# Dynamical processes on complex networks

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# Bibliography


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# Summary

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# Introduction

# Dynamical processes in complex heterogeneous substrates

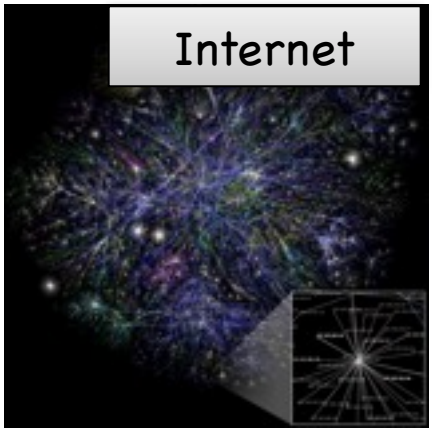
- Many dynamical processes of large theoretical and practical interest take place on top of complex heterogeneous systems

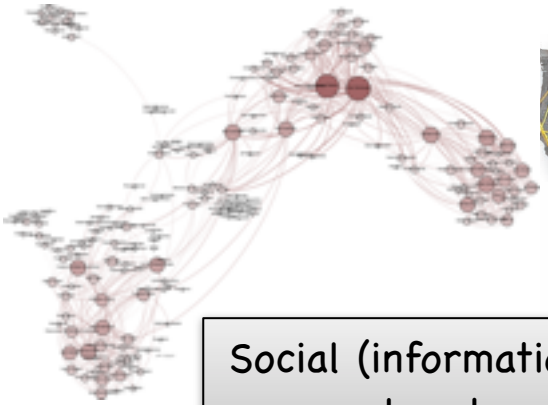
| Dynamical Process | Substrate |
|---|---|
| Spread of diseases | Social Systems |
| Transport of information packets | Internet |
| Transport of nutrients/energy | Food Webs |
| Spread of information/rumours/ opinions | Social Systems |
| Transport of people/goods | Transportation Infrastructures |
| Spread of digital viruses | Communication Infrastructures |

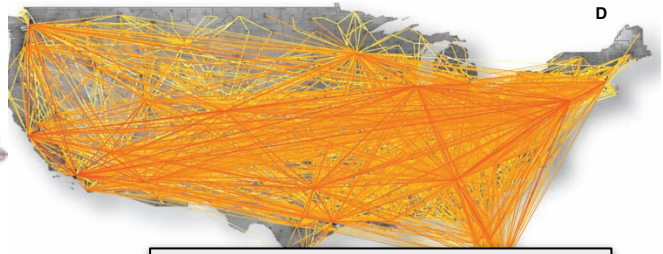
- These are really complex systems, and complex dynamical processes

# Dynamical processes in complex heterogeneous substrates

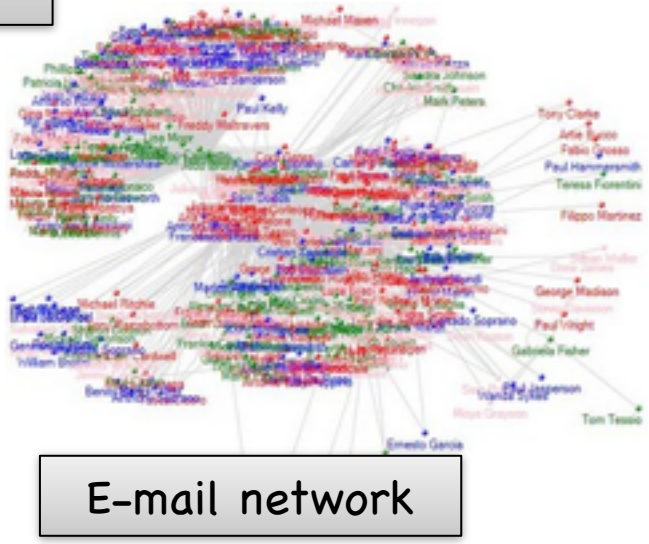
- Interestingly, many of this substrates can be represented as a complex network





Social (information) network





# Dynamical processes in complex heterogeneous substrates

- In order to overcome these complications and obtain information about them we can proceed to make to several simplifications:
  - Represent the complex substrate in terms of a complex networks (simple collection of points connected by lines)
  - Represent the true dynamical process as a discrete stochastic dynamical system (sort of a cellular automata)
- Different levels of realism in the description of the complex network and in the description of the stochastic system can allow for different levels of accuracy in theoretical/numerical predictions of dynamical behavior

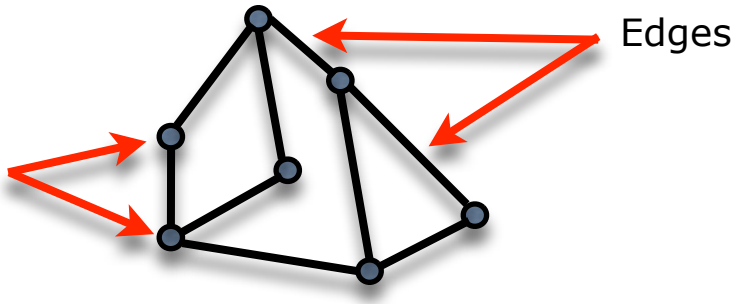
# Purpose of the lectures

- We will focus in the study of simple (but not trivial) dynamical processes
  - Non-equilibrium processes only
- We will focus on networks with simple topological properties
  - Will see what this means right now
- You will learn how to solve analytically these dynamical processes, within certain approximations (mean-field theories)
  - We will see how these approximations sometimes fail and why
- You will (hopefully) learn some “tricks of the trade”
- Final objective:
  - You should be able to attack and solve other models using the tools presented here

# Introduction
# I Networks at the very basic

# Complex networks: Strict characterization

- Network given by the
  - Set of vertices $V=\{1, \ldots, N\}$
  - Set of edges $E=\{(i,j)\}$




- Fully characterized by the adjacency matrix

$$a_{ij} = \begin{cases} 1 & \text{if} \quad (i,j) \in E \\ 0 & \text{if} \quad (i,j) \notin E \end{cases}$$

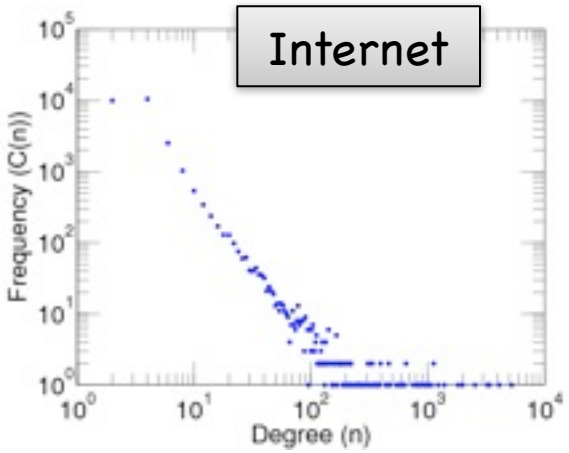
- We will consider simple, non-directed networks ($a_{ij} = a_{ji}$)
  - More realistic cases:
    - Directed nets, weighted nets, etc.

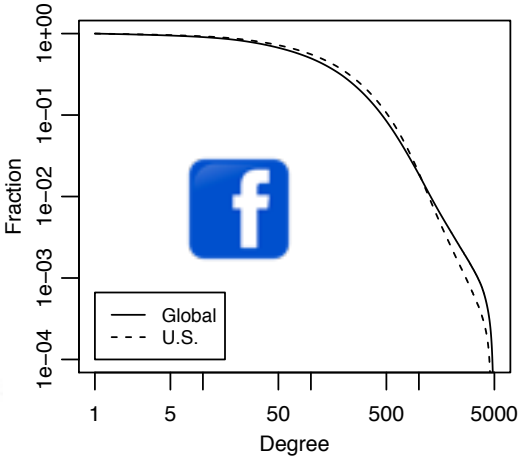
# Complex networks: Statistical characterization

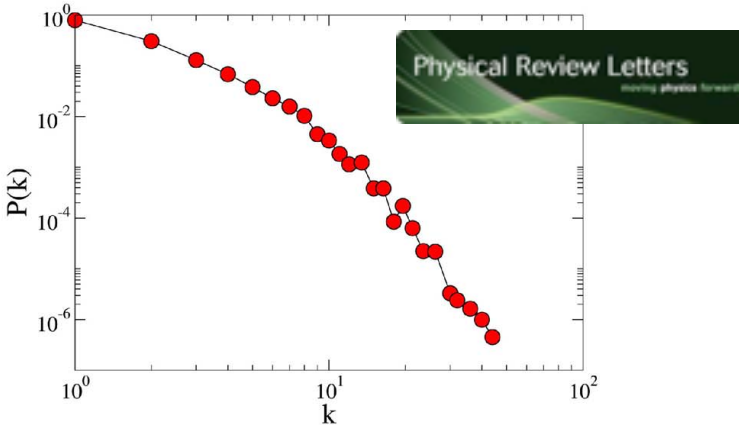
- Alternative statistical characterization in terms of some statistical distributions
  - Degree k of a vertex:
    - Number of other nodes that are connected to it
  - Degree distribution P(k):
    - Probability that a randomly chosen vertex has degree k

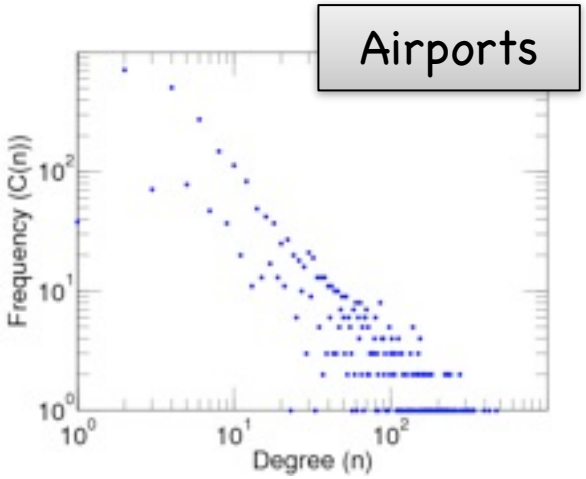
# Empirical observations

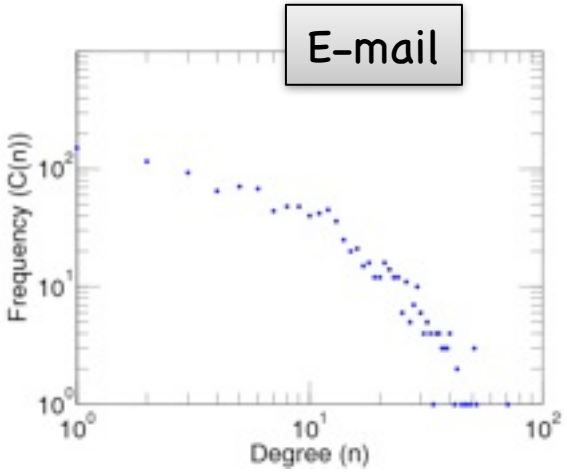
- Most real networks have a degree distribution scaling as a power-law




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

Scale-free (SF) networks

# Complex networks: Statistical characterization

- Degree correlations P(k'|k):
  - (Conditional) probability that an edge that departs from a vertex of degree k arrives at a vertex of degree k'
- Basic useful property:

$$k'P(k')P(k|k') = kP(k)P(k'|k)$$

  - Degree detailed balance condition
- Mostly interested in degree uncorrelated networks with

$$P(k'|k) = \frac{k'P(k')}{\langle k \rangle}$$

- We will not consider more complex properties such as large clustering, non-trivial correlations, etc.

# Quenched vs. Annealed networks

- Quenched networks:
  - A standard real network: Edges between vertices are fixed and do not change in time: $a_{ij}$ takes constant values
- Annealed networks:
  - Time varying network: Edges are rewired in the network at a time scale much sorter than that of any dynamical process, while preserving the degree of each vertex (the degree distribution) and the degree correlations
    - P(k) and P(k'|k), which were statistical properties of a quenched network, become the very definition of an annealed one
  - From a practical point of view: A neighbors of a vertex k is a vertex of degree k' chosen at random with probability P(k'|k)
    - Probability k'P(k')/<k> in uncorrelated networks

# The annealed network approximation

- In annealed networks, the adjacency matrix is defined only in a statistical sense
  - Probability that vertices i and j are joined by an edge

$$\bar{a}_{ij} \to \bar{a}_{kk'} = \frac{1}{NP(k)} \frac{1}{NP(k')} \sum_{n \in k} \sum_{m \in k'} a_{nm} \equiv \frac{k' P(k|k')}{NP(k)} = \frac{kk'}{N\langle k \rangle}$$

  - Annealed network approximation

Uncorrelated networks

- Annealed networks can be considered as:
  - Abstraction from a real network (rewiring)
    - Useful for calculations, as we will see
  - Representation of real time-varying networks
    - Social networks: We have a certain number of friends, but we don't see all of them every day

# Network models for numerical checks

- We want to make computer simulations of our models, in order to check the predictions of possible theoretical solutions or to make direct numerical explorations
- Using real networks is problematic:
  - They are usually too small
    - N ~ $10^4$, $10^5$
  - They come on fixed sizes
    - We cannot check the effects of changing network size
  - The are loaded with correlations, communities and other topological oddities
    - We have no idea (in the general case) how to treat those analytically
- The best option is to perform numerical simulations in statistically controlled network models

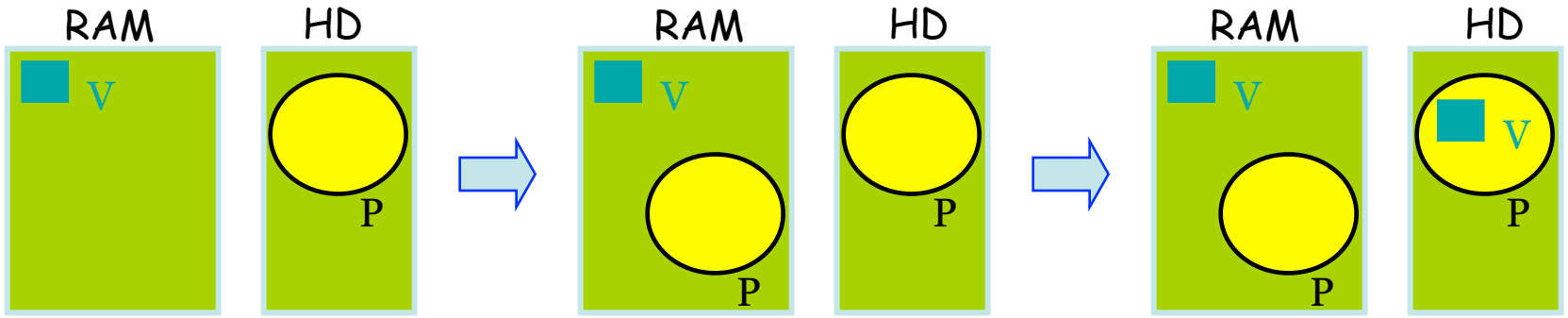
# Network models for numerical checks

- Basic models for numerical simulations
  - Configuration model (CM)
    - Degrees $k_i$ are assigned to nodes, extracted from an a priori degree distribution P(k); edges are randomly created between nodes, respecting the preassigned degrees
      - Creates correlations in SF networks for $\gamma < 3$
  - Uncorrelated configuration model (UCM)
    - As the CM, but degrees are restricted by $k_i < N^{1/2}$
      - No correlations
  - Barábasi-Albert model (BA)
    - Growing network model: A new node is assigned every time step, with m edges that are connected to old nodes with probability proportional to $k_i + a$
      - Degree distribution SF with $\gamma = 3 + a/m$

# Motivation:
# I Epidemic spreading of computer viruses

# Definition of computer viruses

- Definition: A computer virus is a computer program that can copy itself and infect a computer without permission or knowledge of the user
- Classical transmission mechanism: copying into a program



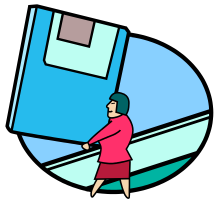

- Usually viruses contain additional instructions designed to interrupt or damage the computer
  - Flash funny messages on the screen
  - Overwrite files
  - Overwrite the FAT of the hard drive
  - Completely erase the hard drive

# Types of computer viruses (strains)

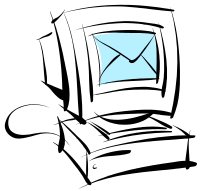
According to the mechanism of transmission:

- File viruses: Infect programs. When the user executes the program, the virus is installed in the RAM and copies itself on any executed program

- Boot viruses: Infect the boot sector of hard drives and floppies. On booting, the virus is installed in the RAM and can infect programs and new floppies



- Macro viruses: Infect data files (documents), such as word documents, using the macro instructions inserted in the documents.



# E-mail viruses

- Class of macro viruses that propagate through email
  - You receive a mail with some attachment (the virus)
    - Psychology applied to make you open it: money, sex, girls...
      - The “I-love-you” bug (more on it later)
  - After opening the attachment, the virus reads the list of contacts in your email client (Outlook)
  - The virus sends itself to all the people in your list of contacts (without you realizing it)
  - The infection propagates again from your contacts

# Why study computer viruses?

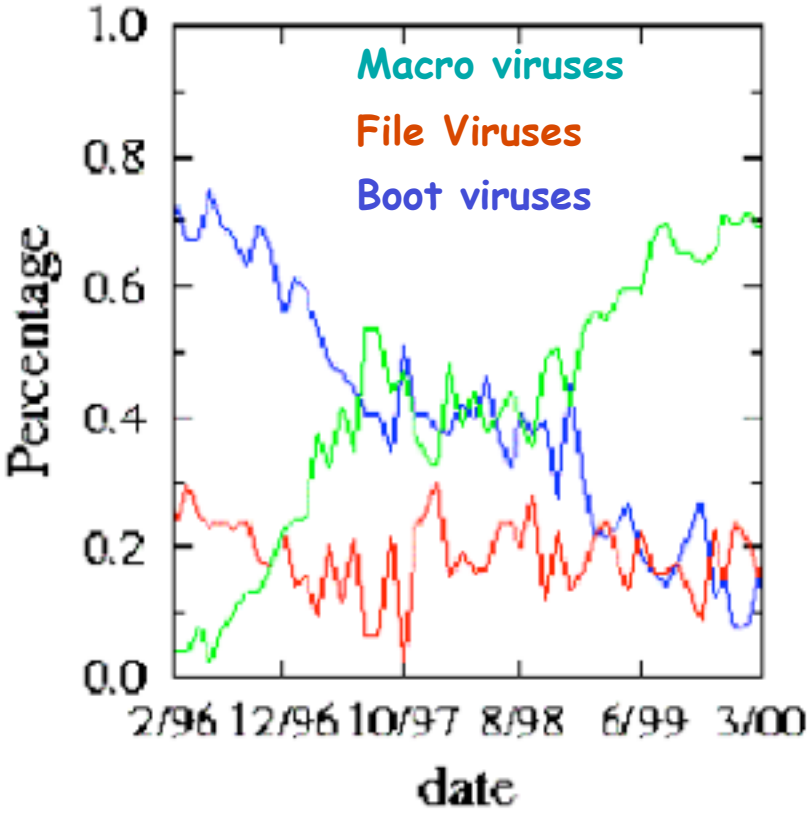
- Economical
  - Viruses cause millions of dollars worth in damaged equipment and downtime
    - March 1999, Melissa virus forced Microsoft and other large companies to completely shut down email service
    - January 2000, Mydoom worm infected 250.000 computers in one day
    - 2000, I-love-you bug produced losses of $8M in a few days
    - January-October 2007, Storm worm infected 50.000.000 computers
  - The antivirus industry moves billions of dollars yearly
- Scientific
  - How similar are cybernetic and biological diseases?

# Computer virus epidemiology

- Based in the analogy with biological epidemiology
- Two possible perspectives:
  - Microscopic level
    - Researches trying to reverse-engineer the source code of computer viruses to design appropriate antivirus software
      - ANALOGY: Quest for new medicines and vaccines
  - Macroscopic level
    - Statistical analysis and modeling of epidemiological data in order to find information and policies aimed at lowering epidemic outbreaks
      - ANALOGY: Macroscopic prophylaxis (vaccination strategies) for the computer community
    - Statistical physics perspective enters here!!
- Focus on the macroscopic level: Statistical analysis and modeling

# Strain data analysis

Analysis of the statistical properties of homogeneous groups of viruses (strains)

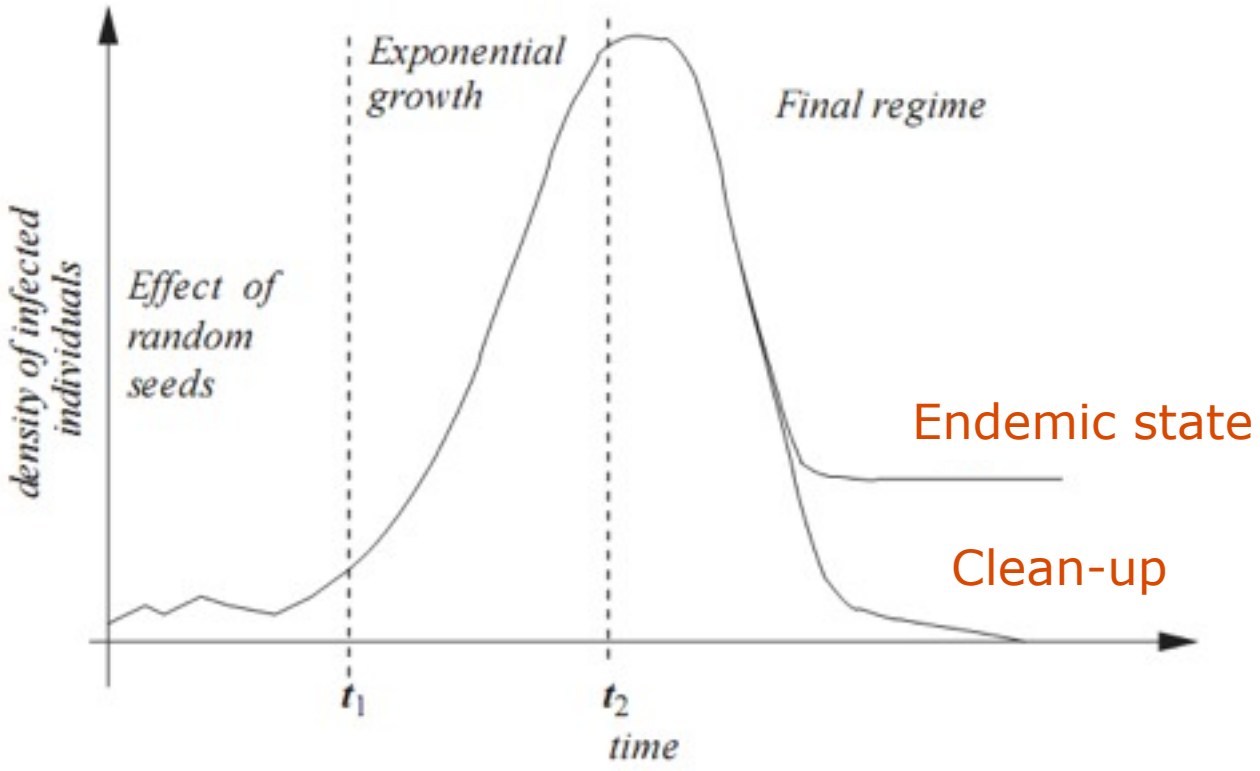



- Decrease of boot viruses
- Steady state for file viruses
- Large increase of macro viruses, especially from computer worms
- Nowadays: macro viruses overwhelmingly dominant

[data from http://www.virusbtn.com]

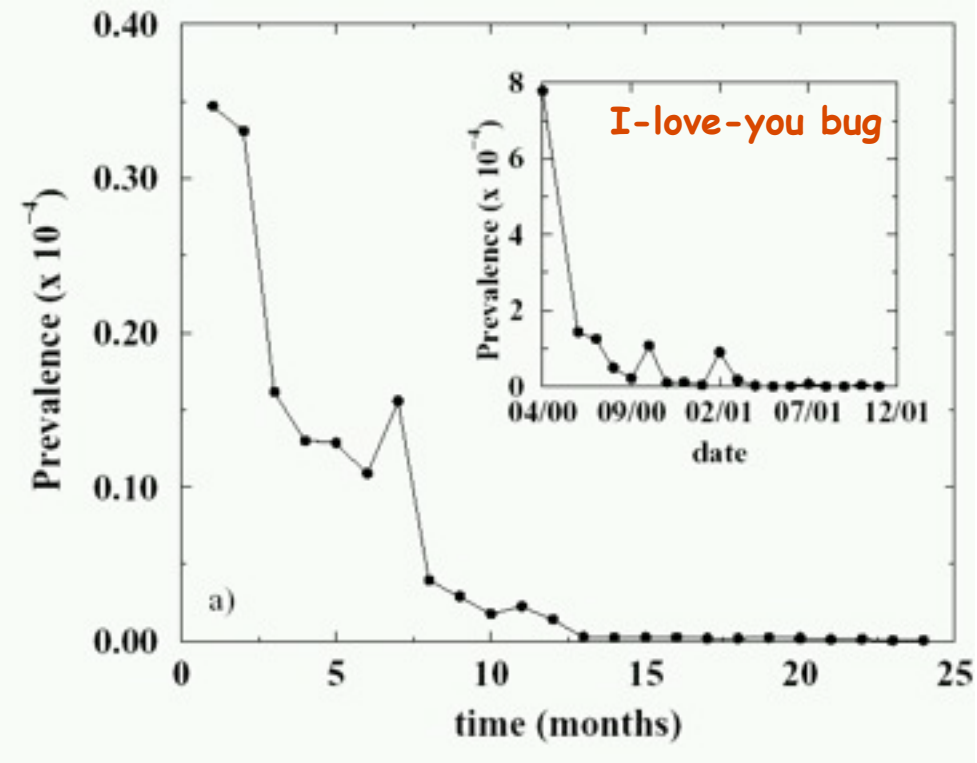
# Epidemic prevalence

- Epidemiologically relevant measures: prevalence (fraction of infected individuals)
- In biological diseases: stages of an epidemic outbreak
  - More on this later on



# Prevalence of individual viruses

Experimental measure of the prevalence for computer worms in the wild

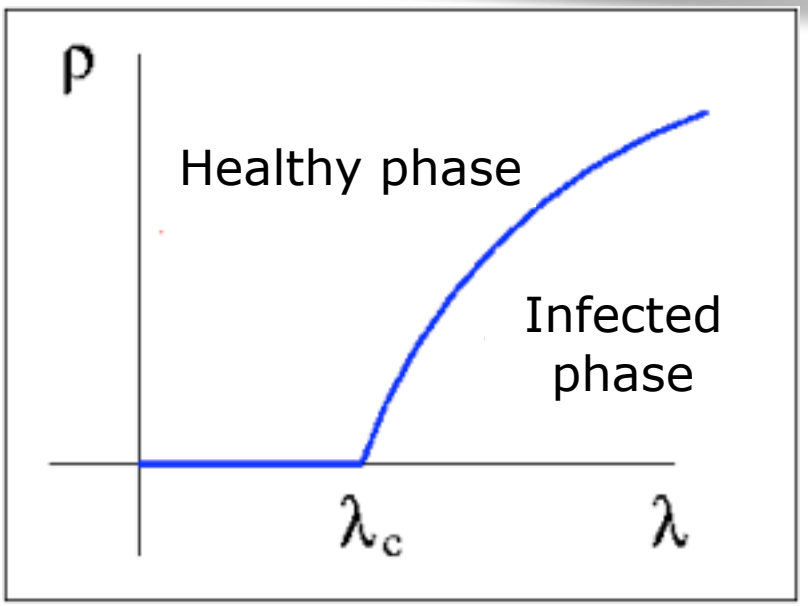



- Very few viruses are able to survive long enough to establish an endemic or stable state (at least at not very large time scales)
- Endemic viruses possess very low ($\rho < 10^{-5}$) but stable prevalence

[data from http://www.messagelabs.com]

# Why is this strange?

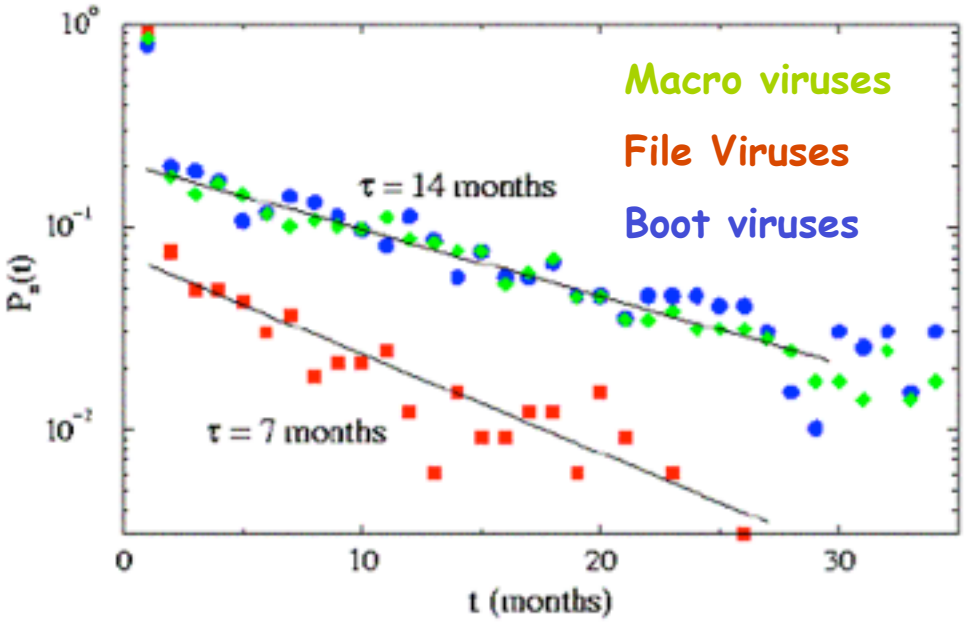
- Classical models of epidemiology predict that the prevalence depend on some parameter λ (spreading rate) measuring the power of infection, and shows a phase transition between an infected and a healthy phase at some finite epidemic threshold $\lambda_c$




- A very low prevalence is only achieved very close to the epidemic threshold
  - Are computer viruses built to be fine-tuned to have a spreading rate very close to the epidemic threshold?

