Cost Balancing Clustering with Unknown Values using Subspace Clustering

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***Abstract*—Clustering is an important technique in machine learning and data mining but traditional distance-based clustering algorithms may have difficulties when values are missing in the dataset. We propose a cost-sensitive subspace clustering model that determines which unknown features should be provided by the user in order to classify a point to its cluster. We then evaluate this model using real-world datasets, and show that it performs comparably to k-means but at a lower cost.**

***Index Terms*—clustering, subspace clustering, machine learning**

I. Introduction

Clustering is one of the fundamental problems in machine learning with many applications in the real world. Most clustering techniques measure the 'likeness' of two points through some distance or proximity metric. This requires all values for every attribute to be known, but this is not always possible as databases are often 'dirty' or the value has not been provided by the user yet. One way to combat this is to have a user input all missing values, but this may be too costly or impossible (for example, confidential information). On the other hand, using a machine learning model to impute the unknown values may produce too many artifacts.

In this paper, we propose a hybrid approach; we will train a model with a complete dataset (no missing values) to learn the boundary between the clusters. Then, given a point with unknown values, this model produces a schedule of features that the user should provide considering the costs associated with updating each value. In other words, the model will guide the users about which features they need to prioritize in order to most accurately find its cluster. This can be used in prognosis to see how similar cases went with minimal costs, or dynamically choose survey questions to find similar consumers.

Learning methods where wide-variety of costs are considered are often referred to as cost-sensitive learning [6] [7], while authors of [8] define methods that consider specifically the cost of finding feature values as test-cost sensitive learning. The main contribution of this paper is to extend such framework, which primarily deals with classifications, to clustering. This is done through two steps:

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- Building a cost considering model which both forms the clusters and stores informations on the boundaries of the clusters.
- Using the above model to suggest order of feature updates and classify points into the preformed clusters.

A. Approach and framework

We begin by assuming the data (represented as feature vectors) is in a metric space and that points that are similar in nature are also close in distance. We further assume that any value of feature f_i may be missing, but can be provided by the user at cost $\mathfrak{C}(f_i)$. For any point p, let $k(p)$ and $u(p)$ be the known and unknown features of p. Finally, we will normalize all values to be between $[0, 1]$, including $\mathfrak{C}(f)$.

In our setting, distance-based clustering becomes problematic. Most obviously, it may be impossible to know *which* centroid is closest to a feature vector with missing values. For example, consider two centroids $c_1 = (1, 0)$ and $c_2 = (2, 2)$ and a point with missing y-coordinate $p = (1, ?)$; we cannot say whether p is closer to c_1 or c_2. However, if we had a conditional dependency of the distribution of the y-coordinate given $x = 1$, then the probability of which cluster p belongs to is not uniform. Precisely, at $p = (1, 5/4)$, p is equidistance to c_1 and c_2; thus if $\Pr(y < 5/4|x = 1) > \Pr(y > 5/4|x = 1)$, then p is more likely to be close to c_1, and vice versa. This is the key idea of subspace clustering.

Subspace clustering algorithms attempt to cluster high dimensional data by projecting different partitions to different subspaces; this allows clustering algorithms to search locally. These algorithms address the *curse of dimensionality* differently from feature selection: rather that judging which features are redundant globally, they attempt to judge if certain features are redundant *conditioned* on being in some subspace [1].

II. Building the model

In this section, we will describe our proposed tree-based unsupervised model: the Cost Balancing Clustering Tree (CBCT). The basic outline follows the well-known decision tree model [3]. Given a dataset D, we choose the 'best' feature and splitting value at each level greedily and recursively partition D until some stopping criteria. This can also be seen

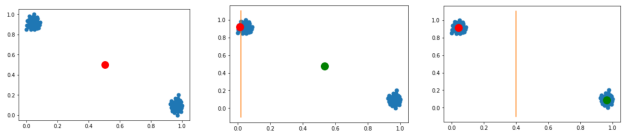
as an extension to the CLusterTree model of [2] which further considers the cost of each split.

A. Reward metric

Given a set of data points D, define c_D as its centroid and δ_D as the average distance between the points in D and c_D. Define a *boundary* to be a pair (f, v), where f is a feature and v is a value in the domain of that feature, and the left partition induced by $b = (f, v)$ to be

$$D_{(b,l)} = \{p | p \in D, p[f] \leq v\}.$$

Finally, the right parition induced by b is $D_{(b,r)} = D \setminus D_{(b,l)}$. We will quantify a boundary b as a good split if the partitions induced by b have lower average distance to their respective centroids compared to the unpartitioned data.



