Unsupervised Classification into Unknown k classes

Abstract

We propose a novel spectral decomposition framework for the unsupervised classification task. Unlike the widely used classification method, this architecture does not require the labels of data and the number of classes. Our key idea is to introduce a piecewise linear map and a spectral decomposition method on the dimension reduced space into generative adversarial networks. Inspired by the human visual recognition system, the proposed framework can classify and also generate images as the human brains do. We build a piecewise linear connection analogous to the cerebral cortex, between the discriminator D and the generator G. This connection allows us to estimate the number of classes k and extract the vectors that represent each class. We show that our framework has the reasonable performance in the experiment.

1 Introduction

Image classification has been one of the most important research in machine learning and artificial intelligence. For the predefined k classes, the classification models based on deep learning have shown the performance that the test accuracy is better than humans (Geirhos et al., 2017; He et al., 2016; Russakovsky et al., 2015; Szegedy et al., 2015). This result is, however, limited to the specific case that the number of classes, k is predefined and we use the supervised learning with entire ground truth labels. The goal of artificial intelligence is that AI systems do real-world tasks as much as humans do. Humans can learn visual information, memorize the compressed information (features) in the brain, imagine the learned objectreconstruct the data in the brain and recognize the difference between objects. This capability allows humans to classify the data of which the number of classes is unknown into the reasonable numbers of classes. How can we enable AI systems to have such capability?

The main contribution of the proposed framework is the following two results. We first showed that there exists a piecewise linear map between two separated neural networks of the Generative Adversarial Networks (GANs). Secondly, we proved the result of the spectral clustering algorithm on a large N data points has the same multiplicity k of the eigenvalue 0 of the graph Laplacian matrix as the problem in the dimension-reduced space. By combining the results, We derive a novel unsupervised classification framework, which estimates the number of classes k and then extract k vectors representing each class. Using our framework, the approximate map of the above piecewise linear map between two networks can induce the information of the spectral decomposed components in the given data graph.

The latent variable model is commonly used in the generative models. Variational Auto-Encoders (VAEs) (Kingma & Welling, 2013) and GANs (Goodfellow et al., 2014) are one of the most famous cases that learn the data distribution successfully. GANs randomly samples the latent variables that are used to train the data distribution so we cannot figure out which latent variable generates a result that we are insterested in. This drawback by random sampling leads to introduce auxiliary conditions into the latent variables (Chen et al., 2016; Mirza & Osindero, 2014). Introducing a label information into the condition of the estimated data probability is powerful to classify where a data point x came from, however this method is not a unsupervised learning. In addition, there are some GANs frameworks that analyze the property of latent spaces (Kumar et al., 2017; Radford et al., 2015).

Spectral clustering is one of the most popular clustering algorithm that outperforms the other well-known clustering algorithms (Ng et al., 2002; Shi & Malik, 2000). Despite the high performance, spectral clustering is hard to apply to cluster the-state-of-the-art dataset because it requires the full dataset that have very large N data points. In this situation, the dimension of the Laplacian matrix is $N \times N$ and it takes at least $O(N^3)$. Therefore, we need a novel dimension reduction technique to widely use the applications of spectral clustering methods (Elhamifar & Vidal, 2009; Ji et al., 2017; Law et al., 2017; Shaham et al., 2018). Especially, we apply the self-expressiveness property (Elhamifar & Vidal, 2009) to the proposed method.

We shortly introduce the main concepts of spectral clustering, GANs and the self-expressiveness property in Section 2. We prove the background propositions that allow us to classify data with the unsupervised learning method in Section 3. Finally, we propose a unsupervised classification algorithm and test our algorithm in Section 4.

Recent image classification methods are based on the supervised learning, in which the learning model takes the whole pairs of an image and an ground-truth label of the given dataset. This training dataset usually consists of more than 10 K data points and lots of participants cross-validate the ground-truth label of each image. Therefore, it takes a lot of costs to produce a reliable training dataset.

2 PRELIMINARIES

In this section, we review cycle-consistent adversarial networks and sparse subspace clustering that we will use when extracting the indicator vectors. We also overview the basic probabilistic property between the classification model and the generative model, which gives us the background to generate indicator vectors.