# Survival probability of strains

Survival probability $P_s(t)$: Fraction of viruses that survive up to a time t after their first appearance




[data from http://www.virusbtn.com]

$$P_s(t) \sim e^{-t/\tau}$$

$\tau$ = average lifetime of each strain

The average life is very large compared with the time scale of viruses or anti-viruses

# Why this peculiar properties?

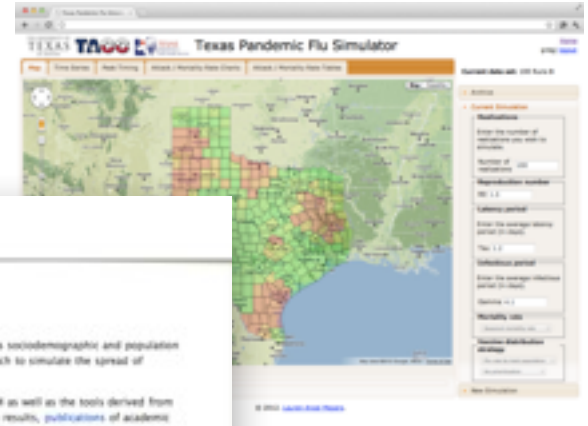
- The observed behavior is not compatible with simple models of epidemic spreading: Why?
- Computer viruses spread in a very particular environment
  - Computer networks (Internet)
  - E-mail (social) networks
- These are complex networks with particular properties
  - They are scale-free
- The scale-free nature of the environment turns out to have very strong effects on the dynamics of virus spreading

# Motivation:
# II Large-scale pandemic forecasting

# Epidemics now

- The study of epidemic spreading is a classical subject, which has attracted in recent years media headlight
  - The 2009 new flu strain H1N1 hit the world, leading a pandemics with a large number of infections, deaths, and panic

| 2009 H1N1 | Mid-Level Range* | Estimated Range* |
|---|---|---|
| **Cases** | | |
| 0-17 years | ~20 million | ~14 million to ~28 million |
| 18-64 years | ~35 million | ~25 million to ~52 million |
| 65 years and older | ~6 million | ~4 million to ~9 million |
| **Cases Total** | ~61 million | ~43 million to ~89 million |
| **Hospitalizations** | | |
| 0-17 years | ~87,000 | ~62,000 to ~128,000 |
| 18-64 years | ~160,000 | ~114,000 to ~235,000 |
| 65 years and older | ~27,000 | ~19,000 to ~40,000 |
| **Hospitalizations Total** | ~274,000 | ~195,000 to ~403,000 |
| **Deaths** | | |
| 0-17 years | ~1,280 | ~910 to ~1,880 |
| 18-64 years | ~9,570 | ~6,800 to ~14,040 |
| 65 years and older | ~1,620 | ~1,160 to ~2,380 |
| **Deaths Total** | ~12,470 | ~8,870 to ~18,300 |

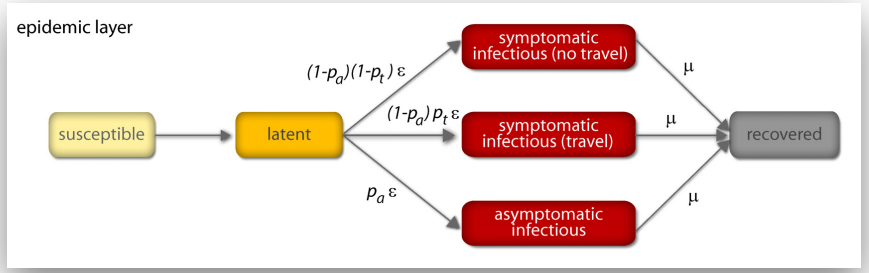


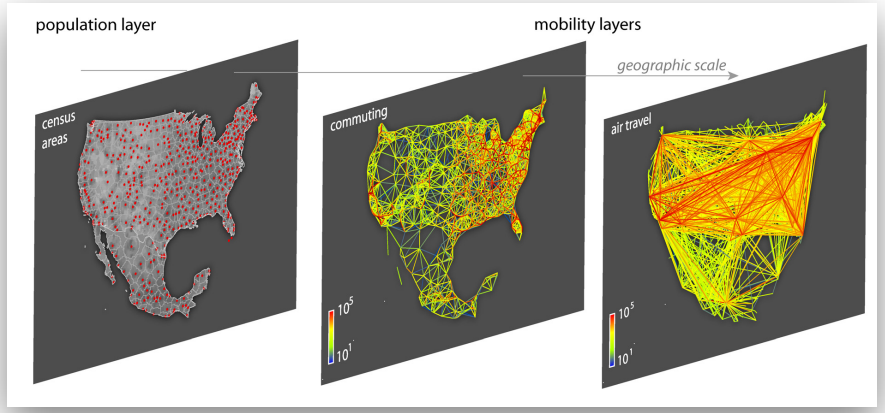


- Several large-scale simulation infrastructures were developed and used at the time, aimed at forecasting the evolution of that and new other pandemics

# How the predicting frameworks work

- Forecasting simulation frameworks are nontrivial systems, implementing:
  - Realistic models of disease propagation, based on real epidemiological data
    - Reaction-diffusion systems with empirically fitted parameters
  - Different layers of social, population and mobility data
    - Substrate for the RD system

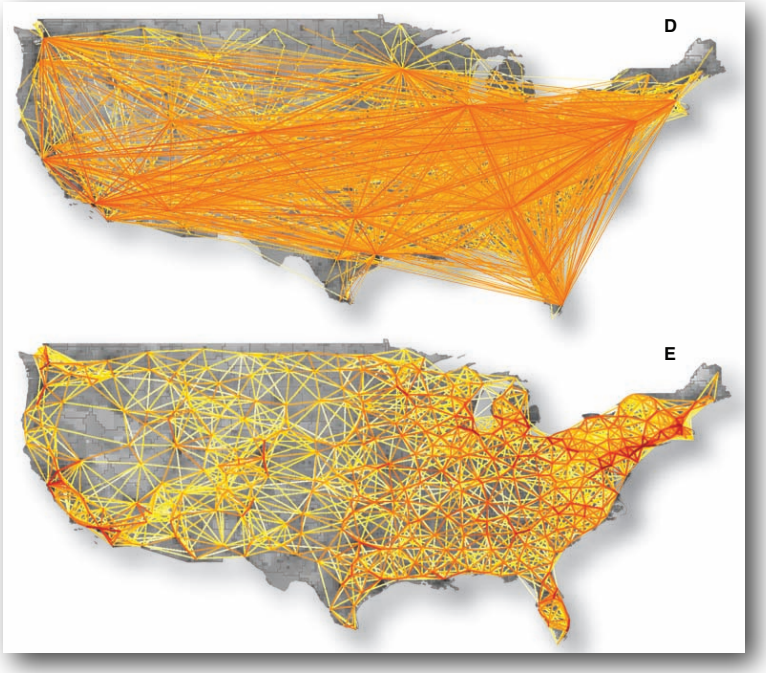



Plus HUGE amounts of supercomputer CPU time ...

# Using the proper substrate

- Small-scale diffusion: Social networks
  - ➡ We don't interact with people in a 2D world, but in a network of acquaintances




- Large-scale diffusion: Transportation networks
  - We move in fast and log-range ways
    - Railroad, commuting, air transportation network

This kind of networks must be implemented in forecasting frameworks

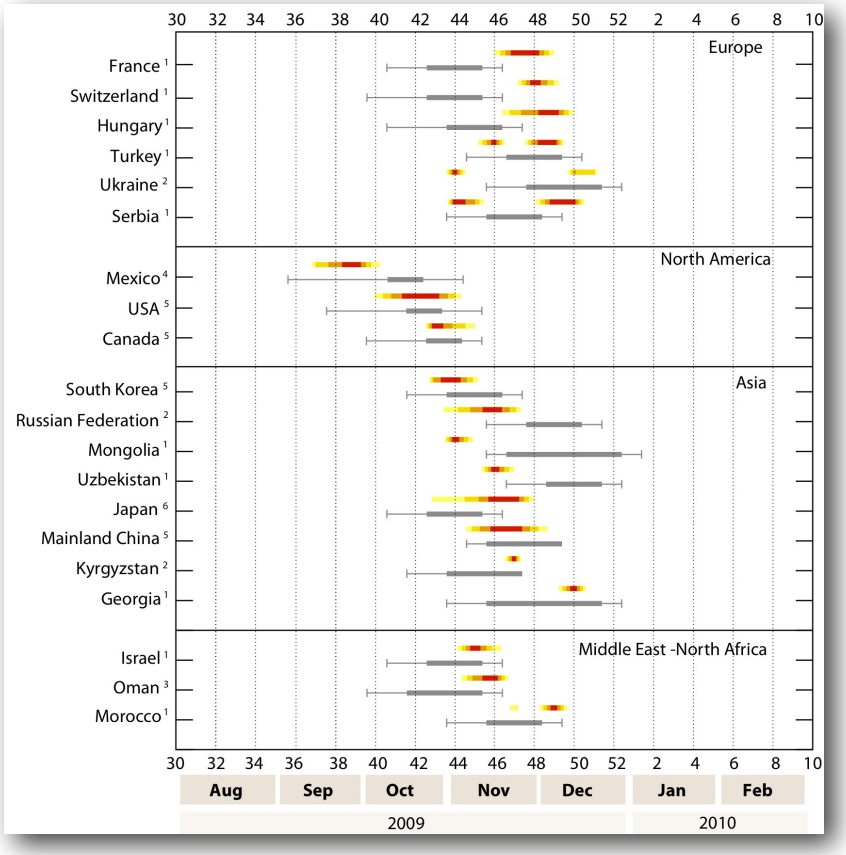
# The importance of being a network

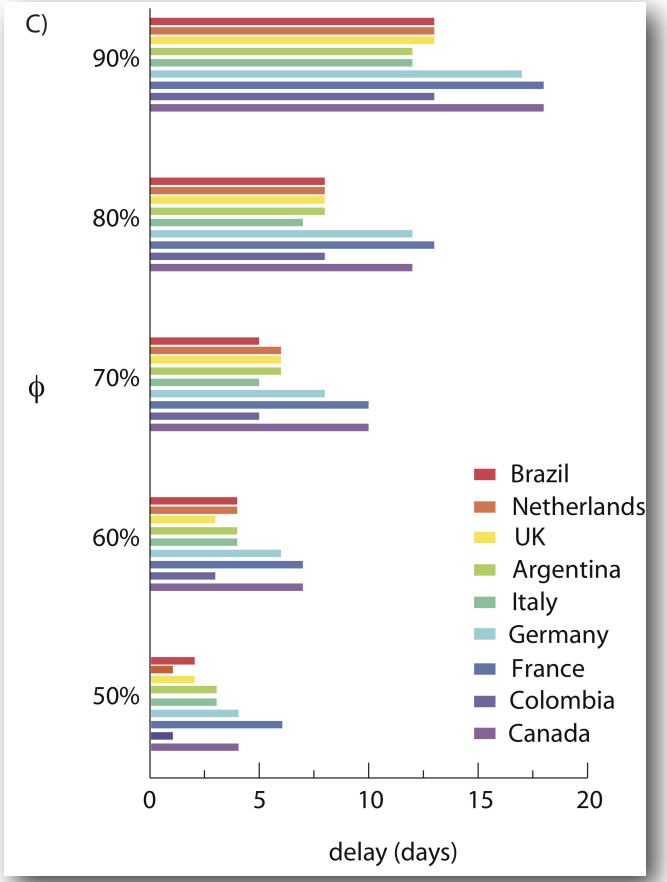
- Strong correlation between transportation powers and epidemic spread
  - XIV century:
    - Black Death pandemics in Europe
      - Crossed Europe in 7 years
  - XX century:
    - 1918 Spanish influenza pandemics
      - Crossed the world in 6 months
  - XXI century:
    - 2009 H1N1 pandemics
      - Crossed the world in less than 2 months
- Particularly important: Air transportation


# Pandemic predictions are possible

- One of the greatest exits of these infrastructures is the ability to make real and practical predictions

Peak of the epidemics on November, instead of February (usual seasonal peak)



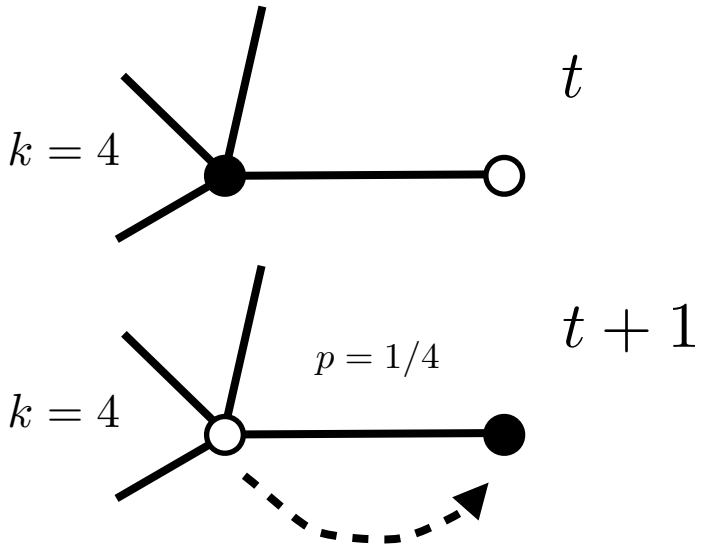




Almost no effect of preventive measures such as airport closing

# A simple model with an exact solution: The random walk

# Diffusion processes: the random walk

- Diffusion processes (random walks) are the simplest dynamics one can consider on any substrate
  - We can start to get a glimpse of the effects of the network complexity in the simplest case
- Additionally, it has relevance in real problems such as searching or traffic in heterogeneous structure
- Simplest realization: the uncorrelated random walk:
  - We have a particle (walker) on an undirected network
  - At time t, it is located on a given vertex of degree k
  - At time t+1 , it hops with probability 1/k to one of the k neighbors of the initial vertex



# Exact solution: Master equation approach

- The random walk can be characterized by the probability P(i,t;j) that a walker starting at node j at time t=0 is at node i at time t
- Simple master equation for this probability in terms of the adjacency matrix $a_{ij}$:

$$P(i,t+1;j) = \sum_n \frac{a_{in}}{k_n} P(n,t;j)$$

- Iterating the equation up to time t

$$P(i,t:j) = \sum_{n_1} \sum_{n_2} \cdots \sum_{n_{t-1}} \frac{a_{in_1}}{k_i} \frac{a_{n_1 n_2}}{k_{n_1}} \cdots \frac{a_{n_{t-1} j}}{k_{n_{t-1}}}$$

- By symmetry

$$k_i P(i,t;j) = k_j P(j,t;i)$$

  - Detailed balance condition

# Exact solution: Master equation approach

- In the steady state (t →∞), where information of the origin is lost

$$P(i) = \lim_{t \to \infty} P(i, t; j)$$

  - Probability that the walker is at vertex i in the steady state
- For this quantity

$$k_j P(i) = k_i P(j)$$

- From here, the normalized probability

$$P(i) = \frac{k_i}{\langle k \rangle N}$$

  - The probability that the walker is at vertex i is proportional to the degree $k_i$

# First passage time

- First passage probability F(i,j,t): probability that a walker starting at i arrives at j for the first time at time t
- Simple equation

$$P(j,t;i) = \delta_{t,0}\delta_{i,j} + \sum_{t'=0}^{t} P(j,t-t';j)F(i,j,t')$$

- In terms of the corresponding Laplace transforms

$$\hat{F}(i,j,s) = \frac{\hat{P}(j,s;i) - \delta_{i,j}}{\hat{P}(j,s;j)}$$

- Look at the mean first passage time to go from i to j

$$\bar{T}(ij) = \sum_{t=0}^{\infty} t^n F(i,j,t) = -\hat{F}'(i,j,s)$$

# Mean first passage time

- Expanding the Laplace transform of P(i,t;j) in powers of s, in introducing in the equation for F(i,j,s) we can obtain the exact result

$$\bar{T}(ij) = \begin{cases} \dfrac{\langle k \rangle N}{k_i} & \text{if} \quad i = j \\ \dfrac{\langle k \rangle N}{k_j} \times \text{corrections} & \text{if} \quad i \neq j \end{cases}$$

- The mean first return time is inversely proportional to the degree
- The mean first passage time is inversely proportional to the degree of the target, times corrections (small) depending on i and j

# Heterogeneous mean-field theory

# Quantitative analysis of dynamical processes on complex networks

- In some cases, an exact solution is possible for simple models on networks; becomes complex for complex processes
- But usually, we must resort to approximate methods
- As in the case of Euclidean lattices, the analytical study of dynamical processes on complex networks in based in the mean-field analysis
- Theoretical framework analogous to the case of Euclidean lattices, based in
  - Homogeneous mixing hypothesis: The mixture of particles is homogeneous and does not depend on space (the particular vertex considered in the case of networks)
- Fundamental difference in the case of networks:
  - Vertices with a different degree can have in principle different dynamical properties (in particular in SF networks)
    - The degree k must be taken explicitly into account in the formulation of mean-field theories
    - This corresponds to a heterogeneous mean-field theory

# Construction of mean-field theories in complex networks

- To construct a heterogeneous MF theory in complex networks we will follow the general procedure:
  - Identify the appropriate set of dynamical variables $\Psi(t)$, characterizing the dynamical system
  - Distinguish the value of the variables in each vertex degree class k, $\Psi_k(t)$
  - Write down the appropriate dynamical equation for each variable $\Psi_k(t)$, starting from the dynamical rules defining the process:

$$\partial_t \mathbf{\Psi}_k(t) = \mathcal{F}[\{\mathbf{\Psi}_{k'}(t)\}]$$

  - In this last step we will be guided by standard MF approximation
    - In many cases, a direct translation adding degree dependence will be enough
    - In others, microscopic deductions are possible
    - In other, intuition

# Heterogeneous mean-field assumptions

- When applying mean-field techniques to complex networks, we will be making several assumptions:
  1) Noise (fluctuations) play no role in the dynamics
     - Usual assumption in standard mean-field treatments
     - Wrong in regular lattices of small dimension
     - In complex networks it is supposed to work due to the small-world property (effective infinite dimensional systems)
       - The diameter of the network is so small that the size of fluctuations cannot be very large, and we can assume than competing fluctuations can cancel each other in very few time steps of the order log N
       - This is in contrast with non-small world networks, such as Euclidean lattices, in which the time to cancel fluctuations scales as $N^{1/d}$

# Heterogeneous mean-field assumptions

2) Lack of dynamical correlations

- We will assume that properties that depend on the state of two vertices can be decomposed in products depending on the state of each individual vertex
  - Example: A system in with nodes can be in state $s_i$

$$\mathrm{Prob}(s_i = \alpha, s_j = \beta) \equiv \mathrm{Prob}(s_i = \alpha) \times \mathrm{Prob}(s_j = \beta)$$

- Sometimes it works, sometimes it does not

# Heterogeneous mean-field assumptions

3) The degree is the only property characterizing the behavior of vertices

- All the vertices with the same degree have the same properties, and can therefore we grouped together
  - Degree coarse-graining
- We will only have to consider equations depending on the degree k, and not on the individual vertices

- This approximation is equivalent to replacing the adjacency matrix by an average at fixed degree
  - The annealed network approximation

- HMF is exact on annealed networks!!

