Thermal Characterisation of Unweighted and Weighted Networks

Jianjia Wang, Hui Wu, Edwin R. Hancock

School of Computer Engineering and Science
Shanghai University
Department of Computer Science, University of York

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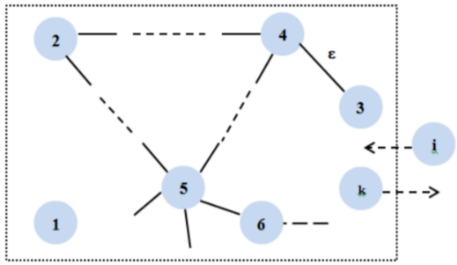
Introduction

Complex network

Thermodynamic analogy



Thermal system

the corresponding partition function

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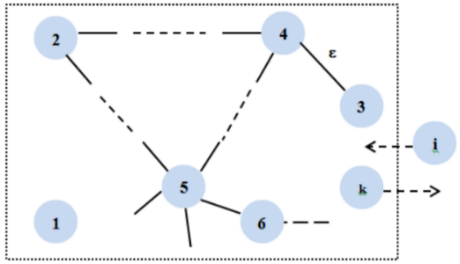
model weighted networks

limit the utility of models for the thermal characterisation of a complex network

Methods

the edges in a network

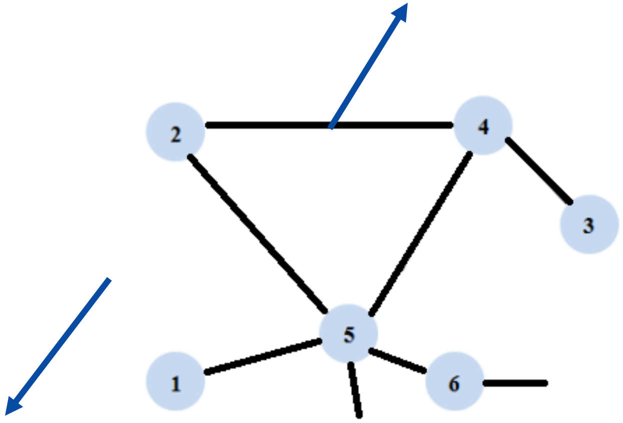


the virtual particles in a thermal system

The particles are in the ground state → $n_i = 0$ → no edge connection between nodes

The particles are in the excited state → $n_i = 1$ → edge connection between nodes

the excited state



the ground state

Temperature in networks

A network is represented by a $|V| \times |V|$ adjacency matrix whose elements indicate the existence or otherwise of edges $|E|$. We denote the weight of each edge is ω so that the total energy is that $U = \omega|E|$.

- the entropy $$S = k_B \ln W = -|V|^2 k_B [\frac{|E|}{|V|^2} \ln \frac{|E|}{|V|^2} + \left(1 - \frac{|E|}{|V|^2}\right) \ln(1 - \frac{|E|}{|V|^2})]$$

where k_B is Boltzmann constant

- the corresponding temperature $$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{N,E} = \frac{k_B}{\omega} \ln(\frac{|V|^2}{|E|} - 1)$$

- the standard deviation for the node degree $$\sigma_d = \sqrt{\sum_{i=1}^{|V|} (d_i - \langle d \rangle)^2} = \sqrt{\sum_{i=1}^{|V|} \left(d_i - \frac{|V|}{Z} e^{-\beta\omega}\right)^2}$$

Canonical ensembles

the traditional approach

- Measure a property of a network several times without controlling the microscopic states
- Complex

the Gibbs approach

- Introduce the concept of an ensemble
- A statistical ensemble is a probability distribution for the state of the system
- Convenient

- the corresponding free energy

$$F(T,|E|) = -k_B T \ln \mathrm{Q} = -|E|\, k_B T \ln\left[1 + e^{-w/(k_B T)}\right]$$

- the entropy

$$S = -\left(\frac{\partial F}{\partial T}\right)_E = \underbrace{|E|\, k_B \ln\left[1+\mathrm{e}^{-\beta w}\right]}_{-F/T} + \left(\frac{|E|\, w}{T}\right)\frac{\mathrm{e}^{-\beta w}}{1+\mathrm{e}^{-\beta w}}$$

- the average internal energy

$$U = F + TS = \frac{|E|\,\omega}{1 + e^{\omega/(k_B T)}}$$

- the heat capacity

$$C = \left(\frac{\partial U}{\partial T}\right)_E = |E|\, \frac{k_B (\beta w)^2 e^{\beta w}}{\left[1 + e^{-\beta w}\right]^2} = |E|\, k_B \left(\frac{\beta w}{Z}\right)^2 e^{\beta w}$$

Weighted networks

A weighted network contains a weighting function for the edges. We take the edge weights to be analogous to the energy states. The distribution of weights is mapped to the density of microstates (DOS) in the networks. This is closely related to the degree distribution.

