

Clustering with Neural Network and Index

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ABSTRACT

A new model called Clustering with Neural Network and Index (CNNI) is introduced. CNNI uses a Neural Network to cluster data points. Training of the Neural Network mimics supervised learning, with an internal clustering evaluation index acting as the loss function. An experiment is conducted to test the feasibility of the new model, and compared with results of other clustering models like K-means and Gaussian Mixture Model (GMM). The result shows CNNI can work properly for clustering data; CNNI equipped with MMJ-SC, achieves the first parametric (inductive) clustering model that can deal with non-convex shaped (non-flat geometry) data.

KEYWORDS

Clustering; Neural Network; MMJ-SC; Clustering Evaluation; K-means; Gaussian Mixture Model; Self-Organizing Map

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1 INTRODUCTION

Cluster analysis is the grouping of objects such that objects in the same cluster are more similar to each other than they are to objects in another cluster. Clustering is a type of unsupervised learning method of machine learning. In unsupervised learning, the inferences are drawn from the data sets which do not contain labeled output variable. Due to its intensive applications in data analysis, people have developed a wide variety of clustering algorithms. Such as K-Means, Gaussian mixtures, Spectral clustering [23], Hierarchical clustering [13], DBSCAN [28], BIRCH [37] etc.

Evaluation (or “validation”) of clustering results is as difficult as the clustering itself [26]. Popular approaches involve “internal” evaluation and “external” evaluation. In internal evaluation, a clustering result is evaluated based on the data that was clustered itself. Popular internal evaluation indices are Davies-Bouldin index [25], Silhouette coefficient [3], Dunn index [5], and Calinski-Harabasz index [21] etc. In external evaluation, the clustering result is compared to an existing “ground truth” classification, such as the Rand index [35].

There have been proposed several types of Artificial Neural Networks (ANNs) with numerous different implementations for clustering tasks. Most of these Neural Networks apply competitive learning rather than error-correction learning as most other types of Neural Networks do.

Unlike Neural Networks used in competitive learning, CNNI mimics an error-correction learning model.

2 RELATED WORK

2.1 Internal clustering evaluation index

Calinski-Harabasz index [21], Silhouette coefficient [3], and Davies-Bouldin index [25] are three of the most popular techniques for internal clustering evaluation.

Besides the three popular ones, numerous criteria have been proposed in the literature [4, 6, 22, 31, 36]. Such as DBCV [22], Xie-Beni (XB) [33], CDbw [11], S_Dbw [10], and RMSSTD [9]. Besides, new cluster validity indices keep emerging, such as the CVNN [19], CVDD [12], DSI [7], SCV [34], AWCD [15] and VIASCKDE [29]. The author also proposed one [17].

Because only Silhouette coefficient is used in this paper, following is some detailed recount about it.

2.2 Silhouette coefficient (SC)

The Silhouette coefficient for a single sample is given as:

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

where a is the mean distance between a sample and all other points in the same class. b is the mean distance between a sample and all other points in the next nearest cluster. The Silhouette coefficient for a set of samples is given as the mean of Silhouette coefficient for each sample. The range of Silhouette coefficient is $[-1, 1]$. A higher Silhouette coefficient score relates to a model with better defined clusters.

2.3 Artificial Neural Network

Artificial Neural Networks (ANNs), usually simply called Neural Networks (NNs) or neural nets, are based on a collection of connected units or nodes called artificial neurons, which loosely model the neurons in a biological brain [2, 8]. Typically, neurons are aggregated into layers. Different layers may perform different transformations on their inputs. Signals travel from the first layer (the input layer), to the last layer (the output layer), possibly after traversing the layers multiple times.

Training of a Neural Network is usually conducted by determining the difference between the processed output of the network (often a prediction) and a target output [20]. This difference is the error. The network then adjusts its parameters (weights and biases) according to a learning rule and using this error value. Successive adjustments will cause the Neural Network to produce output which is increasingly similar to the target output. After a sufficient number of these adjustments the training can be terminated based upon certain criteria. This is known as supervised learning.

