Information theoretical clustering is hard to approximate *

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Abstract

An impurity measures $I : \mathbb{R}^d \mapsto \mathbb{R}^+$ is a function that assigns a *d*-dimensional vector **v** to a non-negative value $I(\mathbf{v})$ so that the more homogeneous **v**, with respect to the values of its coordinates, the larger its impurity. A well known example of impurity measures is the entropy impurity. We study the problem of clustering based on the entropy impurity measures. Let *V* be a collection of *n* many *d*-dimensional vectors with non-negative components. Given *V* and an impurity measure *I*, the goal is to find a partition \mathcal{P} of *V* into *k* groups V_1, \ldots, V_k so as to

minimize the sum of the impurities of the groups in \mathcal{P} , i.e., $I(\mathcal{P}) = \sum_{i=1}^{k} I\left(\sum_{\mathbf{v}\in V_i} \mathbf{v}\right)$.

Impurity minimization has been widely used as quality assessment measure in probability distribution clustering (KL-divergence) as well as in categorical clustering. However, in contrast to the case of metric based clustering, the current knowledge of impurity measure based clustering in terms of approximation and inapproximability results is very limited.

Here, we contribute to change this scenario by proving that the problem of finding a clustering that minimizes the Entropy impurity measure is APX-hard, i.e., there exists a constant $\epsilon > 0$ such that no polynomial time algorithm can guarantee $(1+\epsilon)$ -approximation under the standard complexity hypothesis $P \neq NP$. The inapproximability holds even when all vectors have the same ℓ_1 norm.

This result provides theoretical limitations on the computational efficiency that can be achievable in the quantization of discrete memoryless channels, a problem that has recently attracted significant attention in the signal processing community. In addition, it also solve a question that remained open in previous work on this topic [Chaudhuri and McGregor COLT 08; Ackermann et. al. ECCC 11].

1 Introduction

Data clustering is a fundamental tool in machine learning that is commonly used to coherently organize data as well as to reduce the computational resources required to analyse large datasets. For comprehensive descriptions of different clustering methods and their applications refer to [16, 18]. In general, clustering is the problem of partitioning a set of items so that, in the output partition, similar items are grouped together and dissimilar items are separated. When the items are represented as vectors that correspond to frequency counts or probability distributions many clustering algorithms rely on so called impurity measures (e.g., entropy) that estimate the dissimilarity of a group of items (see, e.g., [15] and references therein). In a simple example of this setting, a company may want to group users according to their taste for different genres of movies. Each user

^{*}This paper was presented in part at the 36th International Conference on Machine Learning ICML 2019 [13].

u is represented by a vector, where the value of the *i*th component counts the number of times u watched movies from genre *i*. To evaluate the dissimilarity of a group of users we calculate the impurity of the sum of their associated vectors, and then we select the partition for which the sum of the dissimilarities of its groups is minimum. The design of clustering methods based on impurity measures is the central theme of this paper.

1.1 Problem Description.

An impurity measure $I : \mathbf{v} \in \mathbb{R}^d_+ \mapsto I(\mathbf{v}) \in \mathbb{R}_+$ is a function that maps a vector \mathbf{v} to a non-negative value $I(\mathbf{v})$ so that the more homogeneous \mathbf{v} with respect to the values of its coordinates, the larger its impurity. One of the most popular/studied impurity measures, henceforth referred to as the *Entropy impurity* is based on the Shannon entropy function and it is defined by

$$I_{Ent}(\mathbf{v}) = \|\mathbf{v}\|_1 \sum_{i=1}^d \frac{v_i}{\|\mathbf{v}\|_1} \log \frac{\|\mathbf{v}\|_1}{v_i}$$

In the PARTITION WITH MINIMUM WEIGHTED IMPURITY PROBLEM (PMWIP), we are given a collection of n many d-dimensional vectors $V \subset \mathbb{R}^d$ with non-negative components and we are also given an impurity measure I. The goal is to find a partition \mathcal{P} of V into k disjoint groups of vectors V_1, \ldots, V_k so as to minimize the sum of the impurities of the groups in \mathcal{P} , i.e.,

$$I(\mathcal{P}) = \sum_{i=1}^{k} I\left(\sum_{\mathbf{v}\in V_i} \mathbf{v}\right).$$
(1)

In this paper, our focus is on the Entropy impurity I_{Ent} as defined above. We use PMWIP_{Ent} to refer to PMWIP with impurity measure I_{Ent} .

1.2 Applications

This kind of clustering is used in a number of relevant applications such as: (i) attribute selection during the construction of random forest/decision trees [8, 9, 12, 14, 23]; (ii) clustering of words based on their distribution over a text collection for improving classification tasks [7, 15] and (iii) quantization of memoryless channels/design of polar codes [32, 22, 21, 29, 27]. The last application will be discussed more thoroughly in the related work section.

Another interesting application, also mentioned in [10, 4], is the compression of a large collection of n short files (e.g. tweets) using entropy encoding (e.g. Huffman or Arithmetic coding). Compressing each file individually might incur a huge overhead since we would need to store the compression model (e.g. alphabet + codewords) for each of them. Thus, a natural idea is to cluster them into $k \ll n$ groups and then compress files in the same cluster using the same model. This approach leads to an instance of PMWIP_{Ent} since it is possible to generate encodings for probability distributions whose sizes are arbitrarily close to their Shannon entropy, so that the objective function in (1) is the total size of the compressed collection ignoring the compression model for each of the clusters.

Despite of its wide use in relevant applications, clustering being a fundamental problem and entropy being an essential measure in Information Theory as well as considerably important in Machine Learning, the current understanding of PMWIP from the perspective of approximation algorithms is very limited as we detail further. This contrasts with what is known for clustering in metric spaces where the gap between the ratios achieved by the best known algorithms and the largest known inapproximability factors, assuming $P \neq NP$, are somehow tight (see [6] and references therein). Our study contributes to reducing this gap of knowledge.

1.3 Our Results and Techniques

Our main contribution is a proof that $PMWIP_{Ent}$ is APX-Hard even for the case where all vectors have the same ℓ_1 -norm. In other words, we show that there exists $\epsilon > 0$ such that one cannot obtain in polynomial time an $(1 + \epsilon)$ multiplicative approximation for $PMWIP_{Ent}$ unless P = NP. Our result implies on the APX-Hardness of MTC_{KL} , the problem of clustering *n* probability distributions into *k* groups where the Kullback-Leibler divergence is used to measure the distance between each distribution and the centroid of its assigned group. With this result, we settle a question that remained open in previous work on the MTC_{KL} problem [10, 2]. Finally, our inapproximability result contributes to the understanding of a problem that has recently attracted significant attention in the signal processing community, as it provides a theoretical limit, under the perspective of computational complexity, on the possibility of efficiently quantizing discrete memoryless channels. In fact, as we explain in Section 2.1, the quantization problem can be formulated as the PMWIP_{Ent}.

Our proof follows the approach employed by Awasthi [6] to show the APX-hardness of the kmeans clustering problem. As in [6], it consists of mapping hard instances from the minimum vertex cover problem in triangle-free bounded degree graphs into instances of the clustering problem, in our case the PMWIP_{Ent}. However, in order to deal with the entropy impurity, we have to overcome a number of technical challenges that do not arise when one considers the ℓ_2^2 distance employed by the k-means problem.

1.4 Paper Organization

The paper is organized as follows: in Section 2 we discuss works that are related to ours. More specifically, we discuss existing work on the problem of quantizing discrete memoryless channels and on the the problem of clustering probability distributions using Kullback-Leibler divergence. In Section 3 we present some technical background that is useful to derive our main result. Section 4 is dedicated to our main contribution. Section 5 concludes the paper with some final remarks and open questions.

2 Related Work

2.1 Connections to quantizer design

Quantization is a fundamental part of digital processing systems used to keep complexity and resource consumption tractable. Quantization refers to the mapping of a large alphabet to a smaller one. A typical example is given by making the output of a channel $X \mapsto Y$ with a large output alphabet travel through an additional channel $Y \mapsto Z$ (the quantizer) whose output is from a small alphabet without affecting too much the capacity of the quantized channel $X \mapsto Z$ with respect to the capacity of the original channel $X \mapsto Y$. To formalize the connection between our problem and the one of designing optimal quantizers, let us consider a discrete memory channel (DMC). Let the input be $X \in \mathcal{X} = \{1, \ldots, d\}$ with distribution $p_x = Pr(X = x)$. Let the channel output be $Y \in \mathcal{Y} = \{1, \ldots, n\}$ and the channel transition probability be denoted by $P_{y|x} = Pr(Y = y \mid X = x)$. The channel output is quantized to $Z \in \mathcal{Z} = \{1, \ldots, k\}$ for some $k \leq n$, by a possibly stochastic channel (quantizer) defined by $Q_{z|y} = Pr(Z = z \mid Y = y)$, so that the conditional probability distribution of the quantizer output Z w.r.t. the channel input X is $T_{z|x} = Pr(Z = z \mid X = x) = \sum_{y \in Y} Q_{z|y} P_{y|x}$.

