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Random thoughts on random walks: networks, centrality, and tracking the spread of disease

## networks

, fancy word for graphs: nodes = vertices, connections = edges
, typically directed (Twitter) or undirected (Facebook)
> connectedness/giant component, irreducibility


## adjacency matrix

, 1 if edge from ito $j$ (0 otherwise)
, symmetric for undirected graphs
> makes counting easier
> degree of node $i: \quad d_{i}=\sum_{j} a_{i j}$
》 \# of walks of length $t$ starting from node $i$ :


Undirected Graph

| (1) (2) (3) (4) (5) (6) |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| (1) 0 | 1 | 1 | 0 | 0 | 0 |
| (2) 1 | 0 | 0 | 1 | 0 | 0 |
| (3) 1 | 0 | 0 | 1 | 0 | 0 |
| (4) 0 | 1 | 1 | 0 | 1 | 0 |
| (5) 0 | 0 | 0 | 1 | 0 | 1 |
| (6) 0 | 0 | 0 | 0 | 1 | 0 |

Adjacency Matrix

$$
M_{i}(t)=\sum_{i_{1}, i_{2}, \ldots, i_{t}} a_{i i_{1}} a_{i_{1} i_{2}} \cdots a_{i_{t-1} i_{t}}
$$

〉 \# of 3-cycles in entire network (triple counting):

$$
C^{(3)}=\sum_{i}\left(A^{3}\right)_{i i}=\operatorname{Tr}\left(A^{3}\right)
$$

## centrality


, what does it mean to be central within a network? context-dependent!

〉 create your own...

## centrality


, what does it mean to be central within a network? context-dependent!

〉 create your own...

## centrality

- \{in-, out-, undirected-\} degree centrality
"How many \{followers, followees, friends\} do I have?"
> eigenvector centrality
"How influential am l?"
> Katz centrality/PageRank
"If my friends are important, doesn't that make me important?"
> closeness centrality
"How close am I to everyone else, on average?"
, betweenness centrality
"How many chains of connections include me?"


## degree centrality

$c_{i}^{\text {deg }}=d_{i} / \sum_{i} d_{i}$
, normalization doesn't matter
, defined using only local information (up to scaling)

## eigenvector centrality

〉 defined recursively/iteratively: requires global knowledge of network

$$
c_{i}^{\prime} \longleftarrow \sum_{j} a_{i j} c_{j}
$$

> equivalent to dominant eigenvector of adjacency matrix (hence the name)

$$
A \mathbf{v}=\kappa \mathbf{v}
$$

## PageRank

〉 similar to eigenvector centrality, but using normalized adjacency matrix

$$
p_{i j}=\frac{a_{i j}}{d_{i}}
$$

- defined using global information (as before)

$$
P \pi=\pi
$$

> add a damping factor to ensure everyone ends up with at least some centrality

- i.e., interpolate original graph with complete graph


## (a disservice to) Markov chains

- transition probabilities of going from $i$ to $j$

stationary distribution satisfies $\sum_{i} \pi_{i} p_{i j}=\pi_{j} \quad$ (i.e., $\pi P=\pi$ )
, rate of convergence given by second largest eigenvalue of transition matrix
- example: simple random walk on finite set of states


## PageRank + random walks

- interpretation: proportion of time random walker spends at each node, assuming at each step neighbor selected at random
- i.e., stationary distribution of Markov process on graph with uniform transition probabilities
> technical details: irreducibility, aperiodicity, ergodicity
- damping factor ensures these properties hold

〉 note for later: only local information used at each step in walk...

