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Automatic Clustering with Single Optimal Solution

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Abstract

Determining optimal number of clusters in a dataset is a challenging task. Though some methods are available, there is no algorithm that produces unique clustering solution. The paper proposes an Automatic Merging for Single Optimal Solution (AMSOS) which aims to generate unique and nearly optimal clusters for the given datasets automatically. The AMSOS is iteratively merges the closest clusters automatically by validating with cluster validity measure to find single and nearly optimal clusters for the given data set. Experiments on both synthetic and real data have proved that the proposed algorithm finds single and nearly optimal clustering structure in terms of number of clusters, compactness and separation.

Keywords: Clustering, Optimal clusters, Cluster validity measure, Automatic clustering, Single Optimal Solution, Closest clusters.

1. Introduction

Jain (2010) specified that the partitional clustering technique, k-means, is the most computationally simple and efficient clustering method. Wu et al. (2008) have shown that the k-means was one of the top ten algorithms in data mining. Although the k-means method has a number of advantages over other data clustering methods, the specification of number of clusters is a priori, which is usually unknown.

Discovering an optimal number of clusters in a large data set is usually a challenging task. Jain (2010) shown a number of methods to determine k in k-means type algorithms.. Cheung (2005) studied a rival penalized competitive learning algorithm, and Xu (1997, 1996) has demonstrated a very good result in finding the cluster number. The algorithm is formulated by learning the parameters of a mixture model through the maximization of a weighted likelihood function. In the learning process, some initial seed centers move to the genuine positions of the cluster centers in a data set, and other redundant seed points will stay at the boundaries or outside of the clusters. Guo et.al (2002) have provided a unified algorithm for both unsupervised and supervised learning for solving the problem of selection of the cluster number. Lee and Antonsson (2000) used an evolutionary method to dynamically cluster a data set. Sarkar, et al., (1997) and Fogel, Owens, and Walsh (1966) are proposed an approach to dynamically cluster a data set using evolutionary programming, where two fitness functions are simultaneously optimized: one gives the optimal number of clusters, whereas the other leads to a proper identification of each cluster's centroid. Recently Swagatam Das and Ajith Abraham (2008) proposed an Automatic Clustering using Differential

Evolution (ACDE) algorithm by introducing a new chromosome representation. The majority of these methods to determine the best number of clusters may not work very well in practice. The clustering algorithms are require to be run several times for good solution, and model-based methods, such as cross-validation and penalized likelihood estimation, are computationally expensive. All these algorithms cause different solutions in different independent runs. There is no single clustering algorithm that finds unique set of optimal clusters automatically. This paper proposes a new clustering algorithm Automatic Merging for Single Optimal Solution (AMSOS) is a parameter free, simple finds unique and nearly optimal clusters for large data set automatically.

The proposed Automatic Merging for Single Optimal Solution (AMSOS) is a two-phase iterative procedure. Karteeka et al. (2010) have proposed Single Pass Seed Selection algorithm to initialize seeds for k-means. In the first phase, it produces single set of optimal clusters by initializing initial seeds using SPSS. In the second phase, iteratively a low probability cluster is merged with its closest cluster using average linkage after validating with cluster validity metric. The proposed AMSOS is aimed to meet requirements as 1) nearly optimal clusters and 2) unique clustering solution. Experiments on both synthetic and real data sets from UCI prove that the proposed algorithm finds nearly optimal results in terms of compactness and separation.

Section (2) deals with formulation of the proposed algorithm, while section (3) illustrates the effectiveness of the new algorithm experimenting results on synthetic, real, and micro array data sets. Comments on the results of AMSOS are included in Section (4) and finally concluding remarks are included in section (5).

2 Materials and Methods

Let $P = \{P_1, P_2, \dots, P_m\}$ be a set of m objects in which each object P_i is represented as $[p_{i,1}, p_{i,2}, \dots, p_{i,n}]$ where n is the number of features .

2.1 Automatic Merging for Single Optimal Solution

The choice of the initial seeds was done by SPSS in AMSOS. The SPSS is an optimal seed selection algorithm that produces unique set of initial seeds to k-means type algorithms and is a modification to k-means++ proposed by Arthu and Vassilvitskii (2007). Thus the AMSOS produces single and nearly optimal clustering solution. In the clustering literature Pal and Bezdek (1995) reported that the number of clusters in the data set is in the range from 2 to \sqrt{m} . The AMSOS algorithm first finds $k_{max} = \sqrt{m}$ clusters using k-means and iteratively merges the lower probability cluster with its closest cluster according to average linkage and validates the merging result using Rand Index which is proposed by Rand (1971). The probability of cluster A is as follows.