The aim of quantizer's design is to guarantee that the mutal information I(X;Z) between X and Z is as large as possible, i.e., as close as possible to the mutual information I(X;Y) between the input and the non quantized output Y.

It is known that there is an optimal quantizer that is deterministic (see, e.g., [22]), i.e., for each $y \in Y$ there is a unique $z \in Z$ such that $Q_{z|y} = 1$. Therefore, the quantizer design problem can be cast as finding the k-partition $\mathcal{C} = C_1, \ldots, C_k$ of \mathcal{Y} such that $T_{z|x} = \sum_{y \in C_z} P_{y|x}$ guarantees the maximum mutual information

$$I(X;Z) = \sum_{z \in \mathcal{Z}} \sum_{x \in \mathcal{X}} p_x T_{z|x} \log \frac{T_{z|x}}{\sum_{x'} p_{x'} T_{z|x'}}$$

If for each $y \in \mathcal{Y}$ we define the vector $\mathbf{v}^{(y)} = (v_1^{(y)}, \dots, v_d^{(y)})$ with $v_x^{(y)} = p_x P_{y|x}$ and let $\mathbf{c}^{(z)} = \sum_{u \in C_z} \mathbf{v}^{(y)}$, we have that

$$T_{z|x} = \sum_{y \in C_z} P_{y|x} = \sum_{y \in C_z} \frac{v_x^{(y)}}{p_x}.$$

Hence,

$$I(X,Z) = \sum_{z} \sum_{x} p_{x} \sum_{y \in C_{z}} \frac{v_{x}^{(y)}}{p_{x}} \log \left(\frac{\sum_{y \in C_{z}} \frac{v_{x}^{(y)}}{p_{x}}}{\sum_{x'} p_{x'} \sum_{y \in C_{z}} \frac{v_{x'}^{(y)}}{p_{x'}}} \right)$$

$$= \sum_{x} \sum_{z} c_{x}^{(z)} \log \frac{c_{x}^{(z)}}{p_{x} \| \mathbf{c}^{(z)} \|_{1}}$$

$$= \sum_{x} \sum_{z} c_{x}^{(z)} \log \frac{1}{p_{x}} - \sum_{z} \| \mathbf{c}^{(z)} \|_{1} \sum_{x} \frac{c_{x}^{(z)}}{\| \mathbf{c}^{(z)} \|_{1}} \log \frac{\| \mathbf{c}^{(z)} \|_{1}}{c_{x}^{(z)}}$$

$$= \sum_{x} p_{x} \log \frac{1}{p_{x}} - \sum_{z} I_{Ent}(C_{z}) = H(X) - \sum_{z=1}^{k} I(C_{z}).$$

Therefore, an optimal quantizer that maximizes the mutual information, is obtained by the clustering of minimum impurity

$$\sup_{Q_{z|y}} I(X;Z) = H(X) - \inf_{(C_1,\dots,C_k)} \sum_{z=1}^{k} I(C_z).$$

Efficient techniques for maximizing mutual information in channel output quantization have been the focus of several recent papers as the problem plays an important role in making the implementation of polar codes tractable [30, 28, 31, 21]. The objective in these papers is the minimization of the additive loss in terms of mutual information due to the quantization, i.e., the minimization/approximation of the objective function I(X,Y) - I(X,Z) that (by proceeding as above) is equivalent, in our notation, to the minimization/approximation of

$$\Delta_k(X;Y) = I(X,Y) - I(X,Z) = \sum_z I(C_z) - \sum_y I(v^{(y)}).$$

A main result of [21] is that for arbitrary joint distribution P_{XY} it holds that $\Delta_k(X;Y) = O(k^{-2/(d-1)})$. In [30] it is shown that there exist channels $X \mapsto Y$ such that $\Delta_k(X;Y) = \Omega(k^{-2/(d-1)})$. The papers [28, 31, 21] also provided polynomial-time approximation algorithm for designing such quantizers. In addition, for binary input channels $(|\mathcal{X}| = 2)$ an optimal algorithm is given in [22] and [17].

We note that, although the optimal clustering provides an optimal quantizer, in terms of approximation, because of the additional term in the objective function $\Delta_k(X;Y)$ we have that an approximation guarantee for $\Delta_k(X;Y)$ also gives an approximation guarantee on the optimal impurity, but not vice versa. On the other hand, our inapproximability result for PMWIP_{Ent} implies the same inapproximability result for the problem of optimizing $\Delta_k(X;Y)$.

A different perspective has been taken in [27] where the multiplicative loss I(X; Z)/I(X; Y) has been studied, with the aim of characterizing the fundamental properties of the quantizer attaining the minimum I(X; Z). In particular the authors of [27] study the infimum of I(X; Z) taken with respect to all joint distributions with input alphabet \mathcal{X} of cardinality d and *arbitrary* (possibly continuous) output alphabet \mathcal{Y} such that the mutual information I(X; y) is at least β , where β is a given parameter.

2.2 Clustering with Kullback-Leibler Divergence

PMWIP_{Ent} is closely related to MTC_{KL} defined in [10] as the problem of clustering a set of n probability distributions into k groups minimizing the total Kullback-Leibler (KL) divergence from the distributions to the centroids of their assigned groups. Mathematically, we are given a set of n points $p^{(1)}, \ldots, p^{(n)}$, corresponding to probability distributions, and a positive integer k. The goal is to find a partition of the points into k groups V_1, \ldots, V_k and a centroid $c^{(i)}$ for each group V_i such that

$$\sum_{i=1}^{k} \sum_{p \in V_i} KL(p, c^{(i)})$$

is minimized, where $KL(p,q) = \sum_{j=1}^{d} p_j \ln(p_j/q_j)$ is the Kullback-Leibler divergence between points p and q.

It is known that in the optimal solution for each i = 1, ..., k the centroid $c^{(i)} = (c_1^{(i)}, ..., c_d^{(i)})$ is given by $c_j^{(i)} = \sum_{p \in V_i} p_j / |V_i|$, for each j = 1, ..., d. Thus, MTC_{KL} is equivalent to the problem of

finding a partition that minimizes

$$\sum_{i=1}^{k} \sum_{p \in V_i} KL(p, c^{(i)}) = \sum_{i=1}^{k} \sum_{p \in V_i} \sum_{j=1}^{d} p_j (\ln p_j - \ln c_j^{(i)}) =$$
(2)

$$\sum_{i=1}^{n} \sum_{j=1}^{d} p_j^{(i)} \ln p_j^{(i)} - \sum_{i=1}^{k} \sum_{p \in V_i} \sum_{j=1}^{d} p_j \ln c_j^{(i)} =$$
(3)

$$\sum_{i=1}^{n} \sum_{j=1}^{d} p_j^{(i)} \ln p_j^{(i)} - \sum_{i=1}^{k} \sum_{j=1}^{d} \left(\sum_{p \in V_i} p_j \right) \ln \frac{\left(\sum_{p \in V_i} p_j \right)}{|V_i|} =$$
(4)

$$-\frac{1}{\log e} \sum_{i=1}^{n} I_{Ent}(p^{(i)}) + \frac{1}{\log e} \sum_{i=1}^{k} I_{Ent}\left(\sum_{p \in V_i} p\right)$$
(5)

Therefore, the optimal solution of MTC_{KL} is equal to the optimal one of the particular case of $PMWIP_{Ent}$ in which $\mathbf{v}_i = p_i$ for i = 1, ..., n. While their optimal solutions match in this case, $PMWIP_{Ent}$ and MTC_{KL} differ in terms of approximation since the objective function for MTC_{KL} has an additional constant term $-\sum_{i=1}^{n} I_{Ent}(p^{(i)})$ so that an α -approximation for MCT_{KL} problem implies an α -approximation for PMWIP_{Ent} while the converse is not necessarily true.

In [10] an $O(\log n)$ approximation for MTC_{KL} is given. Some $(1+\epsilon)$ -approximation algorithms were proposed for a constrained version of MTC_{KL} where every element of every probability distribution lies in the interval $[\lambda, v]$ [3, 1, 4, 25]. The algorithm from [3, 4] runs in $O(n2^{O(mk/\epsilon \log(mk/\epsilon))})$ time, where *m* is a constant that depends on ϵ and λ . In [1] the running time is improved to $O(ngk + g2^{O(k/\epsilon \log(k/\epsilon))} \log^{k+2}(n))$ via the use of weak coresets. Recently, using strong coresets, $O(ngk + 2^{poly(gk/\epsilon)})$ time is obtained [25]. We shall note that these algorithms provide guarantees for μ -similar Bregman divergences, a class of metrics that includes domain constrained *KL* divergence. By using similar assumptions on the components of the input probability distributions, Jegelka et. al. [19] show that Lloyds *k*-means algorithm—which also has an exponential time worst case complexity [33]—obtains an $O(\log k)$ approximation for MTC_{KL} . For PMWIP_{Ent}, an $O(\log^2 \min\{k, d\})$ is presented in [13].