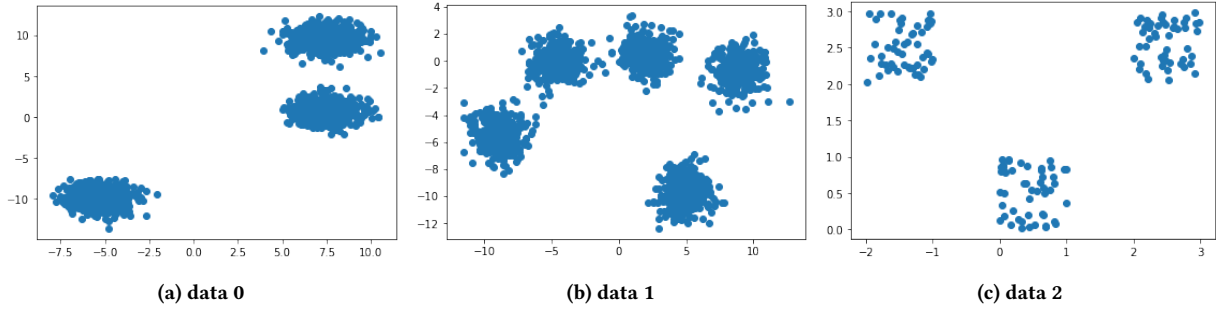


Figure 1: Three datasets for Experiment I

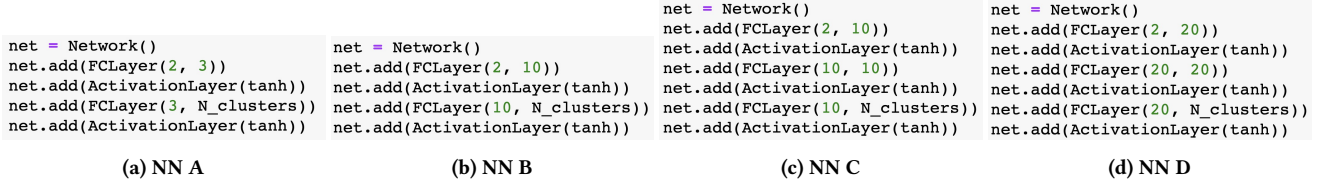


Figure 2: Four Neural Networks

2.4 Self-Organizing Map

Probably, the most popular type of neural nets used for clustering is called Self-Organizing Map (SOM), also known as Kohonen network [14]. “There are many different types of Kohonen networks. These Neural Networks are very different from most types of Neural Networks used for supervised tasks. Kohonen networks consist of only two layers”. The structure of SOM may look like perceptrons. “However, SOM works in a different way than perceptrons or any other networks for supervised learning”.

In a SOM, each neuron of an output layer holds a vector whose dimensionality equals the number of neurons in the input layer. “In turn, the number of neurons in the input layer must be equal to the dimensionality of data points given to the network”.

“When the network gets an input, the input is traversed into only one neuron of the output layer, whose value is closer to the input vector than the values of other output neurons. This neuron is called a winning neuron or the best matching unit (BMU). This is a very important distinction from many other types of Neural Networks, in which values propagate to all neurons in a succeeding layer. And this process constitutes the principle of competitive learning”.¹

CNNI is also a Neural Network for clustering, but it works like Neural Networks for supervised learning. The only difference is that we use an internal clustering evaluation index as the loss function, adjust the weights of the Neural Network to reduce the loss (improve the value of the index).

2.5 Deep Clustering

Deep clustering models use a Deep Neural Network (DNN) to transform high dimensional data into more clustering-friendly representations without manual feature extraction, then use a classic

clustering model to cluster the transformed data [1, 27, 38]. In these models, a Neural Network is used as a helper for clustering, the “clustering” part of these models is still accomplished by classic clustering models, such as K-means, Agglomerative clustering etc. In CNNI, no other classic clustering models are needed.

3 THE STRUCTURE OF CNNI

The structure of CNNI is simple: a Neural Network for supervised learning plus an internal clustering evaluation index. The index acts as the loss function, because there is no target output associated with each input data point in clustering scenario.

The number of neurons in the input layer of CNNI equals to the dimension of the data points given to the network. The number of neurons in the output layer of CNNI equals to number of K clusters we want to classify. By comparing values of output neurons, label of one data point is obtained (e.g., find out the maximum of output neurons).

Training of CNNI has some difference from other supervised learning Neural Networks. We need to compute each data point’s label according to the Neural Network’s current state, then calculate the value of the clustering evaluation index, according to the labels of all data points. Adjustment of the weights of the Neural Network is based on the value of the index.

4 EXPERIMENTS

We tested the practicability of CNNI with several experiments. In the experiments, six synthetic datasets are to be clustered by four simple feed-forward Neural Networks (FNNs) with different model capacity (Figure 2). All the synthetic datasets are generated with library functions from the scikit-learn project [24].

Coordinate descent is used to train the Neural Networks.

