EK-Means: Towards Making Ensemble *K*-Means Work for Image-Based Data Analysis Without Prior Knowledge of *K*

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Keywords: K-Means, DCAS, Clustering, Cluster Number, Malware Detection.

Abstract: Despite its widespread application, *K*-means is significantly constrained by its dependence on the prior knowledge and its limitations in handling irregular data patterns, which restrict its performance in practical scenarios such as malware detection. To address these shortcomings, a novel EK-means algorithm is proposed. It introduces a dynamic cluster adaptation strategy (DCAS) to leverage similarity and separation measures in the pre-clustering phase to enable adaptive splitting and merging of clusters. The continuous refinement of cluster compactness and centroid representativeness in this approach facilitates the discovery of clusters with arbitrary shapes and the automatic discovery of the true number of clusters. Experimental results show that EK-means achieves high clustering accuracy across multiple datasets, including Fashion-MNIST, Virus MNIST, BIG 2015, and Malimg. It notably excels in malware detection tasks, outperforming some existing mainstream *K*-means enhancement methods.

1 INTRODUCTION

Cluster analysis groups data points to maximize intra-cluster similarity and minimize inter-cluster similarity. Traditional methods like *K*-means and its extensions are popular for their simplicity and efficiency (Liu et al., 2023). However, they struggle with determining the optimal number of clusters, *K*, and assume spherical, evenly distributed clusters, which limits their performance on non-spherical or irregular data distributions (Ikotun et al., 2023).

Current methods address these limitations with various strategies. Heuristic approaches, based on empirical rules, are computationally efficient but often lack consistency and objectivity. Evaluation metrics, such as the Silhouette Coefficient (Bagirov et al., 2023), Dunn Index (Sary et al., 2024), and Davies-Bouldin Index (Sowan et al., 2023), assess clustering quality but are sensitive to initial conditions, often yielding inconsistent results, especially with noisy or complex data. Hypothesis testing methods, relying on distributional assumptions (e.g., Gaussian), struggle with data that deviates from these assumptions or contains mixed structures (Zhao et al., 2008). Common techniques like the Silhouette Coefficient, and information criteria (e.g., AIC/BIC) (Hajihosseinlou et al., 2024) perform well with spherical distributions but fail to capture the complexities of non-spherical or irregular data.

To address these challenges, we propose EK-means, an ensemble *K*-means method that automatically identifies the optimal number of clusters, enhancing performance on non-spherical and irregularly distributed data. We also introduce DCAS, a strategy that adapts the clustering process to the data's distribution, improving flexibility and robustness. The main contributions are as follows.

- The DCAS is designed to enable the automatic discovery of the actual number of clusters through splitting and merging operations.
- A similarity measure called the Local Compactness Measure (LCM) is proposed, which is designed to assess intra-cluster similarity and effectively reduce computational complexity.
- By conducting a series of experiments, we demonstrate that EK-means prove exceptional accuracy and robustness across multiple image datasets. Furthermore, it effectively discovers the true number of clusters in malware detection, achieving a high accuracy rate.

The paper is structured as follows: Section 2 reviews advancements in *K*-means extensions to address its limitations; Section 3 presents the EK-means

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Niu, D., Ping, Y., Liu, Y., Wei, F. and Wu, W.
EK-Means: Towards Making Ensemble K-Means Work for Image-Based Data Analysis Without Prior Knowledge of K.
DOI: 10.5220/0013250100003899

In *Proceedings of the 11th International Conference on Information Systems Security and Privacy (ICISSP 2025) - Volume 2*, pages 575-584
ISBN: 978-989-758-735-1; ISSN: 2184-4356

approach and its implementation; Section 4 provides experimental results and compares EK-means with other methods; Section 5 concludes with key findings.

2 RELATED WORK

K-means is a widely used unsupervised clustering method valued for its efficiency and simplicity. However, it has several limitations: (1) the number of clusters *K* must be predefined, which is often difficult in real-world datasets (José-García and Gómez-Flores, 2016); (2) it assumes spherical clusters, limiting its performance on irregular or non-spherical data (Daud et al., 2024); (3) it is sensitive to outliers and noise, which can distort results (Gan and Ng, 2017); and (4) its sensitivity to initial centroid placement can lead to local optima (Ahmed et al., 2020). To overcome these challenges, various improvements have been proposed to eliminate the need for predefined *K* and to handle non-spherical clusters. The following sections outline key advancements in these areas.

