Belief propagation for graph partitioning

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Abstract
We study the belief-propagation algorithm for the graph bi-partitioning problem, i.e. the ground state of the ferromagnetic Ising model at a fixed magnetization. Application of a message passing scheme to a model with a fixed global parameter is not banal and we show that the magnetization can in fact be fixed in a local way within the belief-propagation equations. Our method provides the full phase diagram of the bi-partitioning problem on random graphs, as well as an efficient heuristic solver that we anticipate to be useful in a wide range of application of the partitioning problem.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Graph partitioning problem was one of the first optimization problems treated with methods of statistical mechanics of disordered systems [1, 2]. Since then other applications of the theory of spin glasses in hard optimization and constraint satisfaction problems attracted a lot of interest and many remarkable results were obtained. As anticipated in the early works [2, 3], understanding of the energy landscape and the phase transitions in the space of solutions leads to the understanding of algorithmic hardness of the problems [4, 5], and even more remarkably it leads to the development of a new class of heuristic algorithmic techniques [4]. Nowadays, the cavity method [6] serves as a state of art technique for understanding random optimization problems, and its application on given instances of the problem is a base for a class of one of the most promising heuristic solvers, known as message passing algorithms in computer science.

Despite all these activities in the field, neither the phase diagram nor a message passing algorithm for partitioning a graph into two groups of a given size has been worked out. The
main reason why the graph partitioning is a tricky problem to treat is the existence of a global constraint that fixes the size of the two groups. The aim of this article is to fill this gap, and give the phase diagram of the graph bi-partitioning on sparse random graphs and an associated belief-propagation algorithm.

1.1. Partitioning problem: setting and applications

A graph $G(V, E)$ is given by the set of vertices $V$ and edges $E$. If an element $(i, j)$ belongs to the set of edges we say that vertices $i$ and $j$ are connected. The graph bi-partitioning problem consists of dividing vertices of the graph into two disjoint sets of a given size, so as to minimize the number of connections between vertices from different groups. The problem is known to be NP-complete [7], and hence there is a good reason to believe that no exact polynomial algorithm exists.

The graph partitioning problem is encountered in many important applications. Here are a few examples: in an electric circuit design one needs to know on which board to place the different components to minimize the number of links between different boards [8]. In parallel computing one has to partition data and tasks among several processors in order to minimize the communication between them [9]. Partitioning is also closely related to data clustering and community detection [10]. The list could continue for long, and it is hence crucial to develop efficient heuristic algorithms that give good solutions to the problem.

A large volume of literature on heuristic methods for graph partitioning exists. One of the early fundamental works in the field is [11], its running time is, however, $O(N^2)$ so it is no longer used in practice. Simulated annealing techniques can be used, see e.g. [12, 13]. A local search based methods such as the extremal optimization of [14] were suggested. There is a whole class of spectral partitioning methods that use the eigenvectors of the Laplacian of the connectivity graph, see e.g. [15]. However, the current state of art method for partitioning, that is used in most practical applications, is based on the multi-level programming: the nodes are grouped into super-nodes and the super-nodes grouped again, at the end the system size is very small and the problem is solved exactly and the grouping of nodes is then unwrapped. The multi-level programs use elements from many other approaches, see [16] for an excellent review.

We do not anticipate that belief propagation developed in this paper will be, by itself, competitive with the highly tuned implementations of the multi-level methods. However, we do anticipate that it can be used as a component of these implementations. For example, in the multi-level algorithms one needs to estimate the probability that two nodes can be grouped in the same super-node—this is exactly what belief propagation is designed to compute very fast and efficiently.

The graph bi-partitioning problem is equivalent to finding the ground state of the Ising model with fixed magnetization. The energy in the Ising model is given by the following Hamiltonian:

$$H = - \sum_{(ij) \in E} S_i S_j,$$

where $S_i$ is the Ising spin (either +1 or -1) on the $i$th vertex of the graph. The magnetization $m, -1 \leq m \leq 1,$ is given by

$$\frac{1}{N} \sum_i S_i = m,$$

where $N$ is the number of vertices. Therefore, the problem of finding a configuration of spins that minimizes (6) while demanding magnetization $m$ to be fixed is equivalent to dividing
vertices into two groups of size $N(1 + m)/2$ and $N(1 - m)/2$ such that the number of links between them is minimal. For $m = 0$, the graph is divided into two groups of equal size, i.e. the graph bisection. The cost of a graph partitioning at a given magnetization, that we call $b(m)$, is given as the number of edges between different groups divided by the total number of vertices. The relation between $b(m)$ and ground-state energy $E(m)$ of the Ising model at magnetization fixed to $m$ is

$$b(m) = \frac{E(m) + M}{2N},$$

where $N$ is the number of nodes, and $M$ the number of edges.

1.2. Previous results on bi-partitioning random graphs

In graph theory estimating the asymptotic size of the bisection width in random regular graphs, i.e. graphs of a fixed degree chosen uniformly at random from all the possible ones, is a classical question. Many upper and lower bounds were derived. The currently best-known upper and lower bounds on bisection width in random regular graphs are by [17–21] and we summarize their numerical values in table 1 and figure 4.

