FUB-Clustering: Fully Unsupervised Batch Clustering

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Abstract: Traditional methods for unsupervised image clustering such as K-means, Gaussian Mixture Models (GMM), and Spectral Clustering (SC) have been proposed. However, these strategies may be time-consuming and labor-intensive, particularly when dealing with a vast quantity of unlabeled images. Recent studies have proposed incorporating deep learning techniques to improve upon these classic models. In this paper, we propose an approach that addresses the limitations of these prior methods by allowing for the association of multiple images at a time to each group and by considering images that are extremely close to the images that are already associated to the correct cluster. Additionally, we propose a method for reducing and unifying clusters when the number of clusters is deemed too high by the user, utilizing four different heuristics while considering the clustering as a single element. Our proposed method is able to analyze and group images in real-time without any prior training. Experiments confirm the effectiveness of the proposed strategy in various setting and scenarios.

1 INTRODUCTION

Unsupervised image clustering is a task that aims to group unlabeled images based on their visual characteristics. As individuals are now exposed to a vast quantity of unlabeled images, the process of manually labeling this data can be time-consuming and, in some cases, incredibly labor-intensive. One of the earliest proposed clustering methods is the K-means algorithm (MacQueen, 1967), which utilizes the Euclidean distance between points in a given feature space. Variations of the K-means algorithm have been proposed, such as those in (De la Torre and Kanade, 2006) and (Ye et al., 2007) , which incorporate dimensionality reduction and clustering jointly. Other popular clustering methods include Gaussian Mixture Models (GMM) (Bishop and Nasrabadi, 2006) and Spectral Clustering (SC) (Ng et al., 2001). Spectral Clustering variants have gained popularity due to their ability to outperform K-means algorithms (Von Luxburg, 2007).

Recent studies have proposed incorporating deep learning techniques to improve upon classic models. These approaches often involve the combination of stacked autoencoders (Vincent et al., 2010) with classic methods such as K-means, GMM, and Spectral Clustering. The authors of (Xie et al., 2016) proposed a method that simultaneously learns features and performs clustering by combining stacked autoencoders with clustering algorithms. The paper in (Li et al., 2018) proposed a method based on autoencoder that works on two parts, one fully convolutional autoencoder that extract the features and the other part that is a fully convolutional encoder and a soft K-means to perform the clustering. The work described in (Jiang et al., 2016) proposed an unsupervised generative clustering framework that combines Variational Deep Embedding (VAE) with a Gaussian Mixture Model (GMM). Another approach was proposed by (Yang et al., 2016) in which they join the process of representation and image clustering during the training as one process.

The authors of (Van Gansbeke et al., 2020) proposed a two step methods that learn feature representation and find the meaningful nearest representation. In (Park et al., 2021) a method that assist other existing method to find a better clustering solution is proposed. The paper in (Niu et al., 2022) presents a three steps method that divide the clustering in feature model that measure the instance level of similarity, "clustering head" that measure the cluster level discrepancy and both previously step jointly

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Deep learning approaches have been shown to produce good results, but they require a time-consuming training process. Our goal is to develop an approach that can analyze and group images in real-time without any prior training, nor any prior knowledge on the number of elements, number of clusters, features or semantic categories of elements to be clustered. In particular, the authors of (Ortis et al., 2017) proposed a clustering method for clips of videos extracted from different sequences recorded at different times, that exploits a pre-trained CNN to extract features and determine similarity without any prior training. The main advantage of (Ortis et al., 2017) is its generalizability, and the fact that the algorithm is fully unsupervised, without any prior on the clustering problem setting. However, this method can only associate one image at a time to each group, which may lead to some samples being placed in different clusters when the dataset is rather large.

Our proposed approach build on (Ortis et al., 2017), but it extends this method by allowing for the association of multiple images at a time to each group (i.e., batch clustering). Additionally, our approach adds a clustering reduction step to the pipeline, when the number of clusters is deemed too high. In the experiments, we tested four different approaches for the clusters reduction.

In the following sections, we will present our proposed method, showcase the results we obtained, and compare them with state-of-the-art techniques.

