A DEEP CONVOLUTIONAL AUTO-ENCODER WITH EMBEDDED CLUSTERING

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ABSTRACT

In this paper, we propose a clustering approach embedded in a deep convolutional auto-encoder (DCAE). In contrast to conventional clustering approaches, our method simultaneously learns feature representations and cluster assignments through DCAEs. DCAEs have been effective in image processing as it fully utilizes the properties of convolutional neural networks. Our method consists of clustering and reconstruction objective functions. All data points are assigned to their new corresponding cluster centers during the optimization, after that, clustering centers are iteratively updated to obtain a stable performance of clustering. The experimental results on the MNIST dataset show that the proposed method substantially outperforms deep clustering models in term of clustering quality.

Index Terms— Deep Learning, Deep Convolutional Auto-Encoder, Embedded Clustering.

1. INTRODUCTION

Clustering is an unsupervised machine learning approach. It aims to group a set of unlabelled data based on homogeneous patterns in a given feature space. Traditional clustering algorithms attain a limited performance as the dimensionality goes higher. Dealing with high-level representation provides beneficial components, benefiting the achievement of such a clustering task. As there is no supervising knowledge to provide information about categories labels, representative features with compact clusters are much more beneficial. Deep auto-encoders (DAEs) and deep convolutional auto-encoders (DCAEs) are unsupervised models for representation learning. They map inputs into a new representation space, allowing one to obtain useful features through the encoding procedure. The data is projected into a set of feature spaces, using the encoding part, from which the decoding part reconstructs the original data. The training is performed in an unsupervised manner by minimizing the differences between original data and reconstructed data with distance metrics. The major difference between a DAE and a DCAE is that the former adopts fully-connected layers to reconstruct the signal globally while the latter utilizes local information to achieve the same objective. DCAEs can benefit from a local model. These methods have been exploited for the purpose of clustering, where features learned through deep networks (e.g. AE or CAE) provide an abstracted latent representation which is used for clustering analysis. Existing works can be classified into four categories summarized in Table 1. *Huang et al.* [2]

Method	Separated Clustering	Embedded Clustering
AE	*Tian* [1], *Huang* [2]	*Song* [3], *Xie* [4]
CAE	*Li et al.* [5]	*Guo et al.* [6]

Table 1. Deep Clustering Methods

and *Tian et. al* [1] used AEs to learn a lower dimensional representation space, to obtain effective features used for clustering; thereafter, K-means is applied to cluster the obtained features. *Lia at el.* [5] utilizes the CAE to learn representation, thereafter, the decoder part is neglected and a soft K-means model is added on top of the encoder to make a unified clustering model. Even though such a scheme takes advantages of a deep neural network to map the original data into a representative feature space followed by clustering analysis, feature space learning and clustering are two separate procedures, the objectives of which are not optimized jointly. *Song et al.* [3] and *Xie et al.* [4] embedded a clustering objective into an AE framework, while *Guo et al.* [6] recently propose clustering with a CAE. Developing an embedded clustering approach in a deep network allows extracting latent features and clustering assignments simultaneously. This scheme usually leads to a more compact latent feature space.

In this paper, we present a clustering approach embedded into a DCAE framework which aims to learn feature representation and cluster assignment simultaneously. In contrast to conventional clustering approaches, our method makes use of representation learning with deep neural networks, which helps to find compact and representative latent feature spaces for further recognition tasks. Most of existing methods fundamentally rely on pre-training the parameters, using different settings, while we train our model in an end-to-end way with fixed settings without any pre-training or fine-tuning procedures, enabling a faster training process. In contrast to Guo et al.'s work, our proposed method differs in several key respects. First, for the clustering approach, instead of clustering with KL divergence, we apply an objective function that restricts the distance between learned feature representations, in a latent space, and their identical centroids, producing a stable

representation, which is appropriate for clustering process. Accordingly, the centroids are iteratively updated. Second, our work differs particularly in terms of architecture, cost functions, and optimization. Finally, our results show that our model yields a substantially better performance for both reconstruction and clustering quality. We evaluate our proposed model on the MNIST data-set and compare our method with three baselines, showing that our method substantially outperforms others in both reconstruction and clustering quality.

