Stochastic Processes on Complex Networks

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ver. 1

Overview

Objective

- Some analytic approaches to stochastic processes on complex networks
- Some of the effects of the heterogeneous connectivity on dynamics
- Limitations of the approximate analytic approaches

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Branching processes

Galton-Watson branching process

The problem of extinction of families (1874)

Let $q_0, q_1, q_2, \ldots$ be the respective probabilities that a man has $0, 1, 2, \ldots$ sons and each son have the same probability for sons of his own. What is the probability that the male line is extinct after r generations, and what is the probability for any given number of descendants in the maie line in any given generation?

- To examine the hypothesis that distinguished families are more likely to die out than ordinary ones, a first step would be to determine the probability that an ordinary family will disappear
- R.A. Fisher used this model to study the survival of the progeny of a mutant gene (1922-1930)
- The probability of extinction was given by J.F.F. Steffensen (1930) and the asymptotic form of the probability that the family is still in existence was determined by A. Kolmogorov (1938).
- After 1940, interest in the model increased because of the analogy between the growth of families and nuclear chain reactions

Definition

- The number of individuals in a given generation n : $s(n)$
  $s(0) = 1, s(1), s(2), \ldots$: the number of individuals in the 0−th, first, second, ... generations
- For given $s(n)$, $s(n+1) = k_1 + k_2 + \cdots k_{s(n)}$ with the number of children k's following independently a branching probability q_k
- Branching probability $q_k < 1$ for all $k = 0, 1, 2, \ldots$ and $q_0 + q_1 < 1$
- Branching ratio $\kappa = \langle k \rangle = \sum_k k\, q_k < \infty$
- A Markov process with the transition probability
  $P_{\ell j} = P(s(n+1) = \ell | s(n) = j) =$
  $\sum_{k_1=0}^{\infty} \sum_{k_2=0}^{\infty} \cdots \sum_{k_j=0}^{\infty} q_{k_1} q_{k_2} \cdots q_{k_j} \delta_{k_1+k_2+\cdots+k_j,\ell}$

Number of individuals in a given generation

- Probability to find ℓ individuals in generation $n+1$: $P(s(n)=\ell)$
- Time evolution $P(s(n+1)=\ell)=\sum_j P_{\ell j}P(s(n)=j)$
- Generating function of $P(s(n+1))$: $f_{(n+1)}(z)\equiv\sum_\ell P(s(n+1)=\ell)z^\ell$ satsfies the recursive relation

$$f_{(n+1)}(z)=f_{(n)}(f(z))=f(f_{(n)}(z))$$

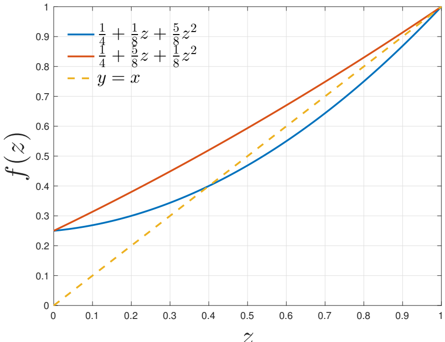
$f_{(n+1)}(z)=\sum_\ell\sum_j P_{\ell j}P(s(n)=j)z^\ell=\sum_\ell\sum_j P(s(n)=j)\sum_{k_1=0}^{\infty}\sum_{k_2=0}^{\infty}\cdots\sum_{k_j=0}^{\infty}q_{k_1}q_{k_2}\cdots q_{k_j}\sum_\ell\delta_{k_1+k_2+\cdots+k_j,\ell}z^\ell=\sum_j P(s(n)=j)\left(\sum_k q_k z^k\right)^j=f_{(n)}\left(f(z)\right)$

- Generating function of the branching probability $f(z)=\sum_k q_k z^k$
- $f(0)=q_0, f(1)=1$, and $f(z)$ is a convex function if $q_0+q_1<1$
- $f_{(n)}(z)=f_{(n-1)}(f(z))=f_{(n-2)}(f(f(z)))=\cdots=f_{(1)}(f_{n-1}(z))=f_n(z)$ where $f_n(z)$ the n-th iterate of $f(z)$.

Probability of extinction

- The probability of extinction in a given generation n : $P(s(n)=0)=f_n(0)$
- $f_n(0)$ increases with n :
  $P(s(n)=0)=\mathrm{Prob.}(s(1)=0\bigcup s(2)=0\bigcup\cdots\bigcup s(n)=0)$
- Extinction probability $r=\lim_{n\to\infty}P(s(n)=0)=\lim_{n\to\infty}f_n(0)$
- Self-consistent equation for r : $f_n(0)=f(f_{n-1}(0))\to$

$$r=f(r)$$



- Whether the branching ratio $\kappa=f'(1)$ is larger or smaller than 1 distinguishes whether $y=f(z)$ meets $y=z$ not only at $z=1$ but also at $z<1$.
- The extinction probability

$$r=\begin{cases}1 & (\kappa=f'(1)\le 1)\\ <1 & (\kappa=f'(1)>1)\end{cases}$$

Instability of the number of individuals

- The sequence $\{s(n)\}$ either goes to ∞ or goes to 0

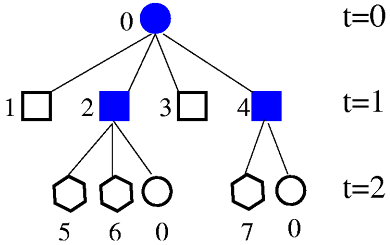
Theorem

$\lim_{n\to\infty} P(s(n) = \ell) = 0$ *for given* $\ell = 1, 2, \ldots$; $s(n) \to 0$ *with probability* r *and* $s(n) \to \infty$ *with probability* $1 - r$.

$$P(s(n+n') = \ell | s(n) = \ell) = \begin{cases} q_1^{n'} < 1 & \text{if } q_0 = 0 \\ < 1 - q_0^{n'} < 1 & \text{otherwise} \end{cases}$$

Distribution of finite tree size I

- The probability that the total number of individuals in a tree grown by a branching process is equal to s in generation n : $P_n(s)$
- Time (n) evolution of $P_n(s)$:



$P_n(s) = \sum_{k=0}^{\infty} q_k \prod_{j=1}^{k} P_{n-1}(s_j)\delta_{s_1+s_2+s_k,s-1}$,
where k is the number of children of the root and s_j is the size of the tree rooted in the j-th child of the root.

Distribution of finite tree size II

- Generating function $F_n(z) = \sum_{s=1}^{\infty} P_n(s) z^s$ satisfies the recursive relation

$$F_{n+1}(z) = z\, f(F_n(z))$$

with $f(z)$ the generating function of the branching probability.
$F_{n+1}(z) =$
$\sum_s \sum_{k=0}^{\infty} q_k \sum_{s_1=1}^{\infty} \sum_{s_2=1}^{\infty} \cdots \sum_{s_k=1}^{\infty} P_n(s_1) P_n(s_2) \cdots P_n(s_k) \delta_{s_1+s_2+s_{s(1)}, s-1} z^s =$
$\sum_k q_k z \left(\sum_s P_n(s) z^s\right)^k = z\, f(F_n(z))$

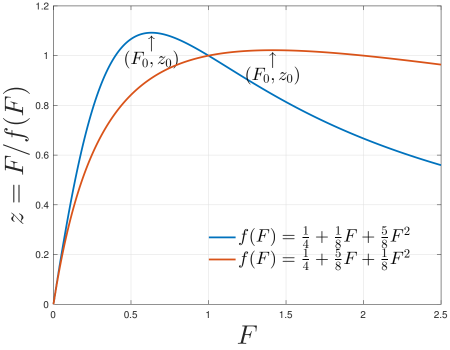
- Stationary distribution $P(s) = \lim_{n\to\infty} P_n(s)$ and its generating function $F(z) = \lim_{n\to\infty} F_n(z)$ satisfies

$$F(z) = z\, f(F(z))$$

- $F(1) = \sum_s P(s)$ is the probability to find a finite tree and the solution of the self-consistent equation $F(1) = f(F(1))$, equal to the extinction probability r.

Asymptotic behavior of the stationary tree-size distribution I

- The singular behavior of $F(z)$ can inform of the large-s behavior of $P(s)$.



- The plots of $z = F/f(F)$ versus F represent the inverse of $F(z)$.
- If the derivative $\frac{dz}{dF} = \frac{f(F) - Ff'(F)}{f(F)^2}$ is zero at F_0, then $F(z)$ is singular there: $F_0\, f'(F_0) = f(F_0)$ and $z_0 = F_0/f(F_0)$

Asymptotic behavior of the stationary tree-size distribution II

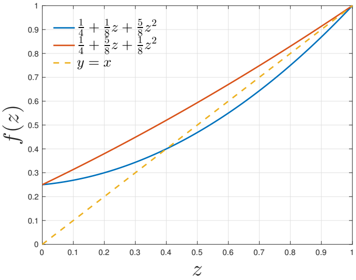
- Assuming that $f(F)$ is analytic for $0 \le F < F_0$, we see that around (F_0, z_0),
$z \simeq z_0 + \frac{dz}{dF}|_{F_0}(F-F_0) + \frac{1}{2}\frac{d^2z}{dF^2}_{F_0}(F-F_0)^2 + \cdots = z_0 - \frac{1}{2}F_0\frac{f''(F_0)}{f(F_0)^2}(F-F_0)^2 + \cdots$
- We are interested in the regime $F < F_0$:

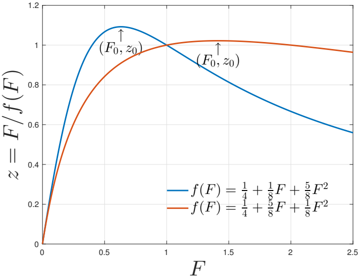
$$F(z) \simeq F_0 - \left(\frac{2f(F_0)^2}{F_0 f''(F_0)}\right)^{1/2}(z_0 - z)^{1/2}$$

- Expand $F(z)$ around $z = 0$ as $F(z) = \sum_s P(s)z^s$ to obtain $P(s)$:
$(1-x)^{1/2} = -\sum_{s=0}^{\infty}\frac{1}{s!}\frac{(2s-2)!}{2^{2s-1}(s-1)!}x^s$ for $|x| < 1$
$F(z) \simeq F_0 + \left(\frac{2f(F_0)^2}{F_0 f''(F_0)}\right)^{1/2} z_0^{1/2}\sum_{s=0}^{\infty}\frac{1}{s!}\frac{(2s-2)!}{2^{2s-1}(s-1)!}\left(\frac{z}{z_0}\right)^s$
- Using Stirling's formula $s! \simeq s^s\sqrt{2\pi s}e^{-s}$, we obtain

$$P(s) \simeq \left(\frac{2f(F_0)^2}{F_0 f''(F_0)}\right)^{1/2} z_0^{1/2} z_0^{-s}\frac{1}{s!}\frac{(2s-2)!}{2^{2s-1}(s-1)!} \simeq \left(\frac{f(F_0)}{2\pi f''(F_0)}\right)^{1/2} z_0^{-s} s^{-3/2} \text{ for } s \gg 1$$

Subcritical, critical, and supercritical phase





- The location of the singular point (F_0, z_0) varies depending on the form of f.
- Subcritical phase : the branching ratio $\kappa < 1$: $z_0 > 1$ and $F_0 > 1$: $P(s)$ decays exponentially $P(s) \sim e^{-s/s_0}$ with the characteristic scale $s_0 = 1/\ln z_0$
- Critical phase : $\kappa = 1$: $z_0 = 1$ and $F_0 = 1$: $P(s)$ is a power-law $P(s) \sim s^{-3/2}$
- Supercritical phase : $\kappa > 1$: $z_0 > 1$ and $F_0 < 1$: $P(s)$ decays exponentially $P(s) \sim e^{-s/s_0}$ with the characteristic scale $s_0 = 1/\ln z_0$

Discrete Tauberian theorem

Theorem (Discrete Tauberian theorem)

$\sum_{n=0}^{\infty} a_n z^n \sim (1-z)^{-\rho} L\left(\frac{1}{1-z}\right)$ as $z \to 1^-$
$\iff$
$a_n \sim \frac{n^{\rho-1}}{\Gamma(\rho)} L(n)$ as $n \to \infty$
if $\rho > 0$, a_n monotonic, and $L(x)$ is slowly varying for x large such that $L(\lambda x)/L(x) \to 1$ as $x \to \infty$.

