Diffusion on complex networks: algorithmic foundations

Anil Kumar S. Vullikanti Dept. of Computer Science and Virginia Bioinformatics Institute Virginia Tech





Acknowledgements

Joint work with:

- NDSSL members including: Madhav Marathe Henning Mortveit, Maleq Khan, Zhao Zhao, Chris Kuhlman, Samarth Swarup
- □ S. S. Ravi, SUNY Albany
- Dan Rosenkrantz, SUNY Albany
- □ Aravind Srinivasan, University of Maryland
- Rajmohan Rajaraman, Northeastern University
- □ Ravi Sundaram, Northeastern University

Diffusion models and applications



Graph connecting different entities
 Nodes change state based on their neighbors' states



Wide variety of models for different applications

Broad goals

Motivation: wide variety of diffusion processes are used in different applications

 Can be formulated by similar fundamental questions in terms of graph dynamical systems

Goals:

- Modeling and analysis of complex networks
- Characterize dynamical properties, especially in terms of the underlying graph structure
- Techniques to optimize and control dynamics

Challenges

Underlying complex networks

- Analytical approaches based on renormalization and differential equation methods not easily applicable
- Network structure not well understood need for better models
- □ Characterization of dynamical properties
 - Need to identify new properties
- □ Need for new scalable computational approaches
 - Poor locality
 - High expansion and large separators
 - Dynamics on and of networks
 - Co-evolution between networks and diffusion process
 - Behavioral changes

Models of Complex Networks



- Very simple models
- Main goal: capture degree distribution
 well understood analytically

 Based on hypotheses of social evolution ("rich get richer", etc.) Combination of optimization
 objectives with
 random evolution

Most realistic

 Useful for network/policy planners

 Need lot of data, models and HPC tools



[Li, et al., 2005]



[Borner, et al., 2007]





Beyond degree distributions

□ Edge swap operations

- Preserves degree distribution
- Polynomial time mixing [Feder et al., 2005]

 Disease dynamics not completely determined by degree distribution
 Need random graph models to preserve non-local properties







Changes in disease dynamics with edge swaps

Outline for the rest of the talk

- Part I: Modeling and analysis of complex networks
 - Map-reduce based algorithms for relational subgraph analysis
- Part II: Dynamical properties: mathematical and computational aspects
 - Characterize different local diffusion models and techniques for controlling dynamical properties
- □ Part III: Simulation tools for diffusion models
 - Malware spread in large proximity networks

PART I: MODELING AND ANALYSIS OF VERY LARGE GRAPH PROPERTIES

Summary of contributions

- "First principles" approach for synthetic social and infrastructure networks
 - Integrates a large number of diverse public and commercial data sets
 - Stochastic models that capture properties of real networks
- □ Computing properties of very large networks
 - Efficient sampling based approaches for computing structural properties
 - Mapreduce/Hadoop based for relational subgraph analysis
 - New parallel algorithms for dynamical properties

General goal



Non-induced embedding:

 $f: V' \to V$ such that $(u, v) \in E' \Rightarrow (f(u), f(v)) \in E$

Goal: find one or more embeddings of labeled subgraph H in G

Motivation and applications: data mining, social networks, Semantic web



[Brochelor et al]: query of the form $\mathbf{v_1}, \mathbf{v_2}, \mathbf{v_3}, \mathbf{p}$ such that $\mathbf{v_1}$ is a faculty member at UMD, $\mathbf{v_2}$ is an Italian university, who is a friend of $\mathbf{v_1}$ and $\mathbf{v_3}$ has commented on paper p by $\mathbf{v_1}$



- Detecting fraud in financial transactions [Bloedorn et al.]
- Other applications: connection subgraphs [Faloutsos, et al.]

Motivation and applications: systems, networking and software engineering

d



- [Maxwell et al.] discovering graph grammars corresponding to memory leaks
- Automatic custom instruction set generation by enumerating convex subgraphs [Bonzini et al.]
- Mining call graphs to localize software bugs [Eichiner et al.]
- Other applications: anomaly detection in networks through subgraph analysis [Noble et al.]