2.1 Addressing the Pre-Specified Cluster Number Problem

In *K*-means clustering, determining the optimal number of clusters has been a key research challenge. Early approaches used evaluation metrics like silhouette scores and the elbow method to estimate cluster counts. Teklehaymanot et al.(Teklehaymanot et al., 2018) proposed a two-step method that estimates the number of clusters while analyzing data structure, improving model selection accuracy. However, these methods are often limited by subjective thresholds and specific data distributions, reducing their applicability. Later, algorithms were developed to dynamically adjust the number of clusters. For example, X-means (Pelleg and Moore, 2000) uses BIC to evaluate models with different *K* values, optimizing cluster count. Fahim and Ahmed (Fahim, 2021) introduced a DBSCAN-*K*-means hybrid, where DBSCAN estimates cluster count and *K*-means refines intra-cluster consistency. Yang et al. (Yang and Hussain, 2023) developed a *K*-means variant that autonomously identifies the number of clusters. Rykov et al. (Rykov et al., 2024) extended the elbow method with inertia-based techniques for better cluster selection. However, these methods still struggle with highly mixed datasets, revealing room for improvement. Despite these advances, these methods often assume normality, incur high computational costs in high-dimensional data, and lack scalability, pointing to the need for further optimization.

2.2 Strategies for Addressing Non-Spherical Clusters

In *K*-means clustering, the assumption of spherical clusters with equal variance limits its performance on non-spherical or irregular data. Several approaches have been proposed to improve *K*-means' adaptability to complex data distributions. Early methods like DBSCAN (Deng, 2020) use density-based clustering to detect irregular clusters and remove noise. However, DBSCAN struggles with varying cluster densities and is sensitive to parameter settings. To address this, GriT-DBSCAN (Huang et al., 2023) introduces grid-based partitioning, improving efficiency for high-dimensional datasets. Morii et al. (Morii and Kurahashi, 2006) enhanced *K*-means by splitting and merging decision regions to improve clustering accuracy. However, these methods incur high computational costs and rely on selecting appropriate kernels. G-means dynamically adjusts cluster boundaries based on Gaussian distribution assumptions and statistical tests, enabling effective handling of irregular shapes and automatic determination of the cluster count. The *K*-Multiple-Means method (Nie et al., 2019) addresses non-convex clusters by introducing multiple centroids, but it remains computationally expensive and sensitive to parameter settings. Despite these advancements, these methods still struggle with high-dimensional data and parameter sensitivity, indicating the need for further optimization.

To overcome these limitations, EK-means has undergone several key optimizations:

- EK-means automatically determines the cluster count using an ensemble approach, removing the need for a pre-specified *K*. It dynamically refines the final number of clusters without assuming normality.
- EK-means enhances clustering performance on complex data distributions without assuming spherical clusters. By combining similarity and dissimilarity metrics, it adaptively optimizes the cluster structure, achieving high accuracy and robustness on non-spherical datasets.

3 EK-MEANS

In this section, we present the EK-means algorithm. The process begins with an initial clustering step, where the data is partitioned into multiple clusters based on a predefined *K* value. Next, each cluster undergoes decomposition using the DCAS strategy to evaluate whether sub-clusters should be retained.

After completing the decomposition phase, the algorithm enters the merging stage, where DCAS is again applied to determine whether clusters should be merged. This iterative process of decomposition and merging continues until no further changes are needed. We first describe the adaptive strategy for cluster handling, then provide a detailed explanation of the decomposition and merging steps, followed by an overview of the entire EK-means implementation.

3.1 DCAS

This section introduces the DCAS, focusing on how it enables adaptive clustering by optimizing both intra-cluster structure and inter-cluster relationships. As shown in Figure 1, the algorithm evaluates the proximity between clusters based on the similarity of data points within them, determining whether to perform splitting or merging operations. EK-means facilitates the dynamic decomposition and merging of clusters by incorporating inter-cluster compactness. The primary objective is to identify sparse regions within the dataset and partition the data accordingly. This approach eliminates the reliance on initial parameters, enabling real-time adjustments for a more accurate representation of the data structure.

In our adaptive clustering strategy Algorithm 1, we consider two clusters with centroids C_1 and C_2, and corresponding data point sets P_1 and P_2. To evaluate cluster compactness, we randomly sample nn data points from each cluster, forming subsets $S_t = \{x_{t1}, x_{t2}, \ldots, x_{tn}\}$, where $t \in \{1,2\}$ is the cluster index. The set $T = \{n, n_n, n_s\}$ represents the hyperparameters used in EK-means. Here, n is the number of randomly selected data points from a cluster, n_n is the number of nearest neighbors for each point, and n_s is the number of segments between the centroids of the two clusters.

Definition 3.1 (Euclidean Distance)**.** *The $Ed(\cdot,\cdot)$ denotes the Euclidean distance. For two data points x and y, their Euclidean distance $Ed(x,y)$ is computed as:*

$$Ed(x,y) = \sqrt{\sum_{k=1}^{nu} (x_k - y_k)^2} \quad (1)$$

where x_k and y_k are the coordinates of x and y in the k-th dimension, and nu is the number of dimensions.