In terms of computational complexity, Chaudhuri and McGregor [10] proved that the variant of MTC_{KL} where the centroids must be chosen from the input probability distributions is NP-Complete. The NP-Hardness of MTC_{KL} , that remained open in [10], was established in Ackermann et. al. [2], where it is also mentioned that the APX-hardness of k-means in \mathbb{R}^2 would imply the same kind of hardness for MTC_{KL} . However, it is not known whether the former is APX-Hard. Our result provides an important progress in this line of investigation since it establishes the APXhardness of MTC_{KL} . We shall mention that, in terms of restricted instances, one of the authors proved recently that PMWIP_{Ent} is NP-Complete, even when k = 2, via a simple reduction from PARTITION [23].

3 Preliminaries

In this section we introduce some notation and discuss some technical material that will be useful to establish our main result. We start with some notation.

3.1 Notation

Let G = (V, E) be a simple undirected graph. A vertex cover in G is a set of vertices S such that each edge $e \in E$ is incident to some vertex of S. A vertex cover S is minimal if for every $v \in S$, $S \setminus \{v\}$ is not a vertex cover. A star in G is a subgraph G' of G such that there exists one vertex in G', the centre of the star G', that is incident to all edges in G'. If a star G' has p edges we say that it is a p-star.

We say that G is a D-bounded degree graph if for each vertex $v \in V$ the degree of v is at most D. We say that G is D-regular, if for each $v \in V$ the degree of v is D. A triangle in G is a set of three vertex u, v and w such that $uv, uw, vw \in E$. We say that G is triangle-free if it has no triangle.

For a set of vectors C we use $I_{Ent}(C)$ to denote the impurity of C, that is, $I_{Ent}(C) = I_{Ent}(\sum_{\mathbf{v}\in C} \mathbf{v})$.

We define the entropy impurity of a set of edges C from a graph G, over the vertex set $V = \{v_1, \ldots, v_n\}$, as follows:

$$I_{Ent}(C) = 2|C| \cdot H\left(\frac{d^{C}(v_{1})}{2|C|}, \dots, \frac{d^{C}(v_{n})}{2|C|}\right)$$
(6)

where H() denotes the Shannon entropy and $d^{C}(v)$ denotes the number of edges of C incident in v

3.2 Bounds on the Entropy Impurity for Graphs

We now present bounds on the entropy impurity of sets of edges focussing in particular on subsets of edges from triangle-free graphs, which will be the basis of our hardness proof in the next section.

Fact 1. If C is a set of edges forming a p-star, then we have $I_{Ent}(C) = 2p + p \log p$.

We also have that the 3-bounded triangle-free graphs with *p*-edges have impurity at least $2p + p \log p$ as recorded in the following Lemma 1.

To establish the lemma we will exploit Facts 2 and 3 presented in the sequel. The former is a direct consequence of the Schur concavity of the Shannon entropy function (see, e.g., [26]) while the latter is a special case of Turan's and Mantel's theorem about triangle-free graphs (see, e.g., [20]).

Fact 2. Let $\mathbf{p} = (p_1, \dots, p_n)$ and $\mathbf{q} = (q_1, \dots, q_n)$ be probability distributions such that for each $i = 1, \dots, n-1$ it holds that

- $p_i \ge p_{i+1};$
- $q_i \ge q_{i+1};$
- $\sum_{j=1}^{i} p_i \leq \sum_{j=1}^{i} q_i.$

Then, $H(\mathbf{p}) \geq H(\mathbf{q})$.

Fact 3. Let n and m denote the number of vertices and edges of a triangle-free graph. Then $n \ge \lfloor \sqrt{4m} \rfloor$.

Lemma 1. Let C be a set of p edges from a 3-bounded degree triangle-free graph. Then $I_{Ent}(C) \ge 2p + p \log p$.

Proof. Recalling the definition in (6) with |C| = 2p and denoting by $d^{C}(v)$ the number of edges of C incident in v and by v_1, \ldots, v_n the vertices of the underlying graph, we have

$$I_{Ent}(C) = 2pH\left(\frac{d^C(v_1)}{2p}, \dots, \frac{d^C(v_n)}{2p}\right),\tag{7}$$

where H() denotes the Shannon entropy. Since the entropy function is invariant upon permutations of the components, for the rest of this proof, we will assume w.l.o.g., that the vertices are sorted in non increasing order of degree, i.e., $d^{C}(v_{i}) \geq d^{C}(v_{i+1})$ for $i = 1, \ldots, n-1$. Let \tilde{n} denote the number of vertices incident on edges in C. Equivalently, under the standing assumption, \tilde{n} is the largest index i such that $d^{C}(v_{i}) > 0$.

The desired result will follow from showing that the entropy on the right hand side of (7) is lower bounded by $1 + \frac{\log p}{2}$. We will split the analysis into several cases.

Case 1. $p \ge 9$.

Since the edges in C are from a 3-bounded degree graph, we have $d^{C}(v_{i}) \leq 3$ for i = 1, ..., n. Hence,

$$H\left(\frac{d^{C}(v_{1})}{2p}, \dots, \frac{d^{C}(v_{n})}{2p}\right) = \sum_{j=1}^{\tilde{n}} \frac{d^{C}(v_{i})}{2p} \log \frac{2p}{d^{C}(v_{i})} \ge \sum_{j=1}^{\tilde{n}} \frac{d^{C}(v_{i})}{2p} \log \frac{2p}{3} = 1 + \log \frac{p}{3} \ge 1 + \frac{1}{2} \log p,$$

where, in the first inequality we are using $d^{C}(v_{i}) \geq 3$ and the last inequality follows from $p \geq 9$. Case 2. $\tilde{n} \geq p+1$.

By the standing assumptions, we have $d^{C}(v_{1}) \geq \cdots \geq d^{C}(v_{p+1}) > 0$. Therefore, by Fact 2, we have that

$$H\left(\frac{d^{C}(v_{1})}{2p}, \dots, \frac{d^{C}(v_{n})}{2p}\right) \ge H\left(\frac{p}{2p}, \frac{1}{2p}, \dots, \frac{1}{2p}, 0, \dots, 0\right) = 1 + \frac{1}{2}\log p.$$
(8)

By Fact 3, for p = 3, we have that the triangle-free condition implies $\tilde{n} \ge 4 = p + 1$, hence the last case also covers p = 3.

Under the condition in Fact 3, it remains to consider the cases $4 \le p \le 8$ with $\lceil \sqrt{4p} \rceil \le \tilde{n} \le p$, i.e., (i) $p = 4, \tilde{n} = 4$, (ii) $p = 5, \tilde{n} = 5$, (iii) $p = 6, \tilde{n} \in \{5, 6\}$, (iv) $p = 7, \tilde{n} \in \{6, 7\}$, and (v) $p = 8, \tilde{n} \in \{6, 7, 8\}$. For each one of these cases we shall show a probability distribution $\mathbf{w}^{(p,\tilde{n})}$ such that the inequality $H(\mathbf{w}^{(p,\tilde{n})}) \ge 1 + \frac{\log p}{2}$ holds and by Fact 2 also $H(\mathbf{w}^{(p,\tilde{n})}) \le H\left(\frac{d^C(v_1)}{2p}, \ldots, \frac{d^C(v_n)}{2p}\right)$ holds for every choice of a triangle-free set C with p edges incident to \tilde{n} vertices.

Case 3. p = 4, $\tilde{n} = 4$. The only triangle-free graph on $\tilde{n} = 4$ vertices with p = 4 edges is given by a polygon with 4 vertices, i.e., $d^{C}(v_{i}) = 2$, for i = 1, 2, 3, 4. In this case we have

$$H\left(\frac{d^{C}(v_{1})}{2p},\ldots,\frac{d^{C}(v_{4})}{2p}\right) = H\left(\frac{2}{8},\frac{2}{8},\frac{2}{8},\frac{2}{8}\right) = 2 = 1 + \frac{\log p}{2},$$

as desired.

Case 4. $p = 5, \tilde{n} \ge 5$.

By by the assumptions $3 \ge d^C(v_1) \ge \cdots \ge d^C(v_5) > 0$, and Fact 2, we have that

$$H\left(\frac{d^{C}(v_{1})}{2p},\ldots,\frac{d^{C}(v_{n})}{2p}\right) \ge H\left(\frac{3}{10},\frac{3}{10},\frac{2}{10},\frac{1}{10},\frac{1}{10},0,\ldots,0\right) = \log 5 + \frac{8}{10} - \frac{6}{10}\log 3 \ge 1 + \frac{\log 5}{2}$$
(9)

The desired result now follows by noticing that the last quantity in (9) is equal to $1 + \frac{1}{2} \log p$. Case 5. p = 6, $\tilde{n} \in \{5, 6\}$.