2.1 CYCLE-CONSISTENT ADVERSARIAL NETWORKS

Generative Adversarial Networks (GANs) is a generative model that a generator network learns a data distribution implicitly (Goodfellow et al., 2014). GANs is a two player minimax game with two neural networks, a discriminator D and a generator G. The discriminator $D(\mathbf{x})$ is a probability measure that an input x is in the data distribution $p_{data}(\mathbf{x})$ rather than the generator's distribution p_g. The generator G is a mapping from the latent space $\mathbf{z} \sim p_{\mathbf{z}}$ to the data space. This minimax game can be represented as a stochastic optimization problem with value function,

$$\min_G \max_D V(D,G) = \mathbb{E}_{x \sim p_{data}(\mathbf{x})} \left[\log D(\mathbf{x}) \right] + \mathbb{E}_{z \sim p_z(z)} \left[\log \left(1 - D \left(G \left(\mathbf{z} \right) \right) \right) \right]. \quad (1)$$

The cycle-consistent adversarial networks (cycleGANs) is a variant of GANs, which learns how to translate an representation from a source domain S to a target domain T without the paired dataset (Zhu et al., 2017). The cycle-consistency states that two mappings $G : S \to T$ and $F : T \to S$ encode the right permutation of images in S and T, so that, for an arbitrary data point $s \in S$, the mapping from S to T and back again, $F(G(s))$, should be the same as s. This property encourages adversarial networks G and D to have a connection between generated images and input data. We adopt two cycle consistency loss for the forward map and the backward map to learn a connection between two high-level representation domain in G and D.

2.2 SPARSE SUBSPACE CLUSTERING

Sparse subspace clustering is one of the clustering algorithm that is based on spectral clustering. Spectral clustering has many variants of which similarity measures are, for example, Gaussian kernel similarity function (Ng et al., 2002), k-nearest neighbor graphs, ϵ-neighborhood graph. Similarity measure defined on the similarity graph $G = (V, E)$ is a pairwise metric between two data points (nodes) for all possible pair in the dataset and the similarity w_{ij} of two data points x_i, x_j is equal to or greater than 0. The similarity w_{ij} is also same as w_{ji} because the above similarity graph is defined as an undirected graph. The similarity matrix W is composed of the elements which correspond to the similarity measure w_{ij} respectively and then W is symmetric. We can define the graph Laplacian matrix of the similarity graph G as $L = D - W$, where D is the degree matrix and defined as a diagonal matrix that the diagonal elements is given by $d_i = \sum_j w_{ij}$. The multiplicity k

Figure 1: (a) shows the mappings relation in our proposed method. (b) shows the architecutre of the our networks.

of the eigenvalue 0 of L is the number of connected components $A_1, \cdots, A_k$ in the similarity graph. Each connected component is a partition of the similarity graph G and considered as a subgraph, i.e., a cluster. See more details in (Von Luxburg, 2007).

The proper design of weight measure $w : X \times X \to \mathbb{R}^+$ is a key to clustering data very well because the graph Laplacian matrix L is based on a similarity matrix W. Sparse subspace clustering (Elhamifar & Vidal, 2009) uses a novel similarity matrix that is based on the self-expressiveness property. When we assume that the data space is a union of linear subspaces $S = \cup_{l=1}^k S_l$, we can express an arbitrary data point in the dataset as a linear combination of other data points in the dataset, where the coefficients of the data points in the same subspace are non-zero and others should be 0 (Elhamifar & Vidal, 2009; Ji et al., 2017). This property is called self-expressiveness property. Formally, each data point $\mathbf{y}_i \in S$ can be reconstructed as $\mathbf{y}_i = \sum_{j=1}^N c_{ij}\mathbf{y}_j = \mathbf{Y}\mathbf{c}_i$, where $c_{ii} = 0$, N is the size of the dataset, $\mathbf{c}_i := [c_{i1}\ c_{i2}\ \cdots\ c_{iN}]^T$ is the coefficient vector of $\mathbf{y}_i$ and $\mathbf{Y} = [\mathbf{y}_1\ \mathbf{y}_2\ \cdots\ \mathbf{y}_N]$ is the dictionary matrix. The sparse solution of $\mathbf{c}_i$ indicates that the node i is in the same subspace as the node j if the element c_{ij} is non-zero. In this paper, we expand the notion of the self-expressiveness property to reduce the dimensionality of L in Section 3.3.

