

Random walks and diffusion on networks

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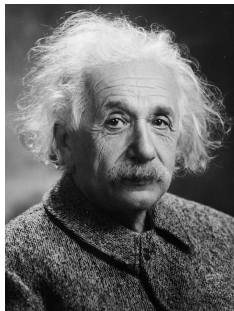
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Talk plan

- Random walks and diffusion
- 1-dim
- Networks
- Applications of RWs on networks

Diffusion is a broad term

- Diffusion of innovation
- Biological diffusion



Background

- Gamblers ruin: Pascal, Fermat, Huygens, Bernoulli,
- Term random walk was coined by Karl Pearson (1905).
- Brownian motion of particles colliding with atoms and molecules (Einstein, 1905)
- Applications: locomotion and foraging of animals, neuronal firing, decision-making in the brain, population genetics, polymer chains, financial markets, sports statistics
- Relevant theoretical research areas: probability theory (in maths), CS, statistical physics, OR,

Why do we study RWs on networks?

- Theoretical interest
- Applications. Especially, RWs lie at the core of many algorithms
 - PageRank
 - community detection
 - core-periphery structure
 - diffusion map
 - respondent-driven sampling
 - consensus algorithms

1-dim

- Assume the continuous space (\mathbb{R}^1)
 - Discrete-space case is similar
- Assume discrete-time RW
- In each time step, a walker at x moves to the interval $[x + r, x + r + \Delta r]$ with probability $f(r)\Delta r$. Then, the master equation is given by

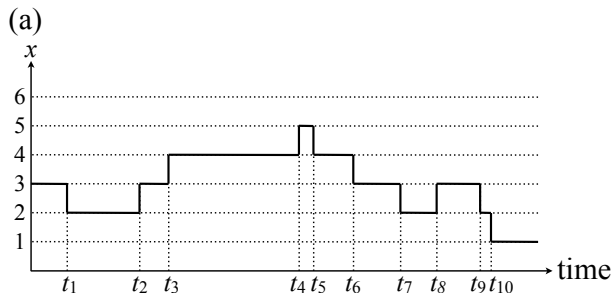
$$p(x; n) = \int_{-\infty}^{\infty} f(x - x')p(x'; n - 1)dx'.$$

- As time n tends to ∞ ,

$$p(x; n) = \frac{1}{(2\pi Dn)^{1/2}} e^{-\frac{(x - vn)^2}{4Dn}},$$

where $v \equiv \langle r \rangle$ and $D \equiv \langle (r - \langle r \rangle)^2 \rangle / 2$.

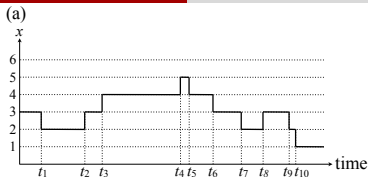
Continuous-time RW



(b)

steps (n)	0	1	2	3	4	5	6	7	8	9	10
x	3	2	3	4	5	4	3	2	3	2	1

(This fig assumes a discrete space)



(b)

steps (n)	0	1	2	3	4	5	6	7	8	9	10	
x		3	2	3	4	5	4	3	2	3	2	1

$$p(x; t) = \sum_{n=0}^{\infty} p(x; n) p(n, t)$$

where x : position, t : time, n : number of moves made

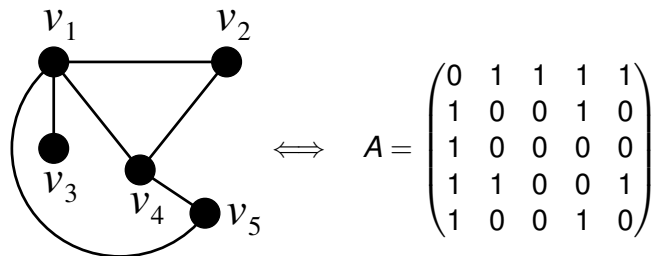
$$\langle n \rangle = \frac{t}{\langle \tau \rangle}, \quad \text{where } \tau \text{ is inter-event time}$$

$$\text{E.g., } \psi(\tau) = \beta e^{-\beta\tau} \rightarrow p(n, t) = \frac{(\beta t)^n}{n!} e^{-\beta t}$$

✓ Full soln in terms of the Laplace and Fourier transforms

RWs on networks

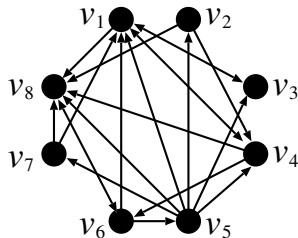
Adjacency matrix



- We allow directed and weighted adjacency matrices.

