

Simulations in Statistical Physics

Course for MSc physics students

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Algorithmically defined models

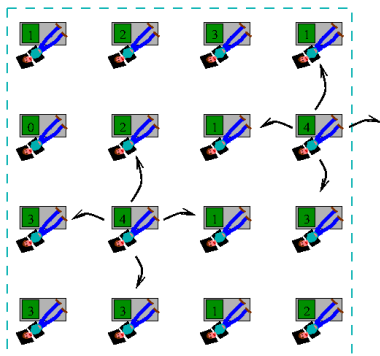
- ▶ Self-Organized Criticality
 - ▶ Bak-Tang-Wiesenfeld model
 - ▶ Forest fire model
 - ▶ Bak-Sneppen model of evolution
- ▶ Traffic models
- ▶ 1d driven systems

Self-Organized Criticality

- ▶ Critical state: inflection point in the critical isotherm
- ▶ Power law functions of correlation length, relaxation time
- ▶ Control parameter, generally temperature
- ▶ Critical point as an attractor?
- ▶ Why? Power law: We see many cases
 - ▶ $1/f$ noise (music, ocean, earthquakes, flames)
 - ▶ Lack of scales (market, earthquakes)
- ▶ Underlying mechanism?

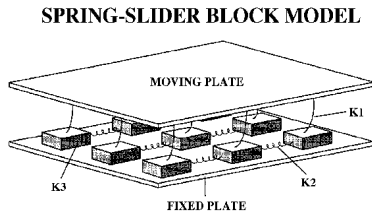
Bak-Tang-Wiesenfeld model

- ▶ Originally a sandpile model
- ▶ Better explained as a *Lazy Bureaucrat model*:
 - ▶ Bureaucrats are sitting in a large office in a square lattice arrangement
 - ▶ Occasionally the boss comes with a dossier and places it on a random table
 - ▶ The bureaucrats do *nothing* until they have less than 4 dossiers on their table
- ▶ Once a bureaucrat has 4 or more dossiers on its table starts to panic and distributes its dossiers to its 4 neighbors
- ▶ The ones sitting at the windows give also 1 dossier to its neighbors and throw the rest out of the window.



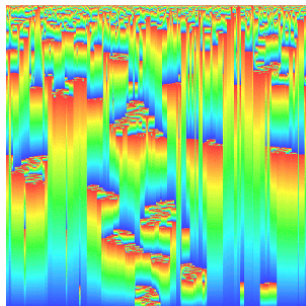
Bak-Tang-Wiesenfeld model

- ▶ Originally a sandpile model
- ▶ Better explained as a *Lazy Bureaucrat model*:
- ▶ Best application: Spring block model of earthquakes:
 - ▶ Masses sitting on a frictional plane in a grid are connected with springs to each other and to the top plate
- ▶ Top plate moves slowly, increasing the stress on the top springs slowly and randomly
- ▶ If force is large enough masses move which increases the stress on the neighboring masses



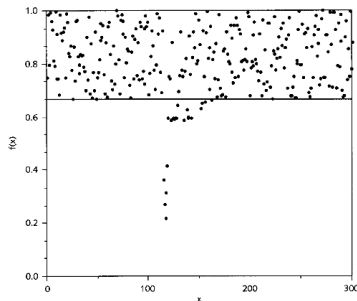
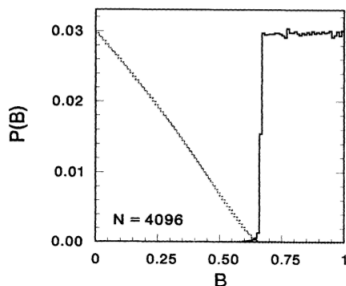
Bak-Sneppen model of evolution

- ▶ N species all depends on two other (ring geometry)
- ▶ Each species are characterized by a single *fitness*
- ▶ In each turn the species with the lowest fitness dies out and with it its two neighbors irrespective of their fitness
- ▶ These 3 species are replaced by new ones with random fitness
- ▶ Initial and update fitness is uniform between $[0, 1]$