Definition 3.2 (Nearest Neighbor)**.** *$NN_b(x_{tj})$ denotes the b-th nearest neighbor of x_{tj}, where x_{tj} represents the j-th randomly selected sample from cluster t.*

For each randomly sampled data point $x_{tj} \in S_t$ in cluster C_t, we compute the average distance to its nearest neighbors, denoted as D-ANND(t, j), as defined below:

Definition 3.3 (Average Nearest Neighbor Distance)**.** *Given a data point x_{tj} and its nearest neighbors, the average nearest neighbor distance D-ANND(t, j) is:*

$$D\text{-}ANND(t,j) = \frac{1}{n_n} \sum_{b=1}^{n_n} Ed(x_{tj}, NN_b(x_{tj})) \quad (2)$$

where x_{tj} represents the j-th randomly selected sample from cluster t.

Definition 3.4 (LCM)**.** *The $LCM(\cdot)$ is the mean of the average distances to the nearest neighbors of randomly sampled points within a cluster, calculated as:*

$$LCM(t) = \frac{1}{n} \sum_{j=1}^{n} D\text{-}ANND(t,j) \quad (3)$$

where t is the cluster index, and j is the j-th randomly selected point in that cluster.

The *LCM* captures the local density of points within a cluster, providing a better reflection of regional structure compared to global metrics like the within-cluster sum of squares (WCSS). By evaluating the neighborhood distances of randomly sampled points, we reduce computational complexity, ensuring efficiency for large datasets. The sample size is typically set to 5 points based on the total number of data points in the cluster. This measure is key to understanding the local structure within each cluster and evaluating the connectivity between clusters. After calculating the compactness measure *LCM*, we divide the line segment between the centroids C_1 and C_2 into n_s equally spaced points.

Definition 3.5 (Position of P_a for Cluster Separation)**.** *The position P_a of a point along the line segment between the centroids C_1 and C_2 is defined as:*

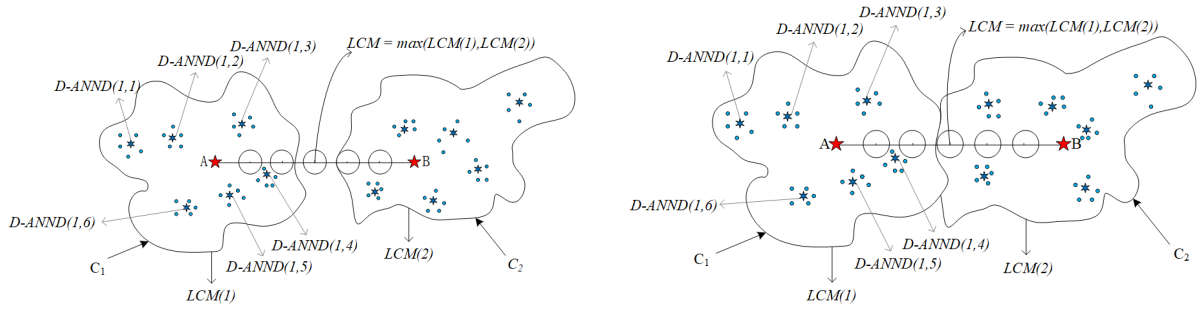
$$P_a = C_1 + a \cdot \frac{|C_1 - C_2|}{n_s}, \quad a = 1,2,\ldots,n_s - 1 \quad (4)$$

where a denotes the index of the point along the segment, n_s is the total number of segments, and $|C_1 - C_2|$ is the distance between the centroids C_1 and C_2.

For each point P_a, a circle with radius d is drawn. If all circles contain a data point, the clusters are connected and merged; if any circle is empty, the clusters remain separate.

3.2 Adaptive Decomposition and Merging

We propose a clustering strategy based on inter-cluster similarity and separability, designed to better explore cluster structures and data point distribution. This approach improves clustering accuracy and data representation effectiveness.



(a) Cluster decomposition

(b) Cluster merging

Figure 1: Adaptive Cluster Decomposition and Merging: Random data points from each cluster are selected to calculate the average distance to nearest neighbors, yielding $LCM(1)$ and $LCM(2)$ for clusters $C1$ and $C2$. The larger LCM value serves as the partition threshold. A line AB is drawn between the centroids, and we check if any data points lie within a circle centered at the partition point on AB. This decides whether to merge or split the clusters.

Algorithm 1: DCAS.