Motivation and applications: bioinformatics



[Alon et al.] Characterization of protein-protein interaction networks based on differences in counts of trees on 9 nodes





Variations: subgraph enumeration problems

□ Functions on the space of embeddings

- Existence and counting all occurrences
- Functions of labels as part of embeddings
- Approximate embeddings
- Relational queries
 - Involving node and edge labels
 - Specified by graph grammars
- □ Motifs and most frequent subgraphs
 - Contrast with random graphs with similar properties

Graphlets

Generalization of degree distribution

Summary of results

- □ SAHad: randomized Hadoop based algorithm for enumerating trees and tree-like subgraphs
 - For given ε , δ : produces (1± ε) approximation with probability ≥ 1- δ
 - Worst case work complexity bound of $O(2^{2k}m f(\varepsilon, \delta))$
 - Scales to graphs with over 500 million edges and templates of size up to 12
 - Color-coding technique for approximate enumeration
- Heterogeneous computing environments
 - Different clusters and amazon EC2 without any system level optimization

Summary of results (continued)

□ Broad class of relational subgraph queries

- Node and edge labeled subgraphs
- Extension to tree-width bounded subgraphs (low treewidth = like trees)
- Can easily compute classes of distributive functions on the space of embeddings
- Can extend to weighted and approximate matches
- Systematic approach to handle queries specified by a class of tree grammars (chain grammars)
- Graphlets and motifs

Prior approach and challenges

- □ Large literature on frequent subgraph enumeration and variations: Apriori, FSG,...
 - Maintain candidate matches for subgraphs with k-1 edges, and extend to subgraph with k edges
 - Backtracking/extensive bookkeeping to ensure valid matches
 - Scales to ~100,000 node graphs, not clear how to parallelize
 - No rigorous worst case bounds
- Database techniques: preprocessing based on fixed distribution of queries
- Dynamic programming based on color-coding
 - No prior parallelization

Attempt: divide and conquer



Could identify embeddings of $\rm H_1$ and $\rm H_2$ and put them together?

But ... overlaps possible





Need to keep track of extra information to avoid overlaps between embeddings of sub-templates

Color-coding idea



[Alon, Yuster, Zwick, 95]

- Basic idea: color graph with k = |H| distinct colors and only count colorful embeddings.
- Dynamic programming to count number of colorful embeddings.
- If G is colored uniformly at random, number of embeddings is proportional to #colorful embeddings:

Pr[given embedding of H is colorful] = $\frac{k!}{k^k}$ $E[\# \text{ colorful embeddings of } H \text{ in } G] = \frac{k!}{k^k}(\# \text{ embeddings})$

Dynamic programming for paths

- Let col(v) denote color of node v
- Let C(v, S) be the number of embeddings of colorful paths of length |S| using set S of colors, that end at node v.

$$C(v, \{\ell\}) = \begin{cases} 1 & \text{if } col(v) = \ell \\ 0 & \text{else} \end{cases}$$

$$C(v,S) = \sum_{w:(v,w)\in E} C(w,S - \{col(v)\})$$

Goal: compute
$$\frac{1}{2}\sum_{v}C(v,\{1,\ldots,k\})$$



Dynamic programming for paths

- Let col(v) denote color of node v
- Let C(v, S) be the number of embeddings of colorful paths of length |S| using set S of colors, that end at node v.

$$C(v, \{\ell\}) = \begin{cases} 1 & \text{if } col(v) = \ell \\ 0 & \text{else} \end{cases}$$

$$C(v,S) = \sum_{w:(v,w)\in E} C(w,S - \{col(v)\})$$

Goal: compute
$$\frac{1}{2}\sum_{v}C(v,\{1,\ldots,k\})$$



Mapreduce/Hadoop



- D Powerful framework for processing large amount of streaming data
 - Developed by Google for web applications [Dean and Ghemavat, 2005]
 - Open source implementation: Hadoop
- Mapreduce internally sorts key-value pairs and reorganizes items with same key value for reducer
 - Mapper produces key-value pairs for each data item
 - Reducer processes all elements with same key
 - Can be repeated multiple times
 - System takes care of producing data streams and sorting

