Entropy inflection and first-order phase transition to disordered ground states

Hai-Jun Zhou[1]

[1] Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China (zhouhj@itp.ac.cn)

Lower temperature leads to a higher probability of visiting low-energy states. This intuitive belief underlies most physics-inspired strategies for addressing hard optimization problems. For instance, the popular simulated annealing (SA) dynamics is expected to approach a ground state if the temperature is lowered appropriately. Here we demonstrate that this belief is not always justified.

Specifically, we employ the cavity method of spin glass to analyze the minimum strong defensive alliance (SDA) problem and discover a bifurcation in the solution space, induced by an inflection point in the entropy–energy profile (see curve B of Fig. 1). Given a graph G of N vertices and M edges, a non-empty subset A of vertices is regarded as an alliance if and only if at least half of the nearest neighbors of every vertex $i \in A$ are also in A (Fig. 1). The SDA problem aims to construct an alliance of smallest cardinality, which requires a careful choice of vertices because SDA is a collective property of all vertices involved. It is a prototype of problems concerning densely connected subgraphs.

We demonstrate that while easily accessible SDA configurations are associated with the lower-free-energy branch, the low-energy configurations are associated with the higher-free-energy branch within the same temperature range. There is a discontinuous phase transition between the high-energy configurations and the amorphous ground states, which generally cannot be followed by SA. We introduce an energy-clamping strategy to obtain superior solutions by following the higher-free-energy branch, overcoming the limitations of SA.

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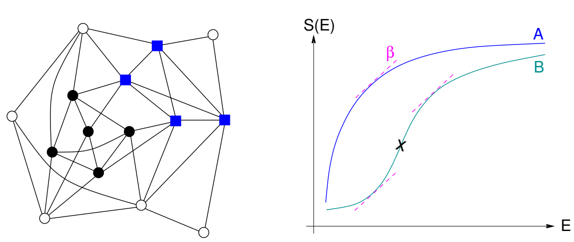

Figure 1: (left) Two strong defensive alliance solutions for a small graph: the one denoted by filled circles has energy $E=5$; the other denoted by filled squares is the minimum alliance, $E=4$. (right) Two qualitatively different entropy curves $S(E)$: curve A is concave, its slope $\beta(E)$ decreases with energy E; curve B is non-concave, it has an inflection point ('X') at which the slope β attains the maximum value.