# The random walk revisited

# HMF theory of the random walk

- Let us consider again the random walk problem, from the perspective of HMF theory
  - See if we can recover the previous exact results
- Characterization of diffusion given by $\rho_i(t)$: Probability that the walker is in vertex i at time t
  - Equivalent to the probability P(i, t; j); we disregard effectively the starting point t
- Within a heterogeneous MF approach, we assume that this quantity depends exclusively on the degree k, $\rho_k(t)$: Probability that the walker is at a given vertex of degree k at time t
  - Occupation probability

# Occupation probability rate equation

- The occupation probability fulfills the rate equation

$$\frac{\partial \rho_k(t)}{\partial t} = -\rho_k(t) + k\sum_{k'} \frac{P(k'|k)}{k'}\rho_{k'}(t)$$

Destruction term

Creation term

- In the steady state $\partial_t \rho_k(t) = 0$, the solution of this equation is

$$\rho_k(t) = \frac{k}{\langle k \rangle N}.$$

  - For any correlation pattern P(k'|k)
    - Universality in the solution

## Other properties accessible via HMF: Random Walk Coverage

- A quantity of immediate interest, related to the speed at which the walker explores the network, is the coverage S(t)
  - Number of different vertices visited by a walker at time †, averaged for different random walks starting from different starting points
- At MF level, we define first $s_k(t)$
  - Fraction of vertices of degree k visited by the random walker at least once
  - Obviously

$$S(t) = N \sum_k P(k) s_k(t)$$

## Other properties accessible via HMF: Random Walk Coverage

- At MF level, we have the rate equation

$$\frac{\partial s_k(t)}{\partial t} = k[1 - s_k(t)] \sum_{k'} \frac{P(k'|k)}{k'} \rho_{k'}(t).$$

- Substituting the steady state approximation $\rho_k(t) = \frac{k}{\langle k \rangle N}$.

$$\frac{\partial s_k(t)}{\partial t} = [1 - s_k(t)] \frac{k}{\langle k \rangle N},$$

- Solution for the initial condition $s_k(0)=0$

$$s_k(t) = 1 - \exp\left( - \frac{kt}{\langle k \rangle N} \right).$$

## Other properties accessible via HMF: Mean-first passage time

- More information about the dynamics of random walks can be extracted from the analysis of the mean first passage time (MFPT) $\vec{\tau}(i)$, defined as the average time that a random walker takes to arrive for the first time at vertex i, starting from a random origin
- At a very MF level
  - The probability for the walker to arrive at a vertex i, in a hop following a randomly chosen edge, is given by $q(i) = k_i / N \langle k \rangle$.
  - Therefore, the probability of arriving at vertex i for the first time after t hops is $P_a(i ; t)=[1-q(i)]^{t-1} q(i)$
  - The MFTP to vertex i can thus be estimated as the average

$$\vec{\tau}(k_i) = \sum_t t P_a(i;t) = \frac{\langle k \rangle N}{k_i}.$$

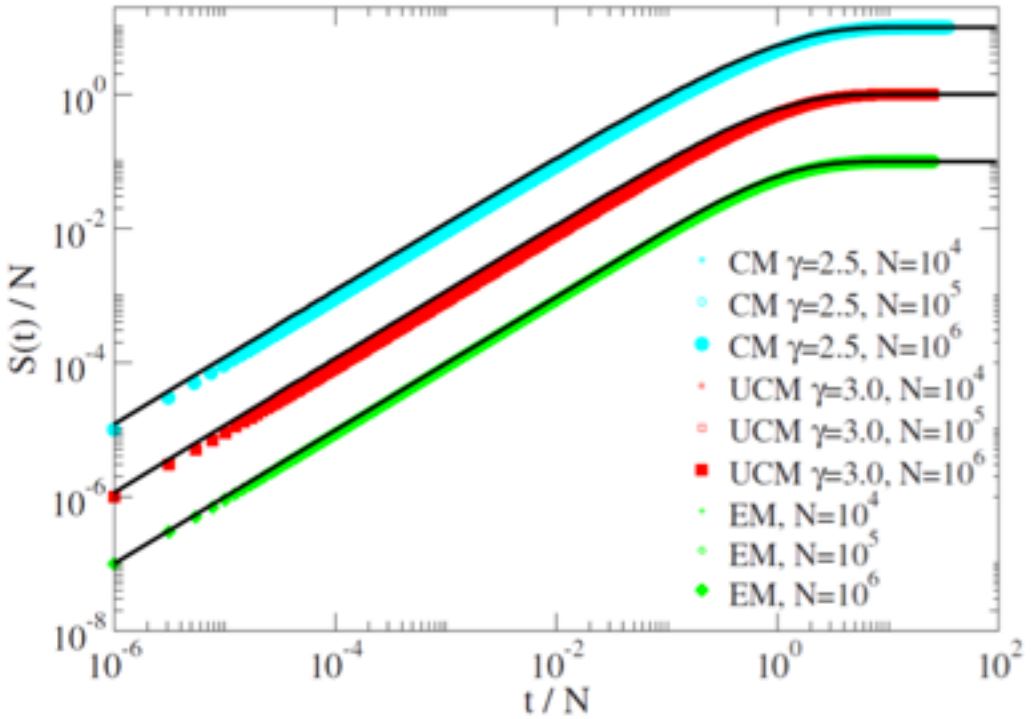
# Numerical checks: Coverage

- MF solution takes the scaling form

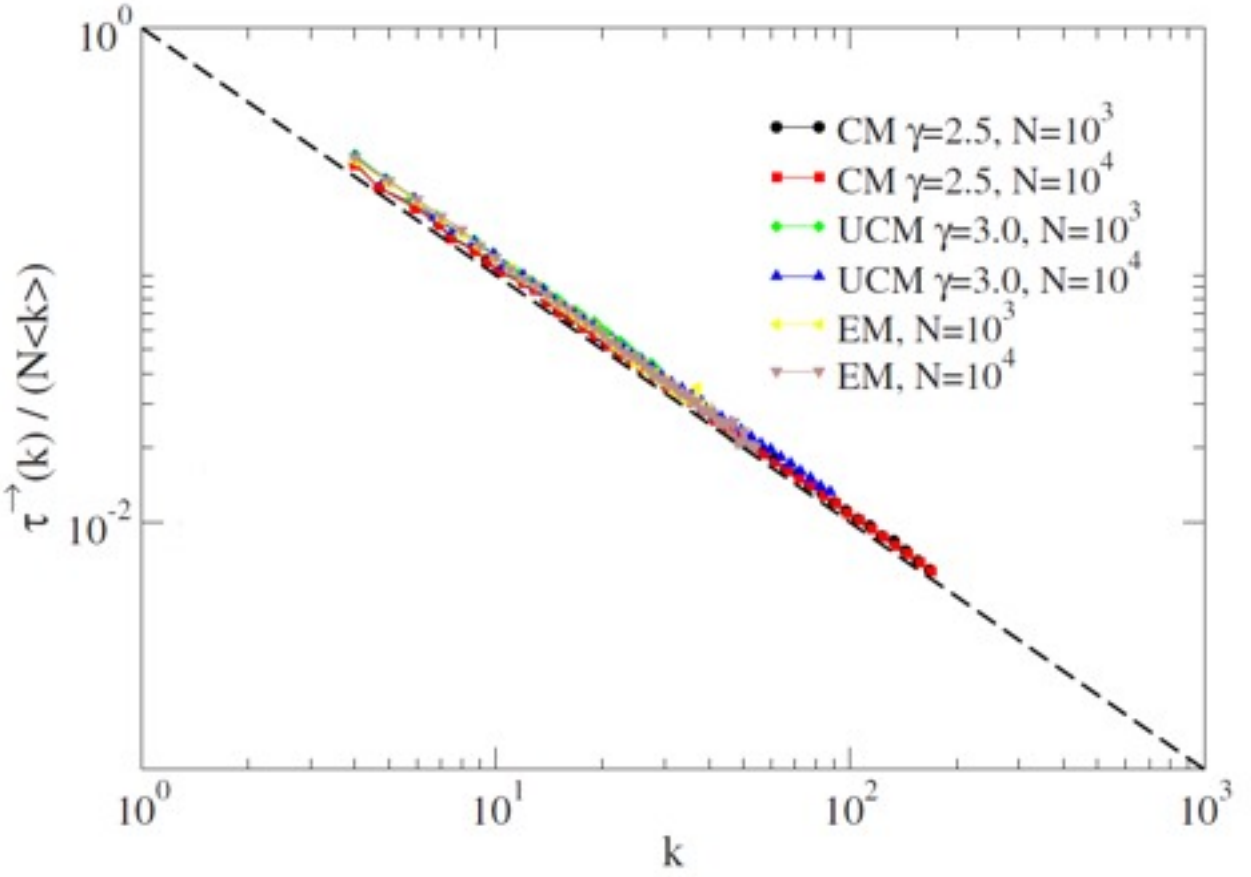
$$\frac{S(t)}{N} = 1 - \sum_k P(k) \exp\left(-\frac{kt}{\langle k \rangle N}\right) \equiv f\left(\frac{t}{\langle k \rangle N}\right)$$

  - Where the scaling function f(x) depends on degree distribution

Numerically, works perfectly for all kinds of networks



# Mean-first passage time

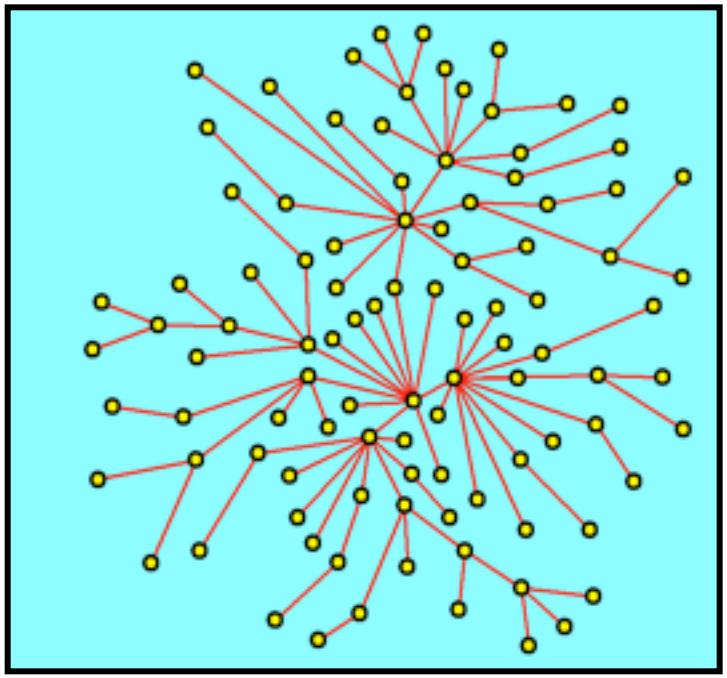



- Numerical simulations provide a perfect fit with MF prediction

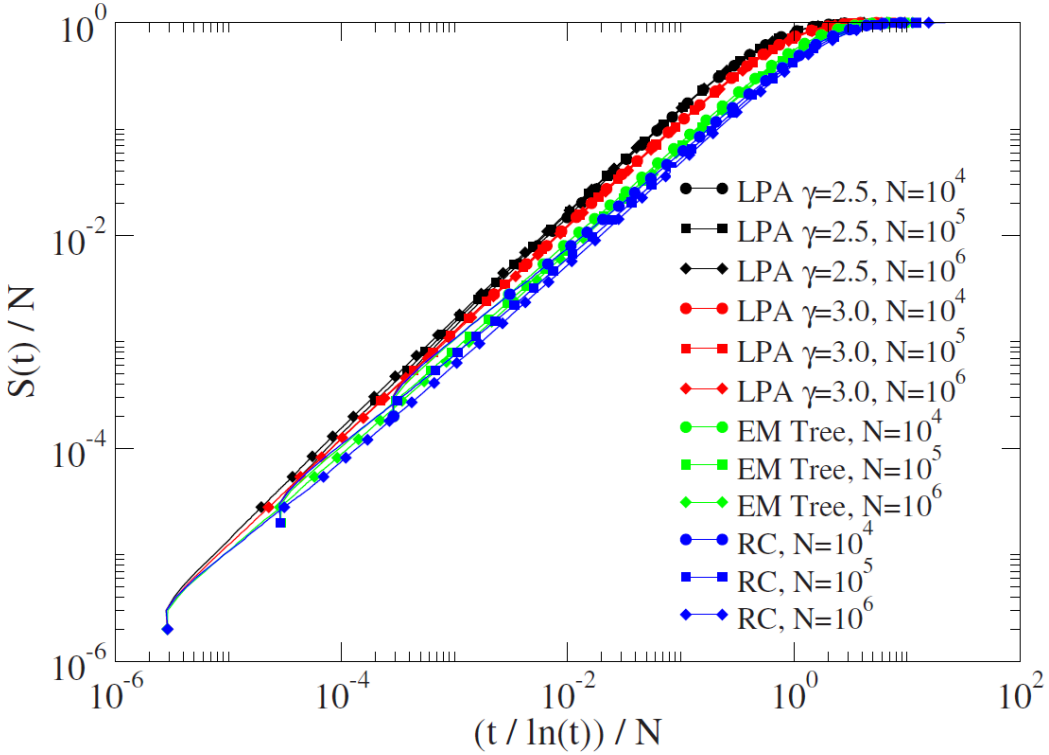
# A caveat: Does HMF always work?

- Mean-field seems to work perfectly for the networks considered
  - One main reason is the lack of dynamical correlations (linear equation)
  - But does it always work for all kinds of networks?

- Consider for example a particular type:
  - Tree networks:
    - Networks such that cutting a single edge divides the network in two disconnected components
- What about diffusion in this particular kind of topology?



# Coverage in trees

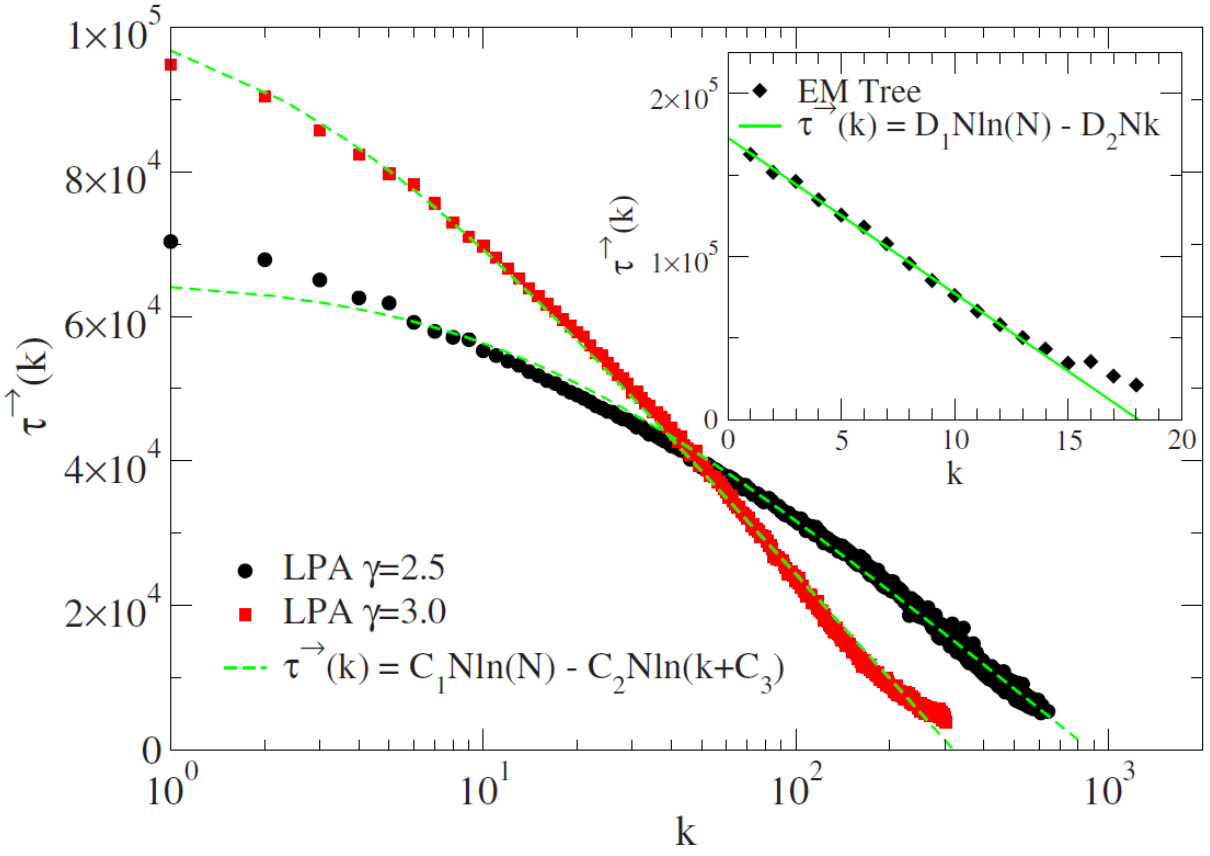



- Numerical simulations show that the predicted scaling in HMF is not fulfilled, observing instead a form that can be numerically fitted to

$$S_T(t) = Nf\left(\frac{t}{\ln(t)N}\right),$$

- No explanation...

# Mean first passage time in trees



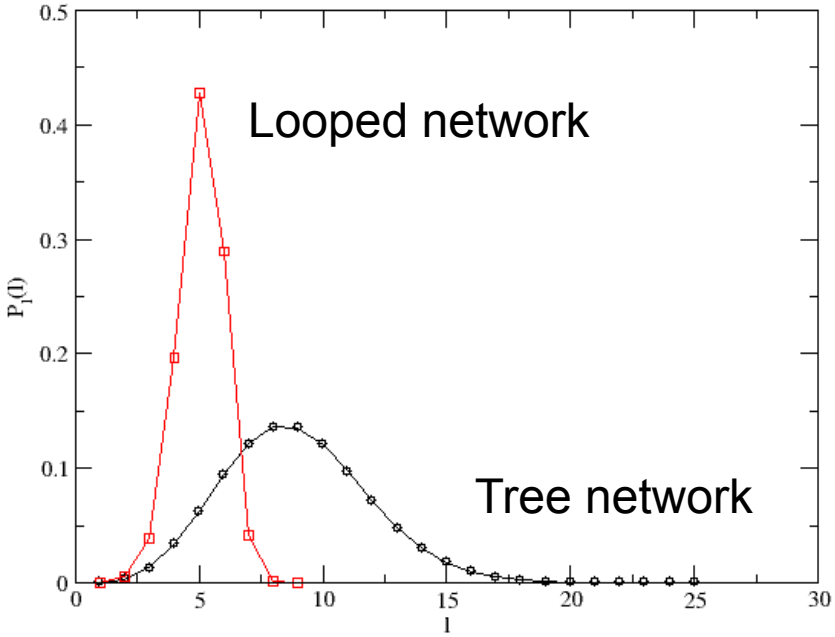

- Again MF does not work in trees, with complex expressions for the MFPT, according to the topological properties of the networks

# Why trees are different?

- We can get an idea of why trees are different looking at the shortest path distribution in two networks with the same size

- Average shortest path length is a well defined quantity in looped networks
  - Very narrow distribution
  - "Strong" small-world

- In trees, however, there are large variations in shortest path, beyond average value
  - "Weak" small-world
  - Distance can influence the behavior of discovery times or MFTP's, yielding larger values



# The random walk revisited
# I Extension of the random walk

# Generalizations of the random walk

- HMF allows to consider in a simple way generalizations of the random walk which are not easily accessible through exact solutions
- Simplest generalization: random walk with heterogeneous transition rates
  - At time t, the walker is at vertex i
  - It chooses at random a neighbor j
  - With a given probability r(i→j), the transition rate, the walker hops from i to j
  - Time is updated t→t+1

- At a degree coarse-grained level, the probability r(i→j) defines a transition rate

$$W_{kk'} = P(k'|k)r(k \to k').$$

# Generalizations of the random walk

- Time evolution of the probability P(k,t) of finding the walker at *any node* of degree k: Simple master equation

$$\frac{dP(k,t)}{dt} = -\sum_{k'} W_{kk'} P(k,t) + \sum_{k'} W_{k'k} P(k',t)$$

- In the steady state, $P^{\infty}(k) = P(k,t\to\infty)$

$$\sum_{k'} [-W_{kk'} P^{\infty}(k) + W_{k'k} P^{\infty}(k')] = 0,$$

- Can be solved imposing a detailed balance condition

$$W_{kk'} P^{\infty}(k) = W_{k'k} P^{\infty}(k'), \qquad \forall k, k'.$$

# Generalizations of the random walk

- With the form of $W_{k\,k'}$:

$$\frac{P^{\infty}(k)}{P^{\infty}(k')} = \frac{W_{k'k}}{W_{kk'}} = \frac{P(k|k')r(k' \to k)}{P(k'|k)r(k \to k')} = \frac{kP(k)}{k'P(k')}\frac{r(k' \to k)}{r(k \to k')},$$

  - Interestingly independent of degree correlations

- Explicit solutions for particular forms of r(k→k′):

$$r(k' \to k) = f(k')g(k)s(k', k).$$

- In this case

$$P^{\infty}(k) = \frac{1}{\mathcal{Z}} kP(k)g(k)/f(k)$$

# Glassy behavior

- This kind of models represent simple examples of dynamical systems with glassy behavior: Very slow relaxation time towards equilibrium
- Example: $r(k \to k') = r_0 \exp(-\beta\, h(k))$
  - Arrhenius rate with energy a function of degree [$\beta = 1/T$]
- Choosing $h(k) = E_0 \log(k)$ and a SF network

$$P^{\infty}(k) = \frac{k^{1-\gamma+\beta E_0}}{\zeta(-1+\gamma-\beta E_0)}$$

  - $\zeta(z)$ Riemann zeta function
- $\zeta(z)$ only converges for $\gamma - \beta E_0 > 2,$
- Glass transition at a critical temperature

$$T_{\mathrm{c}} = \frac{1}{\beta_{\mathrm{c}}} = \frac{E_0}{\gamma - 2}.$$

  - Below $T_c$, there is no steady state in the thermodynamic limit; it is reached very slowly in finite networks, at time scales $t_{\mathrm{eq}} \sim N^{\beta_{\mathrm{c}}/2}$

# Epidemic processes:
# I The SIS model

# SIS model

- The Susceptible-Infected-Susceptible (SIS) model is the simplest epidemiological model, capable to sustain a stationary or endemic state
  - Such as influenza, gonorrhea, computer viruses, etc.

- Definition
  - Individuals are either is a susceptible (S) state or in an infected (I) state
  - Susceptible individuals become infected ($S \rightarrow I$) with probability $\nu$ if they are connected to other infected individuals
  - Infected individuals spontaneously recover ($I \rightarrow S$) with probability $\delta$
  - Characteristic parameter: spreading rate $\lambda = \frac{\nu}{\delta}$

# Numerical implementation on the SIS model on networks

- Numerical algorithm on any network defined as follows:
  - At each time step, we compute the number of infected nodes, $N_i$, and links emanating from them, $N_n$
  - With probability $N_i/(N_i + \lambda N_n)$ a randomly chosen infected vertex becomes susceptible
  - With complementary probability $\lambda N_n/(N_i + \lambda N_n)$, one of the edges is selected and the infection is transmitted through it
  - Numbers of infected vertices and related edges are updated accordingly
  - Time is increase by $t \rightarrow t + 1/(N_i + \lambda N_n)$
  - Iterate this process

# Mean field theory

- The relevant parameter is the density of infected individuals of degree k, $\rho_k(t)$, which fulfills the rate equation

$$\partial_t \rho_k(t) = -\rho_k(t) + \lambda[1-\rho_k(t)]k\sum_{k'} P(k'|k)\rho_{k'}(t)$$

Destruction term

Creation term

- In the creation, the correct term should have been
  - Probability that a susceptible site is connected to an infected and gets the disease from it

# Mean field theory

- We are thus in the situation of having an edge with and S and an I at its extremes

$$P\left\{(S,k) \;\Leftrightarrow\; (I,k')\right\}$$

- Assuming lack of dynamical correlations

$$P\left\{(S,k) \;\Leftrightarrow\; (I,k')\right\} \equiv (1-\rho_k)\; P(k'|k)\; \rho_{k'}$$

  - Decomposed in the properties of independent vertices

# Mean field theory

- Complete equation is quite hard to solve, for general P(k’ | k)
- The most we can do is to perform a stability analysis, to check for the possible presence of non-zero solutions corresponding to an steady state: Linear stability

$$\begin{aligned}
\partial_t \rho_k &= -\rho_k + \lambda(1-\rho_k)k\sum_{k'} P(k'|k)\rho_{k'} \\
&\simeq -\rho_k + \lambda k \sum_{k'} P(k'|k)\rho_{k'} \\
&\equiv \sum_{k'} J_{k,k'}\,\rho_{k'}
\end{aligned}$$

$$J_{k,k'} \equiv -\delta_{k,k'} + \lambda k P(k'|k)$$

Jacobian matrix

# Mean field theory

- Steady states can happen when the largest eigenvalue of $J_{k\,k'}$ is larger than zero
- I.e. when

$$\lambda \leq \lambda_c = \frac{1}{\Lambda_m}$$

  - where $\Lambda_m$ is the largest eigenvalue of the connectivity matrix

$$C_{kk'} = kP(k'|k)$$

# Uncorrelated networks

- In uncorrelated networks, we have P(k′ | k) = k′ P(k′)/<k>
- Therefore we have

$$C_{k,k'} = kk' \frac{P(k')}{\langle k \rangle}$$

- We can check that the only eigenvector of this matrix is $v_k = k$, with an eigenvalue

$$\Lambda_m = \frac{\langle k^2 \rangle}{\langle k \rangle}$$

- Thus

$$\lambda_c = \frac{\langle k \rangle}{\langle k^2 \rangle}$$

# Uncorrelated networks

- The MF equation simplifies to

$$\frac{\partial \rho_k(t)}{\partial t} = -\rho_k(t) + \lambda k \Theta(1 - \rho_k(t))$$

$$\Theta = \frac{1}{\langle k \rangle} \sum_{k'} k' P(k') \rho_{k'}$$

  - Independent of k

- Steady states can be determined by finding the stationary solution and looking for nonzero solutions of the equation

$$0 = -\rho_k(t) + \lambda k \Theta(1 - \rho_k(t))$$

# Mean field predictions in SF networks

- Steady state solution

$$\rho_k = \frac{\lambda k \Theta}{1 + \lambda k \Theta}$$

- Self-consistent equation to solve

$$\Theta = \frac{1}{\langle k \rangle} \sum_k k P(k) \frac{\lambda k \Theta}{1 + \lambda k \Theta}$$

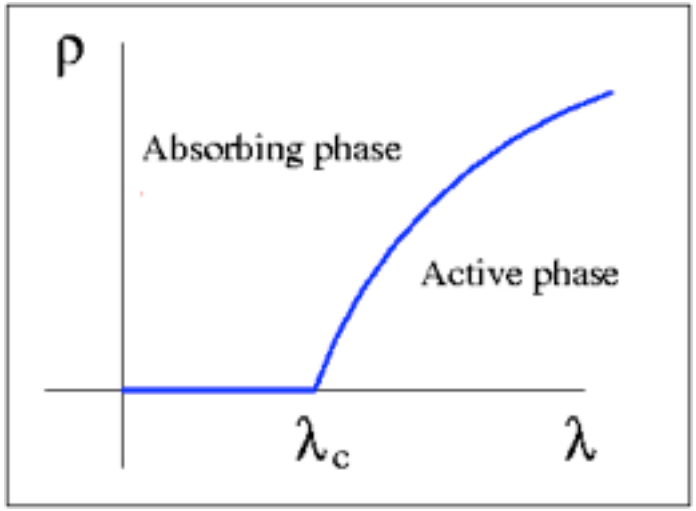
- Solution with non-zero $\Theta$ exist only for:

$$\left. \frac{d}{d\Theta} \frac{1}{\langle k \rangle} \sum_k k P(k) \frac{\lambda k \Theta}{1 + \lambda k \Theta} \right|_{\Theta=0} = \lambda \frac{\sum_k k^2 P(k)}{\sum_k k P(k)} \geq 1 \quad \Rightarrow \quad \lambda > \frac{\langle k \rangle}{\langle k^2 \rangle}$$

# Mean field predictions in SF networks

- There is a phase transition between an active (infected) phase for $\lambda > \lambda_c$ and an inactive (healthy) phase for $\lambda < \lambda_c$
  - Absorbing-state phase transition with an epidemic threshold

$$\lambda_c = \frac{\langle k \rangle}{\langle k^2 \rangle}$$




- For SF networks

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

  - If

$$2 \leq \gamma \leq 3 \Rightarrow \langle k^2 \rangle \to \infty \Rightarrow \lambda_c = 0$$

    - Null epidemic threshold!! : Whatever the virulence λ of the epidemics, it can spread across the whole system

# Mean field predictions in SF networks

- Quantitative prediction for the prevalence (total density of infected individuals in the steady state) in SF networks

$$\rho = \sum_k P(k)\rho_k$$

- In the continuous degree approximation (changing sums by integrals) we have to solve the coupled equations

$$\Theta(\lambda) = \frac{(\gamma-1)m^{\gamma-1}}{\langle k \rangle} \int_m^\infty \frac{k^{-\gamma+2}\lambda\Theta(\lambda)}{1+k\lambda\Theta(\lambda)}$$

$$\rho(\lambda) = (\gamma-1)m^{\gamma-1} \int_m^\infty \frac{k^{-\gamma+1}\lambda\Theta(\lambda)}{1+k\lambda\Theta(\lambda)}$$

# Case γ=3

$$\Theta(\lambda) = \frac{e^{-1/m\lambda}}{\lambda m}\left(1 - e^{-1/m\lambda}\right)^{-1}$$

$$\rho = 2m^2\lambda\Theta(\lambda)\int_m^\infty \frac{k}{k^3(1 + k\lambda\Theta(\lambda))}dk$$

