CSE 847 Project

Yinyang K-means

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1. PROBLEM DESCRIPTION

K-means is a popular machine learning algorithm for clustering. As the amount of data has grown ever larger, the limitation of the classic K-mean algorithm has become more apparent. Specifically, the K-means algorithm is linear in data set size—the number of distance calculations is $O(nkid)$, where n is the number of data points, k is the number of desired clusters, i is the number of iterations, and d is the number of dimensions. This linearity reduces the usability of the algorithm with large datasets. However, Ding *et al.* propose Yinyang K-means [4] which seeks to solve this problem. The authors assert Yinyang K-means can be used in place of classical K-means with no extra conditions or requirements while simultaneously achieving an order of magnitude higher performance. We intend to explore the theoretical properties of this proposed method and verify the authors' claim of a significant speed up.

2. INTRODUCTION

K-means is a venerable clustering algorithm which has gained the trust of researchers through years of use. However, when the dimensionality, data set size, or number of desired clusters is large, K-means becomes prohibitively expensive. Attempts at increasing the performance of K-means mainly fall into two categories: working on improving the core algorithm or improving the performance through some other means (*e.g.* K-means++ [1]). This work focuses on the former method, which includes approximation and optimization. Within this realm, work has been done previously on structural or incremental optimization [9, 6, 5] and on approximation [7, 3, 10, 11, 12]. While this previous work has been of high quality, none of the innovations have gotten much traction or widespread use [4].

In the first category, *Elkan* [6] uses two lemmas to find a lower bound using the triangle inequality:

1. For a point x and centers b and c, if $d(b,c) \geq 2d(x,b)$ then $d(x,c) \geq d(x,b)$.
2. For a point x and centers b and c, $d(x,c) \geq \max\{0, d(x,b) - d(b,c)\}$.

The first lemma is used to avoid calculating distances to centers in cases where $\frac{1}{2}d(c,c') \geq d(x,c)$. The second lemma lets the algorithm use a lower bound $l \leq d(x,b)$, where x is any data point and b is any center. As long as center b does not move too much in an iteration, then l can be used as $d(x,b)$ without actually calculating the distance. Empirically, Elkan's algorithm speeds up K-means by factors of 1.50 to 351. The algorithm performs better with higher k and lower dimensionality: of the four public datasets used in evaluation, performance increased as k varied from 3 to 20 to 100 and dimensionality decreased from 784 to 2.

In one work from the approximation tack, *Sculley* [11] uses mini batches to greatly improve on the accuracy of the online stochastic gradient descent method demonstrated by *Battou and Bengio* [2]. In this approach, Sculley first finds the closest centers to each data point in the mini batch. An array v tracks the number of data points associated with a given center c. The main loop iterates over the data points:

1. Retrieve the center associated with this point.
2. Update $v[c]$.
3. Calculate the center's learning rate as $\eta = \frac{1}{v[c]}$.
4. Perform the gradient step for center c.

Sculley's experiments showed that this mini-batch gradient descent with batch size 1,000 converged orders of magnitude faster than classic K-means while achieving much better accuracy than Bottou and Bengio's method. (Here, the classic algorithm is treated as the ground truth for calculating accuracy.)

In *Drake and Hamerly* [5], the authors keep b lower bounds where $b < k$, k being the number of bounds kept in *Elkan* [6]. These bounds are the distances to the b nearest neighbors of the point in question, and are kept by tracking a point's center and the $1 \leq z \leq b$ closest centers. Of particular note, Drake and Hamerly tune b adaptively as follows: start at $b = \frac{k}{4}$; after each iteration, b becomes the number of useful bounds while staying at least $\frac{k}{8}$. Tests that Drake and Hamerly performed on their algorithm show that for a medium range of dimensions ($\sim$25-125), it out-performs algorithms by Elkan [6], Hamerly [8], and the traditional K-means.

It has been hypothesized that in order to gain popularity in practical use, a replacement for K-means must meet three requirements: equivalent clustering to traditional K-means, consistent and significant performance gains, and simple to use [4].

2.1 Yinyang K-means

The proposed work aims to satisfy those three requirements. It utilizes the triangle inequality in a novel way to keep track of two bounds: the upper bound on the distance from a given point to its assigned cluster center and the lower bound on the distance from the point to any other

center. These two bounds act to reduce the number of distance calculations that need to be performed during the assignment step of K-means. This is achieved through two kinds of filtering: group/global filtering and local filtering. Global filtering works to determine if a point needs to be assigned to a different cluster based on the movement of the cluster centers. If centers change by a large amount, then it is more likely that points need their cluster assignment checked. Group filtering generalizes the global filtering by initially grouping the clusters into groups before the first iteration of K-means and applying the global filter to those groups. Local filtering is performed on any groups of cluster centers that make it through the group filter. Centers that get filtered by the local filter do not have their distances to the data points calculated.

Additionally, a method to optimize the second step of K-means, the center update step, is proposed. The new method updates the cluster centers by modifying them rather than calculating the average across all points contained in that cluster.

3. DATA

The main claim of the authors is the ability to apply the K-means clustering algorithm to data which is large. Thus, our synthetic dataset should attempt to verify this claim by including large amounts of data. It will also be interesting to document how the performance changes as the data size grows. The authors also claim that clustering results of Yinyang K-means is the same as standard K-means. So we vary the "difficulty" of clustering the data by varying the average Euclidean distance of the mean of all of the clusters.

There are four primary parameters that we vary in our synthetic dataset. The first parameter is the number of clusters (N_C) where we use 3 different values: 100, 1,000, and 10,000. The second parameter is the number of features (N_F) where we use 3 different values: 100, 500, and 1,000. The third parameter is the number of samples per cluster (N_S) where we use 3 different values: 100, 500, and 1,000. The fourth and final parameter is the average mean Euclidean distance parameter (μ_{euc}) where we use 3 different values: 100, 500, and 1,000. There are 81 synthetic datasets that we will run both Yinyang K-means and standard K-means on. This information is summarized in Table 1.

We generate the data as multi-variate Gaussian distributions. We first generate an N_C-sized set of means. An overview of this process is shown in Figure 1. We want to vary the average distance between clusters so we introduce an average mean Euclidean distance parameter (μ_{euc}). We then use the `randn` MATLAB function to generate a set of potential means of size $10 * N_C$ each with N_F features. We then sample from the set N_C means and calculate their average Euclidean distance and compare it to μ_{euc}. If it is within the tolerance (δ), we use this as the set of N_C means for a single run.