Transition-probability matrix (of DTRW)

- $i \rightarrow j$ with probability $T_{ij} = \frac{A_{ij}}{s_i^{\text{out}}}$
 where $s_i^{\text{out}} = \sum_{j=1}^N A_{ij}$ is the out-strength of node i .



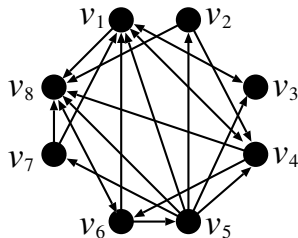
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

- Directed networks allowed
- Weighted networks allowed

Q: Which complicates things more than the other?

Transition-probability matrix (of DTRW)

- $i \rightarrow j$ with probability $T_{ij} = \frac{A_{ij}}{s_i^{\text{out}}}$
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$$B = \begin{pmatrix} 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & 0 & \frac{1}{6} & \frac{1}{6} \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

- Directed networks allowed
- Weighted networks allowed

Q: Which complicates things more than the other?

- Conservation: $\sum_{j=1}^N T_{ij} = 1$
- Dynamics: $p_j(n+1) = \sum_{i=1}^N p_i(n) T_{ij} \quad (j \in \{1, \dots, N\})$

Note that $\sum_{i=1}^N p_i(n) = 1$

- With vectors, $\mathbf{p}(n+1) = \mathbf{p}(n) T$
where $\mathbf{p}(t) = (p_1(n), \dots, p_N(n))$
- $\mathbf{p}(n) = \mathbf{p}(0) T^n$. That's it.

Q: linear or nonlinear?

Two main Qs for RWs

- Both in theory and applications, we are mostly concerned with either (or both) of the following questions
 - Stationary density (infinite-time behaviour)
 - Relaxation time (asymptotic behaviour)
 - First-passage time (finite-time behaviour)
- Other important questions:
 - Flow
 - Other finite-time behaviour (esp. in community detection)
 - (Loss of) detailed balance

Two main Qs for RWs

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 - Stationary density (infinite-time behaviour)
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- Other important questions:
 - Flow
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Stationary density of DTRWs

$$\mathbf{p}(n+1) = \mathbf{p}(n)T$$

$$\mathbf{p}(n) = \mathbf{p}(0)T^n$$

$$\text{Let } p_i^* = \lim_{n \rightarrow \infty} p_i(n)$$

$$\mathbf{p}^* = \mathbf{p}^* T$$

The stationary density is the left eigenvector of T with eigenvalue 1.
The corresponding right eigenvector is: $(1, \dots, 1)^\top$.

Relaxation: $\mathbf{p}(n) \approx \mathbf{p}^* + \lambda_2^n \mathbf{u}_2^L \langle \mathbf{p}(0), \mathbf{u}_2^R \rangle$

where λ_2 is the 2nd largest eigenvalue (in modulus) of T

Stationary density for undirected networks

Central result: $p_i^* = \frac{s_i}{\sum_{\ell=1}^N s_\ell}$ ($i \in \{1, \dots, N\}$)

where $s_i = \sum_{j=1}^N A_{ij} = \sum_{j=1}^N A_{ji}$ is the strength (i.e., weighted degree) of node i

Proof: Use $\mathbf{p}^* = \mathbf{p}^* T$, or $p_i^* = \sum_j p_j^* T_{ji}$ (for each i).

What does $p_i^* = \frac{s_i}{\sum_{\ell=1}^N s_\ell}$ mean?

