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A PTAS for the Classical Ising Spin Glass Problem on the Chimera Graph Structure

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Abstract

We present a polynomial time approximation scheme (PTAS) for the minimum value of the classical Ising Hamiltonian with linear terms on the *Chimera* graph structure as defined in the recent work of McGeoch and Wang [MW13]. The result follows from a direct application of the techniques used by Bansal, Bravyi and Terhal [BBT09] who gave a PTAS for the same problem on planar and, in particular, grid graphs. We also show that on Chimera graphs, the trivial lower bound is within a constant factor of the optimum.

1 Introduction

The classical Ising spin glass problem is defined as follows. Given a graph $G(V, E)$ along with real numbers d_u for all vertices u and c_{uv} for all edges (u, v), the classical Ising spin glass problem is to the minimize the following Hamiltonian,

$$H(S) := \sum_{(u,v)\in E} c_{uv} S_u S_v + \sum_{u\in V} d_u S_u, \tag{1}$$

over all $\{-1, 1\}$ assignments to the vertices given by $S = \{S_u \in \{-1, 1\}\}_{u\in V}$. It is useful to note that $\mathrm{E}_S[H(S)] = 0$, and thus the optimum of $H(S)$ is non-positive.

The Ising spin glass problem is used to model the interactions in physical spin systems and its minimum value is a measure of the ground state-energy of the system. As such this computational problem has received significant attention from both, the algorithmic and complexity perspectives. For a detailed discussion on this problem we refer the reader to the related work of Bansal, Bravyi and Terhal [BBT09] who gave a PTAS for this problem on planar graphs. In this work we focus on the approximability of this problem on the *Chimera* graph structure which we formally define below.

The Chimera Graph Structure. We shall work with the Chimera graph structure as defined in [MW13], with a different notation for convenience. For a positive integer r, the Chimera graph G_r is constructed as follows.

Vertices V. The set of vertices V consists of the integer tuples $\{(i, j, k, l) \in \mathbb{Z}^4 \mid 1 \le i, j \le r, 1 \le k \le 4, l = 0, 1\}$. The indices i and j specify the location in a $r \times r$ grid, k indicates one of four possible vertices, and l specifies the *layer* in which the vertex belongs. The number of vertices is $8r^2$.

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Edges E. The edge set is a disjoint union of E_0, E_1 and E_{01}, where E_0 is the set of edges in layer 0, E_1 is the set of edges in layer 1, and E_{01} is the set of edges across the the two layers. These sets of edges are defined as follows:

E_0: For any $1 \leq i \leq r-1$, $1 \leq j \leq r$, and $1 \leq k \leq 4$, E_0 contains an edge between $(i,j,k,0)$ and $(i+1,j,k,0)$.

E_1: For any $1 \leq i \leq r$, $1 \leq j \leq r-1$, and $1 \leq k \leq 4$, E_1 contains an edge between $(i,j,k,1)$ and $(i,j+1,k,1)$.

E_{01}: For any $1 \leq i \leq r$, $1 \leq j \leq r$, $1 \leq k_0 \leq 4$ and $1 \leq k_1 \leq 4$, E_{01} contains an edge between $(i,j,k_0,0)$ and $(i,j,k_1,1)$.

Note that E_0 is a disjoint collection of $4r$ $(r-1)$-length paths, one each for a fixed pair of values for j and k. Similarly, E_1 is a disjoint collection of $4r$ $(r-1)$-length paths, one each for a fixed pair of values for i and k. Also, E_{01} is a disjoint collection of r^2 $K_{4,4}$ graphs, one for each value of (i,j) with the bipartition given by the sets $\cup_{k=1}^{4}\{(i,j,k,0)\}$ and $\cup_{k=1}^{4}\{(i,j,k,1)\}$.

Note that the Chimera graph structure is non-planar as it contains the $K_{4,4}$ graph, as well as a $K_{r,r}$ minor. Thus, the results of Bansal et al. [BBT09] are not directly applicable. However, utilizing the symmetries in the above construction we are able to adapt the techniques of [BBT09] to prove the following algorithmic results.

Our Results. This work shows the existence of a polynomial time approximation scheme (PTAS) for the classical Ising spin glass problem on the Chimera graph structure. Formally we prove the following theorem.