We then generate a random matrix B and then generate a random positive semi-definite matrix $C = B^{\mathrm{T}}B$ that we use as the covariance. We do this for each mean in the run. We use this mean and the covariance as arguments for the `mvnrnd` MATLAB function to generate the data with N_S samples.

To demonstrate the data generation described above, we used the following parameters: $N_C = 5$, $N_F = 2$, and $N_S = 100$. Since the data is two dimensional, we can visualize it.

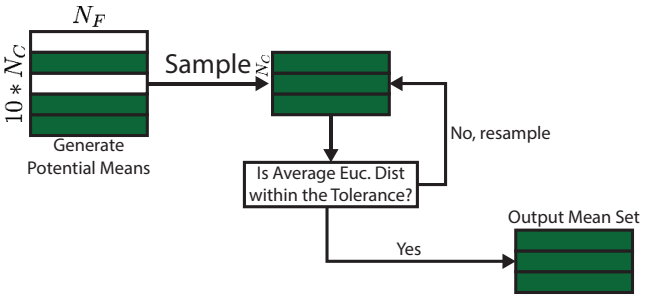


Figure 1: Overview of the mean generation step. A N_C-sized set of means is sampled from the $10 * N_C$-sized set of potential means. If the sample has an average Euclidean distance within the tolerance it is selected. If not, a new sample is selected.

Two examples are shown in Figure 2.

4. YINYANG K-MEANS

4.1 Properties

4.1.1 Definitions

We define the parameters used in the Yinyang K-Means method here. Since Yinyang K-Means is an iterative method, we consider what happens between iterations i and $i+1$ until the convergence condition is met. Let $\mathcal{C}$ be the set of clusters centers at iteration i and $\mathcal{C}'$ be the set of clusters at iteration $i+1$. Let c be a single cluster in $\mathcal{C}$ at iteration i and c' be a single cluster in $\mathcal{C}'$ at iteration $i+1$. Let $b(x)$ be the cluster to which x is assigned at iteration i and $b'(x)$ be the cluster to which x is assigned at iteration $i+1$. Let $\delta(c) = d(c, c')$, that is, the distance a cluster center c travels between iteration i and iteration $i+1$. Let $ub(x) \geq d(x, b(x))$, that is, $ub(x)$ is an upper bound on the distance between x and its assigned cluster. Let $lb(x) \leq d(x, c)\ \forall\ c \in \{\mathcal{C} - b(x)\}$, that is, $lb(x)$ is a lower bound on the distance between x and the closest cluster to which it is not assigned.

4.1.2 Triangle Inequality

The Triangle Inequality is a well-known property used in many Computer Science fields. We document its definition and proof here for completeness.

Theorem: Let $d(a, b)$ represents the distance (in Euclidean space) between a point a and b. If x is data point and b & c are cluster centers, then

$$|d(x, b) - d(b, c)| \leq d(x, c) \leq d(x, b) + d(b, c) \tag{1}$$

Proof:

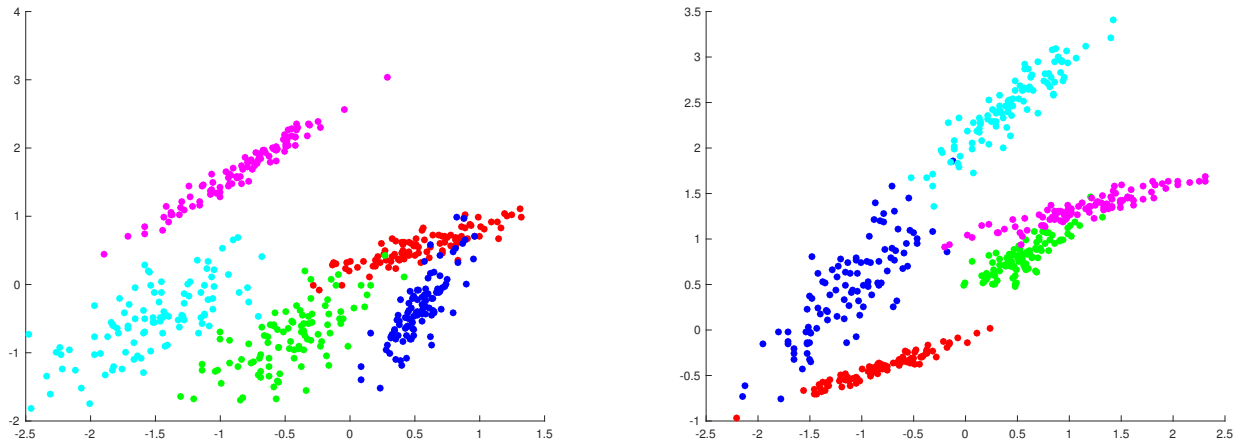
$$\begin{aligned} d(x, c) &= \|x - c\|_2 \\ &= \|x - b + b - c\|_2 \\ &\leq \|x - b\|_2 + \|b - c\|_2 \quad \text{Cauchy–Schwarz Inequality} \\ &= d(x, b) + d(b, c) \end{aligned} \tag{2}$$

Suppose that the left-hand side of Equation 1 is not true, that is

$$d(x, c) < |d(x, b) - d(b, c)|$$

Table 1: Data Parameters

Num. of Clusters	Num. of Features	Num. of Samples Per Cluster	Avg. Euclidean Distance of Means
100	100	100	100
1,000	500	500	500
10,000	1,000	1,000	1,000



(a) Example Data 1

(b) Example Data 2

Figure 2: Examples of generated synthetic data in two dimensions. Each cluster is represented with different colors.