(a) no partition (b) $b_1 = (x, 0.02)$ (c) $b_2 = (x, 0.4)$

Fig. 1: Example of partitions induced by different boundaries

Figure 1 shows a simple dataset with two example boundaries: $D_{(b_1,l)}$ has very few elements very close to $c_{(b_1,l)}$ but $D_{(b_1,r)}$ has many elements very far from $c_{(b_1,r)}$; with b_2, both partitions are close to their respective centroids. Intuitively, b_2 seems to be a better split as the partitions that are induced are uniformly 'tighter'.

Formally, we define the reward of splitting on a boundary b as

$$R(D, b) = p_l(\delta_D - \delta_{(b,l)}) + p_r(\delta_D - \delta_{(b,r)})$$

where $p_* = |D_{(b,*)}|/|D|$. Since $p_l + p_r = 1$, we can simplify the above as $R(D, b) = \delta_D - (p_l\delta_{(b,l)} + p_r\delta_{(b,r)})$.

The reward function is essentially a weighted sum of the decrease in average distance to the centroids induced by a boundary b. The term $\delta_D - \delta_*$ measures the decrease in distance while p_* is the ratio of the number of points in that partition. For $b = (f, v)$, the weigthed sum $p_l(\delta_D - \delta_{(b,l)}) + p_r(\delta_D - \delta_{(b,r)})$ can also be viewed as the *expected* decrease in distance from knowing whether or not $p[f] > v$ as p_l and p_r are estimates of the probability of being in each partition. Finally, we define the *score* of a split as the discounted reward:

$$S(D, b) = R(D, b) - \alpha\mathfrak{C}(f)R(D, b) = R(D, b)(1 - \alpha\mathfrak{C}(f)),$$

where $\alpha \geq 0$ is a hyper-parameter and $\mathfrak{C}(f)$ is the cost of finding the value of feature f.

B. Algorithm for building CBCT

We finally outline a greedy algorithm to build a CBCT given training set D. At each node, we enumerate through the features and evenly spaced values from the domain of each feature in order to find a boundary b that maximizes the score $S(D, b)$. We stop when the number of data points are less than some threshold τ (although other stopping criteria are possible).

In terms of complexity, at each node n, we examine $|D_n|$ elements $|\text{features}(D)||\ell|$ times, where $|\ell|$ is the number of evenly spaced values. At any level, the total number of points in all nodes at that level cannot exceed $|D|$. For a tree of height h, this gives us the upper bound of $O(h|\text{features}(D)||\ell||D|)$. Also note that after using a feature f in a split, we set $\mathfrak{C}(f) = 0$ for descendent nodes.

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build_CBCT(D)
Input: D - dataset
Output: T - resulting tree

1) if $|D| \leq \tau$: return $T = (D, -, -)$
2) for $f \in$ features(D):
   a) $\ell = \text{linspace}(f_{min}, f_{max})$
   b) for $v \in \ell$:
      i) $b_{(f,v)} := (f, v)$
      ii) compute $S(D, b_{(f,v)})$
3) $b_{max} = \arg\max_b S(D, b)$
4) set $\mathfrak{C}(b_{max}.f) := 0$
5) $T_l :=$ build_CBCT$(D_{(b_{max},l)})$
6) $T_r :=$ build_CBCT$(D_{(b_{max},r)})$

III. Guiding the User

Given a point p with $u(p) \neq \phi$ (recall that $k(p)$ and $u(p)$ are known and unknown features of p resp.) and a preconstructed CBCT T, this section will outline the various usages for T to find different information on p.

A. Suggesting next update

From the unknown features, we want to suggest what feature to update next such that if we were to stop updating the tuple after, we would have the best approximation of the remaining unknown features as a function of the known features. Since CBCT places the features that decreases the average distances to centroids (balanced with the cost) the most at the top, we can traverse down T using the known features and stop at the first unknown feature: this is the feature that the model will suggest the user update next.

However, p itself may not follow the hypothesis learned by T and the model should inform this to the user. In particular, traversing down T is essentially finding the cluster that p belongs to; the model has little confidence of its suggestion if p is dislike the found cluster. For some node n, we can define a similarity score of p to the points in that node D_n as

$$\mathscr{S}(D_n, p) = \left(\frac{1}{|D_n|} \sum_{p' \in D_n} \sqrt{\sum_{f \in k(p)} (p'[f] - p[f])^2} \right)^{-1}$$

which is the recipirocal of the average (L2) distance between p and the points of D_n, using only the known features. This value is higher when the distance is smaller (i.e. p is similar to

points D_n). If the distance is zero or there is no known feature, $\mathscr{S} = \infty$ since there is nothing to contradict the model.