Theorem 1.1. *Given a Chimera graph structure G_r on $n = 8r^2$ vertices, the Hamiltonian $H(S)$ can be approximated to $(1-\varepsilon)$ of its minimum value in time $O\left(\varepsilon n \cdot 2^{\frac{32}{\varepsilon}}\right)$.*

The above result is obtained by noting that the graph G_r can be disconnected into constant width *strips* by removing a small fraction of edges from E_0 (or E_1). This allows the application of the partitioning technique used by Bansal et al. [BBT09] for their PTAS on grid graphs. The analysis requires a straightforward lower bound on the magnitude of the optimum value of $H(S)$ in terms of sum of the absolute values of the bilinear coefficients in $H(S)$ corresponding to edges in E_0.

A somewhat more involved analysis yields the following result which shows that the trivial lower bound is within a constant factor of the optimum.

Theorem 1.2. *Let H^* be the optimum value of $H(S)$ on the Chimera graph structure. Then, $H^* \leq -(C/(3C+4))\left[\sum_{(u,v)\in E}|c_{uv}| + \sum_{u\in V}|d_u|\right]$, for some constant $C > \frac{\ln(1+\sqrt{2})}{\pi}$. In particular, the approximation factor is $(3C+4)/C < 17.26$.*

The above result is obtained by extending the straightforward lower bound used to prove Theorem 1.1 with a complementary bound obtained via the Grothendieck constant.

2 PTAS on Chimera Graphs

Let $G_r = G(V,E)$ be the Chimera graph on $n = 8r^2$ vertices and $H(S)$ be the Hamiltonian given in Equation (1) for some real values $\{c_{uv}\}_{(u,v)\in E}$ and $\{d_u\}_{u\in V}$. Recall that E is the disjoint union, $E = E_0 \cup E_1 \cup E_{01}$. For convenience we split $H(S)$ as,

$$H(S) := M_0(S) + M_1(S) + M_{01}(S) + D(S), \tag{2}$$

where,

$$
\begin{aligned}
M_l(S) &:= \sum_{(u,v)\in E_l} c_{uv} S_u S_v, \quad l = 0, 1, \\
M_{01}(S) &:= \sum_{(u,v)\in E_{01}} c_{uv} S_u S_v, \\
D(S) &:= \sum_{u\in V} d_u S_u.
\end{aligned}
$$

We also define the following quantities.

$$
\begin{aligned}
A_l &:= \sum_{(u,v)\in E_l} |c_{uv}| \quad \text{for } l = 0, 1. \\
A_{01} &:= \sum_{(u,v)\in E_{01}} |c_{uv}|. \\
B &:= \sum_{u\in V} |d_u|. \qquad (3)
\end{aligned}
$$

The following lemma follows from the structure of G.

Lemma 2.1. *Let H^* be the minimum value of $H(S)$. Then, $H^* \leq -(A_0 + A_1)$.*

Proof. From the construction of G_r we have that E_0 is a disjoint collection of $4r$ $(r-1)$-length paths in layer 0. Similarly, E_1 is a disjoint collection of $4r$ $(r-1)$-length paths in layer 1. Thus, $E_0 \cup E_1$ is a disjoint collection of $8r$ $(r-1)$-length paths. Thus, there exists an assignment S' such that $M_0(S') = -A_0$ and $M_1(S') = -A_1$. We can ensure that $M_{01}(S') \leq 0$, otherwise the values assigned to all the vertices in layer 0 – i.e. all vertices of the form $(i, j, k, 0)$ – can be flipped which changes the sign of $M_{01}(S')$ while preserving $M_0(S')$ and $M_1(S')$. Thus, we can ensure that $M_0(S) + M_1(S) + M_{01}(S) \leq -(A_0 + A_1)$. Now, if $D(S')$ is positive, then S' can be flipped for all vertices to ensure that $H(S') \leq -(A_0 + A_1)$. □

Let us define a *strip* graph with m levels and width b as any graph which has m levels of b vertices each such that all edges between levels are between adjacent levels. The levels may have edges within them. To be precise, a vertex in level j may have edges only to other vertices in levels j, $(j-1)$ or $(j+1)$. Bansal et al. [BBT09] showed that the problem of minimizing the Hamiltonian on $m \times b$ strip graphs can be solved using dynamic programming in time $O(m4^b)$. The dynamic program computes for level j and each of the 2^b assignments to the vertices in that level, the value of the best solution with that assignment to level j for the Hamiltonian on the subgraph induced by levels $1, \ldots, j$. Going from level j to $j+1$ requires $O(4^b)$ operations, a constant number for each pair of assignments to levels j and $j+1$. Thus, the total time taken is $O(m4^b)$. Our goal in designing the PTAS is to describe a way to decompose the graph G into strip graphs with constant width while not losing much in the objective value. This is similar to the decomposition in [BBT09] for grid graphs with a slightly different analysis.