¹<http://www.kovera.org/neural-network-for-clustering-in-python/>

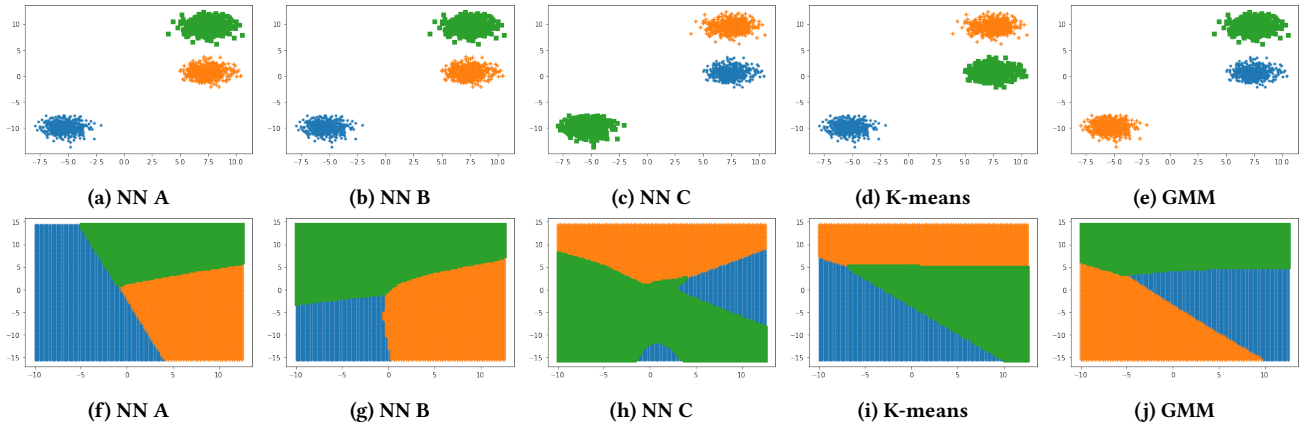


Figure 3: Clustering results and decision boundaries of data 0

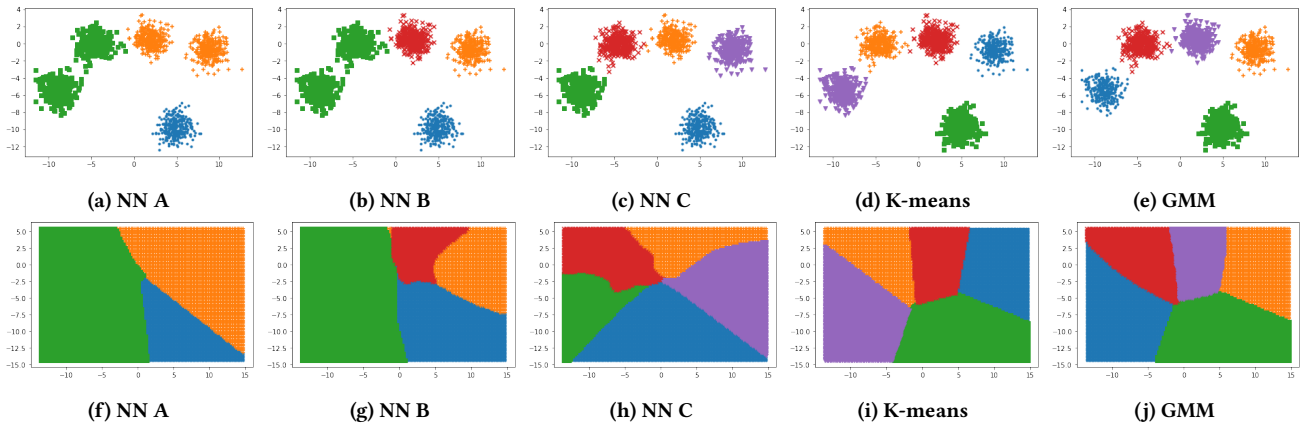


Figure 4: Clustering results and decision boundaries of data 1

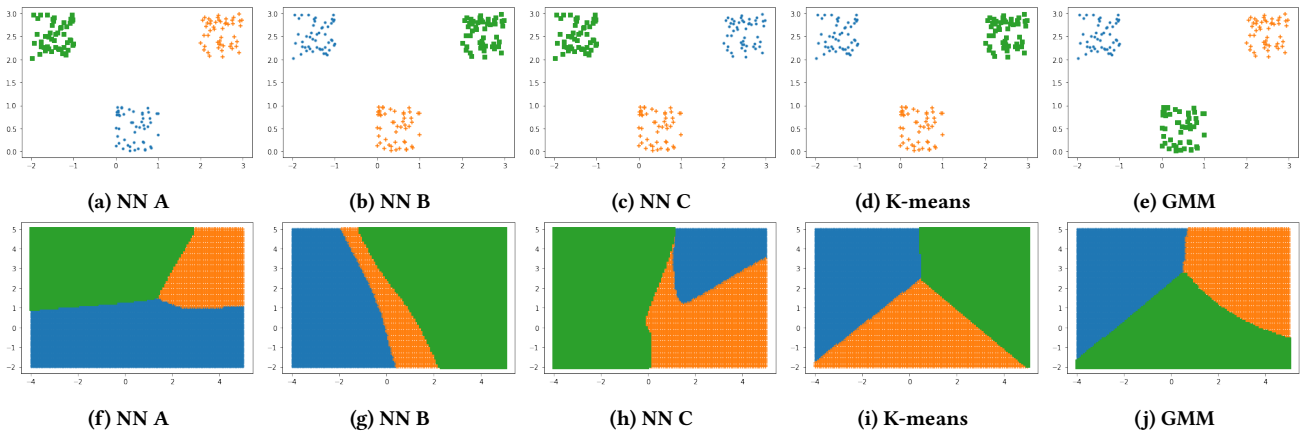


Figure 5: Clustering results and decision boundaries of data 2

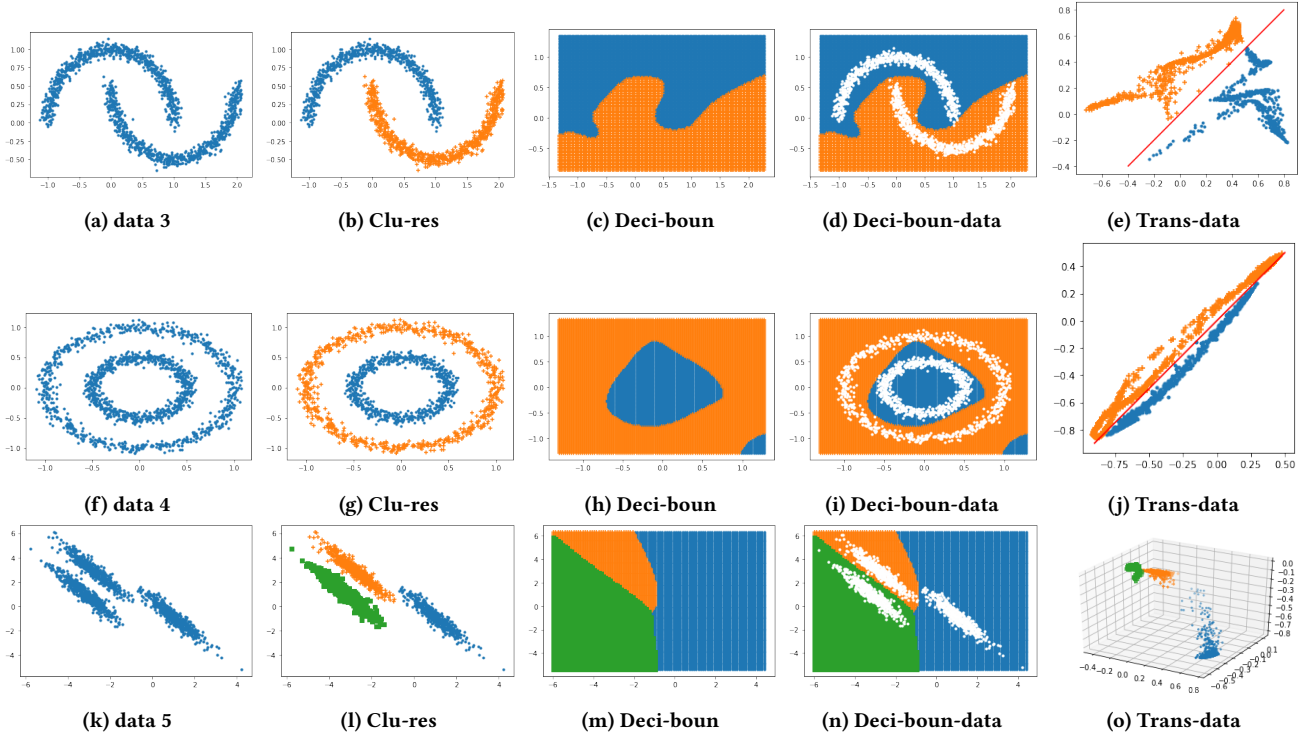


Figure 6: Clustering results, decision boundaries, and transformed data of data 3,4,5

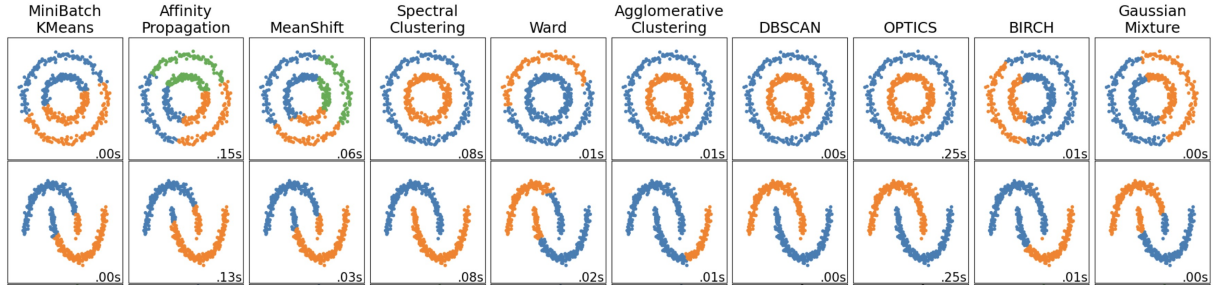


Figure 7: Clustering results of two-moons and two-circles by other models (from the scikit-learn project)

4.1 Coordinate descent

Coordinate descent is an optimization algorithm that successively minimizes along coordinate directions to find the minimum of a function. At each iteration, the algorithm determines a coordinate or coordinate block via some coordinate selection rule, then exactly or inexactly minimizes over the corresponding coordinate hyperplane while fixing all other coordinates or coordinate blocks. A line search along the coordinate direction can be performed at the current iterate to determine the appropriate step size. Coordinate descent is applicable in both differentiable and derivative-free contexts.²

²https://en.wikipedia.org/wiki/Coordinate_descent

In the experiments, we use a naive coordinate descent algorithm (Algorithm 1) for adjusting parameters of the Neural Network. People can test more advanced optimization techniques like gradient descent, genetic algorithms, and particle swarm optimization etc.

4.2 Experiment I

In Experiment I, data 0, 1, and 2 are clustered with Neural Networks A, B, and C. We trained each Neural Network with 30 Epochs for each dataset. After training of the Neural Networks, we predict labels of 10,000 new data points, and plot the decision boundaries of each model. Figure 3, 4, and 5 illustrate the clustering results and decision boundaries discovered by the Neural Networks, for each dataset, and compared with results of K-means and Gaussian Mixture Model (GMM). Note the interesting decision boundaries discovered by different Neural Networks for each dataset.