For Erdős–Rényi random graphs with $N \to \infty$ vertices and mean degree $\alpha$ (every edge is present with probability $\alpha/(N - 1)$), the size of the largest component is $gN + o(N)$, where $g$ satisfies the following equation:

$$g = 1 - e^{-\alpha g}.$$  \hspace{1cm} (4)

In order to divide the graph into two parts of sizes $N(1 + m)/2$ and $N(1 - m)/2$ such that the number of edges between the two is zero, the size of the largest component $g$ must be at maximum $(1 + m)/2$. That is possible for average degree $\alpha < \alpha_s$ where

$$\alpha_s = -\frac{2}{1 + m} \log \frac{1 - m}{2}.$$  \hspace{1cm} (5)

For $\alpha > \alpha_s$, an extensive number of edges needs to be cut in the minimal bipartition. The value $\alpha_s$ is hence in a sense the satisfiability threshold for graph partitioning of Erdős–Rényi random graphs. This is further discussed in [22], where the authors also obtain an interesting upper bound on the bisection width ($m = 0$).

In statistical physics many articles addressed the random graph bi-partitioning problem, see e.g. [2, 12, 23–28], but as far as we can tell they address only cases where (A) the magnetization is fixed to zero, (B) the fluctuations in the degree of the random graph are negligible, i.e. the graphs are either dense or regular. The computational techniques used in the above mentioned papers do not generalize to the non-zero magnetization case nor to graphs with fluctuating degree, as e.g. to the Erdős–Rényi random graphs. We will give a more detailed explanation of why the techniques do not generalize in section 4.3. This also justifies novelty of the approach developed in this article.

1.3. Contribution of this article

If the ground-state energy of the ferromagnetic Ising model (1) was a convex function of the magnetization $m$ then an external magnetic field (playing the role of the chemical potential from the grand-canonical ensemble) could be used to compute $E(m)$ with a standard cavity method [29]. However, random graphs are mean field topologies and the energy at fixed magnetization $E(m)$ does not have to be and in this case is not a convex function, similarly as in the fully connected Curie–Weiss model. The problem of imposing the value of the magnetization is hence more challenging.
A method to explore the non-convex parts of thermodynamical potentials within the Bethe–Peierls (belief-propagation) approximation was suggested in [30], and used later e.g. in [31, 32]. The main idea is to introduce a uniform external magnetic field (or chemical potential) and adjust its value after every update of the local cavity fields. We use this method for partitioning graphs, and we argue that it (or its generalization to the replica symmetry breaking scheme) is asymptotically exact on sparse random graphs.

The main practical contribution of this article is the belief-propagation algorithm for graph partitioning problem that we believe to be of use in the various applications of the problem. We study the behavior and performance of the algorithm on random graphs but we anticipate it will be meaningful and useful for other families of graphs, complex networks for example.

We also compute the phase diagram of (1) at fixed magnetization. In [22] it was argued that in the Erdős–Rényi graphs at zero magnetization the glassy transition happens at some average degree strictly larger than the satisfiability threshold, $\alpha_c > \alpha_s$, we indeed confirm this conjecture, we compute $\alpha_c$ and several other quantities of interest.

An interesting side remark, discussed in section 4.3, concerns the case treated in the previous works: the regular random graphs at zero magnetization. There the average properties of the graph bi-partitioning are equivalent to those of the spin glass problem. We argue why this equivalence does not generalize to non-zero magnetization or non-regular graphs. More detailed discussion about the equivalence can be found in [33].

2. Cavity method at fixed magnetization

As we explained in the introduction, the graph partitioning is equivalent to the ferromagnetic Ising model at fixed magnetization $m^*$. The magnetization will be fixed via an external magnetic field $h$ which appears in the Hamiltonian as

$$H_h = -\sum_{(i,j)\in E} S_i S_j - h \sum_i S_i.$$  \hspace{1cm} (6)

The ground-state energy density of (1) and (6) are related via the Legendre transformation $e(h) = e(m) - hm$, so that the parameter $h$ has to be chosen such that

$$\frac{\partial e(h)}{\partial h} \bigg|_{h^*} = -m^*.$$  \hspace{1cm} (7)

If $e(h)$ is the ground energy density of (6) with field $h$ corresponding to the magnetization $m$, the corresponding partition cost (3) of the graph is

$$b = \frac{e(h) + hm + \frac{\alpha}{2}}{2},$$  \hspace{1cm} (8)

where $\alpha$ is the mean degree of the graph.

2.1. Belief-propagation equations

The Bethe–Peierls approximation, or the belief-propagation equations, aims to describe the Boltzmann measure of (6)

$$\mu([S_i]) = \frac{e^{\beta H_h([S_i])}}{Z},$$  \hspace{1cm} (9)

where $\beta$ is the inverse temperature. The graph partitioning problem corresponds to $\beta \to \infty$. In this section we summarize the well-known belief-propagation equations for this problem. For a detailed derivation see [34, 35].
In the most standard form of belief-propagation equations \[34\] one introduces $\psi_S^{i \rightarrow j}$ to be the probability that variable $i$ takes the value $S_i$ given the interaction on $(ij)$ is absent. On a tree (cycle free) graph then

$$
\psi_S^{i \rightarrow j} = \frac{1}{Z^{i \rightarrow j}} e^{\beta h S_i} \prod_{k \in \partial i \setminus j} \left( \sum_{S_k} e^{\beta S_k S_i} \psi_S^{k \rightarrow i} \right),
$$

where $Z^{i \rightarrow j}$ is normalization ensuring $\psi_S^{i \rightarrow j} + \psi_S^{i \rightarrow j} = 1$. After a fixed point of equations (10) is found the Bethe free energy (or the log-partition function) is given as \[34\]

$$
-\beta F(h) = \log Z = \sum_i \log Z^i - \sum_{(ij)} \log Z^{ij},
$$

where

$$
Z^i = \sum_{S_i} e^{\beta h S_i} \prod_{k \in \partial i} \left( \sum_{S_k} e^{\beta S_k S_i} \psi_S^{k \rightarrow i} \right),
$$

$$
Z^{ij} = \sum_{S_i, S_j} e^{\beta S_i S_j} \psi_S^{i \rightarrow j} \psi_S^{j \rightarrow i}.
$$

