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Report on my stay during March 2016 at the Yukawa Institute for Theoretical Physics

Pan Zhang[1]
[1]Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190 China
E-mail: panzhang@itp.ac.cn

Abstract. In this document I report my research outcome during my stay at the Yukawa Institute of Theoretical Physics from March 1st and March 31st, 2016, which is supported by the International Research Unit of Advanced Future Studies. The report mainly contains a non-technical summary of my recent study on effects of triangles in several network problems including percolation problem and neural network as associative memories.

Keywords: Percolation transition, Neural networks, Non-backtracking matrix, Triangles, Belief Propagation

1. Introduction

I have been visiting at the Yukawa Institute of Theoretical Physics (YITP) from March 1st to March 31st 2016, and was supported by the International Research Unit of Advanced Future Studies. During my stay I have attended a workshop "International Workshop on Advanced Future Studies" from March 14th to March 16th, and gave a talk entitled "Statistical-Physics-based Clustering in Networks". The main research output of my stay during this period is the study on effects of triangles in some network problems, which will be introduced in the following text.

1.1. Background of the problems

Lost of problems of complex systems are defined on a network that represents interactions between agents of the system. For example percolation on a social network gives a simple example of spreading of disease over human contacts. Associative memory models give simple examples to memory stored by neurons connected by synapses in human brain. Many efforts have been devoted to study analytically the statistical property of the system on a given network, especially when network have some good properties like locally-tree like structure. However real-world networks often contain many closed triangles, which contribute to a large clustering coefficient. For example in the social networks we often observe a phenomenon that friends of friends are friends, a typical phenomenon of clustering due to presence of triangles in the network. There are few analytical studies about effects of triangles on the network problems. In this report I give a non-technical summary on my study on effects of triangles for some network problems, including percolation problem, and neural network as associative memory.

1.2. Methods and main results

Our method is based on the belief propagation algorithm considering triangles, and the generalized non-backtracking matrix which is obtained by linearizing the belief propagation algorithm at the factorized fixed point when the system under study has a certain type of symmetry. Our results show that using a simple model for networks, e.g. random networks with local clustering, the effects can be quantitatively studied and are different in different problems: On the percolation problems, considering of triangles gives a tighter lower-bound for the true percolation transition than the lower-bound given by inverse of the leading eigenvalue of the non-backtracking matrix. On the associative memory problem, starting from a locally tree like topology and increasing number of triangles will always harmful to the associative memory and decrease the capacity of the neural network. In the following text we will describe in detail these two problems.

2. Percolation on networks with clustering

Percolation if one of the well-studied problem in statistical physics, and has been used to model many systems including spreading of diseases, attack of Internet, etc. In this (bond percolation) problem, consider a network with n nodes and m edges, each edge is open with probability p, and is closed with probability 1-p. We are interested in the size of connected percolation clusters which is set of nodes connected by open edges. The percolation is a random process, on each realization of the open-close configuration of edges, the percolation cluster could be different. However in the thermodynamic limit (n goes to infinity), the statistical properties of the percolation cluster can be well-characterized. In general with p value there are two situations, one is the non-percolation case that with n goes to infinity, size of the largest percolation cluster is finite, a simple example for this case is with p=0 where all edges are closed and there are n clusters each of which has size 1. The other case is the percolation case where the largest percolation cluster is infinite. In general there is a percolation transition p* separating these two cases. So the size of the largest percolation cluster and the position of the percolation transition, are of great interest in statistical physics, therefore many theory have been proposed to describe these two quantities.

Recently, some progresses have been made (Karrer, 2014; Hamilton, 2014) when the network is sparse and locally-tree like which means short loops (including triangles, quadrangles) in networks are rare. In the paper, authors have made use the Bethe approximation (Bethe, 1935) which assumes the independence of conditional probabilities that is exact when the network is a tree, and is a good approximation when the network is large and sparse. Authors also show that the inverse of the leading eigenvalue of the non-backtracking matrix (Krzakala, 2013) gives a lower bound to the true percolation transition.

However as we have described in the Introduction, most of the real-world networks like the human social networks, are not locally-tree like, as there are many triangles giving the network a high clustering coefficient (Watts, 1998). So the average size of the giant cluster computed in using the Bethe approximation could be a bad approximation to percolation on a network with lots of triangles, thus the lower-bound given by the inverse of the non-backtracking matrix could be a not tight. In this work we propose to improve the approach using the Bethe approximation by considering the effect of triangles. This is actually related to the Kikuchi approximation (also known as cluster expansion approximation) on a general graphs. If we choose a simple random graph model with clustering (Newman, 2009), where loops longer than 4 are, the Kikuchi-related method can be simplified to Bethe approximation considering edges and triangles, and this is the theoretical bases of our analysis.

Assuming the network contains only single edges (i.e., edges do not belong to any triangle) and triangles, first thing we can do is to write out the iterative equations for the marginal probability of a node belonging to a cluster of a particular size s, considering the effects of triangles. However this probability is not solvable in practice because of the larges number of possible cluster size. Fortunately the moment generating function of this probability is solvable and results to belief propagation equations (Yedidia, 2001) using two kinds of messages. One kind of messages is sent along a directed single edge of the graph from one node to another node; the other kind of messages is sent along a triangle to one of its end-point. From a random initial condition, this belief propagation equation will converge to a fixed-point from which we can compute the marginal probability of each node and the size of the giant cluster. Interestingly, belief propagation equations always converge in this case, indicating that there is no one-step replica symmetry breaking effects (Mezard, 2001), as opposed in other problems, e.g. in optimization problems (Zhang, 2009; Barbier, 2013). We think this may be due to the fact that the leading eigenvector always corresponds to one fixed-point of BP, and is always out of the bulk of the spectrum of the non-backtracking matrix as we illustrate below.

