Hybridized Threshold Clustering for Massive Data

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Abstract

As the size $n$ of datasets become massive, many commonly-used clustering algorithms (for example, $k$-means or hierarchical agglomerative clustering (HAC) require prohibitive computational cost and memory. In this paper, we propose a solution to these clustering problems by extending threshold clustering (TC) to problems of instance selection. TC is a recently developed clustering algorithm designed to partition data into many small clusters in linearithmic time (on average). Our proposed clustering method is as follows. First, TC is performed and clusters are reduced into single “prototype” points. Then, TC is applied

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repeatedly on these prototype points until sufficient data reduction has been obtained. Finally, a more sophisticated clustering algorithm is applied to the reduced prototype points, thereby obtaining a clustering on all $n$ data points. This entire procedure for clustering is called iterative hybridized threshold clustering (IHTC). Through simulation results and by applying our methodology on several real datasets, we show that IHTC combined with $k$-means or HAC substantially reduces the run time and memory usage of the original clustering algorithms while still preserving their performance. Additionally, IHTC helps prevent singular data points from being overfit by clustering algorithms.

**Keywords:** Threshold Clustering, Hybridized Clustering, Instance Selection, Prototypes, Massive Data

1. **Introduction**

Clustering, also known as unsupervised learning, is a well-studied problem in machine learning. It aims to group units with similar features together and separate units with dissimilar features (Friedman et al., 2001). Cluster analysis has been used in many fields like biology, management, pattern recognition, etc. Additionally, many methods (for example, $k$-means clustering, hierarchical agglomerative clustering, etc.) have been developed that successfully tackle the clustering problem.

However, enormous amounts of data are collected every day. For example, Walmart performs more than 1 million customer transactions per hour (Cukier, 2010), and Google performs more than 3 billion searches per day (Sullivan, 2015). This becomes a massive accumulation of data. When working with data of such a large size, many of the state-of-the-art clustering methods become intractable. That is, massive data requires novel statistical methods to process this data; research on scaling up existing statistical algorithms and scaling down the size of data without loss of information is of critical importance (Jordan and Mitchell, 2015).

Instance selection is a commonly-used pre-possessing method for scaling down the size of data (Liu and Motoda, 1998; Blum and Langley, 1997; Liu and Motoda, 2002). The goal of instance selection is to shorten the execution time of data analysis by reducing data size $n$ while maintaining the integrity of data (Olvera-López et al., 2010). Instance selection methods rely on sampling, classification algorithms, or clustering algorithms. Previous work has shown methods reliant on clustering have better performance (accuracy) than some methods that rely on classification (Riquelme et al., 2003; Raicharoen and Lursinsap, 2005; Olvera-López et al., 2007, 2008, 2010). However, current instance selection methods that rely on classification often have faster runtimes.

On the other hand, threshold clustering (TC) is a recently developed method for clustering that is extremely efficient. TC is a method of clustering units so that each cluster contains at least a pre-specified number of units $t^*$ while ensuring that the within-cluster dissimilarities are small. Previous work has shown that, when the objective is to minimize the maximum within-cluster dissimilarities, a solution within a factor of four of optimal can often be obtained in $O(t^*n)$ time and space when the $(t^* - 1)$-nearest-neighbors graph is given (Higgins et al., 2016). The runtime and memory usage required for TC is smaller compared to other clustering methods, for example, $k$-means and hierarchical agglomerative clustering (HAC).
In this paper, we propose the use of TC for instance selection. The proposed method, which is called iterated threshold instance selection (ITIS), works as follows. For a given $t^*$, TC is applied on $n$ units to form $n^*$ clusters; each cluster will contain at least $t^*$ units. Then prototypes are formed by finding the center of each cluster. TC is applied again to the $n^*$ prototypes if the data is not sufficiently reduced. Otherwise, the procedure is stopped.

We also propose using ITIS as a pre-processing step on large data to allow for the use of more sophisticated clustering methods. First, ITIS is applied to form a sufficiently small set of prototypes. Then, a more sophisticated clustering algorithm (for example $k$-means, HAC) is applied on this set of prototypes. Finally, a clustering on all $n$ units is obtained by “backing out” the cluster assignments for the prototypes—for each prototype, the units used to form the prototype are determined; these units are assigned to the same cluster assigned to the prototype. This clustering process on all $n$ units is called Iterative Hybridized Threshold Clustering (IHTC).

We show, using simulations and applications of our algorithm to six large datasets, that IHTC combined with other clustering algorithms reduces the run time and memory usage of the original clustering algorithms while still preserving their performance. Additionally, we show IHTC also prevents singular data points from being overfit by desired clustering methods. Specifically, for $m$ iterations of ITIS at size threshold $t^*$, IHTC ensures that each cluster contains at least $(t^*)^m$ units.

The rest of this paper is organized as follows. A brief summary about clustering algorithms ($k$-means, HAC, TC) is given in section 2. Section 3 shows how to extend threshold clustering as an instance selection method and combine the iterated threshold instance selection method with other clustering methods. A simulation study is presented in section 4 and application of our methods on real datasets are presented in section 5. The last section discuss about our method.

2. Notation and Preliminaries

Consider a dataset with $n$ units, numbered 1 through $n$. Each unit $i$ has a response vector $y_i$ and a $d$-dimensional covariate vector $x_i = (x_{i1}, x_{i2}, \ldots, x_{id})$. For each pair of units $i, j$, the dissimilarity between $i$ and $j$, denoted $d_{ij}$, can be computed. Often, the dissimilarity is chosen so that, if units $i$ and $j$ have similar values of covariates $x$, then $d_{ij}$ is small. We assume that $d_{ij} \geq 0$, and that dissimilarities satisfy the triangle inequality; for any units $i$, $j$, $\ell$,

$$d_{ij} + d_{jk} \geq d_{i\ell}$$

(1)

Common choices of dissimilarities include Euclidean distance, Manhattan distance and average distance.

