Minimization of Gini impurity via connections with the \( k \)-means problem

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Abstract

The Gini impurity is one of the measures used to select attribute in Decision Trees/Random Forest construction. In this note we discuss connections between the problem of computing the partition with minimum Weighted Gini impurity and the \( k \)-means clustering problem. Based on these connections we show that the computation of the partition with minimum Weighted Gini is a NP-Complete problem and we also discuss how to obtain new algorithms with provable approximation for the Gini Minimization problem.
1 Introduction

Decision Trees and Random Forests are among the most popular methods for classification tasks. It is widely known that decision trees, specially small ones, are easy to interpret while random forest usually yield to more stable/accurate classifications.

A key decision during the construction of these structures is the selection of the attribute that is used for branching at each node. The standard approach for this selection is to evaluate the ability of each attribute to generate 'pure' partitions, that is, partitions in which each branch is very homogeneous with respect to the class distribution of its examples. To measure how impure each branch is, impurity measures are often employed. An impurity measure maps a vector $u = (u_1, \ldots, u_k)$, counting how many examples of each class we have in a node (branch), into a non-negative scalar. Arguably, two of the most classical impurity measures are the Gini impurity $i_{\text{Gini}}(u) = \sum_{i=1}^{k} u_i \parallel u \parallel_1 \left(1 - \frac{u_i}{\parallel u \parallel_1}\right)$, which is used in the CART package [3], and the Entropy impurity $i_{\text{Ent}}(u) = - \sum_{i=1}^{k} u_i \parallel u \parallel_1 \log \left(\frac{u_i}{\parallel u \parallel_1}\right)$, that along with its variants is used in the C4.5 decision tree inducer [8].

Given an attribute, the goal is then to find a split for the attribute values that induces a partition of the set of examples with minimum weighted impurity, where the weights are given by the number of examples that lie into each of the branches.

Here, we discuss connections between the problem of computing the partition with minimum weighted Gini and the $k$-means clustering problem.

2 Connections between Gini minimization and $k$-means clustering

For a vector $v$ where all components are non-negative the weighted Gini impurity $Gini(v)$ is defined as $Gini(v) = \|v\|_1 \cdot i_{\text{Gini}}(v)$. Let $A$ be a nominal attribute that may take $n$ possible values $a_1, \ldots, a_n$. The $k$-ary Partition with Minimum Weighted Gini Problem ($k$-PMWGP) can be described abstractly as follows. We are given a collection of $n$ vectors $V \subset \mathbb{R}^d$, where the $i$th component of the $j$th vector counts the number of examples in class $i$ for which the attribute $A$ has value $a_j$. The goal is to find a partition $P$ of $V$ into $k$ disjoint groups of vectors $V_1, \ldots, V_k$ so as to minimize the sum of the weighted Gini impurities

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

Recently, we obtained simple constant approximation algorithms for this problem: an $O(n \log n + nd)$ time 2-approximation for the case where $k = 2$ [7] and a linear time 3-approximation for arbitrary $k$ [5]. In fact these papers also handle a more general class of impurity measures that includes the Entropy impurity. The complexity of ($k$-PMWGP) remained open.

\footnote{In the original definition an impurity measure maps a vector of probabilities into a non-negative scalar.}
A problem that is equivalent to the above problem from the perspective of optimality but it is different from the perspective of approximation is the problem of finding the partition $P$ of $V$ into $k$ groups that minimizes

$$Gini(P) - \sum_{v \in V} Gini(v).$$

(2)

Using concavity properties of Gini one can prove that the above expression is always non-negative.

An $\alpha$-approximation with respect to goal (2) implies an $\alpha$-approximation with respect to goal (1) but the converse is not necessarily true, so that approximations with respect to goal (2) are stronger.

In the geometric $k$-means problem we are given a set of vectors $V$ in $\mathbb{R}^d$ and the goal is to find a partition $P$ of $V$ into $k$ groups $V_1, \ldots, V_k$ and set of $k$ centers $c_1, \ldots, c_k$ in $\mathbb{R}^d$ such that

$$Cost_{KM}(P) = \sum_{i=1}^{k} \sum_{v \in V_i} \|v - c_i\|^2_2$$

is minimized.

It is well known that if $U$ is a set of vectors then the vector $c$ for which $\sum_{v \in U} \|v - c\|^2_2$ is minimum is the centroid of $U$, that is, $c = (\sum_{v \in U} v)/|U|$.

We argue that the following connections between $k$-PMWGP and $k$-means hold:

C1 Let $V$ be an instance of $k$-means where all vectors have the same $\ell_1$ norm. If $P$ is an optimal partition for instance $V$ then $P$ is also an optimal partition for instance $V$ of $k$-PMWGP.

C2 there exists a pseudo-polynomial time reduction from $k$-PMWGP to the geometric $k$-means problem.

The key observation for establishing C1 and C2 is the following lemma.

**Lemma 1.** Let $X$ be a set of vectors, all of them with $\ell_1$ norm equal to $L$. Then,

$$Gini\left(\sum_{v \in X} v\right) - \sum_{v \in X} Gini(v) = L \times \left(\sum_{v \in X} \|v - c\|^2_2\right),$$

where $c$ is the centroid of the set of vectors in $X$.

