
Two applications of Min-Max-Jump distance

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Abstract

1 We explore two applications of Min-Max-Jump distance (MMJ distance): MMJ-
2 based K-means and MMJ-based internal clustering evaluation index. K-means and
3 its variants are possibly the most popular clustering approach. A key drawback of
4 K-means is that it cannot deal with data sets that are not the union of well-separated,
5 spherical clusters. MMJ-based K-means proposed in this paper overcomes this
6 demerit of K-means, so that it can handle irregularly shaped clusters. Evaluation (or
7 "validation") of clustering results is fundamental to clustering and thus to machine
8 learning. Popular internal clustering evaluation indices like Silhouette coefficient,
9 Davies–Bouldin index, and Calinski–Harabasz index performs poorly in evaluating
10 irregularly shaped clusters. MMJ-based internal clustering evaluation index uses
11 MMJ distance and Semantic Center of Mass (SCOM) to revise the indices, so that
12 it can evaluate irregularly shaped data. An experiment shows introducing MMJ
13 distance to internal clustering evaluation index, can systematically improve the
14 performance. We also devise two algorithms for calculating MMJ distance.

15 1 Introduction

16 Distance is a numerical measurement of how far apart objects or points are. It is usually formalized
17 in mathematics using the notion of a metric space. A metric space is a set together with a notion of
18 distance between its elements, usually called points. The distance is measured by a function called
19 a metric or distance function. Metric spaces are the most general setting for studying many of the
20 concepts of mathematical analysis and geometry.

21 In this paper, we introduce two algorithms for calculating Min-Max-Jump distance (MMJ distance)
22 and explore two applications of it. Including MMJ-based K-means (MMJ-K-means) and MMJ-based
23 internal clustering evaluation index.

24 MMJ-K-means improves K-means, so that it can handle irregularly shaped clusters. We claim MMJ-
25 CH is the SOTA (state-of-the-art) internal clustering evaluation index, which achieves an accuracy of
26 90/145. MMJ-CH is one of the MMJ-based internal clustering evaluation indices.

27 2 RELATED WORK

28 2.1 Different distance metrics

29 Many distance measures have been proposed in literature, such as Euclidean distance or cosine
30 similarity. These distance measures often be found in algorithms like k-NN, UMAP, HDBSCAN,
31 etc. The most common metric is Euclidean distance. Cosine similarity is often used as a way to
32 counteract Euclidean distance's problem in high dimensionality. The cosine similarity is the cosine
33 of the angle between two vectors.

34 Hamming distance is the number of values that are different between two vectors. It is typically used
35 to compare two binary strings of equal length (1).

36 Manhattan distance is a geometry whose usual distance function or metric of Euclidean geometry
37 is replaced by a new metric in which the distance between two points is the sum of the absolute
38 differences of their Cartesian coordinates (2).

39 Chebyshev distance is defined as the greatest of difference between two vectors along any coordinate
40 dimension (3).

41 Minkowski distance or Minkowski metric is a metric in a normed vector space which can be
42 considered as a generalization of both the Euclidean distance and the Manhattan distance (4).

43 Jaccard index, also known as the Jaccard similarity coefficient, is a statistic used for gauging the
44 similarity and diversity of sample sets (5).

45 Haversine distance is the distance between two points on a sphere given their longitudes and latitudes.
46 It is similar to Euclidean distance in that it calculates the shortest path between two points. The main
47 difference is that there is no straight line, since the assumption is that the two points are on a sphere
48 (6).

49 2.2 K-means

50 K-means (7) and its variants (8; 9; 10) are possibly the most well-liked clustering approach. K-means
51 divides the data into K groups, where K is a hyper-parameter to be optimized. It aims to reduce the
52 within-cluster dissimilarity. While popular, K-means and its variants perform poorly for data sets
53 that are not the union of well-separated, spherical clusters. MMJ-based K-means (MMJ-K-means)
54 proposed in this paper overcomes this demerit of K-means, so that it can handle irregularly shaped
55 clusters.