- Proof in W. Feller, *An introduction to probability theory and its applications* vol II (John Wiley & Sons, 1957)
- $\sum_n n^{\rho-1} e^{-\alpha n} \sim \alpha^{-\rho} \int dy y^{\rho-1} e^{-y}$

When the branching ratio is close to 1

- z_0 and F_0 will be close to 1.
- Let $\Delta \equiv 1-\kappa$. We consider the case of $0<\Delta \ll 1$.
- The branching probability generating function behaves around $z=1$ as

$$f(z) = 1 + \kappa(z-1) + \frac{f''(1)}{2}(z-1)^2 + \cdots \tag{1}$$

  with $\kappa = f'(1)$ if $f''(1) = \langle k^2 \rangle$ is finite. $(f^{(n)}(1) = \langle k^n \rangle)$
- To determine the generating function $F(z)$ of the tree-size distribution $P(s)$

$$z = \frac{F}{f(F)} = \frac{1-(1-F)}{1-\kappa(1-F)+\frac{f''(1)}{2}(1-F)^2+\cdots} \simeq 1 - \Delta(1-F) - \frac{f''(1)}{2}(1-F)^2 + \cdots$$

- $\frac{dz}{dF}\big|_{F_0} = 0$: $F_0 \simeq 1 + \frac{\Delta}{f''(1)}$ and $z_0 = 1 + \frac{\Delta^2}{2f''(1)}$

$$P(s) \sim s^{-3/2}\, e^{-s/s_c} \text{ with } s_c = 1/\ln z_0 \sim \Delta^{-2}$$

Lifetime distribution I

- Extinction probability at generation n: $r(n) = f_n(0) = P(s(n) = 0)$
- Lifetime dsitribution $\ell(n)$: the probability that the tree is terminated at generation n: $\ell(n) = r(n) - r(n-1)$
- Recursive relation $r(n) = f(r(n-1))$
- subcritical or critical phase : $r = \lim_{n\to\infty} r(n) = 1$
- Using the expansion Eq. (1) of $f(z)$ near $z = 1$, we obtain

$$r(n) = 1 + \kappa(r(n-1) - 1) + \frac{f''(1)}{2}(r(t-1) - 1)^2 + \cdots$$

- Let $\tilde{r}(n) = 1 - r(n)$, which is small.
- If the branching ratio κ is significantly smaller than 1, then $\tilde{r}(n) \simeq \kappa\tilde{r}(n-1)$ leading to $\tilde{r}(n) \sim \kappa^n \sim e^{-n/n_c}$ with $n_c \sim 1/|\ln \kappa|$

Lifetime distribution II

- If the branching ratio is close to 1 ($\Delta = 1 - \kappa \ll 1$), then $\tilde{r}(n) = (1-\Delta)\tilde{r}(n-1) - \frac{f''(1)}{2}\tilde{r}(n-1)^2 + \cdots$ or

$$\frac{d\tilde{r}}{dn} \simeq -\Delta\tilde{r} - \frac{f''(1)}{2}\tilde{r}^2 + \cdots$$

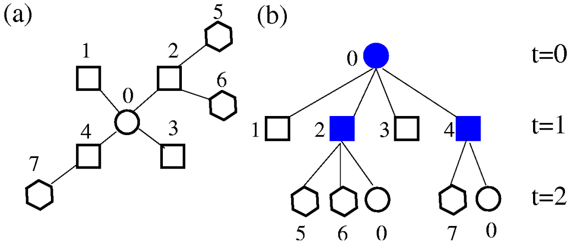
leading to $\tilde{r}(n) \sim \frac{2\Delta}{f''(1)}\frac{e^{-\Delta n}}{1-e^{-\Delta n}} \sim \begin{cases} \Delta e^{-n\Delta} & (n \gg n_c = \Delta^{-1}) \\ \frac{1}{n} & (n \ll n_c) \end{cases}$

- The lifetime distribution $\ell(n) \simeq -\frac{d\tilde{r}}{dn} \sim \begin{cases} \Delta^2 e^{-n\Delta} & (n \gg n_c = \Delta^{-1}) \\ \frac{1}{n^2} & (n \ll n_c) \end{cases}$
- At the critical phase ($\Delta = 0$), the lifetime distribution is a power-law $\ell(n) \sim n^{-2}$.

BTW Sandpile model

- Bak-Tang-Wiesenfeld model for sandpile avalanches
  1. At each time step, a grain is added at a randomly chosen node i.
  2. If the height h_i at the node i reaches or exceeds a threshold $H_i = k_i$ with k_i the degree of the node i, then it becomes unstable and H_i grains at the node topple to its nearest neighbors nodes such that $h_i \to h_i - H_i$ and $h_j \to h_j + 1$ for all neighbor nodes j.
  3. If this toppling causes any of the adjacent nodes unstable, subsequent topplings follow in parallel until there is no unstable node left. This process defines an avalanche.
  4. Repeat 1)-3)
- Avalanche size s: the number of toppling events in an avalanche.
- The duration of an avalanche n
- A cluster of nodes participating in an avalanche can be seen as a tree generated by a branching process
- What is the branching probability q_k for the model on a network?

Critical branching process for the BTW sandpile model I



- After receiving a grain from a neighbor node, grains at a node i topple to its k_i neighbor nodes in an avalanche = node i gives birth to k_i children in the corresponding tree
- The branching probability $q_k = q^{(1)}(k)\, q^{(2)}(k)$ where $q^{(1)}(k)$ is the probability that the node (i) receiving a grain has degree k and $q^{(2)}(k)$ is the probability that toppling indeed occurs.

Critical branching process for the BTW sandpile model II

- $q^{(1)}(k) = \frac{kP_d(k)}{\langle k \rangle}$ where $P_d(k)$ is the degree distribution of the substrate network $P_d(k) = N^{-1} \sum_{i=1}^{N} \delta_{k_i,k}$ and the degree k_i of node i is given by $k_i = \sum_j A_{ij}$ with A_{ij} the adjacency matrix.
- $q^{(2)}(k) = 1/k$ if we assume that the height is uniformly distributed between 0 and $k-1$
- $q_k = \frac{P_d(k)}{\langle k \rangle}$ for $k \geq 1$ and $q_0 = 1 - \sum_k q_k = 1 - \sum_{k \geq 1} \frac{P_d(k)}{\langle k \rangle} > 0$.
- Branching ratio $\kappa = \langle k \rangle = \sum_k q_k = \sum_{k=1}^{\infty} k \frac{P_d(k)}{\langle k \rangle} = 1$ (critical branching processes)

Critical branching processes with diverging moments of q_k

- In scale-free networks with the degree distribution $P_d(k) \sim k^{-\gamma}$, the generating function $f(z) = \sum_{k=0}^{\infty} q_k z^k$ is singular at $z = 1$:
- Let $P_d(k) = \frac{k^{-\gamma}}{\zeta(\gamma)}$ for $k \geq 1$. Then the branching probability $q_k = \frac{k^{-\gamma}}{\zeta(\gamma-1)}$ for $k \geq 1$ and $q_0 = 1 - \frac{\zeta(\gamma)}{\zeta(\gamma-1)}$
- The generating function of q_k behaves around $z = 1$ as

$$f(z = e^{-\alpha}) = \sum_{k=0}^{\infty} q_k e^{-\alpha k} = 1 - \alpha + \frac{\alpha^2}{2} \frac{\zeta(\gamma-2)}{\zeta(\gamma-1)} + \cdots + \frac{\Gamma(1-\gamma)}{\zeta(\gamma-1)} \alpha^{\gamma-1}$$

using the Mellin transform (J.E. Robinson, Phys. Rev. **83**, 678 (1951))
$f(z = e^{-\alpha}) = \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \alpha^n \langle k^n \rangle =$
$1 - \alpha\langle k \rangle + \frac{1}{2}\alpha^2 \langle k^2 \rangle + \cdots + \sum_{n=\lfloor \gamma-1 \rfloor}^{\infty} \frac{(-)^n (\text{const.})}{n!} \alpha^n K^{n-\gamma+1}$ with $\alpha \to 0$, $K \to \infty$ and $K\alpha \to \infty$.

$$f(z) \simeq 1 - (1-z) + \frac{B(\gamma)}{2}(1-z)^2 + \cdots A(\gamma)(1-z)^{\gamma-1}$$

with $A(\gamma) = \frac{\Gamma(1-\gamma)}{\zeta(\gamma-1)}$ and $B(\gamma) = \frac{\zeta(\gamma-2)}{\zeta(\gamma-1)} - 1$

Avalanche size distribution

- Avalanche size distribution $P(s)$
- Its generating function $F(z)=\sum_s P(s)z^s$ satisfies the relation
$z=\frac{F}{f(F)}=\frac{1-(1-F)}{1-(1-F)+\frac{B(\gamma)}{2}(1-F)^2+\cdots+A(\gamma)(1-F)^{\gamma-1}}\simeq$
$\begin{cases} 1-\frac{B}{2}(1-F)^2 & (\gamma>3) \\ 1-A(1-F)^{\gamma-1} & (2<\gamma<3) \end{cases}$
- The singular behavior of the generating function $F(z)$ at $z=1$ is then given by $1-F(z)\sim\begin{cases} \sqrt{\frac{2}{B}(1-z)} & (\gamma>3) \\ A^{-\frac{1}{\gamma-1}}(1-z)^{\frac{1}{\gamma-1}} & (2<\gamma<3) \end{cases}$
- Differentiating the singular terms of $F(z)$ with respect to z, one finds the coefficients to be the tree-size distribution, which is
$P(s)\sim\begin{cases} s^{-3/2} & (\gamma>3) \\ s^{-\frac{\gamma}{\gamma-1}} & (2<\gamma<3) \end{cases}$

Lifetime distribution

- Lifetime distribution $\ell(n) = r(n) - r(n-1) \simeq \frac{dr}{dn}$
- Critical phase : The extinction probability $r = \lim_{n\to\infty} r(n) = 1$
- The extinction probability up to generation n, $r(n)$ satisfies
  $r(n) = 1 - (1 - r(n-1)) + \frac{B(\gamma)}{2}(1 - r(n-1))^2 + \cdots + A(\gamma)(1 - r(n-1))^{\gamma-1}$
- Let $\tilde{r}(n) = 1 - r(n)$.
- $\tilde{r}(n+1) - \tilde{r}(n) \simeq \frac{d\tilde{r}(n)}{dn} \simeq -\frac{B(\gamma)}{2}\tilde{r}(n)^2 + \cdots - A(\gamma)\tilde{r}(n)^{\gamma-1}$
- $\tilde{r}(n) \sim \begin{cases} n^{-1} & (\gamma > 3) \\ n^{-\frac{1}{\gamma-2}} & (2 < \gamma < 3) \end{cases}$
- $\ell(n) \sim \begin{cases} n^{-2} & (\gamma > 3) \\ n^{-\frac{\gamma-1}{\gamma-2}} & (2 < \gamma < 3) \end{cases}$

Random walks

Random walk in discrete space and discrete time

- Occupation probability $P_{ij}(n)$: the probability of being at site i after n steps starting at site j
- Initial condition $P_{ij}(0) = \delta_{ij}$
- Normalization $\sum_i P_{ij}(n) = 1$
- Transition probability (one-step occupation probability) $M_{ij} = P_{ij}(1) = \frac{A_{ij}}{k_j}$ with $A_{ij} = 1$ or 0 the adjacency matrix element and $k_j = \sum_\ell A_{j\ell}$ the number of the nearest neighbors (degree) of site j
- We are interested in $P_{is}(n)$
- Time evolution of $P_{is}(n)$

$$P_{is}(n+1) = \sum_j M_{ij} P_{js}(n)$$

- Generating function of $P_{ij}(n)$: $\mathcal{P}_{ij}(z) = \sum_{n=0}^{\infty} z^n P_{ij}(n)$
- $\mathcal{P}_{is}(z) = \delta_{is} + z \sum_j M_{ij} \mathcal{P}_{js}(z)$

Recurrence

Pólya (1919)

What is the probability that a given site will be ever visited or the starting site will be ever revisited?

- The probability that a site will be visited or the starting site will be revisited at least once in the first n steps increases with n. Then what is the probability in the limit $n \to \infty$?
- First passage time T_{ij}: The time when a walker arrives at i starting at j.
- Reaching or return probability $R_{ij} \equiv \text{Prob.} \ (T_{ij} < \infty)$
- Answer (Pólya's theorem) $R_{ij} = 1$ for $d = 1$ or 2 but less than 1 for $d = 3$

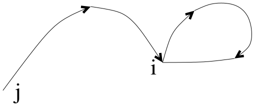
Theorem (Recurrence theorem)

If sites i and j are accessible from each other, i.e., $R_{ij} > 0$ and $R_{ji} > 0$, then either $R_{ii} = R_{jj} = R_{ij} = R_{ji} = 1$ or $R_{ii} < 1, R_{jj} < 1, R_{ij}R_{ji} < 1$.

First-passage probability

- First passage probability $F_{ij}(n) = \text{Prob. } (T_{ij} = n)$: the probability of arriving at site i for the first time on the nth step starting at site j.
- $F_{ij}(0) = 0$.
- $R_{ij} = \text{Prob. } (T_{ij} < \infty) = \sum_{n=1}^{\infty} F_{ij}(n)$, which can be equal to or smaller than 1.
- Relation between the occupation probability and the first-passage probability

$$P_{ij}(n) = \delta_{ij}\delta_{n0} + \sum_{n'=1}^{n} F_{ij}(n')P_{ii}(n-n')$$



- Generating function of $F_{ij}(n)$: $\mathcal{F}_{ij}(z) = \sum_{n=0}^{\infty} z^n F_{ij}(n)$
- $R_{ij} = \mathcal{F}_{ij}(1^-) \equiv \lim_{z\to 1^-} \mathcal{F}_{ij}(z)$
- $\mathcal{P}_{ij}(z) = \delta_{ij} + \mathcal{F}_{ij}(z)\mathcal{P}_{ii}(z)$, leading to

$$\mathcal{F}_{ij}(z) = \frac{\mathcal{P}_{ij}(z)-\delta_{ij}}{\mathcal{P}_{ii}(z)}$$

- Mean first-passage time (MFPT) $\langle T_{ij}\rangle = \mathcal{F}'(1^-)$.

