ECT
Trento, Italy
23 July, 2012

Listen to the Noise:
Bridge dynamics and topology of complex networks

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Location of SINGAPORE in world map
Trento
Shanghai
NUS-Tongji Center for Phononics…
Singapore
Map not to Scale
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Acknowledgement

Financial Support:

Defence Science and Technology Agency, Singapore

Ministry of Education, Singapore

SERC (Singapore Engineering Research Council)

Endowment Fund, NUS

Asian Office of Aerospace R&D (AOARD), the US Air Force

NUS National University of Singapore

Li’s group and some collaborators at NUS

Research Topics:

1. Phononics and Thermoelectrics (theory+experiment)

***Heat conduction in low dimension systems*:**

Necessary and sufficient condition of the Fourier law

Connection between anomalous heat conduction and anomalous diffusion

Effective Phonon theory in 1d nonlinear lattice

Heat conduction in nano scale systems

Phononic devices: thermal diode, transistor, logic gate, and phononic computer …

Thermoelectrics: convert heat into electricity

2. Complex Networks and Systems Biology

dynamics, function and topology structures of biological networks such as metabolic networks, protein-protein interacton networks,

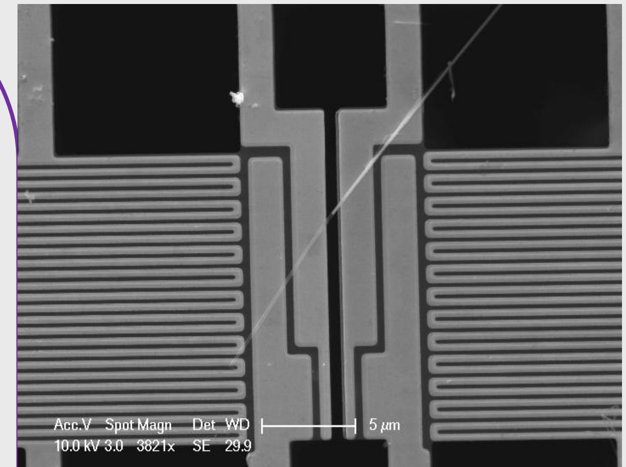
3. Econophysics

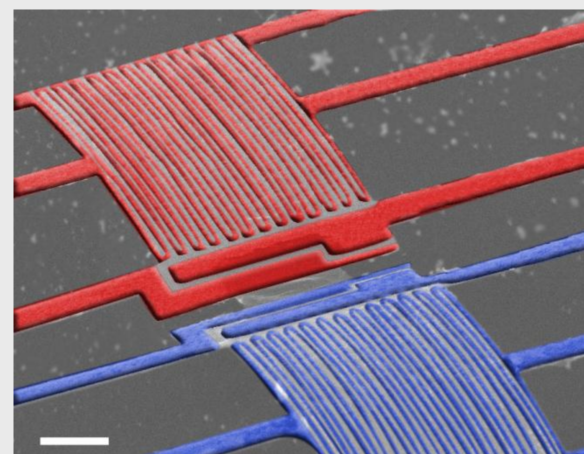
Physical approaches to economy and financial market

NUS National University of Singapore

Experimental Works on Thermal Tranpsort in nanostructures

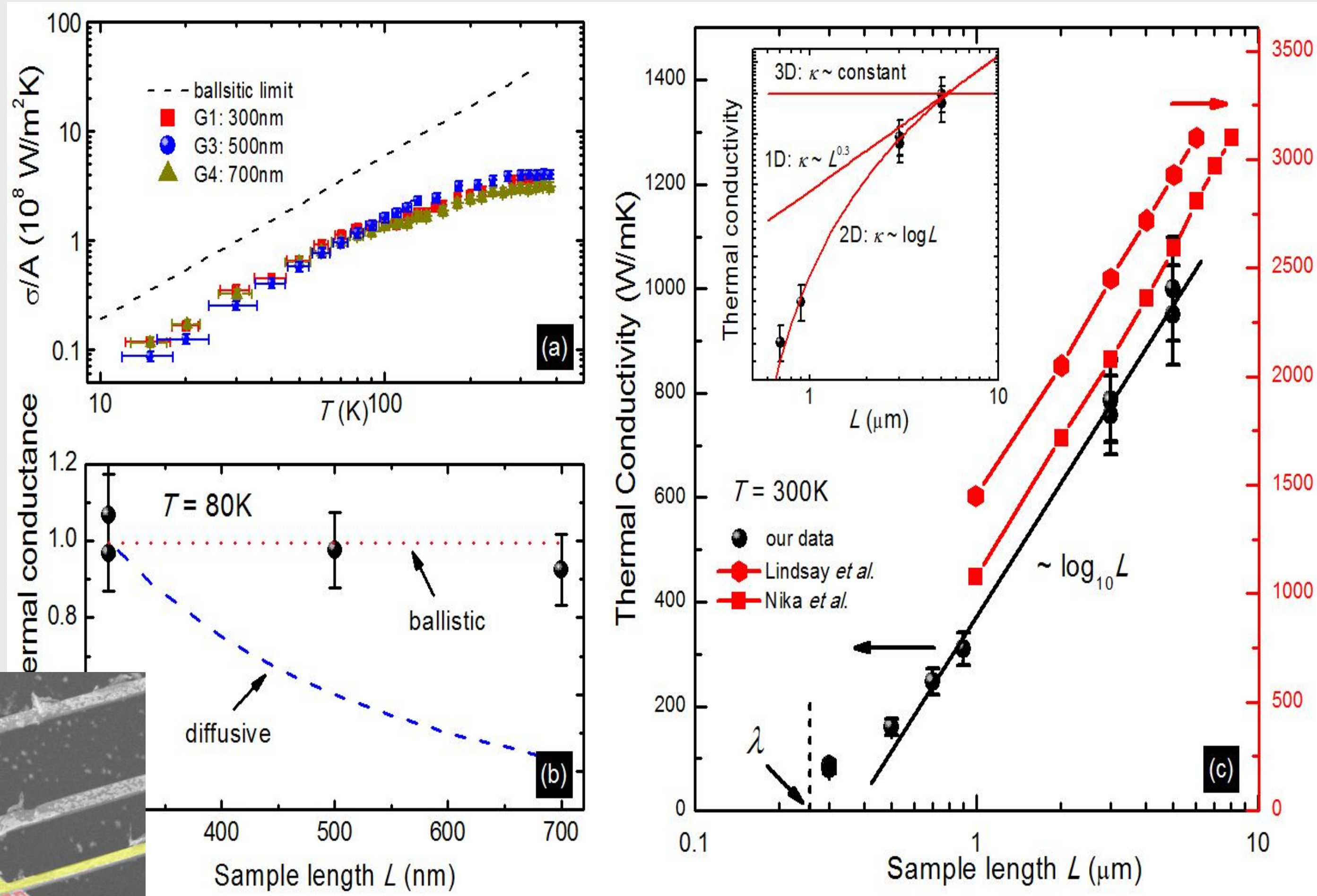
Simultaneous measurement of thermal, electrical conductivity and thermo-power of nanostructures

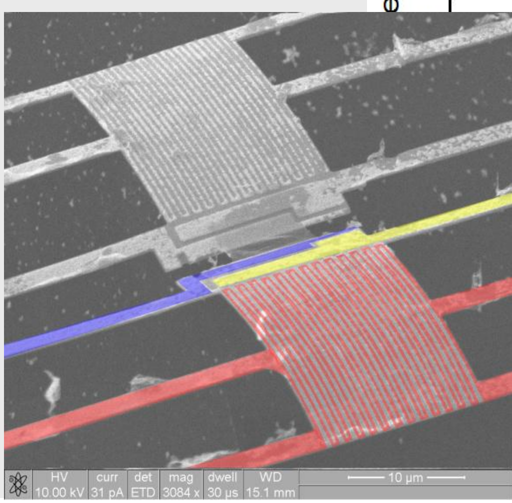




National University of Singapore

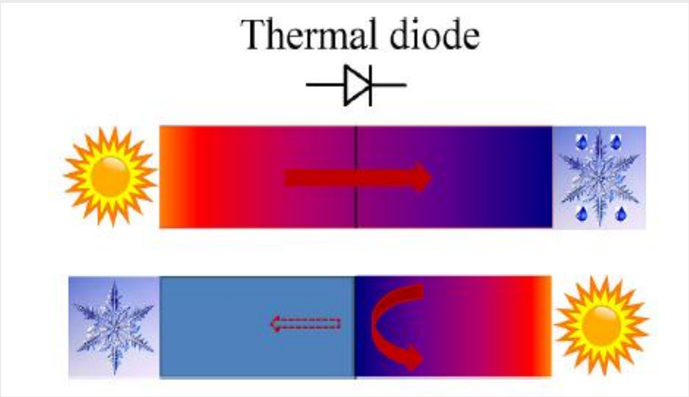
Xu XF…. BL, Barbaros Oezyilmaz (submitted)





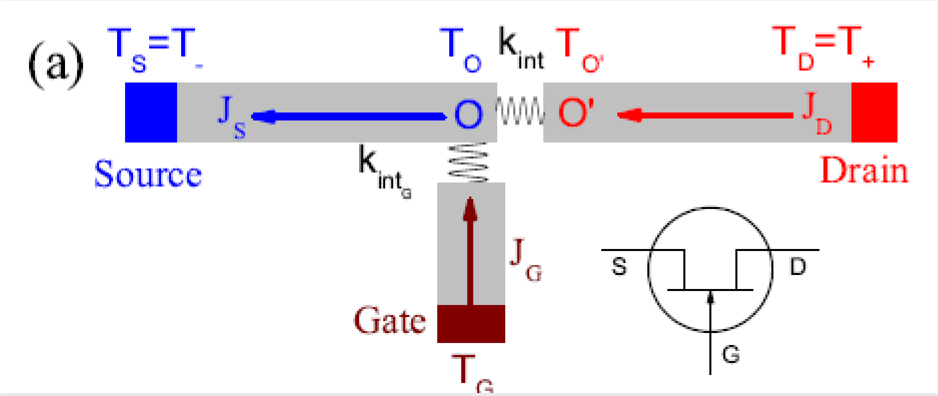
Thermal diode (Theory, NUS)