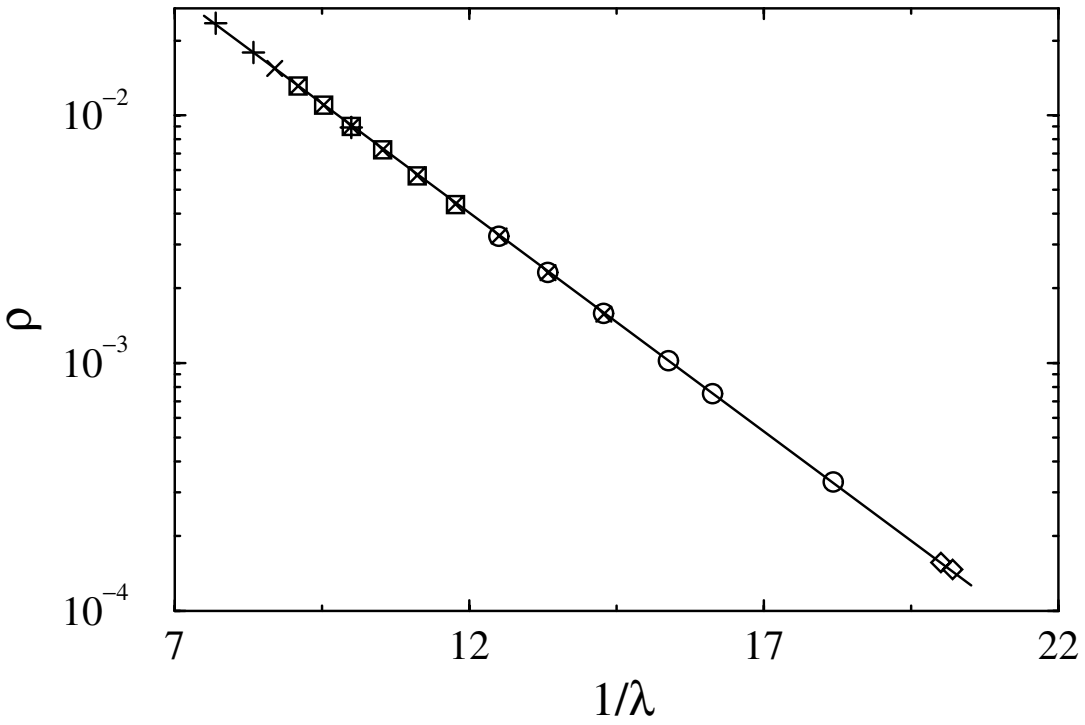
At lowest order

$$\rho \sim 2e^{-1/m\lambda}$$

# Numerical results

- Numerical simulations confirm mean field predictions

$$\gamma = 3, N = 10^8$$




$$\rho \sim 2e^{-1/m\lambda}$$

# General $\gamma$

$$P(k) = (\gamma - 1) m^{\gamma - 1} k^{-\gamma}, \qquad 2 < \gamma$$

$$\Theta(\lambda) = F[1, \gamma - 2, \gamma - 1, -(m\lambda\Theta(\lambda))^{-1}]$$

$$\rho = F[1, \gamma - 1, \gamma, -(m\lambda\Theta(\lambda))^{-1}]$$

F[a,b,c,z] = Gauss hypergeometric function

# General γ

- Close to ρ≈ 0, Θ≈ 0

$$F[1,\alpha,\alpha+1,-(m\lambda\Theta(\lambda))^{-1}]$$
$$\simeq \frac{\alpha\pi}{\sin(\alpha\pi)}(m\lambda\Theta)^{\alpha}+\alpha\sum_{n=1}^{\infty}(-1)^{n}\frac{(m\lambda\Theta)^{n}}{n-\alpha},$$

- Thus

$$\rho\simeq\frac{\gamma-1}{\gamma-2}m\lambda\Theta$$

  - Solution for Θ depends on γ

# General $\gamma$

$$2 < \gamma < 3$$

$$\Theta(\lambda) \simeq \frac{(\gamma-2)\pi}{\sin[(\gamma-2)\pi]}(m\lambda\Theta)^{\gamma-2}$$

Prevalence

$$\rho \sim \lambda^{1/(3-\gamma)}$$

# General $\gamma$

$3 < \gamma < 4$

$$\Theta(\lambda) \simeq \frac{(\gamma-2)\pi}{\sin[(\gamma-2)\pi]}(m\lambda\Theta)^{\gamma-2} + \frac{\gamma-2}{\gamma-3}m\lambda\Theta.$$

Prevalence

$$\rho \sim (\lambda - \lambda_c)^{1/(\gamma-3)} \qquad \lambda_c = \frac{\gamma-3}{m(\gamma-2)}$$

# General $\gamma$

$\gamma > 4$

$$\Theta(\lambda) \simeq \frac{\gamma-2}{\gamma-3} m\lambda\Theta - \frac{\gamma-2}{\gamma-4}(m\lambda\Theta)^2$$

Prevalence

$$\rho \sim \lambda - \lambda_c \qquad \lambda_c = \frac{\gamma-3}{m(\gamma-2)}$$

# General $\gamma$: Summary

$$\rho \sim (\lambda - \lambda_c)^{\beta}$$

☒ $2 < \gamma < 3$

$$\lambda_c = 0 \qquad \beta = \frac{1}{3-\gamma}$$

☒ $3 < \gamma < 4$

$$\lambda_c = \frac{\gamma - 3}{m(\gamma - 2)} \qquad \beta = \frac{1}{\gamma - 3}$$

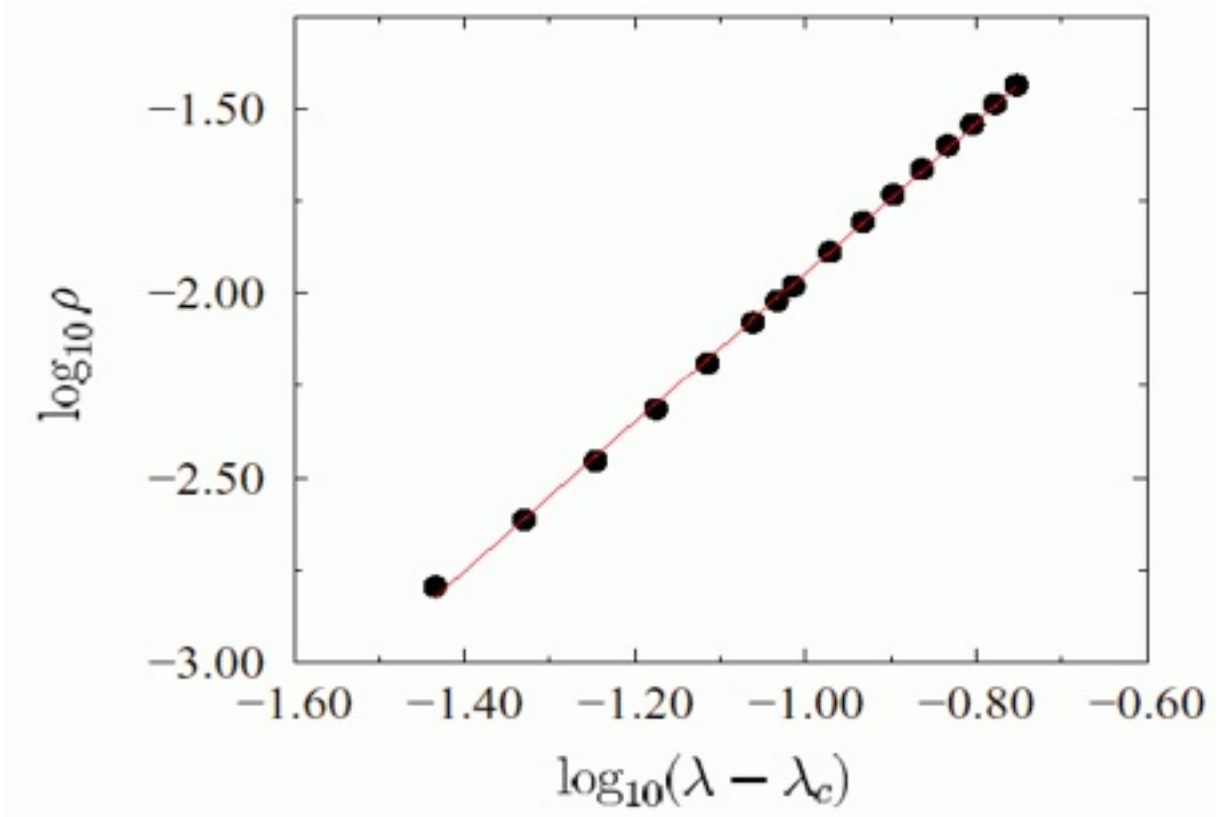
☒ $\gamma > 4$

$$\lambda_c = \frac{\gamma - 3}{m(\gamma - 2)} \qquad \beta = 1$$

# Numerical results

- Numerical simulations confirm mean field predictions

$$\gamma = 2.3, N = 10^5$$



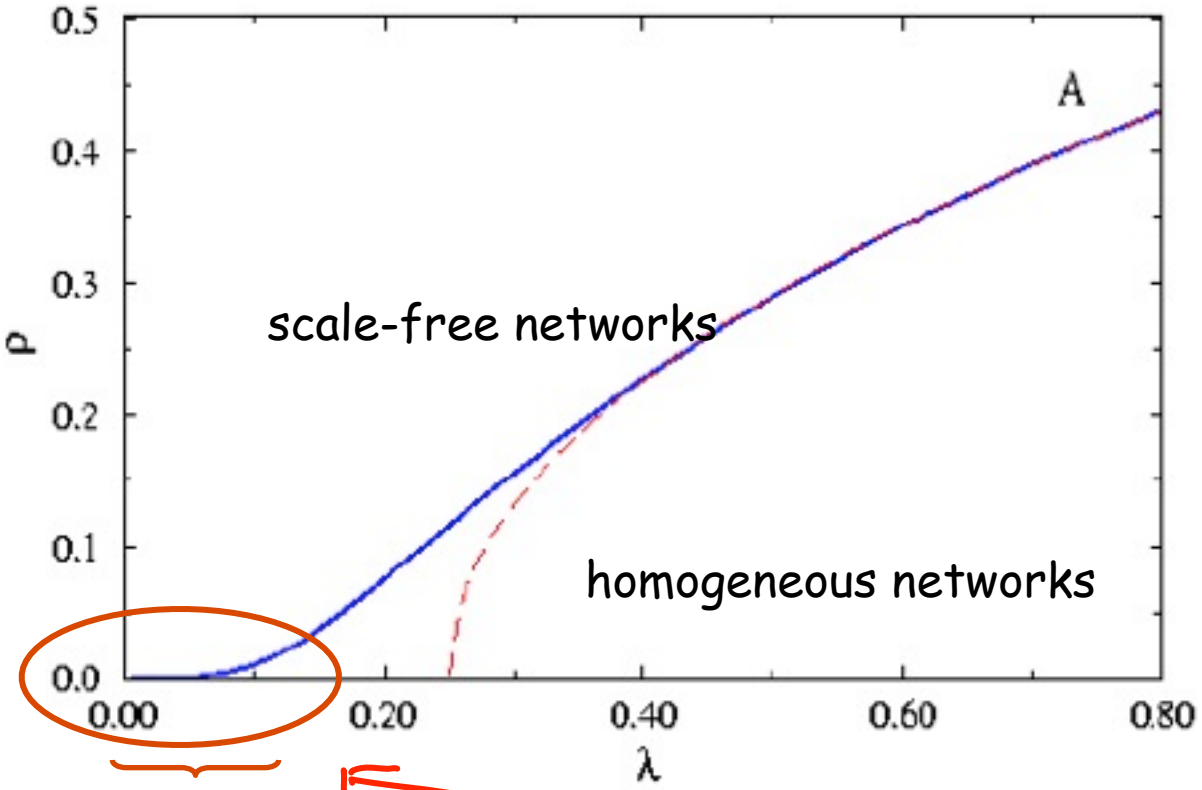

$$\rho \sim \lambda^{1/(3-\gamma)}$$

$$(\beta = 1.8, \lambda_c = 0.07)$$

Simulations on a real Internet map

# Rationalization of computer virus data

- New phase diagram with a null epidemic threshold.
- In contrast with what is obtained for regular networks, there is now a whole region of the phase diagram in which very low prevalence is possible




Low prevalence region!!

Virus can survive in this region

# Epidemic processes:
# II The SIR model

# SIR model

- The Susceptible-Infected-Removed (SIR) model is the simplest epidemiological model, capable an outbreak of a disease that confers immunity
  - Such as measles, chicken pox, etc.
- Definition
  - Individuals are either is a susceptible (S) state, an infected (I) or a removed [immunized] (R) state
  - Susceptible individuals become infected (S $\rightarrow$ I) with probability $\nu$ if they are connected to other infected individuals
  - Infected individuals recover [or die] (I $\rightarrow$ R) with probability $\delta$
  - Characteristic parameter: spreading rate $\lambda = \frac{\nu}{\delta}$

# Numerical implementation on the SIR model on networks

- Numerical algorithm on any network defined as follows:
  - At each time step, we compute the number of infected nodes, $N_i$, and links emanating from them, $N_n$
  - With probability $N_i/(N_i + \lambda N_n)$ a randomly chosen infected vertex becomes removed
  - With complementary probability $\lambda N_n/(N_i + \lambda N_n)$, one of the edges is selected and the infection is transmitted through it
  - Numbers of infected vertices and related edges are updated accordingly
  - Time is increase by $t \rightarrow t + 1/(N_i + \lambda N_n)$
  - Iterate this process

# Mean field theory

- The relevant parameters the density of infected individuals of degree k, $\rho_k(t)$, the density of susceptible $S_k(t)$ and the density of recovered $R_k(t)$
  - Not independent: $\rho_k(t) + S_k(t) + R_k(t) = 1$
    - Only keep track of two

- For uncorrelated networks, the rate equations are

$$\frac{d\rho_k(t)}{dt} = -\rho_k(t) + \lambda k S_k(t)\Theta^{\rm nc}(t),$$

$$\frac{dS_k(t)}{dt} = -\lambda k S_k(t)\Theta^{\rm nc}(t),$$

$$\frac{dR_k(t)}{dt} = \rho_k(t).$$

$$\Theta^{\rm nc}(t) = \frac{1}{\langle k\rangle}\sum_k (k-1)P(k)\rho_k(t).$$

# Uncorrelated networks

- Assuming $\rho_k(0)$ very small, $S_k(0) \cong 1$, $R_k(0)=0$, we can directly integrate to obtain

$$S_k(t) = e^{-\lambda k \phi(t)}, \qquad R_k(t) = \int_0^t \rho_k(\tau)\, \mathrm{d}\tau,$$

$$\phi(t) = \int_0^t \Theta(\tau)\, \mathrm{d}\tau = \frac{1}{\langle k \rangle} \sum_k (k-1) P(k) R_k(t).$$

- Simpler equation for $\phi$(t)

$$\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = 1 - \frac{1}{\langle k \rangle} - \phi(t) - \frac{1}{\langle k \rangle} \sum_k (k-1) P(k) e^{-\lambda k \phi(t)},$$

- Total epidemic prevalence $R_\infty = \sum_k P(k)\, R_k(\infty)$ at very large times

$$R_\infty = \sum_k P(k)(1 - e^{-\lambda k \phi_\infty}).$$

# Uncorrelated networks

- For $\phi_\infty = \lim_{t\to\infty} \phi(t)$

$$\phi_\infty = 1 - \frac{1}{\langle k\rangle} - \frac{1}{\langle k\rangle}\sum_k (k-1)P(k)e^{-\lambda k\phi_\infty}.$$

- Nonzero solutions exist for

$$\frac{\mathrm{d}}{\mathrm{d}\phi_\infty}\left(1 - \frac{1}{\langle k\rangle} - \frac{1}{\langle k\rangle}\sum_k (k-1)P(k)e^{-\lambda k\phi_\infty}\right)\Bigg|_{\phi_\infty=0} \geq 1$$

- That is, for $\lambda > \lambda_c$, with

$$\lambda_c = \frac{\langle k\rangle}{\langle k^2\rangle - \langle k\rangle},$$

Similar structure as in the SIS model

# Solution for γ=3

- In the continuous degree approximation

$$R_\infty = 1 - 2m^2 \int_m^\infty k^{-3} e^{-\lambda k \phi_\infty} dk$$
$$= \lambda^2 \left(-m^2\right) \phi^2 \mathrm{Ei}(-m\lambda\phi) - e^{\lambda(-m)\phi}(1 - \lambda m\phi) + 1$$

- Expanding the exponential integral function in the limit of small λ

$$R_\infty \simeq 2\lambda m \phi_\infty .$$

- Integrating the equation for Φ(t), in the limit of small λ

$$\frac{1}{\lambda m}\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} \simeq \phi\left[1 - \gamma_E - \frac{1}{\lambda m} - \ln(\lambda m \phi)\right].$$

# Solution for $\gamma=3$

- Integrating again

$$\phi(t) \simeq \frac{1}{\lambda m} \exp\left(1 - \gamma_E - \frac{1}{\lambda m} + A\mathrm{e}^{-\lambda m t}\right),$$

- In the stationary regime at large times

$$\phi_\infty \simeq \frac{\mathrm{e}^{1-\gamma_E}}{\lambda m}\mathrm{e}^{-1/\lambda m},$$

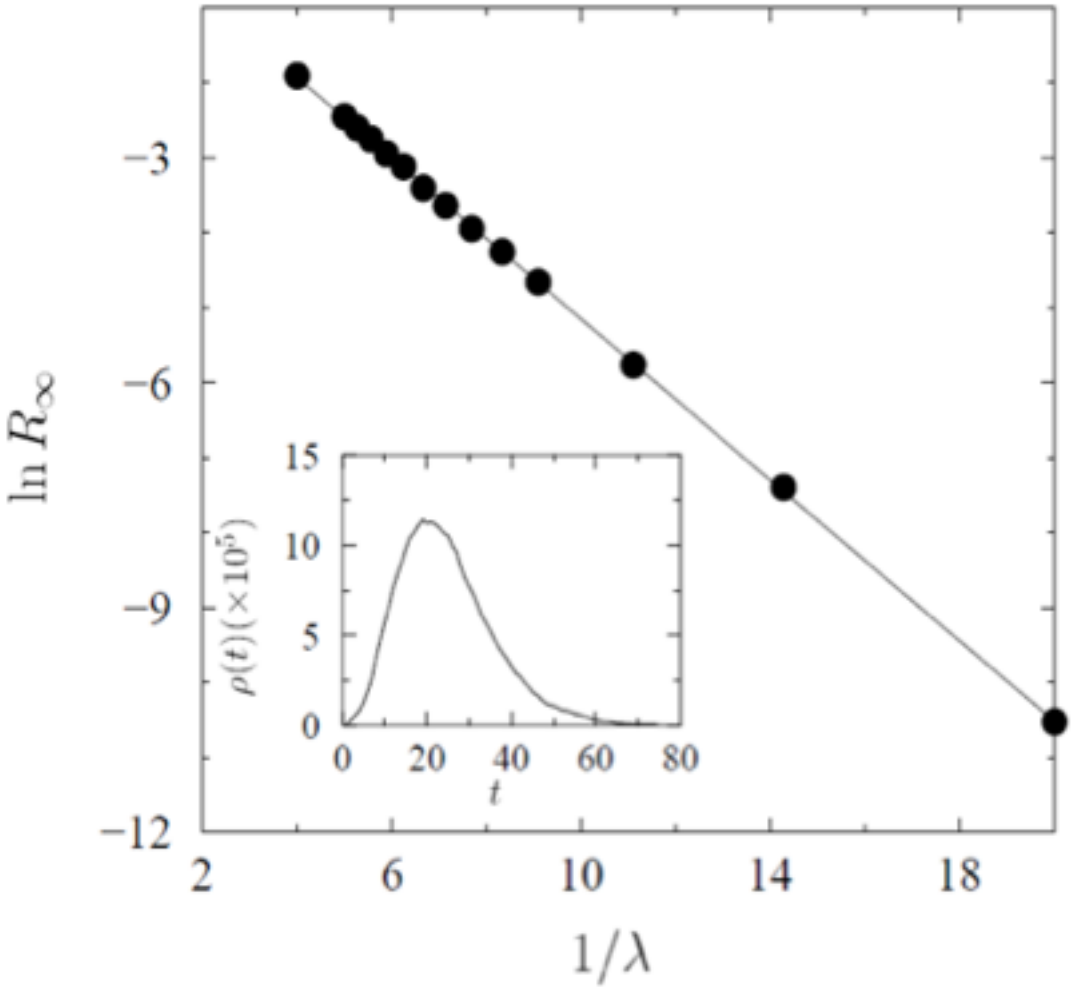
- For the prevalence

$$R_\infty \sim \mathrm{e}^{-1/\lambda m}.$$

# Numerical check

$$R_\infty \sim \mathrm{e}^{-1/\lambda m}.$$

Solution analogous to the SIS model; same happens for other values of γ



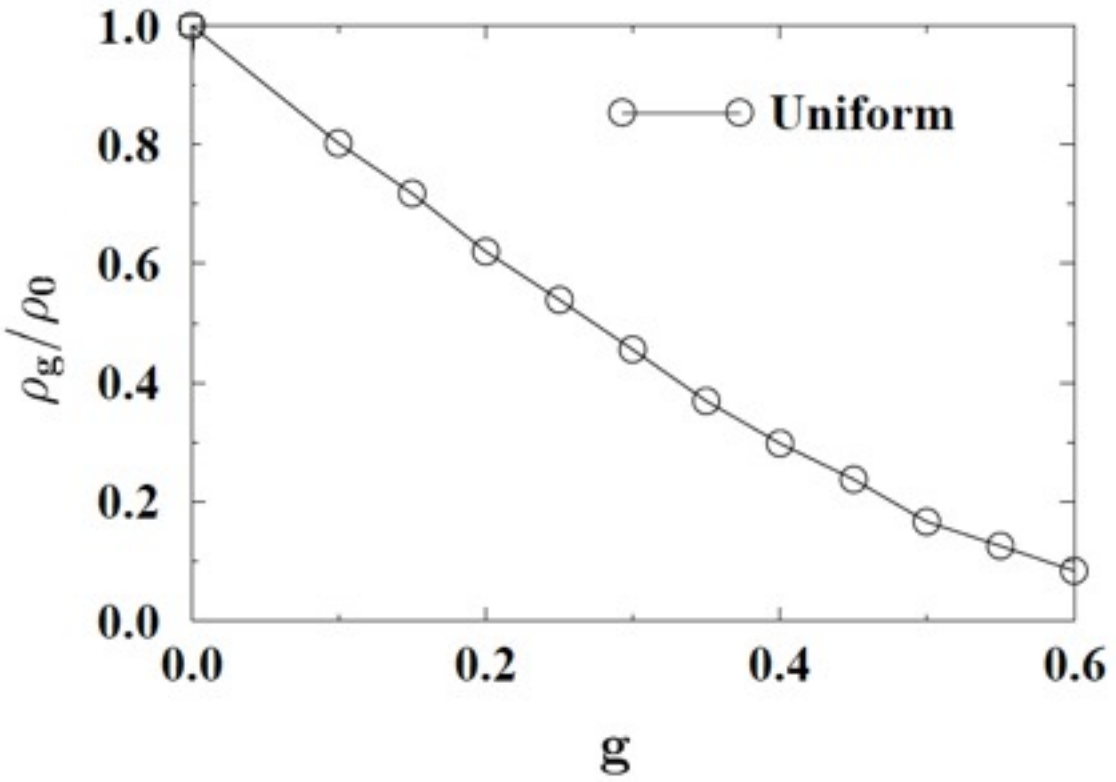
# Epidemic processes:
# III Immunization strategies

# Immunization

- Clearly, epidemics in scale-free networks are really a problem, due to the vanishing epidemic threshold
- Immunization is thus a necessity in order to impede the spreading of infective agents
- Different immunization strategies
  - Immunize everybody
    - Usual choice in biological contexts
      - Extremely expensive
  - A cheaper strategy: Random immunization
    - Immunize a fraction g of individuals selected
    - More or less the strategy used in antivirus software
      - You choose (more or less at random) whether or not install antivirus software

# Random immunization

- Computer simulations in scale-free networks




To complete eradicate the disease, we must immunize a very large fraction of the population; actually the whole population in the limit of an infinitely large network (analytical results …)

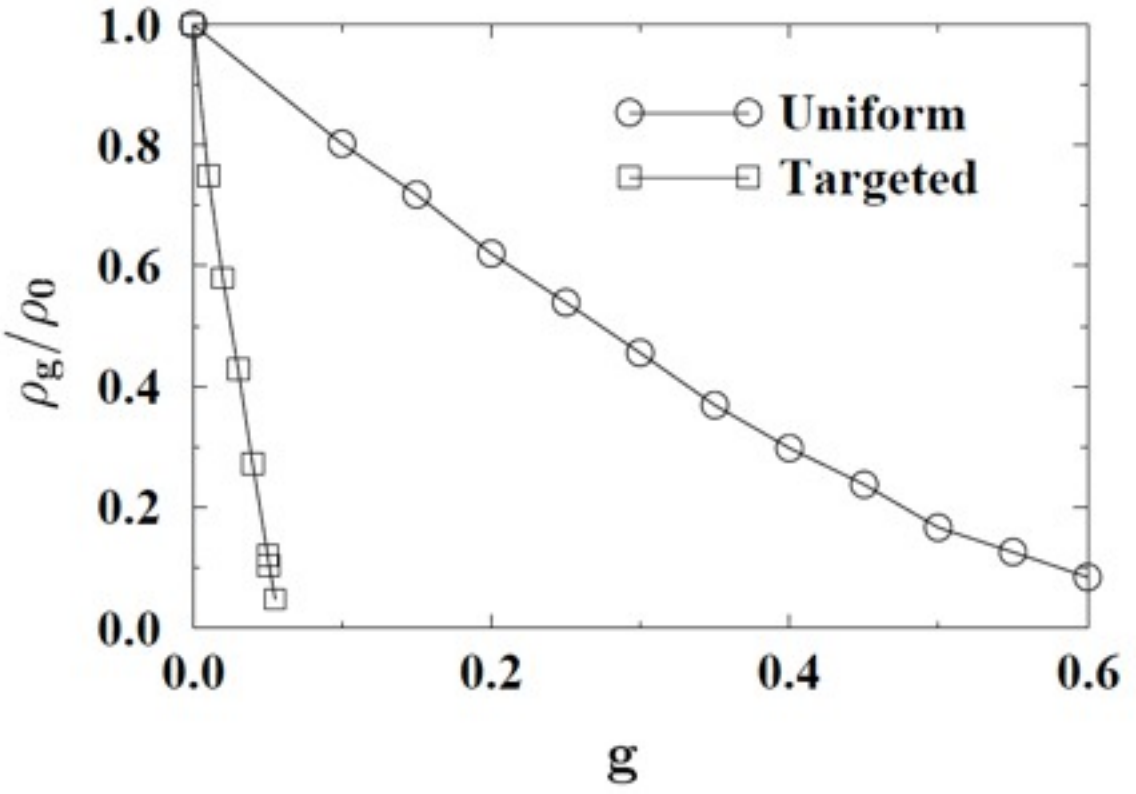
# Targeted immunization

- Thinking a little bit, we can devise more efficient strategies
- The bad effects of scale-free networks arise from a diverging second moment $\langle k^2 \rangle \gg 1$
- This divergence is obviously due to the anomalous amount of vertices with very large degree
- A possible cure could be to immunize just those vertices of large degree