$$P(A) = \frac{|A|}{|X|}$$

where $|A|$ is number of elements belongs to cluster A and $|X|$ is the total number of elements in the original dataset, X. The distance between two clusters is measured using average linkage i.e. the distance between two clusters, $D(C_i, C_j)$ is computed as the average distance between elements from the first cluster and elements from the second cluster and as shown in the following equation.

$$D(C_i, C_j) = \frac{1}{n_i n_j} \sum_{x \in C_i} \sum_{x' \in C_j} |x - x'|$$

Steps:

1. Initialize kmax, number of clusters to the square root of total number of objects
2. Assign kmax objects using SPSS to the cluster centroids
3. Find the clusters using k-means
4. Compute Rand index
5. Find a cluster that has least probability and merge with its closest cluster. Recompute centroids, Rand index and decrement the number of clusters by one. If the newly computed Rand index is greater than the previous Rand index, then update Rand Index, number of clusters and cluster centroids with the newly computed values.
6. If step 5 has been executed for each and every cluster, then go to step7, otherwise got to step5.
7. If there is no change in number of clusters, then stop, otherwise go to step2

2.2 Data sets

The efficiency of new algorithms are evaluated by conducting experiments on four artificial data sets, three real datasets down loaded from the web site UCI and two microarray data sets (two yeast data sets) downloaded from <http://www.cs.washington.edu/homes/kayee/cluster> (Yeung 2001).

The real data sets used:

1. Iris plants database (n = 150, d = 4, K = 3)
2. Glass (n = 214, d = 9, K = 6)
3. Wine (n = 178, d = 13, K = 3)

The real microarray data sets used:

1. The yeast cell cycle data (Cho et al., 1998) showed the fluctuation of expression levels of approximately 6000 genes over two cell cycles (17 time points). We used two different subsets of this data with independent external criteria. The first subset (the 5-phase criterion) consists of 384 genes whose expression levels peak at different time points corresponding to the five phases of cell cycle (Cho et al., 1998). We expect clustering results to approximate this five class partition. Hence, we used the 384 genes with the 5- phase criterion as one of our data sets.
2. The second subset (the MIPS criterion) consists of 237 genes corresponding to four categories in the MIPS database (Mewes et al., 1999). The four categories (DNA synthesis and replication, organization of centrosome, nitrogen and sulphur metabolism, and ribosomal proteins) were shown to be reflected in clusters from the yeast cell cycle data (Tavazoie et al., 1999).

The four synthetic data sets from $Np(\mu, \Sigma)$ with specified mean vector and variance covariance matrix are as follows.

1. Number of elements, m=350, number of attributes, n=3, number of clusters, k =2 with

$$\mu 1 = \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix} \quad \Sigma 1 = \begin{pmatrix} 1 & 0.50 & 0.3333 \\ & 1 & 0.6667 \\ & & 1 \end{pmatrix} \quad \mu 2 = \begin{pmatrix} 7 \\ 6 \\ 9 \end{pmatrix} \quad \Sigma 2 = \begin{pmatrix} 1 & 1 & 1 \\ & 2 & 2 \\ & & 3 \end{pmatrix}$$

2. The data set with m=400, n=3, clusters=4 with

$$\mu 1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \Sigma 1 = \begin{pmatrix} 0.65 & 0 \\ & 0.65 \end{pmatrix} \mu 2 = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \Sigma 2 = \begin{pmatrix} 1 & 0.7 \\ & 1 \end{pmatrix} \mu 3 = \begin{pmatrix} -3 \\ +3 \end{pmatrix} \Sigma 3 = \begin{pmatrix} 0.78 & 0 \\ & 0.78 \end{pmatrix} \mu 4 = \begin{pmatrix} -6 \\ +4 \end{pmatrix} \Sigma 4 = \begin{pmatrix} 0.5 & 0 \\ & 0.5 \end{pmatrix}$$

3. m=300, n=2, k=3;

$$\mu 1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \Sigma 1 = \begin{pmatrix} 1 & 0 \\ & 1 \end{pmatrix} \mu 2 = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \Sigma 2 = \begin{pmatrix} 1 & 0 \\ & 1 \end{pmatrix} \mu 3 = \begin{pmatrix} -3 \\ +3 \end{pmatrix} \Sigma 3 = \begin{pmatrix} 0.7 & 0 \\ & 0.7 \end{pmatrix}$$