Graph algorithms using Mapreduce/Hadoop

- □ Finding paths and diameter
- □ Pagerank and other random walk based measures
- Community detection and clustering problems
- □ Subgraph analysis
 - Counting #triangles: [Pagh et al., 2011], [Suri et al., 2011]
 - Subgraph enumeration to ~100,000 node graphs: [Liu et al., 2009]

Extension to trees

- Partition T into sub-trees T = {T₁, T₂, ..., T_r}. T_i has children child₁(T_i) and child₂(T_i) and root ρ(T_i).
- Recursively compute C(v, ρ(T_i), S): #colorful embeddings of T_i using set S of colors (|S| = |T_i|) in which v is mapped to ρ(T_i) using the following recurrence

$$C(v, \rho(T_i), S) = Z \cdot \sum_{u, S_1, S_2} C(v, \rho(child_1(T_i)), S_1) C(u, \rho(child_2(T_i)), S_2)$$

where the summation is over all valid S_1, S_2, Z is a scaling factor



SAHad: mapreduce implementation

- Partition T into set $T = \{T_1, \ldots, T_r\}$ of sub-trees. Let *child*₁(T_i) and *child*₂(T_i) be child sub-trees of T_i .
- Color each node in G uniformly at random using colors from {1,..., k}
- Repeat for $T_i \in T$
 - Map: takes in input of the form ⟨v, ρ(T_j), C(T_j): count for each subset S ⊂ {1,...,k} with |S| = |T_j|, neighbors of v⟩ Produces key= u, value= C(T_j), for each neighbor u of v
 Reduce: takes in input of the form: key= v, and values C(C₁(T_i)) and C(C₂(T_i)) Use recurrence to compute C(v, ρ(T_i), S) = ∑_{u∈N(v)} ∑_{S1,S2} C(v, ρ(child₁(T_i)), S₁)C(u, ρ(child₂(T_i)), S₂), where summation is over all S₁ ∪ S₂ = S, |S₁| = |child₁(T₁)| and |S₂| = |child₂(S₂)|

Performance analysis

LEMMA

Consider any node v and template T_i .

The input and output sizes for a Counter.Mapper instance, corresponding to v and T_i are O((^k_{|child1(Ti)|}) + (^k_{|child2(Ti)|}) + d(v)) and O(((^k_{|child1(Ti)|}) + (^k_{|child2(Ti)|}))d(v), respectively.
The size of the input to any Counter.Reducer is O(((^k_{|child1(Ti)|}) + (^k_{|child2(Ti)|}))d(v), and the corresponding work complexity is O((^k_{|child1(Ti)|}) (^k_{|child2(Ti)|})d(v)).

THEOREM

For any given $\epsilon, \delta > 0$, SAHAD produces a $(1 \pm \epsilon)$ approximation to the total number of embeddings with probability at least $1 - \delta$, and has a total total work complexity of $O(|E|2^{2k}e^k \log (1/\delta)\frac{1}{\epsilon^2})$.

Experiments: setting

Network	No. of Nodes(in million)	No. of Edges(in million)
Miami	2.1	105.4
Chicago	9.0	537.9
GNP100	0.1	2.0

Different templates



Computing resources

- Athena: 42 node cluster with 32 cores per node
- Amazon EC2

Performance analysis: time & space



Variation with #reducers per node



Total running time vs #reducers per node

Total running time for different tasks

running time (min)

7 reducers on each node 15 reducers on each node number of the reducers number of the reducers **Distribution of total** running time of reducers

running time (min)