56 2.3 Internal clustering evaluation index

57 Evaluation (or "validation") of clustering results is as difficult as the clustering itself (11). Popular
58 approaches involve "internal" evaluation and "external" evaluation. In internal evaluation, a clustering
59 result is evaluated based on the data that was clustered itself. Popular internal evaluation indices
60 are Davies-Bouldin index (12), Silhouette coefficient (13), Dunn index (14), and Calinski-Harabasz
61 index (15) etc. In external evaluation, the clustering result is compared to an existing "ground truth"
62 classification, such as the Rand index (16). However, knowledge of the ground truth classes is almost
63 never available in practice.

64 In Section 5.2, an experiment shows introducing Min-Max-Jump (MMJ) distance to internal clustering
65 evaluation index, can systematically improve the performance.

66 2.4 Path-based distances

67 Euclidean distances are frequently used in machine learning and clustering methods to compare
68 points. However, the distance is data-independent, and not tailored to the geometry of the data. Many
69 metrics that are data-dependent have been devised, such as diffusion distances (17) and path-based
70 distances (18; 19). MMJ distance is a path-based distance.

71 3 Definition of Min-Max-Jump

72 **Definition 1.** *Min-Max-Jump distance (MMJ distance)*

73 Ω is a set of points (at least one). For any pair of points $p, q \in \Omega$, the distance between p and q is
74 defined by a distance function $d(p, q)$ (such as Euclidean distance). $i, j \in \Omega$, $\Psi_{(i, j, n, \Omega)}$ is a path from
75 point i to point j , which has length of n points (see Table 1). $\Theta_{(i, j, \Omega)}$ is the set of all paths from point
76 i to point j . Therefore, $\Psi_{(i, j, n, \Omega)} \in \Theta_{(i, j, \Omega)}$. $\max_jump(\Psi_{(i, j, n, \Omega)})$ is the maximum jump in path
77 $\Psi_{(i, j, n, \Omega)}$.

78 The Min-Max-Jump distance between a pair of points i, j , which belong to Ω , is defined as:

Table 1: Table of notations

Ω	A set of N points, with each point indexed from 1 to N ;
$\Omega_{[1,n]}$	The first n points of Ω , indexed from 1 to n ;
Ω_{n+1}	The $(n + 1)$ th point of Ω ;
C_i	A cluster of points that is a subset of Ω ;
ξ_i	One-SCOM of C_i ;
$\Omega + p$	Set Ω plus one new point p . Since $p \notin \Omega$, if Ω has N points, this new set now has $N + 1$ points;
$\Psi_{(i,j,n,\Omega)}$	$\Psi_{(i,j,n,\Omega)}$ is a sequence from point i to point j , which has length of n points. All the points in the sequence must belong to set Ω . That is to say, it is a path starts from i , and ends with j . For convenience, the path is not allowed to have loops, unless the start and the end is the same point;
$d(i, j)$	$d(i, j)$ is a distance metric between pair of points i and j , such as Euclidean distance;
$max_jump(\Psi_{(i,j,n,\Omega)})$	$max_jump(\Psi_{(i,j,n,\Omega)})$ is the maximum jump in path $\Psi_{(i,j,n,\Omega)}$. A jump is the distance from two consecutive points p and q in the path;
$\Theta_{(i,j,\Omega)}$	$\Theta_{(i,j,\Omega)}$ is the set of all paths from point i to point j . A path in $\Theta_{(i,j,\Omega)}$ can have arbitrary number of points (at least two). All the points in a path must belong to set Ω ;
$MMJ(i, j \Omega)$	$MMJ(i, j \Omega)$ is the MMJ distance between point i and j , where Ω is the <i>Context</i> of the MMJ distance;
$\mathbb{M}_{k,\Omega_{[1,k]}}$	$\mathbb{M}_{k,\Omega_{[1,k]}}$ is the pairwise MMJ distance matrix of $\Omega_{[1,k]}$, which has shape $k \times k$. The MMJ distances are under the <i>Context</i> of $\Omega_{[1,k]}$;
\mathbb{M}_Ω	The pairwise MMJ distance matrix of Ω , $\mathbb{M}_\Omega = \mathbb{M}_{N,\Omega_{[1,N]}}$;

