AFRL-AFOSR-VA-TR-2015-0262

Statistical Inference for Detecting Structures and Anomalies **in Networks**

Cris Moore
SANTA FE INSTITUTE OF SCIENCE INC

08/27/2015
Final Report

Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/ RTC
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
27-08-2015

2. REPORT TYPE
Final

3. DATES COVERED *(From - To)*
9/1/2014 – 5/31/2015

4. TITLE AND SUBTITLE
Statistical Inference for Detecting Structures and Anomalies in Networks

5a. CONTRACT NUMBER
N/A

5b. GRANT NUMBER
FA9550-12-1-0432

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Cristopher Moore

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Santa Fe Institute
1399 Hyde Park Road
Santa Fe, NM 87505

8. PERFORMING ORGANIZATION REPORT NUMBER
Final

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Office of Science and Research
875 Randolph Street
Suite 325 Room 3112
Arlington, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)
AFOSR

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
Final

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for Public Release DISTRIBUTION A

13. SUPPLEMENTARY NOTES

14. ABSTRACT

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15. SUBJECT TERMS
Network data, Social networks, networks of communications and interactions, heath or disease networks, and brain networks

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Cristopher Moore
U	U	U	UU	6	**19b. TELEPHONE NUMBER** *(Include area code)* (505) 946-2763

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Statistical Inference for Detecting Structures and Anomalies in Networks:
Final Report, June 2014–May 2015

Cristopher Moore, Santa Fe Institute
Aaron Clauset, University of Colorado
Mark Newman, University of Michigan

Abstract

Work under this grant focused on methods for extracting hidden information from network data, including data from social networks, networks of communications and interactions, heath or disease networks, and brain networks. During the last 12 months of this project, the funding level was cut substantially. Nevertheless, over this period, our team worked on several substantial projects, including the development of several powerful new algorithms for analyzing networks and their application to specific real-world domains. These efforts produced 8 peer-reviewed papers or new preprints, and more than a dozen invited or contributed presentations on these projects.

We continued to focus on developing powerful and scalable Bayesian statistical and related inference methods for community structure, hierarchies, core-periphery structure, rankings, and other large-scale network structures, and on discovering the fundamental limits of these techniques for inferring such hidden patterns. Additionally, we focused on algorithms applicable to very large networks, networks with auxiliary information (such as annotations, temporal dynamics, or edge weights), and demonstrations of these techniques to domains of interest.

In particular, we discovered new phase transitions in the detectability of hidden community structure in both unsupervised and semisupervised settings, and in time-evolving networks; developed message-passing approaches for models of recurrent epidemics on social networks; demonstrated how our probabilistic models can help distinguish distinct edge formation mechanisms; developed a novel approach to identifying hidden core-periphery structure in networks; and developed a new algorithm for both identifying and characterizing change points in the structural patterns of temporal networks.

No future work is anticipated for this project, as this is the final report for the grant.

Over the past 12 months, we made further progress on our Phase II tasks as described in our proposal and our 2014 statement of work, along with selected ongoing tasks from Phase I and tasks from Phase III for which we made early progress.

1.1 Incorporating auxiliary information
1.2 Scalability
1.4 Ranking in directed networks
1.5 Compensating for partial or noisy data
1.6 Guided exploration of the network
1.7 Anomaly detection in dynamic networks

Our progress on these tasks is detailed below, which has produced 8 peer-reviewed papers or new preprints, as well as numerous colloquia, seminars, and conference presentations.

In particular, we made significant progress on the following problems, models, and algorithms:

- Scalable algorithms for detecting statistically-significant communities and hierarchical structure, using techniques from spin glasses and message-passing for modularity.

- The performance of semisupervised learning in networks, which we discovered undergoes a phase transition in accuracy when the amount of available metadata crosses a critical threshold.
- Inferring social status and niche status in social and ecological networks.
- Inference algorithms for identifying vertices with high centrality or importance, and hidden "core-periphery" structure in networks.
- Detecting "change points" in dynamic networks, where new structural patterns occur.
- Scalable algorithms for detecting community structure in dynamic networks, along with the discovery of a detectability phase transition as a function of the rate of change and the strength of the community structure.
- Efficient modeling and prediction of epidemic models, including threshold models and recurrent disease models such as SIS and SIRS.