Input: C_1, C_2, P_1, P_2, T
Output: flag_m
Randomly select n points: $S_t \leftarrow \{x_{t1}, x_{t2}, \ldots, x_{tn}\}$ from P_t, where $t \in \{1,2\}$
for *each set* S_t **do**
  $LCM(t) \leftarrow \frac{1}{n}\sum_{j=1}^{n} D\text{-}ANND(t,j)$
$LCM \leftarrow \max(LCM(1), LCM(2))$
Calculate $P_a \leftarrow C_1 + a \cdot \frac{|C_1 - C_2|}{n_s}$, $a = 1, 2, \ldots, n_s - 1$
if *Circle*(P_a, LCM) *is not empty for every a* **then**
  flag_m $\leftarrow$ True
else
  flag_m $\leftarrow$ False

Algorithm 2: Adaptive Cluster Decomposition(ACD).

Input: Set of centroids , $C = \{c_1, \ldots, c_K\}$, and its corresponding clustering, $P = \{P_1, \ldots, P_K\}$, T
Output: C', P', flag_EK
flag_EK $\leftarrow$ False
for *each cluster* P_i *in* P **do**
  Apply 2-means clustering:
  $\{P_i^1, P_i^2\} \leftarrow P_i$
  $\{c_i^1, c_i^2\} \leftarrow c_i$
$C' = \emptyset$
$P' = \emptyset$
for *each cluster* P_i *in* P **do**
  flag_m $\leftarrow DCAS(c_i^1, c_i^2, P_i^1, P_i^2)$
  if *flag_m is False* **then**
    $C' \leftarrow C' \cup \{c_i^1, c_i^2\}$
    $P' \leftarrow P' \cup \{P_i^1, P_i^2\}$
    flag_EK $\leftarrow$ True
  else
    $C' \leftarrow C' \cup \{c_i\}$
    $P' \leftarrow P' \cup \{P_i\}$

In contrast to SMKM (Capó et al., 2022), EK-means allows cluster splitting when the DCAS splitting criteria are satisfied and merging according to the DCAS merging criteria. Our method dynamically adjusts the value of K until the true number of clusters is discovered. In comparison, SMKM determines whether to split a cluster based on the reduction in error from adding centroids, splitting only the cluster that results in the maximum error reduction in each iteration. SMKM performs only one split and merge per iteration, maintaining a constant value of K throughout the process.

3.2.1 Adaptive Cluster Decomposition

The adaptive cluster decomposition aims to uncover substructures by iteratively splitting clusters, improving classification accuracy. The process is shown in Algorithm 2. In this phase, we enhance cluster compactness by applying the 2-means algorithm to each cluster P_i, dividing it into two sub-clusters P_i^1 and P_i^2. The connectivity of these sub-clusters is evaluated using an adaptive clustering strategy. If any circle (centered at each sub-cluster point) is empty, it indicates spatial separation between the sub-clusters. This suggests that decomposition improves cluster compactness and classification performance. The variable flag_EK tracks whether a split was performed during the iteration.

3.2.2 Adaptive Cluster Merging

The cluster merging operation enhances compactness and accuracy by identifying structural relationships

Algorithm 3: Adaptive Cluster Merging(ACM).

Input: C, P, T, flag_EK
Output: C', P', flag_EK
merge_found $\leftarrow$ True
$Inter \leftarrow 0$
while *merge_found = True* **do**
  merge_found $\leftarrow$ False
  if $Inter = 1$ **then**
    $C \leftarrow C'$,$P \leftarrow P'$
  $Inter \leftarrow 1$
  $K_{\text{kn}} = |C|$
  while *merge_found = False* **do**
    $(i, j) \leftarrow \arg\min_{1 \le i < j \le K_{\text{kn}}} D_{\text{ij}}$
    flag_m $\leftarrow DCAS(c_{\text{i}}, c_{\text{j}}, P_{\text{i}}, P_{\text{j}})$
    if *flag_m and* $D_{ij} \neq INF$ **then**
      merge_found $\leftarrow$ True
      flag_EK $\leftarrow$ True
      $c' \leftarrow \frac{|P_{\text{i}}| \cdot c_{\text{i}} + |P_{\text{j}}| \cdot c_{\text{j}}}{|P_{\text{i}}| + |P_{\text{j}}|}$
      $C' \leftarrow (C \setminus \{c_{\text{i}}, c_{\text{j}}\}) \cup \{c'\}$
      $P_{\text{i}} \leftarrow P_{\text{i}} \cup P_{\text{j}}$
      $P' \leftarrow (P \setminus \{P_{\text{j}}\}) \cup \{P_{\text{i}}\}$
    else
      $D_{\text{ij}} \leftarrow$ INF

between clusters. In this phase, clusters that are close and structurally similar are merged to optimize the overall cluster shape and centroid representativeness. The merging process, based on density and spatial relationships, is detailed in Algorithm 3. The flag_EK tracks whether a merge occurred during the iteration, and $|C|$ represents the number of centroids in the centroid set C.

