{jis} + \Phi_{jit} \right|$$

and Φ_{ij} is the number of random walkers starting from k passing from j to i after n steps

Betweenness and Currents Summary

- Uses negative random walkers
- Random walker picture works for directed graphs
- Does not use equilibrium eigenvector

 unlike PageRank, Modularity for community detection, ...
- Can introduce distance scale d= p/(1-p)

 Walkers move on with probability p, stop with probability (1-p). Replace T→pT and (1-T)⁻¹→(1-p)/(1-pT)
- Can introduce biased random walks

-e.g.
$$T_{ij} = \frac{lpha_i A_{ij}}{z_j}$$
, $z_j = \sum_i lpha_i A_{ij}$

[Lambiotte et al. 2011]

Betweenness and Currents Summary

Newman suggests a centrality measure of summing over all possible source and sink currents

$$F_i = \sum_{s,t} F_i^{(st)}$$

with
$$F_i^{(st)} = \frac{1}{2} \sum_{j} \left| \Phi_{ijs} - \Phi_{ijt} - \Phi_{jis} + \Phi_{jit} \right|$$

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THANKS

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Considerable input possible from from a mathematical approach to networks

Google "Tim Evans Networks" to find my web pages on networks Average Path Length in MR Random Graph

[Fronczak

Final

et al,

2005]

- Let p_{ii}(x) be the probability that a random walk (never returning along last step) starting at vertex *i* passes through vertex *j* at least once after **x** steps
- Number of different walks of length x from *i* to *j*, *if no loops*, is $W(i,x) = k_i (k_n - 1)^{x-1}$ vertex j

k_n

Initial vertex i k_i

Average Path Length in MR Random Graph (2)

- Probability of *not* arriving at *j* on any one step = $1 (k_j/2E)$
- ⇒ Probability that a random walk does not arrive at j after x steps is

$$p_{ij}(x) = \left(1 - \frac{k_j}{2E}\right)^{W(i,x)} \approx \exp\left\{-\frac{k_i k_j}{2E} z^{x-1}\right\}$$
$$\left(z \coloneqq \frac{\langle k^2 \rangle}{\langle k \rangle} - 1 = \frac{\langle k_n \rangle}{\langle k \rangle} - 1\right)$$

Average Path Length in MR Random Graph (3)

Probability that walker first arrives after x steps
 is p_{ij}(x-1) - p_{ij}(x)

 \Rightarrow Average path length from *i* to *j* is

$$d_{ij} = \sum_{x=1} x \left[p_{ij}(x-1) - p_{ij}(x) \right] = \sum_{x=0} p_{ij}(x)$$

 \Rightarrow Average path length <d>is (after some work) [Fronczak et al,2005]

$$\langle d \rangle \approx \frac{\ln(N) + \ln(z) - \ln(\langle k \rangle) - \gamma}{\ln(z)} + \frac{1}{2}$$

Average Path Length in MR Random Graph (4)

 For *any* random graph has an average shortest length which scales as

$$\langle d \rangle \approx \frac{\ln(N)}{\ln(z)} + c$$