3 GRAPH LAPLACIAN OF THE CONNECTOR NETWORK

We first introduce our proposed architecture of adversarial networks. As point of view as autoencoder, we can consider two adversarial networks as autoencoder. We build a connector network between two networks to improve the cycle consistency and extract the information of connected components. (As shown in Figure 1-b). By training with the cycle-consistency loss, we can make the tuples (Z,X,H) for the whole dataset. Then, we show the relation between the spectral clustering and unsupervised classification. In order to show the relation, we prove the dimension reduction of the mutual expressiveness property in section, and the spectral decomposition of the connector network in section()

3.1 DISENTANGLING UNFOLDS AND EXPANDING THE VOLUME OF MANIFOLD

Deep neural networks learn the high-level abstract representation of the data manifold and the well trained abstraction can disentangle the underlying factors of variation (Bengio et al., 2007). These properties allow interpolating between the data samples more naturally and smoothly. (Bengio et al.,

(a)   (b)

Figure 2: (a) shows the density of h for 1 and 2 MNIST, (b) shows the mean footprint of entire MNIST classes

2013) studied the disentangling effect and proposed three hypotheses about the shape of manifolds in the different representation domains. These hypotheses are verified by several empirical implementations (Goodfellow et al., 2009; Glorot et al., 2011). We can summarize three hypotheses as follows.

- The deeper representations can better disentangle the underlying factors of variation.
- Disentangled representations unfold the manifolds near which raw data concentrates irregularly and expand the relative volume occupied by high-probability points near these manifolds. Then these representations are with greater convexity.
- The underlying class factors of variations will be better disentangled than other factors, so the deeper layer has the better discriminant ability of classes.

In our proposed architecture, there are two high-level (deeper) representation spaces $H and Z$ which is called as feature spaces. These feature spaces fill more uniformly the space than the pixel space X. H and Z also have the smoother density. Therefore, H and Z have greater than convexity than X and it allows the linear combination on these two manifolds in the feature spaces H and Z are and be more convex than the manifold in the pixel space X. By manifold hypothesis, the different class manifolds are well-separated by regions of very low density (Cayton, 2005). The feature spaces are the high-level representation spaces so that the density are unfolded and the linear combinations of features generates more natural results in the pixel space Bengio (2014).

Now, we can define the effective basis of the subspace for each class. In the feature spaces, each class manifold has the enough convexity. The class manifolds are well-separated and show good discriminant ability. Using both properties, we can build the effective basis for each class subspaces and generate the original space by the direct sum of these subspaces, where the subspaces are orthogonal. We empirically tested the effective basis as shown in Figure 3. Randomly sampled features in a subspace of the data space can be an effective basis and be possible to generate all data point in the same subspace. The features in the different subspaces cannot generate the given data samples. We can estimate the effective dimension using the number of the effective basis. Then, we can generate orthogonal subspaces of the entire classes if the effective dimension is small enough than the dimension of feature spaces.

3.2 CONNECTOR NETWORK AND CYCLE CONSISTENCY

We will study the relation between 3 different spaces, Z, X and H in the proposed architecture. As shown in the figure 1-(b), we can consider two adversarial networks as a decoder and an encoder of an auto-encoder respectively (Berthelot et al., 2017; Zhao et al., 2016). The discriminator network D encodes the pixel space X to the feature space H and generator network G decodes the feature space Z to X. We define the connector network C which maps from H to X. The map C between two feature spaces will be trained by the cycle consistency loss to obtain the tuples (Z,X,H) with the correct permutation, where all of elements is in the same-class manifold and shares same learned features.

Figure 3: (a), (b) the generate images using the footprint mask for MNIST and CIFAR10, (c) describes the linear combination using class 2 to generate 1 but failed. (d) is the generated image by the linear combination of the right features h for 1

Cycle consistency loss tends to minimize the difference between an arbitrary point and the returned point after traveling other representation domains. This cycle-consistency objective can allow the inverse maps between all representation spaces. When we apply the forward cycle-consistency loss z C(D(G(z))) and backward cycle consistency loss x G(C(D(x))), the maps between all two spaces become unique. Therefore, we will induce the feature-invariant one-to-one maps G, C, D. We now naturally conjecture an hypothesis.