We define a clustering of a set of units as a partitioning of units such that units within each cluster of a partition have “small dissimilarity” and units belonging to two different clusters have “large dissimilarity.” That is, at minimum, a clustering $v = \{V_1, V_2, \ldots, V_m\}$ will satisfy the following properties:

1. (Non-empty): $V_\ell \neq \emptyset$ for all $V_\ell \in v$.
2. (Spanning): For all units $i$, there exists a cluster $V_\ell \in v$ such that $i \in V_\ell$.
3. (Disjoint): For any two clusters $V_\ell, V_\ell' \in v$, $V_\ell \cap V_\ell' = \emptyset$.
The way of measuring “large” and “small” cluster dissimilarity will vary across clustering algorithms.

There are currently hundreds of available methods for clustering units. Moreover, some of these methods may be combined to construct additional hybridized clustering methods—our procedure for hybridizing is the major contribution of this paper. For brevity, we apply our hybridizing procedure to two clustering methods—$k$-means and hierarchical clustering—with a note that this procedure may be applied to many other types of clustering. We now give a brief summary of these clustering methods.

### 2.1 K-means Clustering

The $k$-means clustering algorithm (Lloyd, 1982) is one of the most widely used and effective methods that attempts to partition units into exactly $k$-clusters.

The $k$-means clustering algorithm proceeds as follows:

1. **(Initialization)** Randomly select a set of $k$ units (referred as centers) from the dataset. $K$ denote the number of clusters and it should be pre-specified.
2. **(Assignment)** Assign all the units to the nearest center, based on squared Euclidean distance, to form $k$ temporary clusters.
3. **(Updating)** Recompute the mean of each cluster. Replace the centers with the new $k$ cluster means.
4. **(Terminate)** Repeat step 2 and 3 until there is no further change for the centers.

The time complexity for the $k$-means clustering algorithm is $O(nkLd)$ and the space complexity is $O((k + n)d)$ (Hartigan and Wong, 1979; Firdaus and Uddin, 2015) where $d$ is the number of attributes for each unit, $L$ is the number of iterations taken by the algorithm to converge.

The $k$-means algorithm suffers from a number of drawbacks (Hastie et al., 2009). First, there tends to be high sensitivity to the selection of initial units in Step 1. Additionally, it tends to overfit isolated units leading to some clusters containing only a few units. Finally, the number of clusters $k$ is fixed; if $k$ is misspecified, $k$-means may perform poorly. In particular, many methods have been developed to mitigate problems due to initialization (Fränti et al., 1997; Frnti et al. 1998 Arthur and Vassilvitskii, 2007; Fränti and Kivijärvi, 2000).

### 2.2 Hierarchical Agglomerative Clustering

Hierarchical agglomerative clustering (HAC) (Ward Jr. 1963) is a ”bottom up” approach that aims to build a hierarchy clusters. It initially treats each unit as a cluster and then continues to merge two clusters together until only one cluster remains. HAC does not require a pre-specified number of clusters; the desired number of clusters can be obtained by using a dendogram—a tree that shows how the units are merged.

The HAC proceeds as follows:

1. **(Initial Clusters)** Start with $n$ clusters, each cluster only contains one unit.
2. **(Merge)** Merge the closest (most similar) pair of clusters into a single cluster.
3. **(Updating)** Recompute the distance between the new cluster and the original clusters.

4. **(Terminate)** Repeat step 2 and 3 until one cluster remains, the cluster contains \( n \) units.

HAC requires linkage criteria to measure inter-cluster distance, but initialization and the choice of \( k \) is no longer a problem. However, the time complexity of HAC is \( O(n^2 \log(n)) \) (Kurita, 1991) and space complexity is \( O(n^2) \) (Jain et al., 1999). This complexity limits its application to massive data. Another hindrance of HAC is that every merging decision is final. Once two clusters are merged into a new cluster, there is no way to partition the new cluster in later steps.

### 2.3 Threshold Clustering (TC)

Our hybridization method makes use of a recently developed clustering method called *threshold clustering* (TC). Initially this method was developed for performing statistical blocking of massive experiments (Higgins et al., 2016). TC differs in two significant ways from traditional clustering approaches. First, TC does not fix the number of clusters formed, but instead, it ensures that each cluster contains a pre-specified number of units. Thus, TC is an effective way of obtaining many clusters, with each containing only a few units. Second, TC ensures the formation of a clustering with a small maximum within-group dissimilarity—more precisely, TC finds approximately optimal clustering with respect to a *bottleneck* objective—as opposed to an average or median within-group dissimilarity. The bottleneck objective is chosen not only to prevent largely dissimilar units from being grouped together, but also because these types of optimization problems often have approximate solutions that can be found efficiently (Hochbaum and Shmoys, 1986).

More precisely, let \( B(t^\ast) \) denote the set of all threshold clusterings—those clusterings \( v \) such that \(|V_\ell| \geq t^\ast\) for each cluster \( V_\ell \in v \). The *bottleneck threshold partitioning problem* (BTPP) is to find the threshold clustering that minimizes the maximum within-cluster dissimilarity. That is, BTPP aims to find \( v^\dagger \in B(t^\ast) \) satisfying:

\[
\max_{V_\ell \in v} \max_{ij \in V_\ell} d_{ij} = \min_{v \in B(t^\ast)} \max_{V_\ell \in v} \max_{ij \in V_\ell} d_{ij} \equiv \lambda; \quad (2)
\]

Here, \( \lambda \) is the optimal value of the maximum within-cluster dissimilarity.