## degree centrality + random walks

, for undirected networks, PageRank (w/o damping) is the simple random walk

- has degree centrality as its stationary distribution if network is connected
, check this yourself! show that

$$
\sum_{j} p_{i j}\left(\frac{d_{j}}{\sum_{i} d_{i}}\right)=\frac{d_{i}}{\sum_{i} d_{i}}
$$

## degree centrality + random walks

, moments of degree distribution: $\left\langle d^{m}\right\rangle=\frac{1}{N} \sum_{i} d_{i}^{m}=\sum_{d} d^{m} P(d)$

- if we sample a node uniformly at random:

$$
P(X=i)=1 / N \Longrightarrow E(\operatorname{deg}(X))=\langle d\rangle
$$

〉 instead, after performing random walk "long enough", we are sampling nodes according to their degree centralities:

$$
P(X=i)=d_{i} / \sum_{i} d_{i} \quad \Longrightarrow \quad E(\operatorname{deg}(X))=\frac{\left\langle d^{2}\right\rangle}{\langle d\rangle}=\langle d\rangle+\frac{\operatorname{Var}(d)}{\langle d\rangle}
$$

, intuition: In the limit, every edge is traversed same proportion of times. So, we are sampling a node at the end of an edge chosen uniformly at random!

## sampling using random walks

- constructive: If we want to sample according to degree centrality, take any node and select neighbor uniformly at random... rinse, repeat...
, principle behind Markov Chain Monte Carlo (MCMC)
- provides way to generate samples from distribution that can't be sampled directly
- need to specify transition probabilities such that stationary distribution of Markov chain is the desired sampling distribution


## real-world implications

> Christakis \& Fowler (2010)
, flu outbreak among Harvard student population from Sep.-Dec. '09

- 2009 H1N1 pandemic: ~60M infected in US, ~300K hospitalizations
> two groups: random vs. friends of random (FoR)
> epidemic curve in FoR tracked progression in random group $\sim 14 d$ in advance

》 deal with it: on average, your friends have more friends than you


## an aside

- long history of using (random) walks to infer properties of the social graph
, Milgram's small-world experiment (1967)
, Watts-Strogatz model: shortcuts in highly clustered networks
, Kleinberg model: distribution of shortcut lengths and efficient routing


## an aside



Erdos-Renyi (tree-like)

## an aside



Erdos-Renyi (tree-like)
small diameter, no clustering

## an aside



Erdos-Renyi (tree-like)
small diameter, no clustering
Watts-Strogatz (lattice + shortcuts)


## an aside



Erdos-Renyi (tree-like)
small diameter, no clustering
small diameter, high clustering
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Kleinberg (distribution of shortcuts)


## an aside



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Kleinberg (distribution of shortcuts) greedy routing finds shortcuts!

## an aside



Erdos-Renyi (tree-like) small diameter, no clustering
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Watts-Strogatz (lattice + shortcuts)


Kleinberg (distribution of shortcuts) greedy routing finds shortcuts!


## disease surveillance

, what do public health officials and CDC care about?
> situational awareness

- early detection of epidemic onset
> peak timing and intensity
, practical reasons
, vaccine supply and distribution
> allowing hospitals to run at high capacity and prepare for large influx of patients
, difficulties both mathematical/statistical and practical


## let's do a little math

, SIR model on a graph (recall Andy's talk!)

$$
\begin{aligned}
\frac{d s_{i}}{d t} & =-\beta \sum_{j} a_{i j} s_{i} x_{j} \\
\frac{d x_{i}}{d t} & =\beta \sum_{j} a_{i j} s_{i} x_{j}-\gamma x_{i} \\
\frac{d r_{i}}{d t} & =\gamma x_{i}
\end{aligned}
$$

## let's do a little math

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$$
\begin{aligned}
\frac{d s_{i}}{d t} & =-\beta \sum_{j} a_{i j} s_{i} x_{j} \\
\longrightarrow \frac{d x_{i}}{d t} & =\beta \sum_{j} a_{i j} s_{i} x_{j}-\gamma x_{i} \\
\frac{d r_{i}}{d t} & =\gamma x_{i}
\end{aligned}
$$

## let's do a little math

, SIR model on a graph (recall Andy's talk!)