Recurrent vs transient

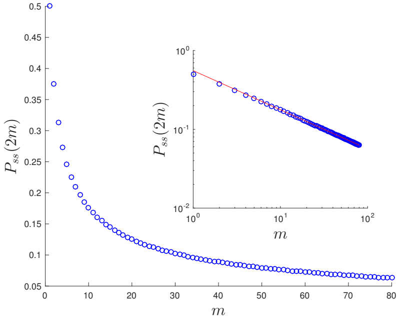
- Return probability $R_{ii} = \sum_{n=1}^{\infty} F_{ii}(n) = 1 - \frac{1}{\mathcal{P}_{ii}(1^-)}$

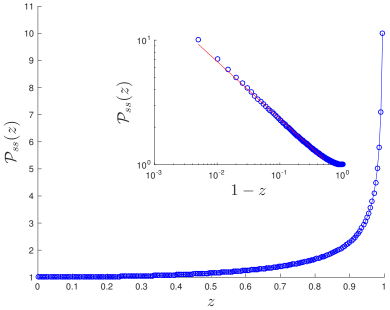
$$\begin{aligned} \text{recurrent}: \; & R_{ii} = 1 \iff \mathcal{P}_{ii}(1^-) = \sum_n P_{ii}(n) \to \infty \\ \text{transient}: \; & R_{ii} < 1 \iff \mathcal{P}_{ii}(1^-) = \sum_n P_{ii}(n) < \infty \end{aligned}$$

Return probability on the 1-dimensional infinite lattice

- Transition probability $M_{ij} = \frac{1}{2}\delta_{i,j\pm 1}$: move to the right or to the left with probability $1/2$.
- Time-dependent return probability
  $P_{ss}(n=2m) = \binom{2m}{m}\left(\frac{1}{2}\right)^m\left(\frac{1}{2}\right)^m \sim_{m\gg 1} (\pi m)^{-1/2} (m! \simeq \frac{m^m}{e^m}\sqrt{2\pi m})$
  $\mathcal{P}_{ss}(z) = \sum_m \binom{2m}{m} 4^{-m} z^{2m} = (1-z^2)^{-1/2}$
- First-passage probability
  $\mathcal{F}_{ss}(z) = 1 - \frac{1}{\mathcal{P}_{ss}(z)} = 1 - (1-z^2)^{1/2}$
  $F_{ss}(2m) = \frac{1}{m!}\frac{d^m \mathcal{F}_{ss}}{d(z^2)^m}\Big|_{z=0} = \frac{1}{2m-1}\binom{2m}{m}\left(\frac{1}{2}\right)^{2m} \sim_{m\gg 1} \frac{\pi^{1/2}}{2} m^{-3/2}$
- Return probability $R_{ss} = \mathcal{F}_{ss}(1^-) = 1 - \frac{1}{\mathcal{P}_{ss}(1^-)} = 1.$

$P_{ss}(z)$ and $\mathcal{P}_{ss}(z)$ in 1d





Reaching probability on the 1-dimensional infinite lattice

- Start at $s=0$.
- $P_{s0}(n+1)=\sum_{s'} M_{ss'}P_{s'0}(n)=\sum_{\ell=-1,1}\frac{1}{2}P_{s-\ell,0}(n)$
- Transition matrix $M_{ij}=\frac{1}{2}\delta_{i,j\pm 1}$ is diagonalized by the plane wave $X_k=(\cdots,e^{iks},e^{ik(s+1)},\cdots)^T$ as $M\,X_k=m(k)X_k$ with the eigenvalue $m(k)=\sum_{\ell=-1,1}\frac{1}{2}e^{i\ell k}=\cos k$ called the structure function of the walk.
- Decomposition in terms of the eigenvectors = Discrete Fourier Transform: $\tilde{P}_k(n)=\sum_s e^{isk}P_{s0}(n)$, $P_{s0}(n)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\,e^{-iks}\tilde{P}_k(n)$.
- $\tilde{P}_k(n+1)=m(k)\tilde{P}_k(n)$, $\tilde{P}_k(0)=1\to\tilde{P}_k(n)=m(k)^n=(\cos k)^n$.
- $\mathcal{P}_{s0}(z)=\sum_{n=0}^{\infty}\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\,e^{-iks}(\cos k)^n z^n=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\,\frac{e^{-iks}}{1-z\cos k}=$ $\frac{1}{2\pi i}\oint_{|r|=1}dz\frac{r^{|s|}}{r-\frac{z}{2}(r^2+1)}=(1-z)^{-1/2}\left\{\frac{1-(1-z^2)^{1/2}}{z}\right\}^{|s|}$
- $\mathcal{F}_{s0}(z)=\frac{P_{s0}(z)}{P_{ss}(z)}=\left\{\frac{1-(1-z^2)^{1/2}}{z}\right\}^{|s|}$

Return probability on the 2-dimensional infinite square lattice

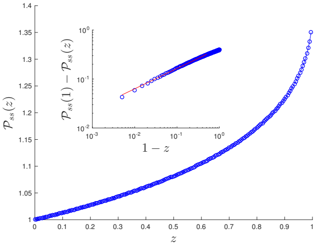
- Transition probability $M_{\vec{r},\vec{r}'} = \frac{1}{4}(\delta_{\vec{r},\vec{r}'\pm\hat{x}} + \delta_{\vec{r},\vec{r}'\pm\hat{y}})$ with the structure function (eigenvalues) $m(\vec{k}) = \frac{\cos k_x + \cos k_y}{2}$
- $\tilde{P}_{\vec{k}}(n) = m(\vec{k})^n = \left(\frac{\cos k_x + \cos k_y}{2}\right)^n$
- Generating function of the occupation probability $\mathcal{P}_{\vec{r},\vec{0}}(z) = \sum_{n=0}^{\infty} \left\{ \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} e^{-i(k_x x + k_y y)} m(\vec{k})^n \right\} z^n = \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \frac{e^{-i(k_x x + k_y y)}}{1 - z\frac{\cos k_x + \cos k_y}{2}}$
- Time-dependent return probability
  $\mathcal{P}_{\vec{r},\vec{r}}(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \frac{1}{\sqrt{(1-\frac{z}{2}\cos k)^2 - (\frac{z}{2})^2}} = \frac{2}{\pi} K(z) \sim_{1-z \ll 1} \frac{1}{\pi} \ln[8(1-z)^{-1}]$
  with the complete elliptic integral of the first kind
  $K(z) = \int_0^1 dx \frac{1}{(1-x^2)^{1/2}(1-z^2x^2)^{1/2}}$
  $P_{\vec{r}\vec{r}}(n = 2m) = \left(\frac{(m-1/2)!}{(-1/2)!m!}\right)^2 \sim_{m \gg 1} (\pi m)^{-1}$
- First-passage probability $\mathcal{F}_{\vec{r}\vec{r}}(z) = 1 - \frac{1}{\mathcal{P}_{\vec{r},\vec{r}}(z)} \sim_{1-z \ll 1} 1 - \frac{\pi}{\ln[8(1-z)^{-1}]}$
- Return probability $R_{\vec{r}\vec{r}} = \mathcal{F}_{\vec{r}\vec{r}}(1^-) = 1 - \frac{1}{\mathcal{P}_{ss}(1^-)} = 1.$

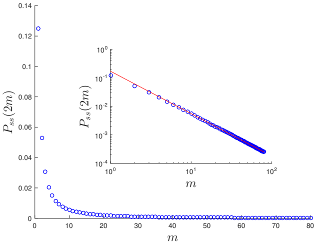
Return probability on the 3-dimensional infinite body-centered cubic lattice

- Transition probability $M_{\vec{r},\vec{r'}} = \frac{1}{8}(\delta_{\vec{r},\vec{r'}+\frac{\hat{x}+\hat{y}\pm\hat{z}}{2}} + \delta_{\vec{r},\vec{r'}+\frac{\hat{x}-\hat{y}\pm\hat{z}}{2}} + \delta_{\vec{r},\vec{r'}+\frac{-\hat{x}+\hat{y}\pm\hat{z}}{2}} + \delta_{\vec{r},\vec{r'}+\frac{-\hat{x}-\hat{y}\pm\hat{z}}{2}})$ with the structure function (eigenvalues) $m(\vec{k}) = \frac{\cos k_x + \cos k_y + \cos k_z}{3}$
- Generating function of the occupation probability $\mathcal{P}_{\vec{r},0}(z) = \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} \frac{e^{-i(k_x x + k_y y + k_z z)}}{1 - z\frac{\cos k_x + \cos k_y + \cos k_z}{3}}$
- Time-dependent return probability $\mathcal{P}_{\vec{r}\vec{r}}(z) = {}_3F_2(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1, ; z^2) \to_{z\to 1} \frac{(-3/4)!^4}{4\pi^3} \simeq 1.3932039\ldots$ with the generalized hypergeometric function ${}_pF_q(a_1, a_2, \ldots, a_p; b_1, b_2, \ldots, b_q; z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \frac{\Gamma(a_1+n)\Gamma(a_2+n)\ldots\Gamma(a_p+n)\Gamma(b_1)\Gamma(b_2)\ldots\Gamma(b_q)}{\Gamma(a_1)\Gamma(a_2)\ldots\Gamma(a_p)\Gamma(b_1+n)\Gamma(b_2+n)\ldots\Gamma(b_q+n)}$
- $P_{\vec{r}\vec{r}}(n = 2m) = \left(\frac{(m-1/2)!}{(-1/2)!m!}\right)^3 \sim_{m\gg 1} (\pi m)^{-3/2}$
- Return probability $\mathcal{P}_{\vec{r}\vec{r}}(z) \sim_{1-z\ll 1} \frac{(-3/4)!^4}{4\pi^3} - \frac{2\sqrt{2}}{\pi}(1-z)^{1/2} \to R_{\vec{r}\vec{r}} = 1 - \frac{1}{\mathcal{P}_{\vec{r}\vec{r}(1-)}} \simeq 0.282230$
- First-passage probability $\mathcal{F}_{\vec{r}\vec{r}}(z) = 1 - \frac{1}{\mathcal{P}_{\vec{r},\vec{r}}(z)} \sim_{1-z\ll 1} R_{\vec{r}\vec{r}} - \frac{1}{\mathcal{P}_{\vec{r}\vec{r}}(1-)^2} \frac{2\sqrt{2}}{\pi}(1-z)^{1/2}$

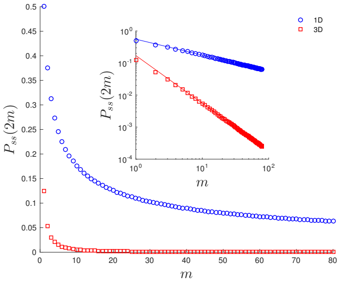
Return-to-origin probabilities

- 3d





- 1d and 3d



Polya's theorem

Theorem (Pólya's theorem)

For the random walks on infinite d-dimensional lattice with finite mean-square displacement and zero mean displacement per step, the walk is recurrent if $d = 1$ or $d = 2$ and transient if $d \geq 3$.

Structure function $m(\vec{k}) = \sum_{\vec{r}} e^{i(\vec{r}-\vec{r}')\cdot\vec{k}} M_{\vec{r},\vec{r}'} \simeq 1 - \frac{1}{2}\sum_{i,j=1}^{d} k_i k_j D_{ij}$ with $D_{ij} = \sum_{\vec{r}} (\vec{r}-\vec{r}')_i (\vec{r}-\vec{r}')_j M_{\vec{r},\vec{r}'}$

$$\mathcal{P}_{\vec{r}\vec{r}}(z = 1^-) = \frac{1}{(2\pi)^d} \int \frac{d^d\vec{k}}{1 - m(\vec{k})} \sim \int_0^{\pi} dk \frac{k^{d-1}}{k^2} \begin{cases} \to \infty & (d \leq 2) \\ < \infty & (d > 2) \end{cases}$$

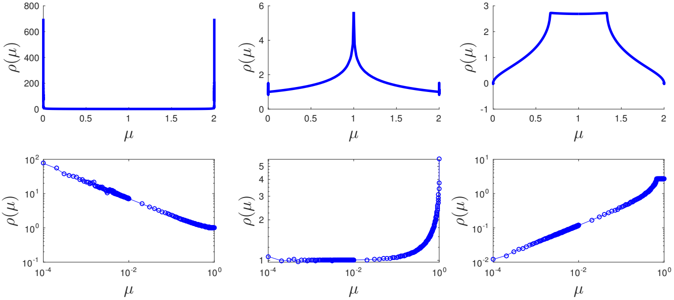
Effects of dimension: Spectral decomposition I