4. m=800, n=2, k=6;

$$\mu 1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \Sigma 1 = \begin{pmatrix} 0.65 & 0 \\ & 0.65 \end{pmatrix} \mu 2 = \begin{pmatrix} -8 \\ -6 \end{pmatrix} \Sigma 2 = \begin{pmatrix} 1 & 0.7 \\ & 1 \end{pmatrix} \mu 3 = \begin{pmatrix} -3 \\ +6 \end{pmatrix} \Sigma 3 = \begin{pmatrix} 0.2 & 0 \\ & 0.2 \end{pmatrix} \mu 4 = \begin{pmatrix} -8 \\ +14 \end{pmatrix} \Sigma 4 = \begin{pmatrix} 0.5 & 0 \\ & 0.5 \end{pmatrix}$$

$$\mu 5 = \begin{pmatrix} 10 \\ 12 \end{pmatrix} \Sigma 5 = \begin{pmatrix} 0.3 & 0 \\ & 0.3 \end{pmatrix} \mu 6 = \begin{pmatrix} +14 \\ -14 \end{pmatrix} \Sigma 6 = \begin{pmatrix} 0.1 & 0 \\ & 0.1 \end{pmatrix}$$

3. Experimental Results

The clustering results of AMSOS are compared with the results of K-means, k-means++, SPSS, a method to obtain robust optimal centroids in a single pass, which is developed by Karteeika (2011), fuzzy-kmeans, and Automatic Clustering using Differential Evolution (ACDE) to determine optimal clusters.

The k-means, k-means++, Fuzzy-k and SPSS algorithms are implemented with the number of clusters as equal to the number of classes in the ground truth.

3.2 Presentation of Results

While comparing the performance of AMSOS with the other techniques (k-means, k-means++, fuzzy-k, SPSS, ACDE) we are concentrating on two major issues: 1) quality of the solution as determined by Error rate and with cluster validity measures Rand, has proposed by Rand (1971), Adjusted Rand, DB, proposed by Davis and Bouldin (1979), CS, is proposed by Chou (2004) and Silhouette is proposed by Rousseeuw (1987) 2) ability to find the optimal number of clusters. Forty independent runs of each algorithm is taken for the algorithms those produce different results in different individual runs. The Rand, Adjusted Rand, DB, CS and Silhouette metrics values and the overall error rate of the mean-of-run solutions provided by the algorithms over the 10 datasets have been provided in Table 1.

The error rate is defined as

$$err = \frac{N_{mis}}{m} * 100$$

where N_{mis} is the number of misclassifications and m is the number of elements of data set original data set X. The best performance values and least performance values that found in 40 independent runs of each algorithm on each dataset is tabulated in Table2 and in Table3. Table 4 contains the obtained centroids from AMSOS for the synthetic datasets and their original cluster centroids.

4. Comments on the results of AMSOS

- In case of Synthetic1, Synthetic2, Synthetic3, Synthetic4 the AMSOS resulting single, robust, optimal clustering solution with least error rates compared to other existing algorithms.
- Table4 demonstrates that the efficiency of AMSOS in determining optimal centroids, which are very close to the original centroids.

- The Automatic Merging for Single Optimal Solution (AMSOS) performs well on different data sets. The misclassification rate of single clustering solution of the AMSOS is either as same as the minimum error rate found in 40 independent runs or nearly equal with the means of different solutions of the existing algorithms for all the data sets. Table 5 shows the error rates of unique solutions of SPSS, AMSOS and means of error rates of forty independent runs of ACDE, k-means, k-means++, fuzzy-k.
- The proposed AMSOS shows an improved performance of 30% over ACDE in terms of error rate.
- For the micro array data sets it is resulting single solution with error rates 35.44, 44.01 for the yeast1 and yeast2.
- The poor performance of AMSOS can be seen in the data sets which contains non separable overlapped clusters.
- The AMSOS produces 82.21% qualitative clusters in terms of Rand validity measure.
- The quality of AMSOS on all data sets is 72.15% in terms of silhouette measure.

Note: Results of CS, ARI, etc., are very much in agreement with above all observations in the performance of AMSOS, hence detailed note with respect to them is not provided to avoid duplication.

5. Conclusions

AMSOS is totally a non-parameter procedure. Unlike the most of the algorithms, it does not require any heuristic parameter values in advance, though it requires k as input the output does not depends on the input. Being the high density point is the first seed, the SPSS (Karteeka 2011) avoids different results that occur from random selection of initial seeds. For the remaining seeds it follows k-means++. The algorithm is insensitive to outliers in seed selection. Thus the AMSOS in combination with SPSS centroids is outlier insensitive and results in single clustering solution. The table 4 demonstrated that the proposed algorithm produce clustering result with optimal centroids and with single solution.