$$
\begin{aligned}
\frac{d s_{i}}{d t} & =-\beta \sum_{j} a_{i j} \xi / x_{j} \\
\longrightarrow \frac{d x_{i}}{d t} & =\beta \sum_{j} a_{i j} \xi_{i} x_{j}-\gamma x_{i} \\
\frac{d r_{i}}{d t} & =\gamma x_{i}
\end{aligned}
$$


for small times, $\mathrm{P}(\mathrm{i}$ is S$)$ is approximately 1
linearized SIR on graph

$$
\frac{d \mathbf{x}}{d t}=\beta A \mathbf{x}-\gamma \mathbf{x}
$$

## linearized SIR on graph

$$
\frac{d \mathrm{x}}{d t}=\beta A \mathbf{x}-\gamma \mathbf{x}
$$

$$
\mathbf{x}(t)=\exp (t(A-\gamma I)) \mathbf{x}(0) \approx e^{(\beta \kappa-\gamma) t} \mathbf{v} \text { cominant e-value of } \mathbf{A}
$$

## linearized SIR on graph

$$
\frac{d \mathbf{x}}{d t}=\beta A \mathbf{x}-\gamma \mathbf{x}
$$

$$
\mathbf{x}(t)=\exp (t(A-\gamma I)) \mathbf{x}(0) \approx e^{(\beta \kappa-\gamma) t} \mathbf{v} \text { cominant e-value of } \mathbf{A}
$$

$$
\text { epidemic takes off if } R_{0}=\frac{\beta}{\gamma}>\frac{1}{\kappa}
$$

early detection + eigenvector centrality

## early detection + eigenvector centrality

$$
\mathbf{x}(t)=\exp (t(A-\gamma I)) \mathbf{x}(0) \approx e^{(\beta \kappa-\gamma) t} \mathbf{v}
$$

## early detection + eigenvector centrality

$$
\begin{aligned}
& \text { dominant e-value of } A \\
& \mathbf{x}(t)=\exp (t(A-\gamma I)) \mathbf{x}(0) \approx e^{(\beta \kappa-\gamma) t} \mathbf{v} \\
& p=\frac{\mathbf{x}\left(\tau_{S}\right) \cdot 1_{S}}{M}=\frac{e^{(\beta \kappa-\gamma) \tau_{S}} \mathbf{v} \cdot 1_{S}}{M} \\
& \text { expected prevalence hits } p \text { in surveillance set } \\
& p=\frac{\mathbf{x}(\tau) \cdot \mathbf{1}}{N}=\frac{e^{(\beta \kappa-\gamma) \tau} \mathbf{v} \cdot \mathbf{1}}{N} \\
& \text { expected prevalence hits } p \text { in entire network }
\end{aligned}
$$

## early detection + eigenvector centrality

$$
\begin{gathered}
\mathbf{x}(t)=\exp (t(A-\gamma I)) \mathbf{x}(0) \approx e^{(\beta \kappa-\gamma) t} \mathbf{v} \\
p=\frac{\mathbf{x}\left(\tau_{S}\right) \cdot \mathbf{1}_{S}}{M}=\frac{e^{(\beta \kappa-\gamma) \tau_{S}} \mathbf{v} \cdot \mathbf{1}_{S}}{M} \quad p=\frac{\mathbf{x}(\tau) \cdot \mathbf{1}}{N}=\frac{e^{(\beta \kappa-\gamma) \tau} \mathbf{v} \cdot \mathbf{1}}{N}
\end{gathered}
$$

expected prevalence hits $p$ in surveillance set
expected prevalence hits $p$ in entire network

$$
\Delta \tau:=\tau_{S}-\tau=\frac{1}{\beta \kappa-\gamma} \ln \left(\frac{c}{c_{S}}\right)
$$

## early detection + eigenvector centrality

$$
\begin{gathered}
\mathbf{x}(t)=\exp (t(A-\gamma I)) \mathbf{x}(0) \approx e^{(\beta \kappa-\gamma) t} \mathbf{v} \\
p=\frac{\mathbf{x}\left(\tau_{S}\right) \cdot \mathbf{1}_{S}}{M}=\frac{e^{(\beta \kappa-\gamma) \tau_{S}} \mathbf{v} \cdot \mathbf{1}_{S}}{M} \quad p=\frac{\mathbf{x}(\tau) \cdot \mathbf{1}}{N}=\frac{e^{(\beta \kappa-\gamma) \tau} \mathbf{v} \cdot \mathbf{1}}{N} \\
\text { expected prevalence hits p in surveillance set } \quad \text { expected prevalence hits p in entire net }
\end{gathered}
$$

expected prevalence hits $p$ in entire network
average e-vector centrality in surveillance set

$$
\Delta \tau:=\tau_{S}-\tau=\frac{1}{\beta \kappa-\gamma} \ln \left(\frac{c}{c_{S}}\right)
$$

## early detection + eigenvector centrality

, problem: not possible* without knowing entire network to begin with!