PRL 98 184301 (2004), 99 104302 (2005)
NUS, theory



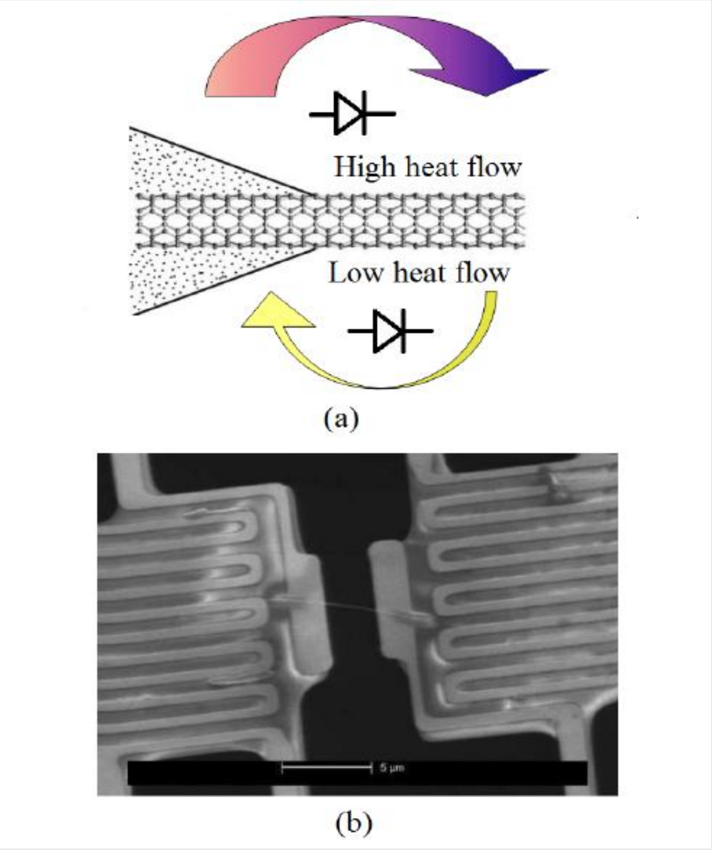
Thermal transistor(theory, NUS)

APL 88, 143501 (2006)



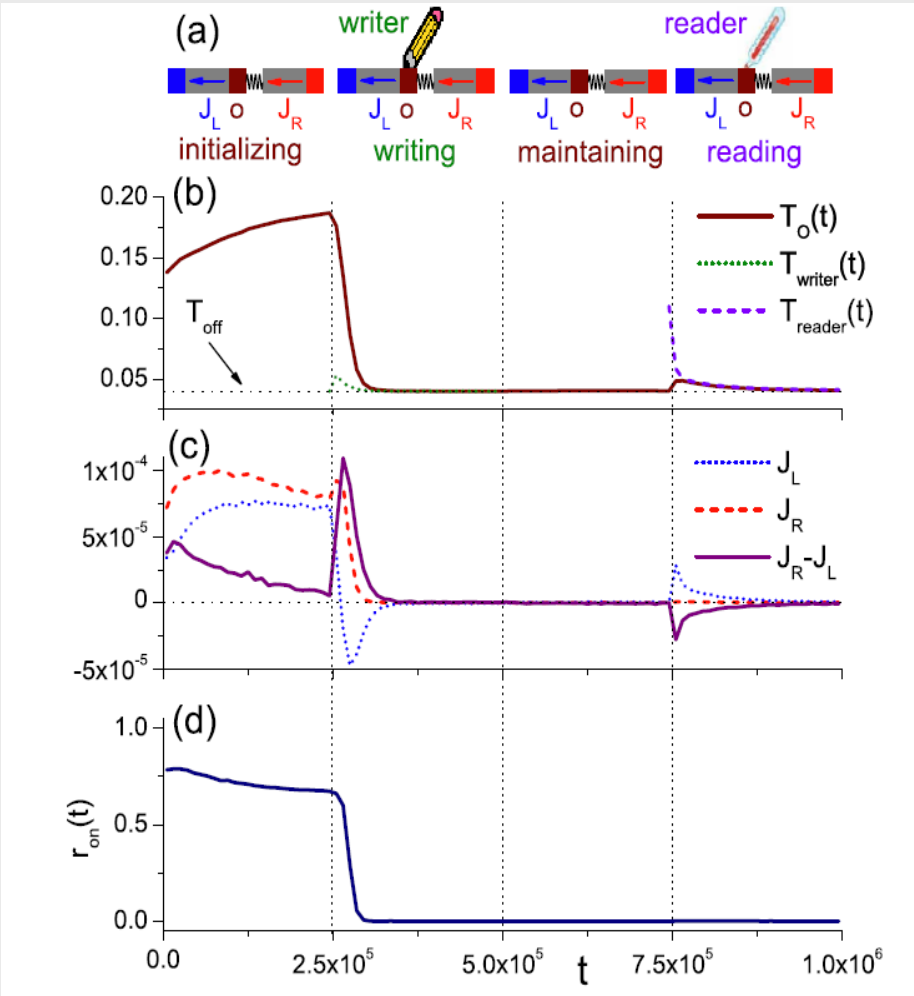
Solid State Thermal Rectifier (Berkeley, Experiment)

Science 314, 1121 (2006)



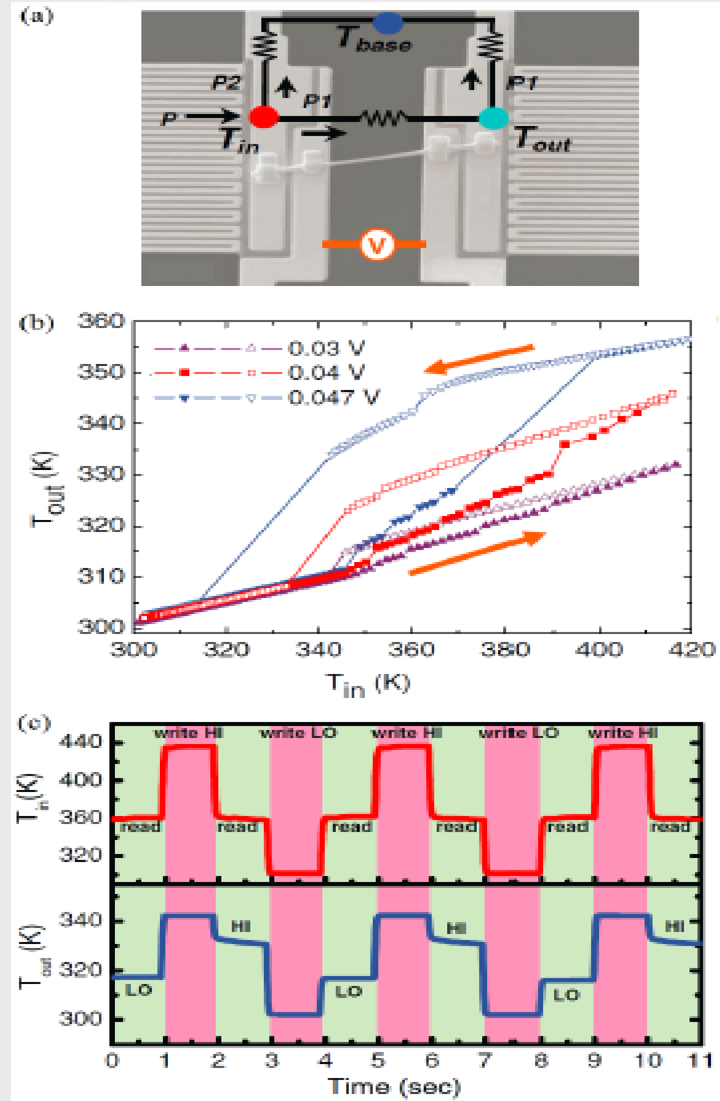
Thermal memory

2008, PRL 101, 267203 , NUS, Theory



Thermal memory: Experiment

2011 Adv Func Mat, NUS



REVIEWS OF MODERN PHYSICS, VOLUME 84, JULY–SEPTEMBER 2012

Colloquium: Phononics: Manipulating heat flow with electronic analogs and beyond

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Gang Zhang

Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, People's Republic of China, and Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, 117546 Singapore

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NUS
...nal University
...gapore

CONTENTS

legitimate then to ask whether p
technology of electronics, prese
Admittedly, it indeed is su
control *a priori* the flow of heat
the flow of electrons. This is b
carriers of heat, the phonons, are
energy bundles that possess ne
charge. Although isolated pho
other, interactions involving ph
in the presence of condensed
come to mind are phonon pola
optical phonons with infrared p
electron interactions occurring
phonon-spin interactions, or ph
the presence of nonlinearity. T
aspects that in many ways are
and matter flow. Nonetheless,
phases many interesting cross
the reciprocal relations of the O
and charge flow, of which ther
Dubi and Di Ventra, 2011) or t
versus its reciprocal Dufour effe
exemplars. Therefore, capitalizi
sities involving phonon transp
successes in nanotechnology m
phononics from a dream into a
In this Colloquium we focus
phononics, i.e., the manipulatio
nanoscale and the objective of pr

Phono
gets h

Scientists Propose Thermal Memory to Store Data - Microsoft Internet Explorer

File Edit View Favorites Tools Help

http://physicsworld.com - Memory device could store data using heat - physicsworld.com - Microsoft Internet ..

新加坡国大两教授创立"声子"理论

未来电脑可能不需电流

早报漫画 ● 梁锡泉

"0" 和 "1"
"0" 表示低
示高温，信
过改变温度
么一来，电
的不再是电
子，或热。
信息的电脑
中撷取热，
啡，而不需
，甚至不需

证明，把热
不同的方式
得到电脑处
的各种热逻
"与" 门、
"非" 门。这
工作为声子
理论基础。
和王博士的
在《物理评
（Physics
ters） 上。
报》是声誉
学期刊，自
美国物理学

理论一方面
传递和处理

李教授举例说，如果能按照热二极管原理设计一种新的隔热材料，就可以让汽车或大厦不会吸收外在环境的热，从而降低车内或室内的空调能耗。现在的超级电脑、服务器等在操作过程中产生大量热，这些热不仅仅对信息处理有害，而且使周围环境温度升高。

这项发明或许有一天可以用来处理、甚至应用这些多余的热能。换句话说，它最终或许能对解决全球暖化作出贡献。

进行10年研究

李保文在这方面的发现并非偶然。他已在这一领域进行了长达10年的研究，一开始的研究是想了解在微观世界比如纳米结构里热是怎样传导的。

德国奥格斯堡大学物理系教授彼得亨吉（Peter Hanggi）博士在回答本报询问的电邮中

他说："控制热流和把热转换成有益电脑的运作，是科学领域最轰动的大事，而且其重要性正在显著地上升。在这个领域里，国大李教授和其研究团队是众人注目的焦点。"

他也说，李保文和研究团队为这个领域创导新风潮。这个领域具备在宏观世界和纳米世界开发全新应用科学的潜能，为理论物理、实验物理和工程科学开拓全新的研究道路。

加州大学伯克利分校机械工程系也对李教授的理论产生兴趣，着手从实验上证明热二极管、热晶体管和热逻辑门的可行性，并已取得一定成果。

早报中英对照

光子学：photonics
光子电脑：Photonic Computer
声子学：phononics
声子电脑：Phononic Computer
声子：phonon
热二极管：thermal diode
热晶体管：thermal transistor
热逻辑门：thermal logic gate
"与" 门：AND gate
"或" 门：OR gate
"非" 门：NOT gate
奥格斯堡大学：

APS NEWS
A PUBLICATION OF THE AMERICAN PHYSICAL SOCIETY • WWW.APS.ORG/PUBLICATIONS/APSNEWS
February 2
Volume 17
www.aps.org/pt
Physics

Thermal Logic Gates

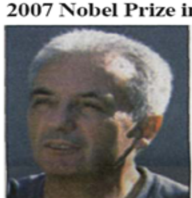
Information processing in the world's computers is mostly carried out in compact electronic devices, which use the flow of electrons both to carry and control information. There are, however, other potential information carriers, such as photons. Indeed a major industry, photonics, has developed around the sending of messages encoded in pulsed light.