Subcase 5.1 p = 6, $\tilde{n} = 5$

By direct inspection, it is not hard to see that there is no triangle-free graph on 5 vertices where three of them have degree 3. Hence, we have that the following conditions must hold

$$3 \ge d^C(v_1) \ge d^C(v_2) > 0$$
 and $2 \ge d^C(v_3) \ge d^C(v_4) \ge d^C(v_5) > 0$

Therefore, by Fact 2, we have

$$H\left(\frac{d^{C}(v_{1})}{2p},\ldots,\frac{d^{C}(v_{n})}{2p}\right) \ge H\left(\frac{3}{12},\frac{3}{12},\frac{2}{12},\frac{2}{12},\frac{2}{12},0,\ldots,0\right) = 1 + \frac{\log 6}{2}$$
(10)

The desired result now follows by noticing that the last quantity in (10) is equal to $1 + \frac{1}{2} \log p$. Subcase 5.2 $\tilde{n} = 6$ By Fact 2 and the assumption $3 \ge d^C(v_1) \ge \cdots \ge d^C(v_6) > 0$, we have

$$H\left(\frac{d^{C}(v_{1})}{2p},\ldots,\frac{d^{C}(v_{n})}{2p}\right) \ge H\left(\frac{3}{12},\frac{3}{12},\frac{3}{12},\frac{1}{12},\frac{1}{12},\frac{1}{12},0,\ldots,0\right) = 2 + \frac{3}{12}\log 3 \ge 1 + \frac{\log 6}{2}$$
(11)

The desired result now follows by noticing that the last quantity in (11) is equal to $1 + \frac{1}{2} \log p$.

Case 6. $p = 7, \tilde{n} \in \{6, 7\}.$

By Fact 2, and the assumption $3 \ge d^C(v_1) \ge \cdots \ge d^C(v_6) > 0$, we have that

$$H\left(\frac{d^{C}(v_{1})}{2p},\ldots,\frac{d^{C}(v_{n})}{2p}\right) \ge H\left(\frac{3}{14},\frac{3}{14},\frac{3}{14},\frac{3}{14},\frac{1}{14},\frac{1}{14},0,\ldots,0\right) = 1 + \log 7 - \frac{6}{7}\log 3 > 1 + \frac{\log 7}{2}$$
(12)

The desired result now follows by noticing that the last quantity in (12) is equal to $1 + \frac{1}{2} \log p$.

Case 7. $p = 8, \tilde{n} \in \{6, 7, 8\}.$

By Fact 2 and the assumption $3 \ge d^C(v_1) \ge \cdots \ge d^C(v_6) > 0$, we have that

$$H\left(\frac{d^{C}(v_{1})}{2p},\ldots,\frac{d^{C}(v_{n})}{2p}\right) \ge H\left(\frac{3}{16},\frac{3}{16},\frac{3}{16},\frac{3}{16},\frac{3}{16},\frac{3}{16},\frac{1}{16},0,\ldots,0\right) = 4 - \frac{15}{16}\log 3 > 1 + \frac{3}{2}$$
(13)

The desired result now follows by noticing that the last quantity in (13) is equal to $1 + \frac{1}{2} \log p$.

4 Hardness of Approximation of PMWIP_{Ent}

The goal of this section is to establish our main result.

Theorem 1. PMWIP_{Ent} is APX-Hard.

This section is split into two subsections. In Section 4.1 we present a gap preserving reduction from vertex cover to our clustering problem. In Section 4.2 we establish its correctness.

4.1 A Gap Preserving Reduction

We start by recalling some basic definitions and facts that are useful for establishing limits on the approximability of optimization problems (see, e.g., [34, chapter 29]).

Given a minimization problem A and a parameter $\epsilon > 0$ we define the ϵ -GAP-A problem as the problem of deciding for an instance I of A and a parameter k whether: (i) I admits a solution of value $\leq k$; or (ii) every solution of I have value $> (1 + \epsilon)k$. In such a gap decision problem it is tacitly assumed that the instances are either of type (i) or of type (ii).

Fact 4. If for a minimization problem \mathbb{A} there exists $\epsilon > 0$ such that the ϵ -GAP- \mathbb{A} problem is NP-hard, then no polynomial time $(1 + \epsilon)$ -approximation algorithm exists for \mathbb{A} unless P = NP.

We will use the following definition of a gap-preserving reduction.

Definition 1. Let \mathbb{A}, \mathbb{B} be minimization problems. A gap-preserving reduction from \mathbb{A} to \mathbb{B} is a polynomial time algorithm that, given an instance x of \mathbb{A} and a value k, produces an instance y of \mathbb{B} and a value κ such that there exist constants $\epsilon, \eta > 0$ for which

- 1. if $OPT(x) \leq k$ then $OPT(y) \leq \kappa$;
- 2. if $OPT(x) > (1 + \epsilon)k$ then $OPT(y) > (1 + \eta)\kappa$;

Fact 5. Fix minimization problems \mathbb{A}, \mathbb{B} . If there exists ϵ such that the ϵ -GAP- \mathbb{A} problem is NPhard and there exists a gap-preserving reduction from \mathbb{A} to \mathbb{B} then there exists η such that the η -GAP- \mathbb{B} problem is NP-hard

We will now specialize the above definitions for a restricted variant of the problem of finding a minimum vertex cover in a graph and for our clustering problem $PMWIP_{Ent}$.

Definition 2. For every $\epsilon > 0$, the ϵ -GAP-MINVC-4 (gap) decision problem is defined as follows: given a 4-regular graphs G = (V, E) and an integer k, decide whether G has a vertex cover of size k or all vertex covers of G have size > $k(1 + \epsilon)$.

Definition 3. For every $\eta > 0$, the η -GAP-PMWIP_{Ent} (gap) decision problem is defined as follows: given a set of vectors U, an integer k, and a value κ , decide whether there exists a k-clustering $\mathcal{C} = (C_1, \ldots, C_k)$ of the vectors in U such that the total impurity $I_{Ent}(\mathcal{C}) = \sum_{\ell=1}^k I_{Ent}(C_\ell)$ is at most κ or for each k-clustering \mathcal{C} of U it holds that $I_{Ent}(\mathcal{C}) > (1 + \eta)\kappa$.

The following result is a consequence of [11, Theorems 17 and 19].

Theorem 2. [11] There are constants $0 < \alpha < \alpha' < 1$ and 4-regular graphs G = (V, E) such that it is NP-Complete to decide whether G has a vertex cover of size $\alpha |V|$ or all vertex covers of G have size $> \alpha'|V|$. Hence for $\epsilon = \frac{\alpha'}{\alpha} - 1$, the ϵ -GAP-MINVC-4 is NP-Complete. In order to show the APX-hardness of $PMWIP_{Ent}$, we employ a gap-preserving reduction from minimum vertex cover (MVC) in 4-regular graphs to $PMWIP_{Ent}$. This reduction is obtained by combining: (i) a gap-preserving reduction from MVC in 4-regular graphs to MVC in 4-bounded degree triangle-free graphs [24]; (ii) an L-reduction from MVC in 4-bounded degree graphs to MVC in 3-bounded degree graphs [5]; (iii) a gap-preserving reduction from instances of MVC in 3-bounded degree triangle-free graphs obtained via (i)-(ii) to instances of PMWIP_{Ent}.

We will first recall the maps at the bases of the reductions (i) and (ii). The proofs that they define gap-preserving reduction (Theorem 3) will be included in the appendix for the sake of self-containment.

From 4-regular graphs to 4-bounded degree triangle-free graphs. Let G' = (V', E') be a 4-regular graph. Let n = |V'| and m = |E'|. Hence m = 2n. Since in every graph there is a cut containing at least half of the edges, we can select $\hat{E} \subseteq E'$ with $|\hat{E}| = m/2 = n$ such that the graph with vertex set V' and set of edges \hat{E} is bipartite and, as a consequence, triangle-free. For each $e = (u, v) \in E' \setminus \hat{E}$ define a new set of vertices $V_e = \{u', v'\}$ and let

$$V_H = V' \cup \bigcup_{e=(u,v)\in E'\setminus \hat{E}} V_e \qquad E_H = \hat{E} \cup \bigcup_{e=(u,v)\in E'\setminus \hat{E}} \{(u,u'), (u',v'), (v',v)\}$$

Finally let $H = (V_H, E_H)$. In words, H is obtained from G' by a double subdivision of the n edges not in \hat{E} .

By construction we have that the graph H has bounded degree 4 and it is also triangle-free.

Let $\mathcal{R}^{(1)}$ be a function that maps a 4-regular graph G' to a 4-bounded degree triangle-free graph H according to the procedure defined above.