- d-dimensional lattice of lateral length L and the total number of sites L^d
- Laplacian matrix $\tilde{L}_{\vec{r},\vec{r}'} = \delta_{\vec{r},\vec{r}'} - M_{\vec{r},\vec{r}'} = \delta_{\vec{r},\vec{r}'} - \frac{1}{2d}\sum_{j=1}^{d}(\delta_{\vec{r},\vec{r}'+\hat{e}_j} + \delta_{\vec{r},\vec{r}'-\hat{e}_j})$
  with the eigenvectors $\langle\vec{k}|\vec{r}\rangle = \phi_{\vec{r}}(\vec{k}) = L^{-d/2}e^{i\vec{k}\cdot\vec{r}}$
  and the eigenvalues $\langle\vec{k}|M|\vec{k}\rangle = \mu(\vec{k}) = 1 - \frac{1}{d}\sum_{j=1}^{d}\cos k_j$
  Ex. $d=1$: $\sum_{r'=0}^{L-1}\tilde{L}_{rr'}f(r') = f(r) - \frac{f(r-1)+f(r+1)}{2} \sim -\frac{1}{2}\frac{d^2f}{dr^2}$ and
  $\mu(k) = 1-\cos k \sim \frac{1}{2}k^2$
- Wave vector $\vec{k}$ under the periodic boundary condition: $\vec{k} = \frac{2\pi}{L}(n_1, n_2, \ldots, n_d)$
  with $n_j = -L/2, -L/2+1, \ldots, -1, 0, 1, \ldots, L/2-2, L/2-1$ for L even and
  $n_j = -(L-1)/2, -(L-3)/2, \ldots, -1, 0, 1, \ldots, (L-3)/2, (L-1)/2$ for L odd.
- Occupation probability $P_{\vec{r}\vec{r}'}(n) = (M^n)_{\vec{r}\vec{r}'} = \sum_{\vec{k}}\{1-\mu(\vec{k})\}^n\frac{1}{L^d}e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')}$
- Time-dependent return probability

$$P_{\vec{r}\vec{r}}(n) = \frac{1}{L^d}\sum_{\vec{k}}\{1-\mu(\vec{k})\}^n$$

Effects of dimension: Spectral decomposition II

- Generating function $\mathcal{P}_{\vec{r}\vec{r}}(z) = \sum_{n=0}^{\infty} \frac{1}{L^d} \sum_{\vec{k}} \{1-\mu(\vec{k})\}^n z^n = \frac{1}{L^d} \sum_{\vec{k}} \frac{1}{1-z+z\mu(\vec{k})}$
- Spectral density function $\rho(\mu) = \frac{1}{L^d} \sum_{\vec{k}} \delta(\mu(\vec{k}) - \mu)$
  $= \frac{1}{(2\pi)^d} \int d^d\vec{k}\, \delta(1 - \frac{1}{d} \sum_{j=1}^{d} \cos k_j - \mu) =$
  $\frac{1}{2\pi} \int_{-\infty}^{\infty} dq e^{iq(1-\mu)} \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} dk\, e^{-i\frac{q}{d}\cos k} \right)^d = \frac{1}{\pi} \int_0^{\infty} \cos[q(1-\mu)]\{J_0(\frac{q}{d})\}^d$



Effects of dimension: Spectral decomposition III

- The convergence/divergence of $\mathcal{P}_{\vec{r}\vec{r}}(1^-) = \frac{1}{L^d}\sum_{\vec{k}} \frac{1}{\mu(\vec{k})} = \int_0^\infty d\mu\, \rho(\mu) \frac{1}{\mu}$ depends on the small-μ behavior of $\rho(\mu)$
- For $\mu \to 0$, $\mu(\vec{k}) \simeq \frac{1}{2d}\vec{k}^2$ and

$$\rho(\mu) = \frac{1}{(2\pi)^d}\int d^d\vec{k}\,\delta(\frac{\vec{k}^2}{2d} - \mu) \simeq \frac{d^{d/2}}{(2\pi)^{d/2}}\frac{\mu^{\frac{d}{2}-1}}{\Gamma(d/2)}$$

- Time-dependent return probability
  - Singularity of the generating function :
    $\mathcal{P}_{\vec{r}\vec{r}}(z) = \int_0^2 d\mu\, \rho(\mu)\, \frac{1}{1-z+z\mu} \simeq_{z\to 1} \int_0^{1-z} d\mu\, \rho(\mu)\, \frac{1}{1-z} + \int_{1-z}^2 d\mu\, \rho(\mu) \frac{1}{\mu} \sim$
    $$\begin{cases} (1-z)^{d/2-1} & (d<2) \\ \ln\left(\frac{1}{1-z}\right) & (d=2) \\ \text{finite constant} & (d>2). \end{cases}$$
  - $P_{\vec{r}\vec{r}}(n) = \frac{1}{(2\pi)^d}\int d^d\vec{k}\,\{1-\mu(\vec{k})\}^n = \int_0^2 d\mu\, \rho(\mu)(1-\mu)^n =$ $(1+(-1)^n)\int_0^1 d\mu\, \rho(\mu)(1-\mu)^n$.
  - For large n, $P_{\vec{r}\vec{r}}(n=2m) \simeq 2\int_0^1 d\mu\, \rho(\mu)\, e^{-\mu n}$ [Laplace transform of $\rho(\mu)$]

Effects of dimension: Spectral decomposition IV

- The behavior of $\rho(\mu)$ for $\mu \to 0$ determines $R(n)$ for $n \to \infty$ such that

$$R(n) \simeq \int_0^\infty d\mu \, \frac{d}{(2\pi)^{d/2}} \frac{\mu^{\frac{d}{2}-1}}{\Gamma(d/2)} e^{-\mu n} \sim n^{-\frac{d}{2}}$$

- Tauberian theorem and the singularity of $\mathcal{P}(z)$ can be used to obtain the same result.

Random walk on a general network

- Random walk on a network which is finite and has no translational invariance
- How fast and far can a random walker go on a network?
- Need to extend the concept of recurrence and transience
- A network of N nodes and L links with the adjacency matrix A_{ij} is considered.
- Transition probability from a node j to i $M_{ij} = \frac{A_{ij}}{k_j}$
- Occupation probability $P_{is}(n)$ evolves with time as $P_{is}(n+1) = \sum_j M_{ij} P_{js}(n)$.

Stationary state on a network

- Fundamental theorem of Markov chains - A finite, irreducible, and aperiodic Markov chain has a unique stationary distribution $P_i = \lim_{n\to\infty} P_{is}(n)$
- irreducible $\sim$ consisting of a single strongly-connected component
- aperiodic $\sim$ without a limiting cycle
- If $M_{ij} = M_{ji}$ for all i and j, it follows that $\sum_j M_{ij} = \sum_j M_{ji} = 1$ leading to $P_i = 1/N$.
- For $M_{ij} \neq M_{ji}$ for some i and j, $P_i = \frac{k_i}{2L}$ (as $\sum_j \frac{A_{ij}}{k_j} P_j = \frac{k_i}{2L}$)
- Detailed balance condition $M_{ij}P_j = M_{ji}P_i$ (implying $(M^n)_{ij}P_j = (M^n)_{ji}P_i$ for all $n \geq 1$)

Return probability on a finite $N = L^d$ lattice

- Time-dependent return probability $R(n) \equiv \frac{1}{N}\sum_s P_{ss}(n) = \frac{1}{N}\sum_{\vec{k}}\{1-\mu(\vec{k})\}^n = \frac{1}{N} + \int d\mu\, \rho(\mu)(1-\mu)^n \sim \frac{1}{N} + (\text{const.})n^{-d/2}$
- Characteristic scale $n_X = N^{2/d}$ such that

$$R(n) \simeq \begin{cases} n^{-d/2} & (n \ll n_X) \\ 1/N & (n \gg n_X) \end{cases}$$

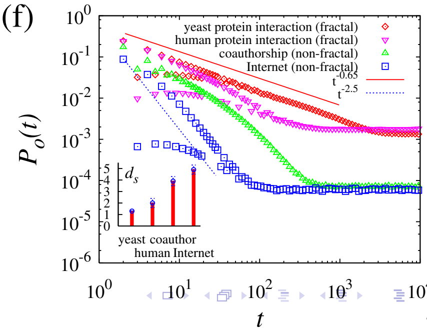
- Generating function
  $\mathcal{R}(z) \equiv \frac{1}{N}\sum_s \mathcal{P}_{ss}(z) = \frac{1}{N(1-z)} + (\text{const.}) + (\text{const.})(1-z)^{d/2-1} + \cdots$.
  The limit $z \to 1^-$ for computing the return probability $R = R(z = 1^-)$ in the infinite lattice ($N \to \infty$) corresponds to the scaling regime $(1-z)N^{2/d} \gg 1$ for $d \leq 2$ and $(1-z)N \gg 1$ for $d > 2$.
- Question: Return probability on complex networks?
  The eigenvalues of the Laplacian matrix of complex networks are not known.
  No translational invariance for complex networks $\to$ $P_{ss}(n)$ for a specific node s can be different from $R(n)$.

Spectral dimension of complex networks

- Laplacian matrix $\tilde{L}_{ij} = \delta_{ij} - \frac{A_{ij}}{k_j}$
- If the spectral density function $\rho(\mu)$ behaves as $\rho(\mu) \sim \mu^{d_s/2-1}$ for small μ, the spectral dimension of this network is d_s.
- How to measure the spectral dimension of an ensemble of networks
  1. Determine numerically the small eigenvalues of $\tilde{L}$ and compute $\rho(\mu) \sim \mu^{d_s/2-1}$.
  2. Obtain the second-smallest eigenvalue μ_2 for different N to estimate d_s by the extreme-value relation $\int_0^{\mu_2} d\mu\, \rho(\mu) \sim 1/N$ or $\mu_2 \sim N^{-2/d_s}$.
  3. Perform the simulation of random walks and obtain $R(n) = \int d\mu\, \rho(\mu) e^{-\mu n} \sim n^{-d_s/2}$

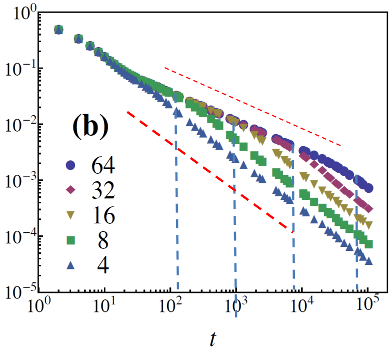
Data	d_s
(u,v) flower network	$\frac{2\ln(u+v)}{\ln uv}$
Yeast ppi	1.30 ± 0.04
Human ppi	2.0 ± 0.4
Coauthorship	3.9 ± 0.4
Internet	4.9 ± 0.4

Table: Spectral dimension



Time-dependent return probability of a specific node

- $P_{ss}(n) \neq R(n)$ for scale-free networks having a power-law degree distribution $P_d(k) \sim k^{-\gamma}$: Simulations show that $P_{ss}(n)$ decays slow with n if the degree of s is large.



- In the stationary state, the probability to cross a link is all the same; $M_{ij}P_{js} = \frac{1}{k_j}\frac{k_j}{2L} = \frac{1}{2L}$.

Idea: Can we represent $P_{ss}(n)$ as the ratio of the effective degree $\hat{k}_s(n)$ to the total number of effective links $\hat{L}(t)$ like $P_{ss}(n \to \infty) = k_s/(2L)$ in the stationary state?

Effective degree I

- For given finite n, a walker has crossed some links and not crossed others.
- $P_{is}(n) = \sum_j M_{ij} P_{js}(n-1)$ = sum of jump probability from the neighbors (j) to i.
- Link accessibility for a link $(j \to i)$

$$W_{ij}(n) = \frac{M_{ij} P_{js}(n-1)}{\max_{ab} M_{ab} P_{ab}(n-1)}$$

  - $W_{ij}(n)$ is between 0 and 1.
  - $\max_{ab} M_{ab} P_{ab}(n-1)$ = that from the first-visited neighbor of s to the starting node $= \langle M_{s\ell} P_{\ell\ell}(n-2) \rangle_{\ell \in \mathrm{n.n.}(s)}$
  - Time evolution of link accessibility :
    $W_{s\ell}(n=2) = \frac{1}{k_s} \frac{1/k_\ell}{\langle (1/k_j) \rangle_{j \in \mathrm{n.n.}(s)}} \simeq \frac{1}{k_s}$ increases to $W_{s\ell}(n \to \infty) = 1$.
    $W_{ij}(n)$ increases from 0 to 1 for $(j \to i)$ far from s.

Effective degree II

- Effective degree

$$\hat{k}_i(t) = \sum_j A_{ij} W_{ij}(n) = \sum_j A_{ij} \frac{\frac{1}{k_j} P_{js}(n-1)}{\langle \frac{1}{k_\ell} P_{\ell\ell}(n-2) \rangle_{\ell \in \mathrm{n.n.}(s)}}$$

increases from 0 or 1 to the full degree k_i.

