REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
07-06-2012	Final Report	1-Oct-2007 - 30-Sep-2011

4. TITLE AND SUBTITLE
Final report: Structure and Dynamics of Complex Networks

5a. CONTRACT NUMBER
W911NF-07-1-0637

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

6. AUTHORS
Jian Liu, Eric Vanden-Eijnden, Weinan E, A. Nadar, Tiejun Li, Hao Shen, D. Crommelin, Jianfeng Lu

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
Princeton University
Office Of Research & Project Administration
The Trustees of Princeton University
Princeton, NJ 08544 -0036

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

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

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
52266-MA.1

12. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
In a series of papers, we have proposed mathematical framework for analyzing community structure in complex networks. Our work is based on analyzing the structure of the Markov chain that arises naturally in such networks. We also proposed the concept of diffusion complex, which is the analog of Witten complex for diffusion processes. This allows

15. SUBJECT TERMS
complex networks, clustering, dynamics, diffusion complex, landscapes

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		Weinan E
					19b. TELEPHONE NUMBER 609-258-3683

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Final report: Structure and Dynamics of Complex Networks

ABSTRACT

In a series of papers, we have proposed mathematical framework for analyzing community structure in complex networks. Our work is based on analyzing the structure of the Markov chain that arises naturally in such networks. We also proposed the concept of diffusion complex, which is the analog of Witten complex for diffusion processes. This allows us to analyze the landscapes of complex networks.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

1. Weinan E and Jianfeng Lu, Diffusion Complexes, submitted.

2. Weinan E, Jianfeng Lu and Yuan Yao, The landscape of complex networks, preprint.

Number of Presentations: 2.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper
2012/06/07 1(3	Madar, A., Greenfield, A., Ostrer, H., Vanden-Eijnden, E. & Bonneau, R. The inferelator 2.0: A scalable framework for reconstruction of dynamic regulatory network models, 31st Annual International Conference of the IEEE Engineering in Medicine and Biology Society: Engineering the Future of Biomedicine. 2009/09/03 00:00:00, . : ,

TOTAL: 1

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
2012/06/07 1(	8	Jian Liu,, Tiejun Li,, Weinan E. Probabilistic framework for network partition, Physical Review E (12 2007)
2012/06/07 1(	5	Sarich, M., , Schütte, C. & , Vanden-Eijnden, E. Optimal fuzzy aggregation of networks, Multiscale Modeling and Simulation (01 2010)
2012/06/07 1(	6	Schütte, C., , Noé, F.,, Lu, J., , Sarich, M. & , Vanden-Eijnden, E. Markov state models based on milestoning, Journal of Chemical Physics (01 2011)
2012/05/31 2(	2	D. Crommelin,, E. Vanden-Eijnden. Data-based inference of generators for markov jump processes using convex optimization", Multiscale Modeling and Simulation, Multiscale Modeling & Simulation (03 2009)

TOTAL: 4

Number of Manuscripts:

Books

Received Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Elected SIAM Fellow, 2009.
Awarded the Kleinman Prize by SIAM, 2009

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Tiejun Li	0.50
Jianfeng Lu	0.10
Frank Noe	0.10
FTE Equivalent:	**0.70**
Total Number:	**3**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Weinan E	0.20	
Eric Vanden-Eljnden	0.20	
FTE Equivalent:	**0.40**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME	
Total Number:	

Names of personnel receiving PHDs

NAME	
Jianfeng Lu	
Lin Lin	
Xiang Zhou	
Total Number:	**3**

Names of other research staff

NAME	PERCENT_SUPPORTED
Jian Liu	0.50
FTE Equivalent:	**0.50**
Total Number:	**1**

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

1. Defined mathematical framework for network partition using the theory of lumpable Markov chains.
2. Defined mathematical framework for probabilistic network partition.
3. Introduced and analyzed diffusion complex.
4. Introduced landscapes for networks. This greatly helped for revealing the structure of the networks.

Technology Transfer

Final Report: Theory and Algorithms for Network Clustering

Weinan E

1 Problem

The main objective of this project is to establish the mathematical foundation and develop efficient numerical algorithms for network clustering or network partition. Network clustering is a rather popular subject in network science. However, with very few exceptions, most work in this area focuses on specific algorithms rather than the mathematical foundation of the problem. In other words, they discuss directly "how to do it" before formulating clearly "what needs to be done". This kind of approach is fairly common in computer science: Much attention is given to developing algorithms rather than formulating clearly the mathematical problem.

Given a complex network, it is of great interest to reduce the network to a much smaller one. In the context of Markov chains, this issue is closely related to the issue of lumpability of a Markov chain: If a Markov chain is lumpable, then the lumped chain can be naturally considered as the reduction of the original Markov chain.