Athena: one disk per node

□ Many reducers: contention for disk

Summary of experimental results

Experiment	Computing resource	Template and network	Key observations
Approximation error	Athena	U7; GNP	Error below 0.5%
Impact of number of data nodes	Athena	U10; Miami, GNP	scale from 4 hours to 30 minutes with data nodes from 3 to 13
Impact of #concurrent reducers	Athena, EC2	U10; Miami	Non-monotone variation in running time
Impact of #concurrent mappers	Athena, EC2	U10; Miami	Time generally constant
Unlabeled/labeled template	Athena, EC2	Varying templates 7-12	< 35 minutes
Graphlets	Athena	U5; Miami, Chicago	< 35 minutes

PART II: DYNAMICS & CONTROL

Diverse diffusion processes

Graph dynamical system: contact graph, node states, local functions, update order



Example: ratcheted threshold-2 model

Model	Description	Example Applications
Percolation and extensions: SI/SIS/SIR/Independent cascades	Each <i>red</i> node infects each <i>blue</i> neighbor independently with some probability	Malware, failures, infections
Complex contagion: threshold and variants	Each <i>blue</i> node switches to <i>red</i> if at least	Spread of innovations, peer pressure
Non-monotone multi- threshold models	Thresholds for switching from <i>blue</i> to <i>red</i> and from <i>red</i> to <i>blue</i>	More complex social behavior
Voter models	Each node picks the state of a random neighbor	Spread of ideologies
Constrained network	Flows with node/link capacities and	Packet flows, traffic,

Key Questions

Understanding Dynamical Properties	Computational aspects	Interventions to control the dynamics
 Existence and characteristics of fixed points E.g.: average #nodes in state 1 in fixed point Transient lengths Stability How do changes in graph, update order or functions alter dynamics? Who becomes "infected"? Impact of network structure 	 Computing different dynamical properties <i>Reachability</i>: does the system reach specific configurations of interest? <i>Predecessor existence</i>: what kind of configurations could lead to the current one? Simulation tools that scale to large systems 	 Forcing node states: changing local functions Freezing selected nodes in a specific state Malware spread (SIS/SIR): anti-virus patches Influence spread (threshold): choose sources to seed spread Voter models: make some nodes stubborn Changes in the graph Add/delete edges to indirectly alter dynamics

Summary of results

- □ Analyzing dynamical properties
 - Stability in threshold systems
 - Characterization of limit cycles and fixed points in bi-threshold systems
 - Impact of structural properties: identifying static graph properties
- □ Efficient algorithms for computing dynamical properties
 - Efficient algorithms and scalable simulation tools for computing dynamical properties
- Control and optimization of the dynamics
 - Influence maximization in voter dynamics
 - Critical sets to control diffusion in SIR (e.g., vaccinations) and threshold models (countering influence)
 - Game theoretical analysis of distributed interventions

Specific results: controlling diffusion in threshold systems

- Goal: choose to remove critical set of at most k nodes/edges so that diffusion starting from set l is minimized
 - Variations: minimize number of infections, maximize number of uninfected nodes, different initial conditions (S chosen from distribution).
- NP-hard to approximate within factor of O(n^δ) for any δ < 1, in general.
- Bicriteria-approximation for threshold 1 (simple contagion): choose k/e nodes to remove, so that number of infections is at most 1/(1 − e) times optimal.
- Threshold more than 1: more complex heuristics that work better than high degree based approaches.

Bicriteria approximation for threshold=1



Flow based algorithm

- Construct flow network with $M = \infty, b = k/OPT$
- Output edges in minimum (s, t)-cut (S, \overline{S})

LEMMA

Let (S, \overline{S}) be the minimum s, t-cut. Then, $|(S - \{s\}, \overline{S} - \{t\})| \le 2k$ and the number of infected nodes, $|S - \{s\}|$ is at most twice the optimal

Suppose (X, \overline{X}) is the optimal cut in the original graph. Then, $|(X \cup \{s\}, \overline{X} \cup \{t\})| \le k + b \cdot OPT$.