Heat pulses, or phonons, rippling through a crystal might also become a major carrier, says Baowen Li of the National University of Singapore. Li, with his colleague Lei Wang, have now shown how circuitry could use heat-energy already present in abundance in electronic devices-to carry and process information.

They suggest that thermal transistors (also proposed by Li's group in Applied Physics Letters, 3 April 2006) could be combined into all the types of logic gates-^uch as OR, AND, NOT, etc.-used *in* conventional processors and that therefore a thermal computer, one that manipulates heat on the microscopic level, should be possible.

Given the fact that a solid state thermal rectifier has been demonstrated experimentally in nanotubes by a group at UC Berkeley (Chang et al., *Science*, 17 November 2006) only a few years after the theoretical proposal of "thermal diode," the heat analog of an electrical diode which would oblige heat to flow preferentially in one direction (Li et al, *Phys. Rev. Lett.* 93, 184301 (2004)). Li is confident that thermal devices can be successfully realized in the foreseeable future. (Wang and Li, *Phys. Rev. Lett.* **99**, 177208 (2007))

2007 Nobel Prize in Physics



Albert Pert

The 2007 Nobel Prize in Physics was awarded to Albert Pert (Universite Paris-Sud, Orsay, France) and Peter Griinberg (Forschungszentrum Julich, Germany) for the discovery of giant magnetoresistance, or GMR for short. GMR is the process whereby a magnetic field, such as that of an oriented domain on the surface of a computer hard drive can trigger a large change in electrical resistance, thus "reading" the data vested in the magnetic orientation.

This is the heart of modem hard drive technology and makes possible the immense hard-drive data storage industry. Pert and Griinberg pioneered the making of stacks consisting of alternating thin layers of magnetic and nonmagnetic atoms needed to produce the GMR effect. GMR is a prominent example of how quantum effects (a large electrical response to a magnetic input) come about through confinement (the atomic layers being so thin); that is, atoms interact differently with each other when they are confined to a tiny volume or a thin plane.

Peter Grunberg

All these magnetic interactions involve the spin of an electron. Still more innovative technology can be expected through quantum effects depending on electrons' spin. Most of the electronics industry is based on manipulating the charges of electrons moving through circuits. But the electrons' spins might also be exploited to gain new control over data storage and

The new nucAides ate not stat>\e, since xncy is pretty long by nuclear standards. Why stud might not exist naturally, the new nuclides sti where heavy elements, including those that mi ated. Thomas Baumann suggests that even he; that it is worth exploring any possible islands i of the periodic table. (Baumann et al., *Nature A*

The Highest-Energy Cosmic Rays

The highest-energy cosmic rays probably coi (AGN), where supermassive black holes are tl the rays across the cosmos. This is the conclus Pierre Auger Observatory in Argentina. This 3000 sq. km of terrain, looks for one thing: cos

These arise when extremely energetic part gush of secondary particles. Many of the rays c pecially from our sun, but many others come fro est-energy showers, with energies above 10" e energy that can be produced in terrestrial accele artifacts offers physicists a tool for studying th«

To arrive at Earth, most cosmic rays will h space, where magnetic fields can deflect them f highest-energy rays, the magnetic fields can't e: the starting point for the cosmic rays can be tra

This allowed the Auger scientists to asse were not coming uniformly from all directii axies with active cores, where the engine ably black holes of enormous size. The those with an energy higher than 57 EeV (J ty well with known AGN's. (Auger collar. Vol. 318. no. 5852, pp. 938-943)

Cooper Pairs in Insulators

Cooper pairs are the extraordinary link-up of flexings of a crystal. They act as the backbone (have also now been observed in a material that i ally an insulator. An experiment at Brown Univ Swiss-cheese-like plank of bismuth atoms made strate with 27-nm-wide holes spaced 100 nm ap perconducting if the sample is many atom-layer! a few atoms thick, owing to subtle effects which

Cooper pairs are certainly present in the su form a non-resistive supercurrent. But how do th in the insulator too? By seeing what happens to is increased.

Biological networks:

OPEN ACCESS Freely available online — PLoS one

Simulating EGFR-ERK Signaling Control by Scaffold Proteins KSR and MP1 Reveals Differential Ligand-Sensitivity Co-Regulated by Cbl-CIN85 and Endophilin

Lu Huang[1,7], Catherine Qiurong Pan[5,7], Baowen Li[6], Lisa Tucker-Kellogg[1,7], Bruce Tidor[1,3,4], Yuzong Chen

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Univers

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Existence of Inverted Profile in Chemically Responsive Molecular Pathways in the Zebrafish Liver

Choong Yong Ung[1,2*], Siew Hong Lam[1], Xun Zhang[3,4], Hu Li[5], Jing Ma[3,4], Louxin Zhang[2,3], Baowen Li[3,4],

1 Depa
Queen
and Ce

Molecular BioSystems

Dynamic Article Links

Cite this: DOI: 10.1039/c2mb05376d

www.rsc.org/molecularbiosystems

PAPER

Metabolic network analysis revealed distinct routes of deletion effects between essential and non-essential genes†

Jing Ma,*[ab] Xun Zhang,[ab] Choong Yong Ung,[d] Yu Zong Chen[abe] and Baowen Li[abc]

Received 19th September 2011, Accepted 13th December 2011

Econophysics:

Linking agent-based models and stochastic models of financial markets

Ling Feng[a,b,c,1], Baowen Li[a,b,1], Boris Podobnik[c,d,e,f], Tobias Preis[c,g,h], and H. Eugene Stanley[c,1]

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Physics and Centre for Computational Science and Engineering, National University of Singapore, Singapore 117542, Republic of S
Polymer Studies and Department of Physics, Boston University, Boston, MA 02215; [d]Faculty of Civil Engineering, University of Rijek
Croatia; [e]Faculty of Economics, University of Ljubljana, 1000 Ljubljana, Slovenia; [f]Zagreb School of Economics and Management, 1
[g]Chair of Sociology, in particular of Modeling and Simulation, Eidgenössische Technische Hochschule Zurich, 8092 Zurich, Switzerla
Capital Asset Management GmbH, 65558 Holzheim, Germany

Contributed by H. Eugene Stanley, March 29, 2012 (sent for review December 6, 2011)

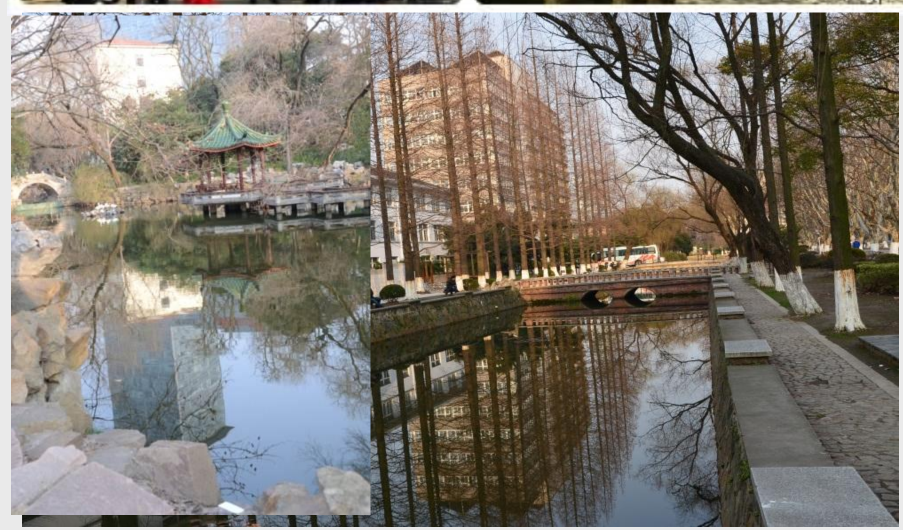
It is well-known that financial asset returns exhibit fat-tailed distributions and long-term memory. These empirical features are the main objectives of modeling efforts using (i) stochastic processes to quantitatively reproduce these features and (ii) agent-based simulations to understand the underlying microscopic interactions. After reviewing selected empirical and theoretical evidence documenting the behavior of traders, we construct an agent-based model to quantitatively demonstrate that "fat" tails in return distributions arise when traders share similar technical trading strategies and decisions. Extending our behavioral model to a stochastic model, we derive and explain a set of quantitative scaling relations of long-term memory from the empirical behavior of individual market participants. Our analysis provides a behavioral interpretation of the long-term memory of absolute and squared price returns: They are directly linked to the way investors evaluate their investments by applying technical strategies at different investment horizons, and this quantitative relationship is in agree-

Market surveys (16–18) also provide clear ev
lence of technical analysis. We consider her
ders, assuming that fundamentalists contrib
noise. Our study is of the empirical data
2006 and ignores the effect of high frequenc
has become significant only in the past 5 y.
vioral agent-based model that is in agreeme
empirical evidence:

i. Random trading decisions made by agent
technical traders use different trading st
decisions to buy, sell, or hold a position a
A trading decision is made daily becau
report the lack of intraday trading pers
trading data (19). Market survey (16) a
managers put very little emphasis on intra
timate the probability p of having daily tr

Wanted!!!