It can be shown that BTPP is NP-hard, and in fact, no \((2 - \epsilon)\)-approximation algorithm for BTPP exists unless \( P = NP \). However, Higgins et al. (2016) develop a threshold clustering algorithm (for clarity, the abbreviation TC refers specifically to this algorithm) to find a threshold clustering with maximum within-cluster dissimilarity at most \( 4\lambda \). That is, TC is a 4-approximation algorithm for BTPP. The time and space requirement for TC are \( O(t^\ast n) \) outside of the construction of a \( t^\ast \)-nearest neighbors graph (Higgins et al., 2016). Constructing a nearest neighbor graph is a well-studied problem for which many efficient algorithms already exist. At worst, forming a \( k \)-nearest neighbor graph requires \( O(n^2 \log n) \) time (Knuth 1998); however, if the covariate space is low-dimensional, this construction may only require \( O(kn \log n) \) time (Friedman et al., 1976; Vaidya, 1989). Hence, TC may be used for large datasets, especially when the threshold \( t^\ast \) and the dimensionality of the covariate space are small.
TC uses graph theoretic ideas in its implementation. See Appendix C for graph theory definitions. TC with respect to a pre-specified minimum cluster size threshold \( t^* \) is performed as follows:

1. **(Construct nearest-neighbor subgraph)** Construct a \((t^* - 1)\)-nearest-neighbors subgraph \( NG_{t^*-1} \) with respect to the dissimilarity measure \( d_{ij} \) (We use Euclidean distance to measure dissimilarity in this paper).

2. **(Choose set of seeds)** Choose a set of units \( S \) such that
   - (a) For any two distinct units \( i, j \in S \), there is no walk of length one or two in \( NG_{t^*-1} \) from \( i \) to \( j \).
   - (b) For any unit \( i \notin S \), there is a unit \( j \in S \) such that there exists a walk from \( i \) to \( j \) of length at most two in \( NG_{t^*-1} \).

   Units in \( S \) are known as *seeds*.

3. **(Grow from seeds)** For each \( \ell \in S \), form a cluster of units \( V^*_\ell \) comprised of unit \( \ell \) and all units adjacent to \( \ell \) in \( NG_{t^*-1} \).

4. **(Assign remaining vertices)** Some units \( j \) may not be assigned to a cluster yet. These units are a walk of length two from at least one seed \( \ell \in S \) in \( NG_{t^*-1} \). Assign the unassigned units to the cluster associated with seed \( \ell \). If there are several choices of seeds, choose the one that with the smallest dissimilarity \( d_{\ell j} \).

The set of clusters \( v = \{ V^*_\ell \}_{\ell \in S} \) form a threshold clustering. Additionally, polynomial-time improvements to this algorithm—for example, in selecting cluster seeds or splitting large clusters—may improve the performance of TC without substantially increasing its runtime. An implementation of TC can be found in the R package *scclust* (Savje et al., 2017).

### 3. Extension of Threshold Clustering

We now describe two extensions of TC: applying TC to instance selection problems and using TC as a preprocessing step for statistical clustering methods.

**3.1 Threshold clustering as instance selection**

Instance selection methods are used in massive data settings to efficiently scale down the size of the data (Leyva et al., 2015). Common techniques for instance selection include subsampling (Pooja, 2013) and constructing *prototypes* (Plasencia-Calaña et al., 2014)—pseudo data points where each prototype represents a group of similar individual units. These methods tend to work quite well for massive data applications.

Suppose the researcher desires to reduce the size of the data by a factor of \( \alpha \). We propose the following method for instance selection, which we call iterated threshold instance selection (ITIS):

1. **(Threshold clustering)** Perform threshold clustering with respect to a small size threshold \( t^* \) (for example, \( t^* = 2 \)) on the \( n \) data points to form \( n^* \) clusters, each containing \( t^* \) or more points.
2. **(Create prototypes)** Compute a center point for each of the $n^*$ groups (for example, centroid or medoid).

3. **(Terminate or continue)** If the data is reduced by a factor of $\alpha$, stop. Otherwise, replace the $n$ data points with the $n^*$ centers and go back to Step 1.

An illustration of the ITIS procedure is given in Figure 1.

Figure 1: An illustration of iterated threshold instance selection (ITIS) with threshold $t^* = 2$ on a sample of $n = 30$ data points drawn from a bivariate Gaussian mixture model. In (2.a), each unit is represented by a point. Applying threshold clustering on the data, 12 clusters are formed in (2.b). A prototype is formed for each of the 12 groups in (2.c). In (2.d), apply threshold clustering on the prototype, 5 clusters are formed. 5 prototypes are formed for the 5 clusters, the results are shown in (2.e). For this illustration, We perform two iterations of ITIS.

Ultimately, the choice of the number of iterations of ITIS $m$ depends on the researcher. For example, a researcher may want to scale down the data as little as necessary in order to perform a computationally intensive statistical procedure on the reduced data. Additionally, the performance of TC may depend on the dissimilarity measure $d_{ij}$; in our experience, using the standardized Euclidean distance tends to work well.

The running time of $m$ iterations of ITIS is $O(t^*mn \log n)$. Moreover, since the size of the data is reduced by a factor of $t^*$ with each iteration, the computational bottleneck of ITIS becomes the construction of a $t^*$–nearest-neighbors graph on all $n$ units. This also
suggests that the computation required of ITIS may be drastically improved through the
discovery of methods for parallelization of threshold clustering.