- Targeted immunization:
  - Immunize a fraction g of the most connected vertices of the network

# Targeted immunization

- Computer simulations in scale-free networks




The eradication of the disease can be achieved by immunizing a very small fraction of the vertices with the largest number of connections. Actually, an exponentially small number of vertices (analytical results …)

# Immunization without global knowledge

- Targeted immunization works extremely well, but suffers from a practical drawback
  - We must have complete knowledge of the network in order to vaccinate the most connected nodes
- Other alternatives have been proposed, requiring less information
- Acquaintance immunization:
  - A fraction g of nodes are selected, and asked to point one of its neighbors
  - The neighbors, and not the nodes, are immunized
  - Why it works?
    - High degree nodes have many edges connected to them; following random edges will find those hubs with high probability

# Reaction-diffusion processes

# Reaction-diffusion processes

- The theory of reaction-diffusion (RD) processes can be used to model a wide variety of dynamical systems

- RD processes are defined in terms of:

  - Set of particles belonging to a certain number of different "species" $A_i$, i=1, …, n
  - Particles diffuse stochastically, jumping at random between nearest neighbor sites
  - Particles react upon contact according to a given set of reaction rules $R_j$, j=1,…,r

- Standard setting: Chemical reactions
  - But they can be used to model general kinds of processes

# Reaction-diffusion processes

- Examples:
  - Diffusion-annihilation process
    - Single type of particles A
    - Particles diffuse, with a diffusion coefficient D
    - Particles experience the reaction

$$A + A \xrightarrow{\lambda} \emptyset$$

  - SIS process
    - Two types of particles S and I
    - Particles diffuse, with possible different coefficients $D_S$, $D_I$
    - Particles experience the reactions

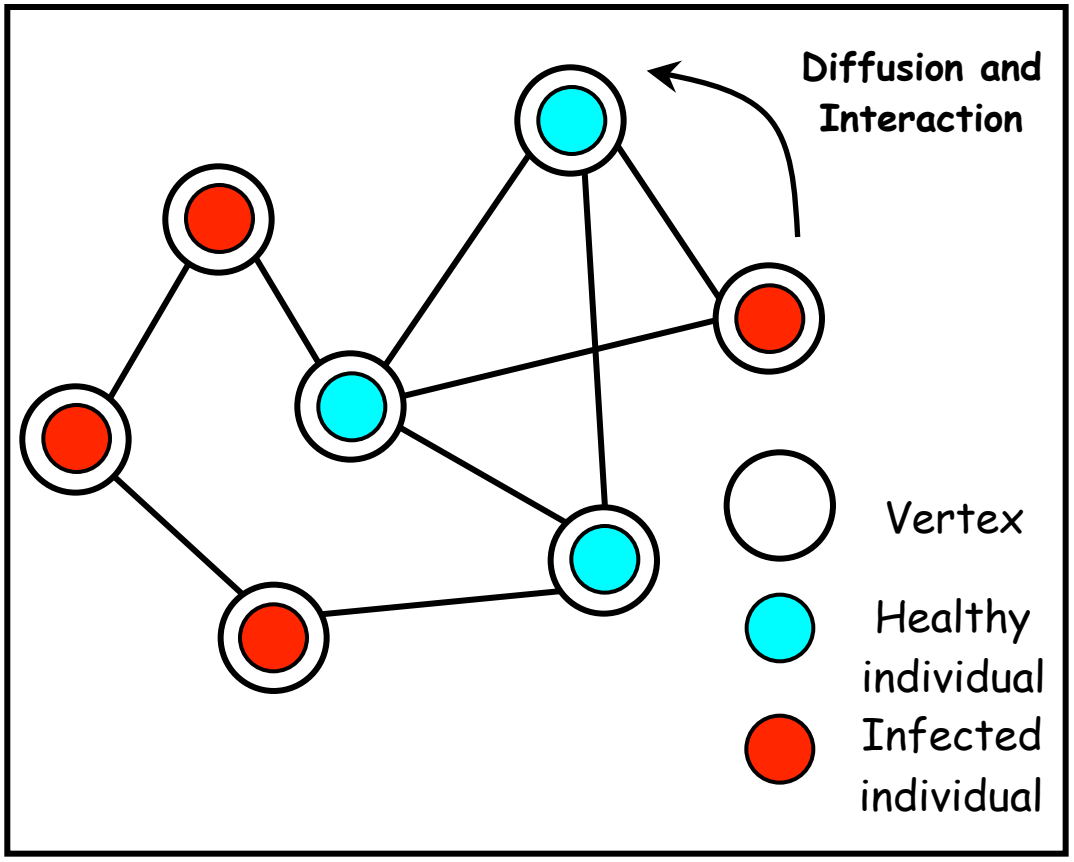
$$S + I \xrightarrow{\delta} 2I,$$
$$I \xrightarrow{\mu} S.$$

# Two basic formalisms

- When considering dynamical processes on complex networks (or regular lattices), two different perspectives are possible:
  - Fermionic systems:
    - Systems with some "exclusion" principle, that limits the number of particles on each vertex
    - Usually, occupation number $n_i(t) = 0, 1$
      - Number of particles inside each vertex is limited to 0 or 1
  - Bosonic formalism:
    - No "exclusion" principles involved
    - Occupation number $n_i(t) = 0, 1, \ldots 1$
      - No limitation in the number of particles on each vertex
- In some cases, the correct formalism arises in a natural way

# Fermionic systems

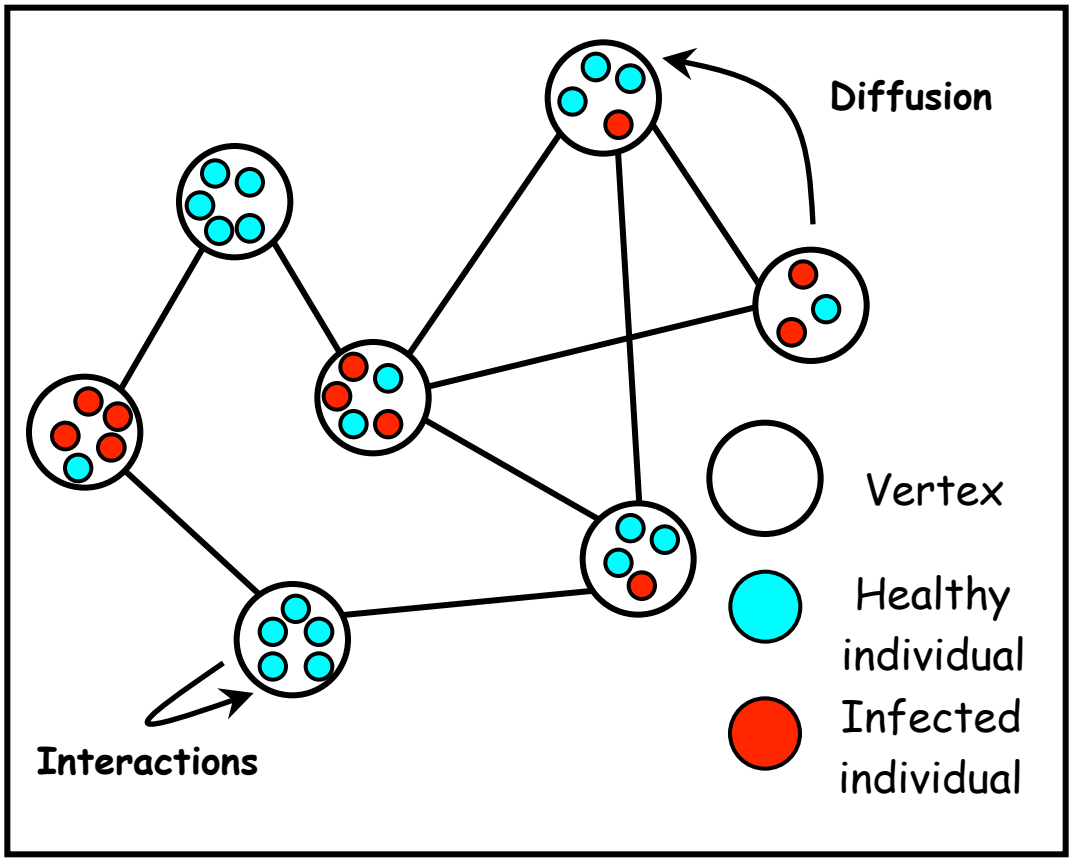
- Example: Small-scale epidemics
  - Spreading in social networks




- Vertices are individuals
- Individuals can be only in one state, healthy or infected
- Each state can be represented by a different kind of particle
- Interactions take place between connected individuals (particles)

# Bosonic systems

- Example: Large-scale epidemics
  - Spreading among cities or countries




- Vertices are cities or countries
- Cities can host many individuals
- Interactions take place inside vertices
- Particles move from vertex to vertex
  - Traveling

# Limitations of both formalisms

- In other cases, there is freedom in the choice of the formalism
- In choosing, consider that both formalisms have some advantages and limitations on complex networks

  - Fermionic formalism:
    - Models generally easy to devise and simulate numerically
    - Analytical theories must be tailored on a case by case approach, based on the particular implementation of the model
    - Usually simple to solve analytically
    - Difficult to implement interactions of more that two particles

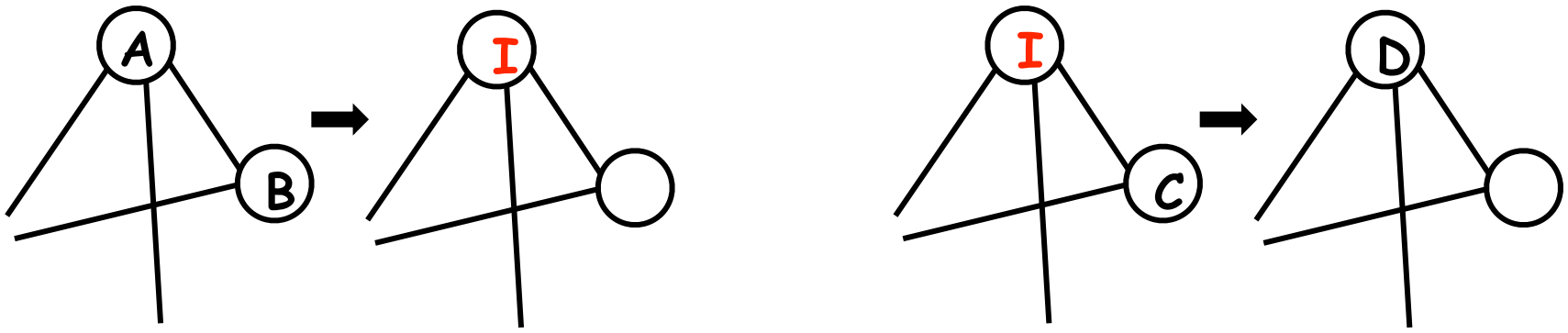
# Limitations of both formalisms

- Ex: What happens with 3 particle interactions?

$$A + B + C \rightarrow D$$

- Solution 1: Use "intermediate" particles

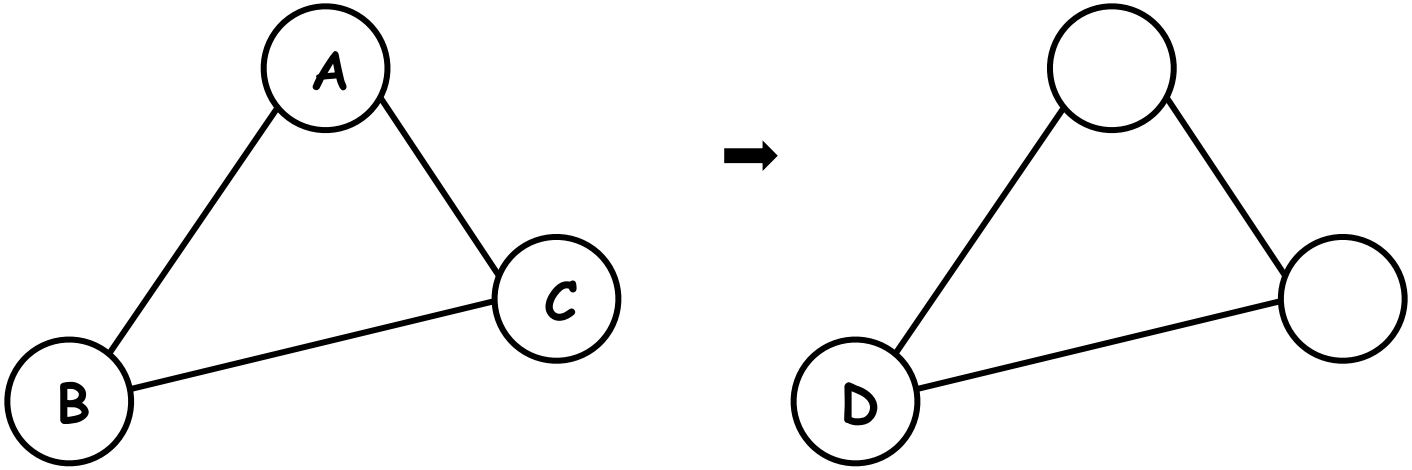
$$A + B + C \rightarrow D \quad \equiv \quad \begin{cases} A + B & \rightarrow & I \\ I + C & \rightarrow & D \end{cases}$$




  - Arbitrary and somewhat artificial

# Limitations of both formalisms

- Solution 2: Interaction among three or more vertices




- Difficult to implement numerically and not general
  - Interactions depend on the degree of the vertices

# Limitations of both formalisms

- Bosonic formalism:
  - No limitation in the order of the interactions
    - Take place inside vertices and do not depend on their connectivity
  - Numerical implementation bit more difficult
    - But however more general
  - Analytical theories can be developed for general classes of models
  - Not so easy to solve
    - Due to the generality of the interactions

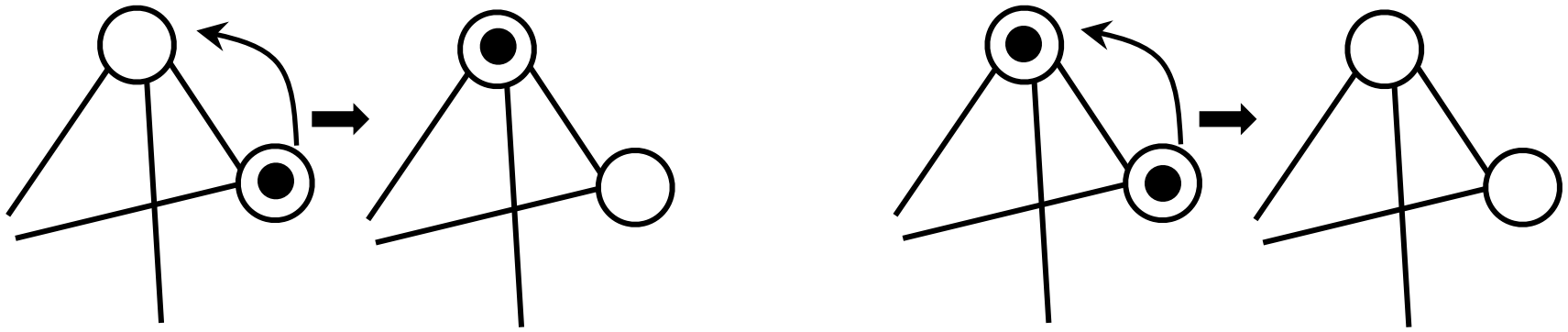
# Reaction-diffusion processes: I Fermionic formalism

# Diffusion-annihilation process

- Choose simplest case: Diffusion-annihilation process

$$A + A \xrightarrow{\lambda} \emptyset$$

- Particles perform an uncorrelated random walk
  - Sequential update, to avoid undefined events
- When one particle lands on top of another, both annihilate



# Heterogeneous mean field theory

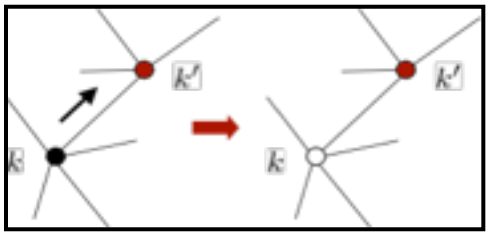
- Dynamical equation for the relative density of particles in the vertices of degree k, $\rho_k(t)$
  - In general networks:

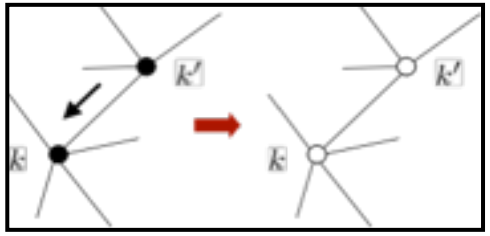
$$\frac{\partial \rho_k(t)}{\partial t} = -\lambda \rho_k(t) - \lambda k \rho_k(t) \sum_k \frac{P(k'|k)}{k'} \rho_{k'}(t) + \lambda k [1 - \rho_k(t)] \sum_k \frac{P(k'|k)}{k'} \rho_{k'}(t)$$

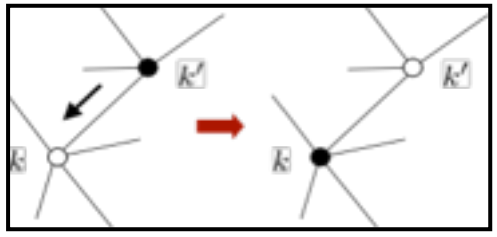
Destruction term by diffusion

Destruction term by reaction

Creation term by diffusion




  - Note: we are neglecting again dynamical correlations between two vertices!!

# Approximate solution in correlated networks

- General equation in correlated networks ($\lambda = 1$)

$$\frac{\partial \rho_k(t)}{\partial t} = -\rho_k(t) + k[1 - 2\rho_k(t)] \sum_k \frac{P(k'|k)}{k'} \rho_{k'}(t)$$

- At very large times, $\rho_k$ becomes very small
  - Diffusion-limited regime (negligible interactions)
  - We can neglect the second order terms in the rate equation

$$\frac{\partial \rho_k(t)}{\partial t} \simeq -\rho_k(t) + k \sum_k \frac{P(k'|k)}{k'} \rho_{k'}(t)$$

    - Old diffusion equation!!
- We have thus the steady state solution

$$\rho_k(t) \simeq \frac{k}{\langle k \rangle} \rho(t)$$

Note the difference with the diffusion problem

# Approximate solution in correlated networks

- Equation for the total density $\rho(t) = \sum_k P(k)\,\rho_k(t)$

$$\frac{d\rho(t)}{dt} = -2 \sum_k P(k)\rho_k(t)\Theta_k(t),$$

$$\Theta_k(t) = \sum_{k'} P(k'|k)\rho_{k'}(t)$$

- Where we have used the degree detailed balance condition
- Inserting the low density approximation, we obtain a solution valid for any correlation pattern

$$\frac{d\rho(t)}{dt} \simeq -2\,\rho(t)^2 \frac{\langle k^2\rangle}{\langle k\rangle^2}, \quad \Rightarrow \quad \frac{1}{\rho(t)} - \frac{1}{\rho_0} \simeq 2\,\frac{\langle k^2\rangle}{\langle k\rangle^2} t,$$

Solution only for finite networks

finite $\langle k^2\rangle$ (more later)

# Uncorrelated networks

- Mean field equation for uncorrelated networks ($\lambda = 1$)

$$\frac{d\rho_k(t)}{dt} = -\rho_k(t) + \frac{k}{\langle k \rangle}[1 - 2\rho_k(t)]\rho(t)$$

- Quasi-stationary approximation

$$\partial_t \rho_k(t) \ll \rho_k(t) \quad \Rightarrow \quad \rho_k(t) \simeq \frac{k\rho(t)/\langle k \rangle}{1 + 2k\rho(t)/\langle k \rangle}$$

- Final equation for the total density

$$\rho(t) = \sum_k P(k)\rho_k(t)$$

$$\frac{d\rho(t)}{dt} = -2\frac{\rho(t)^2}{\langle k \rangle^2} \sum_k \frac{k^2 P(k)}{1 + 2k\rho(t)/\langle k \rangle}$$

# General γ

- Infinite networks

$$P(k) = (\gamma - 1) m^{\gamma - 1} k^{-\gamma},$$

$$\frac{d\rho(t)}{dt} = -2\rho(t)^2 \frac{(\gamma - 1) m^{\gamma - 1}}{\langle k \rangle^2} \int_m^\infty \frac{k^{2-\gamma}}{1 + 2k\rho(t)/\langle k \rangle} dk$$

$$= -\rho(t) F(1, \gamma - 2, \gamma - 1, -(\gamma - 1)/2(\gamma - 2)\rho(t)),$$

$$t = \int_{\rho_0^{-1}}^{\rho(t)^{-1}} \frac{dz}{zF(1, \gamma - 2, \gamma - 1, -(\gamma - 1)z/2(\gamma - 2))}.$$

# General $\gamma$

- Asymptotic expansion

$$F(1,\gamma-2,\gamma-1,-z)\sim z^{2-\gamma},\ z\to\infty,$$

- General solution

$$\frac{1}{\rho(t)}\sim t^{1/(\gamma-2)}.$$

# General γ

- Finite networks of size N

$$\rho_k(t) \simeq \frac{k\rho(t)/\langle k\rangle}{1+2k\rho(t)/\langle k\rangle}$$

  - For $t_c$ such that

$$\frac{2k_c(N)\rho(t_c)}{\langle k\rangle} \ll 1,$$

$$\Theta(t) \approx \frac{\rho(t)}{\langle k\rangle^2}\sum_k k^2 P(k) = \rho(t)\frac{\langle k^2\rangle}{\langle k\rangle^2}. \quad \Rightarrow \quad \frac{1}{\rho(t)} \sim \frac{2\langle k^2\rangle}{\langle k\rangle^2}t,$$

  - In scale-free networks

$$\langle k^2\rangle = \sum_{k=m}^{k_c(N)} k^2 P(k) \sim k_c(N)^{3-\gamma}. \quad \sim N^{(3-\gamma)/2},$$

# Summary for general $\gamma$

- For SF networks we obtain:
  - Solution for infinite networks $N \to \infty$

$$\frac{1}{\rho(t)} \sim t^{1/(\gamma-2)}$$

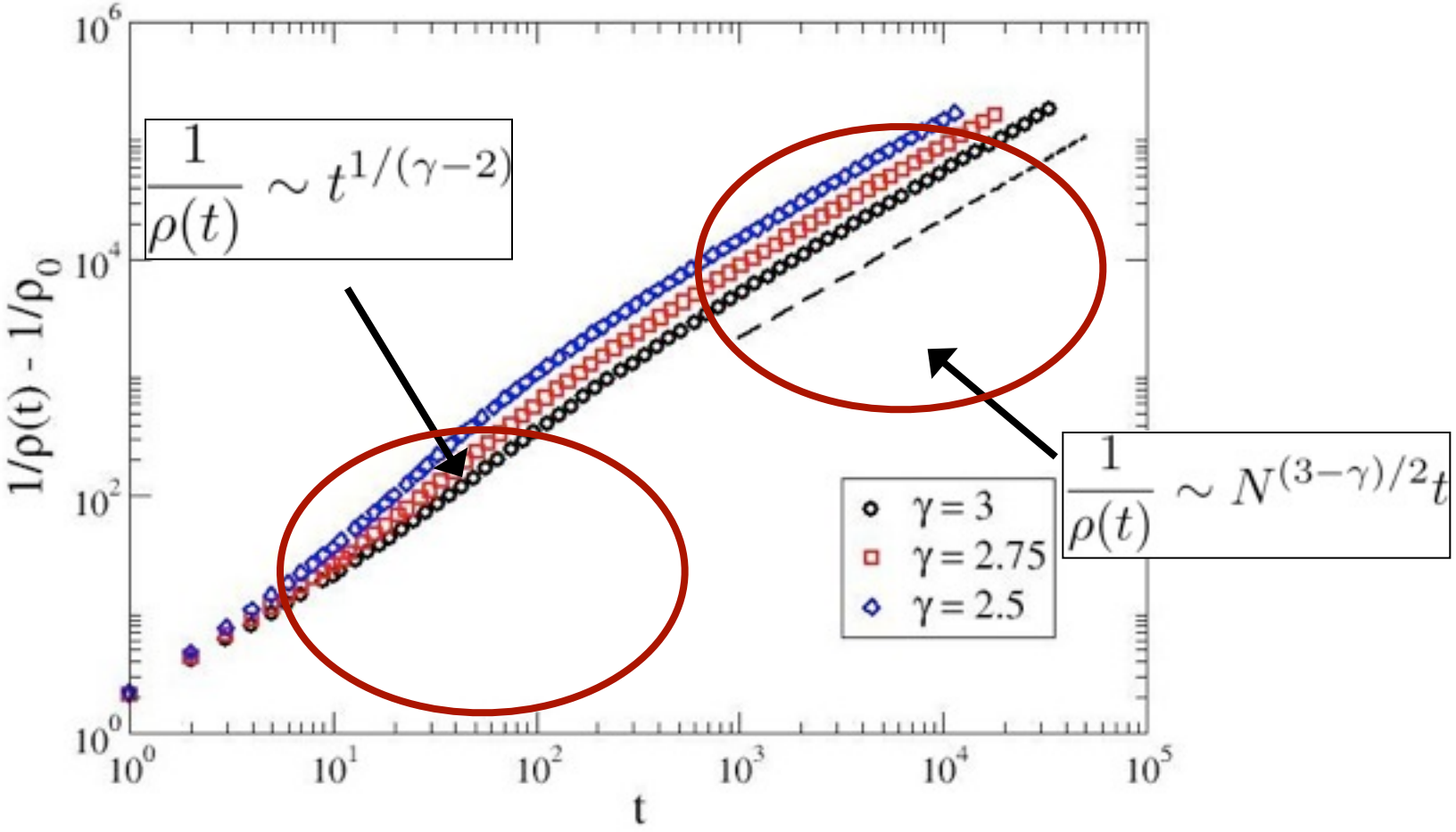
    - Density decays with time as a power-law with an exponent depending on the degree distribution
  - Solution for finite networks $N < \infty$

$$t > t_\times(N) \;\to\; \frac{1}{\rho(t)} \sim N^{(3-\gamma)/2} t$$

    - Above a certain cross-over time, linear behavior with a slope growing with the network size