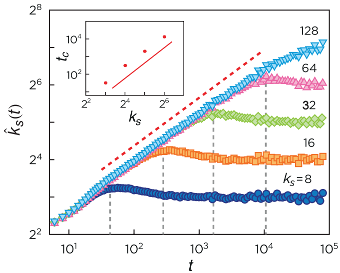
- Total number of effective links

$$2\hat{L}(n) = \sum_i \hat{k}_i(n) = \frac{1}{\langle \frac{1}{k_\ell} P_{\ell\ell}(n-2) \rangle_{\ell \in \mathrm{n.n.}(s)}} \simeq \frac{\langle k \rangle}{R(n-2)} \sim \begin{cases} n^{\frac{d_s}{2}} & (n \ll n_X) \\ 2L & (n \gg n_X) \end{cases}$$

- Occupation probability $P_{is}(n) = \frac{\hat{k}(n)}{2\hat{L}}$

Effective degree III

- Time evolution of the effective degree



- Simulations : $\hat{k}_s(n) \sim n^\theta$ for $n \ll n_c$ and $\hat{k}_s = k_s$ for $n \gg n_c$
- Local-stationary assumption: Link accessibilities $W_{ij}(n)$ are uniform for the links that have been passed $\rightarrow$ Effective degree distribution of the visited nodes $\tilde{P}_d(\hat{k}) \sim \hat{k}^{1-\gamma}$
- In case of the starting node being the hub node, the largest effective degree is that of the starting node $\hat{k}_s$, which satisfies $\int_{\hat{k}_s}^{\infty} \tilde{P}(\hat{k}) \sim 1/\hat{L}$ leading to $\hat{k}_s(n) \sim \hat{L}(n)^{\frac{1}{\gamma-1}}$.

- Scaling behavior of the effective degree

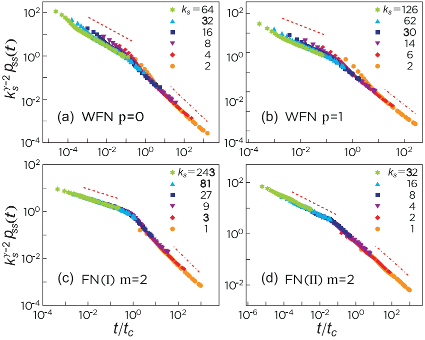
$$\hat{k}_s(n) \sim \begin{cases} n^{\frac{d_s}{2(\gamma-1)}} & (n \ll n_c) \\ k_s & (n \gg n_c) \end{cases} \quad \text{with } n_c \sim k_s^{\frac{2(\gamma-1)}{d_s}}$$

Crossover behavior of the return probability

- Considering the crossover scale $n_c \sim k_s^{\frac{2(\gamma-1)}{d_s}}$ for $\hat{k}_s(n)$ and $n_X \sim L^{\frac{2}{d_s}}$,

$$P_{ss}(n) \sim \begin{cases} n^{-\frac{d_s^{(h)}}{2}} & n \ll n_c \\ k_s n^{-\frac{d_s}{2}} & n_c \ll n \ll n_X \\ \frac{k_s}{2L} & n \gg n_X \end{cases}$$

with the hub spectral dimension $d_s^{(h)} = d_s \frac{\gamma-2}{\gamma-1}$



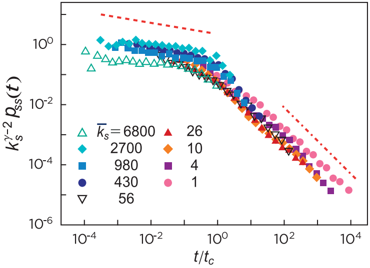


Figure: WWW: $\gamma \simeq 2.2$, $d_s \simeq 1.8$, $d_s^{(h)} \simeq 0.33$

Divergence of the generating function $\mathcal{P}_{ss}(z)$ around $z=1$ I

- Return probability for a specific node $\mathcal{F}_{ss}(1^-) = 1 - \frac{1}{\mathcal{P}_{ss}(1^-)}$
- The generating function for $\epsilon = 1 - z \to 0$,

$$\mathcal{P}_{ss}(z=1-\epsilon) \simeq \sum_n P_{ss}(n) e^{-\epsilon n} \sim$$
$$\int^{n_c} dn\, n^{-\frac{d_s^{(h)}}{2}} e^{-\epsilon n} + \int_{n_c}^{n_X} dn\, k_s n^{-\frac{d_s}{2}} e^{-\epsilon n} + \int^{\infty} dn\, \frac{k_s}{2L} e^{-\epsilon n}$$

- Divergence varies depending on ϵ, the spectral dimension d_s and the hub spectral dimension $d_s^{(h)} = d_s \frac{\gamma-1}{\gamma-2}$:
  1. The first integral diverges if $\min(n_c, \epsilon^{-1})$ is infinitely large and $d_s^{(h)} \leq 2$
  2. The second integral diverges i) if $\min(n_X, \epsilon^{-1})$ is infinitely large and $d_s \leq 2$ or ii) if $d_s > 2$ and $k_s n_c^{1-\frac{d_s}{2}}$ is infinitely large.
  3. The last integral diverges as $\frac{k_s}{2L\epsilon}$ if $\epsilon \ll k_s/(2L)$
  4. $d_s^{(h)} = d_s \frac{\gamma-2}{\gamma-1} = 2\frac{d_s}{d_c}$ with a critical dimension $d_c(\gamma) = 2\frac{\gamma-1}{\gamma-2}$.
  5. $d_s^{(h)} = 2 \Longleftrightarrow d_s = d_c > 2$
  6. $d_s^{(h)} < d_s$.

Divergence of the generating function $\mathcal{P}_{ss}(z)$ around $z = 1$ II

- Characteristic scales $\epsilon_c = n_c^{-1} \sim k_s^{-\frac{2}{d_s}(\gamma-1)}$, $\epsilon_X = n_X^{-1} \sim L^{\frac{-2}{d_s}}$
- $\alpha = (1 - \frac{2}{d})(\gamma - 1)$, which is smaller than 1 for $d < d_c$
- (I) $d_s < 2$:

$$\mathcal{P}_{ss}(z = 1 - \epsilon) \sim \begin{cases} \epsilon^{\frac{d_s^{(h)}}{2} - 1} + \mathrm{const.} & (\epsilon \gg \epsilon_c) \\ k_s \epsilon^{\frac{d_s}{2} - 1} + k_s^{1-\alpha} & (\epsilon_X \ll \epsilon \ll \epsilon_c) \\ \frac{k_s}{2L\epsilon} + k_s L^{\frac{2}{d_s} - 1} & (\epsilon \ll \epsilon_X) \end{cases}$$

- (II) $2 < d_s < d_c$:

$$\mathcal{P}_{ss}(z = 1 - \epsilon) \sim \begin{cases} \epsilon^{\frac{d_s^{(h)}}{2} - 1} + \mathrm{const.} & (\epsilon \gg \epsilon_c) \\ k_s^{1-\alpha} + k_s \epsilon^{\frac{d_s}{2} - 1} & (\epsilon_X \ll \epsilon \ll \epsilon_c) \\ k_s^{1-\alpha} + \frac{k_s}{2L\epsilon} & (\epsilon_* \ll \epsilon \ll \epsilon_X) \\ \frac{k_s}{2L\epsilon} + k_s^{1-\alpha} & (\epsilon \ll \epsilon_*) \end{cases}$$

Divergence of the generating function $\mathcal{P}_{ss}(z)$ around $z = 1$ III

- (III) $d_s > d_c$:

$$\mathcal{P}_{ss}(z = 1 - \epsilon) \sim \begin{cases} (\text{const.}) + \epsilon^{\frac{d_s^{(h)}}{2} - 1} & (\epsilon \gg \epsilon_c) \\ (\text{const.}) + k_s^{1-\alpha} + k_s \epsilon^{\frac{d_s}{2} - 1} & (\epsilon_X \ll \epsilon \ll \epsilon_c) \\ (\text{const.}) + k_s^{1-\alpha} + \frac{k_s}{2L\epsilon} & (\epsilon_* \ll \epsilon \ll \epsilon_X)) \\ (\text{const.}) + \frac{k_s}{2L\epsilon} + k_s^{1-\alpha} & (\epsilon_{**} \ll \epsilon \ll \epsilon_*) \\ \frac{k_s}{2L\epsilon} + (\text{const.}) + k_s^{1-\alpha} & (\epsilon \ll \epsilon_{**}) \end{cases}$$

- Another characteristic scale $n_* = \epsilon_*^{-1} \sim L k_s^{-\alpha}$ and $n_{**} = \epsilon_{**}^{-1} \sim L/k_s$.
- $(1 - z)|_{z=1^-} = \begin{cases} \epsilon_X \sim L^{-\frac{2}{d_s}} & (d_s < 2) \\ \epsilon_* \sim k_s^{\alpha}/L & (2 < d_s < d_c) \\ \epsilon_{**} \sim k_s/L & (d_s > d_c) \end{cases}$

Recurrent vs. transient on heterogeneous networks

- In the limit $N, L \to \infty$ and L/N finite
- With no dominant divergence but $k_s/(2L\epsilon)$, we consider the walk transient.
- Multiple divergence can be observed for the random walks on complex networks.
- (I) $d_s < 2$: the random walk is recurrent for all s in two modes:
  1. Trapping : For $\epsilon \simeq \epsilon_c = k_s^{-\frac{2}{d}(\gamma-1)}$, $\mathcal{P}_{ss}(z=1^-) \sim k_s^{1-\alpha}$ with $\alpha = (1-\frac{2}{d})(\gamma-1) < 0$. This diverges for k_s infinitely large, i.e., $k_s = O(L^\delta)$ with $\delta > 0$.
  2. Returning : At $\epsilon \simeq n_X^{-1} = L^{-\frac{2}{d_s}}$, $\mathcal{P}_{ss}(z=1^-) \sim k_s L^{\frac{2}{d_s}-1}$. This one diverges.
- (II) $2 < d_s < d_c$: the random walk is recurrent for hub starting nodes by trapping :
  1. Trapping: For $\epsilon_* \ll \epsilon \lesssim \epsilon_c$, $\mathcal{P}_{ss}(z=1^-) \sim k_s^{1-\alpha}$ with $0 < \alpha < 1$. This diverges for hub nodes of degree $k_s = O(L^\delta)$ with $\delta > 0$.
- (III) $d_s > d_c$: the random walk is transient for all s. $\alpha > 1$, No divergence.

All-to-one (Global) first-passage probability in networks

- We consider the first-passage probability from all possible starting nodes to a specific target node $F_{m\bullet}(n) = \sum_s \frac{k_s}{2L} F_{ms}(n)$
- weight $k_s/(2L) \rightarrow$ first-passage of the random walkers in the stationary state
- Using $\mathcal{F}_{ms}(z) = \frac{\mathcal{P}_{ms}(z)-\delta_{ms}}{\mathcal{P}_{mm}(z)}$, we find the generating function of $F_{m\bullet}(n)$ represented in terms of $\mathcal{P}_{mm}(z)$ as

$$\mathcal{F}_{m\bullet}(z) = \frac{k_m z}{2L(1-z)} \frac{1}{\mathcal{P}_{mm}(z)}$$

$$\mathcal{F}_{m\bullet}(z) = \frac{k_m}{2L}\left(1 - \frac{1}{\mathcal{P}_{mm}(z)}\right) + \sum_{i\neq m} \frac{k_i}{2L} \frac{\mathcal{P}_{mi}(z)}{\mathcal{P}_{mm}(z)} =$$
$$\frac{k_m}{2L}\left(1 - \frac{1}{\mathcal{P}_{mm}(z)}\right) + \sum_{i\neq m} \frac{k_m}{2L} \frac{\mathcal{P}_{im}(z)}{\mathcal{P}_{mm}(z)} = \frac{k_m z}{2L(1-z)} \frac{1}{\mathcal{P}_{mm}(z)}$$

Global mean first-passage time in networks

- $\langle T_m \rangle = \frac{d}{dz}\mathcal{F}_{m\bullet}(z)|_{z=1^-}$

  $\frac{d}{dz}\mathcal{F}_{m\bullet}(z) = \frac{k_m}{2L(1-z)\mathcal{P}_{mm}(z)} + 2L\, k_m\, z \frac{\mathcal{P}_{mm}(z)-(1-z)\mathcal{P}'_{mm}(z)}{\{2L\,(1-z)\,\mathcal{P}_{mm}(z)\}^2}$

  $\mathcal{P}_{mm}(z) = \frac{k_m}{2L\,(1-z)} +$ (weakly diverging part for $z \to 1$) $\Longrightarrow$

  $2L(1-z)\mathcal{P}_{mm}(z) \to k_m$ and $\mathcal{P}_{mm}(z) - (1-z)\mathcal{P}'_{mm}(z) = \mathcal{P}_{mm}(z) - \frac{k_m}{2L(1-z)}$

  $\mathcal{P}_{mm}(z) = \frac{k_m}{2L(1-z)} + \mathcal{P}^*_{mm}(z)$ with $\mathcal{P}^*_{mm}(z) \equiv \sum_n (P_{mm}(n) - \frac{k_m}{2L})$

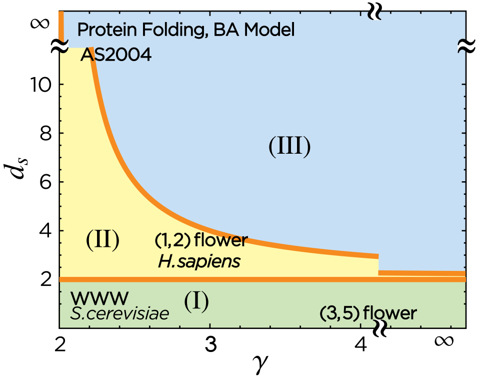
$$\langle T_m \rangle = \frac{2L}{k_m}\mathcal{P}^*_{mm}(1^-) + 1$$

- $$\mathcal{P}^*_{mm}(z=1^-) = \begin{cases} k_m L^{\frac{2}{d_s}-1} & (d_s < 2; z = 1-\epsilon_X) \\ k_m^{1-\alpha} & (2 < d_s < d_c; z = 1-\epsilon_*) \\ \text{const.} & (d_s > d_c; z = 1-\epsilon_{**}) \end{cases}$$

- GMFPT $$\langle T_m \rangle \sim \begin{cases} L^{\frac{2}{d_s}} & (d_s < 2) \\ L k_m^{-\alpha} & (2 < d_s < d_c) \\ L k_m^{-1} & (d_s > d_c) \end{cases}$$

Classification of networks according to the scaling of the GMFPT

- Scaling of $\langle T_m \rangle$ depends both on the spectral dimension d_s and the degree exponent γ
- With small γ (many hubs present), the GMFPT is reduced to $L^{\frac{2}{d_s}} \ll L$ at the hub node of the largest degree $k_m \sim L^{\frac{1}{\gamma-1}}$ in the networks of $2 < d_s < d_c = 2\frac{\gamma-1}{\gamma-2}$.