Without loss of generality, let $d(x,b) > d(b,c)$. Then,

$$d(x,b) - d(b,c) > d(x,c)$$

From Equation 2, we know

$$\begin{aligned} d(b,c) &\leq d(b,x) + d(x,c) \\ &= d(x,b) + d(x,c) \end{aligned}$$

Thus,

$$\begin{aligned} d(x,c) &< d(x,b) - d(b,c) \\ &\leq d(x,b) - (d(x,b) + d(x,c)) \\ &= -d(x,c) \end{aligned}$$

This is a contradiction. Thus, $d(x,c) \geq |d(x,b) - d(b,c)|$. □

4.1.3 *Global-Filtering Condition*

Theorem: A point x in the cluster defined by the cluster center $b(x)$ does not change its cluster after a center update if

$$lb(x) - \max_{c \in \mathcal{C}} \delta(c) \geq ub(x) + \delta(b(x)) \tag{3}$$

Intuition: We know that $lb(x)$ is the distance between x and the closest cluster center to which x is not assigned (i.e. closest cluster center other than $b(x)$). The $\max_{c \in \mathcal{C}} \delta(c)$ term will yield the distance of the farthest-moving cluster from iteration i to iteration $i+1$. We know that $ub(x)$ is the distance between x and its assigned cluster $b(x)$. The $\delta(b(x))$ term will yield the distance x's assigned cluster at iteration i moves between iteration i and iteration $i+1$. The left-hand side of Equation 3, $lb(x) - \max_{c \in \mathcal{C}} \delta(c)$, indicates how close a cluster other than $b(x)$ could possibly be between iteration i and $i+1$. The right-hand side of Equation 3, $ub(x) + \delta(b(x))$, tells us the maximum possible distance between x and the center of $b(x)$ at iteration $i+1$. Thus, $b'(x) = b(x)$ if Equation 3 holds true, otherwise we need to compare the distances between x and all $c \in \mathcal{C}$ to find $b'(x)$. Figure 3 illustrates this concept.

Proof: Let $b(x)$ be x's cluster in iteration i and b' is the same cluster in iteration $i+1$. Let c be any cluster other than $b(x)$ and c' is the same cluster in iteration $i+1$. From the triangle inequality, we have

$$d(x,c') \geq d(x,c) - d(c,c') = d(x,c) - \delta(c)$$

We also know that $\delta(c) \geq \max_{p \in \mathcal{C}} \delta(p)$. Thus,

$$d(x,c') \geq d(x,c) - \max_{p \in \mathcal{C}} \delta(p)$$

We use the fact that $lb(x) \leq d(x,c)$ to acheive the inequality

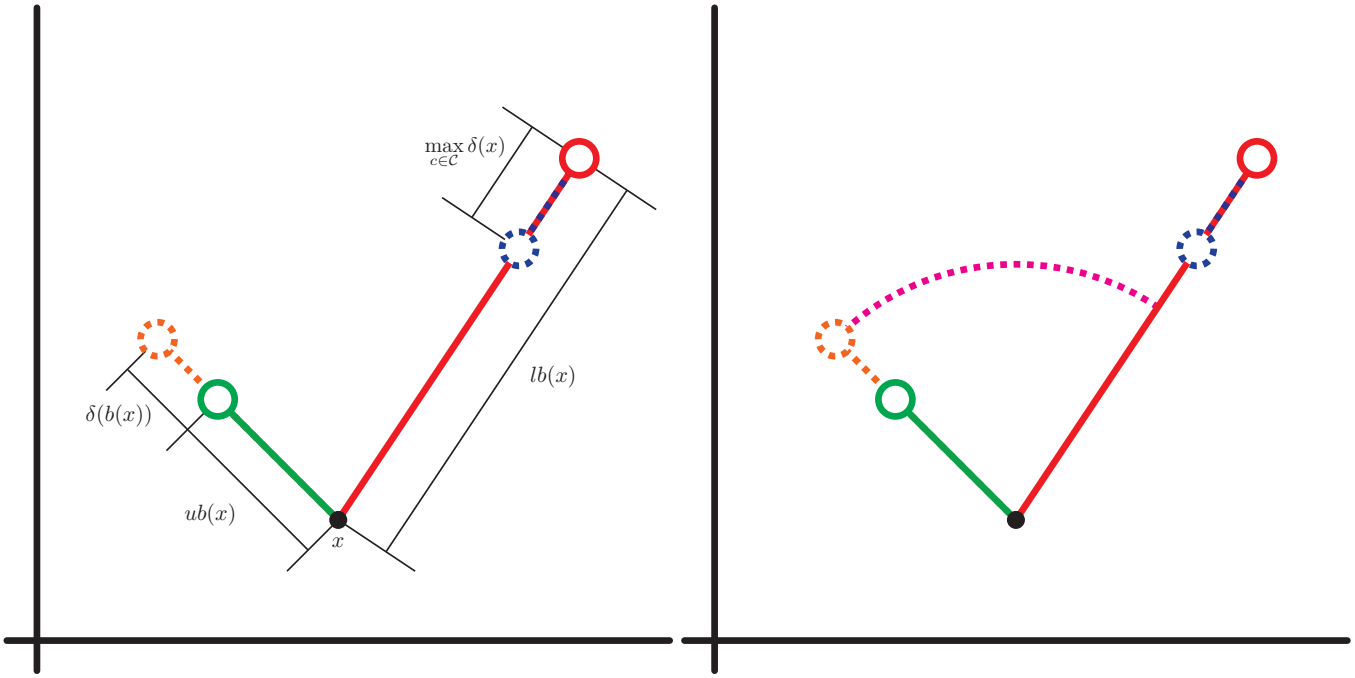
$$d(x,c') \geq lb(x) - \max_{p \in \mathcal{C}} \delta(p)$$

