fMRI Brain Networks as Statistical Mechanical Ensembles

Jianjia Wang*; Hui Wu; Edwin R. Hancock

Introduction

Network neuroscience has been proved to be a sophisticated way to study the intrinsic connectivity in the brain. Tools from statistical mechanics derived from thermal physics have been extensively used to provide an appropriate way of constructing and analysing fMRI networks. According to this viewpoint, we apply ensemble methods from statistical physics to analyse fMRI brain networks for Alzheimer's patients. By mapping the nodes in a network to virtual particles in a thermal system, the microcanonical ensemble and the canonical ensemble are analogous to two different fMRI network representations. The microcanonical ensemble corresponds to a set of networks with a fixed fraction of edges, while the canonical ensemble corresponds to the set networks with edges obtained with a fixed value of the threshold. Ensemble methods describe the macroscopic properties of a network by considering the underlying microscopic characterisations which are closely related to the degree configuration and network entropy. The resulting method turns out to be an effective tool to identify the most salient anatomical brain regions in AD and provides a tool to distinguish groups of patients in different stages of the disease.

Experimental Results

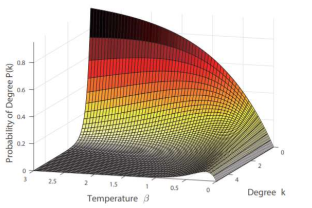

Fig. 1. 3D plot of degree probability with different value of degrees k and the inverse temperature β.

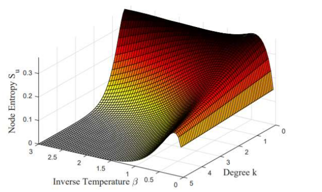

Fig. 2. 3D plot of node entropy from Eq.(26) with different value of degrees k and the inverse temperature β.

In Fig.1, for high degree nodes, the degree probability presents a slight peak in the high-temperature region, but still remaining at a low value of probability. This maximum illustrates that a transition has occurred in the degree distribution with the inverse temperature, and depends on the value of degree at the nodes. For Fig.2, in terms of the temperature, there is a peak that is similar to that observed in the degree probability in the high-temperature region. Thus, there is also a phase transition for the entropy at each node with a varying value of temperature.

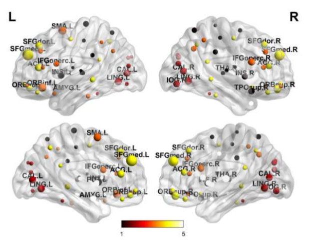

Fig. 3. The significant different of nodal entropy in the anatomical regions in the brain.

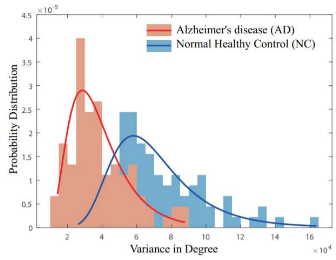

Fig. 4. Probability distribution of degree variance in AD and NC groups

In Fig.3, we explore patients with the depressive neurodegenerative disease have structural and functional inhibition in the frontal lobe and occipital lobe. They are severely damaged by AD with aberrant symptoms that affect recognition, memory and emotional behaviour. Figure 4 shows that the brain networks in AD occupy the lower range of node degree variance compared to the normal subjects.

Methods

A network is represented by $G = (V, E)$, V, E are the number of nodes and edges. We use two different statistical ensembles in the representation of brain functional connectivity networks. In the microcanonical ensemble, a network is regarded as an isolated system with a fixed number of both nodes $|V|$ and edges $|E|$. We denote the weight of each edge is ω so that the total energy is $U = \omega|E|$. The entropy of the network can be written as,

$$S = k_B \ln W = (\mathrm{U} + |\mathrm{V}| - 1)\log(\mathrm{U} + |\mathrm{V}| - 1) \\ - \mathrm{U}\log\mathrm{U} - (|\mathrm{V}| - 1)\log(|\mathrm{V}| - 1)$$

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,

$$\beta = \left(\frac{\partial S}{\partial U}\right)_{|V|} = \frac{1}{\omega} log \frac{U + |V| - 1}{U}$$

The probability distribution for individual node at the energy state can be given by the exponential function,

$$\mathrm{P}(d_u = \mathrm{k}) = \frac{1}{Z} e^{-\beta E_s} = \left(1 - e^{-\beta\omega}\right) e^{-\beta k \omega}$$

$$= \frac{|V| - 1}{\omega|E| + |V| - 1} \left(\frac{\omega|E|}{\omega|E| + |V| + 1}\right)^k$$

where Z is the partition function following the constrain of energy conservation

$$Z = \sum_{\mathrm{k}=0}^{|V|} e^{-\beta \mathrm{k} \omega} = \frac{1 - e^{-|\mathrm{V}|\beta\omega}}{1 - e^{-\beta\omega}} \approx \frac{1}{1 - e^{-\beta\omega}}.$$

when $|V| \gg |E| \gg 1$, i.e., the network is sparse, the degree distribution can be approximated as the power-law,

$$P(k) = \frac{1}{\omega\bar{d}+1} \left(\frac{\omega\bar{d}}{\omega\bar{d}+1}\right)^k \sim c\bar{d}^k;$$

when $|V| \gg |E| \gg 1$, i.e., $\bar{d} \gg 1$, the Taylor expansion of the exponential term is approximated as $e^{-\beta\omega} \approx 1 - e^{-\beta\omega}$

the degree distribution follows the exponential distribution,

$$P(k) = \beta e^{-\beta k}.$$

Conclusion

In this paper, we present a novel way to analyse fMRI networks from the statistical ensembles. Two kinds of ensemble networks, i.e., microcanonical ensemble and canonical ensemble, are studied and suggest different ways of choosing the activation thresholds in fMRI network generation. The microscopic energy states in the thermal system are analogous to the degree of nodes with the unit edge weight. This derives the definition of temperature and partition function used to characterise the structural properties in the network. The degree distribution presents a phase transition with the value of temperature. In experiment, with an expression for the degree distribution to hand, we decompose the global network entropy into contributions associated with each node and use this to identify the most affected anatomical regions in the brain. The variance of associated node degree combined with node entropy work well as the features to classify different groups of patients.

Email

jianjiawang@shu.edu.cn