Exploration and trapping

Mean number of visited sites

- Start at site s
- The number of distinct sites visited in the first n steps of the walk $S_s(n)$
- How fast does $S_s(n)$ grows with n?
- $S_s(n) = \sum_{n'=0}^{n} D_s(n')$ with $D_s(n) = 1$ if the walker arrives at a virgin site and 0 otherwise.
- The mean number of distinct visited sites $\langle S_s(n)\rangle = \sum_{n'=0}^{n} \langle D_s(n')\rangle$
- $\langle D_s(n)\rangle$ = Prob.($D_s(n) = 1$)

Theorem (Lemma of Dvoretzky and Erdös)

For homogeneous lattice walks, $\lim_{n\to\infty}\langle D_s(n)\rangle = 1 - R$ *with the return probability* $R = \mathcal{F}_{ss}(1^-) = 1 - \frac{1}{\mathcal{P}_{ss}(1^-)}$.

leading to

$$\langle S_s(n)\rangle \sim (1-R)n \text{ for } n \to \infty$$

Relation between $\langle S_s(n)\rangle$ and the first-passage probability

- The probability to arrive at a virgin site at the nth step: $\langle D_s(n)\rangle = \sum_{i\neq s} F_{is}(n)$ for $n \geq 1$ and $D_s(0) = 1$.
- $\langle S_s(n)\rangle = \sum_{n'=0}^{n} \langle D_s(n')\rangle = 1 + \sum_{i\neq s}\sum_{n'=1}^{n} F_{is}(n')$
- Generating function of $\langle D_s(n)\rangle - \delta_{n,0}$: $\mathcal{D}_s(z) = \sum_{i\neq s} \mathcal{F}_{is}(z) = \sum_{i\neq s} \frac{\mathcal{P}_{is}(z)}{\mathcal{P}_{ii}(z)} = -1 + \sum_i \frac{\mathcal{P}_{is}(z)}{\mathcal{P}_{ii}(z)}$
- Generating function of $\langle S_s(n)\rangle$:

$$\mathcal{S}_s(z) = \frac{1}{1-z}\sum_i \frac{\mathcal{P}_{is}(z)}{\mathcal{P}_{ii}(z)}$$

$\mathcal{S}_s(z) = \sum_n \langle S_s(n)\rangle z^n = \sum_{n=0}^{\infty}\sum_{n'=0}^{n} \langle D_s(n')\rangle z^n = \sum_{n'=0}^{\infty} \langle D(n')\rangle \sum_{n=n'}^{\infty} z^n = \sum_{n'=0}^{\infty} \langle D(n')\rangle \frac{z^{n'}}{1-z} = \frac{1}{1-z}\{1 + \mathcal{D}_s(z)\} = \frac{1}{1-z}\sum_i \frac{\mathcal{P}_{is}(z)}{\mathcal{P}_{ii}(z)}$

Mean number of visited sites in the infinite lattice

- For homogeneous lattice walks, $\mathcal{P}_{ii}(z) = \mathcal{P}_{ss}(z)$, leading to $\mathcal{D}_s(z) = -1 + \frac{1}{(1-z)\mathcal{P}_{ss}(z)}$ and $\mathcal{S}_s(z) = \frac{1}{(1-z)^2\mathcal{P}_{ss}(z)}$
- Singularity of $\mathcal{S}_s(z)$ as $z \to 1$?
- For homogeneous lattice walks in d dimension,

$$\mathcal{P}_{ss}(z) \simeq \begin{cases} \frac{1}{1-R} & (d > 2) \\ \ln\left(\frac{1}{1-z}\right) & (d = 2) \\ (1-z)^{\frac{d}{2}-1} & (d < 2) \end{cases}$$

- $$\mathcal{S}_s(z) \simeq \begin{cases} \frac{1-R}{(1-z)^2} & (d > 2) \\ \frac{1}{(1-z)^2 \ln\left(\frac{1}{1-z}\right)} & (d = 2) \\ (1-z)^{-\frac{d}{2}-1} & (d < 2) \end{cases}$$
- For $n \to \infty$, $S_s(n) \simeq \begin{cases} (1-R)n & (d > 2) \\ \frac{n}{\ln n} & (d = 2) \\ n^{\frac{d}{2}} & (d < 2) \end{cases}$

The Rosenstock Trapping model

- To model the decrease of the uv-light-irradiated luminescence of the crystals that are first damaged by bombardment with high-energy radiation, Rosenstock proposed a model that a quantum (particle) of energy perform a random walk over molecules until it is absorbed by q fraction of 'bad' molecules that can absorb it or it is emitted as luminescence (1961).
- The survival probability $\phi(n)$: the probability the walker makes at least n steps

$$\phi(n) = \sum_{s=1}^{\infty}(1-q)^s \mathrm{Prob.}(S(n) = s) = \langle (1-q)^{S(n)} \rangle$$

which is the generating function of the probability distribution of the number of distinct visited sites.

Rosenstock (RS) approximation

- A lower bound of the survival probability: $\phi(n) \geq (1-q)^{\langle S(n)\rangle}$ (Jensen's inequality for convex functions)
- Rosenstock (RS) approximation :

$$\phi_{\mathrm{RS}}(n) = (1-q)^{\langle S(n)\rangle}$$

- RS is valid for small q and n : early-time behavior of $\phi(n)$:
  Cumulant expansion:
  $\phi(n) = \exp\left[\ln(1-q)\langle S(n)\rangle + \frac{(\ln(1-q))^2}{2}\sigma^2_{S(n)} + O((\ln(1-q))^3)\right] \simeq (1-q)^{\langle S(n)\rangle} e^{\frac{(\ln(1-q))^2}{2}\sigma^2_{S(n)}}$
- $d=1$: $\langle S(n)\rangle \sim n^{1/2} \to \phi_{\mathrm{RS}}(n) \sim e^{-(\mathrm{const.})q\, n^{1/2}}$
- $d=2$: $\langle S(n)\rangle \sim \frac{n}{\ln n} \to \phi_{\mathrm{RS}}(n) \sim e^{-(\mathrm{const.})q\, \frac{n}{\ln n}}$
- $d=3$: $\langle S(n)\rangle \simeq (1-R)n \to \phi_{\mathrm{RS}}(n) \sim e^{-q(1-R)n}$

Mean lifetime

- $n^\dagger$: the number of steps on which trapping occurs.
- $\mathrm{Prob.}(n^\dagger = n) = \phi(n-1) - \phi(n)$
- Mean lifetime
  $\langle n^\dagger \rangle = \sum_{n=0}^{\infty} n \, \mathrm{Prob.}(n^\dagger = n) = \sum_n n\{\phi(n-1) - \phi(n)\} = \sum_{n=0}^{\infty} \phi(n)$
  average over walk trajectories and trap realizations
- A lower bound : $\langle n^\dagger \rangle \geq \sum_n (1-q)^{\langle S(n) \rangle}$
- Rosenstock approximation $\langle n^\dagger \rangle \simeq \langle n^\dagger \rangle_{\mathrm{RS}} = \sum_n (1-q)^{\langle S(n) \rangle}$
- $d = 1$: $\langle n^\dagger \rangle_{\mathrm{RS}} \sim \int dn \, e^{-q\, n^{1/2}} \sim q^{-2}$
- $d = 2$: $\langle n^\dagger \rangle_{\mathrm{RS}} \sim \int dn \, e^{-q \frac{n}{\ln n}} \sim \frac{1}{q} \ln \left(\frac{1}{q} \right)$
- $d = 3$: $\langle n^\dagger \rangle_{\mathrm{RS}} \sim \int dn \, e^{-q(1-R)n} \sim \frac{1}{(1-R)q}$

The Rosenstock Trapping model on 1d lattice

- Exact mean lifetime in 1d
  - Probability that the closest traps are ℓ units away to the left and r units away to the right of the starting site $f(\ell, r) = q^2(1-q)^{\ell-1}(1-q)^{r-1}$
  - Mean lifetime $\langle n^\dagger(\ell, r)\rangle = \ell r$ for given ℓ and r
  - Average over ℓ and r : $\langle n^\dagger\rangle = \sum_{\ell=1}^{\infty}\sum_{r=1}^{\infty} \ell\, r\, f(\ell, r) = 1/q^2$.
- Survival probability in 1d
  $\phi(n) = \sum_{\ell=1}^{\infty}\sum_{r=1}^{\infty} \phi(n; \ell, r) f(\ell, r)$
  - The conditional survival probability for large n
    $\phi(n; \ell, r) \sim P_{-\ell<x<r}(n) = \sum_{\mu>0} e^{-\mu n}\langle(-\ell, r)|\mu\rangle\langle\mu|0\rangle \sim e^{-\mu_2 n}$
    with $\mu_2 \propto (\ell + r)^{-2}$ the smallest positive eigenvalue of the Laplacian $\tilde{L}$
  - Then we see

$$\phi(n) \sim \sum_{\ell,r} q^2 \exp\left\{-(\mathrm{const.})\frac{n}{(\ell+r)^2} - q(\ell+r)\right\} \sim_{\ell+r=x}$$
$$q^2 \int x\,dx\, e^{-(\mathrm{const.})\frac{n}{x^2} - q\,x} \sim_{x_*\sim(n/q)^{1/3}} q\, n^{1/2} \exp(-(\mathrm{const.}) q^{2/3} n^{1/3})$$

The long-time behavior of the survival probability: Donsker-Varadhan (DV) limit I

Theorem (Theorem of Donsker and Varadhan)

For random walks on d-dimensional lattices of N nodes, $\lim_{n\to\infty} \frac{1}{n^{d/(d+2)}} \ln\langle e^{-KS(n)}\rangle = -K^{2/(d+2)} \left(\frac{d+2}{2}\right) \left(\frac{2a}{d}\right)^{\frac{d}{d+2}}$ *with the infimum of the second smallest eigenvalue of the Laplacian matrix* $\mu_2 \simeq a\, N^{-2/d}$

Grassberger and Procaccia's argument (1982) according to Barkema *et al.* in PRL 87, 170601 (2001)

Consider rare but large trap-free regions where walkers can survive for a long time. With increasing time ever larger trap-free regions become dominant; the probability of finding such regions decreases exponentially with their d-dimensional volume, but the decay rate of particles moving within such a region is inversely proportional to the square of its diameter. The optimal choice of this diameter gives rise to the stretched exponential behavior

The long-time behavior of the survival probability: Donsker-Varadhan (DV) limit II

- $\phi(n) = \langle e^{-KS(n)} \rangle$ with e^{-K} the probability that a site is trap-free.
- Probability of finding trap-free region of volume V : $P(V) = e^{-K\,V}$
- Probability to survive in the region of volume V until the n'th step : $\phi(n;V) = \sum_\mu e^{-\mu n} \langle V|\mu\rangle\langle\mu|0\rangle \sim e^{-\mu_2 n}$ with $\mu_2 \simeq a\,V^{-2/d}$ under the boundary condition $\phi(n;V) = 0$ on the boundary of V. a is a constant.
- $\phi(n) = \sum_V P(V)\phi(n;V) \sim \sum_V \exp\left(-KV - a\,n\,V^{-2/d}\right)$
- valid in the long-time limit

Crossover from the RS to the DV behaviors I

- q small
- RS for n small and DV for n large
- $d = 1$: $-\ln\phi(n) \sim \begin{cases} q\, n^{1/2} & (n \ll n_1) \\ q^{2/3}\, n^{1/3} & (n \gg n_1) \end{cases} = \Psi_{1d}(q^2 n)$ with

  $\Psi_{1d}(x) \sim \begin{cases} x^{1/2} & (x \ll 1) \\ x^{1/3} & (x \gg 1) \end{cases}$
- $d = 2$: $-\ln\phi(n) \sim \begin{cases} q\, \frac{n}{\ln n} & (n \ll n_2) \\ q^{1/2}\, n^{1/2} & (n \gg n_2) \end{cases} = \ln n\, \Psi_{2d}(\sqrt{q\, n}/\ln n)$ with

  $\Psi_{2d}(x) \sim \begin{cases} x^{2} & (x \ll 1) \\ x^{1} & (x \gg 1) \end{cases}$

Crossover from the RS to the DV behaviors II

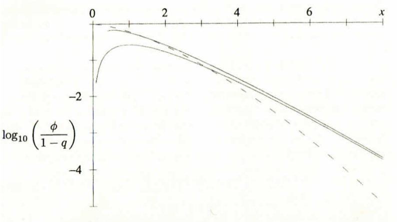


FIG. 6.1. Asymptotic solution of Rosenstock's trapping model for a one-dimensional Pólya walk. We show here three approximations for the survival probability ϕ_n, with $\log_{10}\phi_n/(1-q)$ plotted as a function of $x=\{\pi\log[(1-q)^{-1}]\}^{2/3}n^{1/3}$. The broken line is the large-x form of Rosenstock's approximation (6.310), in the limit of small q so that the factor of $(1-q)$ in the denominator of Eq. (6.310) can be discarded. The lower continuous curve corresponds to the asymptotic form (6.299) established in Anlauf's theorem, while the upper continuous curve corresponds to the 4-term expansion (6.308).