We also know that

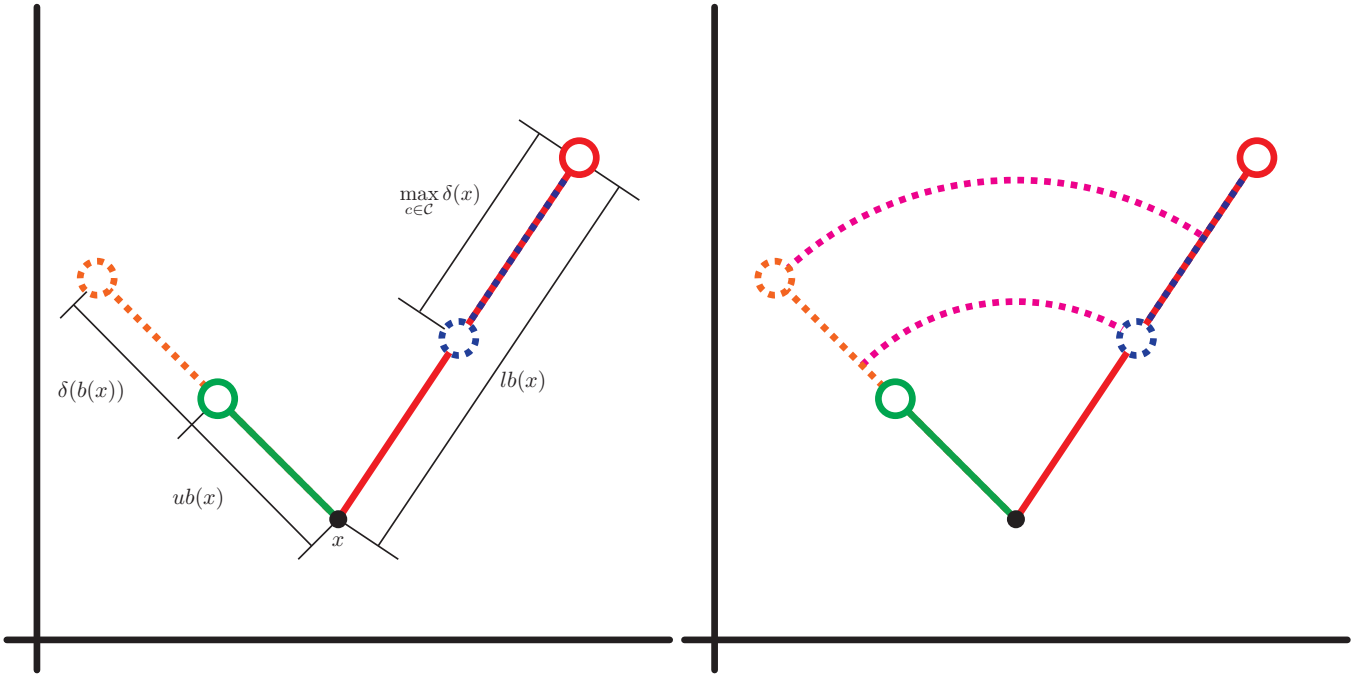
$$d(x,b') \leq d(x,b(x)) - d(b(x),b') = d(x,b(x)) - \delta(b(x))$$

By definition, $d(x,b(x)) \leq ub(x)$. Thus,

$$d(x,b') \leq d(x,b(x)) - \delta(b(x)) \leq ub(x) - \delta(b(x))$$



(a) Success Case



(b) Failure Case

Figure 3: The Global-Filtering Condition tests whether we need to compare x to all the new centroid update or leave it assigned to the same cluster. If the test is successful (i.e. Equation 3 holds), then $b'(x) = b(x)$. If the test fails (i.e. Equation 3 does not hold), then we must calculate the distance between x and all $c \in \mathcal{C}$ to find $b'(x)$.

Therefore, b' remains the closest cluster provided that

$$lb(x) - \max_{c \in \mathcal{C}} \delta(c) \geq ub(x) + \delta(b(x))$$
$$d(x, c') \geq d(x, b') \qquad \square$$

Potential Problem: The Global-Filtering Condition is sensitive to "*big-movers*". That is, if $\max_{c \in \mathcal{C}} \delta(c)$ is large, then Equation 3 will be rarely satisfied. Therefore, we will be forced to calculate the distance between x and *all* of the cluster centers. The speed-up gained by a reduction in the

number of distance calculations will be lost. Classical K-means will yield better performance since the work is the same but the Global-Filtering Condition will incur additional overhead in maintain the upper and lower bounds for each point.

Generalization to Group Filtering: To combat the "*big-movers*" problem, the authors propose a generalization of the Global-Filtering Condition. Instead of applying the Global-Filter to the initial k clusters, the data is split into t groups (this is based on the initial clustering, which is obtained with 5 iterations of classic K-means). The Global-Filtering condition will be applied to each group rather than each cluster.

The number of groups is an important question. The authors suggest $t = \frac{k}{10}$ which they found to give the best overall performance in their experiments. When $t = k$ (i.e. the number of clusters per group is 1), then Group Filtering reduces to Global Filtering. The parameter t makes the algorithm more elastic. That is, if t is large then there are fewer distance calculations but more overhead (to maintain lower bounds). If t is small, then there are more distance calculation but less overhead. Thus, the algorithm is adjustable to fit the needs of the application it will be deployed in.

The grouping is sensitive to a poor initialization. The authors claim that random groups will lead to poor performance. This is because the cluster center in this case are essentially meaningless in the beginning as there is no structure to the groupings. However, if we make an educated guess about the initial groups, then we stand to reduce the chance of a bad initialization. For this reason, the authors suggest grouping based on the initial cluster sets.

4.1.4 Local-Filtering Condition

Theorem: A cluster center $c' \in G'_i$ cannot be the closest center to the point x if there is a center $p' \neq c'$ where $p' \in \left\{G'_i \cup (G'_i)^{\mathrm{C}}\right\}$ such that

$$d\big(x, p'\big) < lb(x, G_i) - \delta(c) \tag{4}$$

Intuition: We know that $lb(x, G_i)$ represents a lower bound on the distance between x and the closest cluster center in G_i to which x is not assigned. The $\delta(c)$ term is the distance the cluster c moves between iteration i and iteration i and $i + 1$. Thus, the right-hand side of Equation 4 represents the smallest possible distance between x and c'. Therefore, c' cannot be the closest cluster if there is a point with a distance smaller than the right-hand side of Equation 4. Figure 4 illustrates this concept.

Proof: From the triangle inequality, we have

$$d\big(x, c'\big) \geq d(x, c) - d\big(c, c'\big)$$

This theorem stems from the fact that $lb(x, G_i) - \delta(c)$ represents the smallest possible distance between x and c'. By definition, we know $d(x, c) \geq lb(x, G_i)$ and $d(c, c') = \delta(c)$. Thus,

$$d\big(x, c'\big) \geq d(x, c) - d\big(c, c'\big) \geq lb(x, G_i) + \delta(c)$$

Therefore c' cannot be the closest center, if there exists a $p' \neq c'$ such that

$$d\big(x, p'\big) < lb(x, G_i) - \delta(c) \qquad \square$$

4.2 Algorithm

Algorithm 1 describes the Yinyang K-means algorithm. It takes X, k, and t as parameters. The X parameter is the data. The k is the number of clusters to partition the data into (same as classic K-means). The t is the number of groups to use. As explained above, if t is large then there are fewer distance calculations but more overhead. If t is small, then there are more distance calculation but less overhead.