$$\Pi = \{max_jump(\epsilon) \mid \epsilon \in \Theta_{(i,j,\Omega)}\} \quad (1)$$

$$MMJ(i, j | \Omega) = \min(\Pi) \quad (2)$$

79 Where ϵ is a path from point i to point j , $max_jump(\epsilon)$ is the maximum jump in path ϵ . Π is the set
80 of all maximum jumps. $\min(\Pi)$ is the minimum of Set Π .

81 Set Ω is called the *Context* of the Min-Max-Jump distance. It is easy to check $MMJ(i, i | \Omega) = 0$.
82

83 In summary, Min-Max-Jump distance is the minimum of maximum jumps of all path between a pair
84 of points, under the *Context* of a set of points.

85 Similar distances have actually been studied in many places in the literature, including the maximum
86 capacity path problem, the widest path problem, the bottleneck edge query problem, the minimax
87 path problem, the bottleneck shortest path problem, and the longest-leg path distance (LLPD)
88 (20; 21; 22; 23).

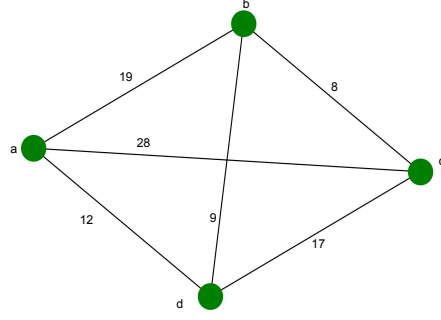


Figure 1: An example

89 There is a minor difference between Min-Max-Jump distance and other similar distances: Min-Max-
 90 Jump distance stresses the *context* of the distance. The *context* is like the condition in conditional
 91 probability. The difference becomes non-trivial when we need to calculate the pairwise MMJ distance
 92 matrix of a set S , under the context of its superset X , such as in Section 6.3 of (24). A set Ω is a
 93 superset of another set B if all elements of the set B are elements of the set Ω .

94 3.1 An example

95 Suppose Set Ω is composed of the four points in Figure 1. There are five (non-looped) paths from
 96 point a to point c in Figure 1:

- 97 1. $a \rightarrow c$, the maximum jump is 28;
- 98 2. $a \rightarrow b \rightarrow c$, the maximum jump is 19;
- 99 3. $a \rightarrow d \rightarrow c$, the maximum jump is 17;
- 100 4. $a \rightarrow b \rightarrow d \rightarrow c$, the maximum jump is 19;
- 101 5. $a \rightarrow d \rightarrow b \rightarrow c$, the maximum jump is 12.

102 According to Definition 1, $MMJ(a, c | \Omega) = 12$.

103 To understand Min-Max-Jump distance, imagine someone is traveling by jumping in Ω . Suppose
 104 $MMJ(i, j | \Omega) = \delta$. If the person wants to reach j from i , she must have the ability of jumping at
 105 least δ . Otherwise, j is unreachable from i for her. Whether the distance to a point is "far" or "near"
 106 is measured by how far (or how high) it requires a person to jump. If the requirement is large, then
 107 the point is "far", otherwise, it is "near."

108 3.2 Properties of MMJ distance

109 **Theorem 1.** Suppose $i, j, p, q \in \Omega$,

$$110 \quad MMJ(i, j | \Omega) = \delta \quad (3)$$

$$111 \quad d(i, p) < \delta \quad (4)$$

$$111 \quad d(j, q) < \delta \quad (5)$$

112 then,

$$112 \quad MMJ(p, q | \Omega) = \delta \quad (6)$$

113 where $d(x, y)$ is a distance function (Table 1).