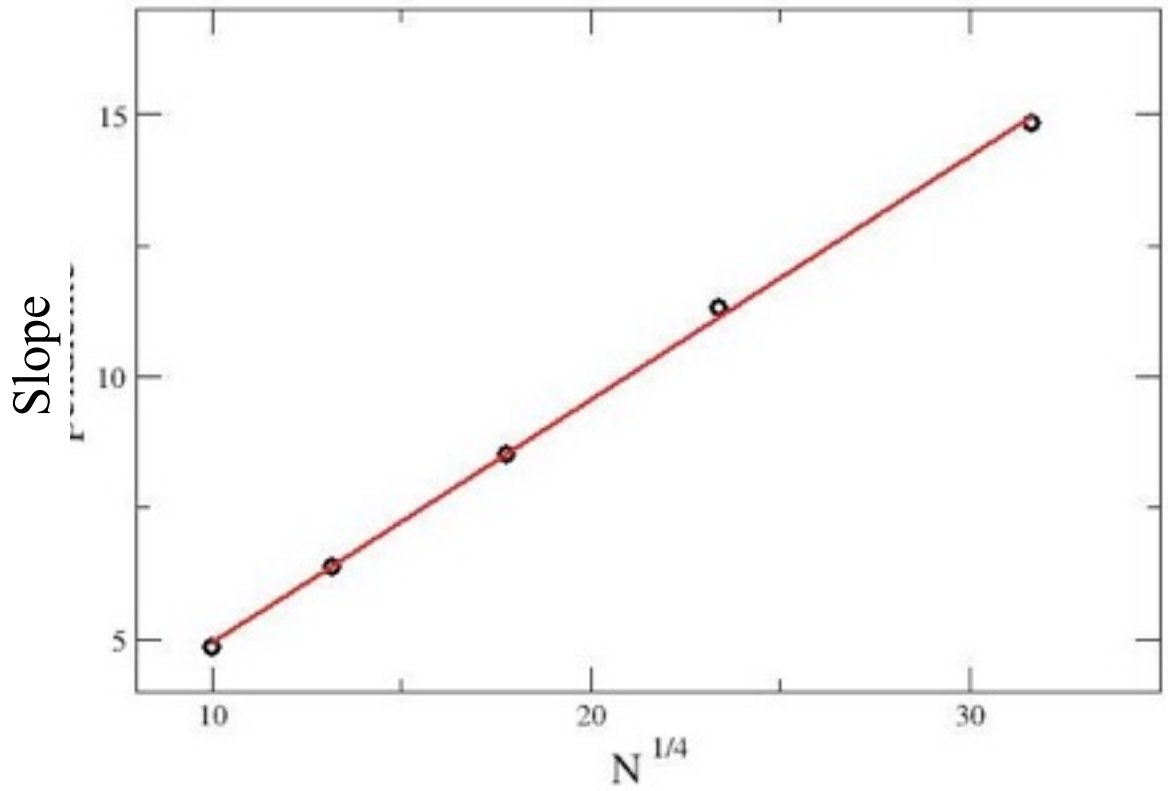
# Numerical results

- Numerical simulations confirm the predictions of mean field theory



# Numerical results

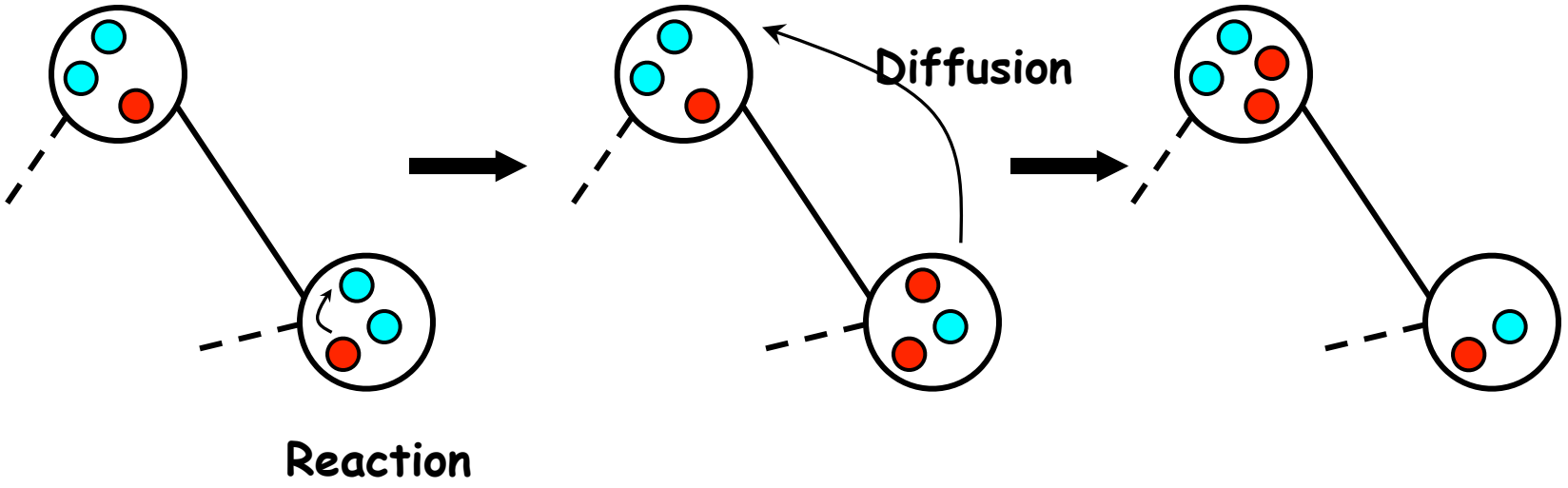
- Further check: for finite networks $\frac{1}{\rho(t)} \sim N^{(3-\gamma)/2} t$
  - If $\gamma = 2.5$ ➡ $\frac{1}{\rho(t)} \sim N^{1/4} t$



# Reaction-diffusion processes: II Bosonic formalism

# Bosonic RD processes in complex networks

- Reactions take place inside vertices
- Only interaction between vertices is by diffusion (random jumping) of particles
  - Same scheme as in Euclidean lattices: the only difference in behavior is the different topology in which diffusion takes place
    - Enough to induce relevant differences



# Bosonic HMF formalism

- Starting point for analytical treatment: MF formalism
  - Particles of different species $A_\alpha$, $\alpha$=1, … , S
  - Particles diffuse (jump to nearest neighbors) with rate $D_\alpha$
  - Reactions $R_r$, r=1, …, R given by the stoichiometric equations

$$\sum_{\alpha=1}^{S} q_\alpha^r A_\alpha \xrightarrow{\lambda_r} \sum_{\alpha=1}^{S} (q_\alpha^r + p_\alpha^r) A_\alpha, \quad r = 1, \ldots, R,$$

$\lambda_r$ = Reaction rate

- MF formalism based on rate equations for the partial densities $\rho_{\alpha,\,k}(t)$ of $A_\alpha$ particles in vertices of degree k

- Two terms
  - Diffusion
    - Random jumps between adjacent vertices
  - Reactions
    - Modeled by the law of mass action

# Bosonic HMF formalism

- For a complex network characterized by P(k) and P(k'|k)
  - Partial densities

$$\frac{\partial \rho_{\alpha,k}(t)}{\partial t} = \underbrace{-D_\alpha \rho_{\alpha,k}(t) + D_\alpha k \sum_{k'} \frac{P(k'|k)}{k'} \rho_{\alpha,k'}(t)}_{\text{Diffusion}} + \underbrace{\sum_r p_\alpha^r \lambda_r \prod_\beta [\rho_{\beta,k}(t)]^{q_\beta^r}}_{\text{Law of mass action}},$$

  - Total densities

$$\frac{\partial \rho_\alpha(t)}{\partial t} = \sum_r p_\alpha^r \lambda_r \sum_k P(k) \prod_\beta [\rho_{\beta,k}(t)]^{q_\beta^r},$$

    - Equation independent of the correlation pattern

- General rate equations, valid of any RD process

# One-species RD processes

- Simplest case S=1 (one single species of particles)
- MF rate equation becomes (D = 1)

$$\frac{\partial \rho_k(t)}{\partial t} = k \sum_{k'} \frac{P(k'|k)}{k'} \rho_{k'}(t) + \sum_{q>0} \Gamma_q [\rho_k(t)]^q, \qquad \frac{\partial \rho(t)}{\partial t} = \rho(t) + \sum_{q>0} \Gamma_q \sum_k P(k) [\rho_k(t)]^q,$$

$$\Gamma_q = -\delta(q,1) + \sum_r p^r \lambda_r \delta(q^r, q),$$

- S=1 RD processes can be classified in two main classes
  - Steady state processes
    - Posses one or more steady states at large time, with possible phase transitions among them
  - Continuously decaying processes
    - Particle density decays continuously with time

# Steady-state bosonic RD processes

- Possibility of steady states and phase transitions
  - Linear stability analysis
- Jacobian matrix for $\Gamma_0 = 0$ (no spontaneous particle creation)

$$L_{kk'} = \Gamma_1 \delta(k', k) + \frac{kP(k'|k)}{k'}.$$

- Unique eigenvector $v_k$=k and eigenvalue

$$\Lambda = \Gamma_1 + 1 \equiv \sum_r p^r \lambda_r \delta(q^r, 1)$$

- If there are steady states and a phase transition
  - $\Lambda > 0$ = steady state $\rho \neq 0$: active phase
  - $\Lambda < 0$ = steady state $\rho = 0$: absorbing phase
    - Absorbing state phase transition

- Threshold $\Lambda_c = 0$, independent of topological heterogeneity

# Diffusion-limited regime

- Information can be obtained for general S=1 RD processes in the very small density regime
- Imposing $\partial_t \rho_k(t)=0$ in uncorrelated networks, and considering $\rho$ very small,

$$\rho_k \simeq -\frac{k}{\langle k \rangle \Gamma_1}\rho,$$

- Inserting in the equation for $\rho$, we obtain, for finite networks

$$\rho \simeq \left( \frac{(\langle k \rangle |\Gamma_1|)^{q_m}}{\langle k^{q_m} \rangle |\Gamma_{q_m}|} \right)^{1/(q_m-1)} \Lambda^{1/(q_m-1)},$$

  - $q_m$=smallest reaction order

- Homogeneous MF solution, with a depressing factor $<k^{q_m}>^{-1/(q_m-1)}$

# On scale-free networks and the value of $\gamma$

- For uncorrelated scale-free networks, $P(k) \sim k^{-\gamma}$

$$\rho \simeq N^{-(q_m+1-\gamma)/(q_m-1)}\ \Lambda^{1/(q_m-1)},$$

- Topological effects play a role for $\gamma < q_m+1$
  - For $\gamma > q_m+1$, homogeneous MF theory applies
  - Conclusion: The previous famous threshold $\gamma = 3$ for the observation of topological effects arises from considering only processes with order $q_m=2$
    - Percolation, contact process, epidemics, Ising model, …
- In the general case, a threshold $\gamma = q_m+1$ is to be expected!

# Monotonously decaying RD processes: Diffusion-limited regime

- For any correlation pattern, and keeping only linear terms

$$\frac{\partial \rho_k(t)}{\partial t} \simeq -\rho_k(t) + k \sum_{k'} \frac{P(k'|k)}{k'} \rho_{k'},$$

- Performing a quasi-static (adiabatic) approximation, we can approximate

$$\rho_k(t) \simeq \frac{k\rho(t)}{\langle k \rangle},$$

- Substituting into the full equation for $\rho(t)$, for finite networks, with any correlation pattern

$$\rho(t) \sim \left( \frac{(q_m - 1)|\Gamma_{q_m}|\langle k^{q_m} \rangle}{\langle k \rangle^{q_m}} \right)^{-1/(q_m - 1)} t^{-1/(q_m - 1)},$$

- Homogeneous MF solution, with a depressing factor $\langle k^{q_m} \rangle^{-1/(q_m-1)}$

# Specific examples

- In order to go beyond the diffusion-limited approximation, specific RD processes must be considered

- Steady state processes
  - Branching-annihilating random walk (BARW)

$$qA \xrightarrow{\lambda} \emptyset$$
$$A \xrightarrow{\mu} (p+1)A \quad ,$$

# Bosonic BARW

- General results
  - For any correlation pattern, the BARW exhibits an absorbing state phase transition at a critical point $\Lambda_c = \mu_c = 0$
  - Diffusion-limited regime (in uncorrelated SF networks)

$$\rho \simeq \left( \frac{[\langle k \rangle p(1-p\mu)]^q}{\langle k^q \rangle q\lambda} \right)^{1/(q-1)} \mu^{1/(q-1)} \sim N^{-\frac{q+1-\gamma}{2(q-1)}} \mu^{1/(q-1)},$$

    - General behavior for finite networks

# Bosonic BARW

- Particular case q=2
  - Steady-state solution ($\partial_t \rho=0$) for uncorrelated networks

$$\rho_k = \frac{|\Gamma_1|}{2|\Gamma_2|}\left(-1+\sqrt{1+\frac{4|\Gamma_2|\rho k}{\langle k\rangle|\Gamma_1|^2}}\right)$$

    - Particular square root behavior at large densities

  - If $\rho < \rho_X$, with $\frac{4|\Gamma_2|\rho_\times k_c}{\langle k\rangle|\Gamma_1|^2}=1,$ where $k_c$ in the network cutoff, then

$$\rho_k \simeq -\frac{k}{\langle k\rangle\Gamma_1}\rho,$$

    - The diffusion-limited regime is recovered

# Bosonic BARW

- For infinite networks, within the continuous degree approximation, self-consistent equation for the density

$$\rho = \frac{|\Gamma_1|}{2|\Gamma_2|}\left(-1+\frac{2(\gamma-1)}{2\gamma-3}\sqrt{\frac{4|\Gamma_2|m\rho}{\langle k\rangle|\Gamma_1|^2}}\times F[-\frac{1}{2},\gamma-\frac{3}{2},\gamma-\frac{1}{2},-\frac{\langle k\rangle|\Gamma_1|^2}{4|\Gamma_2|m\rho}]\right)$$

- Final solution for small $\rho$ ($\mu$)

$$\rho \sim \frac{\tilde{\Gamma}_1^{1/(\gamma-2)}}{|\Gamma_2|} \sim \frac{(p\mu)^{1/(\gamma-2)}}{\lambda},$$

  - We recover the critical point $\mu_c$=0
  - In finite (uncorrelated) networks, it should be observed for

$$\mu > \mu_\times = \frac{k_c^{2-\gamma}}{p} \sim N^{-(\gamma-2)/2}$$

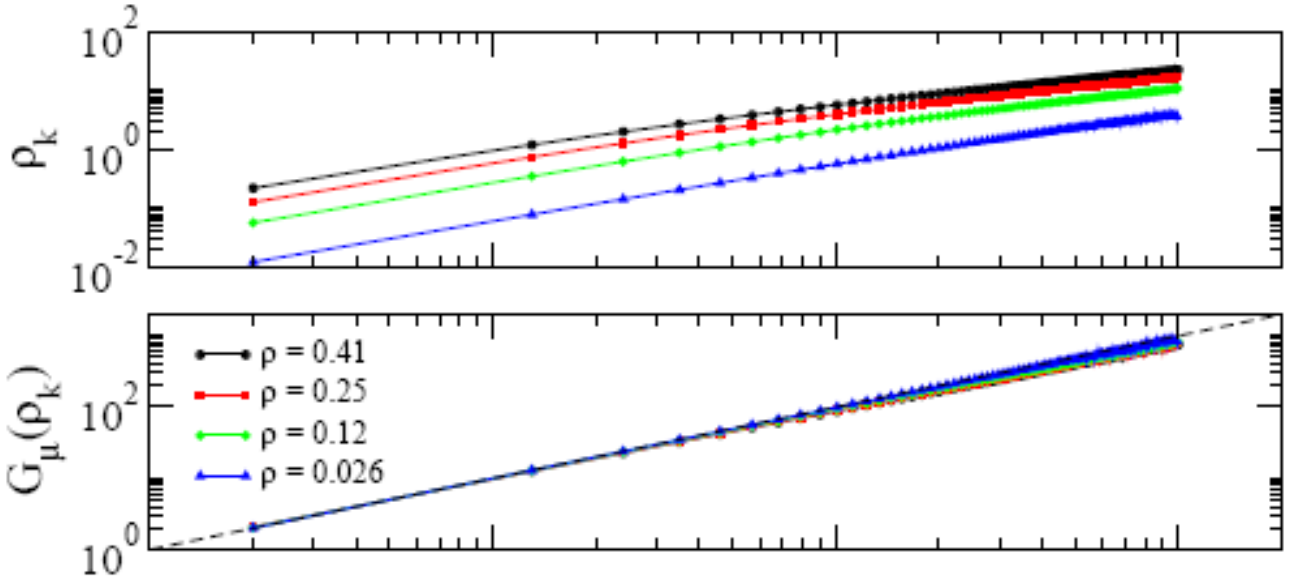
# Bosonic BARW: Numerical check

- Partial densities $\rho_k$ in the steady state, for p=q=2

$$\rho_k = \frac{1-2\mu}{4\lambda}\left(-1+\sqrt{1+\frac{8\lambda\rho k}{\langle k\rangle(1-2\mu)^2}}\right)$$

- Thus

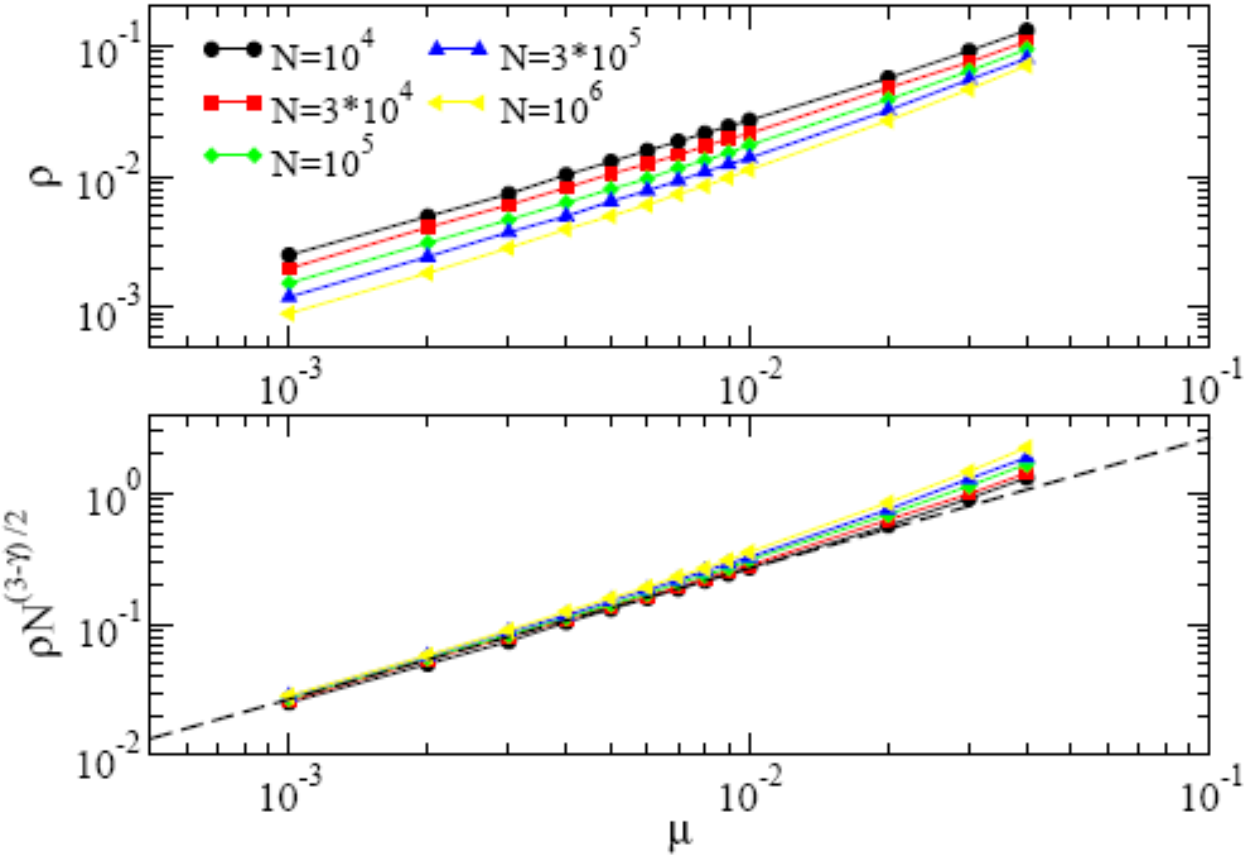
$$G_\mu(\rho_k) \equiv \left[\left(\frac{4\lambda\rho_k}{1-2\mu}+1\right)^2-1\right]\frac{(1-2\mu)^2\langle k\rangle}{8\lambda\rho} \equiv k$$



# Bosonic BARW: Numerical check

- Infinite network solution not observable in finite networks
- For finite networks q=p=2

$$\rho \sim N^{-(3-\gamma)/2}\mu$$



# Specific examples

- In order to go beyond the diffusion-limited approximation, specific RD processes must be considered

- Monotonously decaying processes
  - Diffusion-annihilation process (DA)
    - BARW with p=0

$$qA \xrightarrow{\lambda} \emptyset,$$

# Bosonic DA

- General results
  - For any correlation pattern, in a finite network, at t >> 1 density is dominated by the diffusion-limited regime

$$\rho(t) \simeq \left( \frac{(q-1)q\lambda\langle k^q \rangle}{\langle k \rangle^q} \right)^{-1/(q-1)} t^{-1/(q-1)}, \sim N^{-\frac{q+1-\gamma}{2(q-1)}} t^{-1/(q-1)},$$

# Bosonic DA

- Particular case q=2
  - Performing the adiabatic approximation, partial densities given by

$$\rho_k(t) = \frac{1}{2|\Gamma_2|}\left(-1+\sqrt{1+\frac{4|\Gamma_2|k}{\langle k\rangle}\rho(t)}\right)$$

    - Again, particular square root behavior at large times

  - If $\rho < \rho_f$, with $\rho_\times = \frac{\langle k\rangle}{4|\Gamma_2|}k_c^{-1},$ where $k_c$ in the network cutoff, then

$$\rho_k(t) \simeq \frac{k\rho(t)}{\langle k\rangle},$$

    - The diffusion-limited regime is recovered

# Bosonic DA

- For infinite networks, within the continuous degree approximation, we find the self-consistent equation

$$\frac{\partial \rho}{\partial t} = -\rho - \frac{1}{2|\Gamma_2|} + \frac{\gamma - 1}{|\Gamma_2|(2\gamma - 3)} \sqrt{\frac{4|\Gamma_2| m\rho}{\langle k \rangle}} \times F[-\frac{1}{2}, \gamma - \frac{3}{2}, \gamma - \frac{1}{2}, -\frac{\langle k \rangle}{4|\Gamma_2| m\rho}].$$

- Final solution for large t

$$\rho(t) \sim |\Gamma_2|^{\gamma-2} t^{-1/(\gamma-2)} \sim \lambda^{\gamma-2} t^{-1/(\gamma-2)}$$

  - In finite networks should be observed for

$$t < t_\times \sim k_c^{\gamma-2} \sim N^{(\gamma-2)/2}$$

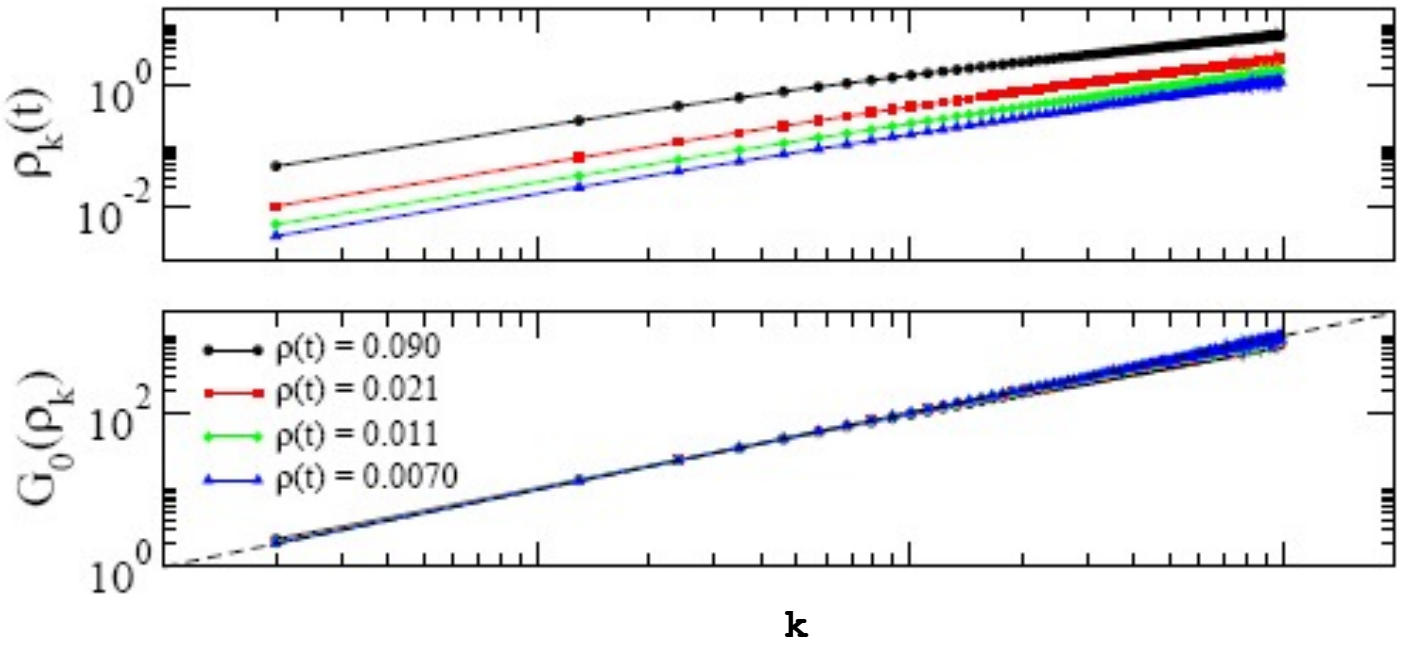
# Bosonic DA: Numerical check

- Partial densities $\rho_k$ in the steady state, for q=2

$$\rho_k(t) = \frac{1}{4\lambda}\left(-1 + \sqrt{1 + \frac{8\lambda k}{\langle k\rangle}\rho(t)}\right)$$