1 Scalable detection of statistically significant communities

Moore, postdoc Zhang
Research Tasks 1.1, 1.3 and 1.5

Modularity is a popular measure of assortative community structure, which measures the number of links internal to communities as compared to what we would expect from a null model where the network is rewired randomly. However, maximizing the modularity can lead to many competing partitions, which have almost the same modularity but which have little in common with each other; it can also overfit, producing illusory "communities" in random graphs where none exist. We address this problem using the tools of statistical physics and spin glass theory. Algorithmically, we use the modularity as a Hamiltonian, compute the marginals of the resulting Gibbs distribution, and assign each node to its most-likely community under these marginals. In contrast to the "ground state" where the modularity is maximized, which is prone to overfitting, this marginal-based partition measures statistically-significant community structure. In essence, it represents the consensus of many high-modularity partitions, as opposed to the single "best" one.

We have derived an efficient Belief Propagation (BP) algorithm to compute these marginals, with a tunable temperature parameter. In random networks with no true communities, the system has two phases as we vary the temperature: a *paramagnetic phase* where all marginals are equal, and a *spin glass phase* where BP fails to converge. In networks with real community structure, there is an additional *retrieval phase* where BP converges, and where the marginals are strongly correlated with the underlying communities. We show analytically and numerically that our algorithm works all the way down to the detectability transition in networks generated by the stochastic block model. Our algorithm is highly scalable: each update takes time linear in the number of edges (with a prefactor proportional to the number of groups) and even on large networks it converges rapidly.

By applying our algorithm recursively, subdividing communities until no statistically-significant subcommunities can be found, we can detect hierarchical structure in real-world networks more efficiently than previous methods. For instance, applied to the popular network data set of political blogs, our algorithm first finds two large communities corresponding to liberals and conservatives, and agreeing with the ground-truth labels on 95% of the nodes. However, our algorithm also finds subcommunities at multiple scales.

We have tested our algorithm against many other popular techniques, including Louvain, Infomap, and OSLOM, and it significantly outperforms them. We also found large statistically-significant communities in several networks where previous literature had claimed they do not exist.

Since the last report, this work has been extended and published.

- P. Zhang and C. Moore, "Scalable detection of statistically significant communities and hierarchies: message-passing for modularity." *Proc. Natl. Acad. Sci. USA* **111** (51), 18144–18149 (2014). Preprint: `http://arxiv.org/abs/1403.5787`

2 Phase transitions in semisupervised learning in networks

Moore, postdoc Zhang, collaborator Zdeborová
Research Tasks 1.1, 1.5 and 1.6

In many networks, nodes have attributes or metadata. If these are known for some subset of the nodes, we would like to be able to make good guesses about the others, filling in our missing information about the network. Our belief propagation algorithms give a scalable and mathematically principled way to do this, in time nearly-linear in the network size. Starting with the known labels, we propagate the probabilities of different labels to the rest of the network, until we reach a fixed point.

We have found that there is often a sudden jump in the accuracy we can achieve, as a function of the fraction of nodes for which the labels are known. When this fraction is too small, we have only local information, about the known nodes and their neighbors. But when this fraction crosses a critical threshold, our knowledge becomes global, percolating throughout the entire network and letting us accurately predict almost all the nodes. Using the cavity method of statistical physics, we have given an efficient BP algorithm for propagating this information, and computed the critical threshold for networks generated by the stochastic block model. With a simplified analysis, we can determine the threshold exactly, showing how the existence of multiple fixed points causes a first-order transition where the accuracy jumps discontinuously. We have found qualitatively similar behavior in real networks.

Since the last report, the final paper on this topic was completed and subsequently published.

- P. Zhang, C. Moore, and L. Zdeborová, "Phase transitions in semisupervised clustering of sparse networks." *Physical Review E* **90**, 052802 (2014). Preprint: `http://arxiv.org/abs/1404.7789`

3 Probabilistic models of status and ranking

Clauset and Moore, grad student Jacobs, collaborator Dunne
Research Tasks 1.4 and 1.6

Characterizing the structural roles of vertices in networks remains an important open problem, with most work focusing on "centrality" heuristics that often have uncertain theoretical relevance to particular networks. In this work, we adapt a flexible probabilistic model of vertex position or status, originally developed in mathematical ecology as a model of food webs and called the probabilistic niche model, to the task of characterizing the positional structure of vertices within arbitrary networks.

We apply a powerful multi-temperature Monte Carlo technique from statistical physics called *parallel tempering* for sampling and optimizing the posterior distribution of models. This technique has not previously been applied to estimating network models, but provides excellent results in this case. We then use this technique to address an outstanding problem in the theory of food webs, namely whether parasites and free-living predators play different structural roles. While ecological networks are not currently an area of DARPA concern, we regard this as valuable test bed for developing techniques and algorithms that can address analogous problems in social, technological, and brain networks: specifically, to test for statistically significant heterogeneities in network structure, based on physical location, social status, or other continuous-valued correlates.

