Graph Evolution Networks

lecture-9

Course on Graph Neural Networks (Winter Term 21/22)

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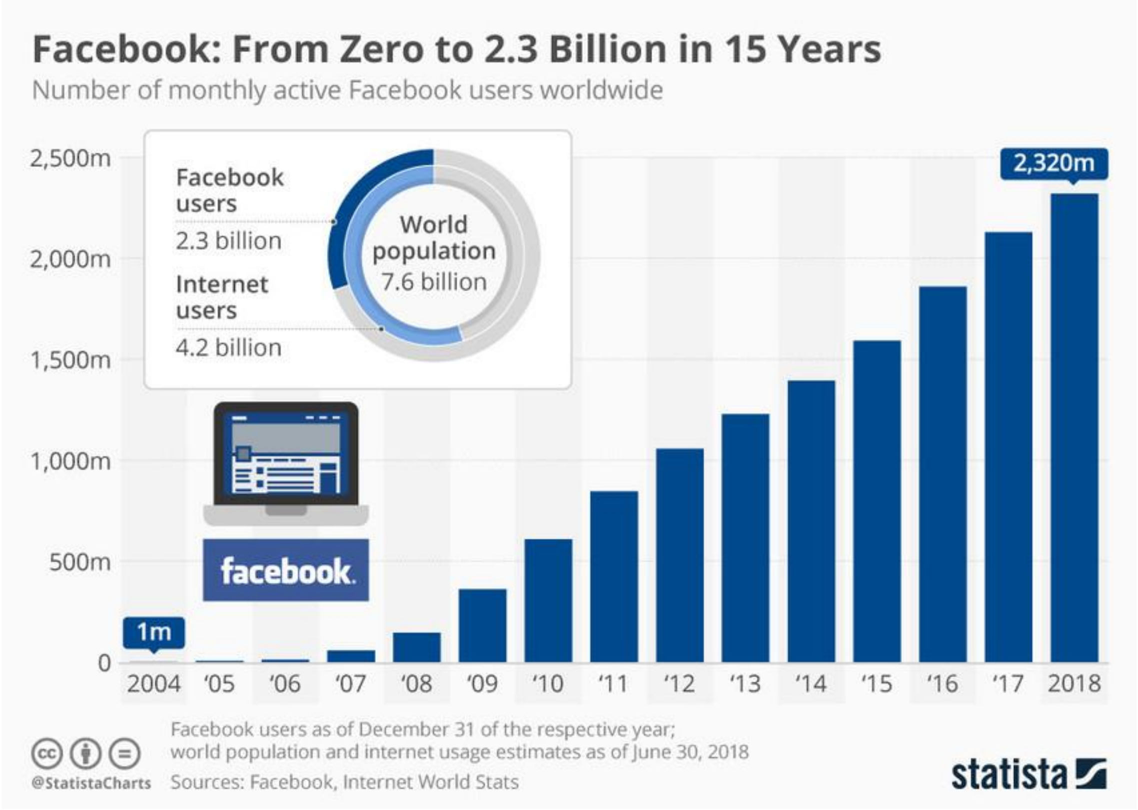
Evolving Networks

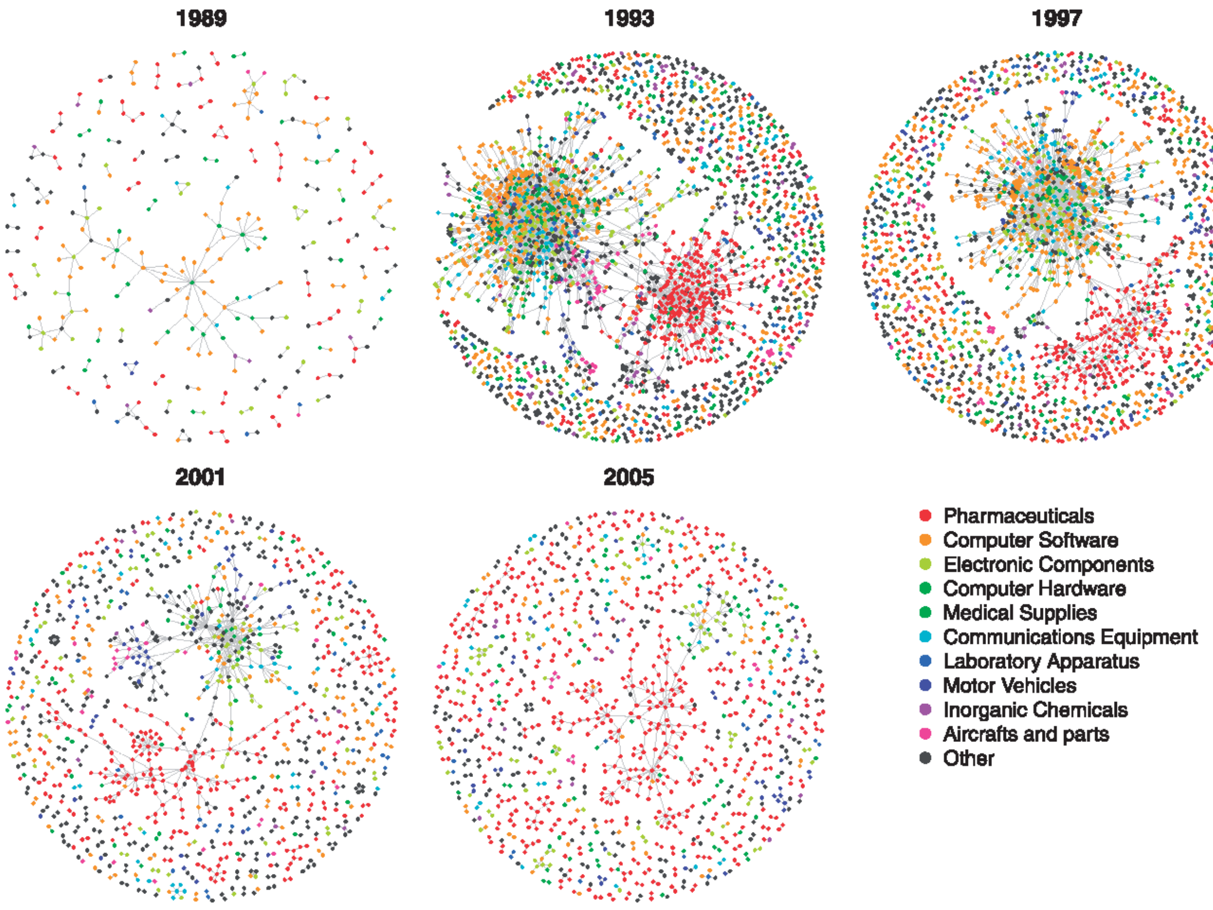
Almost all networks evolve by adding or removing links and node