② $|(S,\overline{S})| = |(S - \{s\}, \overline{S} - \{t\})| + (|S| - |I|)b \le k + b \cdot OPT$, which implies $|(S - \{s\}, \overline{S} - \{t\})| \le 2k$ and $|S| - |I| \le 2OPT$.

Bi-threshold model: limit cycles and fixed points

state of $v = \begin{cases} 1 & \text{if } \geq k^{\uparrow} \text{ 1-neighbors} \\ 0 & \text{if } < k^{\downarrow} \text{ 1-neighbors} \end{cases}$

Non-monotone dynamics: more realistic model of agent behavior



Theorem

Consider a bi-threshold system with thresholds $k^{\uparrow}, k^{\downarrow}$.

- If the system is synchronous, all limit cycles are of length at most 2.
- If the system is asynchronous: if k[↓] k[↑] ≤ 1, all limit sets are fixed points. Otherwise, there can exist arbitrarily long limit cycles (even on a tree).
- If the system is asynchronous and the graph is a tree, with $k^{\uparrow} = 1, k^{\downarrow} = d(v) + 1$, all limit sets are fixed points.

Proof: fixed points for trees

$$k^{\uparrow}=1,k^{\downarrow}=d(v)+1\Rightarrow$$

v switches from 0 to 1 if it has at least one 1-neighbor, and from 1 to 0 if it has at least one 0-neighbor

Proof by induction

- Without loss of generality, can assume permutation π updates nodes level by level, with the higher numbered levels first.
- Inductive hypothesis: if x → x', then for each node v other than the root, x'_v = x_{p(v)}, where p(v) is the parent of v
- Base case. v is a leaf \Rightarrow following cases
 - $x_{p(v)} = 1$: irrespective x_v either 0 or 1, $x'_v = 1$
 - $x_{p(v)} = 0$: irrespective x_v either 0 or 1, $x'_v = 0$
- Inductive step: consider interior node v. For each child w of v, we have x'_w = x_v, by induction. Therefore, as in the case of leaves, we will have x'_v = x_{p(v)}
- Again by induction, it follows that after the *i*th iteration, all nodes in the first *i* levels have the same state as the root.

PART III: EFFICIENT SIMULATION TOOLS

Summary of results: efficient computational tools

- EpiFast: Epidemics on large social-contact networks
- EpiCure: spread of malware in proximity networks
 InterSim: HPC framework based on graph dynamical systems

Malware on hybrid wireless networks

- Malware: from nuisance to a threat
- Challenges and tools needed
 - Multiple scales: Bluetooth to Internet; selfforming; resistant to regulation
 - Need to model mobility, multi-level network representation to capture interactions between humans and devices, and behavioral changes
 - Modeling and simulation of malware spread: more abstract models and efficient simulation tools that scale to large networks

Key questions

- Detect and understand characteristics of the spread of new worms
- Identify vulnerable devices and networks
- Strategies to control the spread: anti-virus patches, quarantining



"Human mobility and wireless networks could abet the spread of mobile malware" – Jon Kleinberg, Nature 2008

Current approaches: broad spectrum

Compartmental model

- Assume complete mixing population
- **G** Random waypoint mobility



Detailed modeling of all device states

Does not scale beyond networks with few hundred devices

Motivating question: approach that captures worm characteristics reasonably well, but scales to very large graphs

Our approach: EpiCure

- Malware modeled as a stochastic diffusion processes.
- High resolution models of synthetic social contact networks, mobility and call behavior
 - First principles based approach, integrates over 14 different public and commercial data sets
 - Detailed model of movement and activities of people in urban regions
 - Can explicitly incorporate behavioral changes in model
- EpiCure: HPC modeling and simulation environment to study mobile malware in large dynamic networks
 - <u>Generic</u>: can work with generic malware models and networks (user inputs)
 - <u>Scalable</u>: Scales to large realistic *dynamic* networks
 - <u>Expressive</u>: Allows one to study a large class of adaptive and non-adaptive responses