2 PROPOSED METHOD

This Section presents the keystone of our approach. Firstly, the images are grouped in non meaningful clusters by means of a fast batch clustering approach, then some images are moved from one cluster to others depending on the mutual similarity between elements of same and other groups. This will produces an high number of cluster. Secondly, the number of clusters is reduced by a proper process detailed in Section 2.2. In particular, we defined four different strategies:

- outlier average;
- outlier maximum;
- maximum average;
- maximum maximum.

2.1 Stochastic Batch Clustering

The n input images are shuffled and then distributed among K non meaningful groups. In the meantime, we arbitrary extract some features from the images. In particular we employed the last Fully Connected layer extracted by the AlexNet CNN pre-trained on ImageNet (Krizhevsky et al., 2017). In general it is possible to extract features with other pre-trained networks or with a custom feature extraction process. Then, the clustering process is refined by moving some specific elements from the initial clusters to others.The specific elements to move will be chosen after the analysis of the similarity as detailed in the following. Given a representation (i.e., a feature) of the image I a cluster $I \in K_I$, we compute the cosine similarity between I and all the images belonging to $K_i, i = 1, ..., N$. This will produce a distribution of cos-similarities. If the involved images are similar one each others, the distribution will be similar to a random uniform like PDF. Otherwise, the presence of outliers will reveal that the group is not uniform. Once we have the group of similarities, we analyse these values and select the upper outliers (i.e., the ones that are out of the distribution due to their high similarity with I), if exist, and then associate them to the same cluster of I. This process is repeated for each image $I_1, ...I_h \in K_1, ..., K_N$ where N is the number of groups. The main advantage of such approach is that the elements move from one cluster to the others depending of mutual similarity with batched elements, rather than considering a trained threshold on the similarity range, which is usually crafted depending on the specific problem or the considered representation feature.

2.2 Clustering Reduction

In the previous section we described how images are initially clustered, however sometimes the granularity of clustering is too high (i.e., it produces too many groups). Then, some elements of the same category are placed in separated groups, often times singleton clusters. Therefore, here we present some strategies to reduce the number of clusters.

However if the initial clustering step is inaccurate, such errors will be propagated in the reduction process and, hence, the quality of the new clustering will be affected. Given a set of groups $C_1, ..., C_n$ where n is the number of groups, we reduce the number of clusters by applying a new fast clustering step, considering each cluster C_j as a single element of the process. Then, we divide the set of clusters in K non meaningful groups. The following paragraphs will describe four different methods for the clustering reduction step.

Given the cluster C_j and the cluster C_k with n and m images respectively, initially the cosine similarity between the images $i_1, ..., i_n \in C_j$ and the images

$i_1,...,i_m \in C_k$ is computed. The results of the computation is a list of similarity values $sim_1,...,sim_{n*m}$. At this point, we propose the following alternatives to calculate the distance between C_j and C_k:

- *Average*: between the similarities is computed the average value $\mu_{j,k}$.
- *Maximum*: between the similarities is searched the maximum value $max_{j,k}$.

Once the distance between the clusters of the K non meaningful group is computed, each cluster is considered as a single entity and needs to be associated to one or more clusters. Given the list of similarities between the cluster C_j considered as single entity in a group $C_j \in K_C$ and all the other clusters C_k considered as single entities that belong to K_i where $i = 1,...,N$, we propose two alternatives:

- *Outlier*: the list of similarities is analysed and the upper outlier is selected from the list. If the upper outliers exist they are associated to the same cluster as C.
- *Maximum*: the list of similarities is analysed and the maximum similarity value is selected. The element that has the maximum similarity value is associated with the cluster C.

So we obtain the four proposed method combining together the method of computation of distance and the association between cluster. Specifically:

- outlier average is the combination of the method "outlier" in the association of elements to a cluster, and the method "average" in the computation of the distance between clusters.
- outlier maximum is the combination of the method "outlier" in the association of elements to a cluster, and the method "maximum" in the computation of the distance between clusters.
- maximum average is the combination of the method "maximum" in the association of elements to a cluster, and the method "average" in the computation of the distance between clusters.
- maximum maximum is the combination of the method "maximum" in the association of elements to a cluster, and the method "maximum" in the computation of the distance between clusters.