Hypothesis. All elements of the cycle consistent tuple (Z, X, H) shares the same class factor and other important factors, such as rotation and brightness.

As shown in fig 1-(a), the linear combinations in the certain class subspace are closed because each class manifold is unfolded and expanded in Z and H. All elements of an arbitrary tuple (Z,X,H) share same class features as shown In figure 2-(b). We can assume that the following proposition

Proposition 3.1. *There exists a linear map C_i from H_i to Z_i, where H_i, Z_i for the manifold of the class i.*

Proposition 3.2. *In addition, the class subspaces can be approximated as orthogonal subspaces as shown in Section 3.1. Then, the map from H to Z can be written as*

$$C = C_1 + \cdots + C_k \tag{2}$$

3.3 MUTUAL EXPRESSIVENESS PROPERTY AND DIMENSION REDUCTION

As we discussed in Section 2, the self-expressiveness property shows that we can express an arbitrary data point as a linear combination of other N data points. Modifying this property slightly, we can write each data point x as a linear combination of N sampled data points $\alpha = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\}$ from the data space X. This fact allows us to generate a set of latent variables, which satisfies the self-expressiveness property. The self-expressiveness property implies that the generated data points are in the global vector space. In the generative model, the latent space is not a global vector space so we need an enormous number of samples to fully cover the latent space. Now, we weaken the self-expressiveness property to generalize the situation of the problem. We divide the latent space H into $H_1, \cdots, H_l$ where the self-expressiveness only satisfies in each H_i not in $H - H_i$.

We also know that it is possible to discard redundant coefficients in the self-expressiveness expression by optimizing the matrix of coefficients (Elhamifar & Vidal, 2009), so there exists at least one sparse solution of x where most coefficients are zero. By observing this property, we can expect that the number of non zero coefficients goes to the dimension of latent space, m. That is because N is much higher than $\dim X$ and X is a m-dimensional manifold. Image clustering methods, for instance, treat the dataset in which the number of data points is much larger than the dimension of data points so we can optimize a solution to have sufficiently enough zero coefficients in the self-expressive linear combination.

Proposition 3.3. *From now on, $Z_i' = C_i' H_i'$ where $Z_i' = (z_1, \cdots, z_{m_i})^T$ and $H_i' = (h_1, \cdots, h_{m_i})^T$.*

Proof. By the observation on GANs, we have N_i latent variables $\beta_i = \{h_{ij}\}_{1 \leq j \leq N_i}$ for each $1 \leq i \leq l$ where $D(x_i) = h_i$ and $N = N_1 + \cdots + N_l$. By the self-expressiveness property in H_i, we can express each $h_i \in H_i$ by the linear combination of $\beta_i' = \{h_1, h_2 \cdots, h_{m_i}, h_{m_i+1}, \cdots h_{N_i}\}$ where β_i' is a reordered set of β_i and the coefficents of the linear combination $\{c_{m_i+1}, c_{m_i+2}, \cdots, c_{Ni}\}$ are zero. In other words, the ordered set $\gamma_i = \{h_1, \cdots, h_{m_i}\}$ is enough to represent all points in the latent space X_i, i.e. $span(\gamma_i) = H_i$. Hence, we can choose C_i' by an $m_i \times m_i$ real matrix. $\square$

This dimension reduction has a crucial role in reducing the dimension of Lapalacian matrix of which similarity matrix is $|C| + |C^T|$

Proposition 3.4. *Suppose that G is an undirected graph with non-negative weights. Then, the number of connected components $A_1, \cdots, A_k$ in G is same as the multiplicity k of the eigenvalue 0 of L. The eigenspace corresponding to the eigenvalue 0 is spanned by the indicator vectors $1_{A_1}, \cdots, 1_{A_k}$ of those components.*

Proof. the proof in (Von Luxburg, 2007). $\square$

3.4 Unsupervised classification and footprint mask

Now, we consider the unsupervised classification problem that is not given even a single ground-truth label for the given dataset. For example, when the cross-entropy loss is applied in the supervised classification, we need pairs of input data and ground-truth probability mass $p = [0, , 1, \cdots, 0]$, which contains single 1 at the i-th element, i.e. the class index $c = i$, to estimate the difference between the prediction and the ground-truth. We can formally write the probabilistic interpretation as

$$P(c = i|\mathbf{x}) = \frac{P(c = i)P(\mathbf{x}|c = i)}{P(\mathbf{x})} \tag{3}$$