114 *Proof.* $MMJ(i, j | \Omega) = \delta$ is equivalent to $\exists P \in \Theta_{(i, j, \Omega)}$, such that $M(P) = \delta$, and $\forall T \in \Theta_{(i, j, \Omega)}$,
 115 $M(T) \geq \delta$, where $\Theta_{(i, j, \Omega)}$ is the set of all paths from point i to point j under context Ω . $M(P)$ is
 116 the maximum jump in path P . We can assume $MMJ(p, q | \Omega) > \delta$ and $MMJ(p, q | \Omega) < \delta$, then
 117 we will arrive to a contradiction in both cases. \square

118 **Theorem 2.** Suppose $r \in \{1, 2, \dots, n\}$,

$$f(t) = \max(d(\Omega_{n+1}, \Omega_t), \text{MMJ}(\Omega_t, \Omega_r \mid \Omega_{[1,n]})) \quad (7)$$

119

$$\mathbb{X} = \{f(t) \mid t \in \{1, 2, \dots, n\}\} \quad (8)$$

120 then,

$$\text{MMJ}(\Omega_{n+1}, \Omega_r \mid \Omega_{[1,n+1]}) = \min(\mathbb{X}) \quad (9)$$

121 For the meaning of $\Omega_t, \Omega_r, \Omega_{[1,n]}$, and $\Omega_{[1,n+1]}$, see Table 1.

122 *Proof.* There are n possibilities of the MMJ path from Ω_{n+1} to Ω_r , under the context of $\Omega_{[1,n+1]}$,
 123 set \mathbb{X} enumerate them all. Each element of \mathbb{X} is the maximum jump of each possibility. Therefore,
 124 according to the definition of MMJ distance, $\text{MMJ}(\Omega_{n+1}, \Omega_r \mid \Omega_{[1,n+1]}) = \min(\mathbb{X})$. \square

125 **Corollary 1.** Suppose $r \in \{1, 2, \dots, N\}, p \notin \Omega$,

$$f(t) = \max(d(p, \Omega_t), \text{MMJ}(\Omega_t, \Omega_r \mid \Omega)) \quad (10)$$

126

$$\mathbb{X} = \{f(t) \mid t \in \{1, 2, \dots, N\}\} \quad (11)$$

127 then,

$$\text{MMJ}(p, \Omega_r \mid \Omega + p) = \min(\mathbb{X}) \quad (12)$$

128 For the meaning of $\Omega + p$, see Table 1.

129 *Proof.* The proof follows the conclusion of Theorem 2. \square

130 **Theorem 3.** Suppose $i, j \in \{1, 2, \dots, n\}$,

$$x_1 = \text{MMJ}(\Omega_i, \Omega_j \mid \Omega_{[1,n]}) \quad (13)$$

131

$$t_1 = \text{MMJ}(\Omega_{n+1}, \Omega_i \mid \Omega_{[1,n+1]}) \quad (14)$$

132

$$t_2 = \text{MMJ}(\Omega_{n+1}, \Omega_j \mid \Omega_{[1,n+1]}) \quad (15)$$

133

$$x_2 = \max(t_1, t_2) \quad (16)$$

134 then,

$$\text{MMJ}(\Omega_i, \Omega_j \mid \Omega_{[1,n+1]}) = \min(x_1, x_2) \quad (17)$$

135 *Proof.* There are two possibilities of the MMJ path from Ω_i to Ω_j , under the context of $\Omega_{[1,n+1]}$:
 136 Ω_{n+1} is in the path or it is not in the path. x_2 is the min-max jump of the first possibility; x_1 is the
 137 min-max jump of the second possibility. Therefore, according to the definition of MMJ distance,
 138 $\text{MMJ}(\Omega_i, \Omega_j \mid \Omega_{[1,n+1]}) = \min(x_1, x_2)$. \square

139 4 Calculation of Min-Max-Jump distance

140 We propose two methods to calculate the pairwise Min-Max-Jump distance matrix of a dataset. There
 141 are other methods for calculating or estimating it, such as a modified SLINK algorithm (25), or with
 142 Cartesian trees (26; 27), or from a sequence of nearest neighbor graphs (23), or a modified version of
 143 the Floyd–Warshall algorithm.