Definition 3.6 (Euclidean Distance Between Clusters)**.** *The distance between two clusters i and j is the Euclidean distance between their centroids C_i and C_j:*

$$D(i, j) = \|C_i - C_j\| \tag{5}$$

where C_i and C_j are the centroids of clusters i and j, and $\|\cdot\|$ denotes the Euclidean norm.

Definition 3.7 (Closest Pair of Clusters)**.** *The indices (i^*, j^*) correspond to the pair of clusters i and j that have the smallest Euclidean distance between their centroids. These indices are defined as:*

$$(i^*, j^*) = \arg\min_{i,j} D(i, j) \tag{6}$$

where $D(i, j)$ is the Euclidean distance between the centroids C_i and C_j of clusters i and j, respectively.

The algorithm begins by identifying the most similar pair of clusters, minimizing the distance $D(i, j)$ to find the target for merging. An adaptive strategy evaluates their connectivity: if both clusters contain data points within the circles, they are considered connected and should be merged. The centroid of the merged cluster is calculated as a weighted average of the original centroids, with weights based on the number of data points in each cluster. The algorithm then iterates, checking for the closest pair of clusters until no further merges are possible. This merging process prioritizes intra-cluster density and spatial relationships. By using *LCM* and assessing spatial split points, the algorithm ensures merging only occurs when sufficient connectivity exists, avoiding unnecessary merges. The process continues until no more clusters can be merged, improving clustering quality, representativeness, and compactness.

3.3 EK-Means Implementation

The EK-means method dynamically optimizes clusters through adaptive strategies, including cluster splitting and merging operations. The overall implementation steps are outlined in Algorithm 4.

The EK-means method begins with pre-clustering using the K-means++ algorithm (Arthur and Vassilvitskii, 2007) with an initial number of clusters K_{start} to obtain the initial centroid set C and cluster set P. This forms the basis for further adaptive adjustments. Next, the algorithm proceeds with cluster decomposition and merging. Initially, each cluster is iteratively split into two sub-clusters using the 2-means algorithm. The connectivity of these sub-clusters is then assessed through adaptive strategies to determine whether they should be retained. After all clusters have been split, the merging operation begins. During merging, the closest pair of clusters is identified, and their connectivity is evaluated. If the merging criteria are not met, the next closest pair is considered. When merging conditions are satisfied, the clusters are combined, and the centroid set C is updated. The process repeats until no pairs of clusters meet the merging conditions. After merging, the splitting and merging steps continue until the stopping criteria are met, such as when no further changes occur, or the maximum number of iterations is reached. Finally, the EK-means algorithm outputs the optimized centroid set C and cluster set P.

4 EXPERIMENTS

We conducted experiments on several image datasets to evaluate EK-means' capability in category discovery and clustering performance. The section be-

Algorithm 4: EK-means.

Input: Dataset D, Initial number of clusters K_{start}, flag_EK, max_iter, T
Output: C , P
Pre-clustering:
$C, P \leftarrow K\text{-means++}(D, K_{\text{start}})$
$i\_iter \leftarrow 0$
Adaptive Strategy:
while $flag\_EK$ ***or*** $i\_iter < max\_iter$ **do**
  $i\_iter \leftarrow i\_iter + 1$
  $C', P', \text{flag\_EK} \leftarrow ACD(C, P, T)$
  $C, P, \text{flag\_EK} \leftarrow ACM(C', P', T, \text{flag\_EK})$

gins with a description of the experimental setup and datasets, followed by an analysis of the algorithm's stability. Finally, we assess EK-means' performance in malware analysis tasks.

4.1 Experimental Setup

The experiments consist of three main assessments:

- **Stability Analysis**: This experiment evaluates the clustering accuracy and stability of EK-means using the Fashion MNIST dataset.
- **Malware Analysis**: This experiment evaluates the performance of EK-means in malware detection using the Virus MNIST (Noever and Noever, 2021), BIG 2015 (Ronen, 2018), and Malimg (Nataraj et al., 2011) datasets.

To compare with EK-means, we selected *K*-means++, X-means, CDKM (Nie et al., 2022), and SMKM. *K*-means++, CDKM, and SMKM require a predefined number of clusters, while X-means and EK-means can autonomously determine the final cluster count based on the initial *K*.

Our experiments assess clustering accuracy and the ability to identify true categories using clustering accuracy as the evaluation metric. Clustering accuracy evaluates the consistency between predicted and true labels. The formula for clustering accuracy is given by:

$$\text{Accuracy} = \frac{\text{Correctly identified class}}{\text{Total number of class}} \times 100 \quad (7)$$

All experiments were performed on a machine running Windows 11 with a 3.20 GHz CPU and 128 GB RAM.

