fMRI Brain Networks as Statistical Mechanical Ensembles

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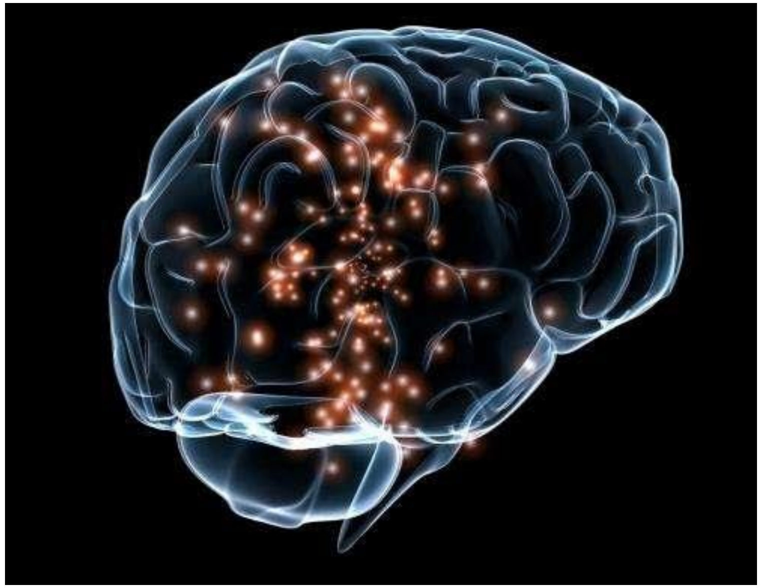
Introduction



the network structure

the neuronal activities

the network characterisations

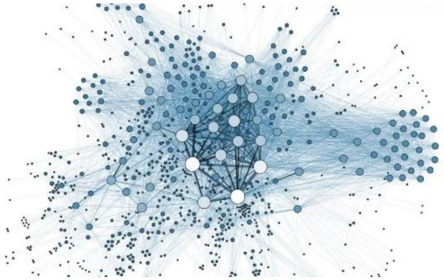
analyse clinical disorders

Alzheimer’s disease(AD)

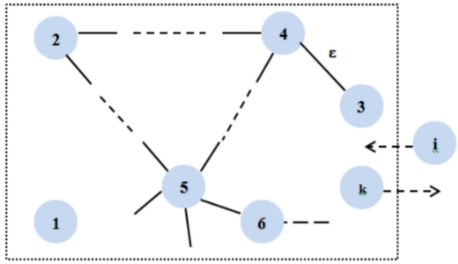
the brain network construction

(no consistent best method)

Thermodynamics and statistical physics



the nodes in a network



the virtual particles in a thermal system

- microcanonical ensemble
- the canonical ensemble

the partition function

thermodynamic characteristics in networks

capture the macroscopic characteristics of networks

temperature, helmholtz free energy, entropy, etc

Statistical Ensembles

➢ The microcanonical ensemble

This is an ensemble of networks which have a fixed number of nodes and edges. Each edge has a unit weight. This gives a preliminary definition of energy and entropy that associate with the network structure.

➢ The canonical ensemble

This is an ensemble of networks which have a fixed number of nodes but a variable number of edges. Each edge has the unit weight. This allows us to introduces the concept of temperature, associated with the variance of the number of edges. The degree of each node is analogous to the energy states of the thermal system.

Methods

In microcanonical ensemble

In the microcanonical ensemble, a network is regarded as an isolated system with a fixed number of both nodes $|V|$ and edges $|E|$.

- the probability distribution for individual node $$P_s = \frac{1}{Z} e^{-\beta E_S}$$ where Z is the partition function $$Z = \sum_{s=0}^{|V|} e^{-\beta E_S}$$

- the average energy $$\bar{U} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta}$$

- the corresponding entropy $$S = -\sum_{s=0}^{|V|} P_S \log P_S = \beta \bar{U} + \log Z$$

Methods

➢ In canonical ensemble

Similar to the microcanonical ensemble, networks in the canonical ensemble have the fixed number of nodes but a variable number of edges.