The iterative nature of ITIS does have a drawback; with each iteration, the prototype
units become less similar to the units comprising the prototype. In particular, the approx-
imate optimality property of TC may not hold if \( m > 1 \). However, simulations suggest
that this issue is not severe in massive data settings. Alternatively, approximate optimality
may be preserved by choosing \( t^* = \alpha \) and running one iteration of ITIS. However, the one
iteration version does not seem to be as promising under massive data settings since the
runtime of TC increases as \( t^* \) increases. See Appendix A for details.

3.2 Iterative Hybridized Threshold Clustering

Often, researchers would like to use certain clustering methods (for example, \( k \)-means, HAC,
etc.) because of favorable or familiar properties of these clustering methods. However,
under massive data settings, using such clustering techniques may not be feasible because
of prohibitive computational costs. We propose the following method for using ITIS as
a pre-processing step on all \( n \) units to allow for the use of more sophisticated clustering
methods. We call this procedure Iterative Hybridized Threshold Clustering (IHTC). It
works as follows:

1. **(Create prototypes)** Perform iterative threshold instance selection with respect to
   a size threshold \( t^* \) on the \( n \) data points \( m \) times to form prototypes.

2. **(Cluster prototypes)** Cluster the prototypes (for example, using \( k \)-means) obtained
   by 1.

3. **("Back out" assignment)** For each prototype, determine which of the original \( n \)
   units contributed to the formation of that prototype and assign these units to the
   cluster belonging to the prototype.

Figure 2 gives an illustration of IHTC with \( k \)-means.

IHTC reduces the size of the data by a factor of \( (t^*)^m \), which can improve the efficiency of
the original clustering algorithm. Additionally, IHTC also prevents overfitting of individual
points, which may lead to a more effective clustering regardless with just a couple iterations
of IHTC. Specifically, for \( m \) iterations of ITIS at size threshold \( t^* \), IHTC ensures that each
cluster contains at least \( (t^*)^m \) units. Finally, we note that IHTC may be applied to most
other clustering algorithms—not just \( k \)-means or HAC.

4. Simulation

We first demonstrate properties of IHTC using simulated data. We apply IHTC to samples
of varying sizes where each data point is sampled from a mixture of three bivariate Gaussian
distributions. Specifically, samples are drawn independently from a distribution with pdf:

\[
f(x) = 0.5p(x|\mu_1, \Sigma_1) + 0.3p(x|\mu_2, \Sigma_2) + 0.2p(x|\mu_3, \Sigma_3)
\]

where \( p(x|\mu_j, \Sigma_j) \) is the pdf of a Gaussian with parameters \( \mu_j \) and \( \Sigma_j \), \( j = 1, 2, 3, \)

\[
\mu_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \mu_2 = \begin{bmatrix} 7 \\ 8 \end{bmatrix}, \mu_3 = \begin{bmatrix} 3 \\ 5 \end{bmatrix}
\]

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Figure 2: An illustration of hybridized threshold clustering with $k$-means on bivariate data: $n = 20, k = 3, t^* = 2$. In graph (3.a), each unit is represented by a point. Applying threshold clustering on the data, 7 clusters are formed in (3.b). A prototype is formed for each of the 7 groups in (3.c). In (3.d), $k$-means clustering is performed on the prototypes. The "backed out" final clustering results are given in (3.e).

$$
\Sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0.5 \end{bmatrix}, \Sigma_2 = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}, \Sigma_3 = \begin{bmatrix} 3 & 0 \\ 0 & 4 \end{bmatrix}.
$$

We use Euclidean distance as our dissimilarity measure. The data size $n$ varies between $10^4$ and $10^8$ observations and each setting is replicated 1000 times. For each simulation, we record the run time in seconds and memory usage in megabytes for the whole procedure.

Algorithms are implemented in the R programming language. We use the scclust package to perform threshold clustering (Savje et al., 2017). The default `kmeans` and `hclust` functions in R are used for $k$-means and hierarchical agglomerative clustering respectively. This simulation was performed on the Beocat Research Cluster at Kansas State University, which is funded in part by NSF grants CNS-1006860, EPS-1006860, and EPS-0919443 (University, 2018). We perform simulations on a single core Intel Xeon E5-2680 v3 with 2.5 GHz processor with 30 GM of RAM at maximum.

4.1 IHTC with K-means Clustering

We perform IHTC with $k$-means with threshold $t^* = 2$ and number of clusters $k = 3$. The run time and memory usage are in Figure 3 and Table 1. Because we simulated data from
a Gaussian mixture model, each cluster roughly should correspond to a different Gaussian distribution. Hence, we can use prediction accuracy to measure the performance of our methods. The prediction accuracy is the number of units correct clustered divided by data size $n$. The prediction accuracy for IHTC with $k$-means are in Figure 4 and Table 1. The first point of each curve (iteration $m = 0$) indicates the performance without pre-processing of the data; that is $m = 0$ indicates where only the original clustering algorithm is applied to the data.