- the partition function $Z_\omega = \int_0^\infty e^{-\beta\omega} D(\omega)\, d\omega$ where $D(\omega)$ is the distribution function for the weights

➢ **Exponential distribution** $D(\omega) = ke^{\alpha\omega}$

- the partition function $Z_\omega^E = \dfrac{k}{\beta-\alpha}, (\beta > \alpha > 0)$
- the internal energy $U_\omega^E = \dfrac{1}{\beta-\alpha}$
- the entropy $S_\omega^E = \log(\dfrac{k}{\beta-\alpha}) + \dfrac{\beta}{\beta-\alpha}$
- the heat capacity $C_\omega^E = \dfrac{\beta^2}{(\beta-\alpha)^2}$

➢ **Power-law distribution** $D(\omega) = c\omega^\gamma$

- the partition function $Z_\omega^P = \dfrac{c\Gamma(\gamma+1)}{\beta^{\gamma+1}}$
- the internal energy $U_\omega^P = \dfrac{\gamma+1}{\beta}$
- the entropy $S_\omega^P = \log(\dfrac{c\Gamma(\gamma+1)}{\beta^{\gamma+1}}) + \gamma + 1$
- the heat capacity $C_\omega^P = \gamma + 1$

Experiment results

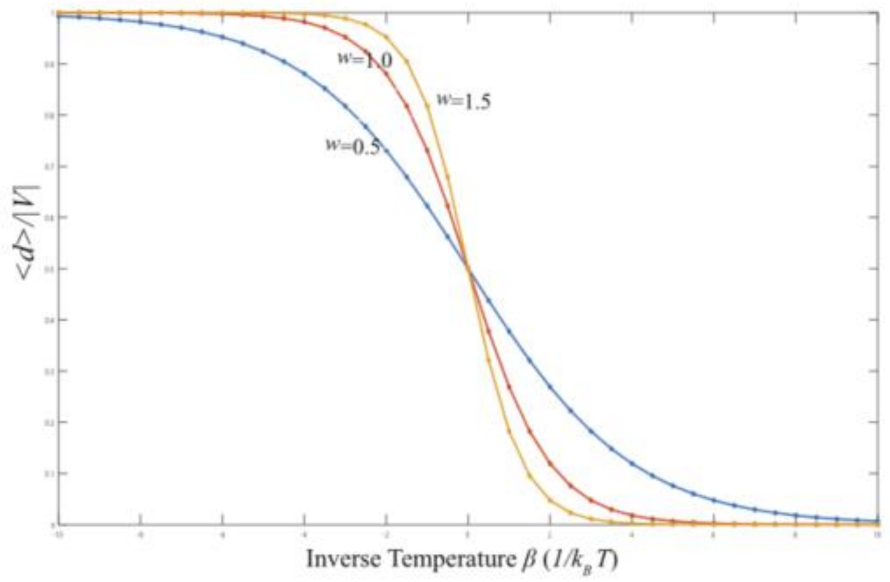


Fig. 1. The behaviour of average degree per node as a function of temperature β

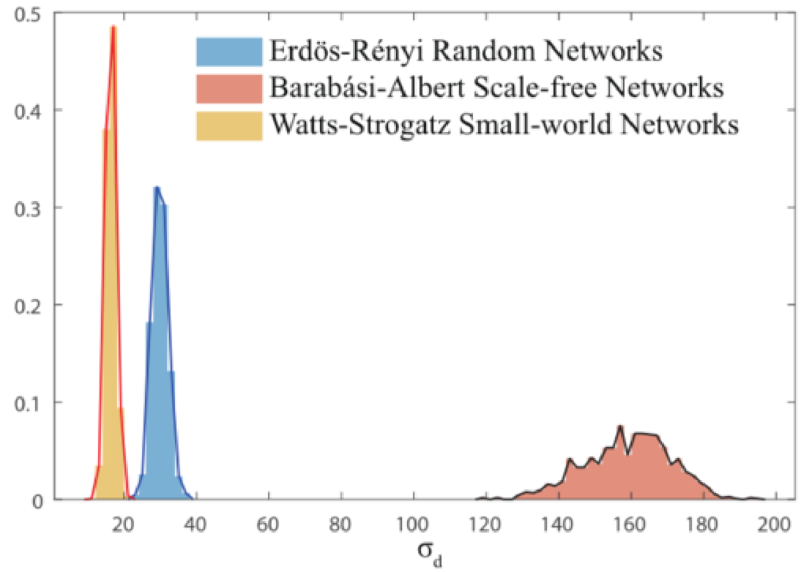


Fig. 2. Histograms of degree fluctuation for three different classes of complex network models(Erdős-Rényi random graph model, the Watts-Strogatz small-world model and the Barabási-Albert scale-free model), $N = 1,000$, $L = 10,000$

The random graphs and small-world networks have narrow bandwidth distribution. However, the scale-free networks exhibit a rather different distribution with a broad bandwidth in the degree fluctuation.

