Thermal Characterisation of Unweighted and Weighted Networks

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Introduction

Thermodynamic characterisations or analogies have proved to provide powerful tools for the statistical analysis of network populations or time series, together with the identification of structural anomalies that occur within them. However, the physical analogy adopted in this analysis is sometimes vague and remains an open question. In this paper, we take a novel view of the thermal characterisation where we regard the edges in a network as the particles of the thermal system. By considering networks with a fixed number of nodes we obtain a conservation law which applies to the particle occupation configuration. Using this interpretation, we provide a physical meaning for the temperature. If we further interpret the elements of the adjacency matrix as the binary microstates associated with edges, this allows us to further extend the analysis to systems with edge-weights. We thus introduce the concept of the canonical ensemble into the thermal network description and the corresponding partition function and then use this to compute the thermodynamic quantities.

Results

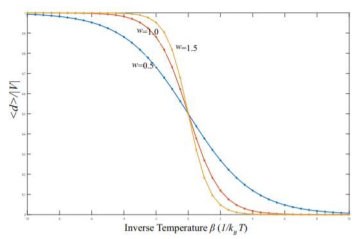

Fig. 1. The behaviour of average degree per node as a function of temperature β

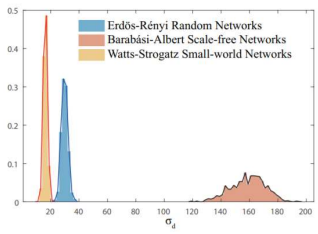

Fig. 2. Histograms of degree fluctuation for three different classes of complex network models(Erdős-Rényi random graph model, the Watts-Strogatz small-world model and the Barabási-Albert scale-free model), $N = 1,000$, $L = 10,000$

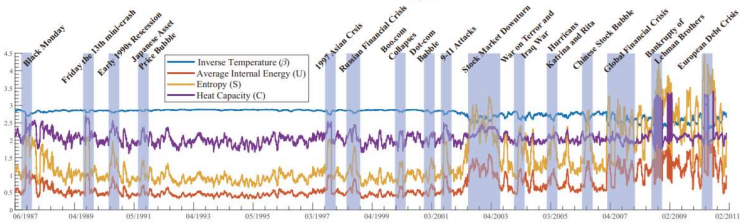

Fig. 3. Thermal quantities in NYSE (1987-2011) derived from directed networks.

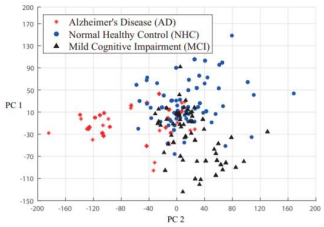

Fig. 7. Visualisation of leading LDA components for thermal features used to classify three groups of patients in the Alzheimer's disease study (AD, NHC, MCI).

In Fig.1 and Fig.2, we explore the utility of the degree fluctuation as a means of distinguishing the three models and find 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. In Fig.3, the sharp peaks in the thermodynamic characterisations indicate significant changes in network structure events during the different financial crises. Fig.7 shows that 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).

Methods

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 of the network can be written as,

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

where k_B is Boltzmann constant. This derives the temperature for the network configuration with the fixed number of nodes $|V|$ and edges $|E|$ as,

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

The standard deviation for the node degree can be regarded as the measure of fluctuation,

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

The network of binary states is analogous to a thermal system forming a canonical ensemble, which means the whole bunch of networks have an identical number of edges and nodes with different configurations of structural connection. The corresponding free energy can be calculated by using the partition function,

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

Then, some thermodynamic quantities, such as the corresponding entropy and the average internal energy, can be easily derived.

For a weighted network, we study two conservative distributions of DOS, namely, the exponential distribution and the power-law. We compute the integral form of the partition function for the weighted network,

$$Z_\omega = \int_0^\infty e^{-\beta\omega} D(\omega)\, d\omega$$

where $D(\omega)$ is the distribution function for the weights.

Conclusion

The main conclusion is that we develop a new thermal network characterisation based on an analogy where the edges are mapped to the particles. The corresponding temperature defines the physical meaning of nodes and edges in the network. We also explore a weighted network representation where the edge weights are the microstate energies. The thermal characterisations are derived from the corresponding partition function and give global properties such as average internal energy, entropy, heat capacity. These are used to interpret the detailed structural connections in the networks. Our experimental results suggest these thermal descriptions are useful to identify fluctuations in network structure and distinguish different kinds of network structures.

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