, where $\mathbf{x}$ is a data point. If we assume that the numbers of data points in the whole classes are same, then $P(c)$ is uniform. Then, for the given point $\mathbf{x}$, $P(\mathbf{x})$ is fixed so the we can measure $P(c|\mathbf{x})$ by the estimating the likelihood $P(\mathbf{x}|c)$. In Section 3.3, we showed that the indicator vectors of the connected components are the eigenvectors of the Laplacian matrix L, which are corresponding to the eigenvalue 0. The components of the indicator vectors span the eigenspaces of the matched connected components respectively. The orders of components for the Laplacian matrix L_C and the connector network C are identical by the definition in Section 3.3. Therefore, for all connected component A_i, the indicator vectors $\mathbf{1}_{A_i} = h \in H_i$ spans the class subspace H_i. The indicator vector itself, however, might not be in the class manifold because it can exist outside the boundary of the manifold. Now we call these identical vectors as the footprint masks. The feature vectors in H have the high density and value at some elements as shown in fig 2. This fact implies that those feature vectors lie in the eigenspace which is spanned by the above indicator vectors. Therefore, the inner-product between indicator vectors and features vectors could be the parameter that estimates the probability of the likelihood $P(x|c \in A_i)$. We now define the probability $P(h \in A_i)$ as

$$P(h \in A_i) = \frac{h \cdot \mathbf{1}_{A_i}}{h \cdot \mathbf{1}_A}, \tag{4}$$

where A denotes $A_1 \cup \cdots \cup A_k$. This definition allows us to classify the give data to the correct label i where $P(h \in A_i)$ is maximized. As we can see the patterns of the feature vectors, we call these feature vectors as the footprints of the input images and the indicator vectors as the the footprint mask.

4 Unsupervised classification into unknown k classes

In this section, we describe the loss function and the training algorithm of unsupervised classification into unknown k classes. Is is known that estimating the number of classes k is hard and heuristic (Von Luxburg, 2007). We find the empirical observation on the hint of k. Using the observation, we suggest a conjecture that helps to estimate the number of classes k in the certain case.

4.1 Training and loss functions

The training procedure of our method is similar with the GANs. We introduce the cycle consistency loss for the discriminator D and the generator G. The connector network $C : H \rightarrow Z$ can be

written as a matrix. The loss function of the connector network is defined as the sum of the forward cycle-consistency loss and the backward loss to encode the right permutation better. We update the connector network last for each iteration because we should apply the change of the permutations (Z, X) and (X, H). After the enough training steps, the feature spaces are trained and the class manifolds in the feature spaces unfolds and expands gradually. Then, the Laplacian matrix become practical so we can extract each eigen-images for the underlying classes. As shown in fig(3), each eigen-image represents each class.

Algorithm 1 Unsupervised Classification into Unknown k Classes (UCUC)

1: **for** the number of iterations **do**
2:    Sample minibatch of m latent vectors $\mathbf{z}^{(0)}, \cdots, \mathbf{z}^{(m)}$ from prior $p_g(z)$
3:    Sample minibatch of m data points $\mathbf{x}^{(0)}, \cdots, \mathbf{x}^{(m)}$ from dataset
4:    Update the discriminator by ascending :

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\mathbf{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\mathbf{z}^{(i)}\right)\right)\right) \right] + \lambda_D \left\| \mathbf{x}^{(i)} - G\left(C\left(D\left(\mathbf{x}^{(i)}\right)\right)\right) \right\|_1 \tag{5}$$

5:    Update the generator and connect by descending their stochastic gradients:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \left[\log\left(1 - D\left(G\left(\mathbf{z}^{(i)}\right)\right)\right) \right] + \lambda_G \left\| \mathbf{z}^{(i)} - C\left(D\left(G\left(\mathbf{z}^{(i)}\right)\right)\right) \right\|_1 \tag{6}$$