〉 never really know the underlying social graph, can only infer global properties from local subnetworks
, is there a random walk whose stationary distribution is eigenvector centrality?


## correlation of centrality measures



〉 could use degree centrality (locally recoverable) as a proxy for eigenvector centrality
> can we do better: is there a random walk whose stationary distribution is eigenvector centrality?

$$
p_{i j}=\frac{a_{i j} v_{j}}{\kappa v_{i}}
$$

transition probabilities

## maximal entropy random walk (MERW)

$$
\begin{gathered}
p_{i j}=\frac{a_{i j} v_{j}}{\kappa v_{i}} \\
\text { transition probabilities }
\end{gathered}
$$

$$
\psi_{i}=v_{i}^{2}
$$

stationary distribution!

$$
p_{i j}=\frac{a_{i j} v_{j}}{\kappa v_{i}}
$$

transition probabilities

$$
\psi_{i}=v_{i}^{2}
$$

stationary distribution!

$$
A \mathbf{v}=\kappa \mathbf{v} \quad \Longrightarrow \quad \sum_{j} p_{i j} \psi_{j}=\frac{1}{\kappa} v_{i} \sum_{j} a_{i j} v_{j}=v_{i}^{2}=\psi_{i}
$$

## maximal entropy random walk (MERW)

$$
p_{i j}=\frac{a_{i j} v_{j}}{\kappa v_{i}}
$$

transition probabilities

$$
\psi_{i}=v_{i}^{2}
$$

stationary distribution!

$$
A \mathbf{v}=\kappa \mathbf{v} \quad \Longrightarrow \quad \sum_{j} p_{i j} \psi_{j}=\frac{1}{\kappa} v_{i} \sum_{j} a_{i j} v_{j}=v_{i}^{2}=\psi_{i}
$$

but transition probabilities given in terms of e-vector centralities!

## maximal entropy random walk

〉 why maximal entropy?
, uniform distribution on a set has maximal entropy among all distributions on that set
, transition probabilities of MERW put equal probability on all paths of length $t$ starting from a given node, as $t$ goes to $\infty$


## entropy rate

$$
S(t)=-\sum_{i_{1}, \ldots, i_{t}} p\left(i, i_{1}, \ldots, i_{t}\right) \ln p\left(i, i_{1}, \ldots, i_{t}\right)
$$

Entropy of set of paths of length $t$ starting at $i$

## entropy rate

$$
S(t)=-\sum_{\text {Entropy of set of paths of length } t \text { starting at } i} p\left(i, i_{1}, \ldots, i_{t}\right) \ln p\left(i, i_{1}, \ldots, i_{t}\right)
$$

$$
h=\lim _{\substack{t \rightarrow \infty \\ \text { entropy rate }}} \frac{\ln S(t)}{t}
$$

## entropy rate

, minimal entropy: all probability is put on one path starting from $i$ :

$$
S(t)=-\sum_{i_{1}, \ldots, i_{t}} p\left(i, i_{1}, \ldots, i_{t}\right) \ln p\left(i, i_{1}, \ldots, i_{t}\right)=0
$$

, maximal entropy: uniform probability on all paths of length $t$ starting from $i$ :

$$
\begin{gathered}
S(t)=-\sum_{i_{1}, \ldots, i_{t}} \frac{1}{M_{i}(t)} \ln \left(\frac{1}{M_{i}(t)}\right)=\ln M_{i}(t) \\
M_{i}(t)=\sum_{i_{1}, i_{2}, \ldots, i_{t}} a_{i i_{1}} a_{i_{1} i_{2}} \cdots a_{i_{t-1} i_{t}}
\end{gathered}
$$