Algorithm 1 Yinyang K-means

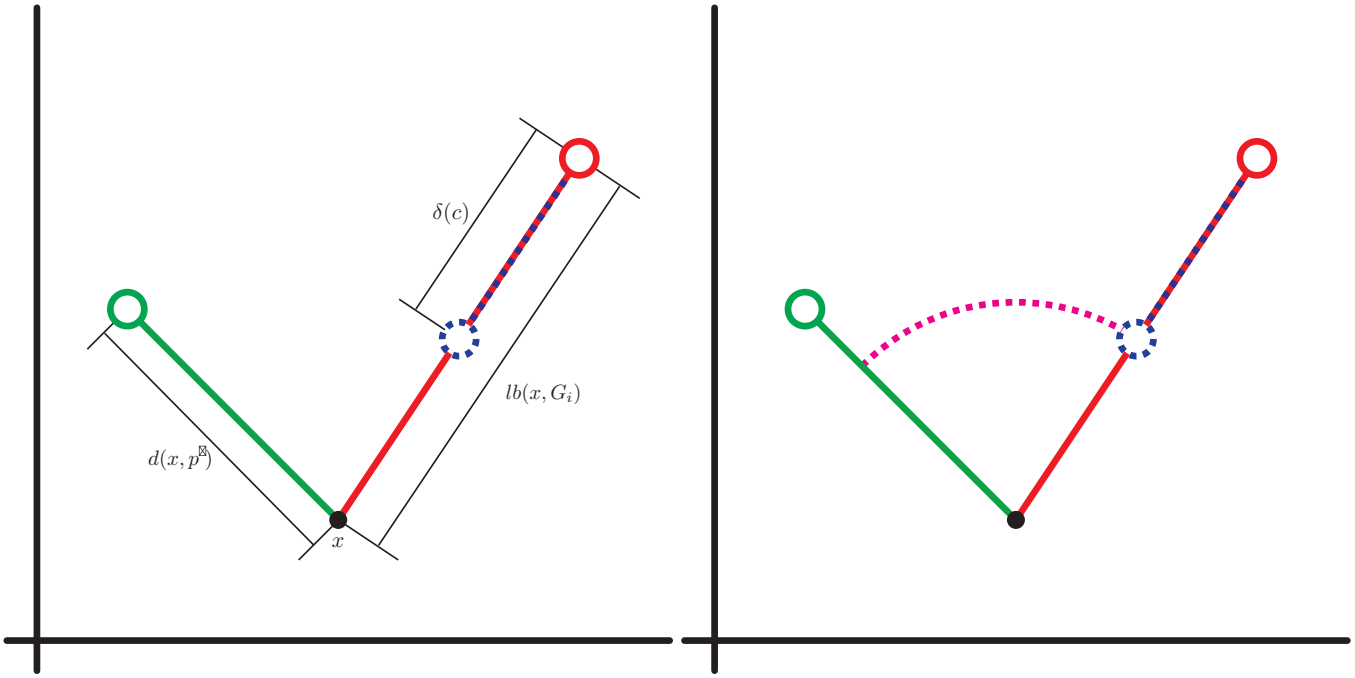
```
1: procedure YYKMEANS(X, k, t)
2:     Split X into t groups with 5 iterations of K-means
3:     Obtain ub and lb ∀ x ∈ X with 2 iter. of K-means
4:     Obtain initial cluster assignments
5:     repeat
6:         Update cluster centers
7:         Obtain max_{c∈G_i} δ(c) ∀ G_i
8:         Update ub(x, G_i) and lb(x, G_i) ∀ G_i
9:         for all x ∈ X do
10:            if Pass Global-Filter then
11:                b'(x) = b(x)
12:            else
13:                if Pass Local-Filter then
14:                    b'(x) = b(x)
15:                else
16:                    Search for b'(x)
17:                end if
18:            end if
19:        end for
20:    until Assignments Unchanged
21:    return Assignments
22: end procedure
```

5. IMPLEMENTATION

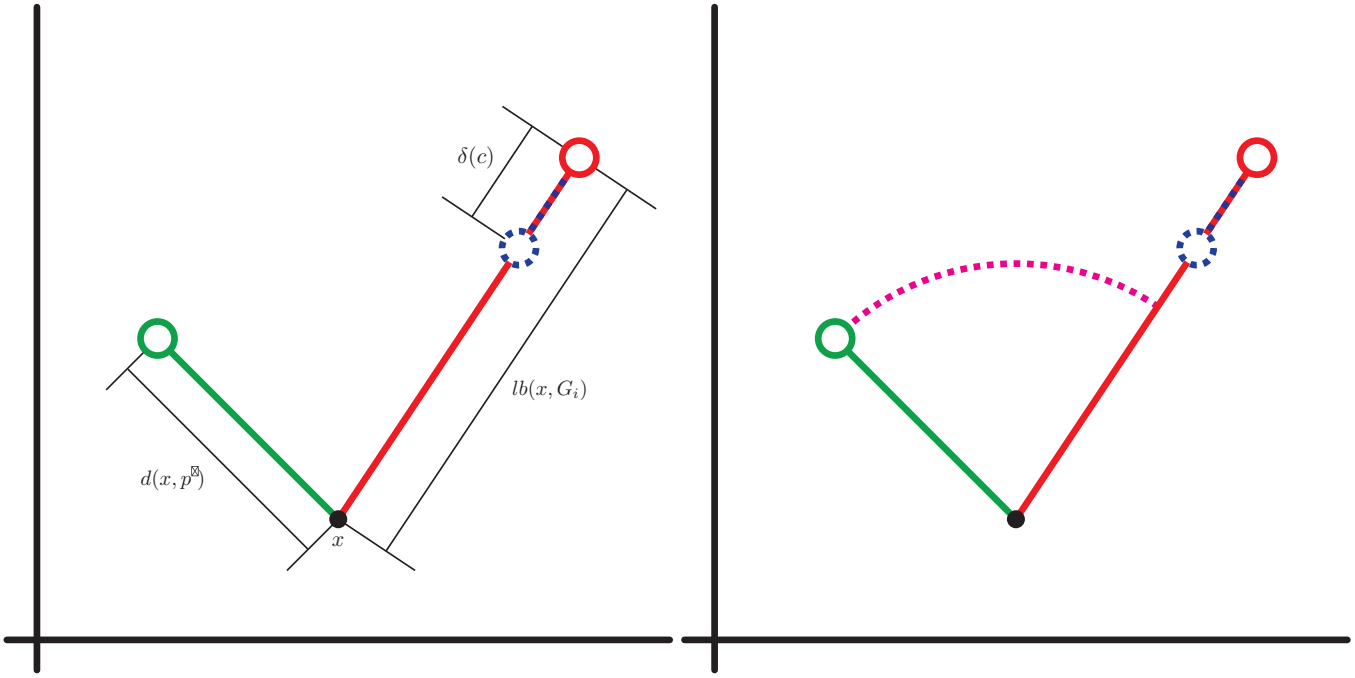
The authors generously provide their code free to use. It is implemented using the C++ library GraphLab. We attempted to build this tool and run the code. However, we were unable to get it to compile. We consulted with Kelly Climer and Antonio Gurgel, the CSE system administrators, but we were still unable to compile the code.