From Figures 3 and 4, and from Table 1, we find that using IHTC with $k$-means decreases the runtime and memory required compared to without IHTC. After one iteration, the runtime and memory usage decreases by about half while the prediction accuracy remains the same. As the number of iterations increases, the additional improvements in runtime and memory usage decrease. After several iterations, runtime and memory usage tend to level off and prediction accuracy slowly decreases.
| Iteration \((m)\) | Run Time (second) | Memory (Mb) | Accuracy |
|-----------------|------------------|-------------|-----------|
|                 | \(10^4\) | \(10^5\) | \(10^6\) | \(10^7\) | \(10^8\) | \(10^4\) | \(10^5\) | \(10^6\) | \(10^7\) | \(10^8\) | \(10^4\) | \(10^5\) | \(10^6\) | \(10^7\) | \(10^8\) |
| 0               | 0.143 | 1.613 | 18.773 | 218.43 | 2815 | 19.39 | 241.64 | 2556 | 27540 | 279346 | 0.9236 | 0.9239 | 0.9239 | 0.9239 | 0.9239 |
| 1               | 0.084 | 0.909 | 10.337 | 119.86 | 1767 | 8.70 | 99.14 | 1019 | 11097 | 110467 | 0.9236 | 0.9239 | 0.9239 | 0.9239 | 0.9239 |
| 2               | 0.072 | 0.647 | 7.886 | 97.07 | 1572 | 3.99 | 44.00 | 488 | 5462 | 54773 | 0.9232 | 0.9238 | 0.9239 | 0.9239 | 0.9239 |
| 3               | 0.058 | 0.550 | 6.975 | 88.52 | 1522 | 1.76 | 23.55 | 253 | 3104 | 31764 | 0.9225 | 0.9237 | 0.9239 | 0.9239 | 0.9239 |
| 4               | 0.053 | 0.502 | 6.534 | 83.86 | 1487 | 0.97 | 14.19 | 166 | 2150 | 21962 | 0.9214 | 0.9234 | 0.9238 | 0.9239 | 0.9239 |
| 5               | 0.053 | 0.497 | 6.332 | 81.46 | 1378 | 0.81 | 8.62 | 130 | 1761 | 17757 | 0.9187 | 0.9229 | 0.9238 | 0.9239 | 0.9239 |
| 6               | 0.051 | 0.487 | 6.272 | 80.90 | 1350 | 0.81 | 7.94 | 112 | 1614 | 16478 | 0.9128 | 0.9216 | 0.9235 | 0.9239 | 0.9239 |
| 7               | -     | 0.487 | 6.263 | 80.62 | 1336 | -     | 7.69 | 106 | 1560 | 15813 | -     | 0.9196 | 0.9231 | 0.9238 | 0.9239 |
| 8               | -     | 0.490 | 6.254 | 80.28 | 1305 | -     | 7.56 | 105 | 1561 | 16005 | -     | 0.9163 | 0.9224 | 0.9236 | 0.9239 |
| 9               | -     | 0.490 | 6.243 | 80     | 1288 | -     | 7.91 | 105 | 1574 | 16099 | -     | 0.9085 | 0.9210 | 0.9234 | 0.9239 |
| 10              | -     | -     | 6.245 | 79.95 | 1252 | -     | -    | 106 | 1596 | 16512 | -     | -     | 0.9184 | 0.9227 | 0.9237 |
| 11              | -     | -     | 6.246 | 79.75 | 1268 | -     | -    | 109 | 1630 | 16587 | -     | -     | 0.9140 | 0.9218 | 0.9235 |
| 12              | -     | -     | 79.72 | 1247  | -     | -     | -    | 1662| 17036| -     | -     | 0.9201 | 0.9233 |

Table 1: Cluster performance of IHTC with \(K\)-means \((k = 3, t^* = 2)\).
4.2 IHTC with HAC

HAC is a computationally expensive algorithm. For example, if data size exceed 65,536 datapoints, the `hclust` function in R will throw an error. We applied IHTC with HAC and consider with respect to threshold \( t^* = 2 \). Comparing the performance with pre-processing and without pre-processing, we found the reduction for runtime and memory requirement is dramatic when we apply IHTC with HAC, while prediction accuracy falls slightly. As the number iterations increase, the improvements in runtime and memory usage decrease, and
after several iterations, runtime and memory tend to a certain stable value and prediction accuracy decreases. Thus, the number of iterations to perform is an unsolved problem. Figures 5 and 6, and Table 2 give the results of IHTC with HAC.

![Figure 4: Prediction accuracy of IHTC with k−means clustering (k = 3, t∗ = 2).](image)

| Iterations | Run Time (second) | Memory (Mb) | Accuracy |
|------------|-------------------|-------------|----------|
|            | 10^1             | 10^2        | 10^3     | 10^4     | 10^5     | 10^6     | 10^7     | 10^8     |
| Null       | 5.425            | -           | -        | 796.46   | -        | -        | -        | -        |
| 1          | 0.940            | 88.619      | -        | 177.27   | 20193    | -        | -        | 0.9122   |
| 2          | 0.220            | 15.755      | -        | 20.49    | 3537.4   | -        | -        | 0.9142   |
| 3          | 0.073            | 2.992       | -        | 7.01     | 459.9    | -        | -        | 0.9121   |
| 4          | 0.048            | 0.752       | 62.28    | 1.11     | 117.9    | 10891    | -        | 0.9091   |
| 5          | 0.044            | 0.393       | 15.41    | 0.73     | 28.7     | 1940     | -        | 0.9012   |
| 6          | 0.045            | 0.350       | 7.44     | 0.74     | 11.2     | 435      | -        | 0.8938   |
| 7          | 0.044            | 0.343       | 6.23     | 0.74     | 9.3      | 165      | -        | 0.8864   |
| 8          | -                | 0.342       | 5.99     | 9.3      | 120      | 2405     | -        | 0.8884   |
| 9          | -                | 0.342       | 5.98     | 90.4     | 9.4      | 115      | 1648     | -        | 0.8896   |
| 10         | -                | 5.99        | 89.2     | 1299     | -        | -        | -        | -        | 0.9012   |
| 11         | -                | 6.04        | 89.7     | 1267     | -        | 118      | 1564     | 19113    | -        |
| 12         | -                | 90.1        | 1288     | -        | 1579     | 16760    | -        | -        | 0.9066   |
| 13         | -                | 89.9        | 1253     | -        | 1604     | 17014    | -        | -        | 0.8991   |
| 14         | -                | -           | 1727     | -        | -        | 17505    | -        | -        | 0.9068   |
| 15         | -                | -           | 1283     | -        | -        | 17784    | -        | -        | 0.8967   |
| 16         | -                | -           | 1288     | -        | -        | 18220    | -        | -        | 0.8950   |