Stationary density for directed networks

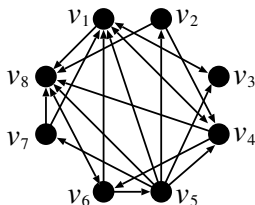
- No such handy results.
- First-order approximation:

$$p_i^* = \sum_{j=1}^N p_j^* \frac{A_{ji}}{s_j^{\text{out}}} \approx (\text{const}) \times \sum_{j=1}^N A_{ji} \propto s_i^{\text{in}}$$

where $s_i^{\text{in}} = \sum_{j=1}^N A_{ji}$ is the in-strength of node i .

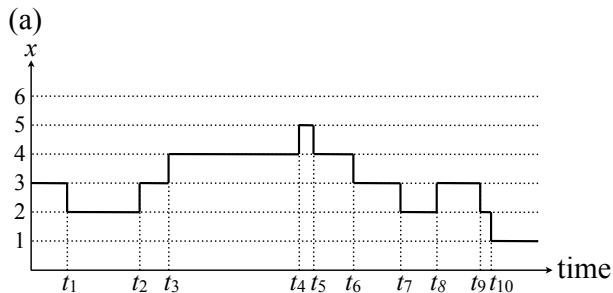
- Accurate in many cases, and inaccurate in many other cases

Example



Node	p_i^*	k_i^{in}	From k_i^{in}	k_i^{out}	From k_i^{out}
v_1	0.2275	5	0.2381	3	0.1429
v_2	0.0140	1	0.0476	2	0.0952
v_3	0.0899	2	0.0952	1	0.0476
v_4	0.0969	3	0.1429	3	0.1429
v_5	0.0843	1	0.0476	6	0.2857
v_6	0.2528	2	0.0952	3	0.1429
v_7	0.0140	1	0.0476	2	0.0952
v_8	0.2205	6	0.2857	1	0.0476

CTRWs on networks



(b)

steps (n)	0	1	2	3	4	5	6	7	8	9	10
x	3	2	3	4	5	4	3	2	3	2	1

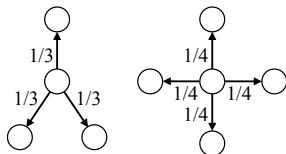
- Node-centric CTRW

- 1 The walker at node i waits an inter-event time τ distributed according to $\psi(\tau)$
- 2 Then, it moves to an (out-) neighbour j with the probability $\propto A_{ij}$

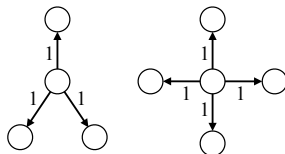
- Edge-centric CTRW:

- 1 Each edge (incident to i) is activated with an inter-event time τ distributed according to $\psi(\tau)$
 - 2 The walker moves the (first) activated edge to a neighbour j
- They are the same only for regular networks (or $s_i^{\text{out}} = (\text{const})$ for directed networks)
 - When $\psi(\tau)$ is a non-Poissonian distribution (cf. temporal networks), things are more complicated. Here we assume a Poissonian $\psi(\tau)$.

(a) Node-centric CTRW



(b) Edge-centric CTRW



(Poissonian) node-centric CTRW

Master equation:

$$\frac{d\mathbf{p}(t)}{dt} = \mathbf{p}(t)(-I + T) \equiv -\mathbf{p}(t)L' = -\mathbf{p}(t)D^{-1}L$$

where

$$L' = I - T = \left(\delta_{ij} - \frac{A_{ij}}{s_i^{\text{out}}} \right) \quad (\text{random-walk normalized Laplacian})$$

$$D = \text{diag}((s_1^{\text{out}}, \dots, s_N^{\text{out}})) \quad (\text{diag}(s_1, \dots, s_N) \text{ if undirected networks})$$

$$L \equiv D - A \quad ((\text{combinatorial}) \text{ Laplacian matrix})$$

Stationary density: $\frac{d\mathbf{p}^*(t)}{dt} = 0$

$\rightarrow \mathbf{p}^* = \mathbf{p}^* T$. Same as DTRW.