From 4-bounded degree graphs to 3-bounded degree graphs. Let $H = (V_H, E_H)$ be a 4bounded degree graph and for each vertex $v \in V_H$ of degree 4, denote the neighbours of v by w_1, w_2, w_3, w_4 . Let G = (V, E) be the graph obtained from H by the following transformation: for each vertex $v \in V_H$ of degree 4: substitute v with a three vertex path whose vertices are denoted by v_a, v_b, v_c and add edges $(v_a, w_1), (v_a, w_2), (v_c, w_3), (v_c, w_4)$.

Let $\mathcal{R}^{(2)}$ be a function that maps a 4-bounded degree graph H to a 3-bounded degree graph G according to the procedure defined above.

Fig. 1 shows an example of the successive application of maps $\mathcal{R}^{(1)}$ and $\mathcal{R}^{(2)}$ starting from a 4-regular graph G' and obtaining a 3-bounded degree and triangle-free graph G.

Definition 4 (3-bounded degree triangle-free hard graphs). Let

$$\mathcal{G}_{\mathcal{R}^{(1)},\mathcal{R}^{(2)}} = \{ G = \mathcal{R}^{(2)}(\mathcal{R}^{(1)}(G')) \mid G' \text{ is a 4-regular graph } \}$$

be the set of 3-bounded degree triangle-free graphs obtained from some 4-regular graph by successively applying functions $\mathcal{R}^{(1)}$ and $\mathcal{R}^{(2)}$.

The following result is a direct consequence of the properties of mappings $\mathcal{R}^{(1)}, \mathcal{R}^{(2)}$, and Theorem 2. Its proof is deferred to the appendix.

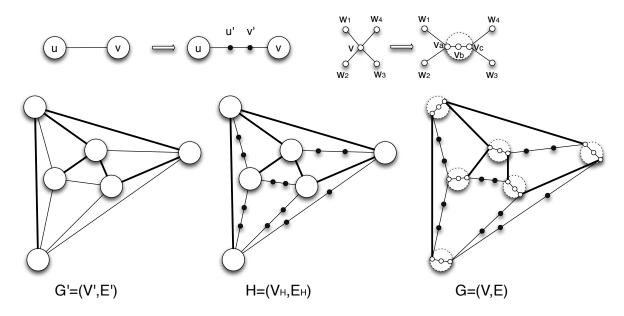


Figure 1: The transformations $\mathcal{R}^{(1)}$ and $\mathcal{R}^{(2)}$. On the left the graph G' = (V, E') with the cut set $\hat{E} \subseteq E'$ in bold. The center picture shows the corresponding graph $H = \mathcal{R}^{(1)}(G')$ obtained by the double subdivision of the edges $E' \setminus \hat{E}$. On the right the graph $G = \mathcal{R}^{(2)}(H)$ obtained by reducing the degree of the 4 degree vertices, using the transformation depicted on top.

Theorem 3. There are constants $0 < \beta < \beta' < 1$ such that it is NP-hard to decide whether a graph $G = (V, E) \in \mathcal{G}_{\mathcal{R}^{(1)}, \mathcal{R}^{(2)}}$ has a vertex cover of size $\beta |V|$ or all vertex covers of G have size $> \beta' |V|$.

From graphs in $\mathcal{G}_{\mathcal{R}^{(1)},\mathcal{R}^{(2)}}$ to PMWIP_{Ent} instances. Let G = (V, E) be a triangle-free and 3bounded degree graph from $\mathcal{G}_{\mathcal{R}^{(1)},\mathcal{R}^{(2)}}$, i.e., obtained from a 4-regular graph via successively applying functions $\mathcal{R}^{(1)}, \mathcal{R}^{(2)}$. Denote by v_1, \ldots, v_n the vertices in V. We construct (in polynomial time) a set of |E| binary vectors $U = \{v^e \mid e \in E\}$, each of them of dimension n, by stipulating that if $e = (v_i, v_j)$ then only the *i*-th and *j*-th components of v^e are 1 and all others are 0.

We denote by $\mathcal{R}^{(3)}$ a function that maps each graph in $\mathcal{G}_{\mathcal{R}^{(1)},\mathcal{R}^{(2)}}$ to a set of vectors U as described above.

Note that if E_C is a set of edges in a graph G with C being its corresponding set of vectors from $U = \mathcal{R}^{(3)}(G)$ then we have that $I_{Ent}(E_C) = I_{Ent}(C)$ as defined in (6).

4.2 A gap preserving reduction based on $\mathcal{R}^{(3)}$

In this section, focussing on set of vectors $U = \mathcal{R}^{(3)}(G)$ obtained from 3-bounded degree trianglefree graphs via the mapping defined in the previous section, we show that there exist η and κ for which it is hard to distinguish whether there is a k-clustering for U with total impurity smaller than κ or all k-clusterings for U have impurity at least $(1 + \eta)\kappa$. In other words, we show that the gap problem η -GAP-PMWIP_{Ent} is NP-hard and, as a consequence, by Fact 4, PMWIP_{Ent} is APX-Hard.

The proof will consists of two parts: first we show how to fix κ so that condition 1) of Definition 1 is satisfied—which we do in Lemma 2 and Corollary 1; and then we derive η so that condition 2) of Definition 1 is also satisfied—which will be done via a series of propositions leading to Lemma 3.

Proving condition 1) of Definition 1. The following lemma, which is key for our development, is based on establishing a relationship between minimal vertex covers and star decompositions in our hard instances for 3-bounded graphs, i.e., graphs from $\mathcal{G}_{\mathcal{R}^{(1)}\mathcal{R}^{(2)}}$.

Given a graph G and the set of vectors $U = \mathcal{R}^{(3)}(G)$ we will find it convenient to visualize vectors in U in terms of their corresponding edges in G. Therefore, for a subset of $C \subseteq U$ we will say that C is a *p*-star if the corresponding set of edges form a star in G, i.e., if |C| = p and there exists a coordinate $j \in [n]$ such that for each vectors $v^e \in C$ the *j*th components of v^e is 1.

Lemma 2. Let G = (V, E) be a triangle-free 3-bounded degree graph in $\mathcal{G}_{\mathcal{R}^{(1)}, \mathcal{R}^{(2)}}$ and let $U = \mathcal{R}^{(3)}(G)$ be the corresponding set of vectors obtained as described in the previous section. If G has a minimal vertex cover of size k then there is a k-clustering \mathcal{C} of U where each $C \in \mathcal{C}$ is either a 2-star or a 3-star.

Proof. Let G' = (V', E') be the 4-regular graph from which we derived G, i.e., $G = \mathcal{R}^{(2)}(\mathcal{R}^{(1)}(G'))$. Recall that each vertex v of G' is replaced with 3 vertices v_a , v_b and v_c in G and there exists a set of |V'|/2 edges $\hat{E} \subseteq E'$ such that each edge $uv \notin \hat{E}$ is replaced with the path uu'v'v.

We first argue that if G admits a minimal vertex cover of size k then there exists a minimal vertex cover S for G, also with size k, that satisfies the following properties:

- 1. For a vertex v in G' exactly one of the following conditions holds: (i) $v_a, v_c \in S$ and $v_b \notin S$ or (ii) $v_a, v_c \notin S$ and $v_b \in S$
- 2. For an edge $e = uv \in E' \setminus \hat{E}$ exactly one vertex in the set $\{u', v'\}$ belongs to S

To see this, we will show that if S is a minimal vertex cover violating these properties then it is possible to locally modify S in order to satisfy then both, hence becoming the desired S.

Let S be a minimal vertex cover of G. Let us first focus on property (1). Fix some vertex v from G'. If $v_b \notin S$, then we must have $v_a, v_c \in S$, for otherwise S does not cover the edges incident in v_b . If $v_b \in S$ we cannot have that both v_a and v_c are in S, for otherwise S would not be minimal since v_b can be removed. Hence, if $v_b \in S$ at most one vertex in $\{v_a, v_c\}$ belongs to S. If this is the case, i.e., S contains v_b and exactly one vertex from $\{v_a, v_c\}$, we can modify S by replacing v_b with the vertex between v_a and v_c which is not in S. The resulting new S is a minimal vertex cover with the same cardinality which also satisfies (1).

For property (2), let us fix an edge $uv \in E' \setminus \hat{E}$, and let u, u', v', v be the corresponding path in G. We first note that at least one of the vertices u', v' must be in S, for otherwise S does not cover edge u'v'. In addition, if both belong to S then neither u nor v can belong to S, for otherwise the cover would not be minimal. In this case, however, we can replace v' with v obtaining a minimal cover with the same cardinality and satisfying (2).

In order to compute the desired clustering for U we work on the graph G_1 obtained from G by undoing the transformation $\mathcal{R}^{(1)}$ that was employed to remove triangles from the 4-regular graph G'. More precisely, $G_1 = \mathcal{R}^{(2)}(G)$. Note that $S_1 = S \cap V(G_1)$ is a minimal cover from G_1 . In fact, if $v_a(v_c)$ is in S_1 then v_b does not belong to S_1 (item 1 above) so that we cannot remove $v_a(v_c)$. Similarly, if $v_b \in S_1$ then $v_a \notin S_1$ so that we cannot remove v_b from S_1 .