Another interesting idea that we have proposed is to endow complex networks with a landscape. Landscape has been a very useful concept for continuous systems arising in physics, chemistry, biology, etc. Building upon the Markov chain structure in networks, we have introduced a way of endowing a landscape to a network. This has proved to be very useful in several different examples arising in social and biological networks.

2 Approach

Our basic starting point is to identify networks with Markov chains so that the issue of network clustering becomes the issue of approximate lumpability of a Markov chain. The latter problem is treated in the following way. For each possible reduced chain on a partition of the state space of the original chain, we can associate a Markov chain on the original state space, which can be considered as the lift of the reduced chain to the original state space. This is done with the help of the invariant measure of the chain. The Hilbert-Schmidt norm of the difference between the transition matrices of the original chain and the lifted chain is a measure of the accuracy of the reduced chain. The optimal reduced chain can be obtained by minimizing this difference.

Questions that we need to address include:

1. How should we decide how big the reduced chain should be, i.e. the size of the partition? In this context, this is the problem of "model selection".

2. Often times it is not a good idea to associate each node to one and only one of the clusters. It is more appropriate to associate a probability distribution for a given node to belong to a certain cluster.

3. A real network has its physical meaning. How do we attach a physical meaning to the reduced network?

In the last decade or so, network has emerged as the appropriate tool for modeling social, economic, biological and physical interactions in a wide range of disciplines. These networks also have many interesting and complex structural and/or dynamic properties which require new understanding. With very few exceptions, the work done in network science is descriptive in nature rather than deductive. Many results are empirical or observational facts rather than consequences of fundamental principles. Much work has to be done in order to establish the mathematical foundation of network science. The present project is a step in that direction.

One can make a comparison with image processing. Image processing has been a subject in computer science for a long time. Many techniques have been developed. However, these techniques do not address the question: What do we want to achieve with these techniques? They simply produce some results without explaining the rationale behind the techniques.

The work of Mumford-Shah, Osher and co-workers changed that. Instead of going directly to the algorithms, one first formulates the objective in terms of a mathematical problem. Algorithms are then developed to solve the mathematical problem. In this way, one has a much better idea of what one is trying to do.

3 Results

So far our accomplishments are as follows:

- We have formulated the mathematical model for network clustering.
- We have formulated a mathematical framework for probablistic clustering, which allows each node to have a certain probability of belonging to a cluster.
- We have developed very efficient numerical algorithms for both deterministic and probabilistic clustering.
- We have tested the algorithms on realistic network models.

We have also introduced the concept of diffusion complex. This is analogous to the Witten complex in quantum mechanics in the context of diffusion process. We are now working on extending this concept to networks. As a first step, we have introduced the concept of landscapes for complex networks. From the invariant distribution of the Markov chain, one can introduce an analog of " free energy" for networks. One can then define local minima and local maxima, as well as saddle points for the free energy on the network. We have tested these concepts on some examples from social and biological networks. The results are very promising: They reveal important information such as "metastable saddles" for protein structure network.

4 Publications

- ELiV08 W. E, T. Li and E. Vanden-Eijnden, "Optimal partition and effective dynamics of complex networks," *Proc. Natl. Acad. Sci. USA*, vol. 105, pp. 7907–7912, 2008.
- Tiejun Li, Jian Liu and Weinan E, "A probablistic framework for network partition", *Phys. Rev. E*, vol. 80, no. 2, 026106, 2009.

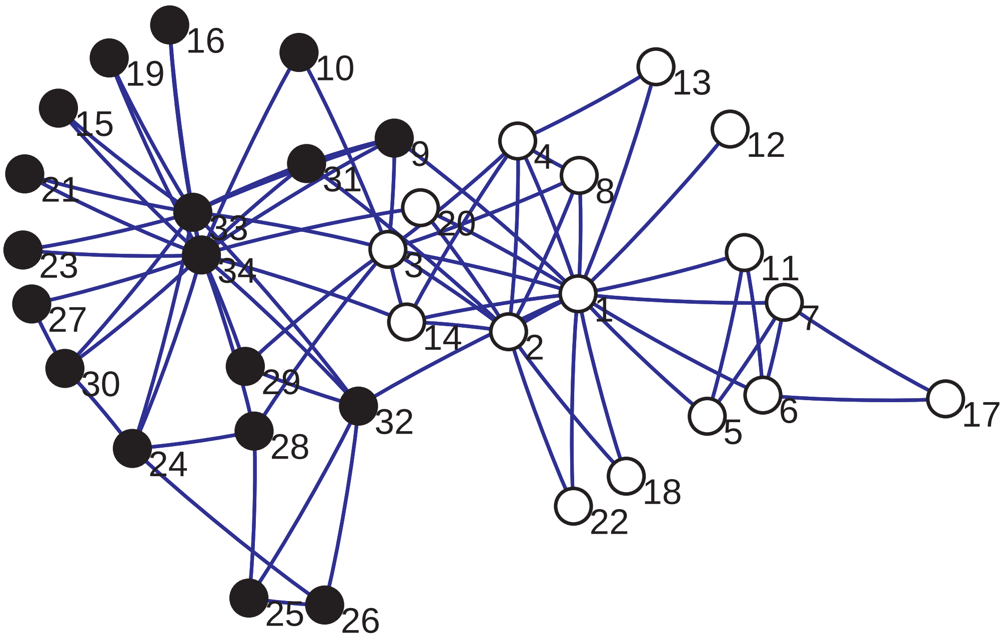

Figure 1: The deterministic partition of the famous Karate club network. This result agrees with the result of Zachary's well-known work.