- Social Networks
- Emails
- News Comments
- Product Evaluations



Evolution of the pooled R&D network

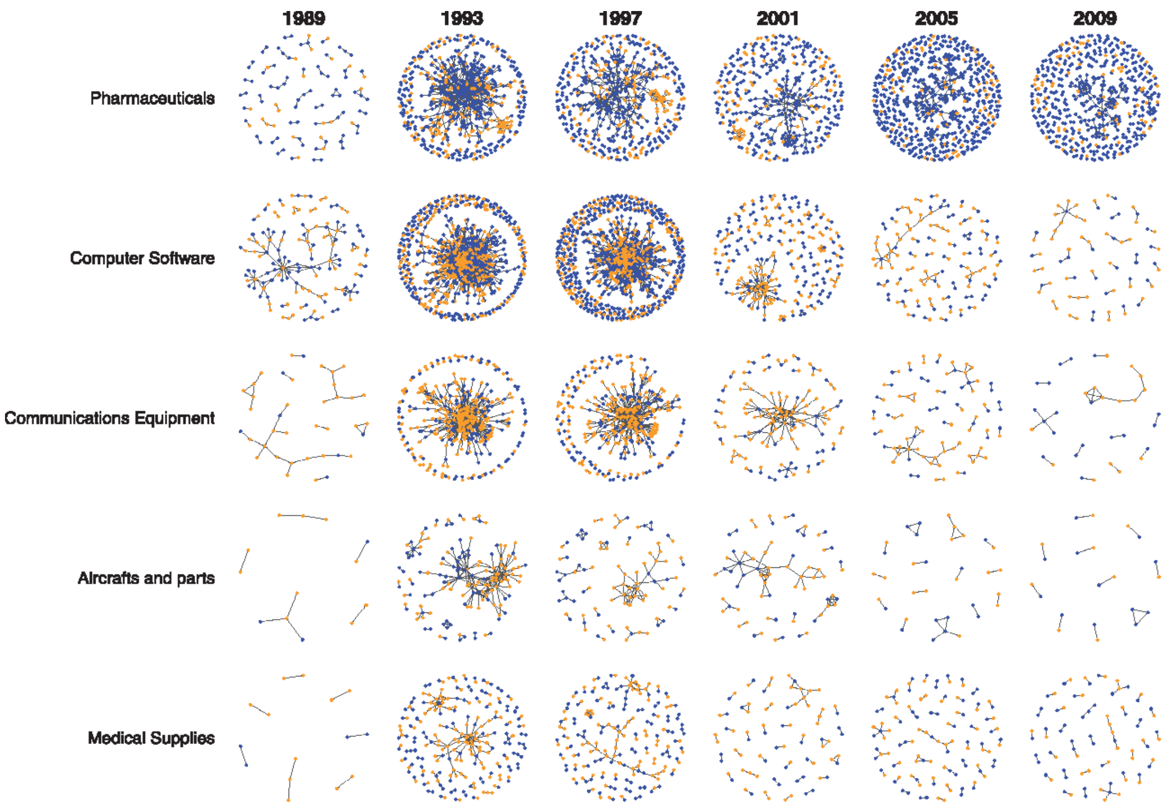
Figure 1. Evolution of the pooled R&D network. Pooled R&D network snapshots in 1989, 1993, 1997, 2001, and 2005. To ...



Ind Corp Change, Volume 26, Issue 4, August 2017, Pages 617–646, https://doi.org/10.1093/icc/dtw041

Evolution of the pooled R&D network

Figure 2. Evolution of five selected sectoral R&D networks. Snapshots in 1989, 1993, 1997, 2001, 2005, and 2009 for ...



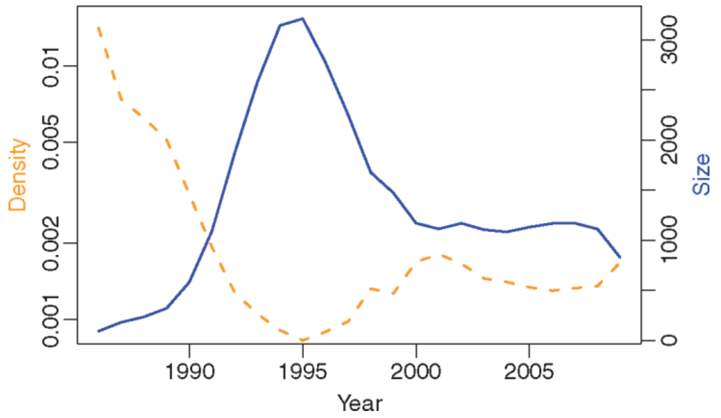


Figure 3. Size and density evolution of the pooled R&D network. Time-evolution of size (solid line, right y-axis) and ...

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Road Map (1/2)

1. Intro and Course Organization
2. Graph Metrics and Random Models
3. Graph Structural Features – Clustering
4. Message Passing & Belief Propagation
5. Graph Embeddings - Message Passing
6. PageRank & Markov Chains & Graph Queries
7. Graph Convolutional Networks
8. Graph Attention Networks
9. Graph Evolution Networks
10. Temporal Graph Networks
11. Deep Graph Generative Models
12. Causal Graph Neural Networks
13. Propagation Graph Neural Networks
    - Network Effects, Cascading and Contagion
    - Outbreak Detection and Influence Maximization

1	**Week-1** Organization	**Objectives** Team building, Setup, Topic
2–4	**Week-2** Description and Feature models	Understand a phenomenon, Extract features, Establish baselines, Preprocessing data
5–7	**Week-3** Basic Prediction models	Predict an outcome, ML architecture and pipeline
8–10	**Week-4** Advanced Prediction models	Training models, Evaluation models
11–13	**Week-5** Generative and Intervention models	Effects of interventions, Risks of confounding, Causal structure

Why do we need Graph Evolution?

Time is a feature of nodes, edges, and graphs

- Frequent versus stale relationships
- Similarity or clustering w.r.t. time

Time itself is a characteristic to be predicted

- Probability of links in time
- Network events (contagion, influence) in time

Brief (incomplete) historical perspective

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2000’s – Measuring network evolution phenomena

- Growth dynamics of the world-wide web [Huberman & Adamic 1999]
- Graphs over time densification laws, shrinking diameters and possible explanations [Leskovec et al. 2005]
- The dynamics of viral marketing [Leskovec, Adamic & Huberman 2007]

2010’s – Generative models for network evolution

- Kronecker graphs an approach to modeling networks [Leskovec et al. 2010]
- Emerging topic detection on twitter based on temporal and social terms evaluation [Cataldi et al. 2010]
- Collaboration over time characterizing and modeling network evolution [Huang et al. 2012]

2020’s – Prediction models of network evolution

- Temporal Graph Neural Networks [Rossi et al. 2020]
- Evolvegraph: Multi-agent trajectory prediction with dynamic relational reasoning [Li et al. 2020]
- Spectral Temporal Graph Neural Network for Multivariate Time-series Forecasting [Cao et al. 2020]

Topics

Structural Evolution

- Densification, Diameter Shrinking

Temporal Evolution Models

- Community Model
- Forest Fire Model
- Temporal PageRank

Temporal Gaph Models (Next Lecture)