If the network is undirected, $p_i^* = s_i / \sum_{\ell=1}^N s_{\ell}$.

(Poissonian) edge-centric CTRW

Master equation:

$$\frac{d\mathbf{p}(t)}{dt} = \mathbf{p}(t)(-D + A) = -\mathbf{p}(t)L$$

Stationary density:

$$\mathbf{p}^* L = 0$$

i.e., zero eigenvector of L

- For undirected networks, $\mathbf{p}^* = \frac{1}{N}(1, \dots, 1)$
- For directed networks, no simple solution but the first-order approximation:

$$p_i^* \approx (\text{const}) \times \frac{s_i^{\text{in}}}{s_i^{\text{out}}}$$

Interim summary

- DTRW
 - driven by transition-probability matrix T
 - $\mathbf{p}^* = \mathbf{p}^* T$
 - $p_i^* \propto s_i^*$ for undirected networks
- CTRW
 - node-centric
 - driven by random-walk normalized Laplacian $L' = I - T$
 - Same \mathbf{p}^* as DTRW
 - edge-centric
 - driven by combinatorial Laplacian $L = D - A$
 - $\mathbf{p}^* L = \mathbf{0}$
 - $p_i^* = 1/N$ for undirected networks
- Undirected vs directed

Applications

- PageRank
- Community detection
- Respondent-driven sampling

PageRank

- Sergey Brin & Larry Page (1998) (but see Pinski & Narin 1976)
Rank websites in Google search!
They were born on 1973.
12th and 13rd richest persons in the world (Nov 2016)
- Other applications: ranking of academic journals and papers, professional sports, disease-gene identification, recommendation systems in online marketplaces, prediction of traffic flow . . .
- It is the stationary density of a DTRW on a network. Why should it be?

The Google logo is displayed in its characteristic multi-colored font.

Web graph

Design principle of the PageRank

The rank of node i should be large when

- i receives many edges (with large weights)
- i received edges from important nodes j
- i receives “exclusive” edges from j

(A)



(B)



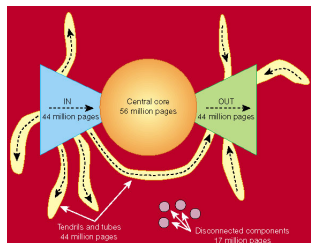
(C)



$$\mathbf{p}^* = \mathbf{p}^* T, \text{ i.e., } p_i^* = \sum_{j=1}^N p_j^* \frac{A_{ji}}{\sum_{\ell=1}^N A_{j\ell}} \text{ fulfills these three criteria.}$$

PageRank math

- Empirical networks (e.g., web graph) are usually not “strongly connected”
 - Sinks (dangling nodes) i.e., $s_i^{\text{out}} = 0$
 - Sources, i.e., $s_i^{\text{in}} = 0$
 - Multiple strongly connected components
 - transient nodes and components



PageRank math

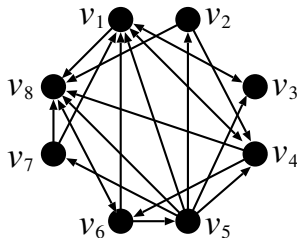
- So, we allow walkers to teleport to other nodes with probability $1 - \alpha$ to make an effective network that is strongly connected.
- Master equation:

$$p_i(t+1) = \alpha \sum_{j=1}^N p_j(t) T_{ji} + (1 - \alpha) u_i$$

where (u_1, \dots, u_N) is the “preference vector” ($\sum_{i=1}^N u_i = 1$)

- A popular choice: $u_i = 1/N$
- At dangling nodes, teleport with probability 1
- A popular choice: $\alpha = 0.85$
- Effective network: $T'_{ij} = \alpha T_{ij} + (1 - \alpha) u_j$ (and correction for dangling nodes)
- PageRank: $\mathbf{p}^* = \mathbf{p}^* T'$