The authors distribute their code with the GraphLab package included. However, the GraphLab package requires the LibEvent package. However, the GraphLab was unable to download this package in its configuration process. This is because in the time since the authors published the Yinyang K-means code, the LibEvent package moved from `sourceforge.com` to `github.com`. So the links were no longer active and GraphLab could no longer download them. We manually edited the GraphLab CMakeFiles to update the `sourceforge` links to `github` links. However, it seems something changed in LibEvent's move as the package downloaded was missing a file that CMake expected to find in the package.

This seemed to become a lost cause, so we next tried to download the latest version of GraphLab and use it with the `yykmeans.cpp` distributed by the authors. However, since the time that the paper was presented in ICML in the summer of 2015, it appears GraphLab was had a significant change to its API. One of the header files used in `yykmeans.cpp` was nowhere to be found in the latest version. Additionally, many of the objects in GraphLab had been changed in the way that they are used. So, it seemed



(a) Success Case



(b) Failure Case

Figure 4: The Local-Filtering Condition tests whether c' has the potential to be $b'(x)$. If the test is successful (i.e. Equation 4 holds), then c' has the potential to be $b'(x)$. If the test fails (i.e. Equation 4 does not hold), then c' cannot be $b'(x)$.

that this option was not viable.

Due to these difficulties, we chose to attempt to implement the algorithm ourselves in MATLAB. We had always planned to implement the algorithm ourselves to increase our understanding of the method, but we thought it would be better to use the author's C++ version for the larger datasets. We found that the algorithm as described is not precise enough for easy implementation; there were even some errors in the paper's description. We consulted one of the authors for assistance and she was kind enough to answer several questions we had while working on our implementation.

In order to make a more fair comparison we implemented our own K-means algorithm to avoid any possible under-the-hood optimizations that may exist in the native MATLAB version. Our own version which allowed us to seed the initial centers as well as record the time per iteration and the number of iterations required to converge.

Despite assistance from the authors, we were unable to successfully implement the algorithm in such a way that replicates the author's results. More details follow in the results section.

6. RESULTS

The authors claim that their algorithm achieves the same clustering results as classic K-means when seeded with the same initial centers. Additionally, they claim that the number of iterations is the same, but each iteration happens 9.36 times faster on average.

Due to the large size of many of our data sets and the difficulties encountered during implementation, we were not able to run comparisons on many data sets above 500 MB in size, which excluded any set with 1,000 or 10,000 clusters.

Our implementation did not see these results come to fruition. Often, our algorithm dropped clusters that the classic K-means did not. For example, on the data set with 100 clusters, 100 samples per cluster, 100 features, and an inter-cluster distance of 100, classic K-means ended with 97 unique indices while our implementation of Yinyang K-means ended with two. Figure 5 shows an example of when a cluster is dropped and when it is not.

Our implementation also did poorly on the number of iterations, often requiring an order of magnitude more iterations than the classic implementation. For example, on the same data set mentioned above, classic K-means took 38 iterations while our implementation took 317 iterations. As a result of the slowness of convergence of our Yinyang implementation, many of the larger data sets that we were able to test did not even see convergence within the limit of 1,000 iterations.

A plot of the number of iterations taken on the largest data sets we ran (100 clusters, 1,000 samples per cluster, 100-1,000 features, and an inter-cluster distance of 100-1,000) can be seen in Figure 6. In this figure, all the blue points are for classic K-means and red points are for Yinyang K-means. The x symbols represent the number of iterations taken on the data set for 100 features, the o symbols are the number of iterations taken for 500 features, and the + symbols are the number of iterations taken for 1,000 features.

Finally, time per iteration was also worse in our implementation than in classic K-means, although the difference was not as great as with the previous metrics. The time difference at the smallest data set tested (100 clusters, 100 samples per cluster, 100 features, and an inter-cluster distance of 100) was 0.098 seconds per iteration compared to 0.327. This difference shrank as the data set got larger: the largest tested sets (100 clusters, 1,000 samples per cluster, 100-1,000 features, and an inter-cluster distance of 100-1,000) saw average per-iteration times of 12.145 seconds for classic K-means and 12.763 seconds for our implementation of Yinyang K-means. These results can be seen in Figure 7. The symbols represent the same data as previously, except the vertical axis shows mean time per iteration (MTPI) in seconds rather than total number of iterations. While previous metrics had dismal results, the MTPI of our implementation of Yinyang K-means approaches that of classic K-means as the data set complexity increases. This shows promise that for very large data or data with many features, our implementation might overtake the classic algorithm in time per iteration. However, the total number of iterations is still problematic, since all nine tests for the largest data sets timed out.

7. CONCLUSION

It is difficult to draw too many conclusions when the algorithm is obviously not working correctly. However, if we assume the authors' method works, then Yinyang K-means does work as a "drop-in" replacement of classic K-means. By maintaining bound for each data point, the number of distance calculations is drastically reduced. In the authors' work, they achieved a speed-up regardless of data set size, number of features, or number of clusters. For these reasons, Yinyang K-means offers an improved clustering method.

8. FUTURE WORK

The most obvious step is to ensure our implementation matches the authors' exactly. This will allow us to determine whether we can replicate the authors results or not. The authors only suggest a value of t, so a more detailed study on this parameter could be useful. As t varies, we could document the tradeoff in overhead versus the number of distance calculations needed. Since amount of data is growing larger and larger, it would be interesting to see if an approximation of the clustering could be used on very large datasets (over 1TB in size). The enormous amount of data is unlikely to achieve the true K-means clustering in a reasonable amount of time. However, an approximation could be useful, especially if it could be computed in reasonable amount of time.