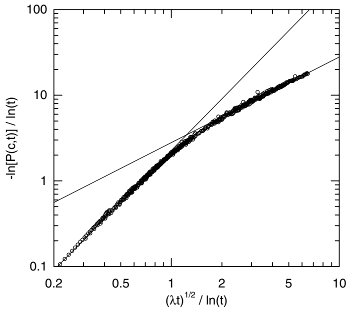


FIG. 3. Collapse of the two-dimensional data: $-\ln[P(c,t)]/\ln(t)$ is plotted as a function of $\sqrt{\lambda t}/\ln(t)$ in a double-logarithmic plot. The solid lines are fits to the data, with slopes 2 and 1. They cross at the point (1.13, 3.5).

Figure: (left) $d=1$ (Hughes, 1995) (right) $d=2$ (Barkema et al., 2001)

Trapping in complex networks I

- KIttas, Carmi, Havlin, and Argyrakis, EPL 84, 40008 (2008).
- Random walk with a number of traps on the largest connected components of the SF networks generated by the Molloy-Reed algorithm for the degree $m \leq k \leq N-1$ with the degree exponent γ.
- The survival probability $\phi(t)$ at a time t depends on the number of nodes N, the fraction of traps q, and the mean connectivity $\langle k \rangle = 2L/N$.
- Mean-field equation $d\phi/dt = -(\mathrm{const.})\phi K/2L$ with K the total number of links incident on the trap nodes, leading to $\phi(t) = \phi(0)e^{-(\mathrm{const.})\frac{K}{2L}t}$
- Corresponding to the RS approximation: $\phi(t) \sim e^{-q(1-R)t}$ with $q = K/(2L)$.
- Simulation results are consistent with the theoretical prediction

Trapping in complex networks II

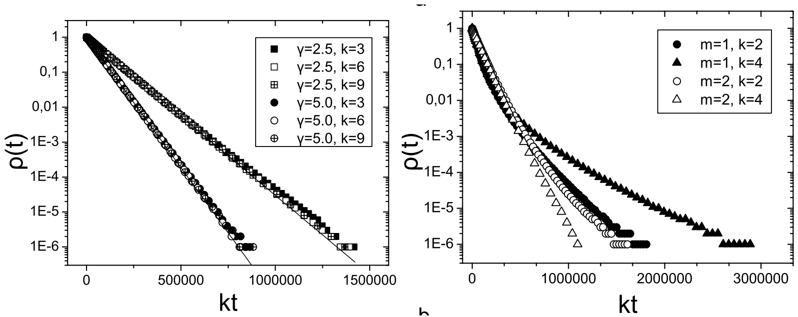


Figure: (left) $\phi(t)$ for $N = 10^4, \gamma = 2.5, m = 3$ and 5 and a single trap on a node of degree k. (b) same as (a) but with $m = 1$ and 2.

Epidemic spreading

Epidemic models

- An individual is in one of three states $X =$ susceptible (S), infectious (I), and recovered (R).
- A population of N individuals is divided into different classes depending on the stage of the disease:
- S, I, R may denote the number of individuals in the corresponding states and $S + I + R = N$.
- 1) spontaneous transition from a state to another such as $I \to R$ or $I \to S$
  2) Contagion of a susceptible individual in interaction with an infectious one $S + I \to 2I$
- SI model: S and I only: $S + I \to 2I$ with the infection rate λ only
- SIS model: S and I only: $S + I \to 2I$ with rate λ and $I \to S$ with rate μ
- SIR model: S, I, and R: $S + I \to 2I$ with rate λ, $I \to R$ with rate μ

Evolution of the number of susceptible, infectious, and recovered individuals I

- The state of an individual j at time t : $x_j(t)$
- We are interested in the ensemble-averaged fraction of each class of individuals: $X(t) = \langle \sum_{j=1}^{N} \delta_{x_j(t),X} \rangle$ with $X = S, I, R$.
- The probability of an individual j to be in state X at time t : $P_j^{(X)}(t) = \langle \delta_{x_j(t),X} \rangle$
- Transition rate of an individual j in a state X to Y at time t: $W_j^{(X \to Y)}(t)$
- SI model:

$$\frac{dI(t)}{dt} = \sum_{j=1}^{N} P_j^{(S)}(t)\, W_j^{(S \to I)}(t),\ S(t) = N - I(t).$$

- SIS model:

$$\frac{dI(t)}{dt} = \sum_{j=1}^{N} \left\{ P_j^{(S)}(t)\, W_j^{(S \to I)}(t) - P_j^{(I)}(t)\, W_j^{(I \to S)}(t) \right\},\ S(t) = N - I(t)$$

Evolution of the number of susceptible, infectious, and recovered individuals II

- SIR model:

$$\frac{dI(t)}{dt} = \sum_{j=1}^{N} \left\{ P_j^{(S)}(t)\, W_j^{(S\to I)}(t) - P_j^{(I)}(t)\, W_j^{(I\to R)}(t) \right\},$$
$$\frac{dS(t)}{dt} = -\sum_{j=1}^{N} P_j^{(S)}(t)\, W_j^{(S\to I)}(t),$$
$$\frac{dR(t)}{dt} = \sum_{j=1}^{N} P_j^{(I)}(t)\, W_j^{(I\to R)}(t)$$

- Transition rates

$W_j^{(S\to I)}(t) = P_j^{(S)}(t)^{-1} \sum_{x_{j_1}, x_{j_2}, \ldots, x_{j_k}} P_j^{(x_j = S, x_{j_1}, x_{j_2}, \ldots, x_{j_k})}(t) \lambda \sum_{\ell=1}^{k} \delta_{x_{j_\ell}, I}$ with

$A_{j\, j_\ell} = 1$ for $\ell = 1, 2, \ldots, k$,

$W_j^{(I\to S)}(t) = \mu$,

$W_j^{(I\to R)}(t) = \mu$

Mean-field approach

- Homogeneous network: all nodes have k neighbors
- Assumptions:
  1. Assume no fluctuations from node to node: all nodes are statistically equivalent: $P_j^{(X)}(t) = P^{(X)}(t) = \frac{X(t)}{N}$: $i(t) = \frac{I(t)}{N}, s(t) = \frac{S(t)}{N}, r(t) = \frac{R(t)}{N}$
  2. Assume no dynamical correlations between the states of different nodes: $P_j^{(x_j=S, x_{j_1}, x_{j_2}, \dots, x_{j_k})}(t) = P_j^{(S)}(t) \prod_{\ell=1}^{k} P_{j_\ell}^{(x_{j_\ell})}(t)$
- Then the transition rates are represented as

$$W_j^{(S\to I)}(t) = \lambda \sum_{\ell=1}^{N} A_{j\ell} \left(\sum_X P_\ell^{(X)} \delta_{X,I} \right) = \lambda \sum_{\ell=1}^{N} A_{j\ell} P_\ell^{(I)} = \lambda\, k_j \frac{I(t)}{N} = \lambda\, k_j\, i(t)$$

Time evolution in the mean-field approach I

- SI model:

$$\frac{di(t)}{dt} = s(t)\lambda\, k\, i(t) = \lambda\, k\, i(t)\{1 - i(t)\} \to i(t) = \frac{i(0)e^{t/\tau}}{1+i(0)(e^{t/\tau}-1)} \text{ with } \tau = \frac{1/k}{\lambda}$$

- SIS model:

$$\frac{di(t)}{dt} = s(t)\lambda\, k\, i(t) - \mu\, i(t) = (\lambda\, k - \mu)\, i(t) - \lambda\, k\, i(t)^2 \to i(t) = \frac{B}{1+(\frac{B}{i(0)}-1)e^{-t/\tau}}$$

$$\text{with } \tau^{-1} = \lambda\, k - \mu \text{ and } B = \frac{1}{\tau\,\lambda\, k} = 1 - \frac{\mu}{\lambda k}$$

- Epidemic threshold: $\tau > 0 (\tau < 0)$ if the infection rate $\lambda\, k$ is larger (smaller) than the recovery rate μ.
- Long-time limit $(t/|\tau| \to \infty)$: $i(\infty) = \begin{cases} B = 1 - \frac{\mu}{\lambda k} & (\lambda\, k > \mu) \\ 0 & (\lambda k < \mu) \end{cases}$
- Early-time regime $(t/\tau \to 0)$, $i(t) \simeq i(0)\left\{1 + t\left(\frac{1}{\tau} - \lambda\, k\, i(0)\right)\right\}$
- Case of $\tau = 0$: $i(t) = \frac{i(0)}{1+i(0)\,\lambda\, k\, t}$

Time evolution in the mean-field approach II

- SIR model:

$$\frac{di(t)}{dt} = \lambda\, k\, s(t)\, i(t) - \mu\, i(t).$$

  - Epidemic threshold: As $s(t) \simeq 1$ initially, whether λk is larger or smaller than μ determines the early-time spread of the considered disease.

Heterogeneous mean-field approach

- Nodes have varying numbers of neighbors k in scale-free networks.
- Assumptions:
  1. No structural or dynamical fluctuations in the set of nodes with the same degree : all nodes with the same degree are statistically equivalent: $P_j^{(X)}(t) = P_{k_j=k}^{(X)}(t) = \frac{X_k(t)}{N_k}$: $i_k(t) = \frac{I_k(t)}{N_k}, s_k(t) = \frac{S_k(t)}{N_k}, r_k(t) = \frac{R_k(t)}{N_k}$ with N_k the number of nodes of degree k
  2. No dynamical correlations between the states of different nodes: $P_j^{(x_j=S,x_{j_1},x_{j_2},\dots,x_{j_k})}(t) = P_j^{(S)}(t)\prod_{\ell=1}^{k} P_{j_\ell}^{(x_{j_\ell})}(t) = P_{k_j}^{(S)}(t)\prod_{\ell=1}^{k} P_{k_{j_\ell}}^{(x_{j_\ell})}(t)$
- Then the transition rates are represented as

$$W_j^{(S\to I)}(t) = \lambda \sum_{\ell=1}^{N} A_{j\ell}\left(\sum_X P_\ell^{(X)}\delta_{X,I}\right) = \lambda \sum_{\ell=1}^{N} A_{j\ell}P_\ell^{(I)} = \lambda k_j \Theta_{k_j}(t) \text{ with}$$

$$\Theta_{k_j}(t) = k_j^{-1}\sum_{\ell=1}^{N} A_{j\ell}P_\ell^{(I)}(t) = \sum_{k'} P(k'|k_j)P_{k'}^{(I)} = \sum_{k'} P(k'|k_j) i_{k'}(t) \text{ with}$$

$$P(k'|k) = \frac{\sum_{\ell=1}^{n}\delta_{k_\ell,k}\sum_{\ell'=1}^{N} A_{\ell\ell'}\delta_{k_{\ell'},k'}}{\sum_{\ell=1}^{n}\delta_{k_\ell,k}\sum_{\ell'=1}^{N} A_{\ell\ell'}}$$

- No degree-degree correlations assumed $\rightarrow A_{\ell\ell'} = \frac{k_\ell k_{\ell'}}{2L} \rightarrow P(k'|k) = \frac{k' P_d(k')}{\langle k\rangle}$

Time evolution in the SI model in the heterogeneous mean-field approach

- SI model :

$$\frac{di_k(t)}{dt} = s_k(t)\lambda\, k\, \Theta_k(t) = \lambda\, k\, \{1 - i_k(t)\}\Theta_k(t) \text{ with}$$
$$\Theta_k(t) = \Theta(t) = \sum_{k'} \frac{k' P_d(k')}{\langle k \rangle} i_{k'}(t)$$

- Early-time regime $(i(t) \ll 1)$: $\frac{di_k(t)}{dt} = \lambda\, k\Theta(t)$ with
$\frac{d\Theta(t)}{dt} = \sum_{k'} \frac{k' P_d(k')}{\langle k \rangle} \frac{di_{k'}(t)}{dt} = \sum_{k'} \frac{k' P_d(k')}{\langle k \rangle} \lambda k' \Theta(t) = \lambda \frac{\langle k^2 \rangle}{\langle k \rangle} \Theta(t)$
  - The probability of a neighbor to be infected $\Theta(t) = i(0)e^{t/\tau}$ with the characteristic time scale $\tau = \frac{\langle k \rangle / \langle k^2 \rangle}{\lambda}$ increases with time exponentially in the initial stage
  - Growth time scale τ is related to the network heterogeneity such that τ goes to zero (fast spread of infection) in strongly heterogeneous networks.
  - $i_k(t) = i_k(0) \left\{ 1 + \frac{k \langle k \rangle}{\langle k^2 \rangle} (e^{t/\tau} - 1) \right\}$
  - $i(t) = \sum_k i_k(t) = i(0) \left\{ 1 + \frac{\langle k \rangle^2}{\langle k^2 \rangle} (e^{t/\tau} - 1) \right\}$