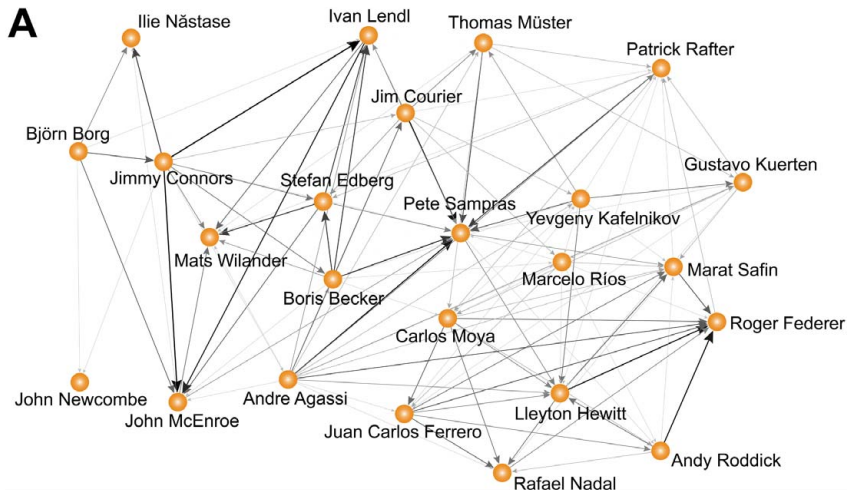
Back to the example



Node	p_i^*	k_i^{in}	k_i^{out}
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v_3	0.0899	2	1
v_4	0.0969	3	3
v_5	0.0843	1	6
v_6	0.2528	2	3
v_7	0.0140	1	2
v_8	0.2205	6	1

- The three criteria are respected?
 - i receives many edges (with large weights)
 - i received edges from important nodes j
 - i receives “exclusive” edges from j

Tennis players on PageRank



(Radicchi, PLOS ONE, 2011)

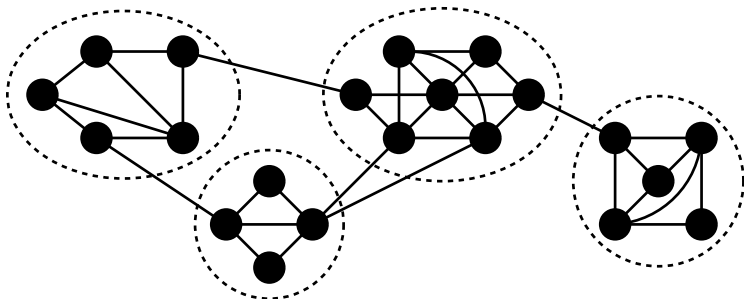
Tennis players on PageRank

Table 1. Top 30 players in the history of tennis.

Rank	Player	Country	Hand	Start	End
1	Jimmy Connors	United States	L	1970	1996
2	Ivan Lendl	United States	R	1978	1994
3	John McEnroe	United States	L	1976	1994
4	Guillermo Vilas	Argentina	L	1969	1992
5	Andre Agassi	United States	R	1986	2006
6	Stefan Edberg	Sweden	R	1982	1996
7	Roger Federer	Switzerland	R	1998	2010
8	Pete Sampras	United States	R	1988	2002
9	Ilie Năstase	Romania	R	1968	1985
10	Björn Borg	Sweden	R	1971	1993
11	Boris Becker	Germany	R	1983	1999
12	Arthur Ashe	United States	R	1968	1979
13	Brian Gottfried	United States	R	1970	1984
14	Stan Smith	United States	R	1968	1985
15	Manuel Orantes	Spain	L	1968	1984
16	Michael Chang	United States	R	1987	2003
17	Roscoe Tanner	United States	L	1969	1985
18	Eddie Dibbs	United States	R	1971	1984
19	Harold Solomon	United States	R	1971	1991
20	Tom Okker	Netherlands	R	1968	1981
21	Mats Wilander	Sweden	R	1980	1996
22	Goran Ivanišević	Croatia	L	1988	2004
23	Vitas Gerulaitis	United States	R	1971	1986
24	Rafael Nadal	Spain	L	2002	2010
25	Raúl Ramírez	Mexico	R	1970	1983
26	John Newcombe	Australia	R	1968	1981
27	Ken Rosewall	Australia	R	1968	1980
28	Yevgeny Kafelnikov	Russian Federation	R	1992	2003
29	Andy Roddick	United States	R	2000	2010
30	Thomas Muster	Austria	L	1984	1999