2. METHOD

The proposed approach embeds K-means clustering algorithm into a DCAE framework which is trained in a fully unsupervised manner. The architecture is shown in Fig. 1. It consists of two objective functions, one minimizes the distance between feature representations and their identical cluster centers, and another minimizes the reconstruction error. The two objectives are simultaneously optimized.

2.1. Deep Convolutional Auto-encoder (DCAE)

In contrast to a DAE model, the DCAE [7] uses convolutional and deconvolutional layers instead of fully connected layers. DCAE can be better appropriate in image-processing tasks because it takes advantage of the properties of a convolutional neural network (CNN) [8]. Local connections and parameter sharing distinguish the CNN to have a property in translation latent features [9]. In the encoding part, convolutional layers are used, as feature extractors, to learn features through mapping the data into an internal layer. A latent representation of the n^{th} feature map of the existing layer is given by the following form:

$$h_n = \sigma(x * W_n + b_n) \tag{1}$$

where W are the filters and b is the corresponding bias of the n^{th} feature map, σ is the activation function (e.g. sigmoid, ReLU), and $*$ denotes the 2D convolution operation.

In contrast, the deconvolutional layers invert this process and reconstruct the latent representation back to its original shape, so this process maps the obtained features into pixels [10] by using the following form:

$$y_n = \sigma(\sum_{n \in H} h_n * \tilde{W}_n + c) \tag{2}$$

where H denotes the group of latent feature maps, $\tilde{W}$ is the flip operation over both dimensions of the weights, c is the corresponding bias, σ is the activation function, and $*$ denotes the 2D convolution operation.

The DCAE extracts latent representations through its internal layer by minimizing the reconstruction error. We use the cross-entropy (logistic) loss via Eq.(3) because experiments have shown that the Euclidean (L2) loss function is not robust to convolutional neural networks designed with deconvolutional layers, and networks trained with perceptual loss tend to produce much better results [11–13]. In a like manner of standard networks, the backpropagation method computes the gradient of the error with respect to all parameters.

$$E_1 = -\frac{1}{N}\sum_{n=1}^{N}\left(y_n \log \widehat{y}_n + (1 - y_n)\log(1 - \widehat{y}_n)\right) \tag{3}$$

Where $\widehat{y}$ is the pixel value of the reconstructed image, and y is the pixel value of the target image. For further detail of CAE, readers can refer to [7].

2.2. Clustering Embedded on Deep Convolutional Auto-encoder

Using the DCAE model described in Section 2.1, we now utilize its strength as a training procedure for feature transformations. The goal of our clustering model is to learn feature representations and cluster assignments simultaneously. Using the DCAE, as feature-extractor, supports the achievement of such a clustering process. This idea allows clustering method to deal with learned features instead of raw data. We follow [3] by developing a deep clustering model, but instead of a classic AE, we apply the DCAE to the clustering task. Although DCAE provides an effective representation in a new latent space, it does not internally impose compact representation constraints using clustering. Therefore, we add a clustering objective function to the DCAE framework, which minimizes the distance between data samples and assigned centroids in latent space as follows [3]:

$$E_2 = \lambda \cdot \frac{1}{2N}\sum_{n=1}^{N} \parallel h^t(x_n) - c_n^* \parallel^2 \tag{4}$$

where N denotes the number of samples, λ is clustering weight-parameter that control the contribution percentage of clustering cost function in the overall cost function (5), $h^t(*)$ is the internal representation obtained by the encoder mapping at the t^{th} iteration, (x_n) is the n^{th} sample in the dataset, and c_n^* is the assigned cluster center to the n^{th} sample. The overall cost function is a combination of two parts: the first part is essentially the cross-entropy loss minimizing the reconstruction error, while the second part is clustering objective function minimizing the distance between data representations in the latent space and their corresponding cluster centers.