Distinguished Foreign Professor
Distinguished (Chair) Professor
Outstanding Young Professor
Professors, Associate Professors
Research Fellows
Visiting Professors



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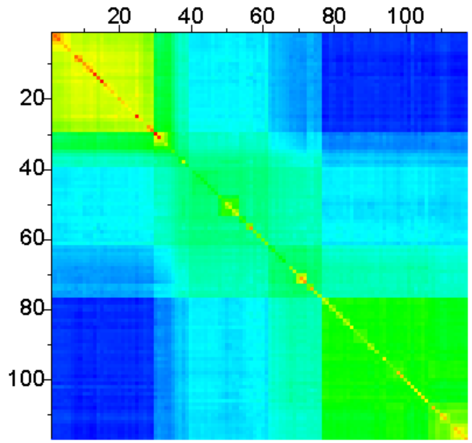
Research Fields

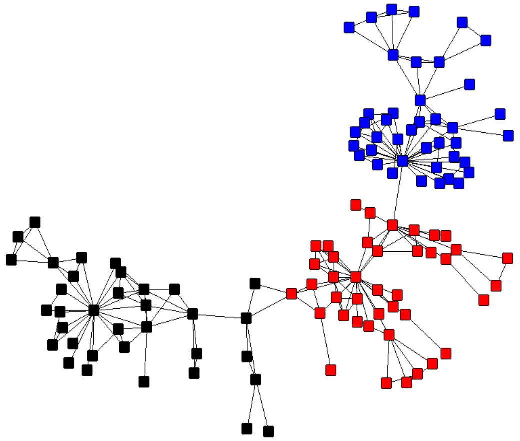
- Non-equilibrium statistical physics
- Phonon/Heat transport in nanoscale
- Phonon-electron interaction and thermoelectrics
- Photon –phonon interaction: solar thermal energy conversion
- Phonon-magnon interaction: phonon Hall effect
- Phononic meta-material: controlling and manipulating vibrational energy
- Heat transfer/manipulation in biological systems
- Phononic devices

NUS National University of Singapore

Listen to the noise:

Bridge dynamics and topology of complex networks





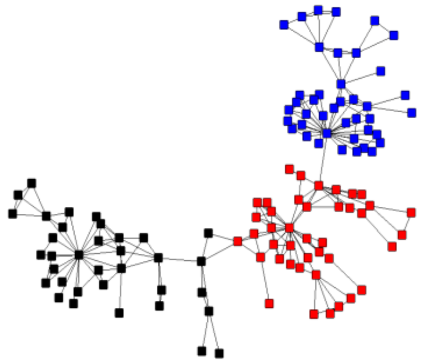
Collaborators:

- Dr Jie Ren (NUS Graduate School for Integrative Sciences and Engineering, Currently a Postdoc at Theory Division, LANL)
- Dr. Wen-Xu Wang (Arizona State University - ASU, currently Professor at Beijing Normal University)
- Prof. Ying-Cheng Lai (ASU)

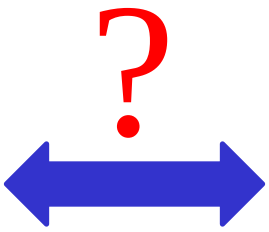
Real-Life Networks

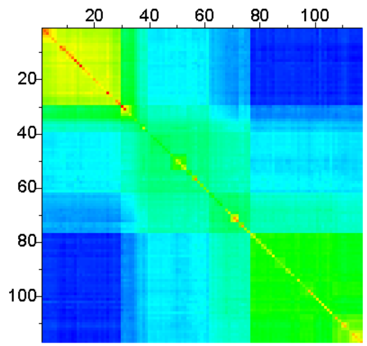
- **Transportation networks**: airports, highways, roads, rail, electric power…
- **Communications**: telephone, internet, www…
- **Biology**: protein's residues, protein-protein, genetic, metabolic…
- **Social nets**: friendship networks, terrorist networks, collaboration networks…

It is well accepted that:
Structure plays a fundamental role in shaping the dynamics of complex systems.
However, the general intrinsic relationship still remains unclear.



Topological structure





Dynamical pattern

Ubiquitous noise has profound effects on dynamical systems and information retrieval.

Outline

- Harmonic Oscillators

- Unified View: a general approach to bridge network topology and the dynamical patterns through noise

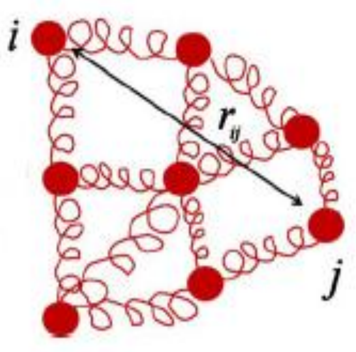
- Application

From topology to dynamics: stability of networks

From dynamics to topology: inferring network structures

Coupled Harmonic Oscillators: Vibrational properties with static structure

Examples: protein's residues interaction, electric circuit, solid lattice…



$$m_i \frac{d^2 x_i}{dt^2} = -c \sum_j L_{ij} \cdot x_j - \gamma \frac{dx_i}{dt} + \eta_i$$

second order time derivative

Thermal noise: $\langle \eta_i(t)\eta_j(t')\rangle = 2k_B T \Gamma_{ij} \delta(t-t')$

Matrix form: $\hat{\mathbf{M}}\ddot{\mathbf{x}} = -c\hat{\mathbf{L}}\mathbf{x} - \hat{\Gamma}\dot{\mathbf{x}} + \eta$

$$C_{ij} = \langle x_i x_j \rangle = \frac{k_B T}{\pi} \int_{-\infty}^{+\infty} d\omega [\hat{\mathbf{G}}(i\omega)\hat{\Gamma}\hat{\mathbf{G}}(i\omega)]_{ij} \qquad \hat{\mathbf{G}}(\pm i\omega) = \frac{1}{-\omega^2 \hat{\mathbf{M}} \pm i\omega\hat{\Gamma} + c\hat{\mathbf{L}}}$$

$$\hat{\mathbf{G}}^{-1}(i\omega) - \hat{\mathbf{G}}^{-1}(-i\omega) = 2i\omega\hat{\Gamma} \qquad \hat{\mathbf{G}}^{-1}(0) = c\hat{\mathbf{L}}$$

Pseudo-inverse:

$$L_{ij}^{\dagger} = \sum_{\alpha=1}^{N-1} \frac{1}{\lambda_\alpha} \psi_{\alpha i}\psi_{\alpha j}$$

$$\hat{\mathbf{C}} = -\frac{k_B T}{i\pi} \int_{-\infty}^{+\infty} d\omega \frac{\hat{\mathbf{G}}(i\omega)}{\omega} = \frac{k_B T}{c} \hat{\mathbf{L}}^{\dagger}$$

$$\sigma^2 = 2k_B T$$

Compact form: $\hat{\mathbf{C}} = \frac{\sigma^2}{2c} \hat{\mathbf{L}}^{\dagger},$

reduce to first order

$$\xi = [x_1, \cdots, x_N, \dot{x}_1, \cdots, \dot{x}_N]^T$$
$$\dot{\xi} = -\hat{\mathbf{A}}\xi + \hat{\mathbf{B}}$$

J. Ren and B. Li, PRE **79,** 051922 (2009)

A General Approach to Bridge Dynamics and Network Topology

Under noise, the dynamics of the general coupled-oscillators can be expressed as:

$$\dot{\mathbf{x}}_i = \mathbf{F}_i(\mathbf{x}_i) - c\sum_{j=1}^{N} L_{ij}\mathbf{H}(\mathbf{x}_j) + \eta_i,$$

Examples: Information flow, synchronization, neurodynamics, biochemical process…

Consensus dynamics

$$\dot{x}_j = c\sum_{l=1}^{N} A_{jl}(x_l - x_j) + \xi_j$$

Kuramoto phase oscillators dynamics

$$\dot{\theta}_j = \omega_j + c\sum_{l=1}^{N} A_{jl}\sin(\theta_l - \theta_j) + \xi_j$$

Chaotic Rössler dynamics

$$\dot{x}_j = -y_j - z_j + c\sum_{l=1}^{N} A_{jl}(x_l - x_j) + \xi_j,$$

$$\dot{y}_j = x + 0.2y_j + c\sum_{l=1}^{N} A_{jl}(y_l - y_j),$$

$$\dot{z}_j = 0.2 + z_j(x_j - 9.0) + c\sum_{l=1}^{N} A_{jl}(z_l - z_j).$$

$$\dot{\mathbf{x}}_i = \mathbf{F}_i(\mathbf{x}_i) - c\sum_{j=1}^{N} L_{ij}\mathbf{H}(\mathbf{x}_j) + \eta_i,$$

Linearization

compact form

$D\hat{\mathbf{F}}$ $D\hat{\mathbf{H}}$ Jacobian matrix

covariance of noise

$\langle \eta(t)\eta^T(t')\rangle = \hat{\mathbf{D}}\delta(t-t')$

$$\dot{\xi} = [D\hat{\mathbf{F}}(\bar{\mathbf{x}}) - c\hat{\mathbf{L}} \otimes D\hat{\mathbf{H}}(\bar{\mathbf{x}})]\xi + \eta,$$

long time limit

$$\xi(t) = \int_{-\infty}^{t} \hat{\mathbf{G}}(t-t')\eta(t')dt'$$

$\hat{\mathbf{G}}(t) = \exp(D\hat{\mathbf{F}}(\bar{\mathbf{x}})t - c\hat{\mathbf{L}} \otimes D\hat{\mathbf{H}}(\bar{\mathbf{x}})t)$

$C_{ij} = \langle \xi_i \xi_j \rangle$

$0 = \langle d(\xi\xi^T)/dt\rangle = -\hat{\mathbf{A}}\hat{\mathbf{C}} - \hat{\mathbf{C}}\hat{\mathbf{A}}^T + \langle \eta\xi^T\rangle + \langle \xi\eta^T\rangle,$

$\langle \xi\eta^T\rangle = \int_{-\infty}^{t} \hat{\mathbf{G}}(t-t')\langle \eta(t)\eta^T(t')\rangle dt' = \hat{\mathbf{D}}/2.$

A general relationship:

$$\hat{\mathbf{A}}\hat{\mathbf{C}} + \hat{\mathbf{C}}\hat{\mathbf{A}}^T = \hat{\mathbf{D}}.$$

where $\hat{\mathbf{A}} = -D\hat{\mathbf{F}}(\bar{\mathbf{x}}) + c\hat{\mathbf{L}} \otimes D\hat{\mathbf{H}}(\bar{\mathbf{x}}).$

C: dynamical correlation

L: the underlying topology

Noise bridges Dynamics and Topology.

Ignoring intrinsic dynamics $DF=0$, $DH=1$, symmetric coupling

$$\hat{\mathbf{C}} = \frac{\sigma^2}{2c}\hat{\mathbf{L}}^{\dagger},$$

The same relationship.