We use three tests: (i) calculated goodness-of-fit measures of learning within-class edges when the model is shown only a single class or shown both classes of vertices together, (ii) comparing network structural statistics between the empirical network and networks generated from the learned models, and (iii) calculated link-prediction accuracy when the model is shown only a single class or shown both classes together. By measuring AUC statistics for link prediction, we are able to assess which types of links are well-fit by the model, and which it considers anomalous.

Since the last report, this paper has been submitted to a journal and is currently being revised for resubmission.

- A. Z. Jacobs, C. Moore, J. A. Dunne and A. Clauset, "Untangling the roles of parasites in food webs with generative network models." Submitted (2015).
  Preprint: `http://arxiv.org/abs/1505.04741`

4 Identifying core-periphery structure in networks

Newman, graduate students Zhang and Martin
Research Tasks 1.2 and 1.4

Many networks can be usefully decomposed into a dense core plus an outlying, loosely-connected periphery. Here we propose an algorithm for performing such a decomposition on empirical network data using methods of statistical inference. Our method fits a generative model of core-periphery structure to observed data using a combination of an expectation–maximization algorithm for calculating the parameters of the model and a belief propagation algorithm for calculating the decomposition itself. We found our method to be efficient, scaling easily to networks with a million or more nodes. We tested it on a range of networks, including real-world examples as well as computer-generated benchmarks, for which it successfully identifies known core-periphery structure with low error rate. We also demonstrated that the method is immune from the detectability transition observed in the related community detection problem, which prevents the detection of community structure when that structure is too weak. There is no such transition for core-periphery structure, which is detectable, albeit with some statistical error, no matter how weak it is.

- T. Martin, X. Zhang, and M. E. J. Newman, "Identification of core-periphery structure in networks." *Physical Review E* **91**, 032803 (2015).
  Preprint: `http://arxiv.org/abs/1409.4813`.

5 Detecting statistically significant structural changes in evolving networks

Clauset, postdoc Peel
Research Tasks 1.1 and 1.7

Relational variables among objects or people are a common form of data, and networks provide a general framework through which to quantify and analyze their patterns. For example, online social interactions, offline friendships, and object-user interactions may all be represented as networks. In many cases, these relations are dynamic, and their evolution over time may be represented as a sequence of networks, each giving the interactions among a common set of vertices at consecutive points in time.

A key task in detecting anomalies in evolving networks is *change-point detection*, in which we (1) identify moments in time across which the large-scale pattern of interactions changes fundamentally and (2) quantify what kind and how large a change occurred. Identifying the timing and shape of such change points divides a network's evolution into contiguous periods of relative structural stability, allowing us to subsequently analyze each period independently, while also providing hints about the underlying processes shaping the data.

We model the network structure with a novel generative model that generalizes the classic hierarchical random graph model (previously developed by Clauset, Moore and Newman, *Nature* 2008). This GHRG model compactly captures nested community structure at all scales in a network. We then use this model in a classic change-point detection framework, in which we compare a change versus a no-change model within a sliding window on the network time series, via a generalized likelihood ratio test, in order to identify statistically significant change points.

Previous approaches to change-point detection in networks involved representing the sequence of networks as a time-series of summary statistics (e.g., mean degree, clustering coefficient, mean geodesic distance). Although useful for detecting some types of change points, we demonstrate that these methods *fail* to detect changes, up to 80% of the time, even when the structural change is large enough that *our approach is able to detect the change 100% of the time*.

We present a taxonomy of different types and sizes of network change points and a quantitative characterization of the difficulty of detecting them, in synthetic network data with known change points. We then test the method on three real, high-resolution evolving social networks of physical and digital interactions (the Enron email corpus, MIT Reality Mining physical proximity networks, and Hypertext 2009 physical proximity network), showing that it accurately recovers the timing of known significant external events.

Since the last report, this paper has been published and we have begun applying the technique to new sources of social and epidemiological network data.