At a given value of the external magnetic field $h$ the average magnetization is computed as

$$
m = -\frac{\partial F(h)}{\partial h}/N; \text{using (11) one obtains}
$$

$$
m = \frac{1}{N} \sum_i \frac{\sum_{S_i} e^{\beta h S_i} \prod_{k \in \partial i} \left( \sum_{S_k} e^{\beta S_k S_i} \psi_S^{k \rightarrow i} \right)}{\sum_{S_i} e^{\beta h S_i} \prod_{k \in \partial i} \left( \sum_{S_k} e^{\beta S_k S_i} \psi_S^{k \rightarrow i} \right)}.
$$

In order to write the zero temperature limit, $\beta \rightarrow \infty$, of the above equations we introduce more suitable messages (usually called cavity fields) $h^{i \rightarrow j}$

$$
e^{2\beta h^{i \rightarrow j}} \equiv \frac{\psi_S^{i \rightarrow j}}{\psi_S^{j \rightarrow i}}.
$$

One then obtains equations equivalent to the replica symmetric equations in \[29\]. The self-consistent equations for messages (10) become

$$
h^{i \rightarrow j} = h + \sum_{k \in \partial i \setminus j} \left[ \max (1 + h^{k \rightarrow i}, 0) - \max (h^{k \rightarrow i}, 1) \right] \equiv F([h^{k \rightarrow i}]).
$$

Note that the term in the sum is $-1$ for $h^{k \rightarrow i} \leq -1$, $+1$ for $h^{k \rightarrow i} \geq 1$, and $h^{k \rightarrow i}$ for $-1 < h^{k \rightarrow i} < 1$. From (12)–(13) we obtain the Bethe estimate of the ground-state energy:

$$
E(h, [h^{i \rightarrow j}]) = \sum_i E^i - \sum_{(ij)} E^{ij},
$$

where from (12)–(13) we obtain

$$
E^i = h + d_i + 2 \sum_{k \in i} \max (0, h^{k \rightarrow i})
$$

$$
-2 \max \left[ h + \sum_{k \in i} \max (1 + h^{k \rightarrow i}, 0), \sum_{k \in i} \max (h^{k \rightarrow i}, 1) \right]
$$

$$
E^{ij} = 1 + 2 \max (0, h^{i \rightarrow j}) + 2 \max (0, h^{j \rightarrow i})
$$

$$
-2 \max (1 + h^{i \rightarrow j} + h^{j \rightarrow i}, 1, h^{i \rightarrow i}, h^{j \rightarrow j}),
$$

where $d_i$ is the degree of node $i$. 

5
Define a total cavity field for node $i$ as

$$h_i = \sum_{k \in \partial i} \left[ \max (1 + h^{k \rightarrow i}, 0) - \max (h^{k \rightarrow i}, 1) \right].$$

(20)

Define $n_+$ as the fraction of sites where $h^+ > 0$, $n_-$ where $h^+ < 0$ and $n_0$ where $h^+ = 0$. From equation (14) we obtain that the total magnetization

$$n_+ - n_- - n_0 \leq m \leq n_+ - n_- + n_0.$$ 

(21)

Let us define a function

$$\mathcal{M}(h, [h^i]) = n_+ - n_-.$$ 

(22)

This concludes the presentation of the zero temperature cavity equations for the ferromagnetic Ising model in the external magnetic field $h$. The solution of these equations is well known and gives $m = 1$ for $h > 0$ or $m = -1$ for $h < 0$, and no edges lying between spins of different sizes. In order to compute the ground-state energy (minimum number of edges between opposite sign spins) at a magnetization $-1 < m^* < 1$ we must adaptively update the value of the external field $h$ after every iteration of the belief-propagation equations (16). We use the current values of messages $h^i$, equation (20), and update the external field in such a way that $m^* = \mathcal{M}(h_{\text{new}}, [h^i])$ where $m^*$ is the desired value of the magnetization. We repeat until convergence or maximum number of iterations is achieved, finally we compute the energy (17).