144 4.1 MMJ distance by recursion

145 The first method calculates \mathbb{M}_Ω by recursion. \mathbb{M}_Ω is the pairwise MMJ distance matrix of Ω (Table
 146 1). $\mathbb{M}_{k, \Omega_{[1,k]}}$ is the MMJ distance matrix of the first k points of Ω (Table 1). Note $\mathbb{M}_{2, \Omega_{[1,2]}}$ is simple
 147 to calculate. $\mathbb{M}_\Omega = \mathbb{M}_{N, \Omega_{[1,N]}}$. \mathbb{M}_Ω is a $N \times N$ symmetric matrix. Rows and columns of \mathbb{M}_Ω are
 148 indexed from 1 to N .

149 Step 7 of Algorithm 1 can be calculated with the conclusion of Theorem 2; Step 12 of Algorithm 1
 150 can be calculated with the conclusion of Theorem 3.

151 Algorithm 1 has complexity of $\mathcal{O}(n^3)$, where n is the cardinality of Set Ω .

Algorithm 1 MMJ distance by recursion

Input: Ω **Output:** \mathbb{M}_Ω

```
1: function MMJ_BY_RECURSION( $\Omega$ )
2:    $N \leftarrow \text{length}(\Omega)$ 
3:   Initialize  $\mathbb{M}_\Omega$  with zeros
4:   Calculate  $\mathbb{M}_{2,\Omega_{[1,2]}}$ , fill in  $\mathbb{M}_\Omega[1, 2]$  and  $\mathbb{M}_\Omega[2, 1]$ 
5:   for  $n \leftarrow 3$  to  $N$  do
6:     for  $r \leftarrow 1$  to  $n - 1$  do
7:       Calculate  $MMJ(\Omega_n, \Omega_r \mid \Omega_{[1,n]})$ , fill in  $\mathbb{M}_\Omega[n, r]$  and  $\mathbb{M}_\Omega[r, n]$ 
8:     end for
9:     for  $i \leftarrow 1$  to  $n - 1$  do
10:      for  $j \leftarrow 1$  to  $n - 1$  do
11:        if  $i < j$  then
12:          Calculate  $MMJ(\Omega_i, \Omega_j \mid \Omega_{[1,n]})$ , update  $\mathbb{M}_\Omega[i, j]$  and  $\mathbb{M}_\Omega[j, i]$ 
13:        end if
14:      end for
15:    end for
16:  end for
17:  return  $\mathbb{M}_\Omega$ 
18: end function
```

152 **4.2 MMJ distance by calculation and copy**

153 According to the conclusion of Theorem 1, there are many duplicated values in \mathbb{M}_Ω . So in the second
154 method we can calculate the MMJ distance value in one position and copy it to other positions in
155 \mathbb{M}_Ω .

156 A well-known fact about MMJ distance is: "the path between any two nodes in a minimum spanning
157 tree (MST) is a minimax path." A minimax path in an undirected graph is a path between two vertices
158 v, w that minimizes the maximum weight of the edges on the path. That is to say, it is a MMJ path.
159 By utilizing this fact, we propose Algorithm 2.

Algorithm 2 MMJ distance by Calculation and Copy

Input: Ω **Output:** \mathbb{M}_Ω

```
1: function MMJ_CALCULATION_AND_COPY( $\Omega$ )
2:   Initialize  $\mathbb{M}_\Omega$  with zeros
3:   Construct a MST of  $\Omega$ , noted  $T$ 
4:   Sort edges of  $T$  from large to small, generate a list, noted  $L$ 
5:   for  $e$  in  $L$  do
6:     Remove  $e$  from  $T$ . It will result in two connected sub-trees,  $T_1$  and  $T_2$ ;
7:     Traverse  $T_1$  and  $T_2$ ;
8:     For all pair of nodes  $(p, q)$ , where  $p \in T_1, q \in T_2$ . Fill in  $\mathbb{M}_\Omega[p, q]$  and  $\mathbb{M}_\Omega[q, p]$  with the
weight of  $e$ .
9:   end for
10:  return  $\mathbb{M}_\Omega$ 
11: end function
```