- the temperature $$T = \left(\frac{\partial U}{\partial S}\right)_{|V|} = \frac{1}{k_B \beta}$$

- the Helmholtz free energy $$F = \bar{U} - TS = -T \log Z$$

- the corresponding entropy $$S = -\left(\frac{\partial F}{\partial T}\right)_{|V|} = \left[\frac{\partial (T \log Z)}{\partial T}\right]_{|V|}$$

Phase Transition in Degree

In the microcanonical ensemble, We denote the weight of each edge is ω so that the total energy is $U = \omega|E|$. 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

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

a) when $|V| \gg |E| \gg 1$, the degree distribution can be approximated as the power-law,

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

b) when $|E| \gg |V| \gg 1$, the degree distribution follows the exponential distribution,

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

Experiment

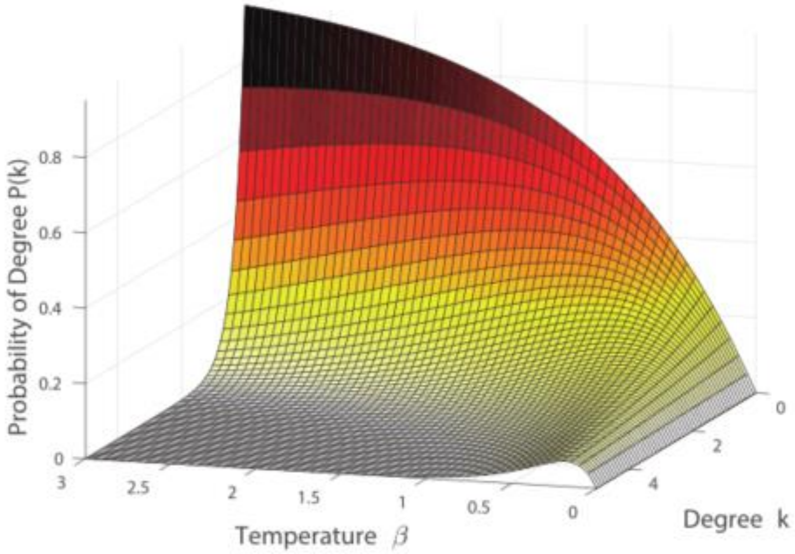


Fig. 1. 3D plot of degree probability with different value of degrees k and the inverse temperature β.

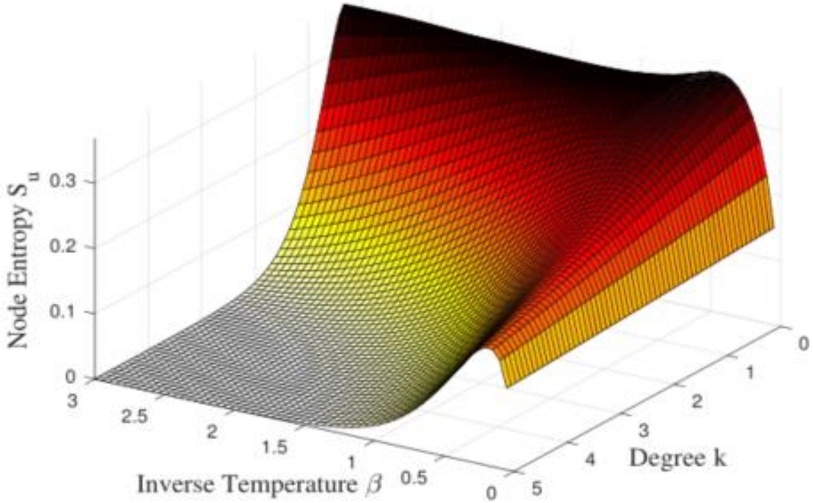


Fig. 2. 3D plot of node entropy from Eq.(26) with different value of degrees k and the inverse temperature β.