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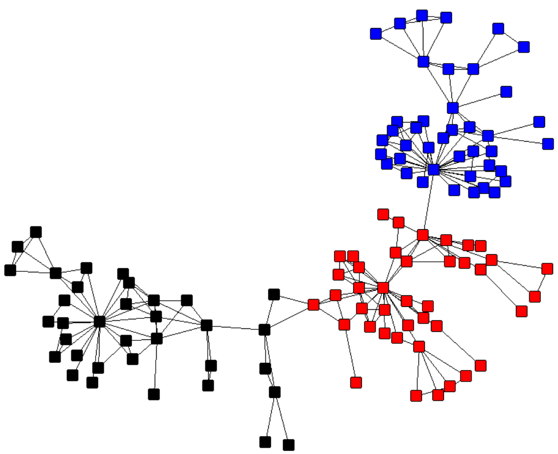
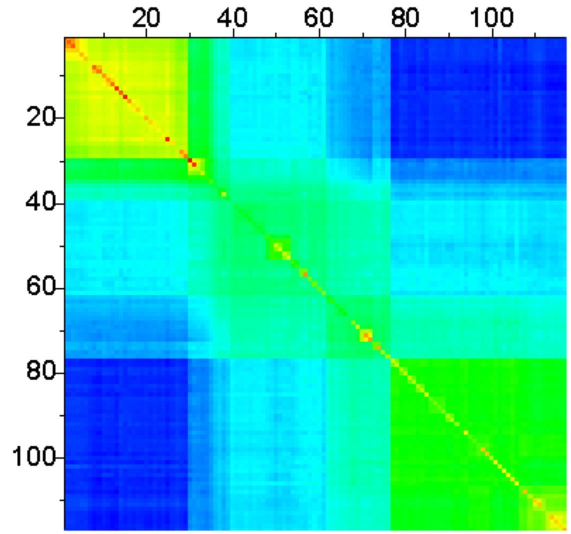
Example:

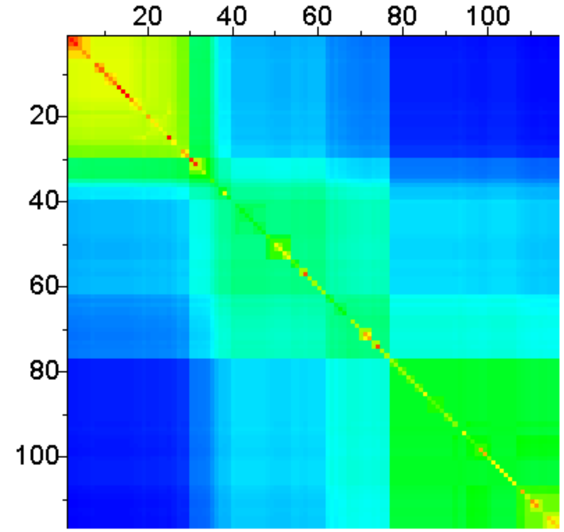


Simulation



Kuramoto model: $C_{ij} = \langle \xi_i \xi_j \rangle$

Theory



Pseudo-inverse: $L_{ij}^{\dagger} = \sum_{\alpha=1}^{N-1} \frac{1}{\lambda_\alpha} \psi_{\alpha i} \psi_{\alpha j}$

Group structures at multi-scale are revealed clearly.

Nodes become strong correlated in groups, coherently with their topological structure.

$$C_{ij} \sim L_{ij}^{\dagger} = \sum_{\alpha=1}^{N-1} \frac{1}{\lambda_\alpha} \psi_{\alpha i} \psi_{\alpha j}$$

The contribution of smaller eigenvalues dominates the correlation **C**

smaller eigenvalues ~ smaller energy ~ large wave length ~ large length scale

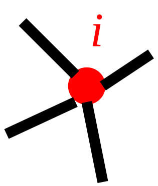
Path-integral (topology) representation of correlations (dynamics)

Decompose $\hat{\mathbf{L}} = \hat{\mathbf{K}} - \hat{\mathbf{P}}$ $\quad \hat{\mathbf{K}} = \mathrm{diag}(k_1, \cdots, k_N)$ $\quad \hat{\mathbf{P}}$ is the adjacency matrix

The correlation matrix **C** can thus be expressed in a series: $\quad \hat{\mathbf{C}} = \frac{\sigma^2}{2c}\hat{\mathbf{L}}^{\dagger},$

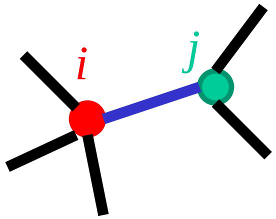
$$\hat{\mathbf{C}} \sim (\hat{\mathbf{K}} - \hat{\mathbf{P}})^{-1} = \hat{\mathbf{K}}^{-1} + \hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1} + \hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1} + \cdots$$

$\hat{\mathbf{K}}^{-1}$



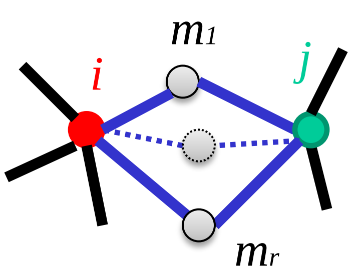
$$\frac{1}{k_i}$$

$\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}$



$$\frac{1}{k_i} \cdot \frac{1}{k_j}$$

$\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}$



$$\frac{1}{k_i} \cdot \Big(\sum_{q=m_1}^{m_r} \frac{1}{k_q}\Big) \cdot \frac{1}{k_j}$$

Path-integral representation:

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$$C_{ij} = \frac{\sigma^2}{2c} \sum_{\mathbf{path}} \prod_{m \in \mathbf{path}} \frac{1}{k_m}$$

Pure dynamical property.

Topology associated property

Application

From topology to dynamics: stability of networks

J. Ren and B. Li, PRE **79,** 051922 (2009)

From dynamics to topology: inferring network structures

J. Ren, W.X. Wang, B. Li, and Y.C. Lai, PRL **104**, 058701 (2010)

W.X. Wang, J. Ren, Y.C. Lai, and B. Li, PRE, under review.

From topology to dynamics: stability of networks

Define the average fluctuation as S:

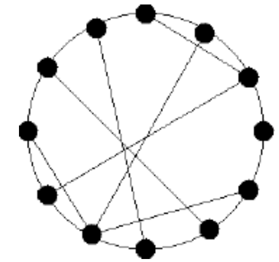
$$S = \frac{1}{N}\sum_{i}^{N}\langle (x_i - \bar{x})\cdot(x_i - \bar{x})\rangle = \frac{1}{N}\mathrm{Tr}(\hat{\mathbf{C}}) = \frac{1}{N}\sum_{\alpha=1}^{N-1}\frac{1}{\lambda_\alpha}$$

$$S = \frac{1}{N}\sum_{\alpha=1}^{N-1}\frac{1}{\lambda_\alpha}$$

Characterize the stability of networks.

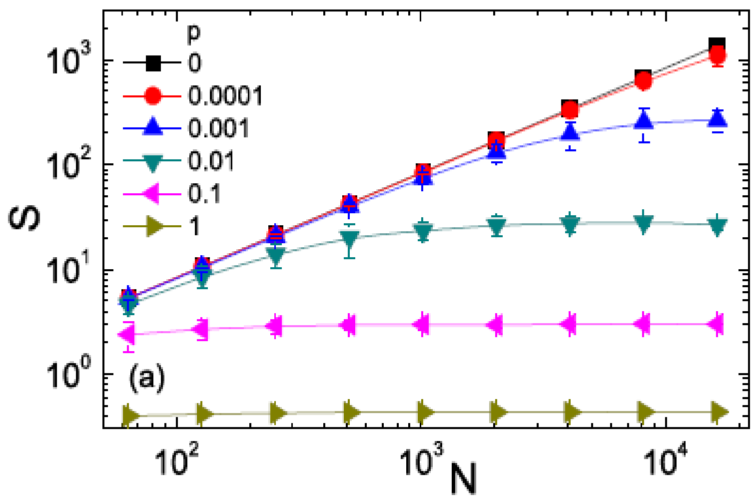
smaller S ~ smaller fluctuations ~ more stable

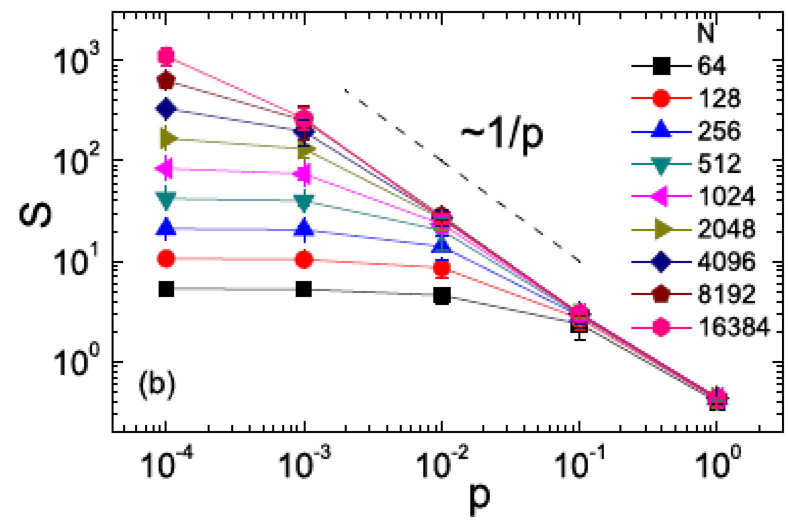
Small-world networks



ring chain + random links

With probability p to add random links to each node.





Perturbation: $L' = L - \Delta$

New correlation: $C' = (I - C\Delta)^{-1}C = C + C\Delta C + C\Delta C\Delta C + \cdots$

Add link (i, j): $S' = \frac{1}{N}\,\mathrm{tr}\,C' = S - \frac{\sum_{k=1}^{N}(C_{ik} - C_{jk})^2}{N(1 + R_{ij})}$

Adding link always decreases S

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From topology to dynamics: stability of networks

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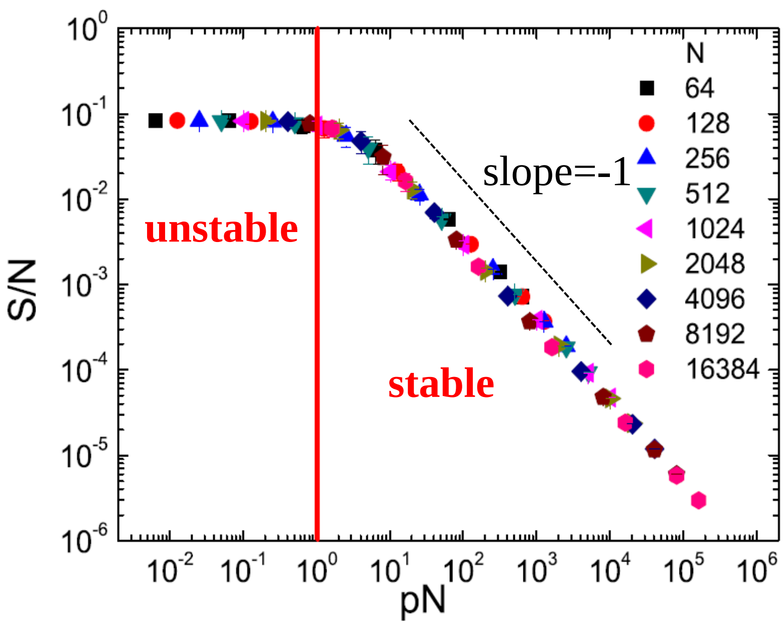
Finite Size Scaling



$$S = \frac{1}{N}\sum_{\alpha=1}^{N-1}\frac{1}{\lambda_\alpha} \xrightarrow{\text{continuous limit}} S = \int \frac{\rho(\lambda)}{\lambda} d\lambda$$

A heuristic argument for the density of state:

For small world networks (1D ring + cross-links), the ring chain is divided into quasi-linear segments.