9. CONTRIBUTIONS

In our opinion, we worked together well on this project. Ben wrote the introduction to this paper. Thomas generated the data and wrote the corresponding section in this paper. Thomas wrote the proof for the Triangle Inequality, Global-Filtering Condition, and Local-Filtering Condition. Ben implemented the algorithm in MATLAB and corresponded with the original authors when our results did not match theirs. We both worked to try and discover any bugs once we obtained results unlike the authors. Thomas prepared the theory section of the presentation while Ben prepared the result section.

10. REFERENCES

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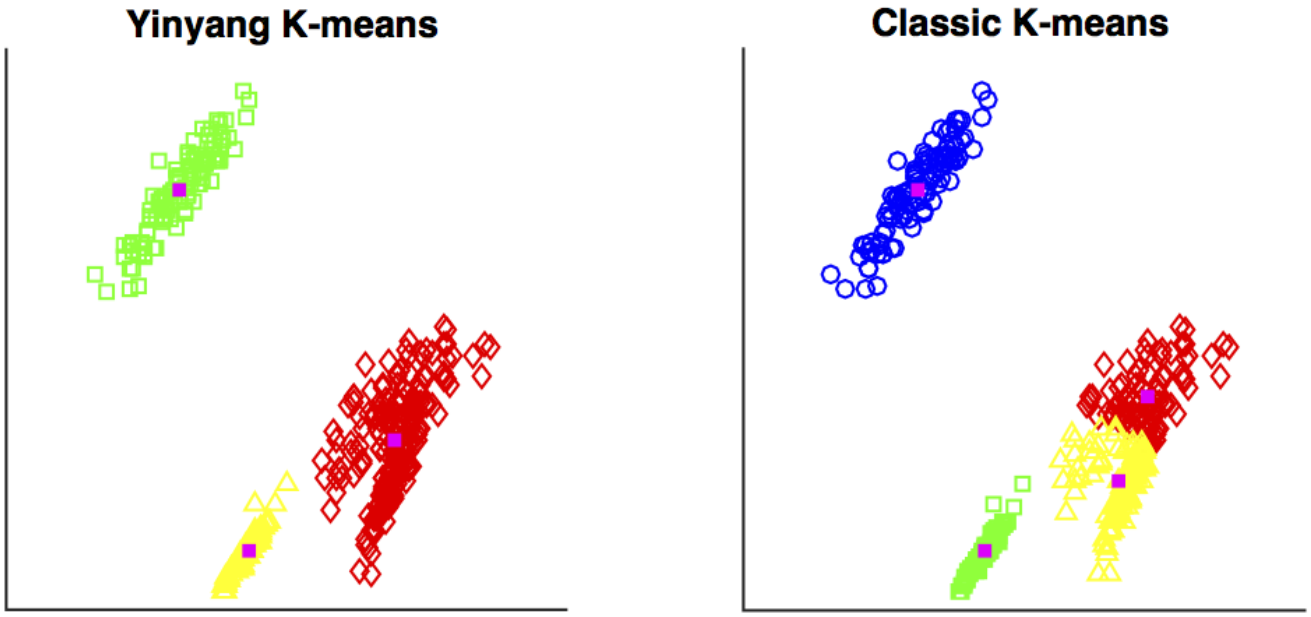
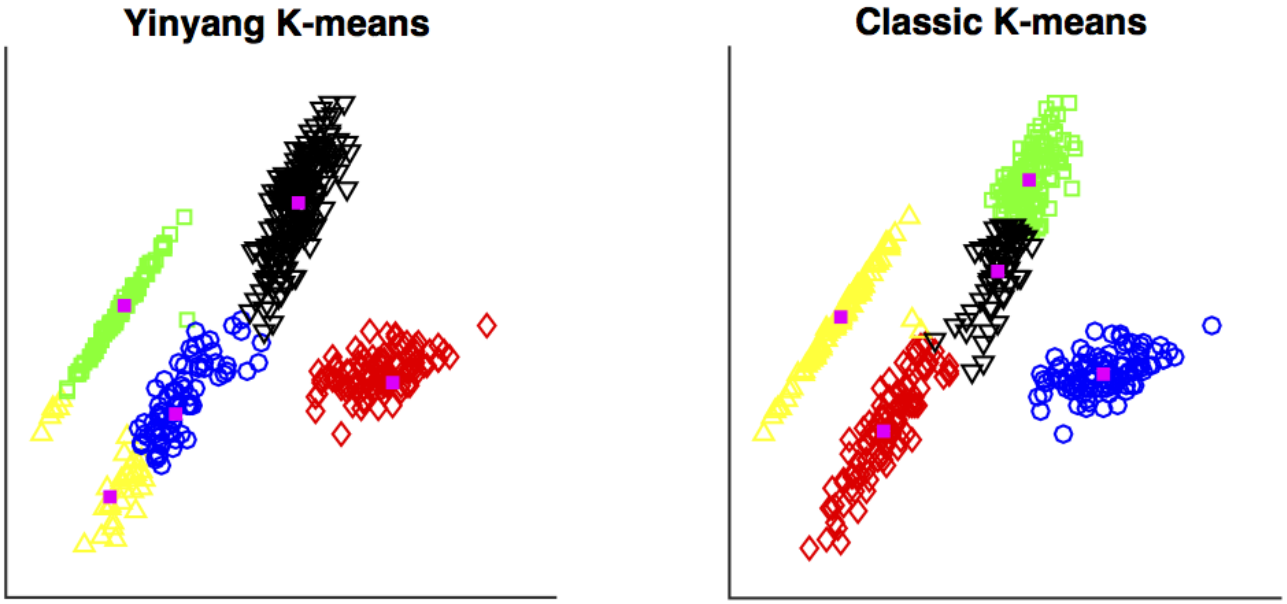


(a) Yinyang K-means drops a cluster ($k = 4$)



(b) Yinyang K-means does not drop a cluster ($k = 5$)