Now we build a star decomposition for G_1 and then we transform it into a star decomposition for G. For every vertex $v \in S_1$ we will construct a set $D_1(v)$ consisting of the edges of the star centred at v.

Let $A = \{ \text{vertices in } S_1 \text{ of degree } 3 \text{ in } G_1 \}$ and $B = \{ \text{vertices in } S_1 \text{ of degree } 2 \text{ in } G_1 \}$. Note that A consists of the vertices of type v_a or v_c while B consists of those of type v_b .

Initially, for every $v \in S_1$ we add to $D_1(v)$ the edges that connect v to the vertices in $V(G_1) \setminus S_1$. Since S_1 is a minimal cover, after this assignment, we have $|D_1(v)| \ge 1$ for every $v \in S_1$. In addition, we also have $|D_1(v)| = 2$ for every node $v \in B$ due to the item 1 above.

We then extend the sets $D_1(v)$ by applying the following procedure:

 $E_1 \leftarrow$ edges with both endpoints in S_1 (those not yet assigned to a set $D_1(v)$) **While** there exists an edge $e = uv \in E_1$, with $|D_1(v)| = 2$ **do** Remove e from E_1 and add it to $D_1(u)$

Let $G'_1 = (S_1, E_1)$, where E_1 is the set of edges left unassigned at the end of the above procedure. Let $v \in A$. If v is isolated in G'_1 then $|D_1(v)| \ge 2$. Otherwise, if v is non-isolated, then its degree in G'_1 is 2. Thus, the non-isolated vertices in G'_1 form a collection of disjoint cycles. Hence, for each v in the cycle we add to $D_1(v)$ exactly one of the two edges incident to it. This way, we increase the cardinality of each v in the cycle by 1 so that $|D_1(v)| \ge 2$ for every $v \in S_1$, that is, they are centres of stars of size at least 2.

From the star decomposition for G_1 we can obtain a family of sets $\{D(v)\}_{v \in V}$ that will induce a star decomposition for G as follows: initially, for $v \in A \cup B$, we set $D(v) = D_1(v)$. Then, for each $e = uv \in E' \setminus \hat{E}$ we proceed as follows: if $uv \in D_1(u)$ we create a star centred at v' with edges vv'and v'u' so that $D(v') = \{vv', v'u\}$. In addition, we set $D(u) = (D(u) \setminus e) \cup \{uu'\}$.

Then, we define the clustering C of vectors in U by creating a cluster for each star in the decomposition of G and putting in the cluster the vectors corresponding to the edges of the star it represents.

Corollary 1. Let G = (V, E) be a triangle-free 3-bounded degree graph from $\mathcal{G}_{\mathcal{R}^{(1)}, \mathcal{R}^{(2)}}$, and let $U = \mathcal{R}^{(3)}(G)$ be the corresponding set of vectors obtained as described in the previous section. If G has a minimal vertex cover of size k then there is a k-clustering \mathcal{C} for U with impurity $I_{Ent}(\mathcal{C}) = 6k + 3(|U| - 2k)\log 3$.

Proof. Let C be the k-clustering given by Lemma 2 and let x and y denote the number of 2-stars and 3-stars in C, respectively. Then 2x + 3y = |U| and x + y = k, whence, x = 3k - |U| and y = |U| - 2k. Finally, from Fact 1 we have

$$I_{Ent}(\mathcal{C}) = 6x + y (6 + 3\log 3) = 6k + 3(|U| - 2k)\log 3.$$

The consequence of the last corollary is that when \mathbb{A} denotes the problem of finding the minimum vertex cover of a graphs in $\mathcal{G}_{\mathcal{R}^{(1)},\mathcal{R}^{(2)}}$ and \mathbb{B} denote the problem PMWIP_{Ent}, the reduction that maps a graphs $G = (V, E) \in \mathcal{G}_{\mathcal{R}^{(1)},\mathcal{R}^{(2)}}$ to the instance (U, k) of PMWIP_{Ent} defined by $U = \mathcal{R}^{(3)}$ satisfies property 1 in Definition 1, with $\kappa = 6k + 3(|E| - 2k) \log 3$.

Proving condition 2) of Definition 1. We now want to show that when the minimum vertex cover of the graph G has size at least $k(1 + \epsilon)$ then the impurity of every k-clustering is at least a constant times larger than $6k+3(|U|-2k)\log 3$, which is the impurity of the clustering in Corollary 1, which exists when the minimum vertex cover of G has cardinality $\leq k$. This will imply that our reduction satisfies also the second property in Definition 1.

In the following, C will denote a clustering of minimum impurity for the instance of PMWIP_{Ent} obtained via the reduction, when, for some constant $\epsilon > 0$, the size of the minimum vertex cover for G is at least $k(1 + \epsilon)$.

We will use the following notation to describe such a clustering C of minimum impurity.

- a: number of clusters in C consisting of a 3-star; we refer to these clusters as the a-group of clusters;
- b: number of clusters in C consisting of a 2-star; we refer to these clusters as the b-group of clusters;
- c: number of cluster in C consisting of a 1-star (single edge); we refer to these clusters as the c-group of clusters;
- d: number of clusters in C consisting of 2 edges without common vertex (2-matching); we refer to these clusters as the d-group of clusters;
- e: number of remaining clusters in C; we refer to these clusters as the e-group of clusters;
- q: number of edges in the e-group of clusters.

In the definitions above the letters a, b, c, d and e are used to denote both the size and the type of a group of clusters. We believe this overloaded notation helps the readability.

In Fig. 2, we summarize the impurities of small clusters significant to our analyses, according to the above grouping.

The following proposition will be useful in our analysis.

Proposition 1. Let $x \ge 2$ and let n_1, n_2 be positive integers. We have that

$$n_1(2x + x\log x) + n_2(2(x+1) + (x+1)\log(x+1)) \ge (n_1 + n_2)(2\overline{x} + \overline{x}\log\overline{x}),$$

where $\overline{x} = (n_1 x + n_2 (x+1))/(n_1 + n_2).$

Proof. It is enough to prove that

$$n_1 x \log x + n_2 (x+1) \log (x+1) \ge (n_1 + n_2) \overline{x} \log \overline{x}.$$

This inequality follows from Jensen inequality since $f(x) = x \log x$ is convex in the interval $[2, \infty]$

The next two propositions give lower bounds on the sum of the impurities of the clusters in the e-group.

Proposition 2. The total impurity of the clusters in the e-group is at least $2q + (q/e)\log(q/e)$.

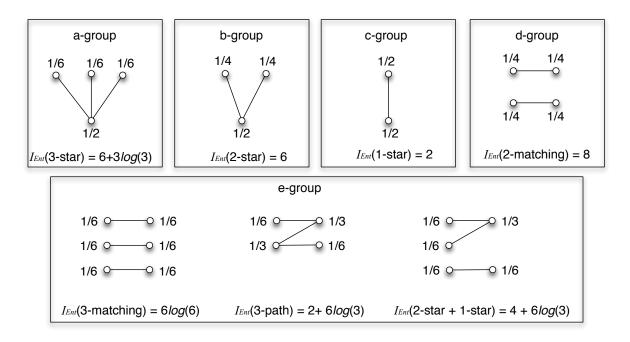


Figure 2: The types of *small* clusters C of edges, $|C| \leq 3$ that we can have from a triangle-free graph, together with the corresponding impurity $I_{Ent}(C)$. The numbers on the vertices form the distribution **q** such that $I_{Ent}(C) = 2|C| \cdot H(\mathbf{q})$ as in (6).

Proof. Let C_1, \ldots, C_e be the clusters in the *e*-group. Note that each one of these clusters has cardinality ≥ 3 . Let $p = \lfloor q/e \rfloor$. Then, we have $p \geq 3$. Suppose that there exist clusters C_i, C_j such that $|C_i| = x$ and $|C_j| = y$ with y > x + 1. Let C'_i be an (x + 1)-star and C'_j be a (y - 1)-star, then we have

$$I_{Ent}(C_i) + I_{Ent}(C_j) \geq 2x + x \log x + 2y + y \log y$$

$$\geq 2(x+1) + (x+1) \log(x+1) + 2(y-1) + (y-1) \log(y-1)$$

$$\geq I_{Ent}(C'_i) + I_{Ent}(C'_j),$$

where the first inequality follows from Lemma 1, the second inequality holds true for each $3 \le x \le y - 2$ and the last inequality follows from Fact 1.