Next, let $\mathscr{N}_f$, for $f \in u(t)$, be the set of nodes that can be reached by following these rules of traversal: at any node n, 1) if the splitting feature is known, go down the appropriate branch; 2) if the splitting feature is f, then go down both branches; 3) otherwise add n to $\mathscr{N}_f$. Intuitively, $\mathscr{N}_f$ is the set of all nodes we could *possibly* end at if f was known and we traverse T until the first unknown feature. Finally, the confidence score of a particular update suggestion is the expected similarity score:

$$\mathscr{C}_1(T, p, f) = \sum_{n \in \mathscr{N}_f} \Pr(\text{terminate at node n}|k(t))\mathscr{S}(D_n, p),$$

where we approximate the probability of terminating at a certain node as $|D_n| / \sum_{i \in \mathscr{N}_f} |D_i|$. The lower this score, the less confident the model is about the suggestion being the most beneficial.

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compute_$\mathscr{N}_f(T, p)$
Input: T - tree; p - point
Output: $\mathscr{N}_f$

1) if T is empty: return $\{\}$
2) if T is a leaf: return $\{T.\text{node}\}$
3) set b to be the boundary at current node
4) if $p[b.f]$ is known:
   a) if $p[b.f] > b.v$: return compute_$\mathscr{N}_f(T.\text{right}, p)$
   b) else: return compute_$\mathscr{N}_f(T.\text{left}, p)$
5) else if $b.f = f$:
   a) $N_f^{(r)} = \text{compute\_}\mathscr{N}_A(T.\text{right}, t)$
   b) $N_f^{(l)} = \text{compute\_}\mathscr{N}_A(T.\text{left}, t)$
   c) return $N_f^{(r)} \cup N_f^{(l)}$
6) else: return $\{T.\text{node}\}$

B. Classifying p's cluster

We will combine two metrics to classify which cluster C_n the point with uncertainty p belongs to: the probability of any point belonging to C_n and the similarity between $k(t)$ and the points in C_n. The reason behind this is simple; suppose C_1 has larger number of points (thus is more frequent) than C_2 but the elements of C_2 are more similar to t, then these two quantities must be balanced in order to effectively judge with cluster p belongs to.

Let $\mathscr{N}$ be the set of nodes reachable probabilistically by using all unknown features (as opposed to $\mathscr{N}_f$ which only used feature f). For each $n \in \mathscr{N}$, we give a confidence score that p belongs to C_n as

$$\mathscr{C}_2(T, p, n) = p_n \mathscr{S}(D_n, p)$$

where $p_n = |D_n| / \sum_{i \in \mathscr{N}} |D_i|$. We then present to the user a list of possible clusters ordered by their $\mathscr{C}_2$ scores. We also supply simple repair functions mean, median, and mode impoutations, akin to [4], which can be used for data cleaning (itself a large field with vast industrial applications).

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compute_$\mathscr{N}(T, p)$
Input: T - tree; t - tuple
Output: $\mathscr{N}$

1) if T is empty: return $\{\}$
2) if T is a leaf: return $\{T.\text{node}\}$
3) let b be the boundary at current node
4) if $t[b.f]$ is known:
   a) if $t[b.f] > b.v$: return compute_$(T.\text{right}, p)$
   b) else: return compute_$(T.\text{left}, p)$
5) else:
   a) $\mathscr{N}^{(r)} = \text{compute\_}(T.\text{right}, p)$
   b) $\mathscr{N}^{(l)} = \text{compute\_}(T.\text{left}, p)$
   c) return $\mathscr{N}^{(r)} \cup \mathscr{N}^{(l)}$

Finally, the difference in $\mathscr{C}_2$ scores before and after an update may be used to catch erroneous updates. If p follows the hypothesis learned by the model, the top confidence score $\mathscr{C}_2$ will increase as we receive more user-provided values. On the other hand, if the model receives a value that was not expected, which makes the hypothesis less likely to apply, then the confidence will decrease. Thus, if an update leads to a large change in the top $\mathscr{C}_2$ score in the negative direction (this is a loss of confidence), we should inform the user. Let p' be a tuple with a single update from p, then report

$$\mathfrak{C}_3(T, p, p') = \max_n \mathscr{C}_2(T, p', n) - \max_n \mathscr{C}_2(T, p, n).$$

IV. Experimental results

The algorithms above were implemented using C++ with the goal of assessing the practical performance using real-life datasets [5]. We divide roughly 90% of the data as the training set and the rest as the test set. We use the training set to build a CBCT and simulate user interaction by dropping random subset of the features for each tuple in the test set and provide those values as needed.