4.2 Experimental Datasets

To evaluate the algorithm's performance, we selected four representative datasets: Fashion MNIST, Virus MNIST, BIG 2015, and Malimg, covering tasks like image clustering and malware analysis. Table 1 presents key statistics for each dataset. Feature extraction is performed using the pre-trained ResNet18 model (He et al., 2015), where images are resized, normalized, and converted into *n*-dimensional feature vectors for analysis.

4.3 Stability Analysis

This section evaluates the stability of EK-means using the Fashion MNIST dataset, focusing on two aspects: (1) the consistency of accuracy and final cluster number *K* across multiple experiments, and (2) the effect of different initial *K* values on the final cluster count and accuracy.

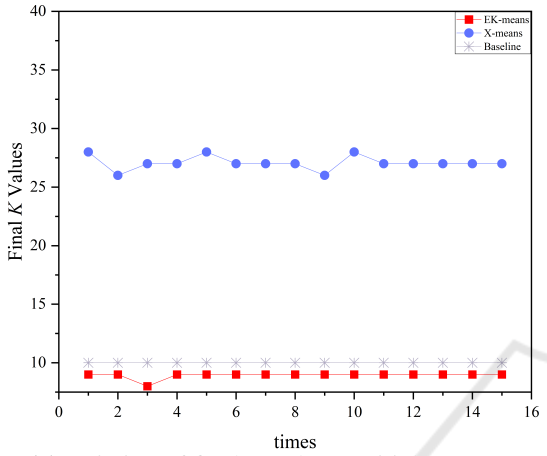
As shown in Figure 2a, with an initial $K = 16$, the final cluster number obtained by EK-means remains close to the actual class count (10) across repeated tests, indicating its ability to capture the intrinsic structure of the data effectively. In contrast, X-means exhibits more significant fluctuations in *K*, with final values consistently above 25, deviating significantly from the ground truth. Figure 2b presents the accuracy of both algorithms under the same initial *K*. EK-means maintains a high accuracy above 0.9 with minimal variance, significantly outperforming X-means, whose accuracy remains below 0.5 with noticeable instability. These results demonstrate the robustness and consistency of EK-means over multiple trials. Furthermore, Figure 3a and 3b explore the influence of varying initial *K* values. In Figure 3a, EK-means shows minimal variation in the final *K*, which consistently approximates the true number of classes. X-means produces significantly fluctuating *K* values, often far exceeding the ground truth. Figure 3b plots the clustering accuracy against the initial *K*. EK-means achieves stable, high accuracy across different initial *K* values, while X-means exhibits larger variations, with accuracy consistently below 0.5. In summary, EK-means demonstrates strong robustness and adaptability, achieving consistent performance across multiple trials and under varying initial conditions.

4.4 Malware Analysis

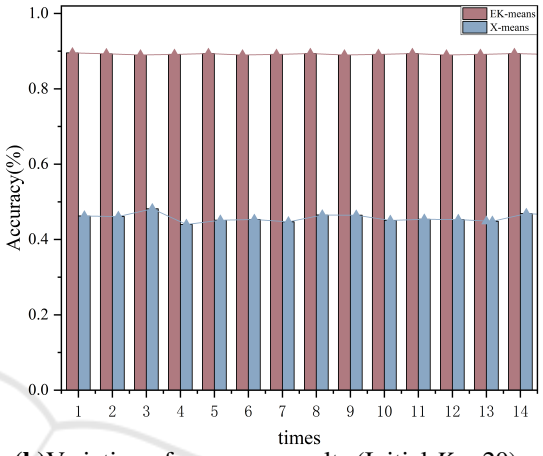
We conducted experiments on the Virus MNIST, BIG 2015, and Malimg datasets to evaluate the effectiveness of EK-means in malware analysis. Figure 4 illustrates the clustering performance of different methods under varying initial *K* values, including the final number of clusters obtained by EK-means and X-means.

Table 1: Description of the benchmark datasets.

Datasets	Dataset Description			
	Dims	Size	# of Classes	Task description
Fashion MNIST	10	70000	10	Image clustering
Virus MNIST	10	50000	10	Malware analysis
BIG2015	10	10868	9	Malware analysis
Malimg	25	9339	25	Malware analysis

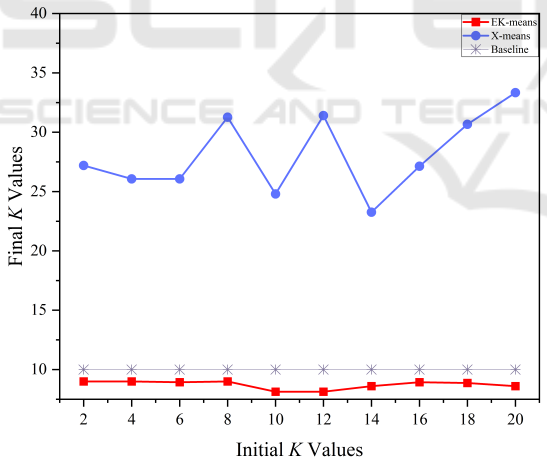


(a) Variation of final K values (Initial K = 20).