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Table 1. Validity measures with error rates

Dataset	Algorithm	No. of clusters, k		Cluster Validity Measures						Mean Error rate
		i/p k	o/p k	ARI	RI	HI	SIL	DB	CS	
Synthetic1	k-means	2	2	0.92	0.96	0.92	0.839	0.467	0.645	0.236
	k-means++			0.925	0.962	0.925	0.839	0.466	0.567	1.914
	fuzk			0.899	0.95	0.9	0.839	0.468	0.52	2.571
	SPSS			0.932	0.966	0.932	0.839	0.465	0.725	1.714
	ACDE	19	3.05	0.85	0.925	0.849	0.643	0.772	1.348	51.56
	AMSOS	19	2	0.932	0.966	0.932	0.839	0.465	0.75	1.714
Synthetic2	k-means	4	4	0.821	0.927	0.854	0.718	0.58	1.178	19.1
	k-means++			0.883	0.953	0.907	0.776	0.519	1.21	7.16
	fuzk			0.944	0.979	0.957	0.791	0.484	0.931	2.2
	SPSS			0.939	0.977	0.953	0.792	0.527	0.812	2.4
	ACDE	22	5.35	0.885	0.957	0.914	0.68	0.674	1.321	58.89
	AMSOS	22	4	0.939	0.977	0.953	0.792	0.527	0.943	2.4
Synthetic3	k-means	3	3	0.957	0.98	0.96	0.813	0.509	0.87	2.242
	k-means++			0.97	0.987	0.974	0.823	0.761	0.92	1
	fuzk			0.97	0.987	0.974	0.823	0.5	0.96	1
	SPSS			0.97	0.987	0.974	0.823	0.507	0.657	1
	ACDE	17	4	0.472	0.777	0.553	0.754	0.461		83.59
	AMSOS	17	3	0.97	0.987	0.974	0.823	0.507	0.768	1
Synthetic4	k-means	6	6	0.816	0.941	0.882	0.82	0.407	0.72	51.27

	k-means++	28	7.9	0.958	0.988	0.976	0.932	0.222	0.62	10.96
	fuzk			0.98	0.994	0.988	0.953	0.183	0.45	8.738
	SPSS			1	1	1	0.975	0.144	0.723	0
	ACDE			0.979	0.994	0.989	0.878	0.308	0.359	53.21
	AMSOS			28	6	1	1	1	0.975	0.144
Iris	k-means	3	3	0.774	0.892	0.785	0.804	0.463	0.607	15.77
	k-means++			0.796	0.904	0.807	0.804	0.461	0.712	13.37
	fuzk			0.788	0.899	0.798	0.803	0.46	0.658	15.33
	SPSS			0.44	0.72	0.441	0.799	0.582	1.962	50.67
	ACDE	12	3.15	0.887	0.95	0.901	0.784	0.435	0.706	10.17
	AMSOS	12	2	0.568	0.776	0.553	0.952	0.233	0.402	33.33
Wine	k-means	3	3	0.295	0.675	0.35	0.694	0.569	0.612	34.58
	k-means++			0.305	0.681	0.362	0.694	0.562	0.678	33.54
	fuzk			0.34	0.7	0.401	0.696	0.566	0.753	30.34
	SPSS			0.337	0.699	0.398	0.696	0.601	0.813	30.34
	ACDE	13	4.45	0.367	0.723	0.447	0.373	0.555	1.626	52.89
	AMSOS	13	2	0.197	0.593	0.186	0.714	0.644	1.024	41.01
Glass	k-means	6	6	0.245	0.691	0.382	0.507	0.901	0.967	55.86
	k-means++			0.259	0.683	0.365	0.548	0.871	1.523	56.1
	fuzk			0.241	0.72	0.44	0.293	0.998	1.613	62.29
	SPSS			0.252	0.722	0.444	0.382	1.061	1.512	45.79
	ACDE	15	5.5	0.309	0.712	0.425	0.338	1.146	2.868	54.35
	AMSOS	15	5	0.27	0.669	0.337	0.639	0.95	1.366	70.56
Yeast1	k-means	4	4	0.497	0.765	0.53	0.466	1.5	1.439	35.74
	k-means++			0.465	0.751	0.503	0.425	1.528	1.678	37.49
	fuzk			0.43	0.734	0.468	0.37	2.012	1.679	39.18
	SPSS			0.508	0.769	0.538	0.464	1.471	1.217	35.44
	ACDE	15	5.55	0.594	0.806	0.612	0.348	2.314	2.669	81.86
	AMSOS	15	4	0.508	0.769	0.538	0.464	1.471	1.515	35.44
Yeast2	k-means	5	5	0.447	0.803	0.607	0.438	1.307	1.721	38.35
	k-means++			0.436	0.801	0.603	0.421	1.292	1.521	40
	fuzk			0.421	0.799	0.598	0.379	1.443	1.341	35.73
	SPSS			0.456	0.804	0.608	0.453	1.236	2.567	43.23
	ACDE	20	6.225	0.537	0.838	0.677	0.363	1.438	2.326	44.95
	AMSOS	20	4	0.469	0.8	0.6	0.506	1.154	1.342	44.01