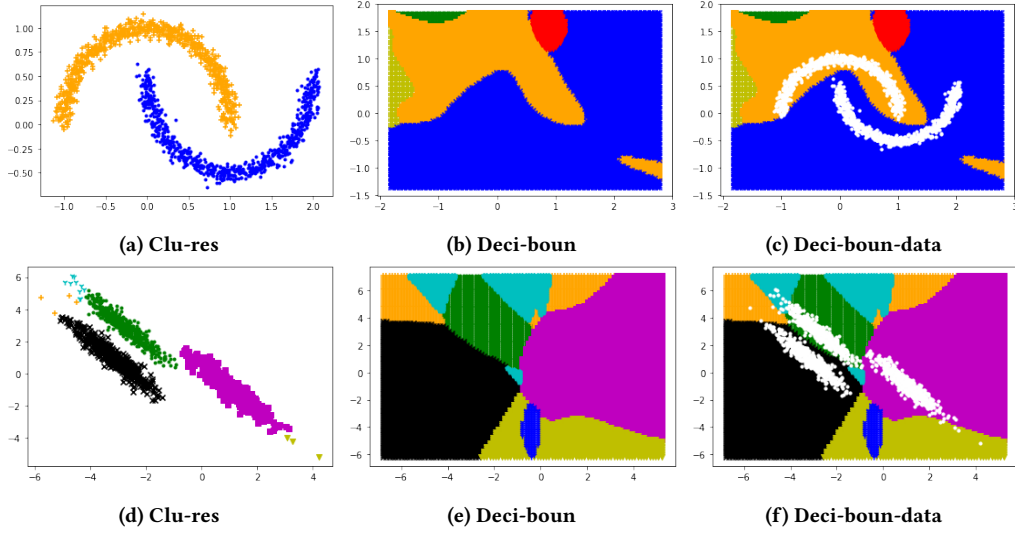


Figure 8: Clustering results and decision boundaries of automatic model selection

Algorithm 1 Naive coordinate descent for CNNI**Require:**Neural Network's parameter set: N , an Index: I , Epochs: E ;**Ensure:**Optimized parameters of N ;

- 1: Randomly initialize each member of N ;
- 2: for e in E ;
- 3: for n in N ;
- 4: Make a random variation to n . If it improves I , keep it. Otherwise, discard it;
- 5: **return** N .

4.3 Experiment II

In another paper [18], we introduced a new internal clustering evaluation index, called MMJ-based Silhouette coefficient (MMJ-SC). In Experiment II, we test CNNI with this new index. In the experiment, data 3 and 4 are clustered with Neural Network D, data 5 is clustered with Neural Network C.

The result is shown in Figure 6. The last column of Figure 6 plots the transformed data by the Neural Networks after convergence. To get a transformed point, after training of a Neural Network, we feed the Network with a data point, the values of the output neurons are the coordinate of the transformed data point. As shown by sub-figure (e) and (j) of Figure 6, linearly non-separable data becomes linearly separable by the line $f(x) = x$, after transformation by the Neural Network.

Figure 7 is clustering results of the two-moons and two-circles data by other models (from the scikit-learn project). It can be seen that only Spectral clustering, Agglomerative clustering, DBSCAN and OPTICS can deal with these non-convex shaped (non-flat geometry) data. However, all these models are non-parametric (transductive). That means we cannot get a set of parameters, and predict the label of a new point based on the parameters. Therefore, we can conclude that: CNNI equipped with MMJ-SC, is the first parametric

(inductive) clustering model that can deal with non-convex shaped (non-flat geometry) data.

5 INDICES BASED ON FUZZY CLUSTERING

Fuzzy clustering (also referred to as soft clustering) is a form of clustering in which each data point can belong to more than one cluster with probability. As a comparison, in non-fuzzy clustering (also known as hard clustering), data are divided into distinct clusters, where each data point can only belong to exactly one cluster. By far we are using indices based on hard clustering, however, Neural Networks can naturally output soft clustering, by applying a Softmax activation to the last layer of a Neural Network.

In this section, we propose two soft clustering based indices and test one of them on two challenging data.

5.1 Two soft clustering indices (SCIs)**5.1.1 SCI V1.**

Definition 5.1. SCI V1

$$I_{sci} = \sum_{l \in L} P(l)I(l) \quad (1)$$

where L is the set of all possible labeling of data X ; l belongs to L ; $P(l)$ is the possibility of labeling l , it is easy to compute when we have soft clustering of data X ; $I(l)$ is an ordinary hard clustering based index, like SC or MMJ-SC.

SCI V1 is very expensive to calculate naively, since there are K^N possible labeling of data X , where N is the number of points in X , K is the number of clusters. Therefore, we do not test it in this paper. Hopefully mathematicians will find a smart way to calculate it efficiently.

5.1.2 SCI V2.

Definition 5.2. SCI V2

$$I = \frac{1}{N} \sum_{x \in X} s(x) \quad (2)$$

$$I_{sci} = \frac{1}{N} \sum_{x \in X} P(x)s(x) \quad (3)$$

SCI V2 revises an ordinary hard clustering based index like SC or MMJ-SC, in which the index for a set of samples is given as the mean of index for each sample (Equation 2).

In the revision, we first determine the label for each sample x , by finding the maximum probability of sample x belonging to a cluster; $P(x)$ is the probability of sample x belonging to the cluster. After labels of all samples are determined, then we can calculate the index value $s(x)$ for each sample x . N is the number of points in data X .

If $P(x) = 1$ for all samples $x \in X$, then $I_{sci} = I$.

5.2 A new optimization algorithm for CNNI

Naive coordinate descent (Algorithm 1) works good for simple clustering task, such as data 0-5 in Experiment I and II. For more challenging clustering tasks like data 6 and 7 in Figure 9, naive coordinate descent seems not works. Therefore, a new optimization algorithm for dealing with these more challenging clustering tasks is designed.

The algorithm is called Step Back to See a Bigger Picture (SBSBP). In SBSBP, we set a criteria to identify a local minima. If the criteria for recognizing a local minima is reached, we randomly step back some steps; making the Neural Network worse for clustering the data judged by the Index, so that the Neural Network can jump out of the local minima region, and try to step to the global minima. The best parameters so far are recorded so that we can restore it after the training.