$$\min_{W,b} E_1 + E_2 \tag{5}$$

2.3. Optimization

At each epoch, our model optimizes two components using stochastic gradient descent and backpropagation: (1) CAE

parameters as well as a mapping function h, and (2) cluster centers c. At each epoch, the model optimizes the mapping function h, while keeps the cluster centers fixed at c. Thereafter, each obtained new internal representation is assigned to the closest centroid. Following [3], this is defined as:

$$c_n^* = arg\min_{c_m^{t-1}} \parallel h^t(x_n) - c_m^{t-1} \parallel^2 \tag{6}$$

where c_m^{t-1} denotes the cluster centers computed at the previous epoch. After each internal representation is assigned to the closest cluster center, the cluster center is updated using the sample assignment computed in the previous epoch via the following equation as [3]:

$$c_m^t = \frac{\sum_{x_n \in c_m^{t-1}} h^t(x_n)}{\sum c_m^{t-1}} \tag{7}$$

where c_m^{t-1} is all samples that belong to the m^{th} cluster at the previous epoch, and $\sum c_m^{t-1}$ is the number of samples that belong to the m^{th} cluster.

2.4. Architecture

We adopt the base architecture proposed in [14]. Our extension to the architecture are the following. Firstly, instead of two loss functions (cross-entropy loss and Euclidean loss) to minimize the reconstruction error, we only use cross-entropy loss, as previous studies have shown that the Euclidean loss function is not robust to convolutional neural networks designed with deconvolutional layers [11–13]. Also with only the cross-entropy loss, our experiments have shown that only cross-entropy reconstruction loss can provide good training convergence. Secondly, we exploit the learned features via the internal layer and feed it to clustering loss which minimizing the distance between data points and their assigned cluster centers, embedding clustering techniques in a DCAE framework. Thirdly, instead of optimizing the CAE to reach optimal reconstruction, we sequentially optimize the mapping function h and cluster centers to obtain efficient clustering results. The final architecture of our model for deep clustering embedded in DCAE is presented in Fig. 1.

The network architecture consists of two convolutional layers with filter sizes of 9×9 with 8 kernels in the first convolutional layer and 4 kernels in the second convolutional layer. This followed by two fully-connected layers, which have 250 neurons and 10 neurons respectively, in the encoding part. In the decoding part, a single fully-connected layer of 250 neurons followed by two deconvolutional layers. The first deconvolutional layer consists of 4 kernels with the size of 12×12, and the second deconvolutional layer consists of 4 kernels with the size of 17×17. As an activation function, a standard sigmoid activation function is utilized.

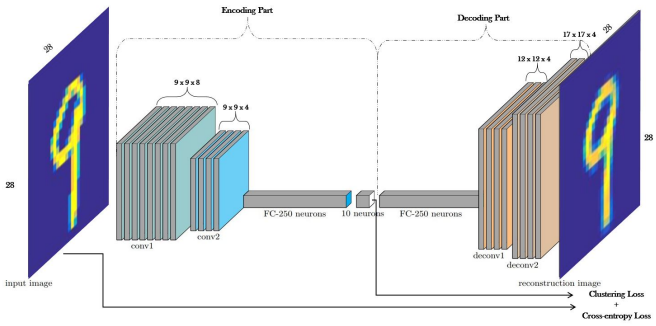

Fig. 1. The architecture of our proposed model.

3. EXPERIMENT AND DISCUSSION

The proposed method was implemented using MatConvNet [15] and evaluated on MNIST dataset. The model was trained end-to-end in an unsupervised manner. There is no pre-training and fine-tuning procedures involved. All weights were initialized using Xavier method [16] and biases were initialized to 0, and the cluster centers are initialized randomly. Stochastic gradient descent was used where each batch contains 100 random shuffled images. An initial learning rate of 0.006 with a momentum of 0.9 and weight decay of 0.0005 was used. We set λ, the clustering weight-parameter that controls the loss contribution percentage of clustering error, to 0.2, and the model converged after 500 epochs.

The CAE is trained to transform the data into latent representation and then reconstruct the original input or obtain an optimal approximation of the underlying data representation by minimizing the reconstruction error. Some examples of original inputs and reconstruction images obtained by our model are demonstrated in Fig. 3, allowing to visually differentiate and evaluate the reconstruction quality of the proposed model. In Fig. 3, the reconstructed images (bottom row) look qualitatively identical to original ones (top row) with certain levels of blurring, which helps to capture common patterns instead of subtle details at local regions for reconstruction. It is noteworthy that due to such smoothness the digit 5 has a similar structure to the digit 6. One reasonable explanation is that the proposed method is designed for unsupervised representation learning with a signal reconstruction objective, where such supervision information, *e.g.* differentiating 5 and 6, are not available to aid the learning of discriminative features.