Recalling the structure of G_r, for any $i = 1, \ldots, r$ let,

$$
E_{i0} := \{((i,j,k,0),(i',j,k,0)) \;\mid\; i' = \{i-1, i+1\} \cap \{1,\ldots,r\},\; 1 \leq j \leq r,\; 1 \leq k \leq 4\}.
$$

In other words, E_{i0} consists of all edges within layer 0 which are incident on the vertices $(i, j, k, 0)$. Let T be a large positive integer which we shall set later. For any $k = 0, 1, \dots, T-1$, let,

$$
\begin{aligned}
E_0^k &:= \bigcup_{\substack{i \equiv k \mod T, \\ 1 \le i \le r}} E_{i0}, \\
A_0^k &:= \sum_{(u,v) \in E_0^k} |c_{uv}|, \\
H_k(S) &:= \sum_{(u,v) \in E_0^k} c_{uv} S_u S_v, \\
H_{sub,k}(S) &:= H(S) - H_k(S).
\end{aligned}
$$

Since every edge in E_0 is present in exactly 2 of the subsets E_0^k, we obtain by averaging that there is a k^* such that $A_0^{k^*} \le (2/T)A_0$. Further, it can be seen that $H_{sub,k}(S)$ is the Hamiltonian on a disjoint collection of at most $\lceil r/T \rceil$ strip graphs of dimensions $r \times 8T$ and at most $\lceil r/T \rceil$ strip graphs of dimensions $r \times 8$. To complete the analysis we first assume because of symmetry that $A_1 \ge A_0$. Thus, by Lemma 2.1, the minimum value of $H(S)$ is at most $-2A_0$. Let S' be the assignment that minimizes the value of H_{sub,k^*}, and S^{opt} the assignment that minimizes the value of $H(S)$. We have,

$$
\begin{aligned}
H_{sub,k^*}(S') &\le H_{sub,k^*}(S^{\text{opt}}) \\
&\le H(S^{\text{opt}}) + A_0^{k^*} \\
&\le H(S^{\text{opt}}) + (2/T)A_0 \\
&\le (1 - 1/T)H(S^{\text{opt}}),
\end{aligned}
$$

and,

$$
\begin{aligned}
H(S') &\le H_{sub,k^*}(S') + A_0^{k^*} \\
&\le (1 - 1/T)H(S^{\text{opt}}) + (2/T)A_0 \\
&\le (1 - 2/T)H(S^{\text{opt}}).
\end{aligned}
$$

Since $H(S') \ge H(S^{\text{opt}})$, from the above we get that $H(S')$ is a $(1 - 2/T)$ approximation to $H(S^{\text{opt}})$. We now set $T = 2/\varepsilon$ to obtain a $(1-\varepsilon)$ approximation to $H(S^{\text{opt}})$. To compute the value $H(S')$, we compute the assignment S' that minimizes $H_{sub,k}(S)$ for each $k = 0, 1, \dots, T-1$, and take the one that gives the minimum value of $H(S')$. For each k, this involves minimizing the Hamiltonian on at most $(2r/T + 2)$ strip graphs of r levels and width at most $8T$. As discussed above, the computation time for one such strip graph is $O(r4^{8T})$ which adds up to $O(r^2 4^{8T}/T)$ time for all the strip graphs. Thus, the total computation time to obtain a $(1-\varepsilon)$ approximation is $O\left(\varepsilon r^2 4^{\frac{16}{\varepsilon}}\right) = O\left(\varepsilon n 2^{\frac{32}{\varepsilon}}\right)$.

3 A constant factor bound

In this section we prove Theorem 1.2. The key ingredient is the following lemma which bounds the bilinear quadratic form on $K_{4,4}$ in terms of the sum of the absolute values of the coefficients.