- L. Peel and A. Clauset, "Detecting change points in the large-scale structure of evolving networks." Proc. of the 29th International Conference on Artificial Intelligence (AAAI), 2914-2920 (2015).
  Preprint: `http://arxiv.org/abs/1403.0989`
  Code: `http://gdriv.es/letopeel/proximitynetwork.html`

6 Detectability thresholds and optimal algorithms for community structure in dynamic networks

Clauset and Moore, grad student Ghasemian, postdocs Zhang and Peel
Research Tasks 1.1, 1.2, and 1.7

Community detection in dynamic networks inherits many of the challenges of community detection in static networks, including learning the number of communities, their sizes and node membership, and the pattern of connections among communities, e.g., assortative, disassortative, core-periphery, etc. It also poses new challenges, because both the network edges and the community memberships may evolve over time. A common approach is to simply take the union of dynamic graphs over a certain time window, and treat the resulting graph with techniques from static network analysis, thereby ignoring the dynamics within the window. In this project, we explicitly model the dynamic nature of these networks and the way community memberships change over time, integrating information about the communities in an optimal way.

Here, we study the fundamental limits on learning latent community structure in dynamic networks. Specifically, we study dynamic stochastic block models where nodes change their community membership over time, but where edges are generated independently at each time step. In this setting (which is a special case of several existing models), we are able to derive the detectability threshold exactly, as a function of the rate of change and the strength of the communities. Below this threshold, we claim that no algorithm can identify the communities better than chance. We then give two algorithms that are optimal in the sense that they succeed all the way down to this limit. The first uses belief propagation (BP), which gives asymptotically optimal accuracy, and the second is a fast spectral clustering algorithm, based on linearizing the BP equations along the lines of previous work under this grant. We verify our analytic and algorithmic results via numerical simulation.

- A. Ghasemian, P. Zhang, A. Clauset, C. Moore and L. Peel, "Detectability thresholds and optimal algorithms for community structure in dynamic networks." Submitted (2015).
  Preprint: `http://arxiv.org/abs/1506.06179`

7 Efficient prediction of epidemic models and threshold models

Moore, grad student Shrestha, collaborator Scarpino
Research Task 1.2 and Uses Cases

Given an epidemic model, we would like to calculate the probability that a given node becomes infected, given a particular initial condition. This initial condition might consist of a set of infected individuals, or the set of initial adopters of a behavior or trend; it might also be probabilistic, assigning each individual some initial probability of being infected. These models are stochastic: each individual passes the infection on to its neighbors at a certain rate, which we model as a Markov process in continuous time. The straightforward way to compute these probabilities is to simulate the model many times, performing many independent runs. However, this is computationally expensive, especially if we also want to sweep the space of parameters or initial conditions: for instance, to fit the model to real-world epidemic data, or to search for effective intervention strategies.

Following Karrer and Newman (*Phys. Rev. E* **82**, 016101 (2010)), we developed a dynamic message-passing (DMP) approach to this problem, that applies also to threshold models of behavior popular in sociology: these are models, first proposed by Granovetter, where each individual has to hear about a trend or behavior from some number of neighbors being adopting it themselves. This work appeared in our previous report.

Since then, we have successfully extended this work to more complex epidemic models, and in particular "recurrent" models such as SIS and SIRS, where multiple waves of infection can pass through the population. In these models, the method of Karrer and Newman cannot be applied directly, since nodes can return to previous states (such as when an infected individual becomes susceptible again). We have developed a new class of differential equations for these models. Our methods are much faster than direct simulation, and they are also more efficient than the so-called "pair approximation" currently used in epidemiology, especially for complex epidemic models where individuals have multiple states.

- M. Shrestha, S. Scarpino, and C. Moore, "Message-passing approach for models of recurrent epidemics in networks." *Physical Review E* **92**, 022821 (2015).
  Preprint: `http://arxiv.org/abs/1505.02192`

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The full title of the funded effort.

Statistical Inference for Detecting Structures and Anomalies in Networks

Grant/Contract Number
AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".

FA9550-12-1-0432

Principal Investigator Name
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Cristopher Moore

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Bhawana Sharma

Reporting Period Start Date

9/1/2014

Reporting Period End Date

5/31/2015

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P. Zhang, C. Moore, and L. Zdeborova, "Phase transitions in semisupervised clustering of sparse networks." Physical Review E 90, 052802 (2014). http://arxiv.org/abs/1404.7789

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C. Aicher, A. Z. Jacobs and A. Clauset, "Learning latent block structure in weighted networks." Journal of Complex Networks 3(2), 221-248 (2015). http://arxiv.org/abs/1404.0431

Changes in research objectives (if any):

N/A

Change in AFOSR Program Manager, if any:

N/A

Extensions granted or milestones slipped, if any:

N/A

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
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