Experiment results

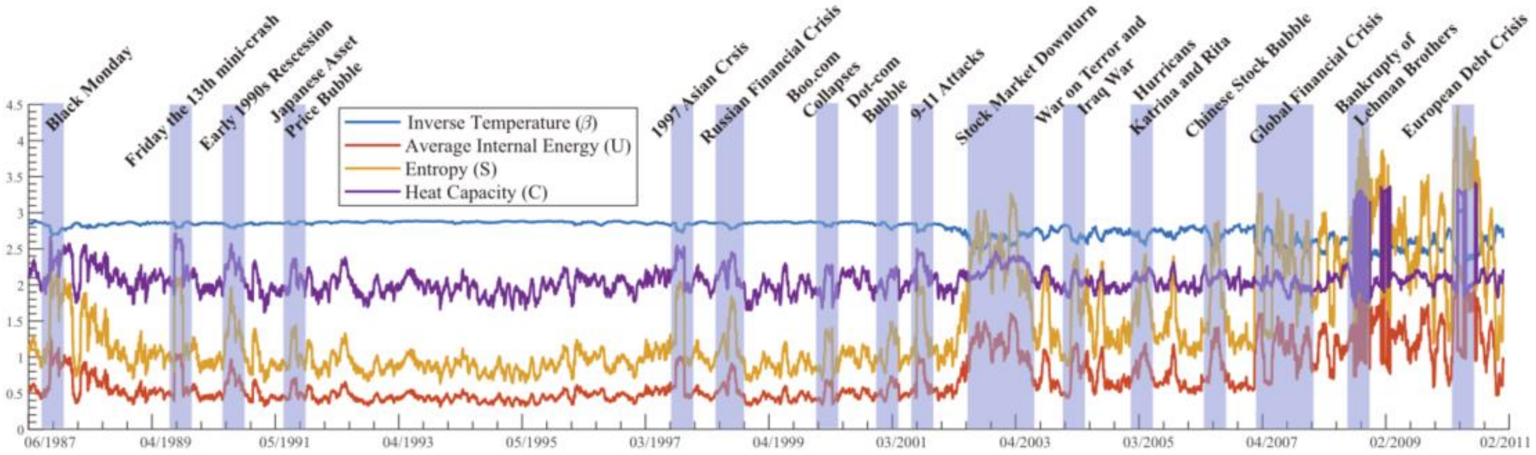


Fig. 3. Thermal quantities in NYSE (1987-2011) derived from directed networks.

The sharp peaks in the thermodynamic characterisations indicate significant changes in network structure events during the different financial crises.

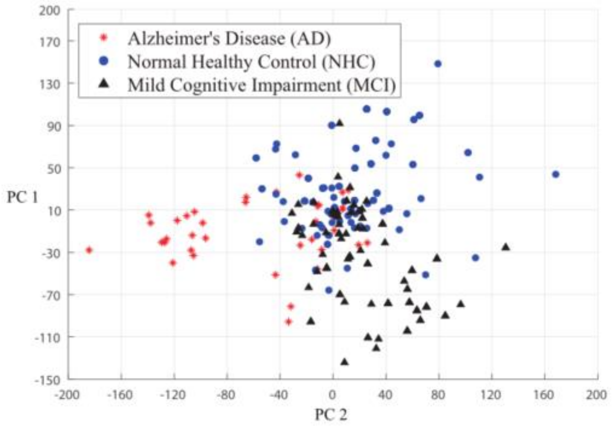


Fig. 7. Visualisation of leading LDA components for thermal features used to classify three groups of patients in the Alzheimer's disease study (AD, NHC, MCI).

Each group of network features forms a cluster in the projection space. This provides a good separation among the three groups of Alzheimer’ s subjects (AD, NHC, MCI).

Conclusions

Innovation

- develop a novel thermodynamic analogy (the edges are mapped to the particles)
- explore a weighted network representation
- the thermal characterisations are derived from the corresponding partition function
- give global properties such as average internal energy, entropy, heat capacity

Utility

- identify fluctuations in network structure
- distinguish different kinds of network structures

Future work

- explore the micro-canonical and grand-canonical ensembles
- break the conservation law underpinning Boltzmann statistics