Lemma 3.1. *Let $G(U, V, E)$ be a $K_{4,4}$ graph with $U = \{u_1, \ldots, u_4\}$ and $V = \{v_1, \ldots, v_4\}$ giving the bipartition and $E = U \times V$ the edge set. There is a universal constant $C > 0$ such that for any real numbers $\{c_{ij} \mid 1 \leq i, j \leq 4\}$,*

$$\min_S \sum_{1 \leq i,j \leq 4} c_{ij} S_{u_i} S_{v_j} \leq -C \sum_{1 \leq i,j \leq 4} |c_{ij}|, \tag{4}$$

where $S = \{S_u \mid u \in U\} \cup \{S_v \mid v \in V\}$ is a $\{-1, 1\}$ assignment to the vertices of G. In particular, the above holds for some $C > \frac{\ln(1+\sqrt{2})}{\pi}$.

Proof. Let us first assign unit vectors x_i for vertices u_i and y_j for vertices v_j ($1 \leq i, j \leq 4$). The seminal work of Grothendieck [Gro53] implies the following:

$$\max_{\substack{x_i, y_j \in \mathbf{S}^7 \\ 1 \leq i,j \leq 4}} \sum_{1 \leq i,j \leq 4} c_{ij} \langle x_i, y_j \rangle \leq K \max_S \sum_{1 \leq i,j \leq 4} c_{ij} S_{u_i} S_{v_j}. \tag{5}$$

Here K is a universal constant for which the above inequality holds for any $K_{t,t}$, wherein our case $t = 4$. Determining the exact value of K has been a major open question. The work of Krivine [Kri77] showed that $K \leq \frac{\pi}{2\ln(1+\sqrt{2})}$ and in more recent work Braverman, Makarychev, Makarychev and Naor [BMMN11] showed that in fact $K < \frac{\pi}{2\ln(1+\sqrt{2})}$. The following claim helps to leverage the above inequality.

Claim 3.2. *There exists a set of unit vectors vectors $\{x_i \mid 1 \leq i \leq 4\} \cup \{y_j \mid 1 \leq j \leq 4\}$ such that,*

$$\sum_{1 \leq i,j \leq 4} c_{ij} \langle x_i, y_j \rangle \geq \left(\frac{1}{2}\right) \sum_{1 \leq i,j \leq 4} |c_{ij}|. \tag{6}$$

Proof. We first set the vectors $\{x_i \mid 1 \leq i \leq 4\}$ to be a set of 4 orthonormal vectors. For $j = 1, 2, 3, 4$ we let the unit vector $y_j = (1/2) \sum_{i=1}^{4} \text{sgn}(c_{ij}) x_i$. It is easy to check that this setting of the vectors satisfies the inequality in the claim. □

Using the above claim in conjunction with Equation (5) along with the bound on the value of K we obtain,

$$\max_S \sum_{1 \leq i,j \leq 4} c_{ij} S_{u_i} S_{v_j} \geq C \sum_{1 \leq i,j \leq 4} |c_{ij}| \tag{7}$$

Reversing the signs of the assignments to the vertices in U, we complete the proof of the lemma. □

The following lemma provides a bound on the minimum value of $H(S)$.

Lemma 3.3. *Let H^* be the minimum value of $H(S)$. Then $H^* \leq A_0 + A_1 - CA_{01}$.*

Proof. Since the set of edges E_{01} is a disjoint collection of r^2 $K_{4,4}$ graphs, using Lemma 3.1 one can set the assignment S such that $M_{01}(S) \leq -CA_{01}$. The maximum values of $M_0(S)$ and $M_1(S)$ are A_0 and A_1 respectively. Also, by flipping the sign of S if necessary, one can simultaneously ensure that $D(S)$ is non-positive. □

Combining the above lemma with Lemma 2.1 we obtain,

$$\begin{aligned}
(C+2)H^* &\le -(C+1)(A_0+A_1)+A_0+A_1-CA_{01},\\
\Rightarrow (C+2)H^* &\le -C(A_0+A_1+A_{01}),\\
\Rightarrow \left(\frac{C+2}{C}\right)H^* &\le -(A_0+A_1+A_{01}).
\end{aligned} \tag{8}$$

Moreover, an appropriate assignment of S ensures that $D(S) = -B$. Thus, we also have the following bound,

$$H^* \le A_0 + A_1 + A_{01} - B.$$

Combining the above with Equation (8) yields,

$$\begin{aligned}
\left(\frac{2(C+2)}{C}+1\right)H^* &\le -2(A_0+A_1+A_{01})+(A_0+A_1+A_{01}-B),\\
\Rightarrow H^* &\le -\left(\frac{C}{3C+4}\right)(A_0+A_1+A_{01}+B)
\end{aligned}$$

which completes the proof of Theorem 1.2.

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