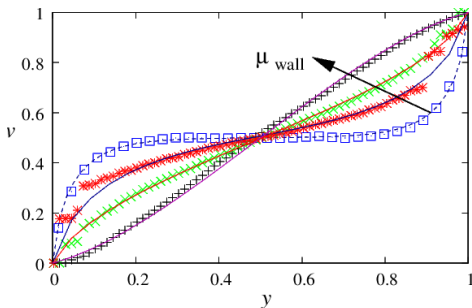
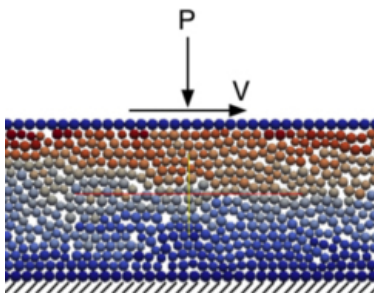
Bak-Sneppen model of evolution: Results

- ▶ Steady state with avalanches
- ▶ Avalanches start with a fitness $f > f_c \simeq 0.66$
- ▶ Avalanche size distribution power law
- ▶ Distance correlation power law



Bak-Sneppen model of evolution an application: Granular shear

- ▶ Fitness \rightarrow Effective friction coefficient
- ▶ Specimen with lowest fitness dies out \rightarrow block is sheared at weakest position (shear band)
- ▶ Neighbors, related species die out and replaced by new species \rightarrow structure gets random around the shear band.

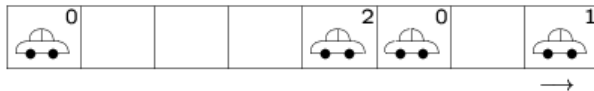


Traffic models



Nagel-Schreckenberg model

- ▶ Periodic 1d lattice (ring) Autobahn
- ▶ discretized in space and time
- ▶ Cars occupying a lattice moving with velocities $v = 0, 1, 2, 3, 4, 5$
- ▶ Remark, if max speed is 126 km/h, then lattice length is 7 m, a very good guess for a car in a traffic jam
- ▶ It uses parallel update: at each timestep all cars move v sites forward



Nagel-Schreckenberg model

► Algorithm:

1. **Acceleration:** All cars not at the maximum velocity increase their velocity by 1
2. **Slowing down:** Speed is reduced to distance ahead (1 sec rule)
3. **Randomization:** With probability p speed is reduced by 1
4. **Car motion:** Each car moves forward the number of cells equal to their velocity.

Configuration at time t :



a) Acceleration ($v_{max} = 2$):



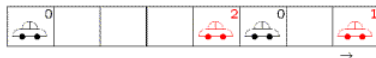
b) Braking:



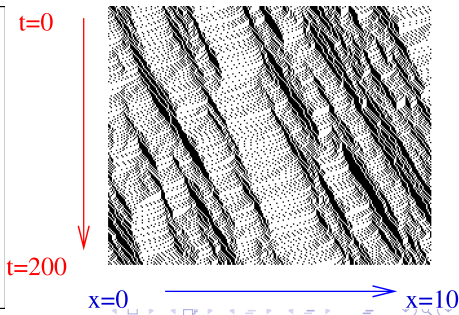
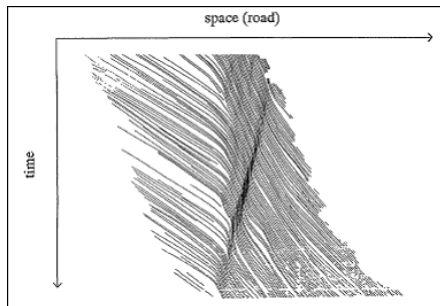
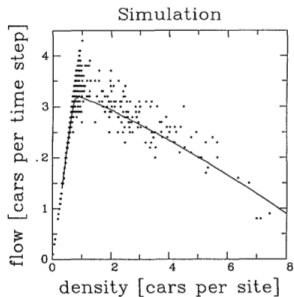
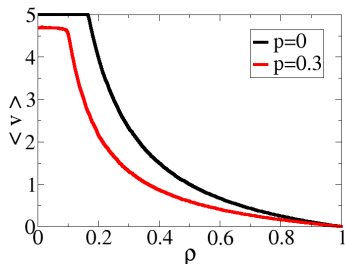
c) Randomization ($p = 1/3$):



d) Driving (= configuration at time $t + 1$):