Table 2. Best Validity indices along with error rate

Dataset	Algorithm	No.	of	Cluster Validity Measures	Minimu
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		clusters, k								m Error rate
		i/p k	o/p k	ARI	RI	HI	SIL	DB	CS	
Synthetic1	k-means	2		0.932	0.966	0.932	0.839	0.465	0.75	1.714
	k-means++			0.932	0.966	0.932	0.839	0.465	0.75	1.714
	fuzk			0.899	0.95	0.9	0.839	0.468	0.732	2.571
	SPSS			0.932	0.966	0.034	0.839	0.465	0.725	1.714
	ACDE	19	2	1	1	1	0.839	0.463	2.13	0
	AMSOS	19	2	0.932	0.966	0.932	0.839	0.465	0.75	1.714
Synthetic2	k-means	4		0.939	0.977	0.953	0.792	0.44	1.821	2.4
	k-means++			0.939	0.977	0.953	0.792	0.44	1.805	2.4
	fuzk			0.944	0.979	0.957	0.791	0.44	0.931	2.2
	SPSS			0.939	0.977	0.023	0.792	0.527	0.812	2.4
	ACDE	22	4	0.939	0.977	0.953	0.79	0.445	2.224	2.4
	AMSOS	22	4	0.939	0.977	0.953	0.792	0.527	0.943	2.4
Synthetic3	k-means	3		0.97	0.987	0.974	0.823	0.474	0.768	1
	k-means++			0.97	0.987	0.974	0.823	0.474	1.701	1
	fuzk			0.97	0.987	0.974	0.823	0.474	0.749	1
	SPSS			0.97	0.987	0.013	0.823	0.507	0.657	1
	ACDE	17	4	0.566	0.836	0.671	0.872	0.19	1.764	50
	AMSOS	17	3	0.97	0.987	0.974	0.823	0.507	0.768	1
Synthetic4	k-means	6		1	1	1	0.975	0.139	0.759	0
	k-means++			1	1	1	0.975	0.142	0.403	0
	fuzk			1	1	1	0.975	0.127	0.412	0
	SPSS			1	1	0	0.975	0.144	0.723	0
	ACDE	28	6	1	1	1	0.975	0.136	0.605	0
	AMSOS	28	6	1	1	1	0.975	0.144	0.233	0
Iris	k-means	3		0.886	0.95	0.899	0.806	0.411	0.753	4
	k-means++			0.886	0.95	0.899	0.806	0.411	0.753	4
	fuzk			0.886	0.95	0.899	0.806	0.411	0.769	4
	SPSS			0.44	0.72	0.28	0.799	0.582	1.962	50.67
	ACDE	12	3	0.904	0.958	0.916	0.806	0.435	1.061	3.333
	AMSOS	12	2	0.568	0.776	0.553	0.952	0.233	0.402	33.33
Wine	k-means	3		0.337	0.699	0.398	0.696	0.447	0.939	30.34
	k-means++			0.337	0.699	0.398	0.696	0.447	0.939	30.34
	fuzk			0.347	0.704	0.408	0.696	0.488	0.929	29.78
	SPSS			0.337	0.699	0.301	0.696	0.601	0.813	30.34
	ACDE	13	2	0.423	0.755	0.511	0.686	0.555	3.368	28.65
	AMSOS	13	2	0.197	0.593	0.186	0.714	0.644	1.024	41.01