3 EVALUATION

3.1 Benchmark Datasets and Evaluation Metrics

We evaluated the performance of our clustering method on four well-known public benchmark datasets: STL-10 (Coates et al., 2011), CIFAR-10 (Krizhevsky et al., 2010a), CIFAR-100/20 (Krizhevsky et al., 2010b) and CIFAR-100 (Krizhevsky et al., 2010b). In Table 1 details the benchmark datasets. In particular, the variability of the number of classes ranges from 10 to 100 categories. Note that the chosen extraction process forces the images to be resized in 224x224 format before the feature extraction. As in (Ortis et al., 2017), we built a confusion matrix from the clustering decisions to better evaluate its performances. In particular, the clustering task can be formalized as a pairing process between each pair of elements in the dataset. Therefore, given a pair of samples of the same category, if they are clustered in the same group we have a True Positive, whereas we count a True Negative decision (TN) if the process assigns two samples of different classes to different clusters. Similarly, a False Positive decision (FP) assigns two different samples to the same cluster and a False Negative decision (FN) assigns two similar images to different clusters. With the above formalization we can compute a confusion matrix related to the pairing task. The metrics we used to evaluate our clustering results are:

Table 1: Employed Benchmark Datasets.

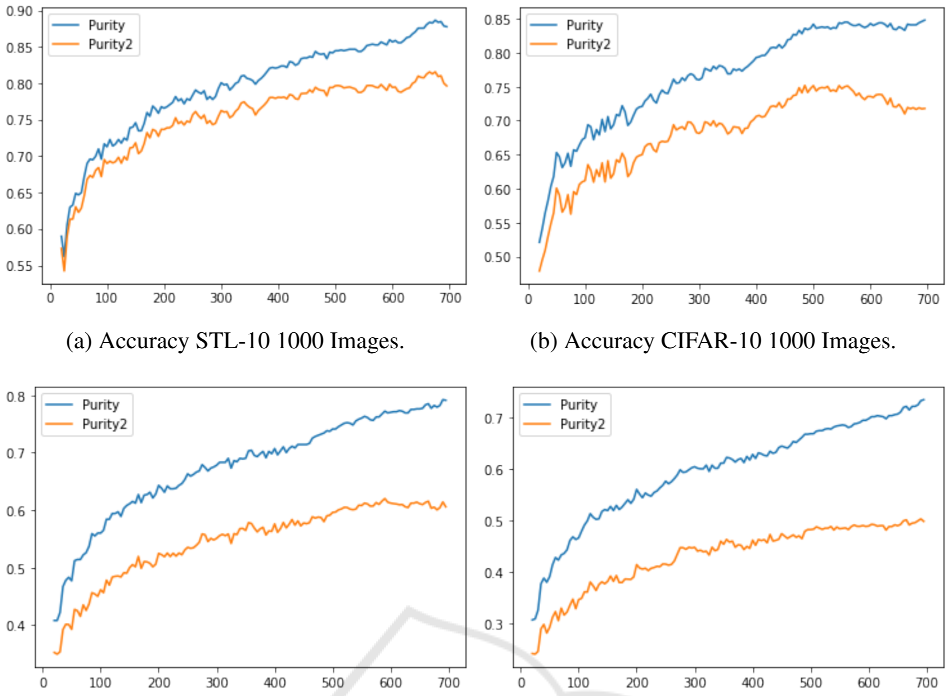
Dataset	Image Size	Images	Classes
STL-10	96x96	13000	10
CIFAR-10	32x32	60000	10
CIFAR-100/20	32x32	60000	20
CIFAR-100	32x32	60000	100

- Rand Index (*RI*) which is the measure of the percentage of correct decision:

$$RI = \frac{TP + TN}{TP + FP + FN + TN}. \quad (1)$$

  where
  - TP is True Positive where two images of the same class has been assigned to the same cluster,
  - TN is True Negative where two images of different class has been assigned to different cluster,
  - FP is False Positive where two images of different class has been assigned to the same cluster,
  - FN is False Negative where two images of the same class has been assigned to different cluster.
- Precision is the positive predictive value:

$$Precision = \frac{TP}{TP + FP}. \quad (2)$$



(a) Accuracy STL-10 1000 Images.