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.

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.

Experiment

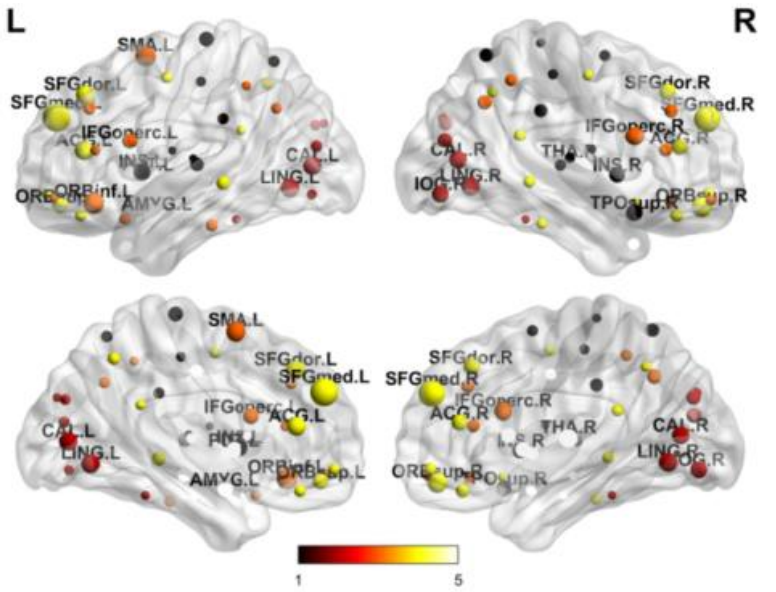


Fig. 3. The significant different of nodal entropy in the anatomical regions in the brain.

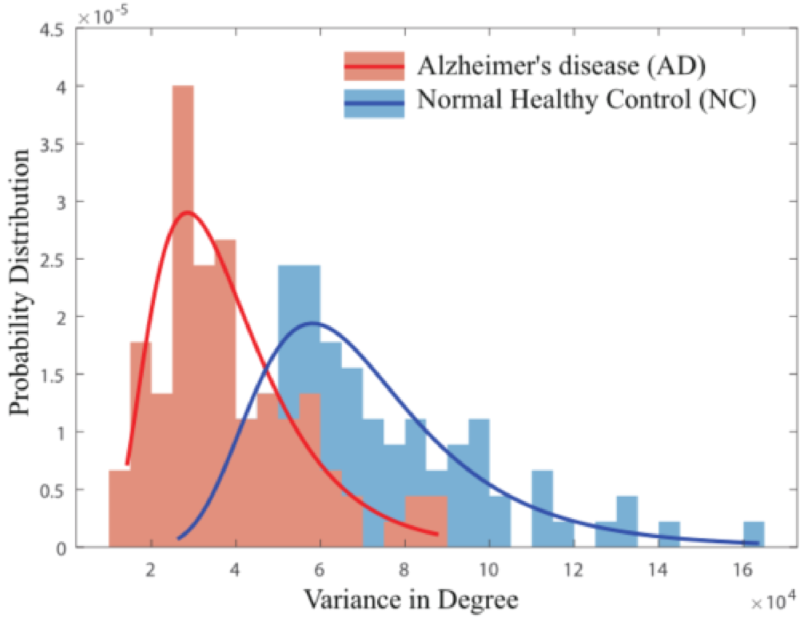


Fig. 4. Probability distribution of degree variance in AD and NC groups

Fig.3 plots patients with the depressive neurodegenerative disease have structural and functional inhibition in the frontal lobe and occipital lobe.

Figure 4 shows that the brain networks in AD occupy the lower range of node degree variance compared to the normal subjects.

Conclusions

- 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,
- The degree distribution presents a phase transition with the value of temperature
- We use this method 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.