6:    Update the connector network C with two cycle-consistency loss

$$\nabla_C \left[\left\| \mathbf{z}^{(i)} - C\left(D\left(G\left(\mathbf{z}^{(i)}\right)\right)\right) \right\|_1 + \left\| \mathbf{x}^{(i)} - G\left(C\left(D\left(\mathbf{x}^{(i)}\right)\right)\right) \right\|_1 \right] \tag{7}$$

7:    Compute the moving average of each i-th eigenvalue of random-walk Laplacian matrix L_{sym} and find the estimated number $\hat{k}$
8: **end for**
9: Compute the footprint masks $\mathbf{1}_{A_i}$ using the spectral clustering algorithm (Ng et al., 2002)
10: Classify the given dataset using the footprint mask.

4.2 ESTIMATING THE NUMBER OF CLASSES k

We found an interesting observation about the number of classes k. The eigenvalue λ of the graph Laplacian matrix equals to Ncut of the given graph (Shi & Malik, 2000). In the ideal cases, we can assume that L is a block-diagonal matrix and each of blocks L_i is a proper sub-graph Laplacian. If there is no connection between subgraphs, then L is a perfect block-digonal matrix and the multiplicity of the eigenvalue 0 is same as the number of blocks. In the real world dataset, there exists quite large off-diagonal noise in the similarity matrix, as shown in the previous result. These non-zero off-diagonal elements make the eigenvalue zero only at the first eigenvalue and increase the Ncut of the graph gradually. We can consider the $i - th$ eigenvalue as the Ncut by the block diagonal matrix with i blocks, which is applied on the perturbed block diagonal matrix of which the underlying connected component is k. Now, we conjecture the pattern of the eigenvalue. We assume that the off-diagonal elements have the same value and the dimension of the all eigenspaces are same. Now, we estimate the number of classes k by starting from $m \ll k$. We can consider the difference of Ncut between k-block diagnoal matrix and m-block diagnoal matrix as the the area of $S_m - S_m \cap S_k$, where $S_m = \frac{n^2}{m}$ and $S_k = \frac{n^2}{k}$ when the matrix size is n. As m increases, the difference of Ncut increases, but at $k = m$ the value have the very small local minimum becuase two matrices are perfectly overlapped. Using this property we can derive the function of the difference of the Ncut over m, as follows.

$$S_m \cap S_k = n^2 \left(\frac{1}{k^2}(k - m + 1) + \sum_{i=1}^{m-1} \left[\left(\frac{i}{m} - \left\lfloor \frac{ik}{m} \right\rfloor \frac{1}{k} \right)^2 + \left(\left(1 + \left\lfloor \frac{ik}{m} \right\rfloor \right) \frac{1}{k} - \frac{i}{m} \right)^2 \right] \right) \tag{8}$$

where $m \leq k$. if $m > k$, swith m and k vice versa. This overlapped area is $\frac{n^2}{k}$ at $m = k$ trivially. The figure of the theoretical conjecture is in 4a. This result can predict the emprical result of the pattern of the eigenvalue. Therefore, we can conjecture that the underlying number of classes is at the second deep local minima.

5 EVALUATION

In this section, we introduce the setting of experiments and the architecture of our adversarial networks. Adversarial networks are based on (Radford et al., 2015). For the smaller size of dataset, such as MNIST and CIFAR10 we reduce the size of kernels properly. We have the result the expectation of the estimated number of k for MNIST is 10.2 and for CIFAR10 10.1. The prediction accuracy for MNIST is 0.874.

| (a) | (b) | (c) |

Figure 4: a shows theoretical result of the estimated eigengap using the overlapped area of block-diagonal matrices and Figure (b) and (c) shows the eigengap $|\lambda_k - \lambda_{k-1}|$ of the MNIST and CIFAR10.

6 CONCLUSION

We have proposed an unsupervised classification method that can estimates the unknown number of classes k and generate the footprint masks representing each class to classify the test data points using those vectors. We expand the self-expressiveness property to the mutual expressiveness property that shows the connection between two different latent spaces. Our method provides the learned class-feature and this implies that the label of the given data point is automatically generated. This fact reduce the tremendous cost of producing the ground-truth label in the very large dataset. Future works of unsupervised classification method may extend to more general cases that a map between target spaces cannot be easily decomposed.

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