160 The complexity of Algorithm 2 is $\mathcal{O}(n^2)$. Because the construction of a MST of a complete graph is
161 $\mathcal{O}(n^2)$. During the "for" part (Step 5 to 9) of the algorithm, it accesses each cell of \mathbb{M}_Ω only once.
162 Unlike Algorithm 1, which accesses each cell of \mathbb{M}_Ω for $\mathcal{O}(n)$ times. The merit of the "Calculation
163 and Copy" method is that it is easier to understand than using the Cartesian trees (26; 27).

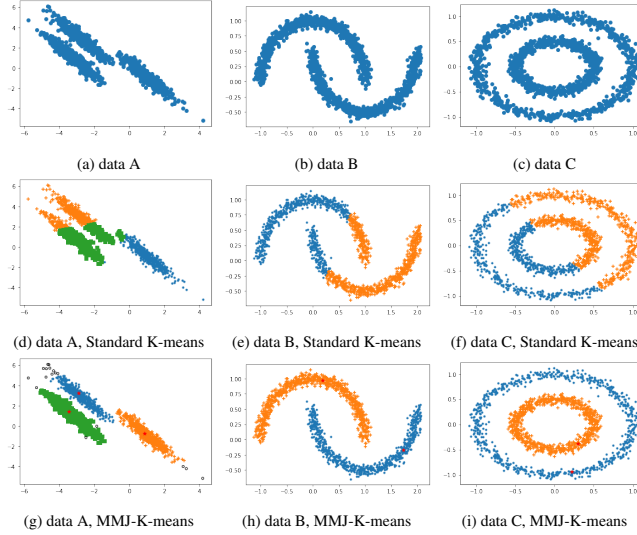


Figure 2: Standard K-means vs. MMJ-K-means

164 5 Applications of Min-Max-Jump distance

165 We explore two applications of MMJ distance, and test the applications with experiments. All the
 166 MMJ distances in the experiments are calculated with Algorithm 1.

167 5.1 MMJ-based K-means

168 K-means clustering aims to partition n observations into k clusters in which each observation belongs
 169 to the cluster with the nearest mean (cluster center or centroid), serving as a prototype of the cluster
 170 (28). Standard K-means uses Euclidean distance. We can revise K-means to use Min-Max-Jump
 171 distance, with the cluster centroid replaced by the Semantic Center of Mass (SCOM) (particularly,
 172 One-SCOM) of each cluster. For the definition of SCOM, see a previous paper (29). One-SCOM is
 173 like medoid, but has some difference from medoid. Section 6.3 of (29) compares One-SCOM and
 174 medoid. In simple terms, the One-SCOM of a set of points, is the point which has the smallest sum
 175 of squared distances to all points in the set.

176 Standard K-means usually cannot deal with non-spherical shaped data, such as the ones in Figure 2.
 177 MMJ-based K-means (MMJ-K-means) can cluster such irregularly shaped data. Figure 2 compares
 178 Standard K-means and MMJ-K-means, on clustering three data which come from the scikit-learn
 179 project (30). Figure 3 are eight more samples of MMJ-K-means. The data sources corresponding to
 180 the data IDs can be found at this URL (temporarily hidden for double blind review).

181 It can be seen MMJ-K-means can (almost) work properly for clustering the 11 data, which have
 182 different kinds of shapes. The black circles are Border points (Definition 2), the red stars are the center
 183 (One-SCOM) of each cluster. During training of MMJ-K-means, the Border points are randomly
 184 allocated to one of its nearest centers.