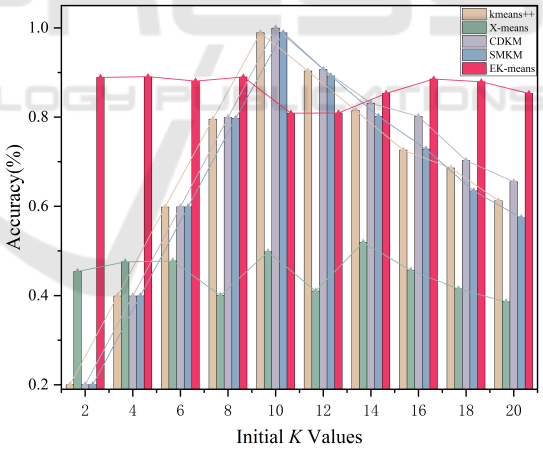


(b) Variation of accuracy results (Initial K = 20).

Figure 2: Comparison of EK-means and X-means clustering performance with initial K=20.



(a) Final K values with varying initial K.

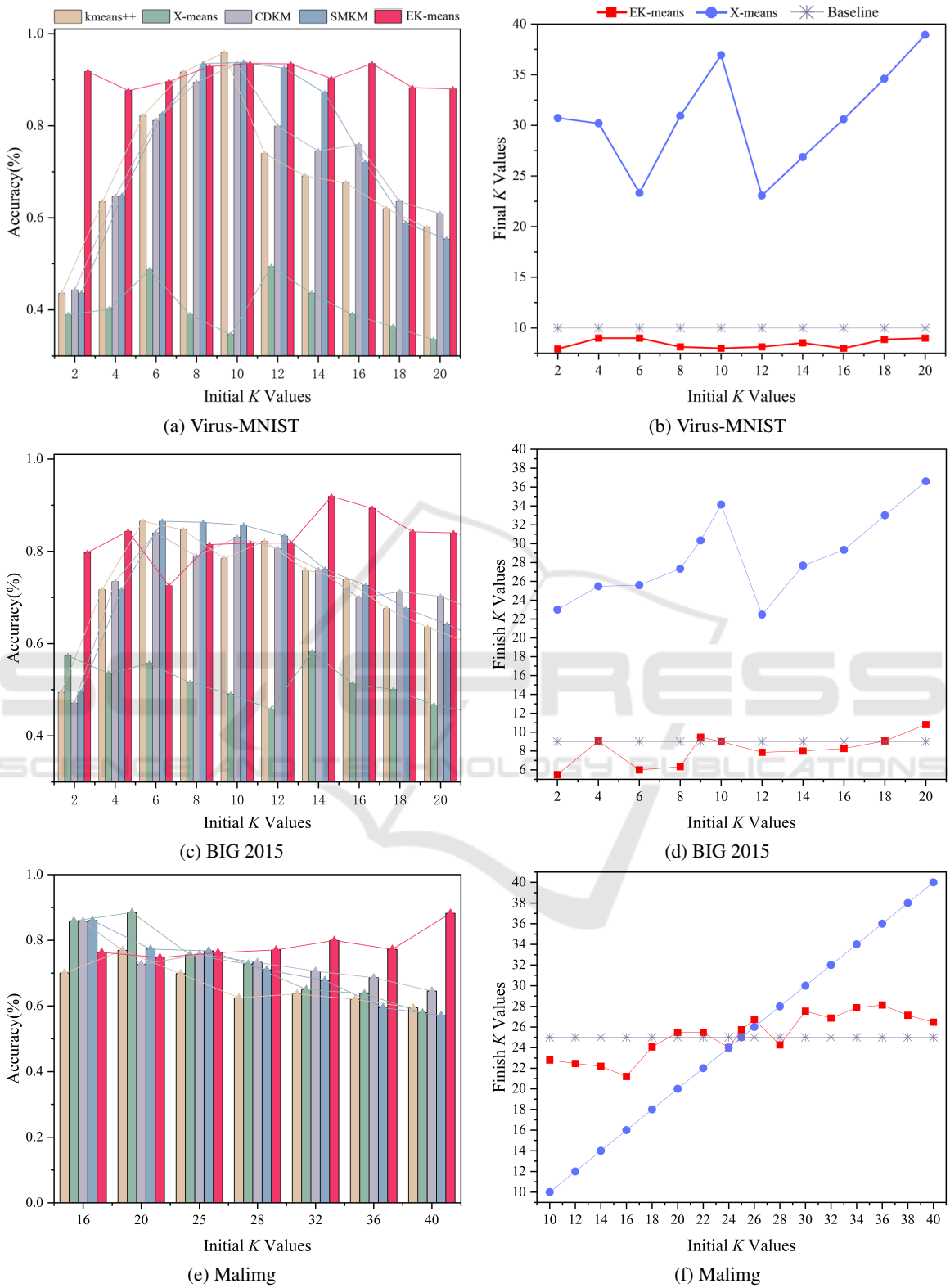


(b) Accuracy results with varying initial K.

Figure 3: Analysis of clustering results with varying initial K values.

Virus-MNIST. In the Virus MNIST dataset, when the initial K deviates from the actual number of clusters, the accuracy of K-means++, CDKM, and SMKM drops significantly, with optimal performance only when K matches the true number of categories. In contrast, EK-means maintains high accuracy across various initial K values, with the final K value remaining close to the actual one, demonstrating its robustness. On the other hand, X-means exhibits substantial fluctuations in the final K value, often exceeding the actual number of categories. This results in a noticeable drop in accuracy, indicating its limitations in identifying actual categories in malware datasets.

BIG 2015. On the BIG 2015 dataset, EK-means performed exceptionally well. As shown in Figure 4(d), when the initial K exceeds 12, the final K value is close to the true number of categories, signif-



(a) Virus-MNIST (b) Virus-MNIST

(c) BIG 2015 (d) BIG 2015

(e) Malimg (f) Malimg

Figure 4: Malware analysis.

icantly improving clustering accuracy. This improvement is attributed to EK-means' strategy of only splitting clusters that meet certain criteria, ensuring more effective partitioning. When the initial K is too low, each cluster may contain multiple categories, leading to poor partitioning and increased computational complexity. Conversely, a larger initial K value enables finer partitioning from the start, improving cluster purity and the accuracy of subsequent splits.

Malimg. On the Malimg dataset, as the initial K value increases, the accuracy of EK-means improves, similar to the findings on the BIG 2015 dataset, which also exhibits significant class imbalance. A larger initial K value proves crucial for improving the clustering effectiveness of EK-means when there are substantial differences between categories. With smaller initial K values, clusters often contain a mix of categories, and the disparities in class sizes make it difficult to differentiate rare categories effectively, leading to a final K value smaller than the true number of categories. To improve EK-means' performance on the Malimg dataset, using a larger initial K value is recommended. Additionally, K-means++, CDKM, and SMKM maintain relatively stable accuracy, with misclassification having minimal impact on overall accuracy even when the K value exceeds the actual number of categories due to class imbalance.