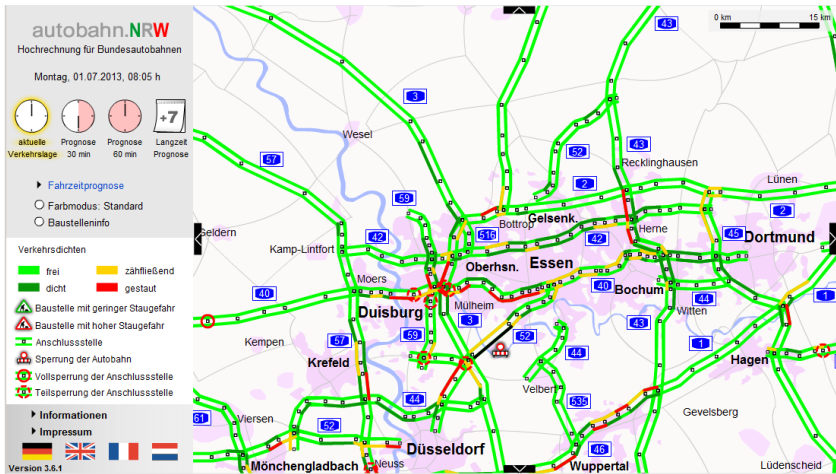


Emergence of traffic jams



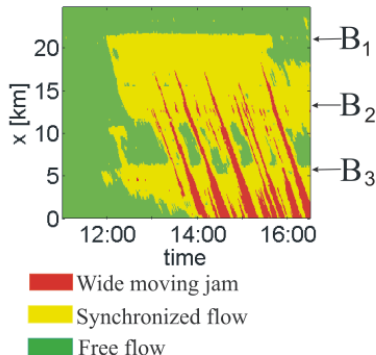
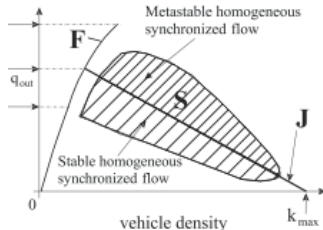
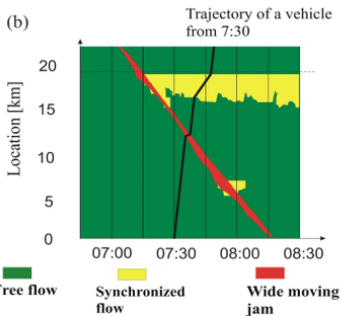
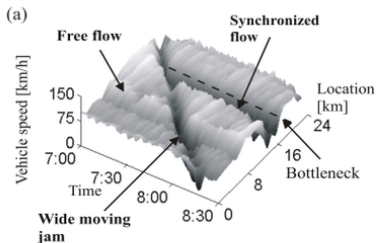
Nagel-Schreckenberg model

- ▶ Transition from free-flow to jammed state
- ▶ Jammed state is a phase-separated phase
- ▶ Without randomization a sharp transition
- ▶ Had been used in NRW to predict traffic jams

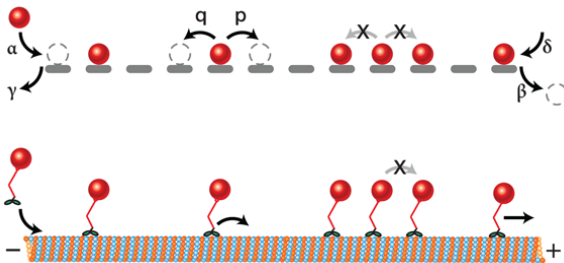


Three-phase traffic theory

Three traffic phases

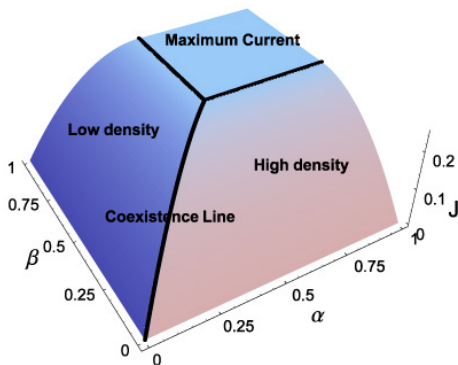
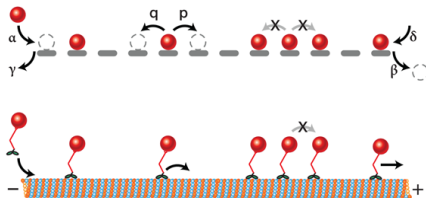