- Thus

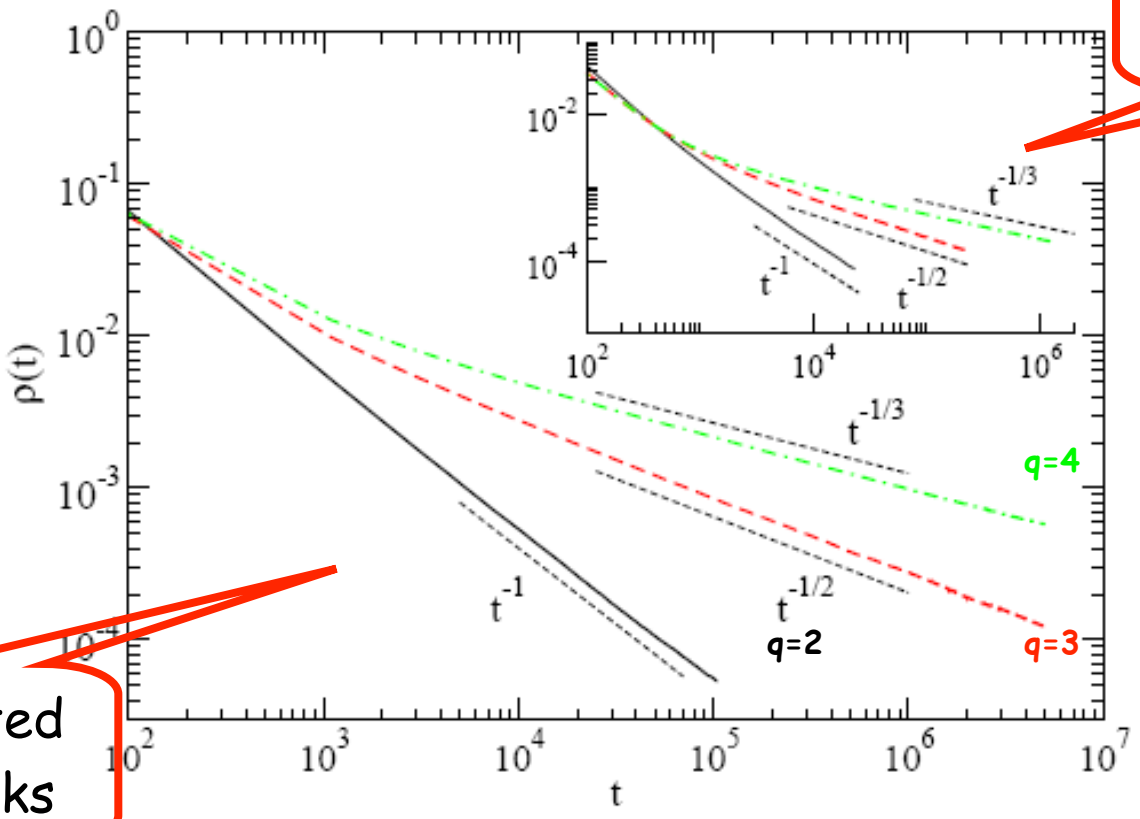
$$G_0(\rho_k) \equiv \left[(4\lambda\rho_k(t)+1)^2 - 1\right]\frac{\langle k\rangle}{8\lambda\rho(t)} \equiv k$$



# Bosonic BA: Numerical

- Infinite network solution not available in finite networks
- For finite networks for any q

$$\rho \sim A(N,\gamma)^{-1/(q-1)} t^{-1/(q-1)}$$



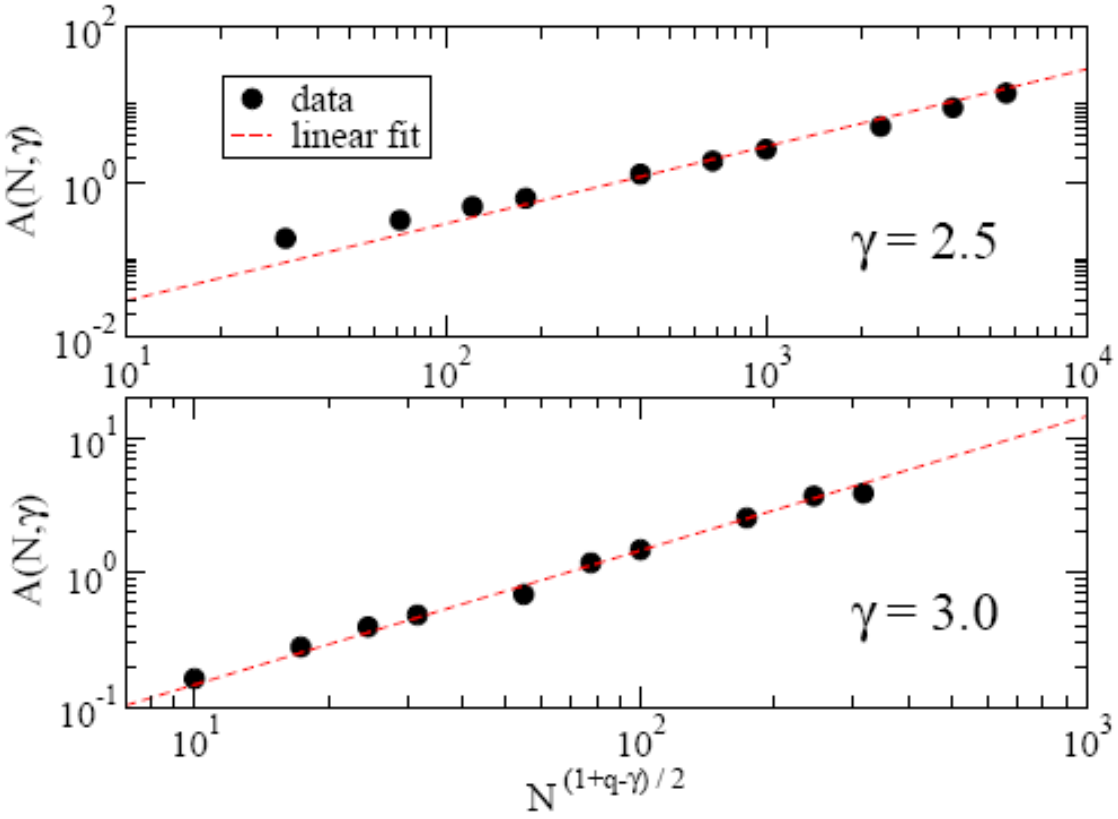

Correlated SF networks

Uncorrelated SF networks

# Bosonic BA: Numerical

- Additionally, for the numerical prefactor

$$A(N,\gamma) \sim N^{(1+q-\gamma)/2}$$



# Ordering dynamics

# Glauber dynamics at T=0

- Ordering dynamics that can model the evolution of systems of social agents (e.g. the opinion of agents with respect to a certain issue) in terms of a binary variable that is updated in response to the pressure of the peers of each individual
- Definition:
  - Ising variables ( $\sigma_i = \pm 1$) in the vertices of a network
  - Spins are updated as a function of the local field

$$h_i = \sum_j a_{ij}\sigma_j$$

$$\sigma_i = +1 \quad \Leftarrow \quad h_i(t) > 0$$

$$\sigma_i = -1 \quad \Leftarrow \quad h_i(t) < 0$$

$$\sigma_i = \pm 1 \quad \Leftarrow \quad \text{With probability } 1/2 \quad h_i(t) = 0.$$

# Mean field theory

- Dynamical equation for the probability that a vertex of degree k is in a +1 state $q_k(t)$

$$\frac{\mathrm{d}q_k(t)}{\mathrm{d}t} = \underbrace{-q_k(t)\mathrm{Prob}[h_k < 0] - q_k(t)\mathrm{Prob}[h_k = 0]\frac{1}{2}}_{\text{Destruction terms}}$$

$$\underbrace{+ (1 - q_k(t))\mathrm{Prob}[h_k > 0] + (1 - q_k(t))\mathrm{Prob}[h_k = 0]\tfrac{1}{2}}_{\text{Creation terms}},$$

$$\frac{\mathrm{d}q_k(t)}{\mathrm{d}t} = -q_k(t) + \mathrm{Prob}[h_k > 0] + \frac{1}{2}\mathrm{Prob}[h_k = 0].$$

# Uncorrelated networks

- Define probability that a vertex is connected to a neighbor in state +1

$$Q = \frac{1}{\langle k \rangle} \sum_k k P(k) q_k.$$

  - Independent of the state of the original vertex
- The local field can be zero only if k is even and exactly half of its edges point to +1 spins.
  - Thus

$$\text{Prob}[h_k = 0] = \left( \begin{array}{c} k \\ k/2 \end{array} \right) Q^{k/2} (1-Q)^{k/2},$$

- The local field can be positive when more than half of its edges point to +1 spins
  - Thus

$$\text{Prob}[h_k > 0] = \sum_{\ell=\lceil (k+1)/2 \rceil}^{k} \left( \begin{array}{c} k \\ \ell \end{array} \right) Q^{\ell} (1-Q)^{k-\ell},$$

# Uncorrelated networks

- Final equation

$$\frac{\mathrm{d}q_k(t)}{\mathrm{d}t} = -q_k(t) + \sum_{\ell=\lceil k/2 \rceil}^{k} \left[1 - \tfrac{1}{2}\delta_{\ell,k/2}\right] \binom{k}{\ell} Q^{\ell}(1-Q)^{k-\ell}.$$

- And for Q

$$\dot{Q} = -Q + \Psi(Q),$$

$$\Psi(Q) = \frac{1}{\langle k \rangle} \sum_{k} kP(k) = \sum_{\ell=\lceil k/2 \rceil}^{k} \left[1 - \tfrac{1}{2}\delta_{\ell,k/2}\right] \binom{k}{\ell} Q^{\ell}(1-Q)^{k-\ell}.$$

- Very tedious equation to solve… but it can be done asymptotically

# Mean field predictions in SF networks

- The systems always orders (all spins +1 or -1 at t = 1)
- Ordering time $t_{ord}$ starting from symmetric initial conditions (disordered system, with zero magnetization)
  - Time $t_{ord}$ till achieve a given magnetization
    - For $2 < \gamma < 5/2$, $t_{ord}$ decreases with N (network size)

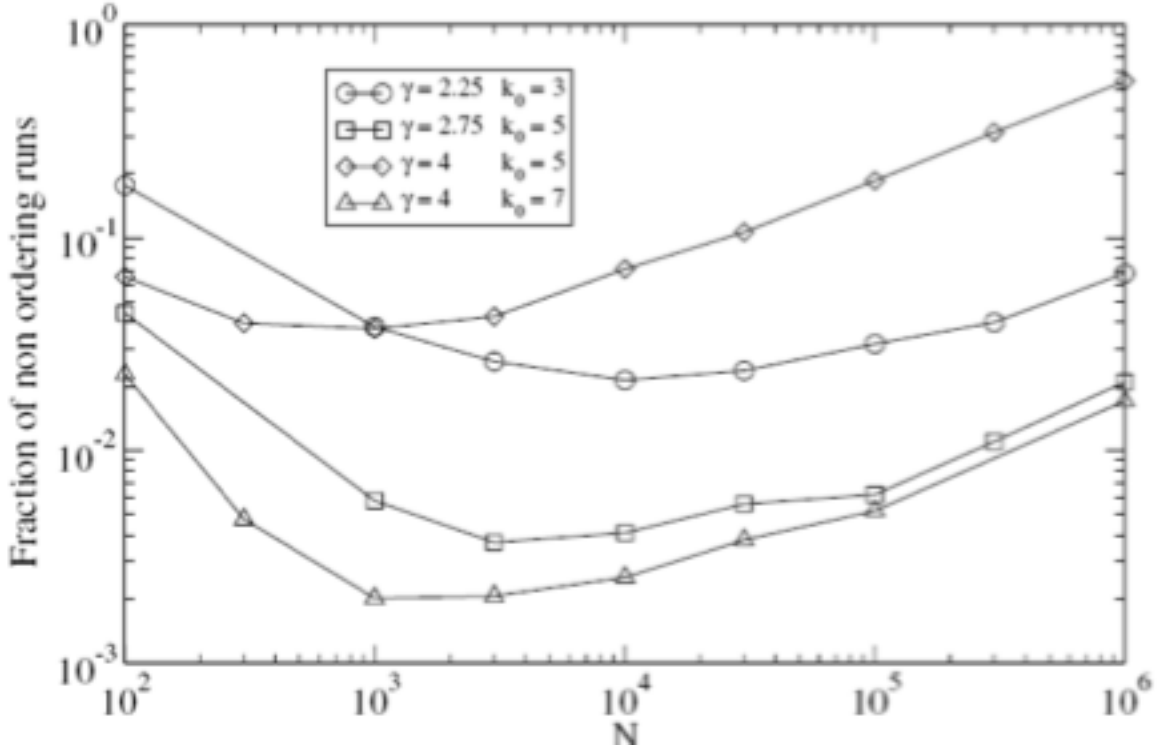
$$t_{\rm ord} \sim N^{(\gamma-5/2)/2} \ln N$$

    - For $\gamma > 5/2$, $t_{ord}$ increases logarithmically with N

$$t_{\rm ord} \sim \ln N$$

# Numerical results

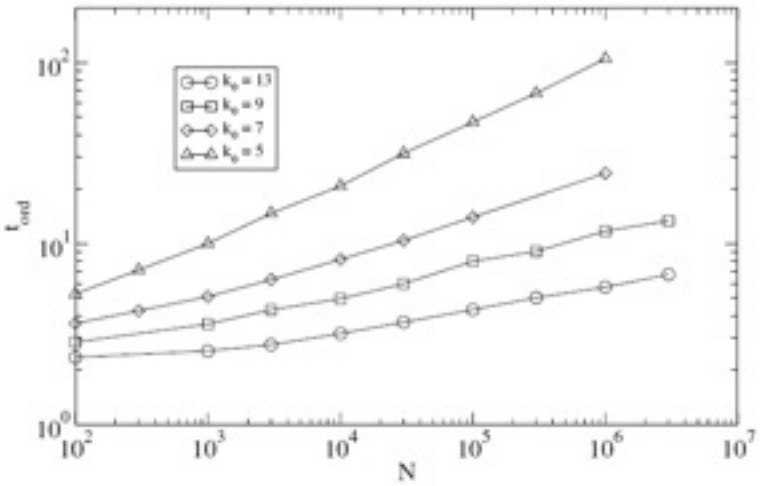
- Not all systems become ordered

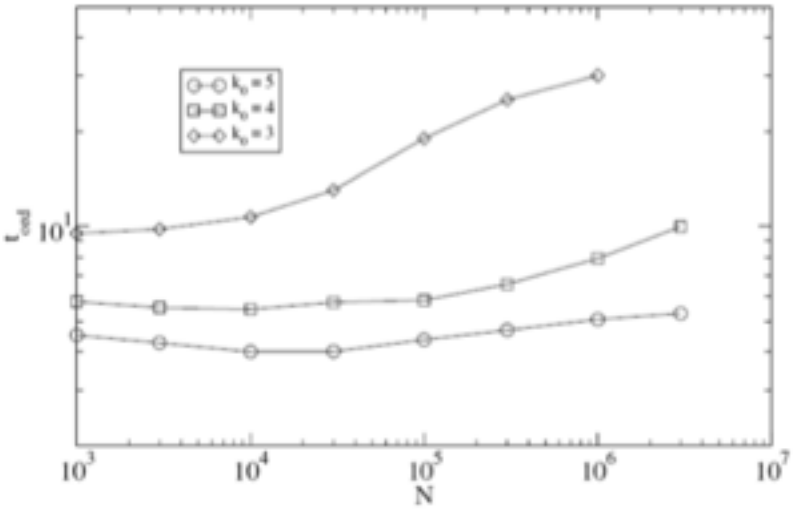



- In the thermodynamic limit, no network is able to order, whatever its value of $\gamma$

# Numerical results

- Ordering time $t_{ord}$ restricted to those runs that get actually ordered




$\gamma = 4 > 5/2$ $\gamma = 2.25 < 5/2$

- For $\gamma > 5/2$ does not grow logarithmically, but as a power law
- For$\gamma < 5/2$ does not decrease, but increases instead

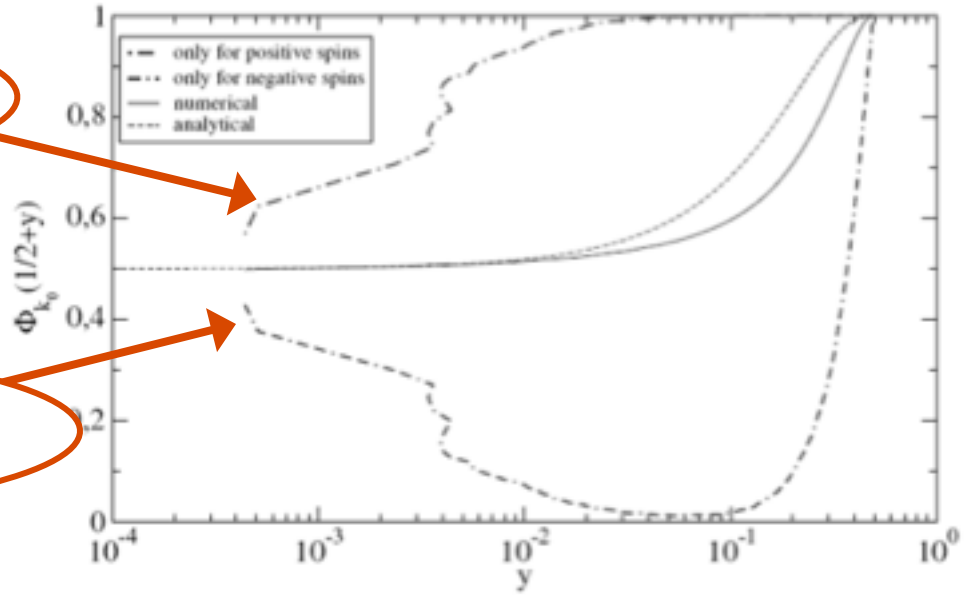
# Why mean field does not work?

- The most relevant mean field assumption turns out to be the following:
  - The probability that a spin $\sigma_i$ is connected to a +1 spin (the dynamical variable Q), is independent of the state of $\sigma_i$
- Numerically, instead strong dynamical correlations appear in the system, invalidating the mean field approximation!!!

...

**Probability that a +1 spin is connected to a +1 spin**

**Probability that a -1 spin is connected to a +1 spin**



# Beyond heterogeneous mean field theory
# I Quenched mean-field theory

# Beyond HMF

- HMF is a simple and tractable theory, but it implies two strong assumptions
  - Neglects dynamical correlations
  - Neglects the actual structure of the network
    - Annealed network approximation
- As we have seen, dynamical correlations can lead to the complete breakdown of HMF theory
- Introduction of dynamical correlations is a highly complex task
  - Although doable is some cases
- Introduction of the actual network structure can be done by means of the Quenched mean field (QMF) theory
- Let us see how it works in the case of the SIS model

# QMF theory for the SIS model

- Continuous time master equation approach for the probability $\rho_i(t)$ that vertex i is infected at time t [μ curation rate, δ infection rate]

$$\rho_i(t+\Delta t) = (1-\mu\Delta t)\rho_i(t) + Q_i(t)[1-\rho_i(t)].$$

  - $Q_i(t)$ = probability that vertex i becomes infected

$$Q_i(t) = 1 - \prod_j [1 - \delta \Delta t A_{ij}\rho_j(t)]$$

- In the limit $\Delta t \to 0$, defining $\lambda = \delta / \mu$

$$\dot{\rho}_i(t) = -\rho_i(t) + \lambda[1-\rho_i(t)]\sum_j A_{ij}\rho_j(t)$$

  - Evident cancelation of dynamical correlations, specially explicit in the second term

# Threshold in QMF theory

- Linear stability analysis
- Linearized equation:

$$\dot{\rho}_i(t) \simeq -\rho_i(t) + \lambda \sum_j A_{ij}\rho_j(t)$$

  - Associated Jacobian:

$$J_{ij} = -\delta_{ij} + \lambda A_{ij}$$

  - Solution $\rho_i = 0$ unstable when the largest eigenvalue of J is positive
    - Threshold QMF

$$\lambda_c^{QMF} = \frac{1}{\Lambda_N}$$

$\Lambda_N$ = largest eigenvalue of the adjacency matrix

# Comparison of QMF and HMF thresholds

- For non SF networks, both thresholds are finite in the limit N → ∞
- In SF networks we observe different scalings with N:
  - Size dependence in uncorrelated networks through largest degree $k_{max}$
    - $k_{max} \sim N^{1/2}$, $\gamma \leq 3$, $k_{max} \sim N^{1/(\gamma-1)}$, $\gamma > 3$
      - $k_{max} \to \infty$ for $N \to \infty$

- HMF threshold (directly)

$$\lambda_c^{HMF} = \frac{\langle k \rangle}{\langle k^2 \rangle} \simeq \begin{cases} k_{max}^{\gamma-3} & \gamma \leq 3 \\ \text{const.} & \gamma > 3 \end{cases} .$$

- QMF: Use mathematical results $\Lambda_N \sim \max[\sqrt{k_{max}}, \langle k^2 \rangle / \langle k \rangle]$

$$\lambda_c^{QMF} = \frac{1}{\Lambda_N} \simeq \begin{cases} \frac{\langle k \rangle}{\langle k^2 \rangle} \sim k_{max}^{\gamma-3} & 2 < \gamma < 5/2 \\ 1/\sqrt{k_{max}} & \gamma > 5/2 \end{cases}$$

# Which theory is more accurate?

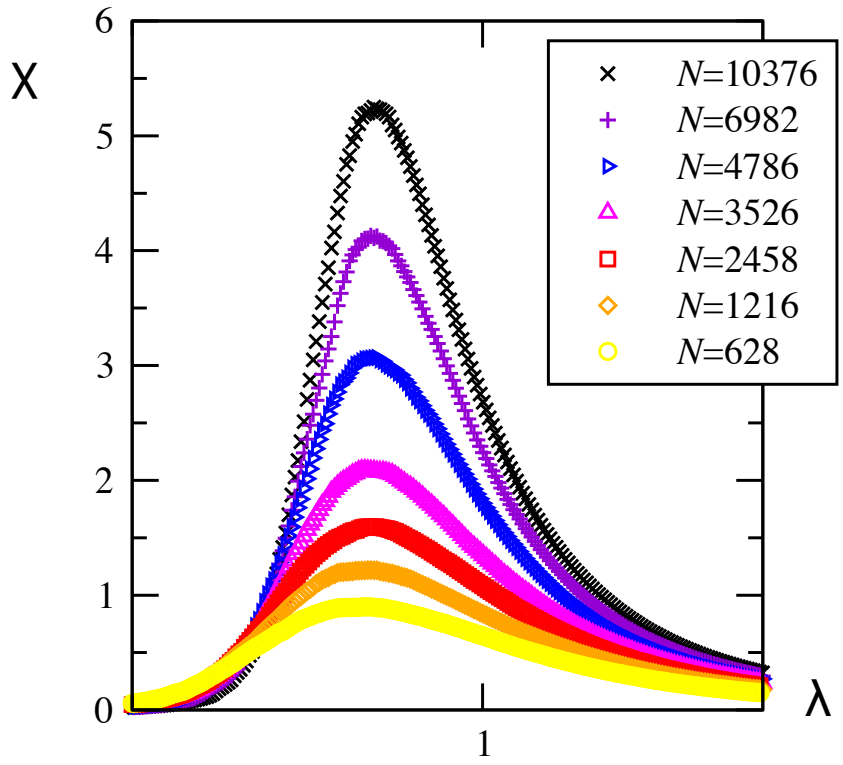
- High precision determination of the critical point: The susceptibility method
- Define susceptibility $$\chi = N \frac{\langle \rho^2 \rangle - \langle \rho \rangle^2}{\langle \rho \rangle}$$
- For fixed N, as a function of λ, susceptibility shows a peak at $\lambda_p(N)$
- In systems with constant $\lambda_c$, peak scales with N

$$\lambda_p(N) - \lambda_c \sim N^{-1/\bar{\nu}}$$

  - Position of the peak tends to the critical point

- Height of the peak also scales

$$\chi_p(N) \sim N^{\gamma/\nu}$$



# Numerical determination of the epidemic threshold

- We will assume the same behavior in the SIS model in networks
  - E.g.