Figure 5: Cluster result

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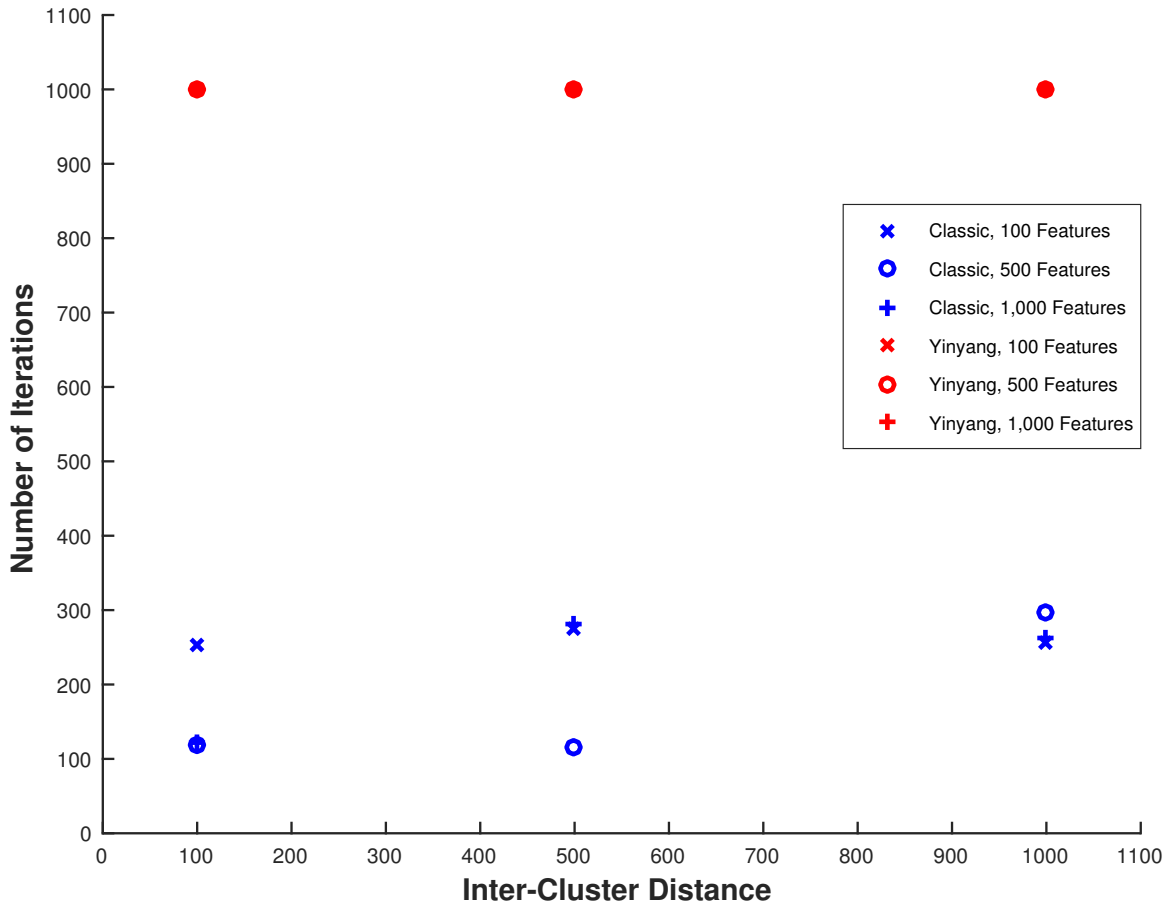

Figure 6: A plot of the number of iterations taken on various data sets.

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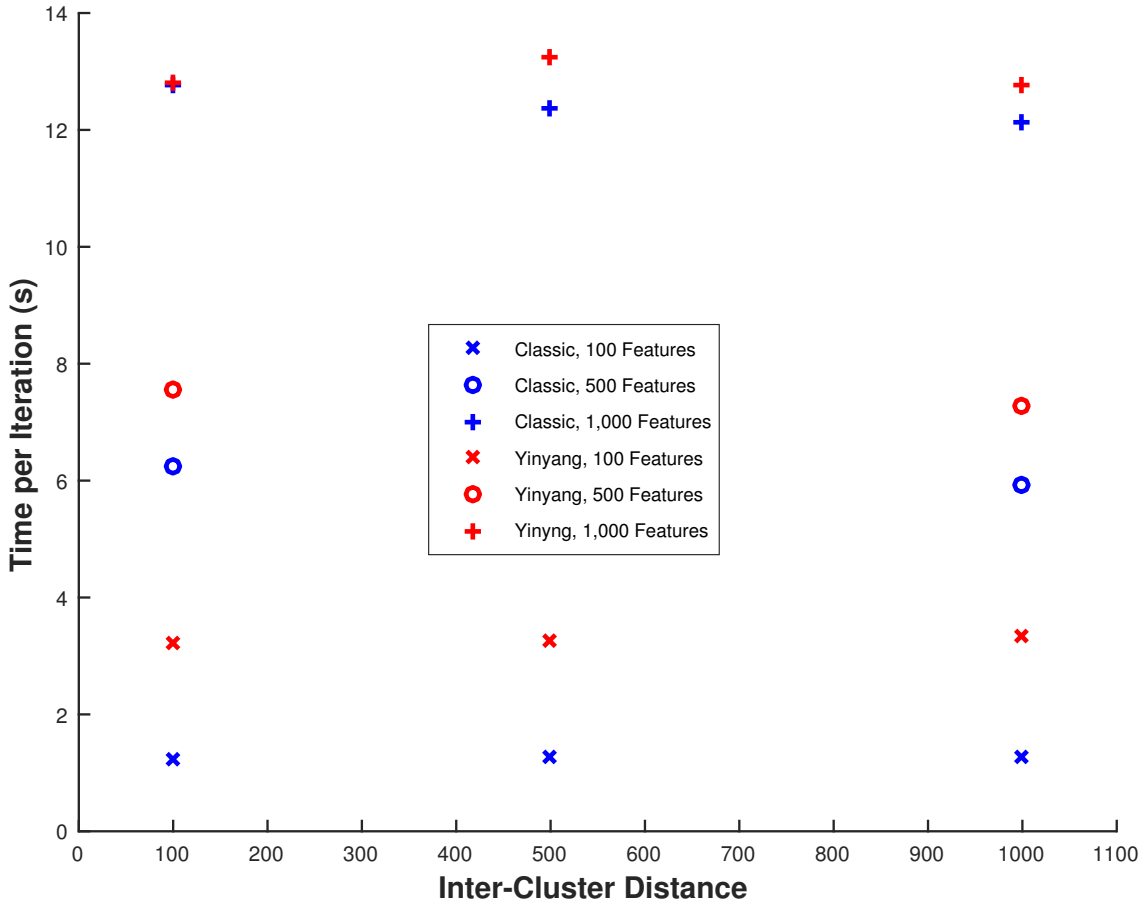

Figure 7: A plot of the time per iterations taken on various data sets.