A local minima is identified if there is no improvement within some steps (Patience).

5.3 Experiment III

In Experiment III, we revise MMJ-SC with SCI V2, and tested it with more challenging clustering tasks of data 6 and 7 in Figure 9. Data 6 and 7 are referred to as Data 45 and Data 106 in [17]. The data sources corresponding to the data IDs can be found at this URL.³

The Neural Network used in Experiment III has similar structure as the Neural Networks in Figure 2, with one layer deeper and more nodes. It has shape $2 \rightarrow 80 \rightarrow 80 \rightarrow 80 \rightarrow 10$, which has 14,010 parameters. The activation to the last layer is changed to Softmax. As mentioned in Section 7.3.1, CNNI has some ability of automatic model selection. Therefore, we set the number of output neurons to 10 and let the Neural Network automatically select the true number of clusters. The Neural Network is optimized with SBSBP.

In the experiment, the *Patience* hyper-parameter is fixed. However, we can also make it dynamic, so that it is larger in later stages of training. When the index is a continuous value, we need to set a *Tolerance* hyper-parameter to decide whether the index has improved, or worsened, or unaffected. In the experiment, the *Tolerance* hyper-parameter is set to 10^{-8} .

Algorithm 2 Step Back to See a Bigger Picture (SBSBP)

Require:

Neural Network's parameter set: N , an Index: I , Maximum steps: M , hyper-parameter: *Patience*;

Ensure:

Optimized parameters of N ;

```

1: Randomly initialize each member of  $N$ ;
2: Calculate the Index  $I$ ;
3:  $Counter \leftarrow 0$ ;
4: for  $i$  in  $M$ ;
5:   Randomly select a parameter  $n$  from  $N$ ;
6:   Generate a random number  $\delta$ ;
7:    $n \leftarrow n + \delta$ ;
8:   Calculate the Index  $I$ ;
9:   If  $I$  improves:
10:     $Counter \leftarrow 0$ ;
11:    Keep the variation to  $n$ , continue;
12:   Elif  $I$  is invariant:
13:     $Counter++$ ;
14:    Restore previous value of  $n$ ,  $n \leftarrow n - \delta$ ;
15:   Else:
16:     $Counter++$ ;
17:    If  $Counter > Patience$ :
18:       $Counter \leftarrow 0$ ;
19:      Randomly_step_back_some_steps;
20:    Else:
21:      Restore previous value of  $n$ ,  $n \leftarrow n - \delta$ ;
22: return  $N$ .
```

Algorithm 3 Randomly_step_back_some_steps

Require:

Neural Network's parameter set: N , an Index: I , hyper-parameter: ρ_1, ρ_2 ;

```

1:  $another\_counter \leftarrow 0$ ;
2:  $Steps \leftarrow random.randint(\rho_1, \rho_2)$ ;
3: while  $another\_counter < Steps$ ;
4:   Randomly select a parameter  $n$  from  $N$ ;
5:   Generate a random number  $\delta$ ;
6:    $n \leftarrow n + \delta$ ;
7:   Calculate the Index  $I$ ;
8:   If  $I$  worsens:
9:      $another\_counter++$ ;
10:    Keep the variation to  $n$ , continue;
11:   Else:
12:    Restore previous value of  $n$ ,  $n \leftarrow n - \delta$ ;
```

As shown by Figure 9, after millions of steps of training, the Neural Network finally clustered the two data correctly, and learned reasonable (although unsatisfactory) decision boundaries.

6 MMJ-K-MEANS LOSS

Section 7.2 mentions we can use other losses like MMJ-K-means loss. In this section, we conduct experiments to test this idea.