Table 2: Cluster performance for IHTC with HAC (t∗ = 2)
Figure 5: Run time and memory usage of IHTC with HAC (t* = 2).
5. Experiments

In this section, we will use our threshold clustering algorithm performance on several publicly available datasets. A brief description of each dataset can be found in Table 3. The Euclidean distance is used to measure the dissimilarity and principal component analysis (Hotelling, 1933; Friedman et al., 2001) is used for each dataset to perform feature selection. The number of classes \( k \) is chosen by the elbow of plot of within-cluster sum of squared distances for different \( k \). All experiments run on a single CPU core laptop.

| Name                        | Instances | Attributes | Classes |
|-----------------------------|-----------|------------|---------|
| PM 2.5 (Havera, 2017)       | 41757     | 5          | 4       |
| Credit Score (Kaggle, 2011) | 120269    | 6          | 5       |
| Black Friday (Dagdoug, 2018)| 166986    | 7          | 4       |
| Covertype (Blackard and Dean, 1999) | 581012   | 6          | 7       |
| House Price (Zillow, 2017)  | 2885485   | 5          | 5       |
| Stock (Brogaard et al., 2014; Carrion, 2013) | 7026593 | 5          | 7       |

Table 3: Data description.

Tables 4, 5, and 6, and Figures 7 and 8 demonstrate results of IHTC with \( k \)-means and HAC for these datasets. Iteration \( m = 0 \) indicates the performance when no pre-processing was conducted; only \( k \)-means clustering was applied to the data. BSS/TSS is the ratio of between cluster sum of squares and total sum of squares. Larger ratio value indicates better cluster performance. The number of prototypes is the size of the reduced data after \( m \) iterations. We found that using IHTC with \( k \)-means or HAC decreases the runtime and memory required compared to without IHTC. After one iteration, the runtime and memory usage decreases by about half while preserving the value of the BSS/TSS ratio. As
the number of iterations becomes large, the improvements in runtime and memory usage
decrease and the BSS/TSS ratio decreases slowly.

To demonstrate the versatility of IHTC, we also consider its performance with the clus-
tering method DBSCAN (Ester et al., 1996). The results of DBSCAN are contained in
Appendix B.
| Name          | Run Time (second) | Memory Usage (Mb) | BSS/TSS     | Number of Prototypes |
|---------------|-------------------|-------------------|-------------|----------------------|
|               | m = 0             | m = 1             | m = 2       | m = 3             | m = 0             | m = 1             | m = 2             | m = 3             | m = 0             | m = 1             | m = 2             | m = 3             |
| PM 2.5        | 0.636             | 0.282             | 0.232       | 0.268             | 71.28             | 25.69             | 3.7             | 5.91             | 0.5347            | 0.5346            | 0.5345            | 0.5344            | 41757             | 17281             | 7166             | 2984             |
| Credit Score  | 2.902             | 2.046             | 2.696       | 2.904             | 244.55            | 23.9             | 13.95           | 17.65            | 0.5187            | 0.5184            | 0.5178            | 0.5169            | 120269            | 49669             | 20471            | 8456             |
| Black Friy    | 2.802             | 0.468             | 0.522       | 0.554             | 317.05            | 32.95            | 24.5          | 28.91            | 0.3493            | 0.3456            | 0.3402            | 0.3226            | 166986            | 11868             | 4914             | 2017             |
| Coverttype    | 22.244            | 10.184            | 11.968      | 13.562            | 1073.9            | 387.66           | 150.46         | 172.78           | 0.4791            | 0.4806            | 0.4741            | 0.4787            | 581012            | 241072            | 99509            | 41102            |
| House Price   | 110.08            | 40.24             | 58.02       | 65.05             | 5178.7            | 881.2            | 726.4          | 859.4            | 0.5589            | 0.5589            | 0.5589            | 0.5587            | 2885485           | 1196674           | 496442           | 206332           |
| Stock         | 262               | 121.82            | 105.98      | 127.62            | 12528.9           | 4545.9           | 1943.8         | 2169.9           | 0.5829            | 0.5828            | 0.5825            | 0.5820            | 7026593           | 2952376           | 1226666         | 508366           |

Table 4: Cluster performance for IHTC with k-means (t* = 2).

| Performance | PM 2.5 | Credit Score | Black Friday |
|-------------|--------|--------------|--------------|
| Run Time (second) | m = 1 | m = 2 | m = 3 | m = 1 | m = 2 | m = 3 | m = 1 | m = 2 | m = 3 |
| Memory Usage (Mb)    |        |        |        |        |        |        |        |        |        |
| BSS/TSS           | 0.4964 | 0.4964 | 0.4964 | 0.4791 | 0.4806 | 0.4741 | 0.3176 | 0.3024 | 0.3142 |
| Number of Prototypes | 17281 | 7166 | 2984 | 20471 | 8456 | 3508 | 11868 | 4914 | 2017 |