Structural Evolution

Macro Evolution

Proportion of number of nodes and edges over time

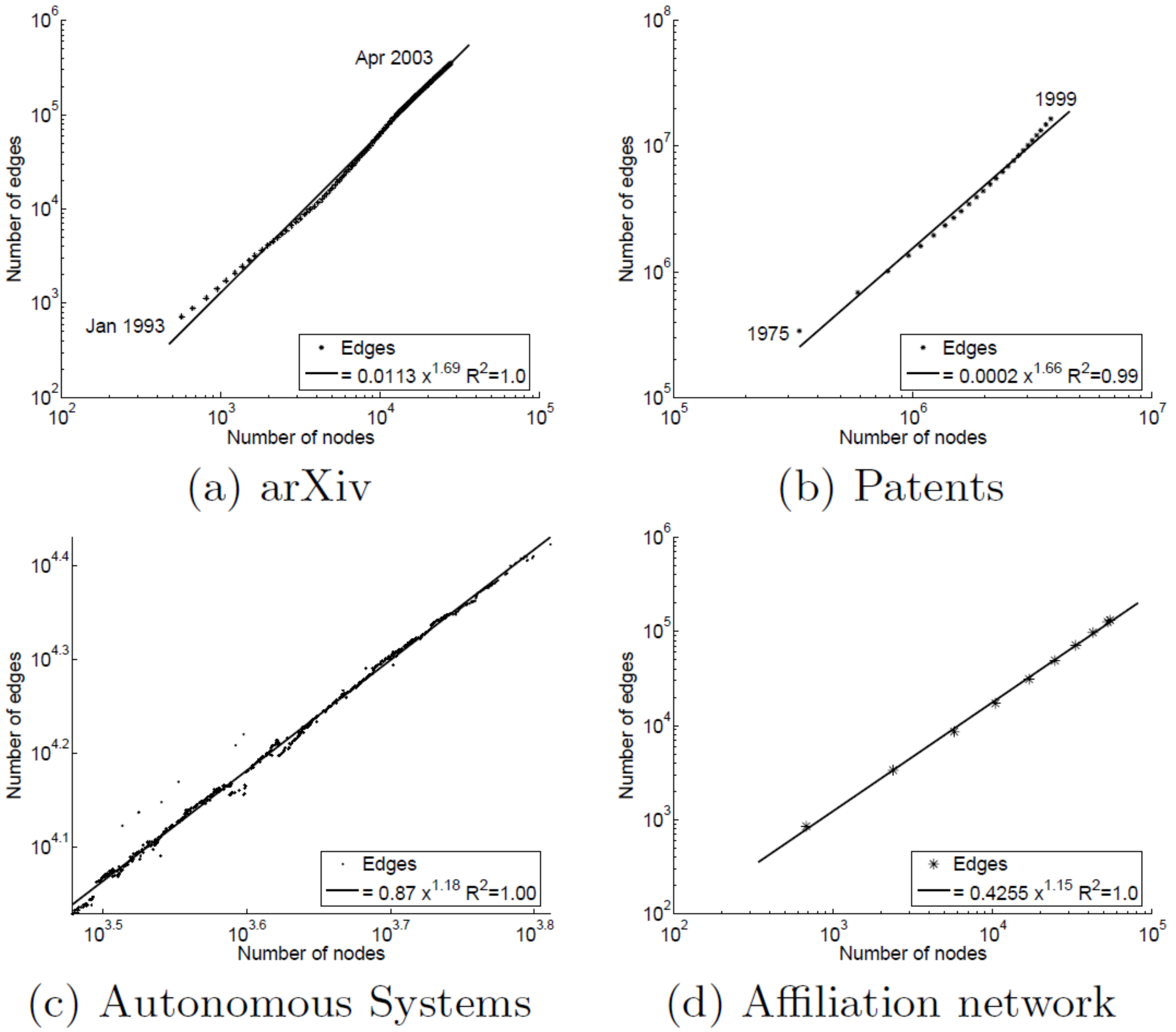
Change in diameter

Degree distribution

Connectivity

[1] https://en.wikipedia.org/wiki/Winograd_Schema_Challenge

Evolution of Edges and Nodes Distribution



Exponential growth of nodes and edges

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2005). Graphs over time: densification laws, shrinking diameters and possible explanations. In *ACM KDD* (pp. 177-187).

Network Diameter (or geodesic distance)

Network diameter $\bar{h}$: average **shortest path** length among all nodes

Path is sequence of nodes that are connected to each other

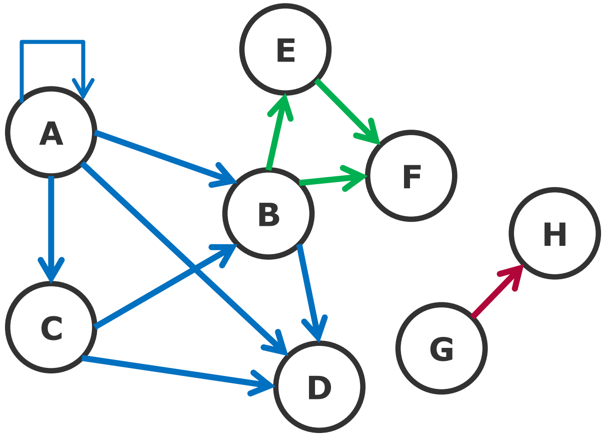
Shortest path h: is the minimal distance between nodes

$$\bar{h} = \frac{1}{2\,E_{max}} \sum_{i,j \neq i} h_{ij}$$

Maximum number of edges:

$$\mathrm{E_{max}} = \binom{N}{2} = \frac{N(N-1)}{2}$$

$h_{\mathrm{i,j}}$ is the distance between nodes *i* and *j*

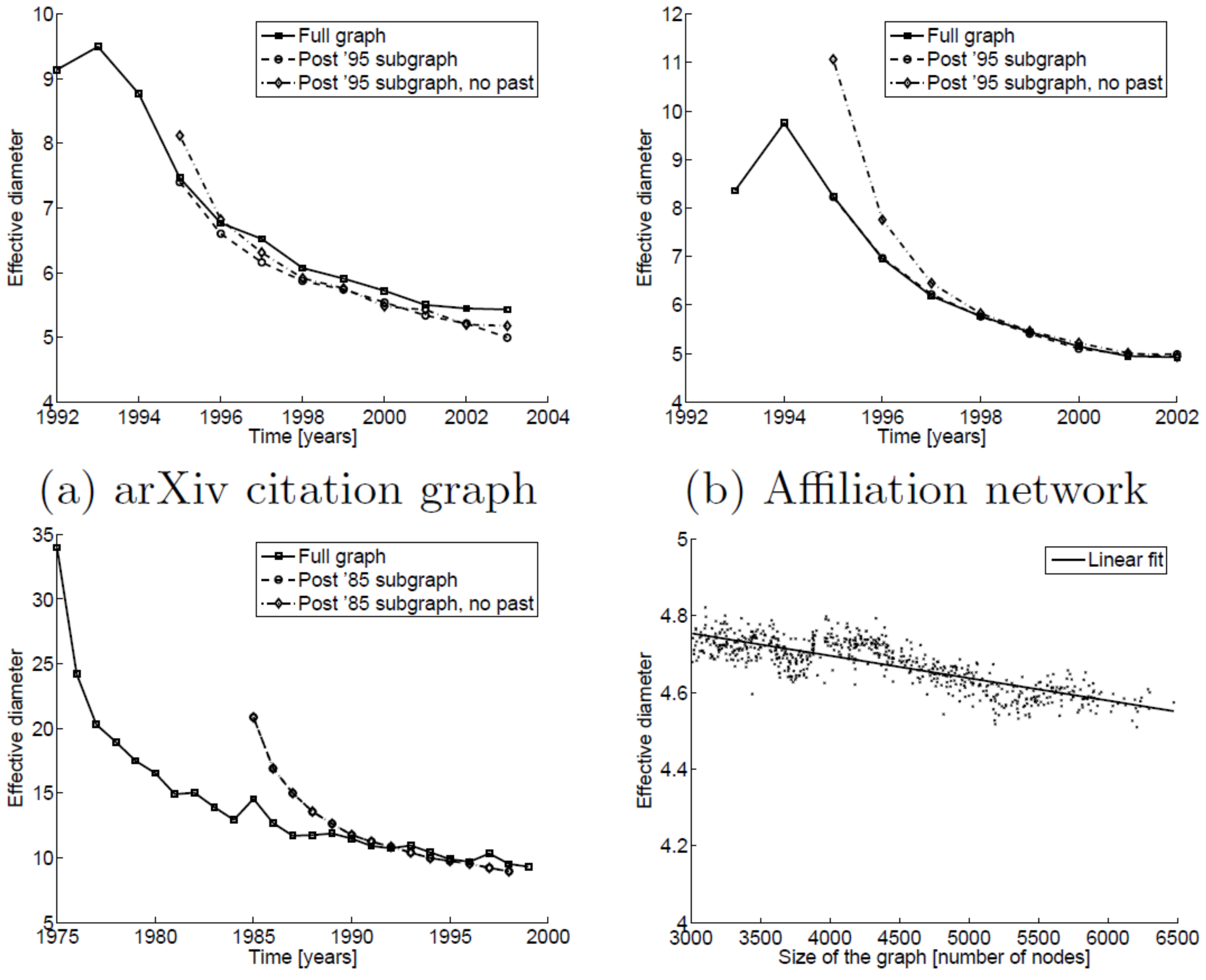


$h_{A,F} = 2$

$h_{F,A} = \infty$

$h_{A,G} = \infty$

Evolution of Diameter



(a) arXiv citation graph
(b) Affiliation network
(c) Patents
(d) AS

Shrinking diameters

AS = Autonomous System

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2005). Graphs over time: densification laws, shrinking diameters and possible explanations. In *ACM KDD* (pp. 177-187).

Evolution of Connectivity - Emergence of giant component

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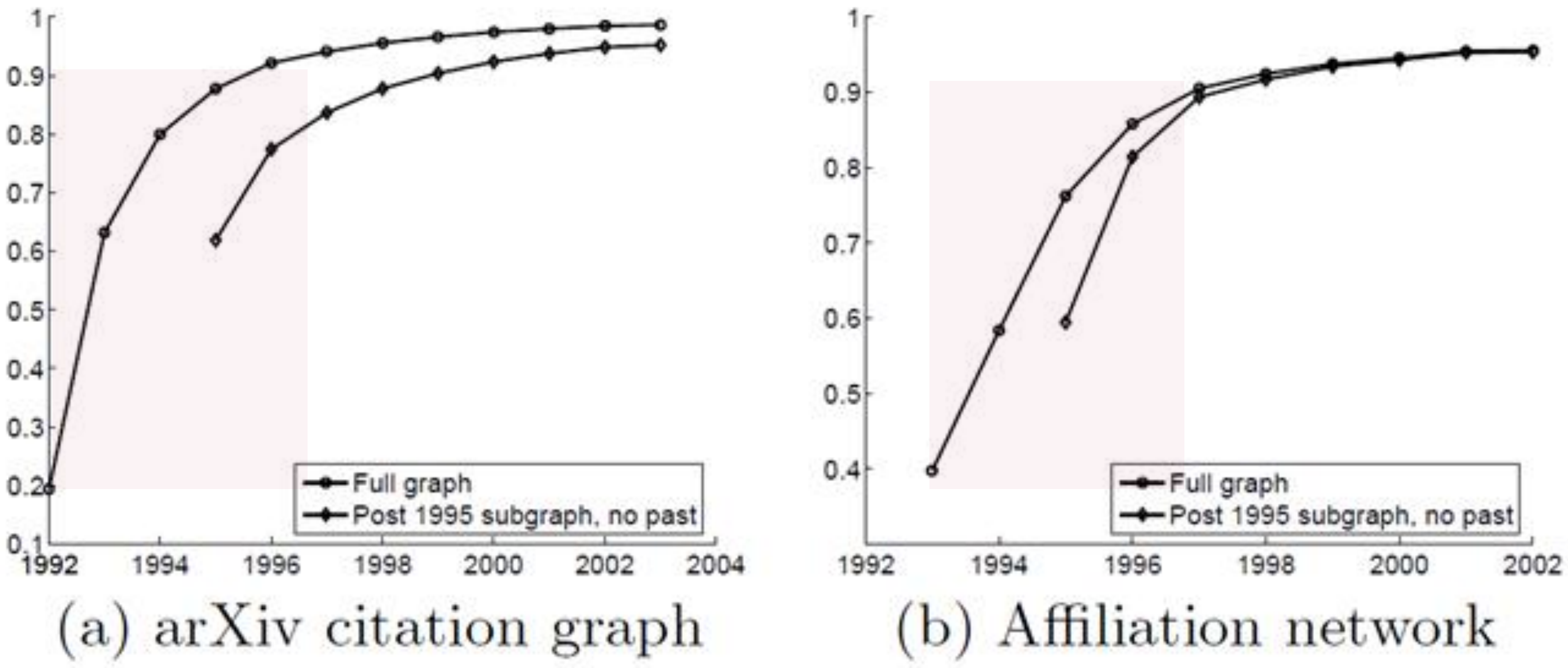
The fraction of the nodes that are part of the giant connected component over time.



After 4 years, 90% of all nodes are connected to the giant component.

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2005). Graphs over time: densification laws, shrinking diameters and possible explanations. In *ACM KDD* (pp. 177-187).

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Distribution of Node Degrees

z = average number of edges
k = degree of an edge

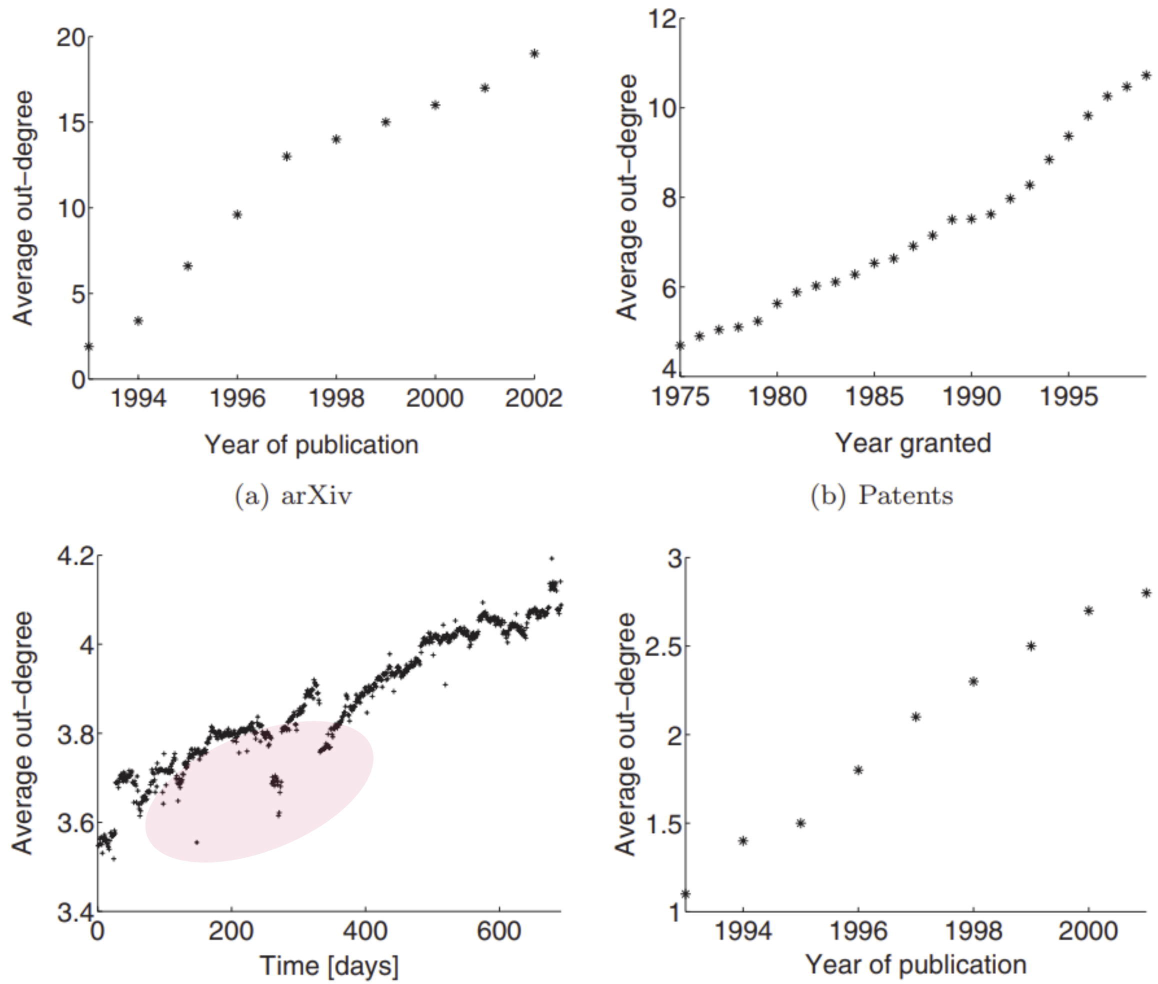
$$p_k = \binom{N}{k} p^k (1-p)^{N-k} \simeq \frac{z^k e^{-z}}{k!},$$