The probability to find length l is, e^{-pl}

Each segment l has small eigenvalue of the order of l^{-2}

$$S = \int \frac{\rho(\lambda)}{\lambda} d\lambda \sim \int_0^N \frac{l^{-2}e^{-pl}}{1/l^2} dl = \frac{1}{p}\left(1 - e^{-pN}\right)$$

When $pN \ll 1,\ S \sim N$; (unstable) while $pN \gg 1,\ S \sim 1/p$ (stable)

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From topology to dynamics: stability of networks

Each protein is a network with residue-residue interaction.

The thermodynamic stability is crucial for protein to keep its native structure for right function.

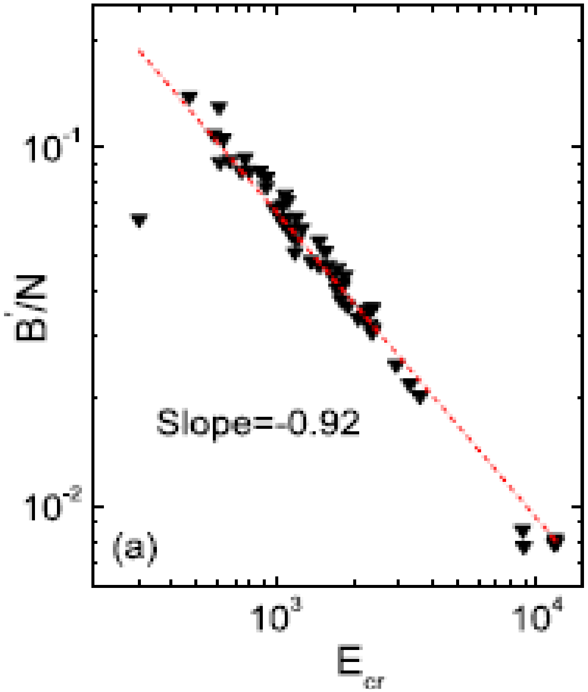
We expect that nature selection forces proteins to evolve into the stable regime:

$$S/N \sim E_{cr}^{-1} = (pN)^{-1}$$

The mean-square displacement of C^{α} *atoms* is characterized by *B* factor. (*B*~*S*)

$$B'/N \sim E_{cr}^{-a}, \quad a = 0.92 \pm 0.01$$

Real protein data follow -1 scaling



E_{cr} is the number of cross-links

Real protein data can be download from Protein Data Bank *www.pdb.org*

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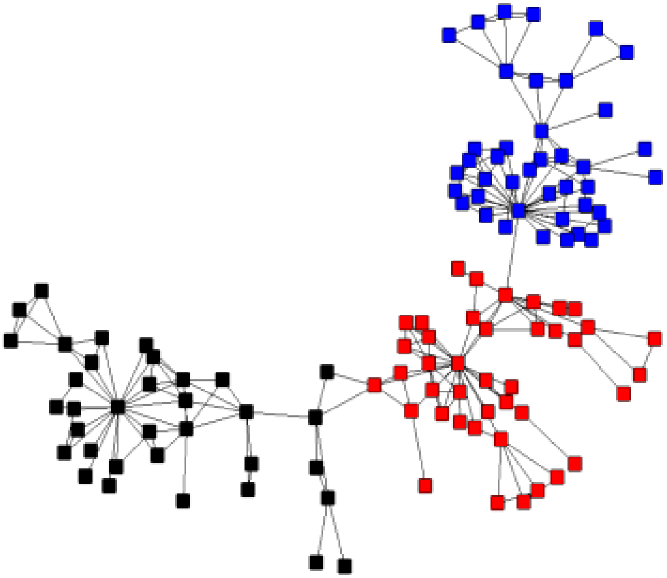
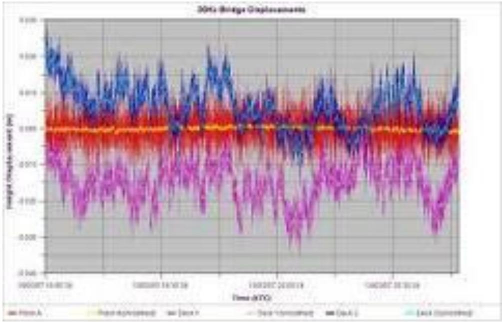
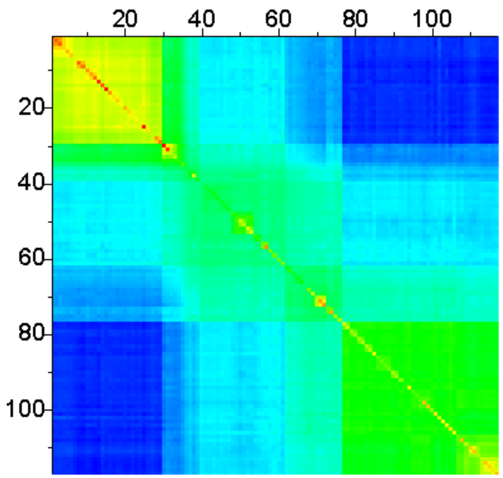




the inverse problem



From dynamics to topology: inferring network structures

$$\hat{\mathbf{C}} = \frac{\sigma^2}{2c}\hat{\mathbf{L}}^{\dagger}, \quad \Rightarrow \quad \hat{\mathbf{L}} = [\sigma^2/(2c)]\hat{\mathbf{C}}^{\dagger} \qquad C_{ij} = \langle [x_i(t) - \bar{x}(t)] \cdot [x_j(t) - \bar{x}(t)] \rangle,$$

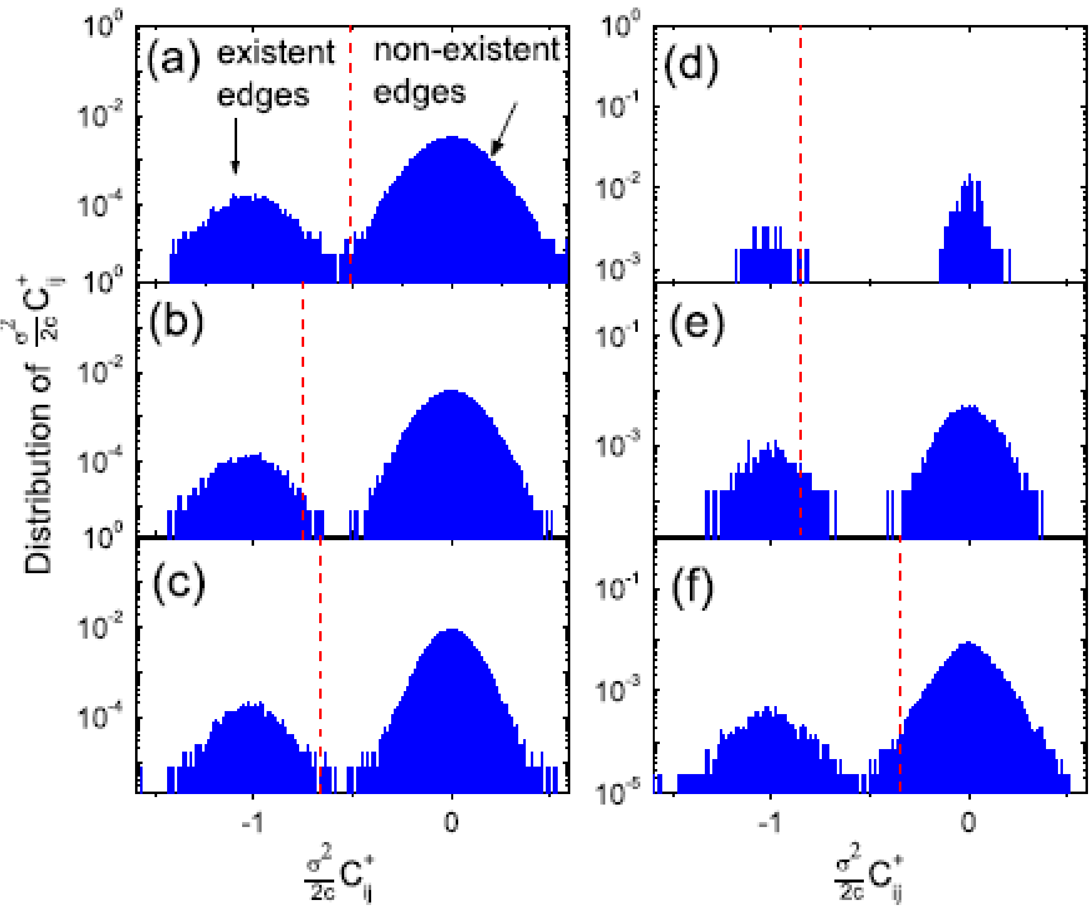


FIG. 1 (color online). Distribution of the values of $[\sigma^2/(2c)]C^{\dagger}_{ij}$, where $C^{\dagger}_{ij}$ are the elements in the pseudo inverse matrix of the dynamical correlation matrix $\hat{\mathbf{C}}$. Consensus dynamics [15] are used for (a) random [21], (b) small-world [22], (c) scale-free model networks [23] and three real-world networks: (d) friendship network of karate club [25], (e) network of American football games among colleges [26], and (f) the neural network of C. Elegans [22]. The theoretical threshold $[\sigma^2/(2c)]C^{\dagger}_{M}$ is marked by red dashed lines. The sizes of model networks are all 500. For random networks, the connection probability among nodes is 0.024. For scale-free networks the minimum degree is $k_{\min} = 6$. For small-world networks, $\langle k \rangle = 12$ and the rewiring probability is 0.1.

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From dynamics to topology: inferring network structures

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To determine the threshold

$$S \equiv \sum_{i=1}^{N} 1/C_{ii} = 2cl^2/[\sigma^2(N + l)]$$

where $l = \sum_{i=1}^{N} k_i = N\langle k\rangle$

$$l = (S\sigma^2 + \sqrt{S^2\sigma^4 + 8cNS\sigma^2})/4c$$

High accuracy

TABLE I. Success rates of existent links (SREL) and of non-existent links (SRNL) [20] with our method for (i) Consensus, (ii) I-Rössler, (iii) N-Rössler, and (iv) Kuramoto dynamics on random [21], small-world [22], scale-free model networks [23], and six real-world networks: network of political book purchases (Book) [24], friendship network of karate club (Karate) [25], network of American football games among colleges (Football) [26], electric circuit networks (Elec. Cir.) [27], dolphin social network (Dolphins) [28], and the neural network of C. Elegans (C. Elegans) [22]. The noise strength is $\sigma^2 = 2$. For the non-identical Rössler system, $\omega = [0.8, 1.2]$ and for the Kuramoto dynamics, $\omega = [0, 0.2]$. Other parameters of model networks are the same as Fig. 1.