In the rest of this paper we concentrate on the random regular and Erdős–Rényi graphs and we observed that in these graph ensembles whenever the cost of the minimal partitioning is non-zero then $n_0 = 0$. This means the algorithm fixes the magnetization to the desired value $m^*$ following equation (21). In some cases, however, the $n_0 > 0$ (for instance on the Erdős–Rényi random graphs for $\alpha < \alpha_s$ – for definition of $\alpha_s$ see section 4). In such cases it is crucial to note that the value of the external magnetic field $h$ is the same for all the magnetizations in interval $\mathcal{M}(h_{\text{new}}, [h^i]) - n_0 < m < \mathcal{M}(h_{\text{new}}, [h^i]) + n_0$. Since the ground-state energy (17) depends only on the values of the local and external fields (and not on the sign of $h^i + h$) then the energy is the same for all magnetizations $\mathcal{M}(h_{\text{new}}, [h^i]) - n_0 < m < \mathcal{M}(h_{\text{new}}, [h^i]) + n_0$. Hence, the method predicts correct ground-state energy (and also other related quantities that do not depend directly on the sign of the local field $h^i + h$) for magnetization fixed to $m^*$ even if $n_0 > 0$. Specific results will be discussed in section 4.

2.2. Population dynamics at fixed magnetization

In order to calculate the average ground-state energy (17), and thus the partitioning cost $b$, for a given ensemble of random graphs one implements the population dynamics method [6, 35].

In the standard population dynamics one keeps a sample of messages $h(i)$. In every step we draw a random number $d$ corresponding to the number of neighbors of one side of a random edge in the graph. We then draw $d$ random messages $h(i)$ and compute a new message using update equations (16) with a given value of the external magnetic field $h$ till convergence or till maximum number of iterations. Finally one computes the ground energy and the corresponding magnetization. If this is done with the above equations for graph bi-partitioning then the resulting magnetization will always be either +1 for $h > 0$ or −1 for $h < 0$. 

6
Algorithm 1. Population dynamics algorithm for BP on $d$-regular random graphs with fixed magnetization $m^*$

\[ h \leftarrow 0 \]
Randomly initialize messages $h(i)$, $i = 1, 2, \ldots, N$

for $j = 1$ to max do

for $i = 1$ to $N$ do

Randomly select $d - 1$ messages $h(k)$ where $k \in 1, 2, \ldots, N$.

Calculate $h(i)$ from $\{h(k)\}$ as $h(i) = \mathcal{F}(\{h(k)\})$ as defined in equation (16)

end for

$h_1 \leftarrow h - 1$

$h_2 \leftarrow h + 1$

while $|h_1 - h_2| < \text{criterion}$ do

for $i = 1$ to $N$ do

Randomly select $d$ messages $h(k)$ where $k \in 1, 2, \ldots N$

Calculate $h^i$ from $\{h(k)\}$ using functional form from equation (20)

if $h^i > 0$ then

$n_+ \leftarrow n_+ + 1$

end if

if $h^i < 0$ then

$n_- \leftarrow n_- + 1$

end if

end for

$m \leftarrow n_+ - n_-$

if $m < m^*$ then

$h_1 \leftarrow h$

end if

if $m > m^*$ then

$h_2 \leftarrow h$

end if

$h \leftarrow (h_1 + h_2)/2$

end while

end for

Follow similar logic of choosing randomly elements of $h(i)$ and calculate $E$ using equations (17–19)

return $E, h$

We, however, want to find the ground-state energy at magnetization values $-1 < m^* < 1$. In order to do that we will not keep the external field $h$ constant. Instead after every iteration of (16) we use the current values of messages $h(i)$ and update the value of $h$ in such a way that $m^* = \mathcal{M}(h_{\text{new}}, \{h(i)\})$ where $m^*$ is the desired value of the magnetization. We use the bisection method in each iteration in order to find the new value of the external magnetic field. As we explained in the case $n_0 > 0$ then every $m^*$ in interval (21) leads to the same value of $h_{\text{new}}$ and the same value of energy. This justifies the use of equation (22).

The resulting population dynamics code is sketched in algorithm 1. Note that in the population dynamics one makes use of equations (16)–(22), but instead of summing over neighborhood nodes on a given graph equations (16)–(22) are regarded as functions of their arguments, where the arguments are the messages $\{h(i)\}$ randomly selected in each iteration of the population dynamics.
2.3. 1RSB at fixed magnetization

As may be anticipated from the relation between graph bisection and the spin glass [2] the belief-propagation equations (replica symmetric approach) are not always asymptotically exact for the graph bi-partitioning. Instead in some regions of parameters the problem is glassy and the replica symmetry breaking approach is needed for an exact solution, just like in the Sherrington–Kirkpatrick model [36, 37]. The 1RSB approach for sparse random graphs was developed in [6, 29] and is well established. Hence, we only point out the difference in the equations that leads to fixing a non-trivial value of the magnetization.

In order to write the 1RSB equations we follow closely the approach of [29]. We introduce a complexity function

\[ \Sigma_1(E) \]

and its Legendre transform

\[ \Phi_1(y) \]

also called the replicated potential

\[ -\frac{y}{\Phi_1(y)} = -\frac{yE}{\Sigma_1(E)}, \]

\[ \frac{\partial y}{\partial E} = E. \]

(23)

Every thermodynamical state has a corresponding value of the cavity field \( h^{i \rightarrow j} \) and according to [29] the self-consistent equation for the distribution of cavity fields over states is

\[ P^{i \rightarrow j}(h^{i \rightarrow j}) = \frac{1}{Z^{i \rightarrow j}} \int \prod_{k \in \partial i \setminus j} dP^{k \rightarrow i}(h^{k \rightarrow i}) e^{-\gamma E^{i \rightarrow j}} \delta[h^{i \rightarrow j} - F(\{h^{k \rightarrow i}\})], \]