(b) Accuracy CIFAR-10 1000 Images.

(c) Accuracy CIFAR-100/20 1000 Images.

(d) Accuracy CIFAR-100 1000 Images.

Figure 1: Accuracy comparison in STL-10, Cifar-10, Cifar-100 and Cifar-100/20. We refer to Purity for the full dataset that contains 1000 images, and to Purity2 for the the dataset without the singleton clusters.

- Recall is the sensitivity:

$$Recall = \frac{TP}{TP+FN}. \quad (3)$$

- Purity Score which is the measure of purity considering each cluster with respect to the most frequent class in the cluster (Li and Ding, 2006) We will refer to this formula as Purity and Accuracy:

$$Accuracy = Purity = \frac{1}{N}\sum_{i=1}^{k} max_j|C_i \cap T_j|. \quad (4)$$

  where N is the number of images, k the number of Cluster, C_i the ith cluster, T_j is the set of element of the class j that are present in the cluster C_j.

- Adjusted Rand Index (ADJ) (Hubert and Arabie, 1985)
- Normalised mutual info (NMI) (Strehl and Ghosh, 2002)

3.2 Analysis of Number of Elements per Group

What this paragraph analyse is the difference between the number of element for each group. To have a significant group of images and at the same a rapid execution it has been choosen to randomly take 1000 images for each dataset and analyse their results considering a number of images for each group from 20 till 700. For the sake of comparison, results are presented also removing singleton cluster. The aim is to see in which case are obtained the optimal results for each dataset. Then next sections present the result reported in Table 2. In the results, we refer to Name_Dataset$_{drop}$ when the dataset has not singleton clusters because they have been removed by the proposed pipeline.

Table 2: Best Accuracy Results.

Dataset	Images per Group	Accuracy
STL-10	675	0.887
STL-10$_{drop}$	675	0.815
CIFAR-10	695	0.848
CIFAR-10$_{drop}$	485	0.751
CIFAR-100/20	690	0.792
CIFAR-100/20$_{drop}$	590	0.620
CIFAR-100	695	0.734
CIFAR-100$_{drop}$	690	0.502

3.2.1 STL-10

As shown in Figure 1a, the accuracy values obtained on STL-10 have a growth almost till the end, when the value starts to slow down again, analysing the number we see that the maximum value of accuracy consider-

Table 3: Results of Clustering with dataset containing all the images and dataset containing only the cluster with at least 2 elements.

Dataset	Max Accuracy	Min Accuracy	Mean Accuracy	Dev Std Accuracy
STL-10	0.890	0.858	0.874	0.008
STL-10$_{drop}$	0.816	0.774	0.795	0.013
CIFAR-10	0.836	0.785	0.813	0.011
CIFAR-10$_{drop}$	0.752	0.680	0.720	0.014
CIFAR-100/20	0.786	0.731	0.759	0.012
CIFAR-100/20$_{drop}$	0.642	0.567	0.605	0.016
CIFAR-100	0.758	0.692	0.730	0.012
CIFAR-100$_{drop}$	0.540	0.471	0.500	0.014

ing all cluster and only the cluster that have at least 2 images is when we have 675 elements per group.

3.2.2 Cifar-10

The results in Figure 1b show that the accuracy values have a growth till the end when we consider every cluster; when we remove the cluster that have only one element the growth is approximately till 550 element per group and the the value starts to go down. Analysing the number we see that the maximum value of accuracy considering all cluster is obtained when there are 695 element per group, and the maximum value of accuracy considering the cluster that have at least more than 2 images is 485.