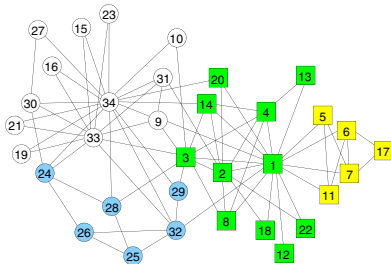
(Radicchi, PLOS ONE, 2011)

Community detection

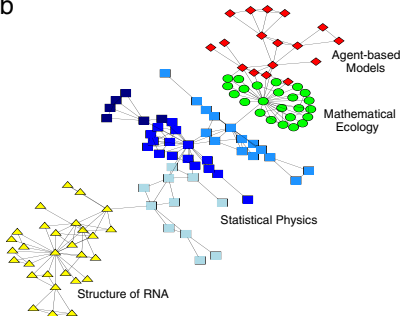


- A very very popular application of network analysis
- Various algorithms to detect communities in unlabeled networks

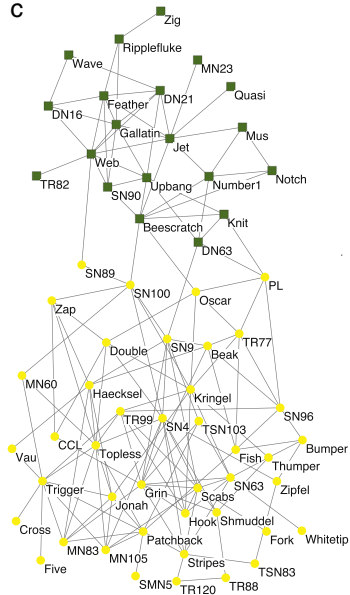
a



b

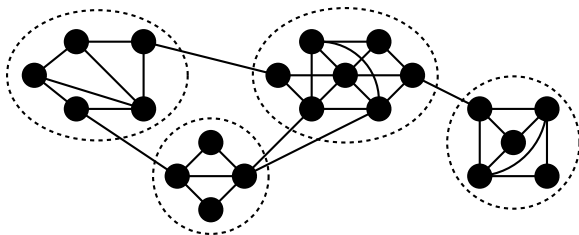


c



Why RWs?

- Idea: A random walker would wander within a community for a long time before transiting to another community.
- Various algorithms based on this idea: Markov stability, Walktrap, InfoMap, Nibble, ...



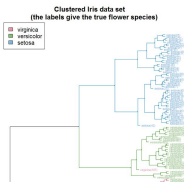
Walktrap (Pons & Latapy, J. Graph Algo., 2006)

- Consider an undirected and unweighted network
- A (DT)RW-based distance between nodes:

$$r_{ij} = \sqrt{\sum_{\ell=1}^N \frac{(T_{i\ell}^n - T_{j\ell}^n)^2}{k_{\ell}}}$$

Physical meaning of r_{ij} ?

- Nodes i and j with small r_{ij} would belong to the same community
- Then run a hierarchical clustering algorithm
- Discounted by k_{ℓ} because $p_{\ell}^* \propto k_{\ell}$
- n should not be too large because $\lim_{n \rightarrow \infty} T_{i\ell}^n = \lim_{n \rightarrow \infty} T_{j\ell}^n = p_{\ell}^*$, implying $r_{ij} \approx 0$



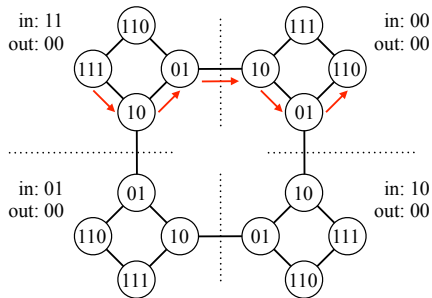
InfoMap (Rosvall & Bergstrom, PNAS 2008)