In the limit when N is very large.
i.e., a Poisson distribution

For the binomial distribution:
Mean $\bar{k} = p(N-1)$
Variance $\sigma^2 = p(1-p)(N-1)$

Newman, Mark EJ, Steven H. Strogatz, and Duncan J. Watts. "Random graphs with arbitrary degree distributions and their applications." *Physical review E* 64.2 (2001): 026118.

Evolution of Average degree - Densification



Linear growth of average out-degree

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2007). Graph evolution: Densification and shrinking diameters. *ACM transactions on Knowledge Discovery from Data (TKDD)*, *1*(1)

Evolution Models

Community Guided Attachment Model

Goal: approximate the power law behavior of densification

Intuitions: $\mathrm{edges(t)} \propto nodes(t)^{a}$

Densification as a process of communities within communities, hence trees.

For nodes added as leaves, $nodes = branchingFactor^{treeHeight}$

$$f(h) = c^{-h}$$

$$\begin{aligned} \bar{d} &= n^{1-\log_b(c)} && if\ \ 1 \leq c < b \\ &= \log_b(n) && if\ \ c = b \\ &= constant && if\ \ c > b \end{aligned}$$

Where:

f: is the difficulty of connecting two nodes

h: is the height of their least common ancestor (height of the smallest sub-tree containing both v and w)

$\bar{d}$: is the expected average out-degree of a node

n: number of nodes in the graph

c: is the Difficulty Constant which captures the difficulty in crossing communities

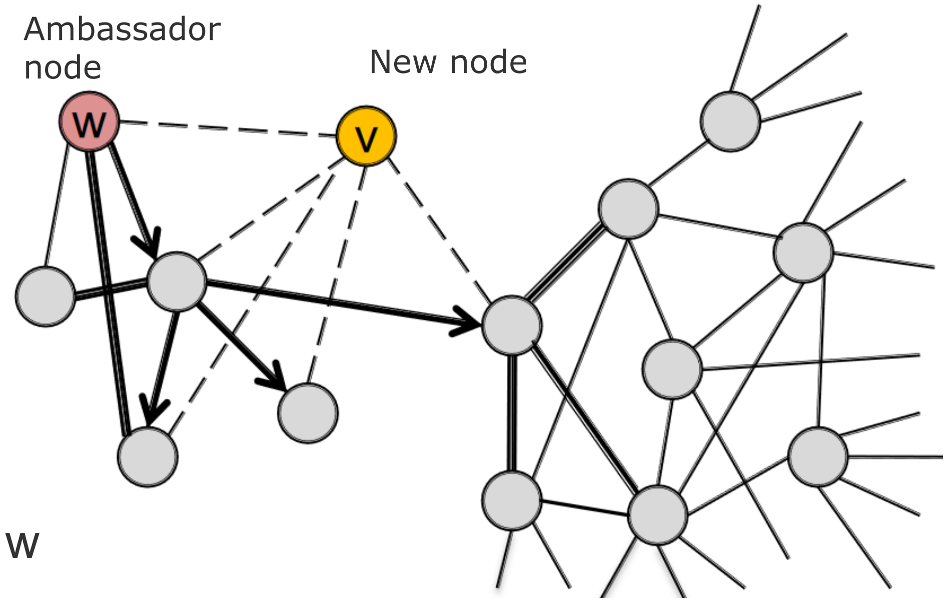
b : is the community branching factor (average number of children per node)

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2005). Graphs over time: densification laws, shrinking diameters and possible explanations. In *ACM KDD* (pp. 177-187).

Forest Fire Model

Goal: generate graphs that densify and have shrinking diameters

Intuition: create new connections by generate a recursive cascade in the graph



Procedure:

1. **Set a fire** - Uniformly at random choose an “ambassador” node w
2. **Spread the fire -** To determine the number of in and out-edges to follow, flip 2 coins sampled from a geometric distribution

   $\Pr(X = k) = (1-p)^{k-1}p$ (based on p and r)

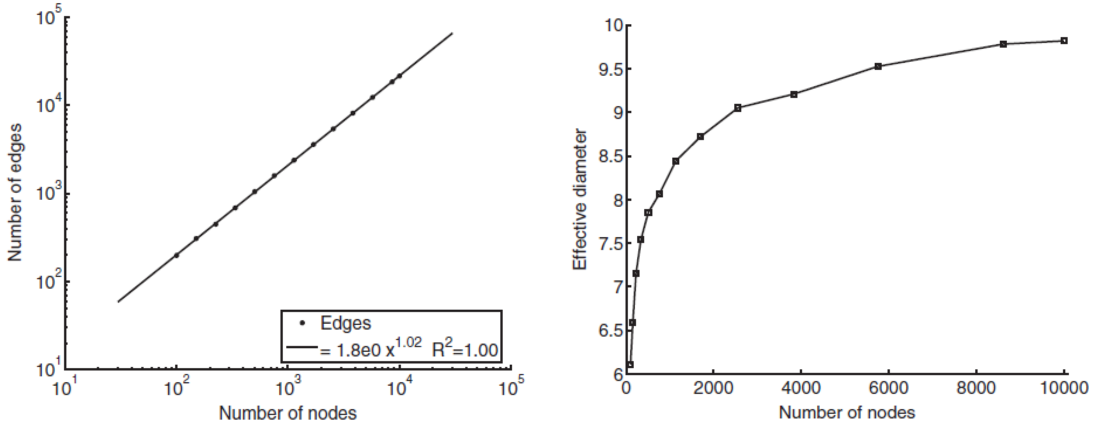
- This “Fire” spreads recursively until it dies