(24)

where \( F(\{h^{k \rightarrow i}\}) \) is defined by equation (16). The reweighting factor is defined by \( E^{i \rightarrow j} = -\lim_{\beta \to \infty} \frac{1}{\beta} \log Z^{i \rightarrow j} \) where \( Z^{i \rightarrow j} \) is the normalization constant in (10) and is given by an equation analogous to (18). Once a fixed point of (24) is found the potential \( \Phi_1(y) \) is computed as follows

\[ \Phi_1(y) = \sum_i \Phi_i - \sum_{ij} \Phi_{ij} \]

with

\[ e^{-\gamma \Phi_i} = \int_{POP} e^{-\gamma E_i}, \]

\[ e^{-\gamma \Phi_{ij}} = \int_{POP} e^{-\gamma E_{ij}}. \]

(25)

where the notation \( \int_{POP} = \int \prod_{k \in \partial i \setminus j} dP^{k \rightarrow i}(h^{k \rightarrow i}) \) and the energy contributions are given by (18)–(19). The energy of the system is then computed according to (23) as

\[ E = \sum E^i - \sum_{ij} E^{ij} \]

with

\[ E^i = \frac{\int_{POP} E^i e^{-\gamma E^i}}{\int_{POP} e^{-\gamma E^i}}, \]

\[ E^{ij} = \frac{\int_{POP} E^{ij} e^{-\gamma E^{ij}}}{\int_{POP} e^{-\gamma E^{ij}}}. \]

(26)

And the magnetization \( m = \sum_i m^i / N \), where

\[ m^i = \frac{\partial E^i}{\partial h} = \frac{\int_{POP} \frac{\partial E^i}{\partial h^i} e^{-\gamma E^i}}{\int_{POP} e^{-\gamma E^i}} + y \frac{\int_{POP} \frac{\partial E^i}{\partial h^i} e^{-\gamma E^i}}{\int_{POP} e^{-\gamma E^i}} - y \frac{\int_{POP} E^i e^{-\gamma E^i}}{\left(\int_{POP} e^{-\gamma E^i}\right)^2}. \]

(27)

Note that \( \frac{\partial E^i}{\partial h^i} = \pm 1 \) depending on the sign of \( h + h^i \), where \( h^i \) is computed from (20). If \( h + h^i = 0 \) then \( -1 < \frac{\partial E^i}{\partial h^i} < 1 \), in (27) we count in such a case \( \frac{\partial E^i}{\partial h^i} = 0 \); just as in the replica symmetric version of the algorithm, this does not change the resulting value of the energy.

Again the only difference between the usual 1RSB and 1RSB at fixed magnetization is that after every iteration the external magnetic field is chosen a new value such that magnetization computed from (27) is equal to the desired value \( m^* \).

Solving the 1RSB equations is often tedious and to obtain the phase diagram it is often sufficient to investigate the convergence of the belief-propagation iterations. This is equivalent to analyzing the local stability of the replica symmetric solution towards replica symmetry.
breaking, as done originally by de Almeida and Thouless [38]. Within the population dynamics we use the noise-propagation method (for a derivation see appendix C of [39]). In the population dynamics algorithm together with cavity fields \( h_i \rightarrow j \), one keeps track of the quantity

\[
\langle v_i \rightarrow j \rangle = \sum_{k \in \partial i \setminus j} \frac{\partial h_i \rightarrow j}{\partial h_k \rightarrow i} \langle v_i \rightarrow i \rangle , \tag{28}
\]

after every sweep of BP iteration we normalize the values \( \langle v_i \rightarrow j \rangle \) by \( \lambda \) in such a way that \( \sum (\langle v_i \rightarrow j \rangle / \lambda)^2 = 1 \). The parameter \( \lambda \) then plays a role of a certain Lyapunov exponent and the belief propagation does not converge if and only if on average \( \lambda > 1 \).

We have found that BP never converges on regular graphs for any value of magnetization \(-1 < m^* < 1\). Nevertheless, the value of the energy calculated with BP gives a lower bound on the actual ground-state energy of the model—this follows from the variational formulation of the replica approach [6], and can be proven in some cases rigorously [40]. Moreover, it is often observed that the BP lower bound is fairly close to the actual value.

For the Erdős–Rényi graphs with given magnetization, we found a phase transition from a replica symmetric region where BP is asymptotically exact to a glassy region where RSB solution would be required to obtain the asymptotically exact value of the ground-state energy (this phase transition is shown in figure 1).

3. BP as a heuristic solver

Equations for the belief propagation derived in the previous section can be used on a given graph as we sketch in algorithm 2.