- Use DTRWs on (generally) directed and weighted networks
- Encode each node into a binary code word
 - Ex: If $v_1 \rightarrow 000$, $v_2 \rightarrow 001$, $v_3 \rightarrow 010$, $v_4 \rightarrow 011$, $v_5 \rightarrow 100$, ..., Trajectory $v_3, v_6, v_3, v_1, v_8, \dots$ is encoded into 010101010000111...
- Unique decoding requires a “prefix-free” coding scheme.
 - : Ex: If $v_1 \rightarrow 000$ and $v_2 \rightarrow 0001$?
 - Huffman code is a famous prefix-free code yielding short binary sequences.
frequently visited node \rightarrow short code word
 - The Shannon entropy gives the lower bound of the mean code word length

$$H = - \sum_{i=1}^N p_i^* \log p_i^*$$

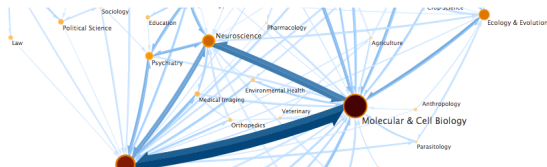
Not about communities so far

- Use coding schemes local to individual communities.
 - Extra workaround to get around entry to and exit from communities
 - But shorter code words if walkers wander within a community
 - Doesn't matter if the same local code word is used in different communities
- Find such a two-layer Huffman code that minimises the mean code word length

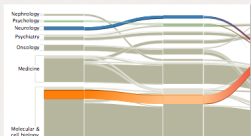


11 111 10 01 00 00 10 01 110 ...

Simplify and highlight important structures in complex networks



Apps »



Code »

```
using infomath::plogp;
for (unsigned int i = 0; i < numNodes; ++i)
{
    enter_log_enter += plogp(m_moduleFlowData[i].enter
    exit_log_exit += plogp(m_moduleFlowData[i].exitFlow
    flow_log_flow += plogp(m_moduleFlowData[i].exitFlow
    enterFlow += m_moduleFlowData[i].enterFlow;
}
enterFlow += exitNetworkFlow;
enterFlow_log_enterFlow = plogp(enterFlow);
```

Publications »

Maps of information flow reveal community structure in complex networks

Martin Rosvall and Carl T. Bergstrom
PNAS **105**, 1118 (2008). [arXiv:0707.0609]



To comprehend the multipartite organization of large-scale biological and social systems, we introduce a new information-theoretic approach to reveal community structure in

News

April 11, 2017 [Source code](#) — [Infomap on Windows](#) — [run Infomap in bash on ubuntu on Windows](#)

Respondent-driven sampling

- Estimate the fraction of infected individuals in a large or difficult-to-reach population.
What would you do?

Respondent-driven sampling

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What would you do?
- Respondent-driven sampling uses edge-tracing in a social network.

Respondent-driven sampling

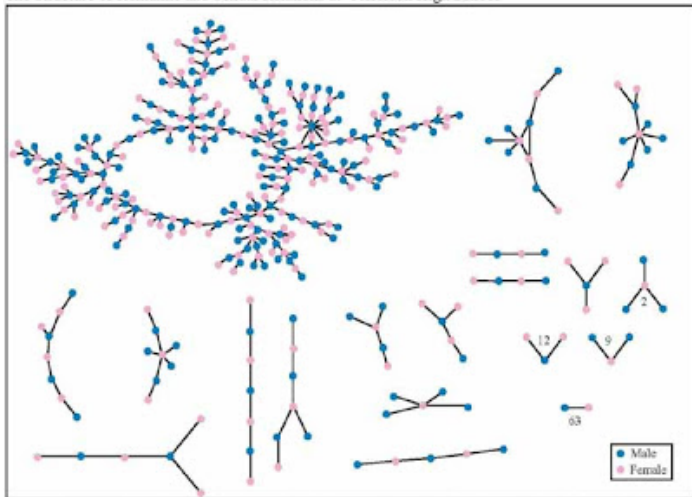
- Estimate the fraction of infected individuals in a large or difficult-to-reach population.
What would you do?
- Respondent-driven sampling uses edge-tracing in a social network.
 - 1 Start from a seed individual
 - 2 He/she recruits neighbours to a survey by passing a coupon to each of them.
 - 3 The successfully recruited individuals then participate in the survey and also pass coupons to their neighbors.
 - 4 Calculate a weighted mean of the samples to derive an estimate