3. **Connect** the new node **v** to all burned nodes

Source: https://web.stanford.edu/class/cs224w/slides/16-evolution.pdf

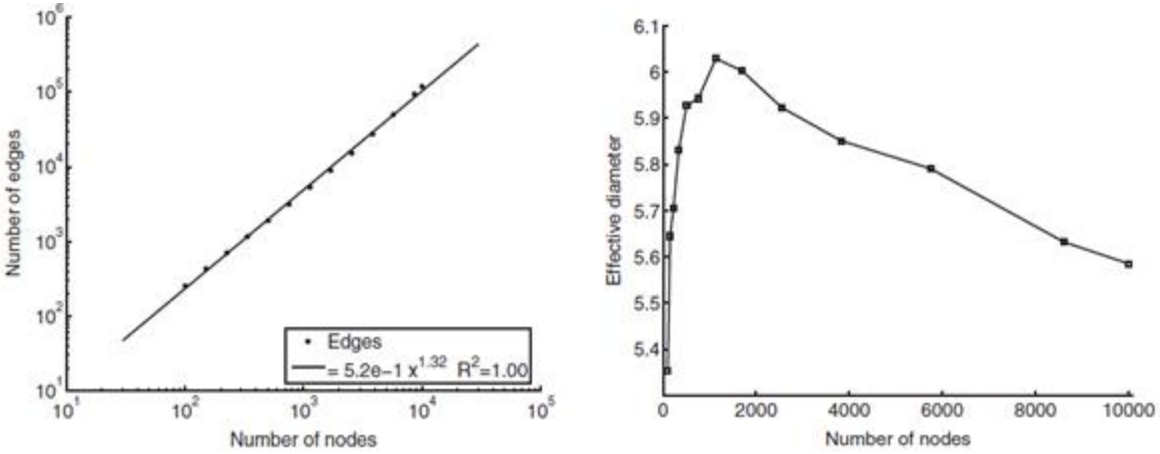
Forest Fire Results - # of edges and Effective Diameter

ARXIV



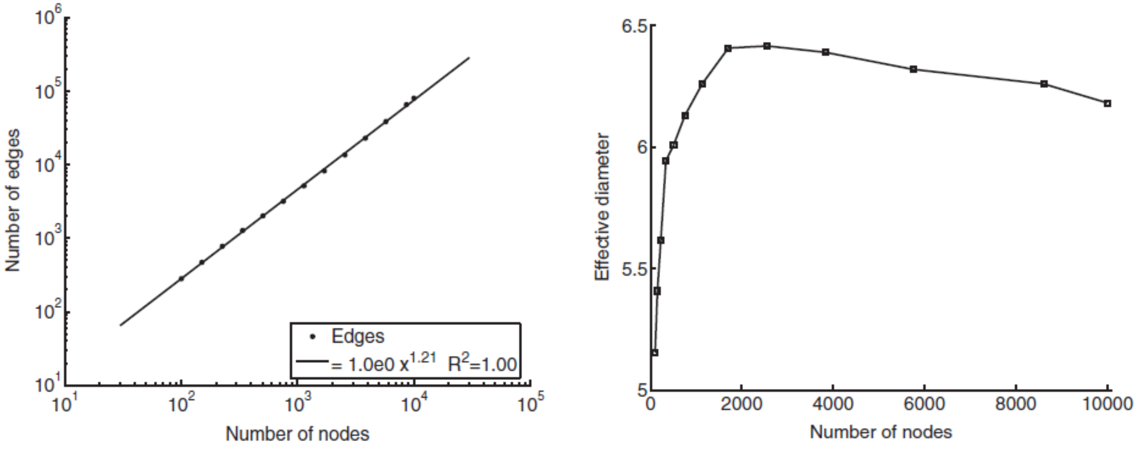
sparse graph (a =**1.01** < 2), with increasing diameter (forward-burning probability: p = 0.35, backward probability: pb = 0.20)

Affiliation Network



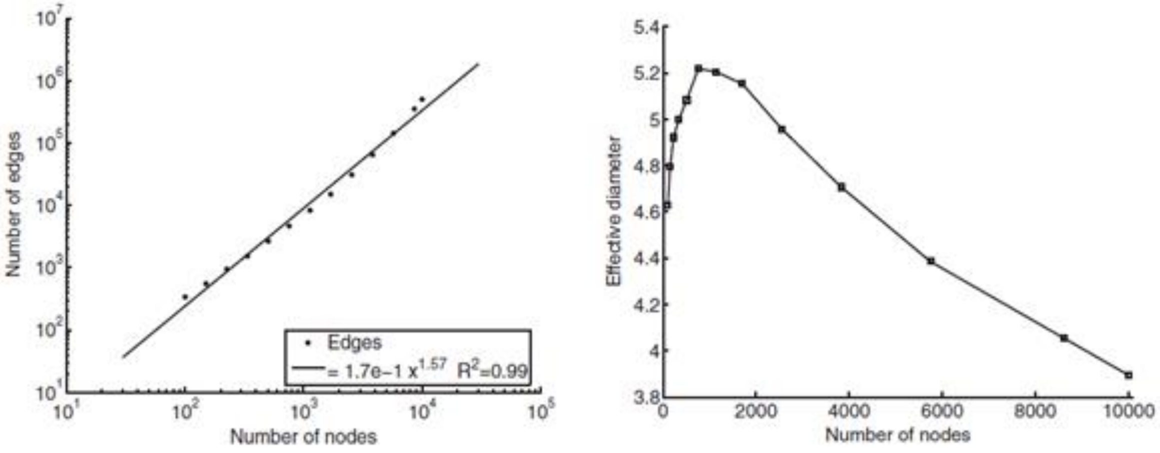
densifying graph ((a = **1.32** < 2) with decreasing diameter (p = 0.37, pb = 0.33)

Patents



densifying graph (a = 1.21 < 2) with slowly decreasing diameter (p = 0.37, p_b = 0.32).