The parameter memory (sometimes referred to as damping), which we set to 0.7 in our simulations, is introduced in order to prevent messages from oscillating. If the algorithm does
Algorithm 2. BP algorithm for partitioning of a given graph

\[ \forall i, j \ \text{initialize messages } h^{i \rightarrow j} \text{ and field } h \text{ randomly} \]
iter \( \leftarrow 0 \)
repeat
\[ \text{for all } i \in V \text{ do} \]
\[ \text{convergence } \leftarrow 0 \]
\[ \text{local_field}[i] \leftarrow \sum_{k \in \partial_i} \left[ \max(1 + h^{k \rightarrow i}, 0) - \max(h^{k \rightarrow i}, 1) \right] \]
\[ \text{for all } j \in \partial i \text{ do} \]
\[ h^{j \rightarrow i}_{\text{new}} \leftarrow h + \text{local_field}(i) - h^{i \rightarrow j} \]
\[ \text{convergence } \leftarrow \text{convergence } + |h^{j \rightarrow i}_{\text{new}} - h^{i \rightarrow j}| \]
\[ h^{j \rightarrow i}_{\text{new}} \leftarrow \text{memory} \ast h^{j \rightarrow i}_{\text{new}} + (1 - \text{memory}) \ast h^{j \rightarrow i}_{\text{old}} \]
end for
end for
sort(local_field)
\[ h = -\text{local_field}[N(1 - m)/2] \]
iter \( \leftarrow \) iter +1
until convergence \(< \varepsilon \) OR iter > maximum iterations
compute \( E \) using equation (17)
return \( E, h \)

Algorithm 3. Decimation algorithm

repeat

Run algorithm 2

Choose a vertex \( i \) such that local_field(\( i \)) is the highest (or lowest if this is an even iteration) and fix all outgoing messages (from this node to +\( \infty \) (−\( \infty \) for an even iteration)). Fix spin in vertex \( i \) to +1 (−1 in even iteration).

until Number of fixed spins to +1 or −1 reaches the value required to fix desired magnetization \( m \)

not converge after a given maximum number of iterations, it is terminated. However, even if the algorithm does not converge, the calculated \( E \) still provides a reasonable estimate of the bisection cost that is asymptotically a lower bound of the true average cost—this last statement is a general property of the replica symmetric solution and in some cases it can be proven rigorously [40].

In the presented algorithm, we introduced a slightly different method to fix the magnetization by manipulating \( h \). In the algorithm 2, we sort all the local cavity fields and set \( h \) so that \( N(1 - m)/2 \) of them are negative (or zero) and the rest positive (or zero). It follows from the definition of messages (15) that the positive value of local cavity field means that spin on this node is to be equal to 1, negative means that the spin is to be −1. If the local cavity field is exactly equal to zero, the spin in a given node is undecided (free). This can be used to actually obtain a graph partition. However, a decimation technique, algorithm 3, achieves much better results in particular when many free or almost free spin are present, reported in figures 3 and 4. The decimation algorithm performs better when it alternates between fixing positive and negative spins. Without this alternation we observed that it first fixes all positive (or equivalently negative) spins and then set all the remaining ones in the opposite direction, which results into higher partition costs.
Note that in the present form the decimation solver has running time quadratic in the size of the system. However, linear running time can be achieved without significant loss of performance by decimating a finite fraction of spins after every iteration, as in the survey propagation algorithm of [4]. It is an interesting open problem to combine the method of reinforcement [41] with our magnetization fixing.

4. Behavior of the method and results

In this section we discuss the behavior of the belief-propagation algorithm of random regular and Erdős–Rényi random graphs. We, however, anticipate that qualitatively similar behavior as on the Erdős–Rényi random graphs will be seen on other graph families.

4.1. Phase diagram of Erdős–Rényi graphs bi-partitioning

The most interesting fact to discuss is the behavior of the algorithm on a given graph and the decimation. In particular: is the function \( M(h, \{ h^{i \rightarrow j} \}) \) (22) continuous in \( h \) such that any value of the magnetization can be fixed? Does the external field \( h \) converge in the iterations? Does the decimation achieve low energy states? We choose typical Erdős–Rényi random graphs to illustrate the behavior and answer these questions.

An Erdős–Rényi random graph of average degree smaller that one, \( \alpha < 1 \), basically looks like a collection of small disconnected trees. Let us hence first discuss how does the algorithm behave on a tree. On a tree the belief-propagation equations (16) have only one possible fixed point for every value of \( h \). For \( h > 0 \) all \( h^{i \rightarrow j} = h + d_i - 1 \), where \( d_i \) is the degree of node \( i \) and magnetization \( m = 1 \), for \( h < 0 \) all \( h^{i \rightarrow j} = h - d_i + 1 \) and \( m = -1 \), and for \( h = 0 \) all \( h^{i \rightarrow j} = 0 \) and \(-1 < m < 1\). In terms of convergence of the algorithm on trees, we observed the following two cases. (A) It converges to the third (\( h = 0 \)) fixed point which predicts the energy cost to be zero for all \(-1 < m^* < 1\). This is the case of Erdős–Rényi graphs with average degree \( \alpha < 1 \). (B) It oscillates between \( h > 0 \) and \( h < 0 \) and does not converge. This is the case e.g. on a star-graph consisting of \( N \) leaves stemming from one node (where the cost is \((1 + |m^*|)/2\)). The qualitative behavior of cases (A) and (B) does not change when we consider the finite-temperature version of the algorithm. Hence, our algorithm does not behave well on some trees, which is a kind of unusual situation for belief propagation. However, on the random graphs that are considered in this paper we never observed the oscillating (i.e. non-converging) behavior in \( h \) as in the case (B). Note that the decimation algorithm works well and is able to obtain reasonably good partitions even on a tree. This is because once a spin is fixed the information propagates and is taken into account basically correctly.