Glass	k-means	6		0.287	0.728	0.456	0.656	0.744	1.917	44.86
	k-means++			0.288	0.725	0.45	0.729	0.522	1.745	46.73
	fuzk			0.263	0.733	0.467	0.317	0.883	3.995	48.13
	SPSS			0.252	0.722	0.278	0.382	1.061	1.512	45.79
	ACDE	15	4	0.331	0.758	0.517	0.636	1.146	3.883	37.38
	AMSOS	15	5	0.27	0.669	0.337	0.639	0.95	1.366	70.56
Yeast1	k-means	4		0.515	0.773	0.545	0.473	1.307	2.117	35.02
	k-means++			0.515	0.772	0.545	0.473	1.376	2.006	35.02
	fuzk			0.453	0.744	0.489	0.396	1.722	16.91	37.55
	SPSS			0.508	0.769	0.231	0.464	1.471	2.012	35.44
	ACDE	15	3	0.661	0.838	0.675	0.418	2.314	4.311	24.47
	AMSOS	15	4	0.508	0.769	0.538	0.464	1.471	1.515	35.44
Yeast2	k-means	5		0.491	0.818	0.635	0.455	1.213	1.217	27.08
	k-means++			0.497	0.82	0.64	0.514	1.092	1.666	26.3
	fuzk			0.478	0.812	0.625	0.43	1.296	6.384	27.86
	SPSS			0.456	0.804	0.196	0.453	1.236	2.567	43.23
	ACDE	20	5	0.551	0.846	0.692	0.428	1.438	3.489	23.18
	AMSOS	20	4	0.469	0.8	0.6	0.506	1.154	1.342	44.01

Table3. Least performance values

Dataset	Algorithm	No. of clusters, k		Cluster Validity Measures						Maximum Error rate
		i/p k	o/p k	ARI	RI	HI	SIL	DB	CS	
Synthetic1	k-means	2		0.91	0.955	0.91	0.839	0.467	0.749	2.286
	k-means++			0.91	0.955	0.91	0.839	0.467	0.749	2.286
	fuzk			0.899	0.95	0.9	0.839	0.468	0.732	2.571
	SPSS			0.932	0.966	0.034	0.839	0.465	0.725	1.714
	ACDE	19	4	0.699	0.849	0.697	0.44	1.275	2.13	96
	AMSOS	19	2	0.932	0.966	0.932	0.839	0.465	0.75	1.714
Synthetic2	k-means	4		0.561	0.82	0.641	0.503	0.904	0.936	67
	k-means++			0.566	0.822	0.643	0.507	0.874	0.936	59.8
	fuzk			0.944	0.979	0.957	0.791	0.528	0.93	2.2
	SPSS			0.939	0.977	0.023	0.792	0.527	0.812	2.4
	ACDE	22	7	0.853	0.945	0.891	0.537	0.865	2.224	96.2
	AMSOS	22	4	0.939	0.977	0.953	0.792	0.527	0.943	2.4
Synthetic3	k-means	3		0.97	0.987	0.974	0.823	0.507	0.749	1

	k-means++			0.432	0.718	0.436	0.44	0.962	0.749	50.67
	fuzk			0.97	0.987	0.974	0.823	0.507	0.731	1
	SPSS			0.97	0.987	0.013	0.823	0.507	0.657	1
	ACDE	17	4	-0.049	0.382	-0.235	0.203	1.078	1.764	87.5
	AMSOS	17	3	0.97	0.987	0.974	0.823	0.507	0.768	1
Synthetic4	k-means	6		0.574	0.851	0.703	0.504	0.727	0.233	0
	k-means++			0.832	0.951	0.902	0.791	0.523	0.233	92.63
	fuzk			0.836	0.952	0.904	0.786	0.503	0.233	94.5
	SPSS			1	1	0	0.975	0.144	0.723	0
	ACDE	28	10	0.944	0.985	0.97	0.736	0.511	0.247	93.88
	AMSOS	28	6	1	1	1	0.975	0.144	0.233	0
Iris	k-means	3		0.44	0.72	0.441	0.798	0.582	0.607	51.33
	k-means++			0.44	0.72	0.441	0.798	0.582	0.607	51.33
	fuzk			0.45	0.725	0.449	0.792	0.576	0.603	56
	SPSS			0.44	0.72	0.28	0.799	0.582	1.962	50.67
	ACDE	12	4	0.795	0.914	0.828	0.623	0.435	0.529	62.67
	AMSOS	12	2	0.568	0.776	0.553	0.952	0.233	0.402	33.33
Wine	k-means	3		0.217	0.628	0.256	0.692	0.608	0.78	42.7
	k-means++			0.217	0.628	0.256	0.687	0.608	0.774	42.7
	fuzk			0.332	0.696	0.392	0.695	0.601	0.914	30.9
	SPSS			0.337	0.699	0.301	0.696	0.601	0.813	30.34
	ACDE	13	8	0.338	0.668	0.336	0.053	0.555	0.647	69.66
	AMSOS	13	2	0.197	0.593	0.186	0.714	0.644	1.024	41.01
Glass	k-means	6		0.152	0.666	0.333	0.207	1.168	0.966	67.29
	k-means++			0.189	0.626	0.252	0.356	1.023	0.722	64.95
	fuzk			0.207	0.707	0.415	0.243	1.178	1.85	66.82
	SPSS			0.252	0.722	0.278	0.382	1.061	1.512	45.79
	ACDE	15	8	0.293	0.646	0.291	0.071	1.146	0.99	86.45
	AMSOS	15	5	0.27	0.669	0.337	0.639	0.95	1.366	70.56
Yeast1	k-means	4		0.246	0.658	0.315	0.184	1.757	1.509	80.17
	k-means++			0.43	0.735	0.47	0.399	2.007	1.509	42.62
	fuzk			0.394	0.721	0.441	0.343	2.239	6.311	80.59
	SPSS			0.508	0.769	0.231	0.464	1.471	1.217	35.44
	ACDE	15	8	0.545	0.786	0.573	0.233	2.314	0.942	97.47
	AMSOS	15	4	0.508	0.769	0.538	0.464	1.471	1.515	35.44
Yeast2	k-means	5		0.361	0.784	0.568	0.339	1.489	1.53	57.03
	k-means++			0.367	0.786	0.572	0.364	1.354	1.21	57.03
	fuzk			0.369	0.769	0.538	0.319	1.819	2.201	53.65
	SPSS			0.456	0.804	0.196	0.453	1.236	2.567	43.23