Asymmetric simple exclusion process



- ▶ $p + q = 1$
- ▶ If $p = q$ then SEP a Markov-process
- ▶ Generally $\gamma = \delta = 0$
- ▶ α and β determines the phase diagram

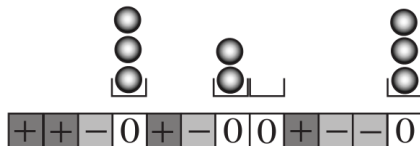
Asymmetric simple exclusion process



Three state ASEP

$$+ \overset{\alpha}{\rightarrow} 0 + \ ; \ 0 \overset{\alpha}{\rightarrow} - 0 \ ; \ + \overset{\frac{1}{q}}{\leftrightarrow} - +$$

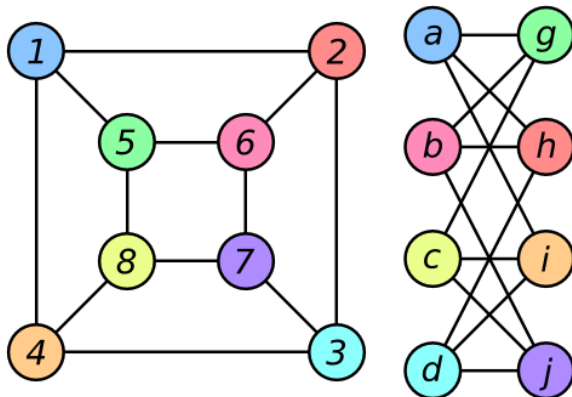
- ▶ If q small three blocks ($00 \dots 00 + + \dots + + - - \dots - -$)
- ▶ Mixed state above $q = 1$
- ▶ Numerical simulations suggested an other phase transition at $q_c < 1$
- ▶ Actually false, correlation length is finite but large $\sim \mathcal{O}(10^{70})$
- ▶ Correspondence to Zero Range Process



Networks

Graphs

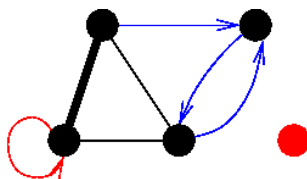
László Babai: algorithm on isomorphism



Networks

Complex networks

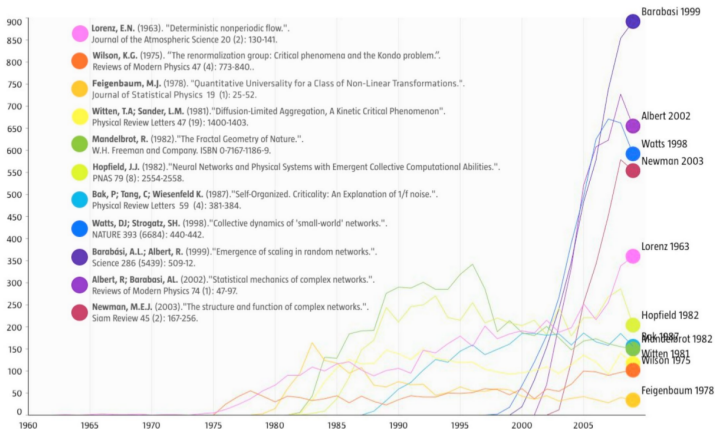
- ▶ Mathematics: Graphs
- ▶ Vertices, nodes, points
- ▶ Edges, links, arcs, lines
 - ▶ Directed or undirected
 - ▶ Loop
 - ▶ Multigraph
 - ▶ Wighted graphs
 - ▶ Connected



Complex networks

Phenomenon	Nodes	Links
Ising	Spins	Interaction(neighbors)
Cell metabolism	Molecules	Chem. reactions
Sci. collaboration	Scientists	Joint papers
WWW	Pages	URL links
Air traffic	Airports	Airline connections
Economy	Firms	Trading
Language	Words	Joint appearance

Complex networks, citations



Random Networks

Generate networks:

- ▶ From data:
 - ▶ Phone calls
 - ▶ WWW links
 - ▶ Biology database
 - ▶ Air traffic data
 - ▶ Trading data
- ▶ Generate randomly
 - ▶ From regular lattice by random algorithm (e.g. percolation)
 - ▶ Erdős-Rényi graph
 - ▶ Configurations model
 - ▶ Barabási-Albert model

Erdős-Rényi

- ▶ P. Erdős, A. Rényi, *On random graphs*, Publicationes Mathematicae Debrecen, Vol. 6 (1959), pp. 290-297 (cit 789)
- ▶ Two variants:
 1. $G(N, M)$: N nodes, M links
 2. $G(N, P)$: N nodes, links with p probability (all considered)
- ▶ Algorithm
 1. $G(N, M)$:
 - ▶ Choose i and j randomly $i, j \in [1, N]$ and $i \neq j$
 - ▶ If there is no link between i and j establish one
 2. $G(N, P)$: (Like percolation)
 - ▶ Take all $\{i, j\}$ pairs ($i \neq j$)
 - ▶ With probability p establish link between i and j

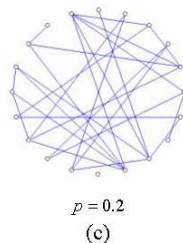
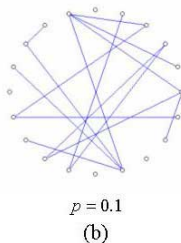
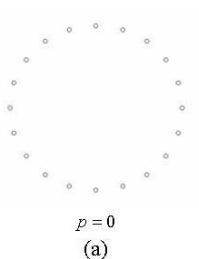
Erdős-Rényi

- Degree distribution

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

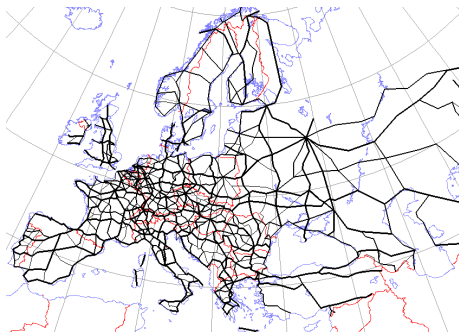
- For large N and $Np = \text{const}$ it is a Poisson distribution

$$P(k) \rightarrow \frac{(np)^k e^{-np}}{k!}$$



Erdős-Rényi

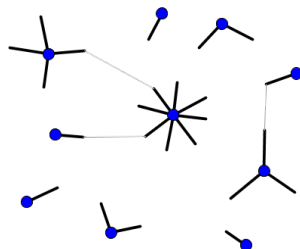
► Real life: Read networks



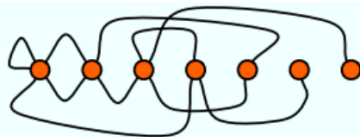
Most networks are different!

Configuration model

- ▶ Get the nodes ready with desired degree distribution
- ▶ Connect them randomly
- ▶ Self loops, and multiple links are created
- ▶ Problems at the end



1 1 1 1 2 2 2 3 3 3 4 4 5 5 6 6

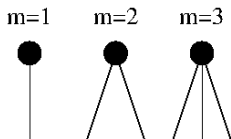


1 4 1 2 2 3 2 5 1 2 3 6 3 4 3 5 1 1 4 5

Preferential attachment

Barabási-Albert graph

- ▶ Initially a fully connected graph of m_0 nodes
- ▶ All new nodes come with m links ($m \leq m_0$)



- ▶ Links are attached to existing nodes with probability proportional to its number of links
- ▶ k_i is the number links of node i , then