But back to the Erdős–Rényi random graphs, for mean connectivities above the percolation threshold but lower than the satisfiability threshold \( 1 < \alpha < \alpha_s \) (given by (5), and depicted in figure 1) one finds that the algorithm 2 converges to a configuration such that on the giant component of the graph all local fields are positive (or negative). Thus all spins on the giant component will be chosen to be +1 (−1). In the rest of the graph (that is all the small components) the local fields as well as the external field \( h \) converge to zero (independently of the graph size). The prediction for the ground-state energy in this case is zero, which is correct in this case as the small components in a random graph are numerous and can be split into two properly sized groups [22]. Again, the decimation algorithm is able to divide small components into (asymptotically) properly sized groups, note that if one spin on a small component is fixed, than all the other vertices orient in the same direction.

After the satisfiability threshold (5), the giant component is bigger than the number of vertices that are in the larger of the two groups, so inevitably one will have neighbors with
Figure 2. The figure shows the partitioning cost $b$ as a function of $m$ for two different Erdős–Rényi graphs with mean connectivities 1.44 and 1.6 (and of sizes $N = 100\,000$). In the simulation, the messages were randomly initialized for $m = -1$ and then $b$ was calculated with algorithm 2. Magnetization was then slightly increased to $m + \Delta m$ and messages $b^{\rightarrow j}$ were initialized with their values from simulation with previous $m$. The dashed curves correspond to the case when the system orients the spins on the small components in the less favorable way (that is, +1 for $m > 0$ and vice versa). The dashed curves end at a spinodal point where the giant component is divided in half.

opposite spins in the ground state. There are two possibilities: (A) BP converges or (B) BP does not converge. If BP does converge, i.e. bellow $\alpha_c$, then it converges to a configuration where the giant component is divided into two groups (positive and negative local fields) and all the other components of the graph are oriented in one direction (the one that has smaller number of vertices on the giant component). In order to fix the proper magnetization on the giant component the external field is nonzero even when the total magnetization $m^* = 0$.

BP does not converge above the replica symmetry breaking threshold $\alpha_c$ depicted in figure 1. But even in such cases if we use the snapshots of fields at a given iteration step the decimation algorithm achieves good energies, as illustrated in section 4.2.

In fact on the Erdős–Rényi random graphs there is a first-order phase transition at zero magnetization. At the transition the derivative of the energy with respect to magnetization has a discontinuity. On both sides of the transition a meta-stable state exists with spinodal points at values of magnetization corresponding to the half-size of the giant component. This phase transition and lines corresponding to the meta-stable state and the spinodal point are illustrated in the figure 2.

How to understand this phase transition: consider large positive magnetization, in the lowest cost solution the giant component and large part of the small components are positive and a small part of the components are negative. As the magnetization is decreased the small components are all turning negative, and also parts of the giant component turn negative. The external field is negative in that region in order to keep the small components negative. Even after half of the spins become negative the system does not realize that it is less costly to turn everybody, instead if the magnetization is slowly decreased further the belief-propagation equations indicate that a larger fraction of the giant component should be negative. As the magnetization is decreased the negative external field becomes closer to zero, at this point the external field flips to positive values the small component turn to positive direction and the system realizes this gives much lower cost. This point corresponds to a spinodal point. Of course this discussion could be repeated by changing the words positive for negative and vice versa. The phase transition, meta-stable state and spinodal point are illustrated in figure 2.
Figure 3. Left: decimation results for 3-regular random graphs of different sizes, compared to presumably exact average ground-state energies as computed from the extremal optimization heuristics by [14], data taken from [33]. Also shown is the asymptotic cost $b = 0.1138$ calculated by the 1RSB method. Note that the decimation algorithm is far better than the best known algorithmic bound $b = 0.16$ [19]. Right: the plot shows replica symmetric (BP) results, 1RSB results and performance of the decimation algorithm for the partition cost $b$ as a function of the magnetization $m$ for 3-regular random graphs. The BP population dynamics algorithm was with $N = 10000$, 1RSB solutions were obtained from a simulation with $N = 30000$. The decimation results were averaged over 10 different graphs, each with $N = 2000$.

If the magnetization is not changed gradually, depending on the initial conditions, the algorithm does converge to one or the other of the two branches. With random initialization we observed in our simulations the lower branch to be more likely (meaning that its basin of attraction is slightly larger). Anyhow, the fact that both the branches are observed with a comparable probability is a nice property as if more stable divisions are present in real networks, our algorithm might be able to find them (or at least those of them with considerably large basin of attraction).

4.2. Performance of the BP decimation

In this section we illustrate accuracy of the decimation BP solver on random 3-regular graphs. Regular graphs are in some sense the hardest case for graph bi-partitioning as they look locally alike from every point and no apparent structure can be explored to decide if two nodes should be in the same group or not.

If figure 3 we show the average bisection cost achieved by the decimation solvers on graphs of different sizes. We compare to the asymptotic value of the cost and to the average values obtained from extremal optimization heuristic of [14, 33]. The extremal optimization algorithm can be thought of as a speeded up simulated annealing that was run long enough for the lowest achieved state to be the ground state, of course the running time is then exponential in the system size, for details see [14, 33]. We see that our decimation solver achieves energies very close to the ground states. In particular, note that the best provable algorithmic bound for 3-regular graph bisection is $b = 0.16$ [19] which is far above what decimation achieves.