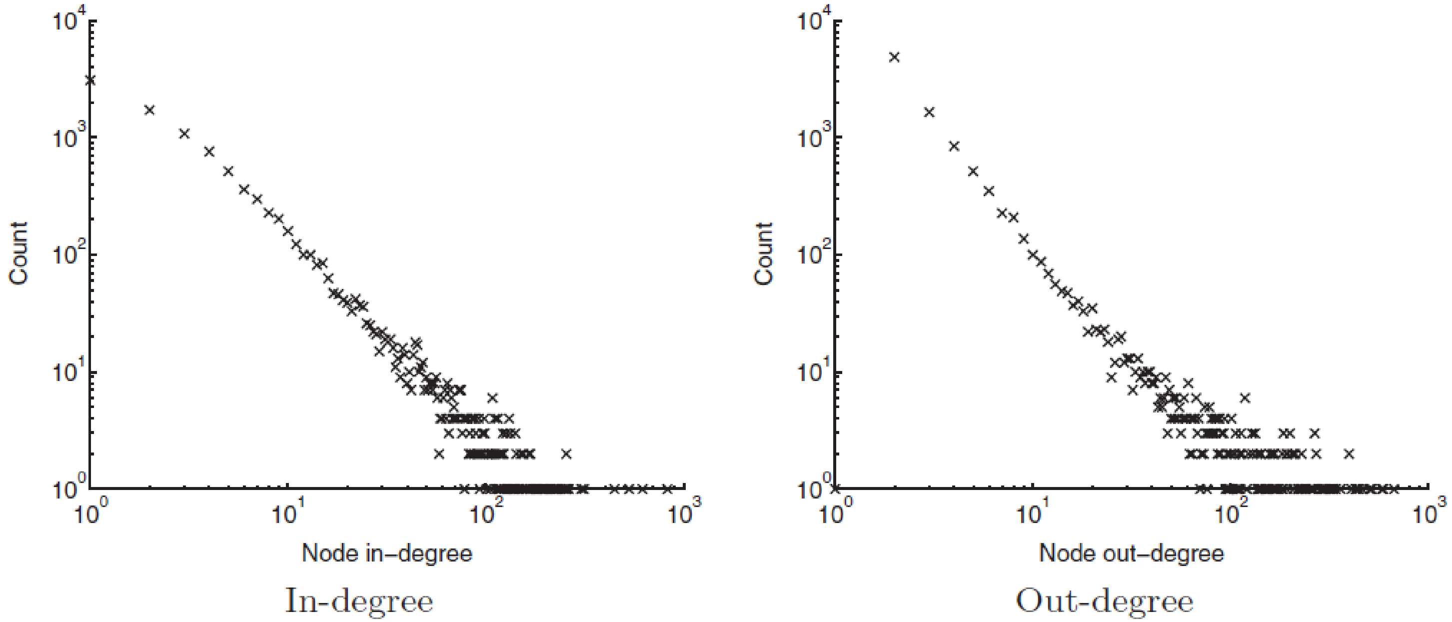
Autonomous Systems (Routers)



dense graph with densification exponent close to 2 (a = 1.57) and decreasing diameter (p = 0.38, pb = 0.35).

Source: https://web.stanford.edu/class/cs224w/slides/16-evolution.pdf

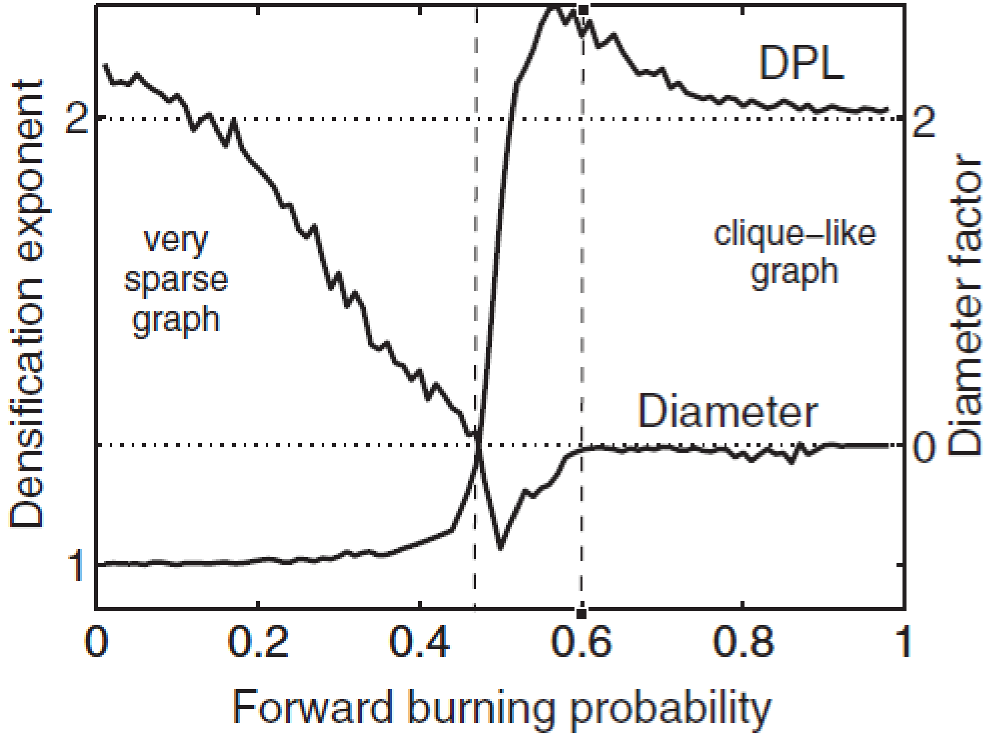
Forest Fire also generates Power law distributions



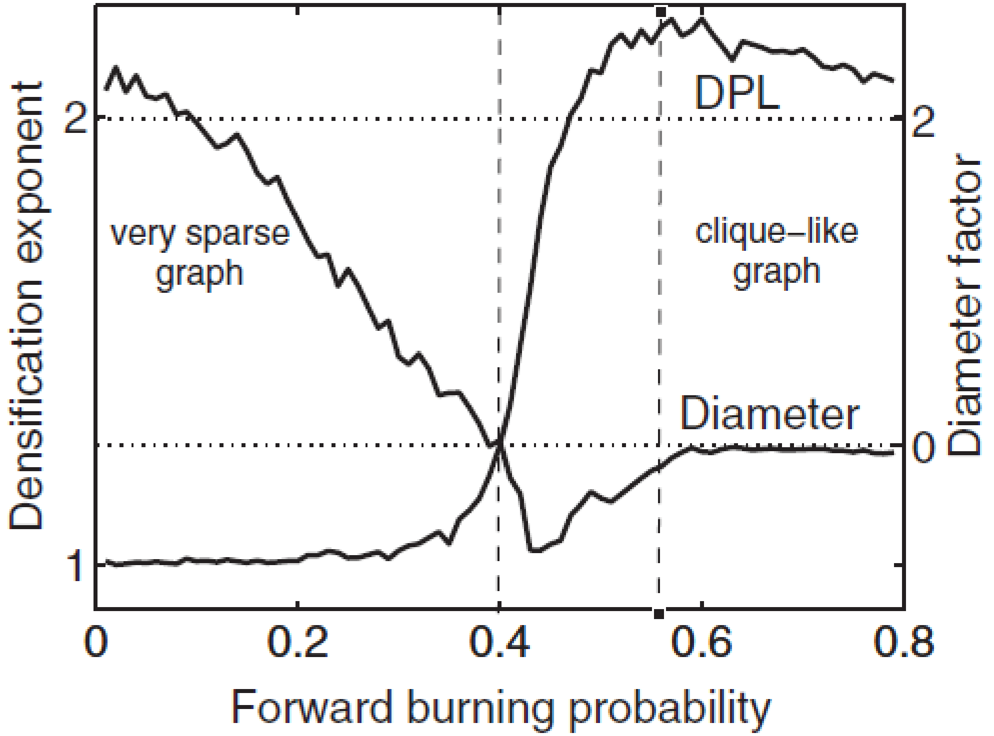
Degree distribution of a sparse graph with decreasing diameter
(forward-burning probability: 0.37, backward probability: 0.32).