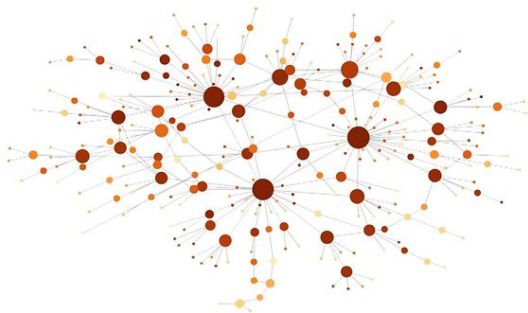
$$p_a = \frac{k_i}{\sum_j k_j}$$

Barabási-Albert graph

- ▶ Degree distribution

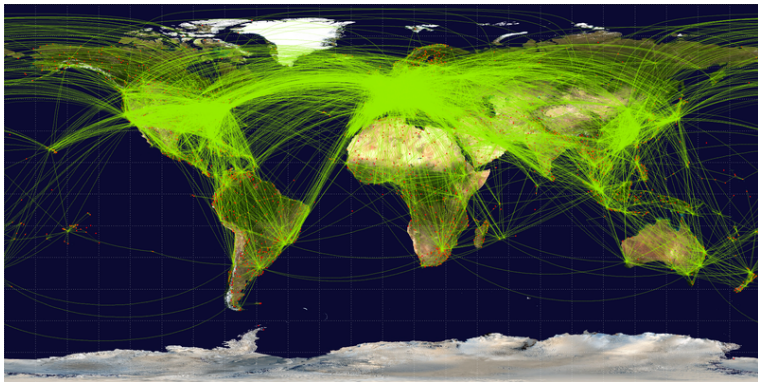
$$p(k) \sim k^{-3}$$

- ▶ Independent of m !

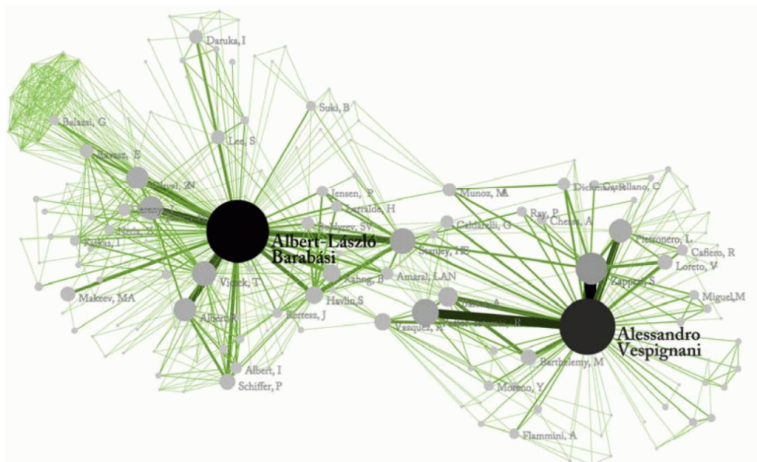


$m = 1$

Scalefree network example: Flight routes



Scalefree network example: Co-authorship

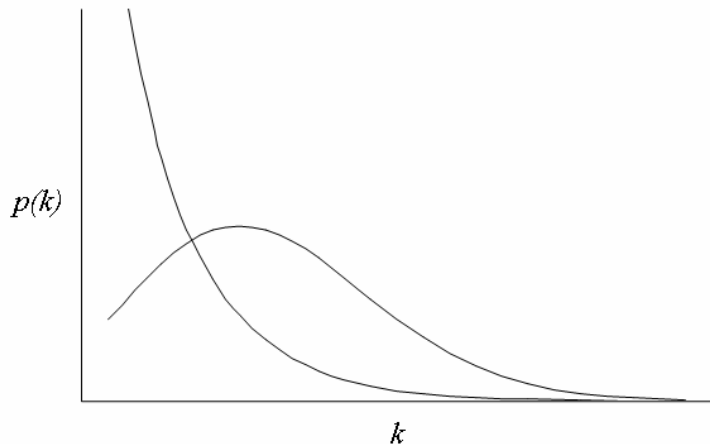


Algorithm for Barabási-Albert graph

1. $n = m_0$ number of existing nodes
2. $K = \sum_j k_j$ total number of connections
3. r random number $r \in [0, K]$
4. Find i_{\max} for which $\sum_{j=0}^{i_{\max}} k_j < r$
5. If there is no edge then add one between nodes $n + 1$ and i_{\max}
6. If node $n + 1$ has less than m connections go to 3.
7. Increase n by 1
8. If $n < N$ go to 2.