First we observe that all messages equal to 1 is always a fixed-point of the belief propagation equation. We call this fixed-point the factorized fixed-point. The point where the factorized fixed-point becomes unstable is our estimate for the percolation transition. The stability analysis of the factorized fixed-point of belief propagation is equivalent to finding the leading eigenvector of a new matrix we call the generalized non-backtracking matrix. As opposed to the non-backtracking matrix (Krzakala, 2013) which is defined on the directed edges of a graph, our generalized non-backtracking matrix is defined on directed edges and triangles of the graph. Since all elements of the matrix are non-negative, Perron-Frobenius applies that the leading eigenvalue is positive, as well as the elements of the elements of the leading eigenvector. Then by constructing a matrix with the same size as the generalized non-backtracking matrix, but has the same non-trivial eigenvalues as the non-backtracking matrix, then we can use the Collatz-Wielandt theorem to prove that the leading eigenvalue of the generalized non-backtracking matrix is always smaller or equal to the leading eigenvalue of the non-backtracking matrix. Further more, we also prove that the threshold given using the generalized non-backtracking matrix is always less or equal to the true percolation transition.

As a summary we show that the percolation transition given by the generalized non-backtracking matrix considering triangles is a lower-bound to the true percolation transition on an infinite connected graph, and is tighter than the bound given by inverse of the non-backtracking matrix.

3. Associative memory networks with clustering

There have been lots of analytical studies on the performance of an associative memory on fully connected graphs and on randomly diluted networks (Amit, 1985; Coolen, 2001; Zhang, 2015). However real neural networks have never been fully connected or randomly diluted. Simulation work reported that clustering is harmful to the performance of associative memory (McGraw, 2003; Kim, 2004), however there has been little study on analytical treatment to this effect. In the previous study we have considered this effect of loops to the dynamics of an associative memory (Zhang 2008), however the equilibrium properties, e.g. the position of the spin glass transition, to our best knowledge, has not been addressed before.

In this work we study the effect of triangles using the similar technics used in the previous section on percolation — the recent developed method of non-backtracking matrices (Krzakala, 2013; Zhang, 2015), but on weighted networks where weights are generated by Hebb's rule (I.e., essentially we are considering the Hopfield model (Hopfield, 1982). The non-backtracking operator for the Hopfield model is exactly the same as that for the Ising model (Zhang, 2015), so as the same procedure in the previous section, we extend this operator to consider the effect of triangles.

Following the belief propagation equation that written out in (Zhang, 2015), which was written out for the Ising model on graphs without (with rare) loops, we modified it into a form considering triangles. In this set of equations, there are still two kinds of messages: one is passing along directed edges (i to j), representing the marginal probability of node j taking value +1; the other kind of message is passing along triangles to one of its end-node, representing the marginal probability which is the expectation of the probability that the triangle ``wants'' its end-node to take +1. These probabilities are also called cavity probabilities in statistical physics. Then we note that when system has no external fields, as in the Hopfield model (Hopfield, 1982), the belief propagation equation has a factorized (paramagnetic) fixed-point where marginal probabilities are zero. This fixed-point reflects only the symmetry in the system: if we change all the +1 to -1 and all -1 to +1 in one configuration, the Hamiltonian of the system does not change at all, due to the symmetric couplings given by the Hebb's rule in the Hopfield model. So we can do exactly the same thing as we did in the last section, for the percolation problem, expanding the belief propagation equation to the first order around this factorized fixed-point, resulting to the generalized non-backtracking matrix as we introduced in the previous section.

However the generalized non-backtracking matrix is different from the one we introduced in last section in several ways: (i) positions of non-zero elements (the topology of the matrix) are the same but the non-zero elements are different. In Hopfield model, elements of the matrix are given by the memorized patterns, while in percolation the elements depends on the edge-open probability. (ii) The generalized non-backtracking matrix for percolation has non-negative elements, thus its leading eigenvalue and eigenvector are non-negative and they are essentially what we want. However in the Hopfield model, the generalized non-backtracking matrix contains negative elements, thus its leading eigenvalue could be negative, or even a complex value.

For Hopfield model, we essentially need first P eigenvalues and eigenvectors with P denoting number of memorized patterns. If there are P real eigenvalues outside the bulk in the spectrum, they correspond to P successfully memorized patterns, and the sign of the eigenvectors can be used to retrieve all patterns simultaneously. If number of patterns that we want to memorize is too large, the leading eigenvalue could be complex, representing the spin-glass state of the system. So the existence of eigenvalues out of the complex bulk tells us that system is in the retrieval phase; otherwise the system is in the spin glass phase. Thus the point when real eigenvalues join the bulk, system has a spin glass phase transition.

Using technics described above, we estimated the phase diagram for Hopfield model in the temperature and pattern-number plane, on networks with only single edges and triangles. And we found that with the same number of edges, the more triangles there are in the network, the smaller retrieval phase there are in the phase diagram. So as a conclusion, clustering is harmful to the performance of Hopfield model.

4. Summary

In this document I have reported two problems that I have been studying during my stay at the Yukawa Institute of Theoretical Physics during March, 2016. Using the similar technique — analysis of the spectrum of generalized non-backtracking matrix considering triangles in the network. We have estimated the effect of the triangles to the phase transitions of the system, and to the performance of the system. The study on the percolation problem will be summarized into a research paper, while the study on the Hopfield model is still in its early stage and needs more work to complete.

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