185 **Definition 2.** *Border point*

186 *A point is defined to be a Border point if its nearest mean (center, centroid, or One-SCOM) is not*
 187 *unique.*

188 Compared with other clustering models that can handle irregularly shaped data, such as Spectral
 189 clustering or the Density-Based Spatial Clustering of Applications with Noise (DBSCAN), the merit
 190 of MMJ-K-means is its simplicity; the logic of MMJ-K-means is as simple as K-means. We just
 191 replace the Euclidean distance with MMJ distance, and the centroid with the Semantic Center of
 192 Mass (SCOM).

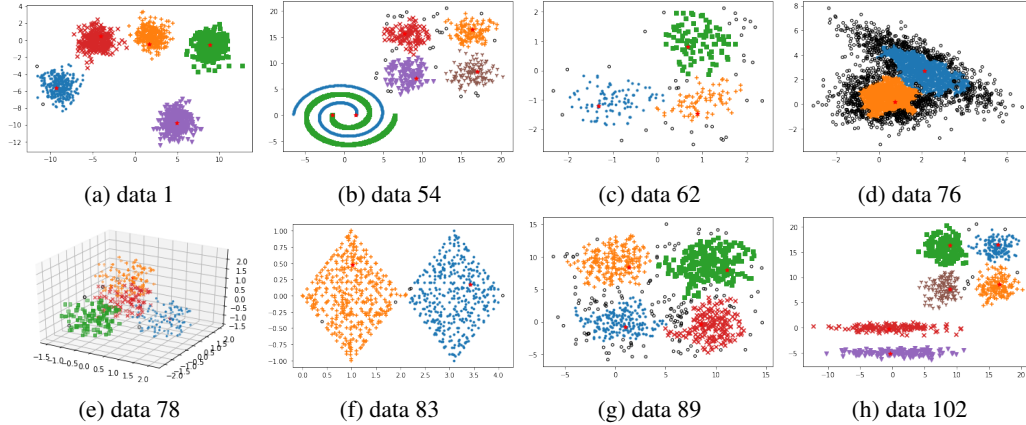


Figure 3: Eight more samples of MMJ-K-means

	CH	SC	DB	CDbw	DBCv	VIASCKDE	New	MMJ-SC	MMJ-CH	MMJ-DB
Accuracy	27/145	38/145	42/145	8/145	56/145	11/145	74/145	83/145	90/145	69/145

Table 2: Accuracy of the ten indices

193 5.2 MMJ-based internal clustering evaluation index

194 Calinski-Harabasz index, Silhouette coefficient, and Davies-Bouldin index are three of the most
 195 popular techniques for internal clustering evaluation. They are used to calculate the goodness of a
 196 clustering technique.

197 The Silhouette coefficient for a single sample is given as:

$$s = \frac{b - a}{\max(a, b)}$$

198 where a is the mean distance between a sample and all other points in the same class. b is the mean
 199 distance between a sample and all other points in the next nearest cluster. The Silhouette coefficient
 200 for a set of samples is given as the mean of Silhouette coefficient for each sample.

201 We can also revise Silhouette coefficient to use Min-Max-Jump distance, forming a new internal
 202 clustering evaluation index called MMJ-based Silhouette coefficient (MMJ-SC). We tested the
 203 performance of MMJ-SC with the 145 datasets mentioned in another paper(31). MMJ-SC obtained
 204 a good performance score compared with the other seven internal clustering evaluation indices
 205 mentioned in the paper(31). Readers can check Table 2 and compare with Table 5 of Liu’s paper(31).

206 MMJ-based Calinski-Harabasz index (MMJ-CH) and MMJ-based Davies-Bouldin index (MMJ-DB)
 207 were also tested. In calculation of these two indices, besides using MMJ distance, the center/centroid
 208 of a cluster is replaced by the One-SCOM of the cluster again, as in MMJ-K-means. It can be seen
 209 that MMJ distance systematically improves the three internal clustering evaluation indices (Table
 210 2). The best performer is MMJ-CH, which achieves an accuracy of 90/145. The accuracy of an
 211 index is computed by evaluating the index’s ability of recognizing the best partition of a dataset from
 212 hundreds of candidate partitions(31).