We employed (batch) MMRS sampling (Johnson et al., 1990) to select data points for calculating intra-cluster compactness, addressing the class imbalance issue, and ensuring the accuracy of the compactness measure. Overall, EK-means outperforms other methods in malware analysis, demonstrating its robustness and accuracy in handling complex datasets. Through its adaptive clustering strategy, EK-means effectively identifies actual categories and adapts to varying data distributions, establishing itself as a powerful tool in malware analysis.

5 CONCLUSIONS

The traditional k-means is widely used for various clustering tasks due to its simplicity, computational efficiency, ease of implementation, and scalability. However, it struggles with automatically discovering the true number of clusters and is ineffective in handling non-spherical and irregularly distributed clusters. To address these issues, we propose a novel method, EK-means. By incorporating DCAS and LCM, EK-means enables the automatic decomposition and merging of clusters, effectively overcoming these challenges. Experimental results demonstrate that the method discovers the true number of clusters in irregular datasets and performs excellently in malware detection tasks. However, EK-means still exhibits certain limitations when dealing with categories with significant substructures. Future research will aim to improve methods for handling complex categories, enhance computational efficiency, improve adaptability to heterogeneous data, and optimize the algorithm's applicability and performance.

ACKNOWLEDGEMENTS

This work is supported by the National Natural Science Foundation of China under Grant no. 62162009, the Key Technologies R&D Program of He'nan Province under Grant No. 242102211065, Postgraduate Education Reform and Quality Improvement Project of Henan Province under Grant Nos. YJS2024AL112 and YJS2024JD38, the Innovation Scientists and Technicians Troop Construction Projects of Henan Province under Grant No. CXTD2017099, and the Scientific Research Innovation Team of Xuchang University under Grant No. 2022CXTD003.

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