³https://github.com/mike-liuliu/Experiment_data_of_a_paper

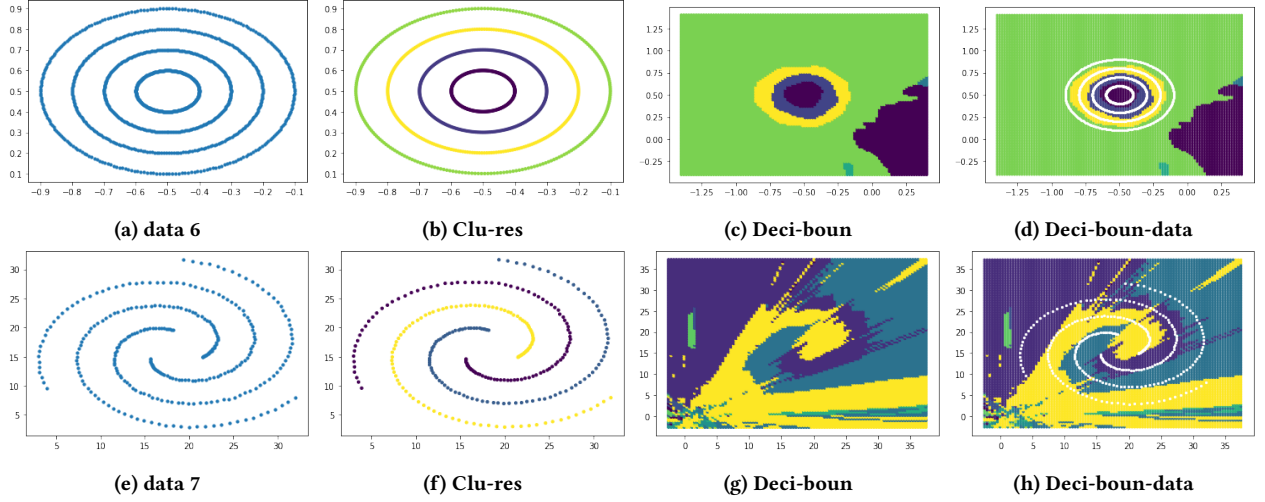


Figure 9: Clustering results and decision boundaries of data 6 and 7

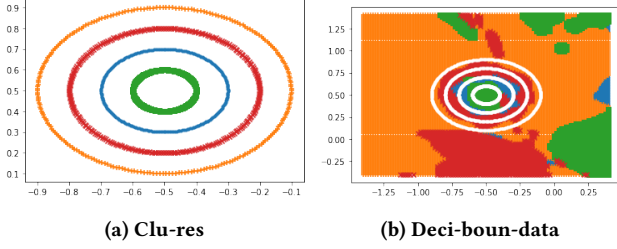


Figure 10: Data 6 trained with MMJ-K-means loss

Equation 4 is the loss of standard K-means.

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2 \quad (4)$$

where N is number of points in data X , K is the number of clusters. μ_k is the centroid of cluster k , c_i is the label of data point x_i .

In MMJ-K-means loss, Euclidean distance is replaced by MMJ distance [18], centroid of a cluster is replaced by the One-SCOM of the cluster [16, 18].

6.1 Experiment IV

In Experiment IV, we tested MMJ-K-means loss with data 6. The Neural Network is optimized with SBSBP. Figure 10 illustrates the clustering result and decision boundary. The result shows MMJ-K-means loss also works for clustering, besides using an index as the loss function.

6.2 MMJ-K-means loss based on Soft Clustering

We can also revise the MMJ-K-means loss to utilize Soft Clustering.

$$\mathcal{L}_s = \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2 (2 - P(x_i)) \quad (5)$$

Equation 5 is similar to SCI V2. We first use Hard Clustering to decide which cluster data point x_i belongs to, then use Soft Clustering to decide the probability of data point x_i belongs to the cluster. $P(x_i)$ is the probability.

If $P(x_i) = 1$ for all samples $x_i \in X$, then $\mathcal{L}_s = \mathcal{L}$.

6.3 Experiment V

In Experiment V, we tested MMJ-K-means loss based on Soft Clustering, with data 3 and 7. Section 7.4 discusses about training the Neural Network with Mini-Batches of data X . In Experiment V, we use a variant of Mini-Batches, and devise a new optimization algorithm (Algorithm 4) for optimizing the Neural Network. In each iteration of Algorithm 4, we first draw a sample from data X , then train the Neural Network with the sample and SBSBP for some steps, then check if the Neural Network has improved for clustering the whole data X . If it is, record the best parameters so far. The MMJ distance matrix of sample S is calculated under the context of data X , not S itself. For the definition of *context* in MMJ distance, see [18].

Algorithm 4 SBSBP and variant of Mini-Batch (MB-SBSBP)

Require:

Neural Network's parameter set: N , Loss: L , Maximum iterations: T , hyper-parameter: M ;

Ensure:

Optimized parameters of N ;

- 1: Randomly initialize each member of N ;
 - 2: for j in T ;
 - 3: Draw a sample S from data X , $S \subseteq X$;
 - 4: Train the Neural Network with sample S and SBSBP for M steps;
 - 5: Calculate the Loss L over the whole data X ;
 - 6: If L improves:
 - 7: Record parameter set N ;
 - 8: **return** Recorded best parameters so far N_{best} .
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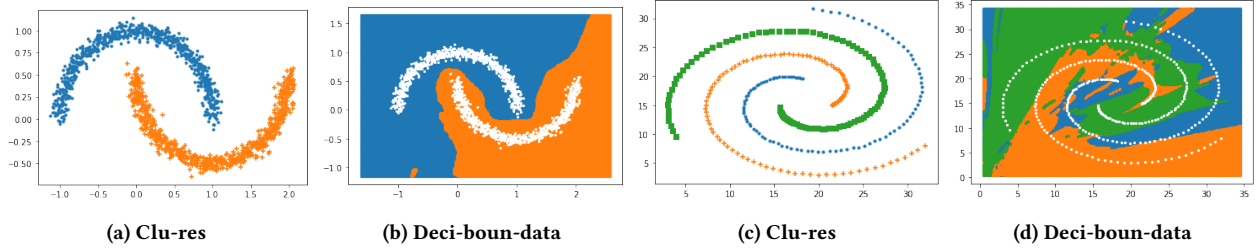


Figure 11: Data 3 and 7 trained with MMJ-K-means loss based on Soft Clustering (Equation 5)

Figure 11 illustrates the clustering results and decision boundaries. The result shows optimizing MMJ-K-means loss based on Soft Clustering also works for clustering.

The Neural Network used in Experiment IV and V has similar structure as the Neural Network used in Experiment III. It has shape $2 \rightarrow 80 \rightarrow 80 \rightarrow 80 \rightarrow N_clusters$. We assume the true number of clusters ($N_clusters$) is known in advance.

Section 6.2 of [18] discusses the issue of “multiple One-SCOMs in one cluster”, in Experiment IV and V, we choose to keep them all.