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2007). Graph evolution: Densification and shrinking diameters. *ACM transactions on Knowledge Discovery from Data (TKDD)*, *1*(1)

Forest Fire Sweet spot



fix burning ratio, *r* = 0.5 and vary forward-burning probability *p*



fix backward-burning probability *pb*= 0.3 *and* vary forward-burning probability *p*

Leskovec, J., Kleinberg, J., & Faloutsos, C. (2007). Graph evolution: Densification and shrinking diameters. *ACM transactions on Knowledge Discovery from Data (TKDD)*, *1*(1)

Temporal Page Rank

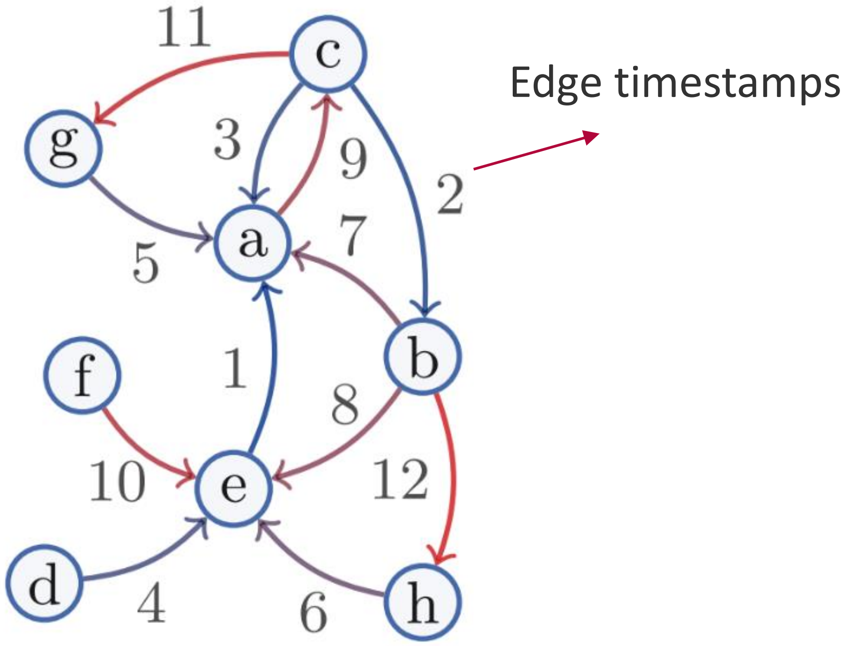
Goal: Make a random walk only on temporal or time-respecting paths

Intuition: Run a regular PageRank on a time-augmented graph

Time stamps increase along the path

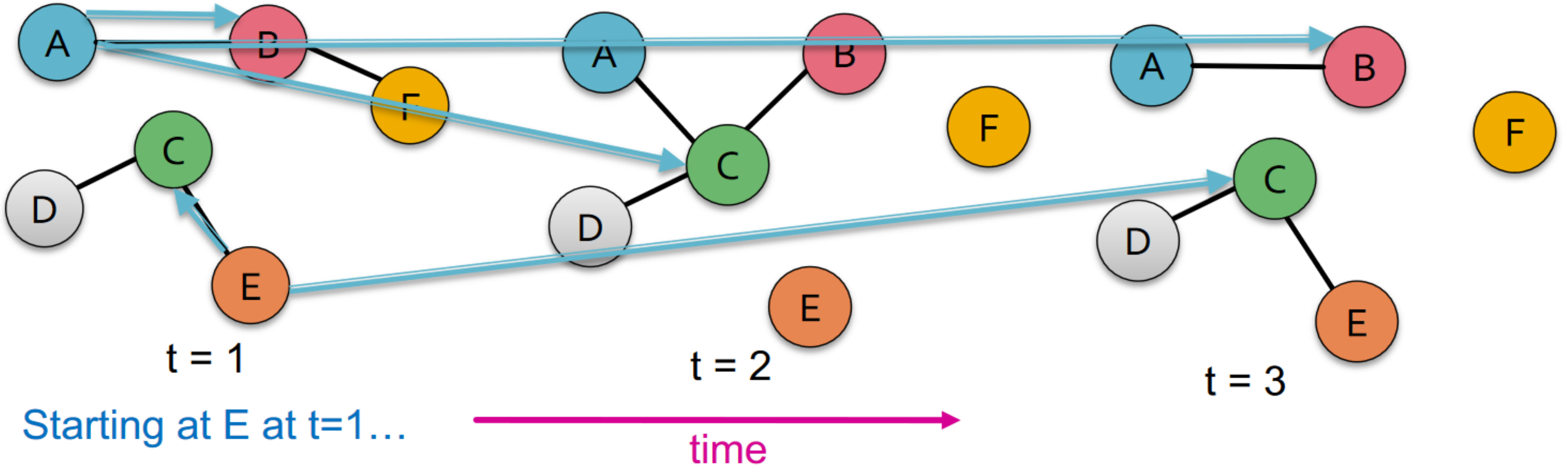
c → b → a → c: time respecting

a → c → b → a: not time respecting



https://web.stanford.edu/class/cs224w/slides/16-evolution.pdf

Temporal PageRank – Augmented Graph

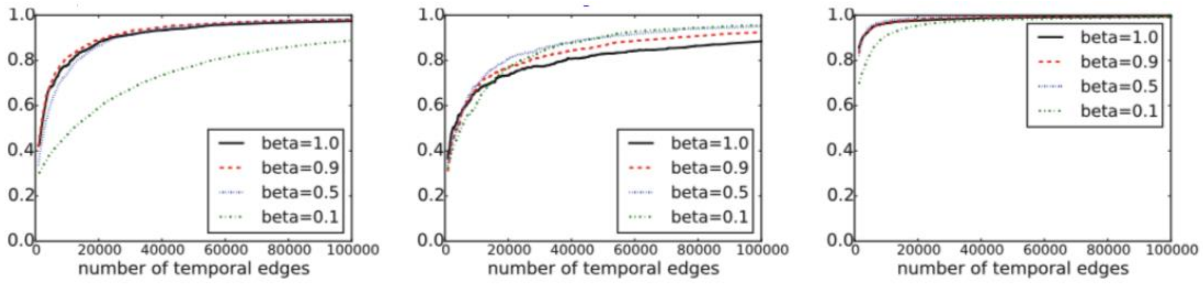


$r(u)$: Temporal PageRank estimate of u

$$r(u,\textcolor{red}{t}) = \sum_{v \in V} \sum_{k=0}^{\textcolor{red}{t}} (1-\alpha)\alpha^k \sum_{\substack{z \in Z(v,u|\textcolor{red}{t}) \\ |z|=k}} P[z|\textcolor{red}{t}]$$

$Z(v,u|t)$ is a set of all possible temporal walks from v to u **until time t**
α is the probability of starting a new walk

Rank quality (Pearson corr. coeff. Between static and temporal PageRank) and transition probability β



(a) *Facebook* (b) *Twitter* (c) *Students*

Smaller β corresponds to slower convergence rate, but better correlated rankings

https://web.stanford.edu/class/cs224w/slides/16-evolution.pdf

Next: Temporal Graph Models

- Temporal Graph Neural Networks [Rossi et al. 2020]
- EvolveGraph: Multi-agent trajectory prediction with dynamic relational reasoning [Li et al. 2020]
- Spectral Temporal Graph Neural Network for Multivariate Time-series Forecasting [Cao et al. 2020]
- Suggestions?

Next and Future Tasks

1. Compute and compare graph metrics (Wednesday, 2.12)
   - Any metrics and networks of your choice
2. First draft of **abstract** (Friday, 4.12)
3. Predictions using traditional method (Wednesday, 9.12)
   - Any two methods of your choice
4. Related work draft (Friday, 11.12)
5. Node and Graph Feature Learning (Wednesday, 16.12)
   - Any two methods of your choice
6. Design alternative pipelines for your GNN (Wednesday, 06.01)
   - Three alternative with different options for embedding, aggregation, and enconding
   - Test at least one.

END