Approach and key techniques for scaling



- □ Approach
 - Network-based representation
 - Probabilistic timed transition system (PTTS) motivated by human epidemics
 - Bluetooth specific states abstracted out
 - State reduction by offline traversal
 - Threading based optimization
 - Error less that 5%
 - Scales to millions of devices



Approach and key techniques for scaling



□ Approach

- Network-based representation
- Probabilistic timed transition system (PTTS) motivated by human epidemics
- Bluetooth specific states abstracted out
- State reduction by offline traversal
- Error less that 5%
- Scales to millions of devices



Sample results: simulation setup

Factorial experiment design		
Network	Area	Chicago Downtown area (zip 60602)
	Demographics	People in age group of 20 – 50 years
	People (devices); locations	30000; 4400
	Smart device ownership	100% - every individual in the demographic has a smart phone
Simulation	Replicates	5
	Duration of Simulation	8 hours (8 AM to 4 PM), typical work schedule
	Initially infected	1%,5%,10%
	Wallclock	Max 2 hours (lower when responses are implemented)
	Infection seed	8 AM
Sensitivity analysis	Malware parameters	Idle time, p _{to}
	Network parameters:	Market share (m), Location Density (d)
Response mechanisms	Static	Degree and Betweenness centrality
	Device-based detection	Passive self detection, local and centralized signature dissemination
Results		Cumulative infection size
		T(q,x): time taken to infect q percent of devices when x is varied

Sample results: mobility matters



Activity-based mobility model



Random Waypoint mobility model





Results: controlling malware spread

Setting: detection by activity monitoring

- □ System call, power signature or behavior based detection
- Require some number of occurrences before detection: "self detection threshold"
- Use self detection for automatic signature generation: local and centralized signature dissemination



Centralized dissemination is more effective than local

Computational contributions

- Speed and Parallelization
 - Sequential EpiCure 300X faster than NS-2
 - Speedups are obtained with <5% loss in accuracy
 - Parallel implementation: Hybrid MPI-threads improves efficiency for multi-core clusters
- Scale and Complexity
 - Scales to 3-5 million devices
 - Heterogeneous and realistic spatial networks
 - Time Varying Networks

	500 Devices	3—5 M devices	
ns-2	45-50 hrs	Cannot Study	
EpiCure	10 minutes (0.1% error, comp. NS-2)	1.5 hrs (<5% error comp. EpiCure v1.0)	

New model reduction and algorithmic techniques needed to scale and parallelize: EpiCure is the first modeling environment that can represent and study malware over urban scale, time varying and heterogeneous networks

Summary of computational contributions

	Simulation based computational models			
Factors	Random Mobility [Yan et al. ACSAC '06, ASIACCS '07]	Real Mobility Data [Wang, Nature '09]	EpiCure Environment	
Scope	1 location	Large area	Large area	
Temporal Scale	ms. / μs.	Time unit (time to infect)	Time units (TUs)	
Spatial Scale	meters	Cell tower region, uniform	meters	
Network size	500 – 1000 devices	6 million	3-5 million	
Within-host Malware Model	Detailed implementation	Compartmental model (SI)	High fidelity malware model, specific to the malware & Bluetooth protocol. Can implement other manifestations.	
Mobility model	Random Waypoint, Random Walk, Random Landmark	Cell tower position from mobile call data	Activity-based mobility model, activity location for each individual	
Device interaction network	Based on mobility models	Homogeneous distribution of devices in each tower region	High resolution network, pair-wise interaction model	
Detection	Can be implemented	Not studied, difficult to implement	Detection based on infection propagation	
Control mechanisms	Can be implemented	Not studied and not easy to implement	Self detection, signature dissemination schemes & co-evolution of networks	
Network co- evolution			Co-evolution of networks can be modeled and studied	

Summary

Graph dynamical systems

- Rich framework to capture a wide variety of diffusion phenomena
- Challenging algorithmic problems, need new computational tools

□ Fundamentally new computational challenges

- Very large heterogeneous graphs
- Cannot be easily partitioned
- Non-uniform communication patterns: difficult to parallelize in conventional models

Thank you