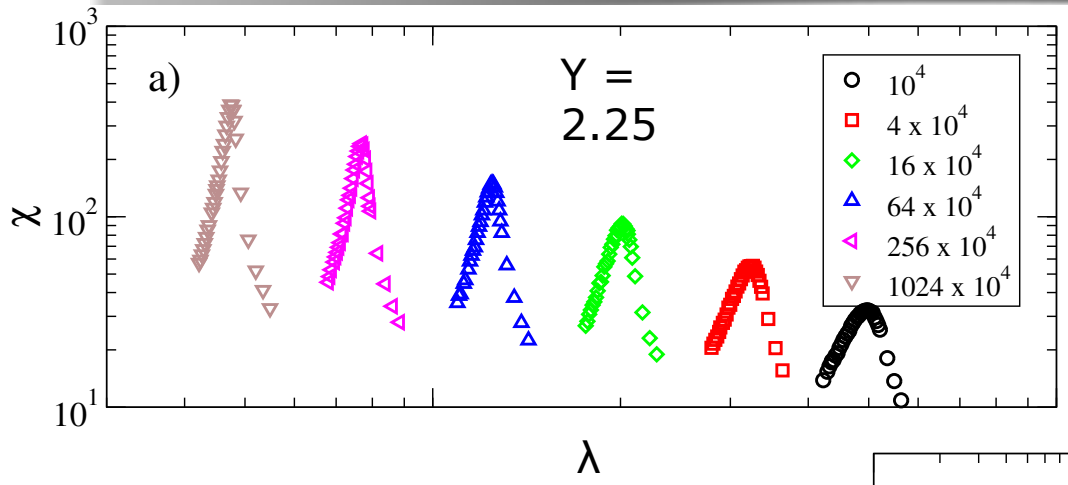
$$\lambda_p(N) - \lambda_c(N) \sim N^{-1/\bar{\nu}}$$

- The peak provides an estimate of the critical point, with an error that depends on N but becomes small for large network size

- Susceptibility height at the peak should also depend on network size

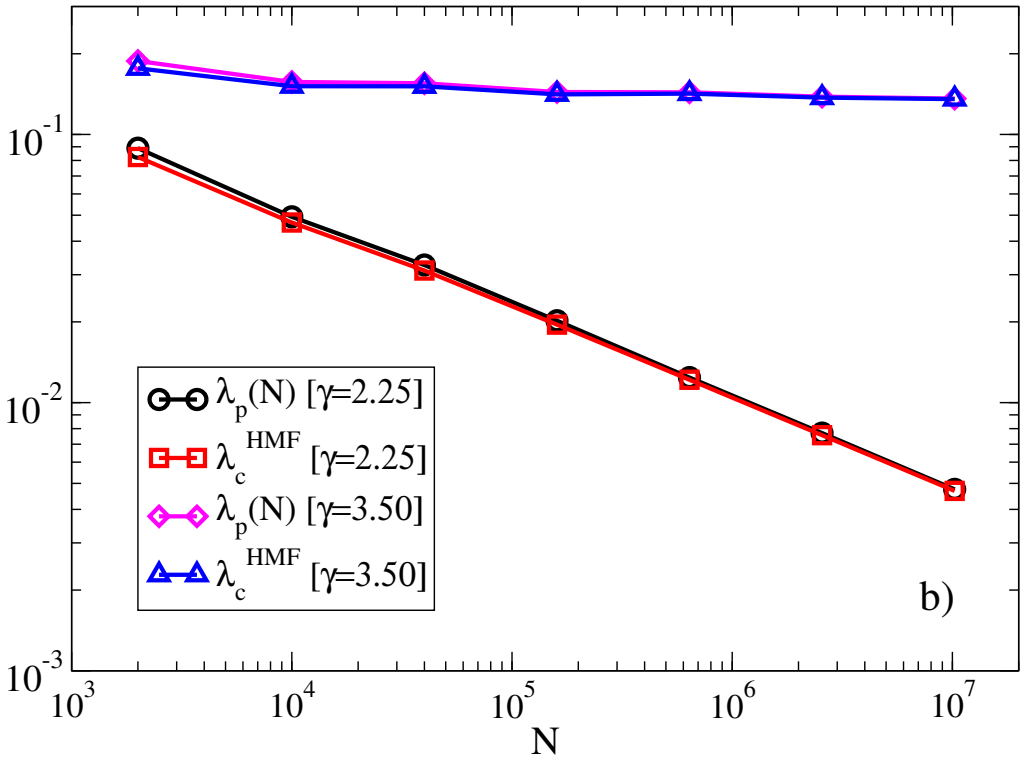
$$\chi_p(N) \sim N^{\gamma/\nu}$$

# Numerical Check: Annealed networks




In annealed networks, HMF theory is exact.
Ideal benchmark

Well defined susceptibility with a peak scaling with network size

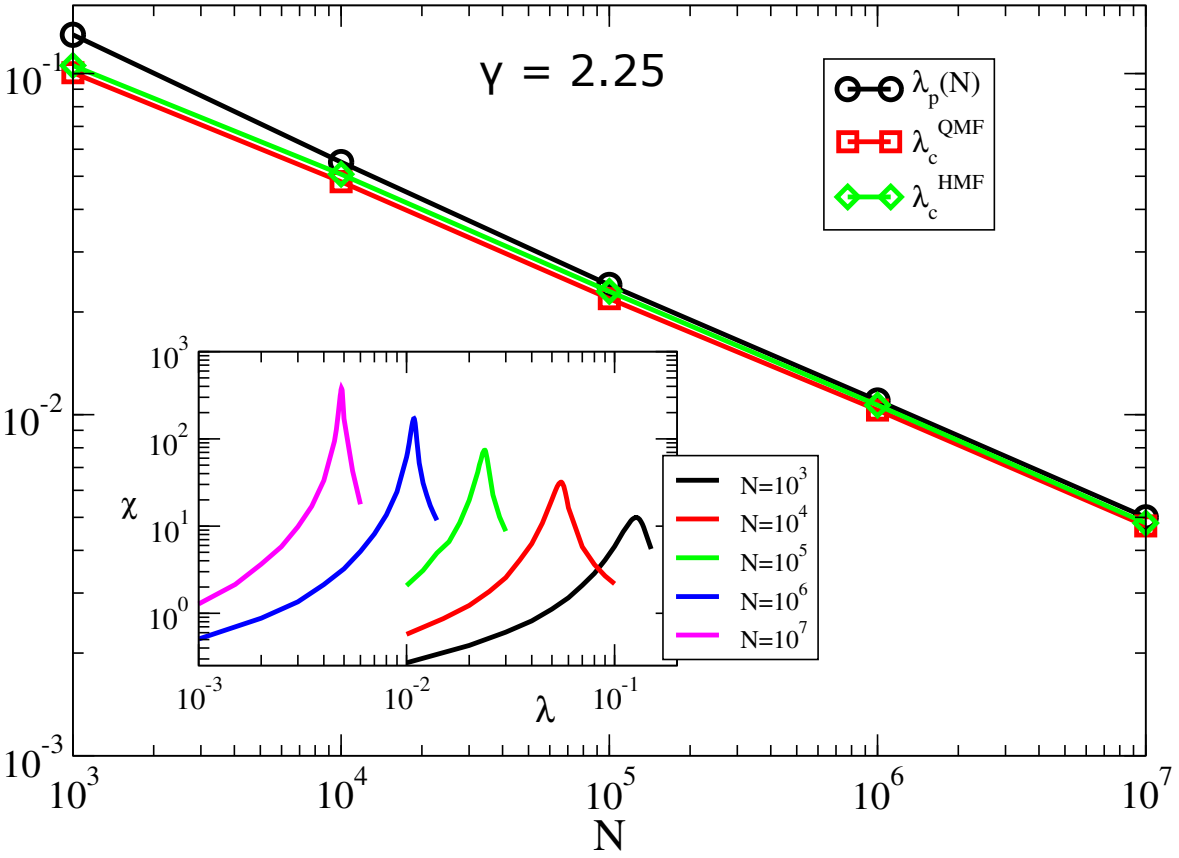



Perfect agreement of theory with susceptibility estimates of thresholds

# Quenched SF networks γ ≤ 5/2

$$\lambda_c^{HM} \sim \lambda_c^{QMF} \sim k_{max}^{\gamma-3}$$

Both HMF and QMF predict the same scaling form of the threshold

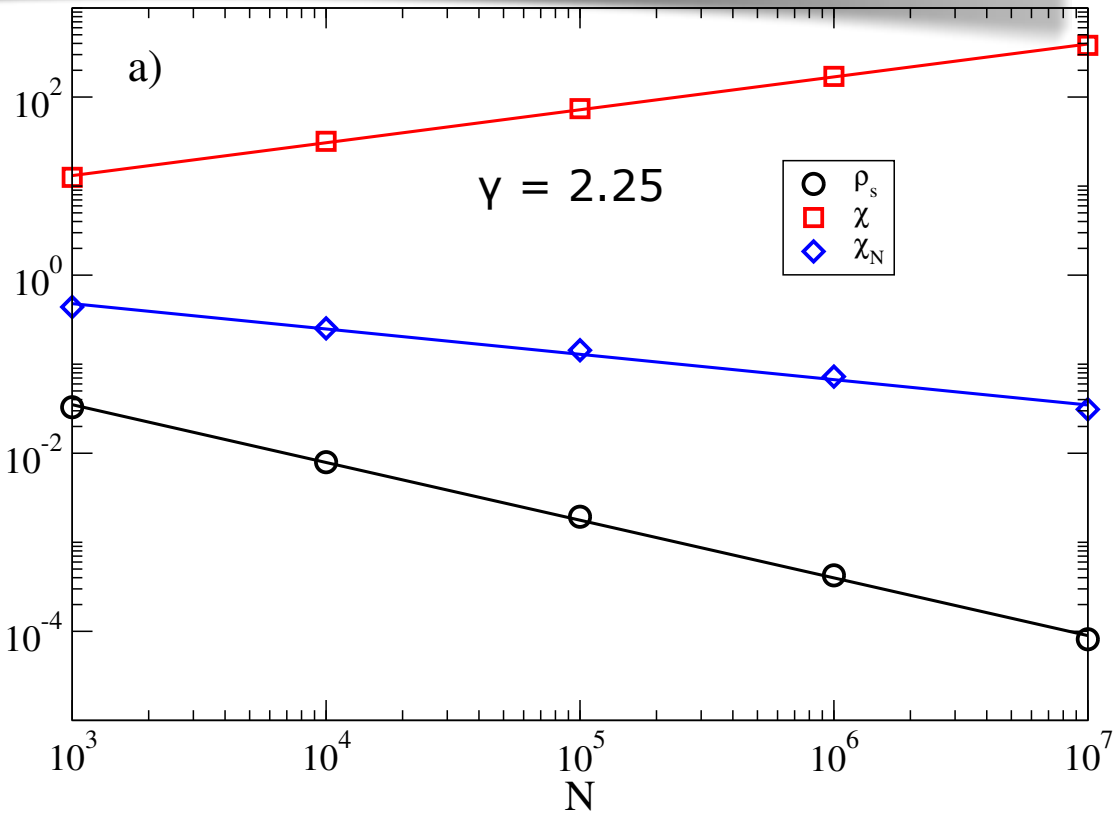



Very good agreement of theory with susceptibility estimates of thresholds at large N

# Quenched SF networks γ ≤ 5/2

Quality of data in this case allows to estimate the scaling exponents

$$\rho_s \sim N^{-\alpha_1}$$
$$\chi \sim N^{\alpha_2}$$
$$\chi_N \sim N^{\alpha_3}$$




Additional comparison with

$$\chi_N = N[\langle \rho^2 \rangle - \langle \rho \rangle^2]$$

Fitted exponents:

$$\rho_s \sim N^{-0.65}$$
$$\chi \sim N^{0.37}$$
$$\chi_N \sim N^{-0.28}$$

Fulfill scaling relation

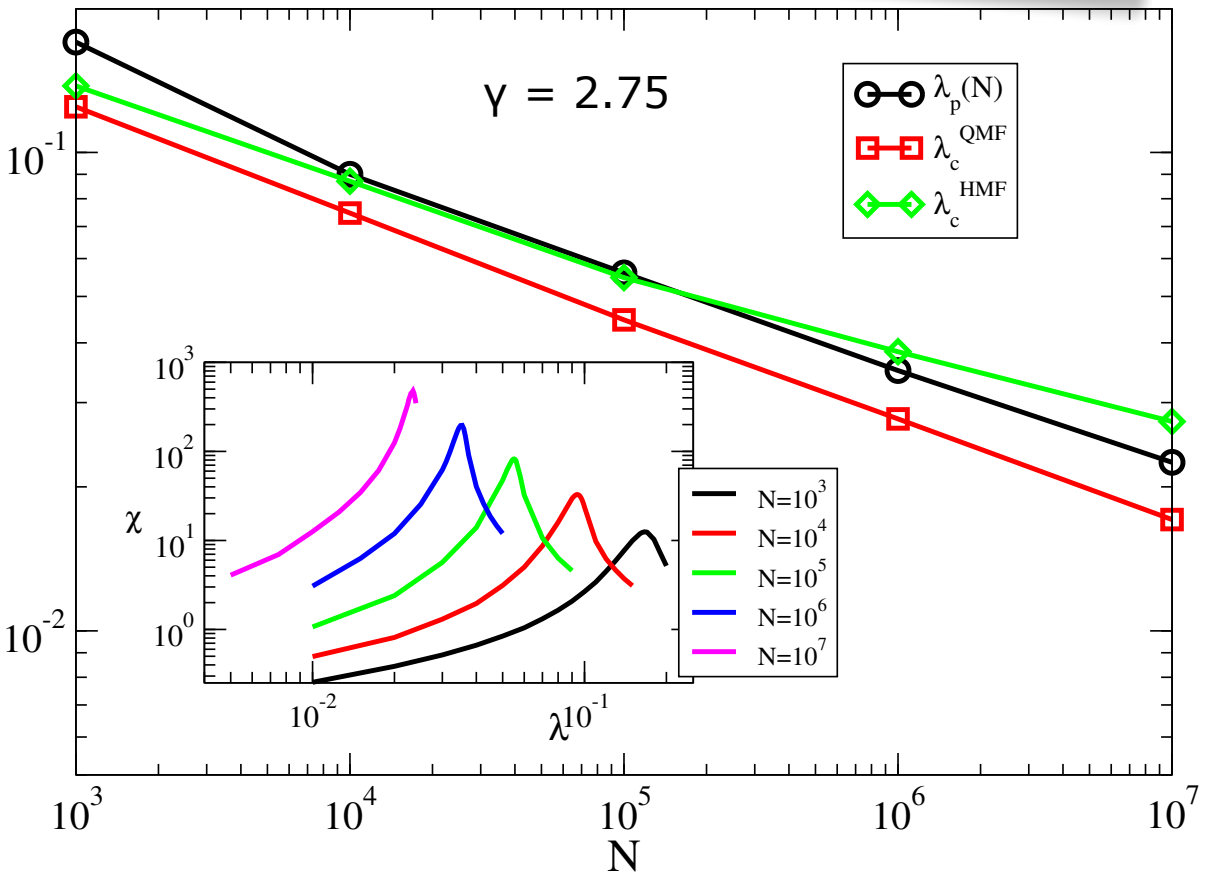
$$\chi_N \sim \chi \times \rho_s$$

# Quenched SF networks 5/2 ≤ γ ≤ 3

$$\lambda_c^{HM} \sim k_{max}^{\gamma-3}$$

$$\lambda_c^{QMF} \sim k_{max}^{-1/2}$$

HMF and QMF predict a different scaling of the threshold with network size



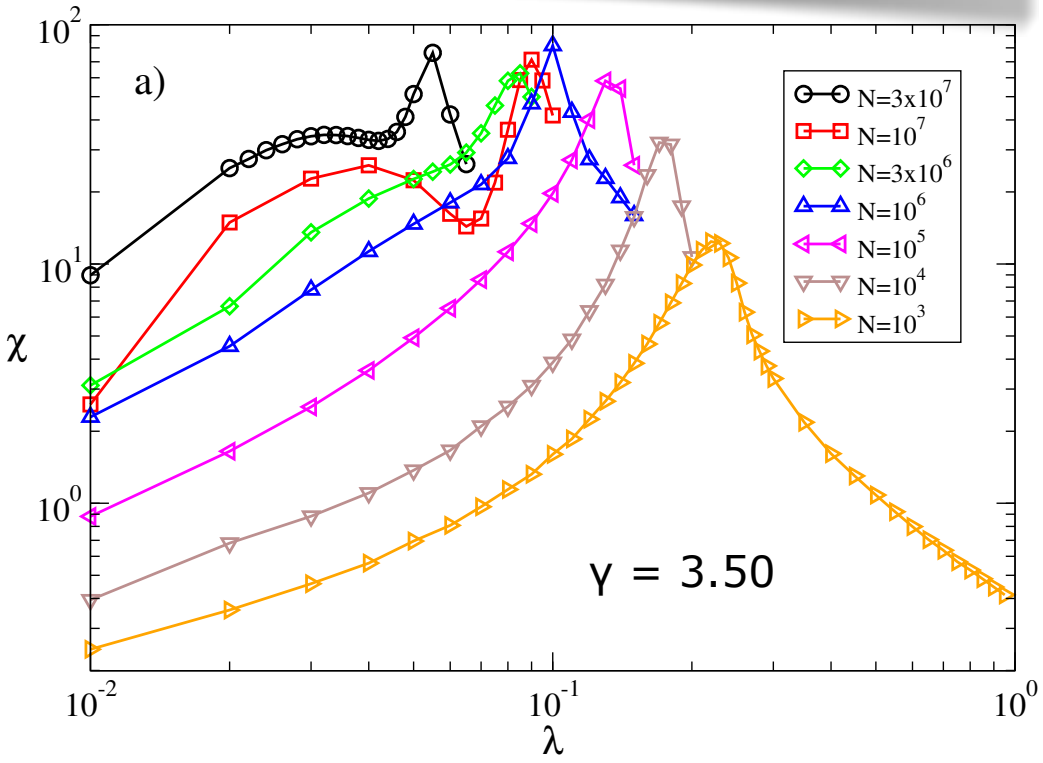

Numerics do not conform to the HMF behavior, specially for large N
QMF theory provides instead the correct scaling of $\lambda_c$ with N, but with a different prefactor (accuracy of estimate ~ 30%)

# Quenched SF networks γ > 3

$$\lambda_c^{HM} \sim \text{const.}$$

$$\lambda_c^{QMF} \sim k_{max}^{-1/2}$$

HMF predicts a finite threshold and QMF a vanishing one

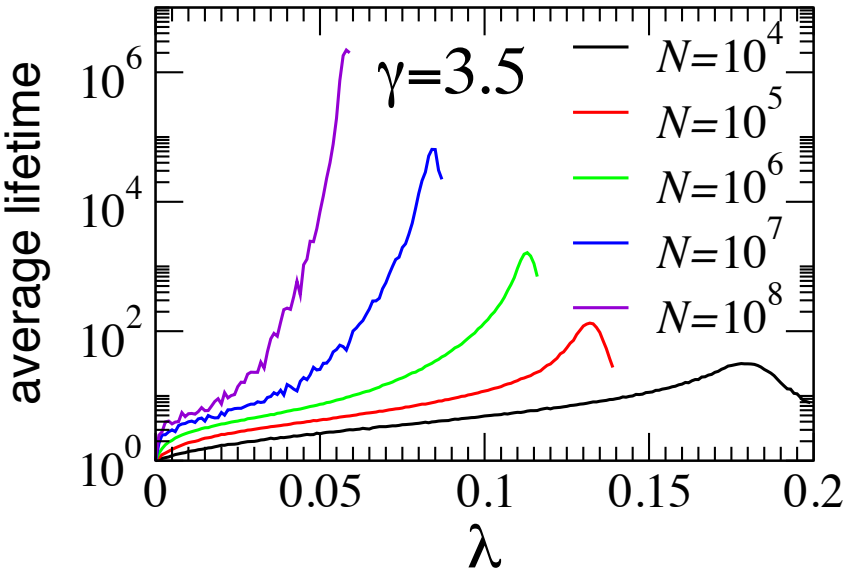



More complex situation:

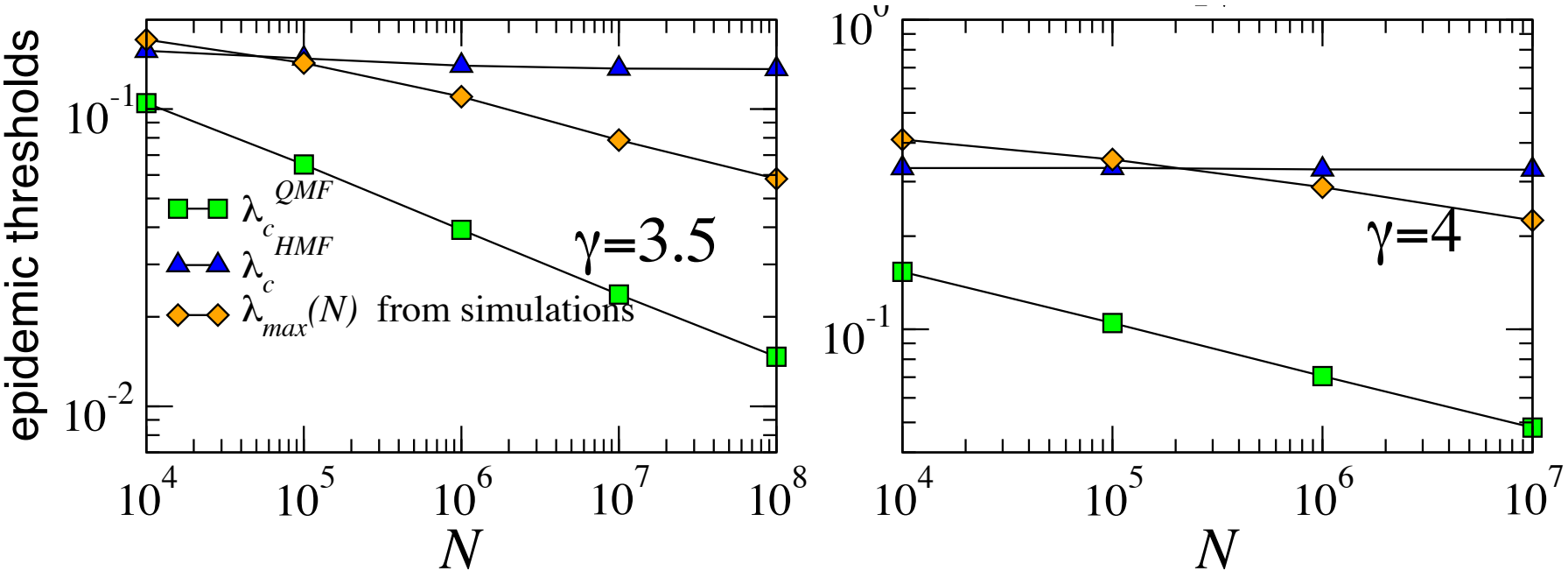
- Small networks lead to a well defined peak for large of λ, at a position quite compatible with the prediction of HMF: $\lambda_c$ constant for large N, although with large fluctuations
- For larger N, another feature emerges for small λ, giving rise to a secondary peak for the largest sizes considered

# A new numerical approach

- We need a different approach to compute the critical point for $\gamma > 3$
- Look at the lifetime T of epidemic outbreaks
- Below $\lambda_c$, T is finite and small; above $\lambda_c$, T is infinite (in infinite networks)
  - That's a problem...
- Fix it looking at the coverage C (fraction of different nodes infected)
- Below $\lambda_c$, C is small; above $\lambda_c$, C=1
- Idea: Look at $T^*$, time till either the infection dies, or $C = C^*$, fixed
  - Below $\lambda_c$, $T^* \sim T$ and is small; above $\lambda_c$ , $T^*$ is small (infection propagates very quickly)
  - Right at $\lambda_c$, $T^*$ should show a peak, that allows to determine the epidemic threshold

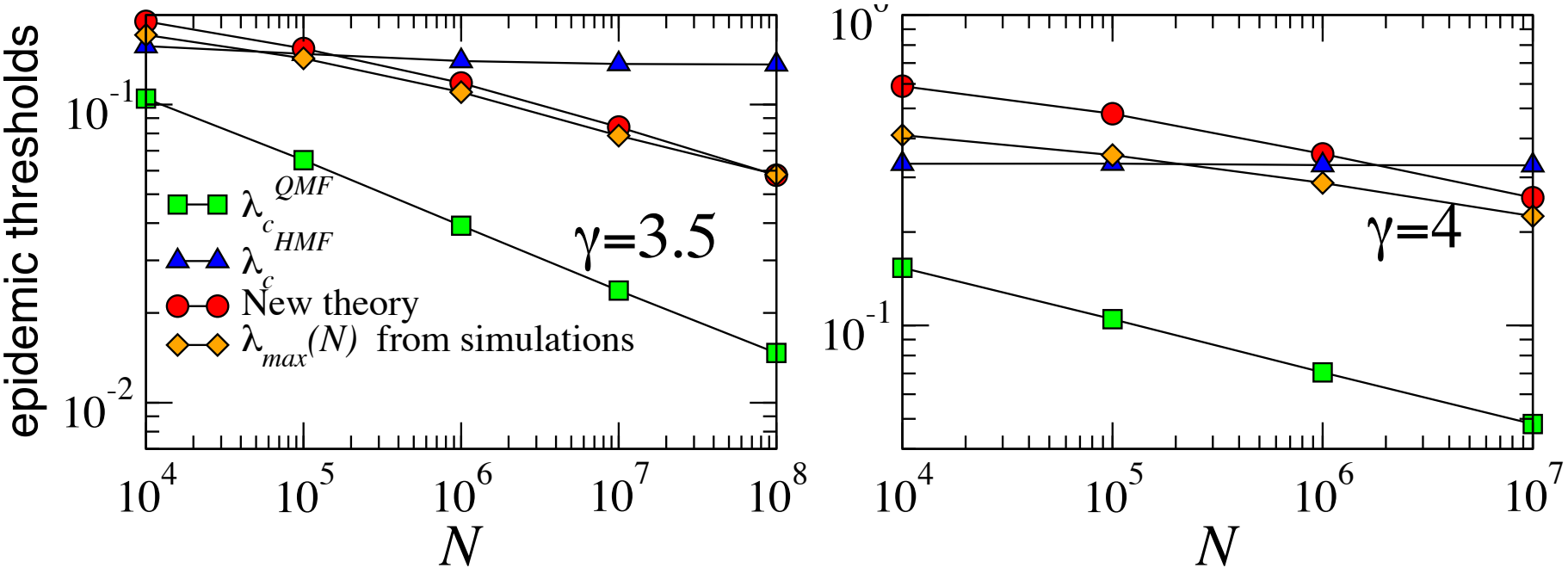


# New threshold for SF networks γ > 3




- The match is not exact, but as in the case of γ < 3, the scaling of the threshold is correctly predicted by QMF

# Further improvements




- More complex theories, including long range dynamical correlations, can give better approximations to the numerical threshold
  - In any case, they represent corrections: The correct scaling is already given by QMF theory

# What we have not seen ...

# Other perspectives, not touched considered here

- Effects of non-trivial correlations
  - Hard task, some results available
- Effects of clustering
  - Doable in simple cases: Percolation
- Effects of long-range dynamical correlations
  - Doable in some cases, such as SIS
- Dynamical processes on small networks
  - HMF will not work
- The effects of a non-static network: The topology (edges) changes with time
  - Temporal networks
- Coupling between dynamical processes and network dynamics
  - Doable with simple models