Table 5: Cluster performance for IHTC with HAC (t* = 2).

| Performance | Covertype | House Price | Stock |
|-------------|-----------|-------------|-------|
| Run Time (second) | m = 4 | m = 6 | m = 6 | m = 7 | m = 8 | m = 7 | m = 8 | m = 9 |
| Memory Usage (Mb)    |        |        |        |        |        |        |        |        |
| BSS/TSS           | 0.4124  | 0.3982  | 0.4144 | 0.5213  | 0.5017  | 0.5017 | 0.4986  | 0.4945  | 0.4993 |
| Number of Prototypes | 17015 | 7015 | 2911 | 15014 | 6268 | 2598 | 15085 | 6267 | 2603 |

Table 6: Cluster performance for IHTC with HAC (t* = 2).
Figure 7: Cluster performance for IHTC with K-means.
6. Discussion

Many clustering methods share one ubiquitous drawback: as the size of the data becomes massive—that is, as the number of units $n$ for the data becomes large—these methods become intractable. Even efficient implementations of these algorithms require prohibitive computational resources under massive $n$ settings. Recently, threshold clustering (TC) has been developed as a way of clustering units so that each cluster contains a pre-specified number of units and so that the maximum within-cluster dissimilarity is small. Unlike many clustering methods, TC is designed to form clustering comprised of many groups.

Figure 8: Cluster performance for IHTC with HAC.
of only a few units. Moreover, the runtime and memory requirement for TC is smaller compared to other clustering methods.

In this paper, we propose using TC as an instance selection method called iterative threshold instance selection (ITIS) to efficiently and effectively reduce the size of data. Additionally, we propose coupling ITIS with other, more sophisticated clustering methods to obtain method to sufficiently scale down the size of data. and introduced IHTC that can efficiently and effectively scale down the size of data so that more sophisticated clustering methods can be applied on the reduced data.

Simulation results and application on real datasets show that implementing clustering methods with IHTC may decrease their runtime and memory usage without sacrificing the their performance. For more sophisticated clustering methods, this reduction in runtime and memory usage may be dramatic. Even for the standard implementation of $k$-means in R, one iteration of IHTC decreases the runtime and memory usage by more than half while maintaining clustering performance.

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Appendix A. Cluster Performance for IHTC with Varying Threshold Size

We compare the cluster performance for IHTC with varying threshold $t^*$ across different data size. For this example, we generate data using the multivariate Gaussian model in Section 4. We set $k = 3$, $n$ is between $10^4$ and $10^8$, and perform one iteration of IHTC ($m = 1$). We analyze performance across different thresholds: $t^* = 2, 4, 8, 16, 32, 64, 128, 256, 512$ and $1024$. The runtime, memory usage and prediction accuracy for IHTC with $k$-means can be found in Figures 9 and 11, and Table 7. Figures 10 and 11, and Table 8 present the cluster performance for IHTC with HAC.

We find, that when the threshold $t^*$ is small, pre-processing the data with IHTC decreases runtime and memory usage compared to without pre-processing, and prediction accuracy fluctuates within a narrow range. When $t^*$ is large, the runtime for our method takes longer than the runtime without pre-processing. In general, across all data sizes, the runtime initially decreases before steadily increasing as $t^*$ increases. On the other hand, despite increasing the threshold $t^*$, the memory usage for IHTC with $k$-means or HAC is continually reducing. Additionally, the prediction accuracy decreases slightly with larger values of $t^*$. 
Figure 9: Run time and memory usage of different $t^*$ with $k$-means ($k = 3, m = 1$).
Figure 10: Runtime and memory usage of for different threshold $t^*$ with HAC ($m = 1$).
Figure 11: Prediction accuracy for different threshold $t^*$ ($m = 1$).
| $t^*$ | Run Time (second) | Memory Usage (Mb) | Accuracy |
|------|-------------------|-------------------|----------|
| None | 0.152 1.44 17.5 214 2697 | 20.37 235.36 2538 27468 278617 | 0.9238 0.9240 0.9239 0.9239 0.9239 |
| 2    | 0.109 0.75 9.6 118 1640 | 9.50 96.73 1014 11085 110919 | 0.9237 0.9240 0.9239 0.9239 0.9239 |
| 4    | 0.067 0.53 7.7 98 1540 | 4.33 48.17 525 5898 59288 | 0.9236 0.9240 0.9239 0.9239 0.9239 |
| 8    | 0.070 0.56 9.4 119 2137 | 1.65 24.50 274 3293 33316 | 0.9233 0.9239 0.9239 0.9239 0.9239 |
| 16   | 0.099 0.86 15.5 197 - | 0.52 11.97 149 1975 - | 0.9230 0.9238 0.9239 0.9239 - |
| 32   | 0.161 1.64 29.8 467 - | 0.20 5.34 90 1314 - | 0.9219 0.9238 0.9239 0.9239 - |
| 64   | 0.297 3.54 62.3 1032 - | 0.10 2.21 59 999 - | 0.9203 0.9233 0.9238 0.9239 - |
| 128  | 0.658 8.72 200.8 - - | 0.04 0.98 41 - - | 0.9174 0.9231 0.9238 - - |
| 256  | 1.565 37.38 546.4 - - | 0.03 0.58 34 - - | 0.9086 0.9221 0.9238 - - |
| 512  | - 100.56 1585 - - | - 0.45 27 - - | - 0.9204 0.9235 - - |
| 1024 | - 384.17 5541 - - | - 0.39 26 - - | - 0.9162 0.9231 - - |