- Weinan E and Tiejin Li, "A unified mathematical framework for network clustering", in preparation.
- Weinan E and Jianfeng Lu, "Diffusion complexes", preprint, submitted to *Comm. Pure Appl. Math.*
- Weinan E, Jianfeng Lu and Yuan Yao, "The landscape of complex networks", preprint.

5 Student/postdoc supported

Students supported:
Xiang Zhou, date of completion of Ph. D. 2009.
Hao Shen, in progress.
Post-docs supported:
Xiang Zhou, September 2009 to August 2011.

6 Awards and honors

- Awarded SIAM Ralph Kleinman Prize.

  Citation: For his extraordinary interdisciplinary contributions and for his exemplary record in mentoring students and postdocs. He has had profound impacts on research in stochastic partial differential equations and turbulence, numerical solution of multiscale problems, dynamics of

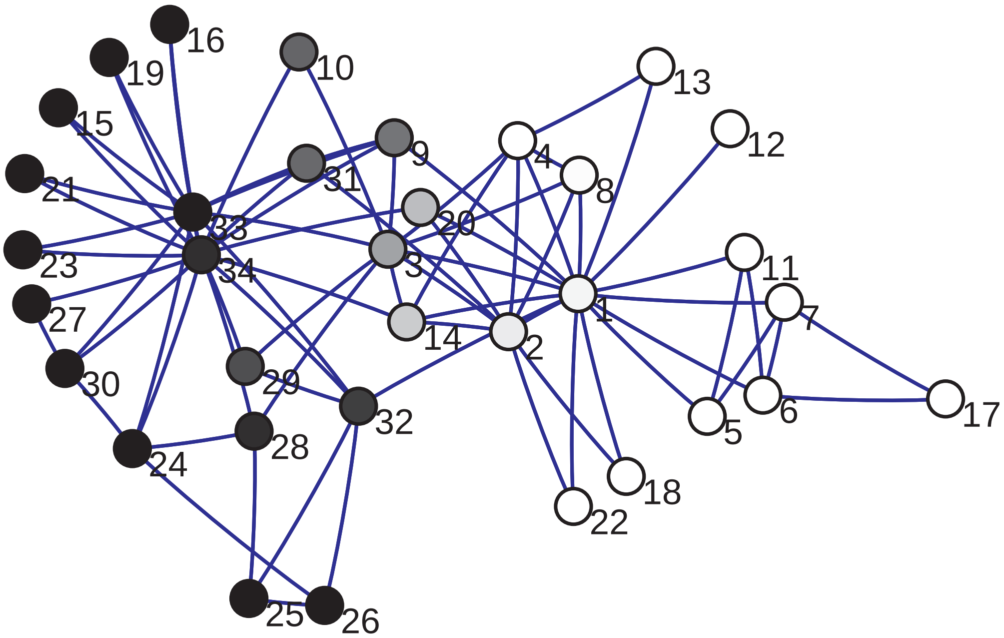

Figure 2: The gray scale plot of ρ_K and ρ_W (which are probabilities for belonging to the two clusters respectively) for each node in karate club network. The darker the color, the larger the value of ρ_K. The transition nodes or intermediate nodes are clearly shown.

interacting dislocations, liquid crystals and polymers, metastability, protein folding, gas dynamics, epitaxial growth, micromagnetics, and superconductivity. His vision and breadth are truly remarkable.

- Elected to the inaugral class of SIAM fellows.

7 Conclusions

- Complex networks is an important subject in many disciplines, particularly in social science.
- Markov chains provide a natural mathematical framework for studying the structure and dynamics of complex networks.
- Network partition (clustering) has been a popular subject in computer science, but it really needs a solid mathematical treatment.
- We have developed the mathematical framework and related algorithms for network partition.

8 Future plans

We intend to continue our study of the dynamics of complex networks, in the same style. In particular, we will investigate the following problems:

1. Diffusion on complex networks. Study how the diffusion process depends on network structure.
2. Stochastic games on complex networks. So far, game theory has only been studied on relatively simple networks. In the same spirit as above, we will study how the network structure affects games on these networks.
3. Physical significance. It is important to relate the mathematical results back to the practical situation in which the networks come about. This requires a deep understanding of the original problem, as well as the mathematical analysis of these networks.