To evaluate the cluster quality, two evaluation metrics, accuracy (ACC) and normalized mutual information (NMI) were computed. We compared our method with three baseline methods: DEC [4], AEC [3] and DCEC [6]. The results are summarized in Table 2. Our proposed method outperforms the baseline methods by a significant margin on both ACC and NMI metrics, where 84.97% and 92.14% were achieved respectively. The proposed method substantially outperforms second place by 6.85 percentage points which also uses CAE

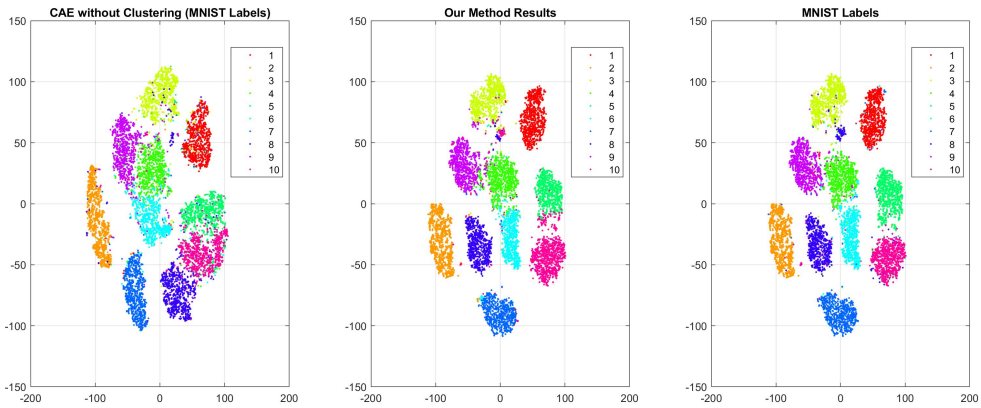

Fig. 2. Visualizations of latent representation on the MNIST testing set. Left: CAE without clustering loss; Middle: CAE with clustering; Right: Ground-Truth.

Fig. 3. Visualizations of input and reconstruction images with respect to digits 0, 3, 5 and 9

approach with jointed clustering loss. Fig. 4 shows both the changes of ACC and NMI with the number of training cycles, which clearly indicates that clustering stably converges using an iterative training scheme.

	NMI	***ACC***
Xie et. al [4], DEC	-	84.30%
Song et. al [3], AEC	66.90%	76.00%
Guo et. al [6], DCEC	-	85.29%
Proposed	**84.97%**	**92.14%**

Table 2. Comparison of clustering quality with baselines.

In addition, we carried out visual assessment where the t-SNE visualization method [17] was applied to evaluate clustering results of the proposed method. Fig. 2 shows a 2D projection of the latent representation of our proposed method, where the clustering results are visualized with color coding using ground truth label. It shows that with jointed clustering loss, the learned latent representation space has more compact structures forming significant clusters which have a better matching with true labels. With jointed clustering loss (Fig. 2, Right), the learned features have larger inter-cluster distances and tighter structures (see the clusters labelled with green, magenta, and dark-blue colors) compared to the method using no clustering constraint (Fig. 2, Left).

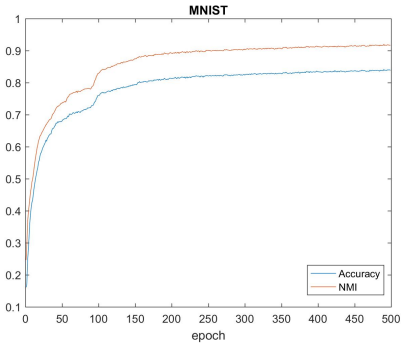

Fig. 4. Changing of accuracy and NMI during training on MNIST

4. CONCLUSION

In this paper, we introduce an unsupervised deep clustering method where a non-linear latent representation and compact clusters are learned jointly. The experimental results have demonstrated the effectiveness of our method to cluster data into appropriate groups. There is a potential for numerous image-processing applications such as representation learning for image classification. Our potential future work is to experiment with more difficult datasets and improve the accuracy of such deep clustering models.

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