The above inequality says that if we replace C_i, C_j with C'_i, C'_j , the impurity of the resulting set of *e* clusters is not larger than the impurity of the original *e*-group. Moreover, the total number of edges has not changed. By repeated application of such a replacement we eventually obtain a group of *e* clusters $\tilde{C} = \{\tilde{C}_1, \ldots, \tilde{C}_e\}$ each of cardinality *p* or *p* + 1 and containing in total *e* edges and such that $\sum_{i=1} I_{Ent}(C_i) \geq \sum_{i=1} I_{Ent}(\tilde{C}_i)$. In particular, the total impurity of such clusters is not larger than the total impurity of the original *e* clusters. Note that these new *e* clusters need not exist and are only used here for the sake of the analysis.

Let n_1 be the number of clusters in $\tilde{\mathcal{C}}$ with p edges and n_2 be the number of clusters in $\tilde{\mathcal{C}}$ with p+1 edges and let $\overline{p} = \frac{n_1 p + n_2(p+1)}{n_1 + n_2}$. Then, $q = n_1 p + n_2(p+1)$ and $e = n_1 + n_2$, hence $\overline{p} = q/e$.

Finally, by applying Proposition 1, we have the desired result:

$$\sum_{j=1}^{e} I_{Ent}(C_i) \geq \sum_{j=1}^{e} I_{Ent}(\tilde{C}_i)$$

= $n_1(2p + p\log p) + n_2(2(p+1) + (p+1)\log(p+1))$
 $\geq (n_1 + n_2)(2\overline{p} + \overline{p}\log\overline{p}) = 2q + \frac{q}{e}\log\frac{q}{e}.$

The following fact that can be proved by inspecting a few cases will be useful.

Fact 6. If a cluster C has 3 edges and it is neither a 3-star nor a triangle then its impurity is at least $2 + 6 \log 3$

Proposition 3. If q < 4e then the total impurity of the clusters in the e-group is lower bounded by $16(q - 3e) + (4e - q) \times (2 + 6 \log 3)$

Proof. We first consider the case where every cluster in the *e*-group has either 3 or 4 edges. Let x and y be the number of clusters with 3 and 4 edges, respectively. Since x + y = e and 3x + 4y = q we get that x = 4e - q and y = q - 3e. It follows from Lemma 1 that the impurity of a cluster with 4 edges is at least 16. Moreover, since triangles and 3-stars are not allowed in a *e*-group, it follows from Fact 6 that the impurity of a cluster with 3-edges is at least $(2 + 6 \log 3)$. Thus, in the case under consideration, the total impurity is lower bounded by $16(q - 3e) + (4e - q) \times (2 + 6 \log 3)$.

Thus, it suffices to show that the *e*-group with q edges and minimum impurity has only clusters with 3 or 4 edges. Let us assume for the sake a contradiction that the *e*-group with minimum impurity has one cluster C with r > 4 edges. In this case, there exist r - 3 clusters of cardinality 3 in the *e*-group, for otherwise the average cardinality would be ≥ 4 , violating the assumption q < 4e. Let $D_1, \ldots D_{r-3}$ be these clusters. Moreover, let C' be a 3-path structure and $D'_1, \ldots D'_{r-3}$ be 4-stars. We have

$$|C'| + \sum_{j=1}^{r-3} |D'_j| = 3 + 4(r-3) = r + 3(r-3) = |C| + \sum_{j=1}^{r-3} |D_j|.$$
 (14)

Furthermore, by definition clusters of cardinality 3 that are in the *e*-group are not 3-stars. Thus, by Fact 6 we have that for each i = 1, ..., r - 3, it holds that $I_{Ent}(D_i) \ge 2 + 6 \log 3$ and by Lemma 1, it holds that $I_{Ent}(C) \ge 2r + r \log r$. Then

$$I_{Ent}(C) + \sum_{j=1}^{r-3} I_{Ent}(D_j) \geq 2r + r \log r + (r-3) (2 + 6 \log 3)$$

> $(2 + 6 \log 3) + 16(r-3)$
= $I_{Ent}(C') + \sum_{i=1}^{r-3} I_{Ent}(D'_i),$

where the second inequality holds for each r > 4.

The above inequalities together with (14) say that if we replace $C, D_1, \ldots D_{r-3}$ with $C', D'_1, \ldots D'_{r-3}$, the impurity of the resulting set of e clusters is smaller than the impurity of the original set of e clusters. Moreover, the total number of edges does not change. Thus, we reach a contradiction, which establishes the proof.

Proposition 4. If the minimum vertex cover for G has size at least $k(1 + \epsilon)$ then the following inequality holds: $c + d + q \ge k\epsilon/2$.

Proof. If it does not hold we could construct a vertex cover of size smaller than $k(1+\epsilon)$ by selecting a vertices to cover the edges of the 3-stars, b vertices to cover the edges of the 2-stars and one vertex per edge of the other clusters. The number of edges in these other clusters is c + 2d + q. Hence, we must have $a + b + c + 2d + q \ge k(1+\epsilon)$. Since $a + b \le k$ we conclude that $c + d + 2q \ge k\epsilon$, so that $c + d + q \ge c/2 + d/2 + q \ge k\epsilon/2$

Let $\mathcal{C}^{(k)}$ denote the k-clustering only consisting of 2-stars and 3-stars described in Lemma 2 and Corollary 1, which exists when the minimum vertex cover of the graph G has size $\leq k$.

We will now show that, if the minimum size of a vertex cover for G is at least $k(1+\epsilon)$ then the impurity of the minimum impurity clustering C (for the instance obtained via the reduction) is at least a constant factor larger than the impurity of $C^{(k)}$.

Lemma 3. Let G = (V, E) be a triangle-free and 3-bounded degree graph and let $U = \mathcal{R}^{(3)}(G)$ be the corresponding set of vectors obtained as described in section 4.1 above. If every vertex cover in G has size $\geq k(1 + \epsilon)$, then there exists a constant $\eta > 0$ such that $I_{Ent}(\mathcal{C}) \geq \kappa(1 + \eta)$, where $\kappa = I_{Ent}(\mathcal{C}^{(k)})$.

Proof. Let E be the sum of the impurities of the clusters in the *e*-group. Then, the impurity of C is given by

$$I_{Ent}(\mathcal{C}) = (6+3\log 3)a + 2c + 8d + 6b + E \tag{15}$$

Since a + b + c + d + e = k and 3a + 2b + c + 2d + q = |U| we get that a = c + 2e + |U| - q - 2kand b = 3k - |U| - 2c - d - 3e + q. Replacing a and b in the righthand side of 15 we get that

$$I_{Ent}(\mathcal{C}) \ge (3\log 3 - 4)c + 2d + (6\log 3 - 6)e - (3\log 3)q + (3\log 3)|U| + (6 - 6\log 3)k + E$$

Thus,

$$I_{Ent}(\mathcal{C}) - I_{Ent}(\mathcal{C}^{(k)}) \ge (3\log 3 - 4)c + 2d + (6\log 3 - 6)e - (3\log 3)q + E$$

Let $\Delta = I_{Ent}(\mathcal{C}) - I_{Ent}(\mathcal{C}^{(k)})$. We split the analysis into two cases according to whether $\overline{p} = q/e \ge 4$ or $\overline{p} = q/e \le 4$

Case 1 $\overline{p} \geq 4$. In this case,

$$\Delta \geq (3\log 3 - 4)c + 2d + [(\log \overline{p} + 2 - 3\log 3)\overline{p} + 6(\log 3 - 1)]e$$
(16)

$$= (3\log 3 - 4)c + 2d + (\log \overline{p} + (2 - 3\log 3) + \frac{6(\log 3 - 1)}{\overline{p}})q$$
(17)

$$\geq (2.5 - 1.5 \log 3)(c + d + q) \tag{18}$$

$$\geq (1.25 - 0.75 \log 3) k\epsilon \tag{19}$$

where the inequality (17)-(18) holds because function $f(x) = (2 - 3 \log 3) + \log x + 6(\log 3 - 1)/x$ is increasing in the interval $[4, \infty]$ and $f(4) = 2.5 - 1.5 \log 3$. The last inequality follows from Proposition 4.

Case 2 $\overline{p} < 4$. We have that

$$\Delta \geq (3\log 3 - 4)c + 2d - (3\log 3)q + (6\log 3 - 6)e + E$$
(20)

 $\geq (3\log 3 - 4)c + 2d + (30\log 3 - 46)e + (14 - 9\log 3)q$ ⁽²¹⁾

$$\geq (3\log 3 - 4)c + 2d + (2.5 - 1.5\log 3)q \tag{22}$$

 $\geq (2.5 - 1.5 \log 3)(c + d + q) \tag{23}$

$$\geq (1.25 - 0.75 \log 3) k\epsilon \tag{24}$$

where (21) follows from (20) due to the lower bound on E given by Proposition 3, (22) follows from (21) because q < 4e and the last inequality follows from Proposition 4.