Time evolution in the SIS model in the heterogeneous mean-field approach I

- SIS model:

$$\frac{di_k(t)}{dt} = s_k(t)\lambda\, k\, \Theta(t) - \mu\, i_k(t) = \lambda\, k\, (1 - i_k(t))\, \Theta(t) - \mu\, i_k(t) \text{ with}$$
$$\Theta_k(t) = \Theta(t) = \sum_{k'} \frac{k' P_d(k')}{\langle k \rangle} i_{k'}(t)$$

- Early-time regime $(i(t) \ll 1)$: $\frac{di_k(t)}{dt} = \lambda\, k\Theta(t) - \mu\, i_k(t)$ $\frac{d\Theta(t)}{dt} = \sum_{k'} \frac{k' P_d(k')}{\langle k \rangle} \frac{di_{k'}(t)}{dt} = \sum_{k'} \frac{k' P_d(k')}{\langle k \rangle} \{\lambda k' \Theta(t) - \mu\, i_{k'}(t)\} = \left\{\lambda \frac{\langle k^2 \rangle}{\langle k \rangle} - \mu\right\} \Theta(t)$
    - Epidemic threshold : $\Theta(t) = i(0) e^{t/\tau}$ with $\tau = \frac{\langle k \rangle / \langle k^2 \rangle}{\lambda - \lambda_c}$ with $\lambda_c = \mu \frac{\langle k \rangle}{\langle k^2 \rangle}$
    - For $\lambda > \lambda_c (\lambda < \lambda_c)$, local infection may spread (decay) exponentially.
    - The epidemic threshold λ_c becomes zero for $\gamma < 3$.
- Long-time limit $(i_k(t) = \text{const.})$: $\frac{di_k(t)}{dt} = \lambda\, k(1 - i_k)\Theta - \mu\, i_k = 0 \rightarrow$ $i_k = \frac{\lambda\, k\, \Theta}{\mu + \lambda\, k\, \Theta} \rightarrow$

Time evolution in the SIS model in the heterogeneous mean-field approach II

- Self-consistent equation

$$\Theta = \sum_k \frac{kP_d(k)}{\langle k \rangle} \frac{\lambda\, k\, \Theta}{\mu + \lambda\, k\, \Theta} \tag{2}$$

- A non-zero solution for Θ exists when the right-hand-side, which increases with Θ as a function of Θ from 0 to a constant smaller than 1, has its derivative larger than 1 at $\Theta = 0$.
- Let $y(\Theta)$ be the right-hand-side of Eq. (2)
- For $\Theta k_{\mathrm{max}} \ll 1$, $y(\Theta) \simeq \frac{\lambda}{\mu} \frac{\langle k^2 \rangle}{\langle k \rangle} \Theta \left\{1 + O(k_{\mathrm{max}} \Theta)\right\}$, which shows that the threshold distinguishing $\Theta > 0$ and $\Theta = 0$ is equal to $\lambda_c = \mu \langle k \rangle / \langle k^2 \rangle$.

Time evolution in the SIS model in the heterogeneous mean-field approach III

- The behavior of Θ as a function of λ close to λ_c can be obtained by analyzing the behavior of $y(\Theta)$ for $\Theta \ll 1$ and $k_{\max}\Theta \gg 1$, which is

$$y(\Theta) \sim \begin{cases} \frac{\lambda}{\lambda_c}\Theta - \frac{\langle k^3\rangle}{\langle k\rangle}\left(\frac{\lambda}{\mu}\right)^2 \Theta^2 + \cdots & (\gamma > 4) \\ \frac{\lambda}{\lambda_c}\Theta - (\text{const.})\left(\frac{\lambda}{\mu}\right)^{\gamma-2} \Theta^{\gamma-2} & (3 < \gamma < 4) \\ \text{const.}\left(\frac{\lambda}{\mu}\right)^{\gamma-2} \Theta^{\gamma-2} & (2 < \gamma < 3) \end{cases} \quad \text{leading to}$$

$$i(t) \sim \Theta \sim \begin{cases} \lambda - \lambda_c & (\gamma > 4) \\ (\lambda - \lambda_c)^{\frac{1}{\gamma-3}} & (3 < \gamma < 4) \\ \lambda^{\frac{1}{3-\gamma}} & (2 < \gamma < 3) \end{cases}$$

Time evolution in the SIR model in the heterogeneous mean-field approach I

- SIR model:

$$\frac{di_k(t)}{dt} = s_k(t)\lambda\, k\,\Theta(t) - \mu\, i_k(t)$$
$$\frac{ds_k(t)}{dt} = -\lambda\, k\, s_k(t)\Theta(t)$$
$$\frac{dr_k(t)}{dt} = \mu\, i_k(t) \text{ with } \Theta_k(t) = \Theta(t) = \sum_{k'} \frac{k' P_d(k')}{\langle k\rangle} i_{k'}(t)$$
$$s_k(t) = e^{-\lambda\, k\, \phi(t)} \text{ with}$$
$$\phi(t) = \int_0^t dt'\, \Theta(t') = \sum_k \frac{kP_d(k)}{\langle k\rangle} \int_0^t dt'\, i_k(t') = \mu^{-1} \sum_k \frac{kP_d(k)}{\langle k\rangle} r_k(t)$$

- Initial condition: $i_k(0) \to 0, s_k(0) \simeq 1, r_k(0) = 0$.
- Early-time regime $(i(t) \ll 1, r(t) \ll 1)$: same as in the SIS model characterized by the same epidemic threshold $\lambda_c = \mu\frac{\langle k\rangle}{\langle k^2\rangle}$
- Long-time limit: $i_k(\infty) \to 0, s_k(\infty) + r_k(\infty) = 1$,

Time evolution in the SIR model in the heterogeneous mean-field approach II

- Self-consistent equation for $t \to \infty$

$$\begin{aligned}\Theta &= \sum_k \frac{kP_d(k)}{\langle k \rangle}\{1 - r_k - s_k\} \\ &= 1 - \mu\phi - \sum_k \frac{kP_d(k)}{\langle k \rangle} e^{-\lambda\, k\, \phi} = 0 \end{aligned} \tag{3}$$

- $r = \sum_k P_d(k) r_k = \sum_k P_d(k)(1 - e^{-\lambda\, k\, \phi})$ represents the fraction of individuals who have been infected, which is positive if $\phi > 0$.
- Rearranging Eq. (3) as $\phi = y(\phi)$ with $y(\phi) = \mu^{-1} \sum_k \frac{kP_d(k)}{\langle k \rangle}(1 - e^{-\lambda\, k\, \phi})$, we find that for $\phi\, k_{\max} \ll 1$, $y(\phi) \simeq \frac{\lambda}{\mu}\frac{\langle k^2 \rangle}{\langle k \rangle}\phi - \frac{1}{2}\frac{\lambda^2}{\mu}\frac{\langle k^3 \rangle}{\langle k \rangle}\phi^2 + \cdots$ giving the same threshold $\lambda_c = \mu\frac{\langle k \rangle}{\langle k^2 \rangle}$

Time evolution in the SIR model in the heterogeneous mean-field approach III

- The behavior of ϕ as a function of λ close to λ_c is obtained by the behavior of $y(\phi)$ for $\phi \ll 1$ and $k_{\max}\phi \gg 1$, which is

$$y(\phi) \sim \begin{cases} \frac{\lambda}{\lambda_c}\phi - \frac{1}{2}\frac{\lambda^2}{\mu}\frac{\langle k^3\rangle}{\langle k\rangle}\phi^2 + \cdots & (\gamma > 4) \\ \frac{\lambda}{\lambda_c}\phi - (\text{const.})\frac{\lambda^{\gamma-2}}{\mu}\phi^{\gamma-2} & (3 < \gamma < 4) \\ \text{const.}\frac{\lambda^{\gamma-2}}{\mu}\phi^{\gamma-2} & (2 < \gamma < 3) \end{cases}$$ leading to

$$r \sim \phi \sim \begin{cases} \lambda - \lambda_c & (\gamma > 4) \\ (\lambda - \lambda_c)^{\frac{1}{\gamma-3}} & (3 < \gamma < 4) \\ \lambda^{\frac{1}{3-\gamma}} & (2 < \gamma < 3) \end{cases}$$

SIS model in the quenched mean-field approach I

- SIS in a given network is considered
- The adjacency matrix A_{ij} is NOT replaced by any probabilistic quantity but preserved in the time evolution equation
- Assumption: No dynamical correlations between the states of different nodes
- The transition probability

$$W_j^{(S\to I)}(t) = \lambda \sum_{\ell=1}^{N} A_{j\ell}\, i_\ell(t)$$

- Evolution of the number of infectious individuals

$$\frac{di_j(t)}{dt} = -\mu\, i_j(t) + \lambda\{1 - i_j(t)\} \sum_\ell A_{j\ell}\, i_\ell(t)$$

- Early-time regime ($i(t) \ll 1$):

$$\frac{di_j(t)}{dt} = -\mu\, i_j(t) + \lambda \sum_\ell A_{j\ell}\, i_\ell(t)$$

SIS model in the quenched mean-field approach II

- With the eigenvalues $\{\Lambda_n | 1 \leq n \leq N\}$'s and the eigenvectors $\{|n\rangle | n = 1, 2, \ldots, N\}$'s of the adjacency matrix A, we find that $i_j(t) = \sum_{n=1}^{N} e^{(\lambda\Lambda_n - \mu)t} \langle j|n\rangle\langle n|i(0)\rangle$.
- If the largest eigenvalue Λ_N satisfies $\lambda\Lambda_N - \mu > 0$, the number of infectious individuals may increase exponentially with time in the early-time regime.
- Epidemic threshold $\lambda_c = \frac{\mu}{\Lambda_N}$
- $\Lambda_N \sim \max\{k_{\max}^{3-\gamma}, k_{\max}^{1/2}\}$ implying $\lambda_c = 0$ for all networks with $k_{\max} \to \infty$
- λ_c from the HMF is not zero but positive.

Dynamical fluctuations in the SIS model I

- Issue: $\lambda_c = 0$ or > 0 in case of $\gamma > 3$
- H.K. Lee, P.-S. Shim, and J.D. Noh, PRE (2013)
  - The modes corresponding to the large eigenvalues of A represents the infection of hubs and their neighbors.
  - For given λ, the eigenmodes satisfying $\lambda\Lambda - \mu > 0$ are activated around the hubs of degree $k > (\mu/\lambda)^2$.
  - Each of those local hub infections will be terminated by all the local infected nodes accidentally becoming susceptible, unless distinct hub infections reinfect one another.
  - Characteristic healing time scale of V infected nodes: $\tau_V \sim e^{a\,V}$
  - In 'unclustered' networks where hubs are sufficiently far from each other, like the (u, v) flower networks, $i(t) \sim \int_{1/\lambda^2}^{\infty} dk\,(\lambda\,k)\,P_d(k)e^{-t/\tau_{\lambda k}} \sim (\ln t)^{2-\gamma} \to 0$ in the long-time limit
- Boguñá *et al.*, PRL (2013) and a comment by Lee, Shim, Noh and the reply.

Dynamical fluctuations in the SIS model II

- Hub-hub reinfection, if any, can be described in the rate equation on a long time scale: $\frac{di_j(t)}{dt} = -\tilde{\mu}_j i_j(t) + \lambda \sum_{\ell=1}^{N} p^{d_{j\ell}} i_\ell(t)$ with $d_{j\ell}$ the distance between j and ℓ, p the infection probability $p = \frac{\lambda}{\lambda+1}$, and $\tilde{\mu}_j = 1/\tau_{\lambda k_j} = e^{-a\lambda k_j}$ the healing rate.
- In random scale-free networks, two nodes j and ℓ whose degrees are k and k' are separated on the average by distance $d_{kk'} = \frac{\ln \frac{2L}{kk'}}{\ln \kappa}$ with $\kappa = \frac{\langle k^2 \rangle}{\langle k \rangle}$ the branching ratio (from $k\kappa^{d_{kk'}} \frac{k'}{2L} \sim 1$)
- For the nodes of given degree k, $\frac{di_k(t)}{dt} = -\tilde{\mu}_k i_k(t) + \tilde{\lambda}_k i_k(t)$ with the effective infection rate $\tilde{\lambda}_k = \lambda N \sum_{k'} e^{\frac{\ln p \, \ln \frac{2L}{kk'}}{\ln \kappa}} P_d(k') \sim \lambda N \sum_{k'} \left(\frac{k\,k'}{2L}\right)^b k'^{-\gamma} \leq \lambda \left(\frac{kk_{\max}}{2L}\right)^b \leq \lambda N^{-\frac{\gamma-3}{\gamma-1}b}$
- Therefore, the nodes of degree k satisfying $\tilde{\lambda}_k > \tilde{\mu}_k$ may remain infectious on a long time scale, which are the nodes of degree $k > \ln N$ but occupy quite small fraction.
- It was claimed that small-degree nodes connecting those hubs are infectious as well
- Numerical results are not so confirming...