**Proof.** Let $u = \sum_{v \in X} v$. We have that

$$Gini(u) - \sum_{v \in X} Gini(v) = \|u\|^1_1 \left(\sum_{i=1}^{d} \left(1 - \frac{u_i}{\|u\|^1_1}\right) \left(\frac{u_i}{\|u\|^1_1}\right) - \sum_{v \in X} \sum_{i=1}^{d} \|v\|^1_1 \left(1 - \frac{v_i}{\|v\|^1_1}\right) \left(\frac{v_i}{\|v\|^1_1}\right)\right)$$

On the other hand,

$$\sum_{v \in X} \|v - c\|^2_2 = \sum_{i=1}^{d} \sum_{v \in X} (v_i - c_i)^2$$

Thus, it suffices to show that for any $i$

$$\|u\|^1_1 \left(1 - \frac{u_i}{\|u\|^1_1}\right) \left(\frac{u_i}{\|u\|^1_1}\right) - \sum_{v \in X} \|v\|^1_1 \left(1 - \frac{v_i}{\|v\|^1_1}\right) \left(\frac{v_i}{\|v\|^1_1}\right) = L \left(\sum_{v \in X} (v_i - c_i)^2\right)$$

Therefore, the key lemma is established.
The left side is equal to
\[ u_i - \frac{(u_i)^2}{\|u\|_1} - \left( \sum_{v \in X} v_i - |X| \right) \frac{\sum_{v \in X} (v_i)^2}{\|u\|_1} = \frac{|X| \sum_{v \in X} (v_i)^2}{\|u\|_1} - \frac{(u_i)^2}{\|u\|_1} = \frac{\sum_{v \in X} (v_i)^2}{L} - \frac{(u_i)^2}{L|X|} \]

Moreover, the righthand side is equal to
\[ \sum_{v \in X} (v_i)^2 - \frac{(\sum_{v \in X} v_i)^2}{|X|} = \sum_{v \in X} (v_i)^2 - \frac{(u_i)^2}{|X|}, \]
which established the lemma.

We should note that the result presented in the previous lemma is mentioned in the appendix of [4] where the Gini index is discussed.

The connection C1 is a direct consequence of Lemma 1 since it implies that for all \( k \)-partitions \( P \) of \( V \)
\[ \text{Gini}(P) = L \cdot \text{Cost}_{KM}(P) + \sum_{v \in V} \text{Gini}(v) \]

From the connection C1 and the hardness of geometric \( k \)-means established in [2] we obtain:

**Theorem 1.** The Partition with Minimum Weighted Gini Problem (PMWGP) is NP-Complete with respect to goal (1) and APX-Hard with respect to goal (2).

**Proof.** The result follows from [2], where a polynomial time reduction from the vertex cover problem on triangle free graphs to the \( k \)-means problem is presented. In this reduction, given a graph \( G = (V, E) \), every edge \( e \) in \( E \) is mapped into a vector \( v \) in \( \mathbb{R}^{|V|} \) where the \( i \)-th component \( v_i \) is 1 if \( i \) is incident on \( e \) and it is 0, otherwise. It is proved that if the minimum vertex cover of \( G \) has size \( k \) then the optimum cost of the corresponding \( k \)-means problem is at most \( |E| - k \) and if the minimum vertex cover has size at least \((1 + \epsilon)k\) then the minimum cost is at least \(|E| - (1 - \Omega(\epsilon))k\).

Our result follows from Lemma 1 and from the fact that in the instance of \( k \)-means above described all vectors have \( \ell_1 \) norm equals 2.

With regards to the connection C2, let \( V \) be an input of \( k \)-PMWGP and let \( V' \) be an instance of \( k \)-means obtained from \( V \) as follows: for each vector \( v \in V \) we add to the input set \( V' \) exactly \( \|v\|_1 \) copies of vector \( v' = v/\|v\|_1 \). Using Lemma 1 and also the fact that in any optimal solution for \( k \)-means identical vectors are in the same partition, we conclude that the optimum value of \( V \) and \( V' \) differ by exactly \( \sum_{v \in V} \text{Gini}(v) \). Note that instance \( V' \) is obtained from \( V \) in pseudo-polytime.

From this reduction one we can obtain new algorithms for \( k \)-PMWGP with provable approximation. As an example, we discuss how to obtain a PTAS for \( k \)-PMWGP with respect to the objective function (2) when \( k \) is fixed. First, in our reduction, we keep each distinct vector and its multiplicity rather than all the \( \sum_{v \in V} \|v\|_1 \) vectors of instance \( V' \). Thus, we can construct the instance \( V' \) from \( V \) in polytime. Next, we run over instance \( V' \) an adapted version of the recursive PTAS for \( k \)-means proposed in [6]. This version efficiently handles copies of the same vector and it is explained referring to the presentation of the PTAS that is given in Figure 1 of [1].

Let \( W = \sum_{v \in V} \|v\|_1 \). The adapted version is as follows:

1. The set of vectors in \( V' \) is represented using the distinct vectors and its multiplicities.
2. In the step 6 of the algorithm described in Figure 1 of [1] a constant number of vectors is sampled from a set of at most \( n \) vectors. In our adaptation we sample from a set of \( W \) vectors, with at most \( n \) of them being distinct. This incurs an extra \( O(\log W) \) factor to the running time.

3. At Step 12 of the same Figure one needs to compute, from a set of vectors \( R \), the \( |R|/2 \) closest vectors to a given set of centroids \( C \). Since this computation can be performed with time complexity proportional to the number of distinct vectors in \( R \), rather than in \( O(|R|) \) time, we do not incur any additional cost.

This adapted version also incurs an extra factor of \( O(\log(W)^k) \) with respect to the original one (executed over \( n \) vectors) due to the number of nodes in the recursion tree. Thus, it runs in polynomial time when \( k \) is fixed. Without efficiently handling the copies we would have a pseudo-polynomial time approximation scheme.

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