Note although K-means loss is used in this section, the K-means model itself is not used. Because a Neural Network can directly output Hard Clustering or Soft Clustering label of a data point, we do not need the K-means model to calculate the label of a data point. We just need the K-means loss.

7 DISCUSSION

7.1 Other choices

Because the purpose of this paper is to introduce CNNI and test its feasibility. We used simple fully connected feed-forward Neural Networks, with fixed activation function Tanh, and fixed clustering evaluation index Silhouette coefficient and MMJ-SC in the experiments. We did not test more advanced Neural Networks like convolutional neural network (CNN) or Bayesian neural network (BNN), and more advanced optimization techniques like dropout [30].

For optimization algorithms, we also tested “Nelder-Mead”, “Powell”, “CG”, and “BFGS” implemented by SciPy [32]. It seems “Powell” works good for CNNI. Other optimization algorithms like gradient descent, genetic algorithms, and other clustering evaluation indices were not tested either.

Further research is necessary to make more elaborate selections of these factors.

7.2 Other losses

With labels of all data points known, another choice is to calculate other losses, such as the likelihood of Gaussian Mixture Model, or the loss of MMJ-K-means [18], then adjust Neural Network parameters by optimizing these losses.

7.3 Model selection

Model selection of CNNI is easy and natural. We test Neural Networks with different structures and different number of output neurons, and pick out the one which obtains the best internal-clustering-evaluation-index value for clustering the given dataset.

7.3.1 Automatic model selection. It seems CNNI has some ability of automatic model selection. Suppose the true number of clusters is K , we can set the number of output neurons to M , where $K \ll M$, hopefully, after training of the Neural Network, the number of active output neurons will degenerate to K . We conducted an experiment to test automatic model selection. In the experiment, we use Neural Network D to cluster data 3 and 5. With the number of output neurons set to 30. The result is shown in Figure 8. It can be seen that in the region where data appears, the number of active output neurons degenerates to K , with some minor error.

7.4 Mini-Batch

Computing the internal clustering evaluation index over the whole dataset may be time-consuming. We can divide the data into M Mini-Batches by random sampling, and use one Mini-Batch for training in one epoch. Or we can train M Neural Networks in parallel with the Mini-Batches, then calculate an average Neural Network, then train the average Neural Network with the whole dataset for several epochs.

7.5 How to understand the learning?

In supervised learning, the learning of the Neural Network is guided by a tutor/teacher/supervisor, which is represented by a training dataset.

How to understand the learning of CNNI? What is guiding the learning? Maybe we can consider the Neural Network is guided by some aesthetic sense, which is represented by an internal clustering evaluation index.

7.6 Overfitting in unsupervised learning

Overfitting is common in supervised learning models. Can overfitting occur in unsupervised learning? Sub-figure 11c and 11d in Figure 11 seems provide a new evidence, of overfitting in unsupervised learning.

As shown by Figure 12, although the Neural Network labeled each training data point correctly, in the region indicated by the two black circles, the Neural Network failed to learn a reasonable decision boundary. It seems the Neural Network just “memorized” the correct labels of training data points, and failed to generalize to new data points in the two regions.

8 CONCLUSION AND FUTURE WORKS

We introduced a new clustering model called Clustering with Neural Network and Index (CNNI). Experiments are conducted to test the

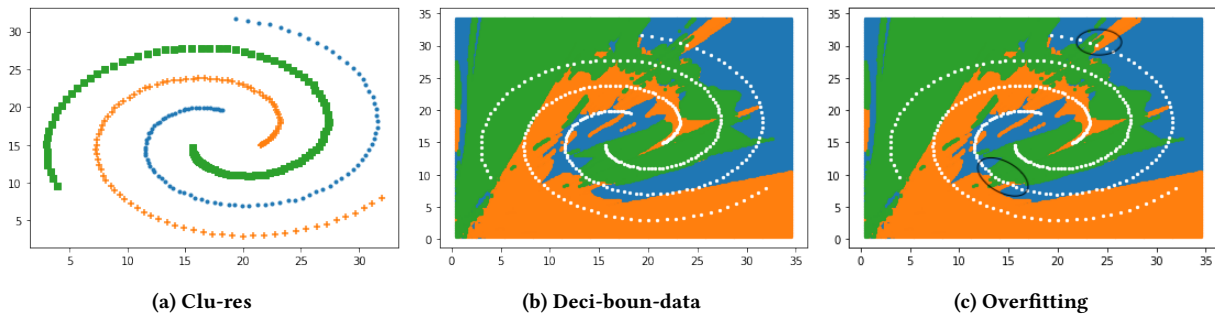


Figure 12: Overfitting in unsupervised learning?

feasibility of CNNI. In the experiments, synthetic datasets were clustered by simple feed-forward Neural Networks (FNNs) with different model capacity. The result shows:

- CNNI can work properly for clustering data.
- Different structures of Neural Networks result in different decision boundaries.
- CNNI equipped with MMJ-SC, achieves the first parametric (inductive) clustering model that can deal with non-convex shaped (non-flat geometry) data.

Further research is necessary to test other types of Neural Networks, optimization techniques, and other clustering evaluation indices. And how CNNI performs in higher dimensions.

A potential advantage of CNNI is its flexibility of model capacity. When the hyperparameter K (number of clusters) is fixed, the model capacity (number of learnable parameters) of other parametric clustering models like K-means and Gaussian Mixture Model (GMM) is fixed. The model capacity of CNNI is flexible due to the utilization of Neural Network.

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