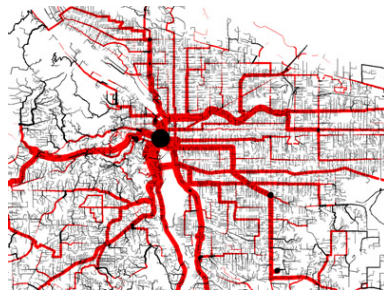
Properties of networks

► Degree distribution



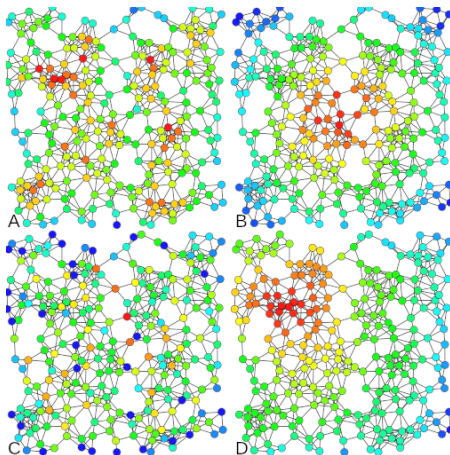
Properties of networks

- ▶ Degree distribution
- ▶ Shortest path



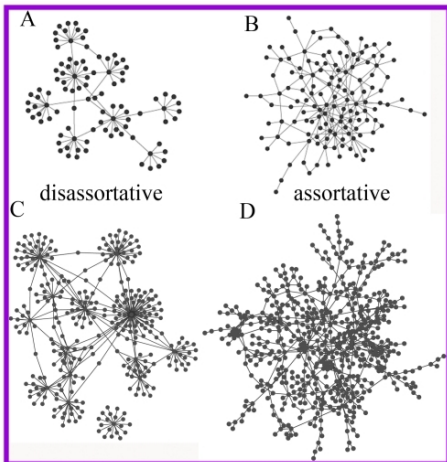
Properties of networks

- ▶ Degree distribution
- ▶ Shortest path
- ▶ **Centrality**
 - ▶ Degree centrality
 - ▶ Closeness centrality
 - ▶ Betweenness centrality
 - ▶ Eigenvector centrality (Page rank)



Properties of networks

- ▶ Degree distribution
- ▶ Shortest path
- ▶ Centrality
- ▶ **Assortativity**



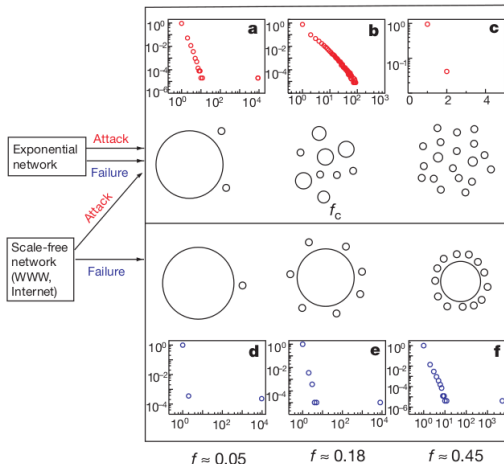
Percolation and attack on random networks

- ▶ Failure: equivalent to percolation: remove nodes at random
- ▶ Attack: remove most connected nodes



Percolation and attack on random networks

- ▶ Failure: equivalent to percolation: remove nodes at random
- ▶ Attack: remove most connected nodes



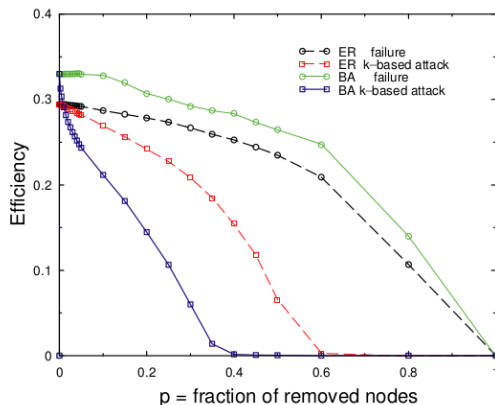
Percolation and attack on random networks

- Efficiency:

$$E(G) = \frac{1}{N(N-1)} \sum_{i \neq j} \frac{1}{t_{ij}}$$

t_{ij} the shortest path between i and j .

- $N = 2000$, $k = 10^4$



Percolation and attack on random networks