213 5.2.1 Using MMJ-SC in CNNI

214 The Clustering with Neural Network and Index (CNNI) model uses a Neural Network to cluster
 215 data points. Training of the Neural Network mimics supervised learning, with an internal clustering
 216 evaluation index acting as the loss function (24). CNNI with standard Silhouette coefficient as the
 217 internal clustering evaluation index, cannot deal with non-flat geometry data, such as data B and
 218 data C in Figure 2. MMJ-SC gives CNNI model the capability of processing non-flat geometry data.
 219 E.g., Figure 4 is the clustering result and decision boundary of data B by CNNI using MMJ-SC.
 220 It uses Neural Network C of the CNNI paper (24). CNNI equipped with MMJ-SC, achieves the

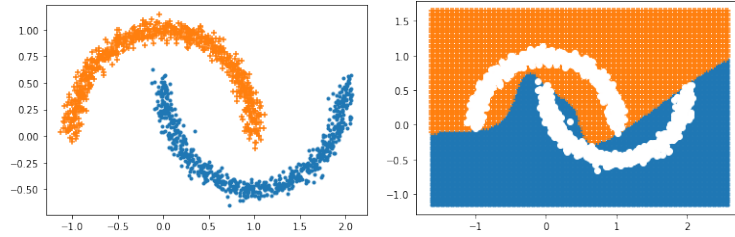


Figure 4: Clustering result and decision boundary of data B by CNNI using MMJ-SC

221 first inductive clustering model that can deal with non-flat geometry data (24). For the definition of
 222 non-flat geometry data, see this¹ Stackexchange question.

223 6 Discussion

224 6.1 Using PAM

225 Since One-SCOM is like medoid, in MMJ-K-means, we can also use the Partitioning Around Medoids
 226 (PAM) algorithm or its variants to find the One-SCOMs (32).

227 6.2 Multiple One-SCOMs in one cluster

228 There might be multiple One-SCOM points in a cluster, which have the same smallest sum of squared
 229 distances to all the points in the cluster. Usually they are not far from each other. We can arbitrarily
 230 choose one or keep them all. If we keep them all, then the One-SCOM of a cluster is not a point, but a
 231 set of points. If the One-SCOM is a set, when calculating a point's MMJ distance to the One-SCOM
 232 of a cluster, we can select the minimum of the point's MMJ distances to all the One-SCOM points.

233 6.3 Differentiating border points

234 Border points defined in Definition 2 can further be differentiated as weak and strong border points.

235 **Definition 3.** *Weak Border Point (WBP)*

236 *A point is defined to be a WBP if its nearest mean (center or One-SCOM) is not unique but less than*
 237 *K , where K is the number of clusters.*

238 **Definition 4.** *Strong Border Point (SBP)*

239 *A point is defined to be a SBP if its nearest mean (center or One-SCOM) is not unique and equals K ,*
 240 *where K is the number of clusters.*

241 Then we can process different kinds of border points with different strategies. E.g., deeming the
 242 Strong Border Points as outliers and removing them.

243 7 Conclusion and Future Works

244 We proposed two algorithms for calculating Min-Max-Jump distance (MMJ distance), and tested
 245 two applications of it: MMJ-based K-means and MMJ-based internal clustering evaluation index.
 246 MMJ-K-means overcomes a big drawback of K-means, improving its ability of clustering, so that it
 247 can handle irregularly shaped clusters. We claim MMJ-CH is the SOTA (state-of-the-art) internal
 248 clustering evaluation index, which achieves an accuracy of 90/145. To thoroughly test the internal
 249 clustering evaluation indices, we conducted an experiment on a set of 145 datasets. A normal
 250 Machine Learning paper usually uses several or dozens of datasets to test their models or algorithms.
 251 In summary, MMJ distance has good capability and potentiality in Machine Learning. Further
 252 research may test its applications in other models, such as other clustering evaluation indices.

¹<https://datascience.stackexchange.com/questions/52260/terminology-flat-geometry-in-the-context-of-clustering>

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