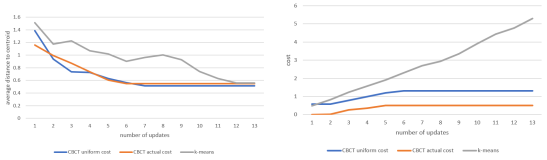
A. Case study I

For the first case study, we used the Heart Disease UCI . This dataset has 13 features related to test results and a label indicating the presence of heart disease in patients. To avoid overfitting, we also prune the tree such that the height does not exceed 7, which was found to work well using cross-validation.

First, we will compare the performance of CBCT with uniform costs to k-means. For CBCT, we measure the distance from p to the centroid of the cluster with the highest $\mathscr{C}_2$ score. From k-means, we will use the training set to $k = 50$ centroids (again chosen through cross-validation) then measure the minimal distance between p and a centroid only using $k(p)$. Figure 2 shows that the average distance decrease faster for the CBCT than k-means but the minimum distances achieved in both clustering algorithm is comparable. The flattening of the curve for the CBCT is due to the pruning.

Next, we compare the performances of a CBCT built with uniform costs to one built with (normalized) costs provided

from the Ontario Health Insurance Plan's fee schedule. Certain tests are 'grouped', meaning performing a test provides values for multiple features. Figure 2 shows that using uniform cost and the actual cost performs similarly (decreasing faster than k-menas), but the average cost is noticibly smaller with the actual cost compared to the uniform cost, which itself is smaller compared to k-means.



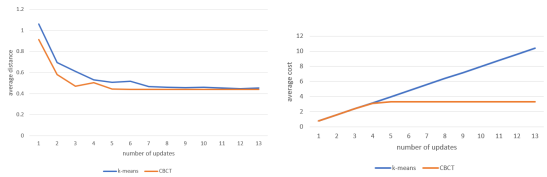
(a) average distances (b) average costs

Fig. 2: CBCT uniform cost vs CBCT actual cost vs k-means

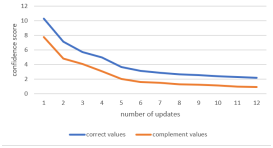
B. Case study II

For this case study, we use the Wine Data Set, which has 13 features. In this dataset, the cost is not provided, so we will set each cost to be the same value. Recall that the score of the split $S(D, b)$ is the discounted reward and that after a feature f is used, $\mathfrak{C}(f)$ is set to zero. This means that at uniform cost, the value we set is essentially the 'willingness' to use an unused feature for the next split. In order to be cost-efficient, we will set the cost to be high (at 0.8).

Again, figure 3 shows that using the updates suggested by a CBCT decreases the average distances faster and more cost efficiently than randomly choosing features. This is especially evident for the first update in this dataset.



(a) average distances (b) average costs



(c) average costs

Fig. 3: CBCT uniform cost vs k-means

Finally, figure 3 also by shows the confidence score of the update suggestions ($\mathscr{C}_1$) when: 1) the correct values are given; 2) the complement values are given. In the latter case, the points generated tend to be dissimilar to other points, thus does not follow closely the hypothesis learned by the model. In both cases, the confidence that an update will help drops as we supply more values (as expected), but it decreases more slowly with the correct values.

V. Discussion and Future Works

When trying to classify a point p to a cluster, the CBCT attempts to improve two aspects: giving better update suggestions than randomly choosing features, and finding and judging possible clusters that p could belong to. The experimental results of the previous section suggest that the CBCT performs similarly to k-means with complete datasets, but reaches the minimum distances faster and more cost efficiently.

These improvements are best used in situations where there is a large repository of complete historical data, yet obtain new data is expensive such as in healthcare or education. This could be of particular interest in education as the advent of online learning has allowed for more personalized learning, but this requires fast identification of classes of learners, that is identify the cluster which the learner belongs to.

There are several avenues to investigate in the future. First, we can see how different reward functions affect the choice of splits. For example, rather than minimizing the distances induced by a boundary, we can maximize the purity of the partition using the Gini impurity, which has already been used in decision tree classifiers as an alternative to entropy.

There is also an alternative way to view this problem. If we view the specific combination of $(k(p), u(p))$ as a state, then finding the next feature update could be stated as a Markov Decision Process (MDP) problem. This idea was used in [9] and [8] for classification, and it would be interesting to find a parallel in clustering.

Finally, it is intersting to consider how human-in-the-loop feature updates can interact with completely automatic repairs. The features at higher in the CBCT are deemed to carry more importance; thus, knowing them should theorectically also assist other algorithms. We could, for instance, see if following the schedule of updates given by the CBCT improves the performance of a matrix completion algorithm compared to randomly supplying values.

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