SREL/SRNL	Consensus	I-Rössler	N-Rössler	Kuramoto
Random	1.00/1.00	1.00/1.00	0.995/1.00	0.977/0.999
Small-world	0.993/1.00	0.988/1.00	0.979/1.00	0.982/1.00
Scale-free	0.995/1.00	0.990/1.00	0.980/1.00	0.978/1.00
Book	0.971/1.00	0.977/1.00	0.964/1.00	0.967/1.00
Karate	0.962/1.00	0.962/1.00	0.936/1.00	0.949/1.00
Football	0.938/1.00	0.932/1.00	0.928/1.00	0.927/1.00
Elec. Cir.	0.976/1.00	0.973/1.00	0.971/1.00	0.965/1.00
Dolphins	0.984/1.00	0.981/1.00	0.984/1.00	0.973/1.00
C. Elegans	1.00/0.997	1.00/0.996	1.00/0.997	0.993/0.997

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From dynamics to topology: inferring network structures

Path-integral representation

$$C_{ij} = \frac{\sigma^2}{2c} \sum_{\text{path}} \prod_{m \in \text{path}} \frac{1}{k_m},$$

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$$C_{ii} = \frac{\sigma^2}{2c}\left(\frac{1}{k_i} + \frac{1}{k_i^2}\sum_{q\in\Gamma_i}\frac{1}{k_q}\right) \simeq \frac{\sigma^2}{2ck_i}\left(1 + \frac{1}{\langle k\rangle}\right) \qquad (7)$$

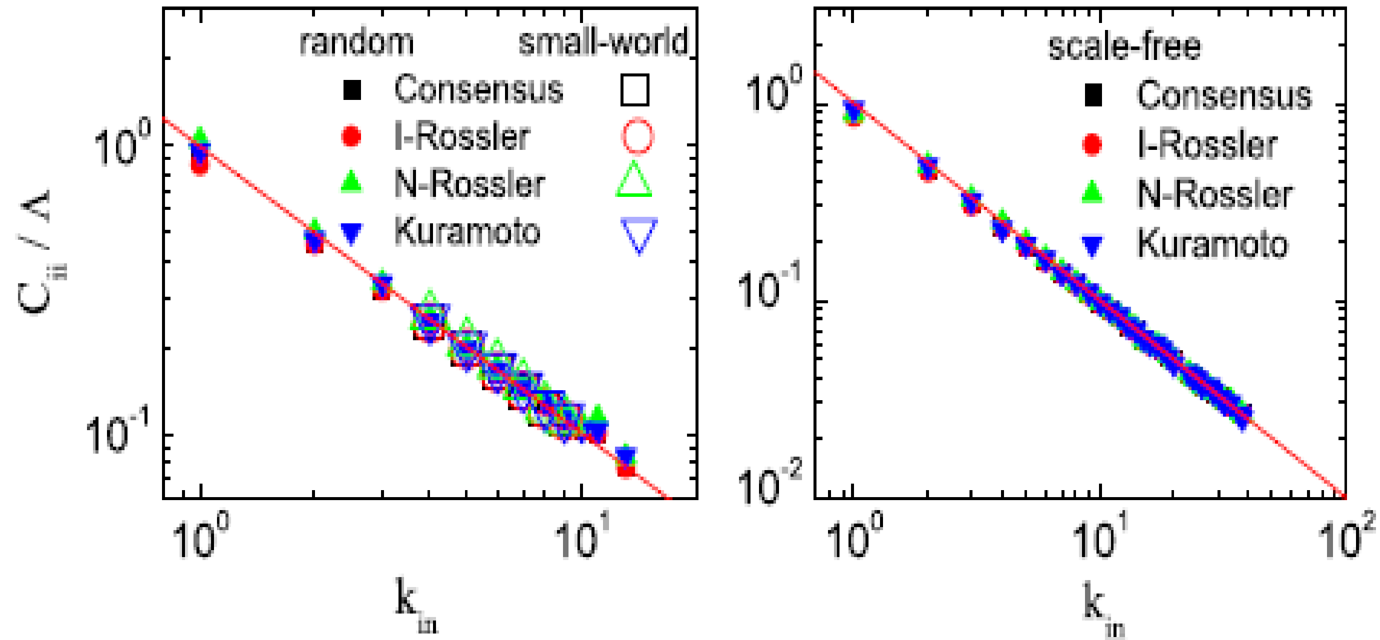


FIG. 2 (color online). C_{ii} as a function of node in-degree k_{in} for different node dynamics for directed networks where each link is assigned a random direction, and $\Lambda = \sigma^2(1 + 1/\langle k\rangle)/2c$. Other network parameters are the same as in Fig. 1. The lines are predictions from Eq. (7).

Networks with Time-delay Coupling

$$\dot{\mathbf{x}}_i(t) = \mathbf{F}_i[\mathbf{x}_i(t)] - c\sum_{j=1}^{N} L_{ij}\mathbf{H}[\mathbf{x}_j(t-\tau)] + \eta_i(t),$$

$$\mathbf{x}_i = \bar{\mathbf{x}}_i + \xi_i$$

$$\dot{\xi}_i(t) = D\mathbf{F}_i \cdot \xi_i(t) - c\sum_{j=1}^{N} L_{ij} D\mathbf{H} \cdot \xi_j(t-\tau) + \eta_i(t),$$

$$\epsilon_\alpha = \sum_i \psi_{\alpha i}\xi_i, \quad \zeta_\alpha = \sum_i \psi_{\alpha i}\eta_i, \quad D\mathbb{F}_{\alpha\beta} = \sum_i \psi_{\alpha i} D\mathbf{F}_i \psi_{\beta i},$$

$\psi_{\alpha j}$ the αth normalized eigenvector of L

λ_α the corresponding eigenvalue. $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots \lambda_{N-1}$.

$$\dot{\epsilon}_\alpha(t) = \sum_\beta D\mathbb{F}_{\alpha\beta} \cdot \epsilon_\beta(t) - c\lambda_\alpha D\mathbf{H}\epsilon_\alpha(t-\tau) + \zeta_\alpha(t).$$

$D\mathbf{F}_i \approx D\mathbf{F}$ so that $D\mathbb{F}_{\alpha\beta} = D\mathbf{F}\delta_{\alpha\beta}$.

$$\dot{\epsilon}_\alpha(t) = D\mathbf{F}\epsilon_\alpha(t) - c\lambda_\alpha D\mathbf{H}\epsilon_\alpha(t-\tau) + \zeta_\alpha(t).$$

Assuming small time delay, we can apply the first-order approximation: $\epsilon(t-\tau) = \epsilon(t) - \tau\dot{\epsilon}(t)$. This yields

$$(1 - c\tau\lambda_\alpha)\dot{\epsilon}_\alpha(t) = (D\mathbf{F} - c\lambda_\alpha D\mathbf{H})\epsilon_\alpha(t) + \zeta_\alpha(t).$$

W.X. Wang, J. Ren, Y.C. Lai, and B. Li, PRE, under review.

From dynamics to topology: inferring network structures

Assuming small time delay, we can apply the first-order approximation: $\epsilon(t-\tau)=\epsilon(t)-\tau\dot{\epsilon}(t)$. This yields

$$(1-c\tau\lambda_\alpha)\dot{\epsilon}_\alpha(t)=(D\mathbf{F}-c\lambda_\alpha D\mathbf{H})\epsilon_\alpha(t)+\zeta_\alpha(t).$$

$$\langle\epsilon_\alpha^2\rangle=\frac{\sigma^2}{(1-c\tau\lambda_\alpha)\left[c\lambda_\alpha(D\mathbf{H}+D\mathbf{H}^T)-(D\mathbf{F}+D\mathbf{F}^T)\right]}$$

$$C_{ij}\;=\;\langle\xi_i\xi_j\rangle=\textstyle\sum_{\alpha=1}^{N-1}\psi_{\alpha i}\psi_{\alpha j}\langle\epsilon_\alpha^2\rangle$$

$$C_{ij}=\frac{\sigma^2}{2c}\sum_{\alpha=1}^{N-1}\frac{\psi_{\alpha i}\psi_{\alpha j}}{(1-c\tau\lambda_\alpha)\left[\lambda_\alpha\frac{D\mathbf{H}+D\mathbf{H}^T}{2}-\frac{D\mathbf{F}+D\mathbf{F}^T}{2c}\right]}.$$

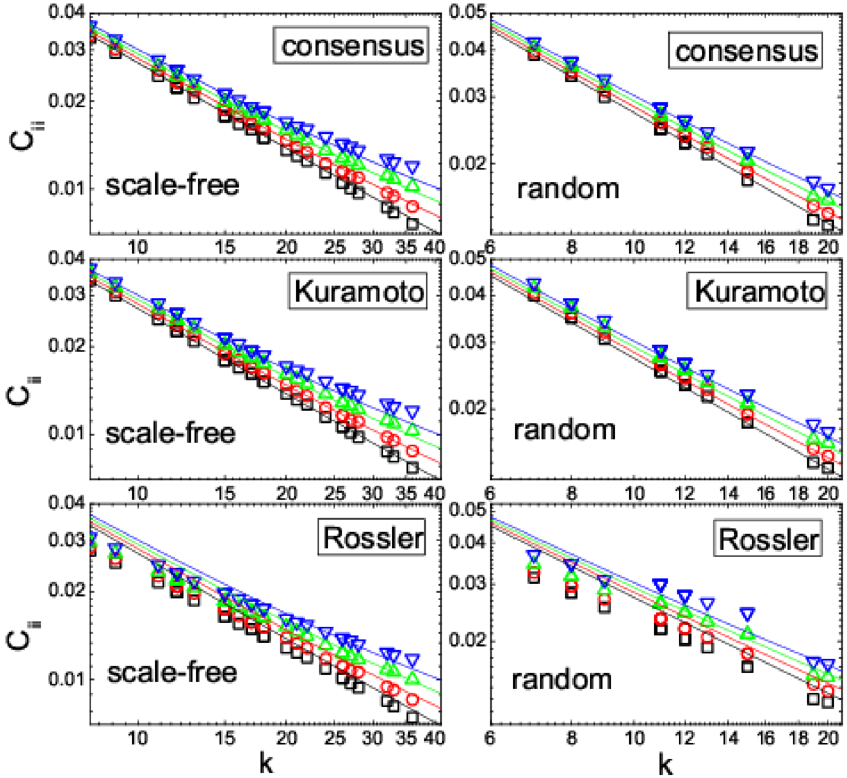
$$C_{ij}\approx\frac{\sigma^2}{2c}\sum_{\alpha=1}^{N-1}\frac{1+c\tau\lambda_\alpha}{\lambda_\alpha}\psi_{\alpha i}\psi_{\alpha j}=\frac{\sigma^2}{2c}[\hat{\mathbf{L}}^\dagger+c\tau\hat{\mathbf{I}}]_{ij},$$