In the right part of figure 3 we compare the partition cost as a function of the magnetization $m$ as obtained from (a) the population dynamics solving the BP equations, (b) solution of the 1RSB equations from section 2.3 under the assumption that for every edge the distribution of fields $P^{i,j}(h^{i,j})$ is the same—this being called the factorized solution in [29], and (c) decimation solver run on graphs of size $N = 2000$. 

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Table 1. This table summarizes the best-known lower bound (second column, [17, 18], Bollobas’s bound \( d/4 - \sqrt{d \ln 2}/2 \) is the best known for \( d \geq 5 \)) and the upper bound (third column, [19–21]) bounds for random regular graph bisection. In the fourth column we give results for the bisection from the population dynamics for belief propagation, these numbers are identical to the ones obtained in [26] with non-integer cavity fields. The fifth column gives results of the 1RSB calculation with integer fields as developed in [29]. And the final column shows performance of our implementation of the BP decimation algorithm for graphs of size \( N = 2000 \).

| \( d \) | \( b_{\text{low}} \) | \( b_{\text{up}} \) | \( b_{\text{RS}} \) | \( b_{\text{1RSB}} \) | \( b_{\text{BPdec}} \) |
|---|---|---|---|---|---|
| 3 | 0.101 | 0.1665 | 0.1125(2) | 0.113 846 | 0.1180(3) |
| 4 | 0.22 | 0.3333 | 0.2579(2) | 0.263 527 | 0.272(1) |
| 5 | 0.3192 | 0.5028 | 0.4072(3) | 0.412 398 | 0.422(2) |
| 6 | 0.4803 | 0.6674 | 0.5756(3) | 0.585 414 | 0.5975(9) |
| 7 | 0.6486 | 0.8502 | 0.7430(4) | 0.752 171 | 0.766(2) |
| 8 | 0.8226 | 1.0386 | 0.9232(3) | 0.936 595 | 0.955(2) |
| 9 | 1.0012 | 1.2317 | 1.1022(4) | 1.11453 | 1.133(1) |

4.3. Random regular graphs at zero magnetization

In this subsection we want to discuss the bisection (zero magnetization) of random regular graphs. This case has been treated in [2, 23–26, 28] using analogy with spin glasses, i.e. the Hamiltonian

\[
H_{SG} = - \sum_{(ij) \in E} J_{ij} S_i S_j ,
\]

(29)

with random \( J_{ij} = \pm 1 \) has been solved instead of fixing magnetization to zero via an external field.

Indeed, note that in random regular graph it is more than reasonable to assume that the two groups in graph bisection have exactly the same properties and hence the first-order phase transition that we have seen at \( m = 0 \) in the Erdős–Rényi graph is expected to disappear. Consequently, the slope of the ground state energy \( e(m) \) at \( m = 0 \) is expected to be zero, and hence also the value of external field to which our algorithm converges is zero \( h = 0 \).

We remind that cavity fields \( h_{\to j} \) can be interpreted as a change in the ground-state energy of (6) when link \((ij)\) is removed from the graph. If \( h \) is an integer then also all \( h_{\to j} \) have to be integers in the the final solution of the problem. The cavity equations can then be parameterized by fraction of negative, positive and zero cavity fields \( h_{\to j} \). The only way to achieve zero magnetization is then to set the fraction of negative and positive cavity fields equal. And this leads exactly to the same equations as Mézard and Parisi obtained in [29] and justifies the approach of [2, 23–26, 28]. Consequences and generalization of this equivalence will be described in [33].

We want to stress that at non-zero magnetization the corresponding external field \( h \) does not take an integer value and hence no straightforward relation to the spin glass problem exists. Also as long as the degree of the graph is not constant there might be a room for a first-order phase transition at \( m = 0 \) due to asymmetries between the two groups in the bisection—as illustrated in the Erdős–Rényi graphs. If the first-order phase transition is present that at \( m = 0 \) the external field \( h \neq 0 \) and hence again no straightforward analogy with the spin glass problem exists. Thus, the approach developed in this paper is the only one known that is able to treat non-regular graphs or non-zero values of the magnetization.

In table 1 and figure 4 we summarize the known rigorous bounds for bisection widths in random regular graphs. We also summarize results of belief propagation obtained from our
population dynamics, and the results from 1RSB calculation using integer values of the cavity fields. Both the latter are only approximation to the full-step replica symmetry breaking result that would presumably be exact in this case. Finally, we compare with performance of our decimation BP solver. In particular, figure 4 illustrates how accurate the decimation solver is. Note that the true value of the bisection width is expected to lie between the decimation and 1RSB data points, since the 1RSB result gives generically a lower ground-state energy than the full-RSB solution [6].

5. Discussion

The main practical contribution of this article is the belief-propagation algorithm for graph partitioning problem that we anticipate to be useful in the various applications of the partitioning problem. We studied the behavior and performance of the algorithm on random graphs but we anticipate it will be meaningful also for other families of graphs, complex networks in particular. Compared to other partitioning algorithms BP has the advantage that it provides information about probability with which a certain node is in a certain group. It is also possible to see different locally stable divisions of the graph—as illustrated by the first-order phase transition in Erdős–Rényi graphs at zero magnetization. In real world networks the partitioning cost at different values of magnetization $m$ may lead to a non-trivial information about communities in the network and information about their significance. Note also that our approach is straightforwardly generalizable to $k$-partitioning the graph into $k$ groups of a fixed size.

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