Respondent-driven sampling

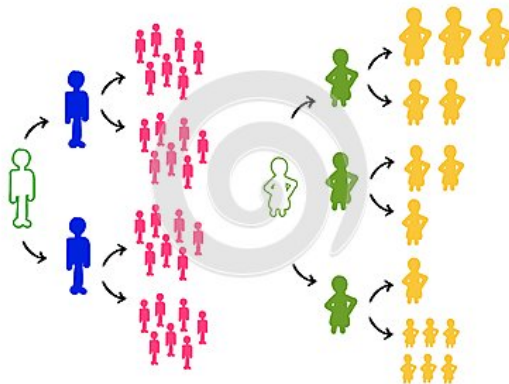
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 - 3 The successfully recruited individuals then participate in the survey and also pass coupons to their neighbors.
 - 4 Calculate a weighted mean of the samples to derive an estimate
- Don't forget to reward participants

- Useful for difficult-to-reach populations

The Structure of Romantic and Sexual Relations at "Jefferson High School"



- RDS = “snowball sampling” + mathematics



(www.dreamstime.com)

Q: Why a “weighted” mean?

- y_i : quantity assigned to node i (e.g., infected or not, age, opinion)
- N_S : number of samples S
- $p_i^* \propto k_i$
- Estimator: $\langle \hat{y} \rangle = \frac{1}{N_S} \sum_{v_i \in S} \frac{y_i}{N \hat{p}_i^*}$
because $N \hat{p}_i^*$ is normalised ($\langle N \hat{p}_i^* \rangle = 1$)
- Use $\hat{p}_i^* = \frac{k_i}{N \langle k \rangle}$ to rewrite

$$\langle \hat{y} \rangle = \frac{1}{N_S} \sum_{v_i \in S} \frac{y_i \langle k \rangle}{k_i}$$

- What's all this mess?

- y_i : quantity assigned to node i (e.g., infected or not, age, opinion)
- N_S : number of samples S
- $p_i^* \propto k_i$
- Estimator: $\langle \hat{y} \rangle = \frac{1}{N_S} \sum_{v_i \in S} \frac{y_i}{N \hat{p}_i^*}$
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$$\langle \hat{y} \rangle = \frac{1}{N_S} \sum_{v_i \in S} \frac{y_i \langle k \rangle}{k_i}$$

- What's all this mess?
We do not know the value of p_i^* or $\langle k \rangle$. We have to estimate them.

We use

$$\langle \hat{k} \rangle = \frac{\sum_{v_i \in S} \frac{k_i}{Np_i^*}}{\sum_{v_i \in S} \frac{1}{Np_i^*}} = \frac{N_S}{\sum_{v_i \in S} (k_i)^{-1}}$$

$$\langle \hat{y} \rangle = \frac{1}{N_S} \sum_{v_i \in S} \frac{y_i \langle \hat{k} \rangle}{k_i} = \frac{\sum_{v_i \in S} (k_i)^{-1} y_i}{\sum_{v_i \in S} (k_i)^{-1}}$$

(RDS II estimator. Volz & Heckathorn, J Official Stat, 2008)

E.g., proportion of nodes that have a discrete type A (e.g., infected):

$$\hat{P}_A = \frac{\sum_{v_i \in A \cap S} (k_i)^{-1}}{\sum_{v_i \in S} (k_i)^{-1}}$$

Resources

Masuda, Porter & Lambiotte, arXiv:1612.03281

- Other topics covered:
 - Fourier and Laplace transforms
 - First-passage times
 - Fractal networks
 - Multilayer networks
 - Temporal networks
 - Discrete-choice models
 - More on community detection
 - Diffusion maps
 - Opinion formation models