3.2.3 Cifar-100/20

In this Section we will talk about the results on the dataset CIFAR-100/20. As we can see in Figure 1c the accuracy values has a growth till the end when we consider every cluster like it happened in Cifar-10; when we remove the cluster that have only one element the growth is approximately till 600 element per group then the values seems to be stable but lower than the maximum value. Analysing the number we see that the maximum value of accuracy considering all cluster is obtained when there are 690 element per group, and the maximum value of accuracy considering the cluster that have at least more than 2 images is 590.

3.2.4 Cifar-100

In this Section we will talk about the results on the dataset CIFAR-100. As we can see in Figure 1d the accuracy values has a growth till the end when we consider every cluster like it happened in Cifar-10 and Cifar-100/20; but unlike Cifar-10 and Cifar-100/20 the growth is till the end even when we remove the cluster that have only one element. Analysing the number we see that the maximum value of accuracy considering all cluster is obtained when there are 695 element per group, and the maximum value of accuracy considering the cluster that have at least more than 2 images is 690.

Table 4: Results of Clustering reduction with the 4 methods: out_max, out_avg, max_max, max_avg iterated 5 times.

Method	STL-10	Cifar-10	Cifar-100/20
FUB	0.874±0.008	0.813±0.011	0.759±0.012
FUB$_{out_max_1}$	0.800±0.035	0.709±0.020	0.667±0.054
FUB$_{out_avg_1}$	0.803±0.039	0.703±0.018	0.663±0.059
FUB$_{max_max_1}$	0.846±0.021	0.741±0.019	0.710±0.036
FUB$_{max_avg_1}$	0.848±0.020	0.743±0.019	0.709±0.038
FUB$_{out_max_2}$	0.735±0.031	0.639±0.024	0.575±0.039
FUB$_{out_avg_2}$	0.752±0.038	0.641±0.021	0.565±0.041
FUB$_{max_max_2}$	0.808±0.019	0.695±0.020	0.636±0.029
FUB$_{max_avg_2}$	0.808±0.018	0.697±0.018	0.630±0.030
FUB$_{out_max_3}$	0.691±0.029	0.588±0.022	0.516±0.039
FUB$_{out_avg_3}$	0.719±0.025	0.597±0.023	0.510±0.035
FUB$_{max_max_3}$	0.778±0.018	0.659±0.024	0.584±0.026
FUB$_{max_avg_3}$	0.779±0.019	0.659±0.018	0.572±0.024
FUB$_{out_max_4}$	0.653±0.030	0.551±0.022	0.478±0.033
FUB$_{out_avg_4}$	0.701±0.023	0.567±0.025	0.478±0.029
FUB$_{max_max_4}$	0.757±0.016	0.629±0.024	0.541±0.025
FUB$_{max_avg_4}$	0.753±0.014	0.624±0.019	0.525±0.020
FUB$_{out_max_5}$	0.626±0.032	0.521±0.025	0.446±0.030
FUB$_{out_avg_5}$	0.678±0.026	0.543±0.025	0.458±0.026
FUB$_{max_max_5}$	0.735±0.020	0.602±0.023	0.507±0.023
FUB$_{max_avg_5}$	0.734±0.011	0.602±0.021	0.489±0.019

3.3 Stochastic Batch Clustering and Clustering Reduction

Each dataset has been divided in random groups of 1000 images; in each group the clustering algorithm is been executed using as number of images per group the optimal value that came out from the analysis of the previous section. In Table 3 is reported a summary of the results.

As observed earlier, the results may contain singleton clusters. So to the results it has been applied the clustering reduction in order to achieve the merging between singleton clusters and other clusters. After the reduction of number of cluster it is expected to

Table 5: Comparations of the results of state of art algorithm and our algorithm.