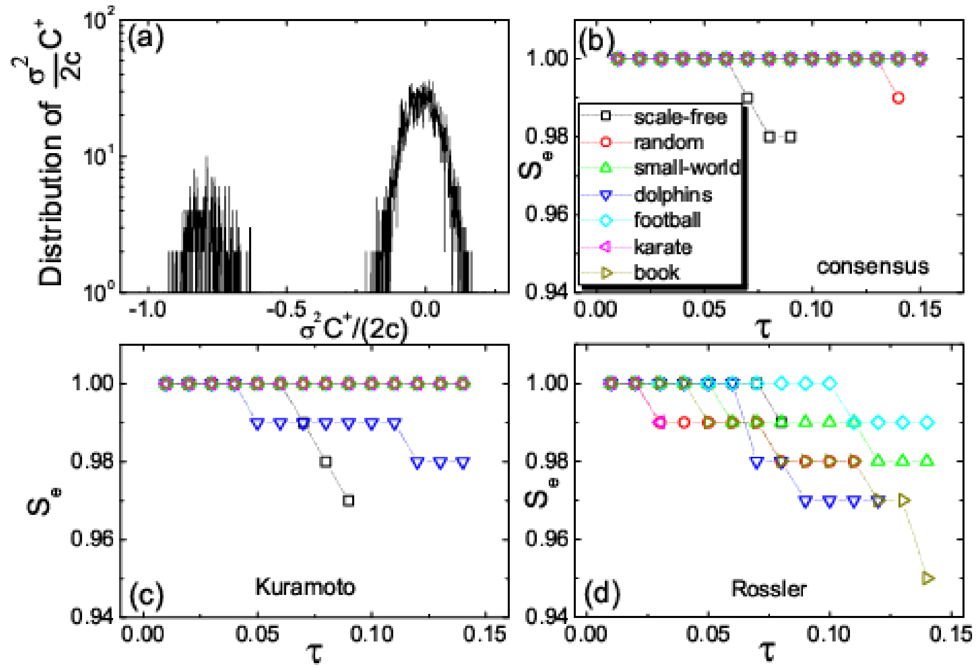
$$C_{ii}\;\approx\;\frac{\sigma^2}{2c}[\hat{\mathbf{K}}^{-1}+\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}+\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}\hat{\mathbf{P}}\hat{\mathbf{K}}^{-1}]_{ii}+\frac{\sigma^2\tau}{2}\;\approx\;\frac{\sigma^2}{2ck_i}\left(1+\frac{1}{\langle k\rangle}\right)+\frac{\sigma^2\tau}{2}$$

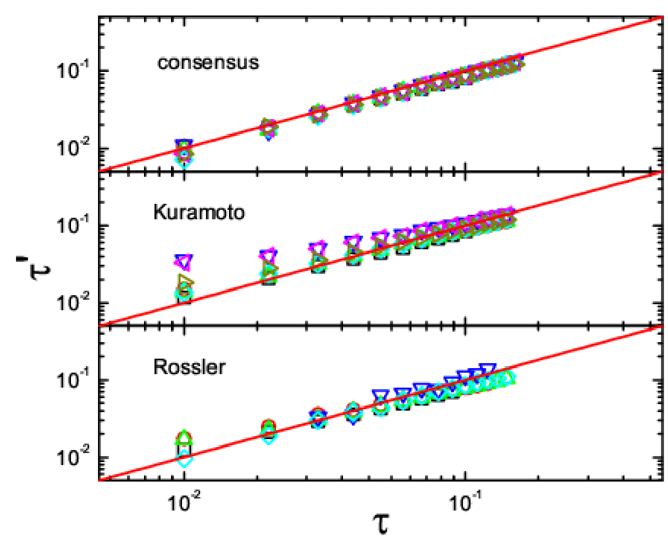
From dynamics to topology: inferring network structures

$$C_{ij} \approx \frac{\sigma^2}{2c}[\hat{\mathbf{L}}^{\dagger} + c\tau\hat{\mathbf{I}}]_{ij}$$

$$C_{ii} \approx \frac{\sigma^2}{2ck_i}\left(1 + \frac{1}{\langle k \rangle}\right) + \frac{\sigma^2 \tau}{2},$$

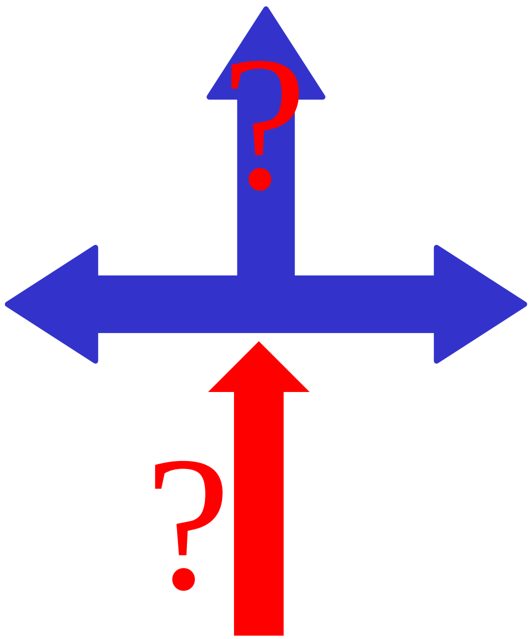




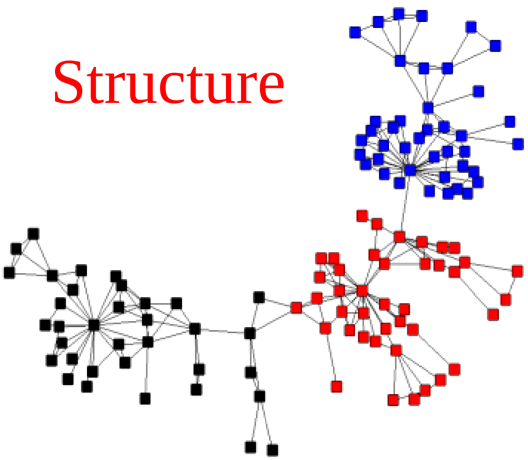


W.X. Wang, J. Ren, Y.C. Lai, and B. Li, arXiv:1101.6074.

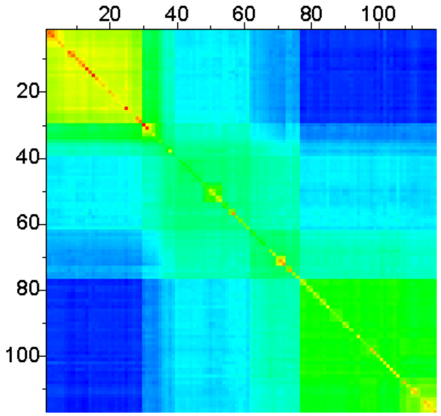
Function



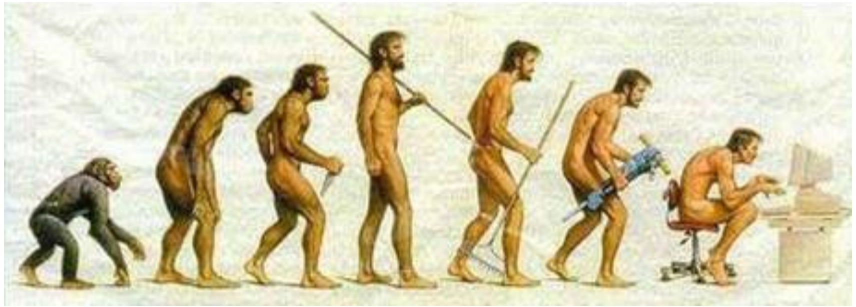
Structure



Dynamics

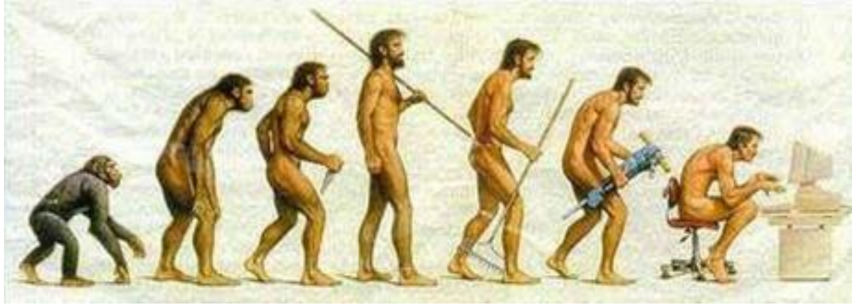


How are they canalized by Evolution?



Uncovering evolutionary ages of nodes in complex networks

By Guimei Zhu Thursday, 15:30pm



THANK YOU!

Consensus Dynamics

Examples: Internet packet traffic, information flow, opinion dynamics…

$$\dot{x}_i = -c\sum_{j=1}^{N} P_{ij}\cdot(x_i - x_j) + \eta_i,$$

P: adjacency matrix

L: laplacian matrix

Or: $\dot{x}_i = -c\sum_{j=1}^{N} L_{ij}\cdot x_j + \eta_i,$ $\langle \eta_i(t)\eta_j(t')\rangle = \sigma^2\delta_{ij}\delta(t-t'),$

Denote $\psi_{\alpha j}$ the αth normalized eigenvector of L

λ_α the corresponding eigenvalue. $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots \lambda_{N-1}.$

Transformation to eigen-space, using $\epsilon_\alpha = \sum_j \psi_{\alpha j} x_j$ $\zeta_\alpha = \sum_j \psi_{\alpha j}\eta_j$

$$\dot{\epsilon}_\alpha = -c\lambda_\alpha\epsilon_\alpha + \zeta_\alpha$$

solution: $\langle \epsilon_\alpha(t)^2\rangle = \frac{\sigma^2}{2c\lambda_\alpha}(1 - e^{2c\lambda_\alpha t})$

Transform back to real-space: $\langle (x_i - \bar{x})(x_j - \bar{x})\rangle = \sum_{\alpha=1}^{N-1}\psi_{\alpha j}\psi_{\alpha j}\langle \epsilon_\alpha(\infty)^2\rangle = \frac{\sigma^2}{2c}\sum_{\alpha=1}^{N-1}\frac{1}{\lambda_\alpha}\psi_{\alpha i}\psi_{\alpha j}$

Compact form: $\hat{\mathbf{C}} = \frac{\sigma^2}{2c}\hat{\mathbf{L}}^\dagger,$

Pseudo-inverse: $L^\dagger_{ij} = \sum_{\alpha=1}^{N-1}\frac{1}{\lambda_\alpha}\psi_{\alpha i}\psi_{\alpha j}$

J. Ren and H. Yang, cond-mat/0703232