## transition probabilities of MERW

$$
\begin{gathered}
p\left(i, i_{1}, \ldots, i_{t}\right)=\frac{a_{i i_{1}} a_{i_{1} i_{2}} \ldots a_{i_{t-1} i_{t}}}{\sum_{i_{1}, i_{2}, \ldots, i_{t}} a_{i i_{1}} a_{i_{1} i_{2} \ldots a_{i_{t-1} i_{t}}}^{\text {uniform probability on all paths }}} \\
\pi\left(i_{1} \mid i\right)=\lim _{t \rightarrow \infty} \frac{a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}}{\sum_{i_{1}} a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}} \\
\text { corresponding transition probabilities! }
\end{gathered}
$$

## transition probabilities of MERW

$$
\pi\left(i_{1} \mid i\right)=\lim _{t \rightarrow \infty} \frac{a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}}{\sum_{i_{1}} a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}}
$$

## transition probabilities of MERW

$$
\begin{aligned}
& \quad \pi\left(i_{1} \mid i\right)=\lim _{t \rightarrow \infty} \frac{a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}}{\sum_{i_{1}} a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}} \\
& \pi^{0}\left(i_{1} \mid i\right)=\frac{a_{i i_{1}}}{\sum_{i_{1}} a_{i i_{1}}} \\
& \text { Oth-order approximation } \\
& \text { "How many friends do I have?" }
\end{aligned}
$$

## transition probabilities of MERW

$$
\begin{gathered}
\pi\left(i_{1} \mid i\right)=\lim _{t \rightarrow \infty} \frac{a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}}{\sum_{i_{1}} a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}} \\
\pi^{0}\left(i_{1} \mid i\right)=\frac{a_{i i_{1}}}{\sum_{i_{1}} a_{i i_{1}}} \\
\text { Oth-order approximation } \\
\text { "How many friends do I have?" } \quad \pi^{1}\left(i_{1} \mid i\right)=\frac{a_{i i_{1}} k\left(i_{1}\right)}{\sum_{i_{1}} a_{i i_{1}} k\left(i_{1}\right)} \\
\text { 1st-order approximation }
\end{gathered}
$$

## transition probabilities of MERW

$$
\begin{gathered}
\pi\left(i_{1} \mid i\right)=\lim _{t \rightarrow \infty} \frac{a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}}{\sum_{i_{1}} a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} \ldots \sum_{i_{t}} a_{i_{t-1} i_{t}}} \\
\pi^{0}\left(i_{1} \mid i\right)=\frac{a_{i i_{1}}}{\sum_{i_{1}} a_{i i_{1}}} \\
\begin{array}{l}
\text { Oth-order approximation } \\
\text { "How many friends do I have?" }
\end{array} \\
\pi^{1}\left(i_{1} \mid i\right)=\frac{a_{i i_{1}} k\left(i_{1}\right)}{\sum_{i_{1}} a_{i i_{1}} k\left(i_{1}\right)} \\
\text { 1st-order approximation }
\end{gathered}
$$

$$
\begin{aligned}
\pi^{2}\left(i_{1} \mid i\right) & =\frac{a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} k\left(i_{2}\right)}{\sum_{i_{1}} a_{i i_{1}} \sum_{i_{2}} a_{i_{1} i_{2}} k\left(i_{2}\right)} \\
& =\frac{a_{i i_{1}} k\left(i_{1}\right) k_{n n}\left(i_{1}\right)}{\sum_{i_{1}} a_{i i_{1}} k\left(i_{1}\right) k_{n n}\left(i_{1}\right)}
\end{aligned}
$$

## 2nd-order approximation

"What is the average degree of my friends' friends?"

## approximated MERW



## performance on Montreal network

Performance of MERW approximations for scale-free networ Performance of MERW approximations for scale-free networ

k-step subset


## recap

〉 can use random walks to sample nodes with desired properties
> how to incorporate into a realistic sampling methodology?
> network models are fun to work with!