Table 7: Cluster performance for iterate once with $k$-means ($k = 3, m = 1$).

| $t^*$ | Run Time (s) | Memory Usage (Mb) | Accuracy |
|------|--------------|-------------------|----------|
| Null | 5.366 - - | 764.5 - | 0.9111 - - |
| 2    | 0.984 115.9 - | 184.8 20196 - | 0.9113 0.9140 - |
| 4    | 0.246 22.59 - | 24.84 4992 - | 0.9113 0.9127 - |
| 8    | 0.095 5.491 - | 12.46 1230 - | 0.9118 0.9135 - |
| 16   | 0.091 2.047 165.8 | 1.720 298.4 29701 | 0.9106 0.9131 0.9075 |
| 32   | 0.153 2.035 65.59 | 0.066 73.78 7207 | 0.9093 0.9127 0.9117 |
| 64   | 0.297 3.919 69.05 | 0.018 19.17 1813 | 0.9078 0.9123 0.9125 |
| 128  | 0.697 9.522 201.3 | 0.005 3.517 466.2 | 0.9076 0.9121 0.9143 |
| 256  | 1.662 40.73 534.3 | 0.004 0.561 130.2 | 0.9056 0.9105 0.9112 |
| 512  | - 105.2 1630 | - 0.325 47.29 | - 0.9096 0.9139 |
| 1024 | - 401.4 6042 | - 0.241 26.97 | - 0.9049 0.9115 |

Table 8: Simulation result for different threshold $t^*$ with HAC ($m = 1$).
Appendix B. Experiment for IHTC with DBSCAN

Table 9 shows the result on the four datasets with the fewest instances. The parameters $\epsilon$ and $Minpts$ are decided by subsample of size 1000 of each dataset with a 10-fold cross-validation method. Comparing the performance for DBSCAN with and without IHTC, we find that IHTC with DBSCAN has shorter runtime but higher memory usage than DBSCAN itself. Total sum of squares (TSS) is equal to between-cluster sum of squares (BSS) plus within-cluster sum of squares. Higher ratio of BSS and TSS indicates the clusters are more compact. We found that the ratio of BSS and TSS is higher when applying IHTC, which shows our method has comparable clustering performance.

| Name      | Run Time (second) | Memory Usage (Mb) | BSS/TSS |
|-----------|-------------------|-------------------|---------|
|           | $m = 0$ | $m = 1$ | $m = 2$ | $m = 0$ | $m = 1$ | $m = 2$ | $m = 0$ | $m = 1$ | $m = 2$ |
| PM 2.5    | 3.96   | 0.9    | 0.26    | 0.8    | 0.4    | 0.2    | 0.5036 | 0.5627 | 0.5336 |
| Credit Score | 25.78  | 4.16   | 2.66    | 3.3    | 1.2    | 38     | 0.4731 | 0.6015 | 0.6441 |
| Black Fridy | 9.26   | 0.64   | 0.56    | 13.5   | 62.1   | 66.2   | 0.3103 | 0.9657 | 0.9985 |
| Covertype  | 233.9  | 223.8  | 231.4   | 13.3   | 15.6   | 15.6   | 0.1785 | 0.1785 | 0.1785 |

Table 9: Cluster performance for IHTC with DBSCAN ($t^* = 2$).
Appendix C. Graph theory definitions

Let $G = (V, E)$ denote an undirected graph.

Definition 1. Vertices $i$ and $j$ are adjacent in $G$ if the edge $ij \in E$.

Definition 2. A set of vertices $I \subseteq V$ is independent in $G$ if no vertices in the set are adjacent to each other. That is, for all $i,j \in I$, $ij \notin E$.

Definition 3. An independent set of vertices $I$ in $G$ is maximal if, for any additional vertex $i \in V$, the set $i \cup I$ is not independent. That is, for all $i \in V \setminus I$, there exists $j \in I$ such that $ij \in E$.

Definition 4. For $i,j \in V$, a walk from $i$ to $j$ of length $m$ in $G$ is a sequence of $m + 1$ vertices $(i = i_0, i_1, \ldots, i_m = j)$ such that the edge $i_{\ell-1}i_\ell \in E$.

Note that, if $(i = i_0, i_1, i_2, \cdots, i_m = j)$ is a walk of length $m$ from $i$ to $j$ and the edge weights of $G$ satisfy the triangle inequality (1), then the weight $w_{ij}$ satisfies the inequality:

$$w_{ij} \leq m \max_\ell (w_{i_{\ell-1}i_\ell}).$$

(3)

Definition 5. The $d^{th}$ power of $G$, denoted $G^d = (V, E^d)$, is a graph such that an edge $ij \in E^d$ if and only if there is a walk from $i$ to $j$ of length at most $d$ in $G$.

Definition 6. The $k$-nearest-neighbors subgraph of $G$ is a subgraph $NG_k = (V, NE_k)$ where an edge $ij \in NE_k$ if and only if $j$ is one of the $k$ closest vertices to $i$ or $i$ is one of the $k$ closest vertices to $j$. Rigorously, for a vertex $i$, let $i(\ell)$ denote the vertex that corresponds to the $\ell^{th}$ smallest value of $w_{ij}, ij \in E$, where ties are broken arbitrarily: $w_{ii(1)} \leq w_{ii(2)} \leq \cdots \leq w_{ii(m)}$. Then

$$NE_k \equiv \left\{ ij \in E : j \in (i(\ell))_{\ell=1}^k \text{ or } i \in (j(\ell))_{\ell=1}^k \right\}.$$  

(4)