Method	STL-10	Cifar-10	Cifar-100/20
K-Means (MacQueen, 1967)	0.192	0.229	0.130
SC (Ng et al., 2001)	0.159	0.247	0.136
AC (Franti et al., 2006)	0.332	0.228	0.138
NMF (Cai et al., 2009)	0.180	0.190	0.118
AE (Bengio et al., 2006)	0.303	0.314	0.165
SDAE (Vincent et al., 2010)	0.302	0.297	0.151
DCGAN (Radford et al., 2015)	0.298	0.315	0.151
DeCNN (Zeiler et al., 2010)	0.299	0.282	0.133
VAE (Kingma and Welling, 2013)	0.282	0.291	0.152
JULE (Yang et al., 2016)	0.277	0.272	0.137
DEC (Xie et al., 2016)	0.359	0.301	0.185
DAC (Chang et al., 2017)	0.470	0.522	0.238
DeepCluster (Caron et al., 2018)	0.334	0.374	0.189
DDC (Chang et al., 2019)	0.489	0.524	N/A
IIC (Ji et al., 2019)	0.610	0.617	0.257
DCCM (Wu et al., 2019)	0.482	0.623	0.327
DSEC (Chang et al., 2018)	0.482	0.478	0.255
GATCluster (Niu et al., 2020)	0.583	0.610	0.281
PICA (Huang et al., 2020)	0.713	0.696	0.337
CC (Li et al., 2021)	0.850	0.790	0.429
IDFD (Tao et al., 2021)	0.756	0.815	0.425
SCAN (Van Gansbeke et al., 2020)	0.809	0.883	0.507
SCAN + RUC (Park et al., 2021)	0.867	0.903	0.533
SPICE (Niu et al., 2022)	0.938	0.926	0.538
FUB-Clustering	0.874±0.008	0.81±0.011	0.759±0.012
FUB-Clustering$_{drop}$	0.795±0.013	0.72±0.140	0.605±0.016
FUB-Clustering$_{out_max_1}$	0.800±0.035	0.709±0.020	0.667±0.054
FUB-Clustering$_{out_avg_1}$	0.803±0.039	0.703±0.018	0.663±0.059
FUB-Clustering$_{max_max_1}$	0.846±0.021	0.741±0.019	0.710±0.036
FUB-Clustering$_{max_avg_1}$	0.848±0.020	0.743±0.019	0.709±0.038

observe a lower accuracy because of the merging of different cluster that not always are 100% accurate so the errors are also merged; another reason why it is expected a lower accuracy is that the singleton cluster have accuracy 100% that will not be considered anymore unless it joins a cluster that is already 100% accurate. In Table 4 there is a summary of the results of the clustering reduction. As expected the results observed have lower accuracy. It is possible to notice also that the methods "out_max" and "out_avg" have lower accuracy than "max_max" and "max_avg", however the reason is related to the number of cluster left, "out_max" and "out_avg" reduce the number of cluster so much more than the other two methods.

3.4 Comparison with the State of the Art

The performance of the FUB-Clustering has been evaluated on three commonly used dataset: STL-10, CIFAR-10, CIFAR-100/20. In Table 5 we compare the results of the different version of FUB and the result of other state-of-art algorithms. From the results we can observe that SPICE(Niu et al., 2022) outperform FUB in the clustering of the Datasets STL-10 and Cifar-10. However SPICE require a training and during the train is known the number of cluster, instead in FUB the number of cluster is not known. Our results are still competitive and outperform other state-of-art methods. Regarding the Cifar 100/20 Datasets FUB outperforms all the other state-of-art methods with all the FUB methods, even the method that drop the singleton clusters.

4 CONCLUSIONS

In this study, we proposed different ways on how to do clustering using features without prior knowledge of the number of cluster, K. Our studies have been performed on images, however this algorithm can be used with other kinds of data as well. The experimental results show that FUB-Clustering is competitive as it outperforms most of the existent state of the art algorithms on two well known dataset (STL-10 and Cifar-10) and outperform all the existent state of art algorithm in the well known dataset Cifar-100/20. It is worth to highlight that FUB is fully unsupervised, so it does not have any prior knowledge on the clustering problem it is applied to (e.g., number of clusters, kind of input data, dimensionality of the space, etc.). Other than clustering single images we are also able to cluster group of images, however if the group of images is not accurate 100% accurate, we might obtain a some errors in our clustering. Despite FUB-Clustering is already able to obtain competitive results, we aim to improve the computational complexity in pursuance of a faster computation.

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