	ACDE	20	8	0.513	0.83	0.659	0.238	1.438	1.713	86.46
	AMSOS	20	4	0.469	0.8	0.6	0.506	1.154	1.342	44.01

Table4. AMSOS efficiency in finding optimal Centroids

Data set	Original Centroids	Obtained Centroids by AMSOS
Synthetic1	7 6 9	7.0783 5.9625 9.0975
	2 3 4	2.0289 3.0849 4.1540
Synthetic2	-6 4	-5.9234 4.0052
	2 2	1.8901 1.9421
	-1 -1	-0.9611 -1.2146
	-3 -3	-2.7994 2.9561
Synthetic3	-3 3	-3.1959 2.9669
	-1 -1	-0.8401 -1.1502
	2 2	2.0215 1.8696
Synthetic4	-8 14	-8.0344 14.0421
	10 12	10.0285 12.0065
	14 -14	13.9763 -13.9768
	-1 -1	-1.1876 -0.9205
	-3 6	-2.9580 6.0961
	-8 -6	-7.9533 -6.0640

Figure 1: AMSOS efficiency in clustering the Yeast2 dataset

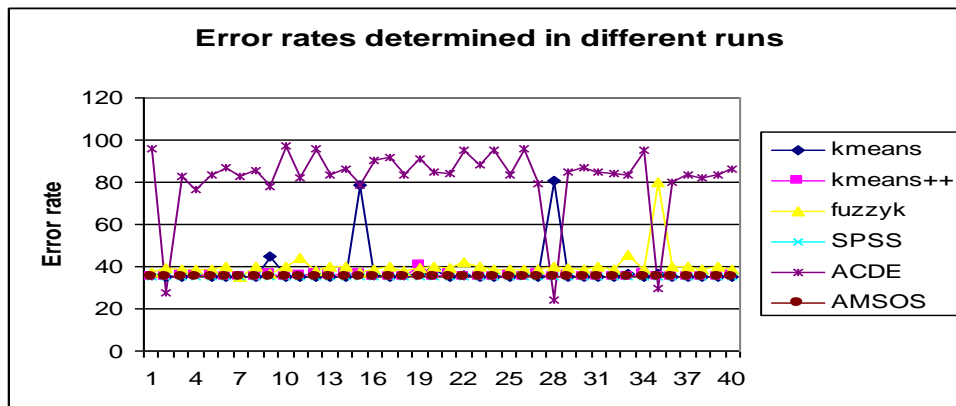
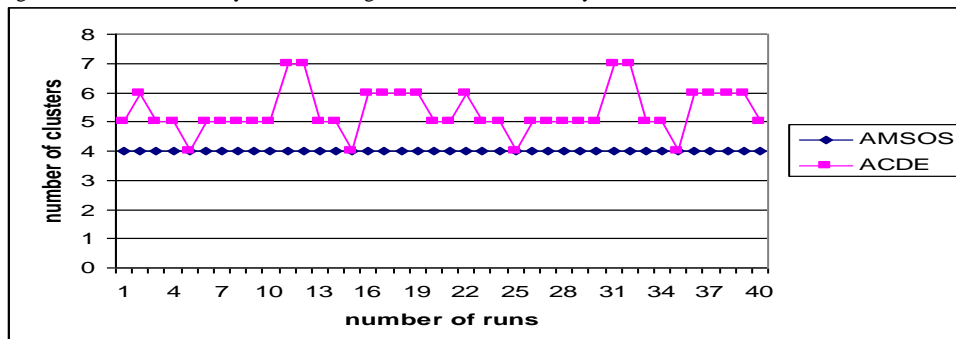