From the inequalities (16)-(19) and (20)-(24) we have

$$\frac{I_{Ent}(\mathcal{C})}{I_{Ent}(\mathcal{C}^{(k)})} \ge \frac{I_{Ent}(\mathcal{C}^{(k)}) + (1.25 - 0.75\log 3)k\epsilon}{I_{Ent}(\mathcal{C}^{(k)})} \ge 1 + \frac{(1.25 - 0.75\log 3)\epsilon}{(6 + 3\log 3)},$$

where the last inequality follows because $I_{Ent}(\mathcal{C}^{(k)}) = 6k + 3(|U| - 2k)\log 3$ and $|U| \leq 3k$ so that $I_{Ent}(\mathcal{C}^{(k)}) \geq (6 + 3\log 3)k$. Thus, we can set

$$\eta = \frac{(1.25 - 0.75 \log 3)\epsilon}{(6 + 3 \log 3)},\tag{25}$$

Proof of Theorem 1. Let $0 < \beta < \beta'$ be the constant in Theorem 3 and $\epsilon = \frac{\beta'}{\beta} - 1$.

By the previous lemma, there exists an $\eta = \eta(\epsilon) > 0$ (as in (25)) such that for every graph $G = (V, E) \in \mathcal{G}_{\mathcal{R}^{(1)}, \mathcal{R}^{(2)}}$ and k, the set of vectors $U = \mathcal{R}^{(3)}(G)$ produced according to our reduction is such that if G has a vertex cover of size $\leq k$ then U has a k-clustering of impurity $\leq \kappa$ and if all vertex covers of G have size $> (1 + \epsilon)k$ then all k-clustering of U have impurity $> (1 + \eta)\kappa$, where $\kappa = 6k + 3(|E| - 2k) \log 3$

This, together with Theorem 3 implies that the η -GAP-PMWIP_{Ent} is NP-hard. Hence, by Fact 4, if $P \neq NP$ there is no polynomial time $(1 + \eta)$ -approximation algorithm for PMWIP_{Ent}.

The same arguments in our reduction can also be used to show the inapproximability of instances where all vectors have ℓ_1 norm equal to any constant value, and in particular 1, i.e., the case where PMWIP_{Ent} corresponds to MTC_{KL}. In summary we have the following.

Corollary 2. MCT_{KL} is APX-Hard.

5 Conclusions

In this paper we proved that $PMWIP_{Ent}$ is APX-Hard even for the case where all vectors have the same ℓ_1 -norm. This result implies that MTC_{KL} is APX-Hard resolving a question that remained open in previous work [10, 2]. Since there exist logarithmic approximations for both $PMWIP_{Ent}$ and MTC_{KL} (under different parameters) [10, 13], the main question that remains open is whether a constant approximation factor for these problems is possible.

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Proof of Theorem 3

Proof. The proof consists in showing that we can obtain a gap preserving reduction from ϵ -GAP-MINVC-4 by composition of the function $\mathcal{R}^{(1)}$ and $\mathcal{R}^{(2)}$ defined in Section 4.1.

Let G' = (V', E') be a 4-regular graph. Let n = |V'| and m = |E'|. Hence m = 2n. Let $H = (V_H, E_H) = \mathcal{R}^{(1)}(G')$. By definition, H has bounded degree 4 and it is also triangle-free. Let $N = |V_H|$ and $M = |E_H|$. We have N = 3n and M = 4n.

With reference to the definition of the function $\mathcal{R}^{(1)}$ in the Section 4.1, let \hat{E} be the set of n edges from E' such that the graph $\hat{G} = (\hat{V}, \hat{E})$ induced by \hat{E} is bipartite and H is obtained from G' by a double subdivision of the edges in $E' \setminus \hat{E}$.

Observation 1. Let $A' \subseteq V'$ be a minimal vertex cover of G'. Then, $A_H = A' \cup \bigcup_{e=(u,v) \in E' \setminus \hat{E}} \{f(e)\}$ with

$$f(e) = \begin{cases} v' & u \in A' \\ u' & u \notin A' \end{cases}$$

is a minimal vertex cover of H of size |A'| + n.

Observation 2. Let A_H be a minimum size vertex cover of H. Then, for each $e = (u, v) \in E' \setminus \hat{E}$ we have that if both u' and v' are in A_H then neither u nor v are in A_H , for otherwise, the minimality of A_H would be violated. Let $\tilde{E} = E' \setminus \hat{E}$. Then, the set

$$A'_{H} = \left(A_{H} \setminus \bigcup_{e=(u,v)\in \tilde{E}|u',v'\in A_{H}} \{u',v'\}\right) \cup \bigcup_{e=(u,v)\in \tilde{E}|u',v'\in A_{H}} \{u,v'\}$$

is a vertex cover of H of size equal to $|A_H|$, hence minimum.

Notice that for every edge $e = (u, v) \in \tilde{E}$ exactly one vertex between u' and v' and at least one between u, v is contained in A'_H . Therefore $A' = A'_H \cap V'$ is a vertex cover of G' of size $|A'_H| - n$. Moreover, A' is a minimum size vertex cover of G' for otherwise (by Observation 1) there would be a vertex cover of H of size smaller than $|A'| + n = |A_H|$.

Putting together the above observations, we have the following.

Claim 1. For $0 < \alpha < \alpha'$, if G' has a (minimum) vertex cover of size αn then H has a vertex cover of size $(\alpha + 1)n = \frac{\alpha+1}{3}N$; and if all vertex covers of G' have size $> \alpha' n$ then every vertex cover of H has size $> (\alpha' + 1)n = \frac{\alpha'+1}{3}N$.

Now let $G = (V, E) = \mathcal{R}^{(2)}(H)$. Since H has n = N/3 vertices of degree 4 and G is obtained from H by adding, for each vertex of degree 4 in H, two new vertices and two new edges, we have that $|V| = |V_H| + 2n = 5n = (5/3)N$ and $|E| = |E_H| + 2n = 6n = 2N = (6/5)|V|$.

Observation 3. Let C_H be a vertex cover of H. Let $C_H(4)$ be the set of vertices of H which have degree 4 and are in C_H . Let $U_H(4)$ be the set of vertices of H of degree 4 which are not in C_H . Then there is a vertex cover C of G defined by

$$C = (C_H \setminus C_H(4)) \cup \bigcup_{v \in C_H(4)} \{v_a, v_c\} \cup \bigcup_{v \in U_H(4)} \{v_b\},\$$

and $|C| = |C_H| - |C_H(4)| + 2|C_H(4)| + |U_H(4)| = |C_H| + |C_H(4)| + |U_H(4)| = |C_H| + N/3$, since the number of vertices in H of degree 4 is equal to N/3.

Observation 4. Let C be a minimum size vertex cover of G. Notice that for each $v \in V_H$ of degree 4 either $|\{v_a, v_b, v_c\} \cap C| = 2$ or $\{v_a, v_b, v_c\} \cap C = \{v_b\}$. Then, let $V_H(4)$ be the set of vertices in V_H of degree 4. We have that, setting

$$C^{-} = \bigcup_{\substack{v \in V_{H}(4) \\ |\{v_{a}, v_{b}, v_{c}\} \cap C| = 2}} (\{v_{a}, v_{b}, v_{c}\} \cap C) \cup \bigcup_{\substack{v \in V_{H}(4) \\ \{v_{a}, v_{b}, v_{c}\} \cap C = \{v_{b}\}}} \{v_{b}\}$$

and

$$C^{+} = \bigcup_{\substack{v \in V_{H}(4) \\ |\{v_{a}, v_{b}, v_{c}\} \cap C| = 2}} \{v\},\$$

the set of vertices

$$C_H = (C \setminus C^-) \cup C^+$$

is a vertex cover of H of size $|C_H| = |C| - |V_H(4)| = |C| - N/3$.

By using the same argument employed before (counter-positive) if all vertex covers of H have size > cN, for some constant 0 < c < 1, then every vertex cover of G have size > (c + 1/3)N.

Putting together Claim 1 and Observations 3 and 4 we have the following.

Claim 2. If G' has a (minimum) vertex cover of size αn then G has a vertex cover of size $\frac{\alpha+2}{3}N = \frac{\alpha+2}{5}|V|$. Moreover, if all vertex covers of G' have size $> \alpha' n$ then every vertex cover of G has size $> \frac{\alpha'+2}{3}N = \frac{\alpha'+2}{5}|V|$.

Fix $\beta = \frac{\alpha+2}{3}$ and $\beta' = \frac{\alpha'+2}{3}$, with α, α' from Theorem 2. By Claim 2 and Theorem 2, we have that there are constants $0 < \beta < \beta' < 1$ such that it is *NP*-hard to decide whether a triangle-free 3-bounded degree graphs G = (V, E) in family $\mathcal{G}_{\mathcal{R}^{(1)}, \mathcal{R}^{(2)}}$ has a vertex cover of size $\beta |V|$ or all vertex covers of *G* have size $> \beta' |V|$. The proof is complete.