Figure 2: AMSOS efficiency in determining number of clusters for synthetic2 dataset



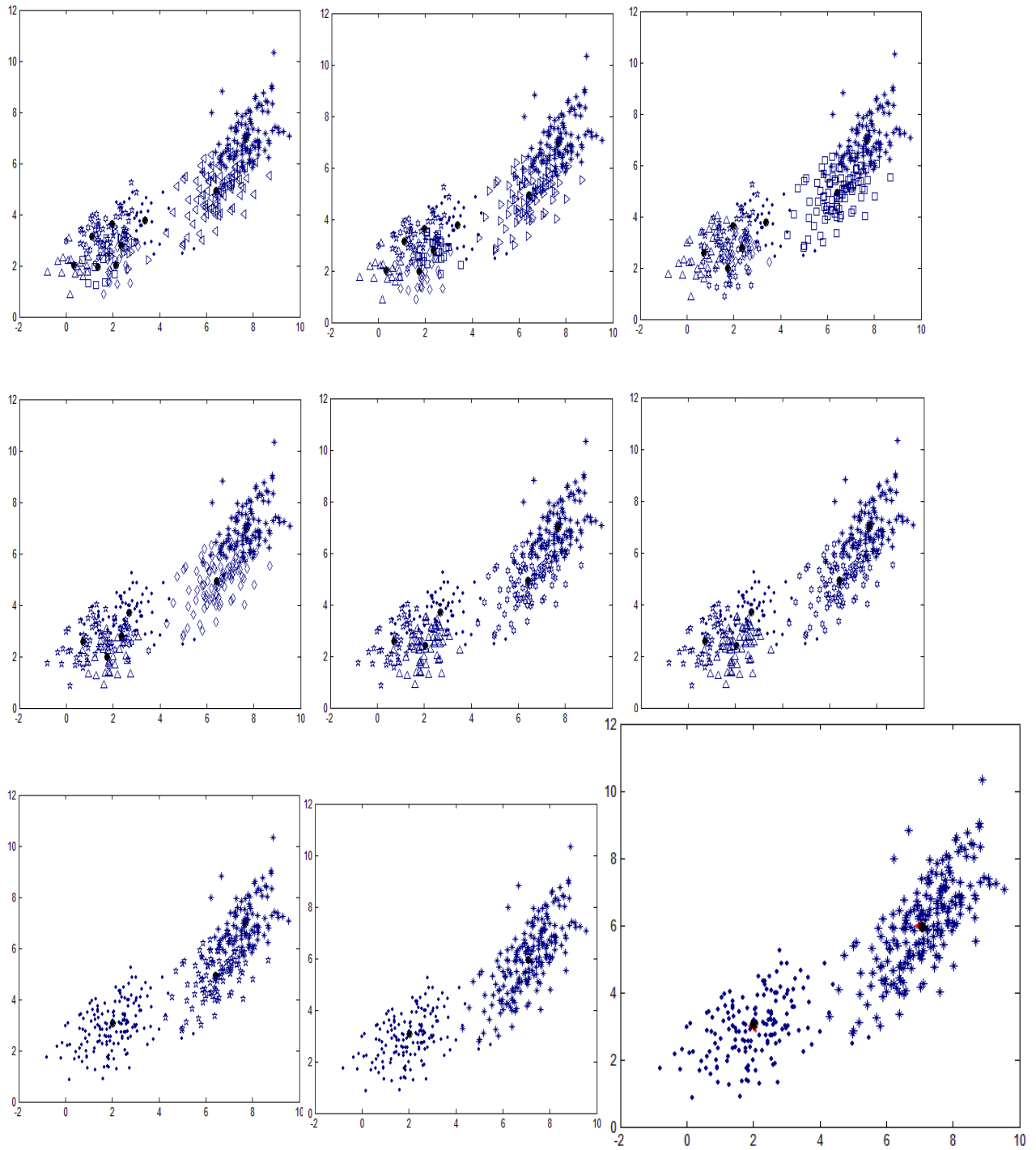


Figure 3. The results obtained by AMSOS for the Synthetic1 data set when initial $k=9$. Starting with initial clusters to final clusters and their obtained centers. The obtained centers are marked with '●' whereas original centers are marked in red colored triangles.

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