Learning Self-Expression Metrics for Scalable and Inductive Subspace Clustering

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Subspace clustering has established itself as a state-of-the-art approach to clustering high-dimensional data. In particular, methods relying on the self-expressiveness property have recently proved especially successful. However, they suffer from two major shortcomings: First, a quadratic-size coefficient matrix is learned directly, preventing these methods from scaling beyond small datasets. Secondly, the trained models are transductive and thus cannot be used to cluster out-of-sample data unseen during training. Instead of learning self-expression coefficients directly, we propose a novel metric learning approach to learn instead a subspace affinity function using a siamese neural network architecture. Consequently, our model benefits from a constant number of parameters and a constant-size memory footprint, allowing it to scale to considerably larger datasets. In addition, we can formally show that our model is still able to exactly recover subspace clusters given an independence assumption. The siamese architecture in combination with a novel geometric classifier further makes our model inductive, allowing it to cluster out-of-sample data. Additionally, non-linear clusters can be detected by simply adding an auto-encoder module to the architecture. The whole model can then be trained end-to-end in a self-supervised manner. This work in progress reports promising preliminary results on the MNIST dataset. In the spirit of reproducible research, we make all code publicly available.

In future work we plan to investigate several extensions of our model and to expand experimental evaluation.

1 Introduction

Subspace clustering [Vidal, 2011] assumes the data to be sampled from a union of low-dimensional subspaces of the full data space. The goal is to recover these subspaces and to correctly assign each data point to its respective subspace cluster. As a state-of-the-art approach to clustering high-dimensional data, it enables a multitude of applications, including image segmentation [Ma et al., 2007; Yang et al., 2008], motion segmentation [Kanatani, 2001; Elhamifar and Vidal, 2009; Ji et al., 2016], image clustering [Ho et al., 2003; Elhamifar and Vidal, 2013] and clustering gene expression profiles [McWilliams and Montana, 2014]. For instance, face images of a subject under fixed pose and varying lighting conditions [Basri and Jacobs, 2003] or images of handwritten digits with different rotations, translations and other natural transformations [Hastie and Simard, 1998] have been shown to lie in low-dimensional subspaces.

Recently, self-expressiveness-based methods [Elhamifar and Vidal, 2009; Liu et al., 2010; Lu et al., 2012; Elhamifar and Vidal, 2013; Liu et al., 2013; Wang et al., 2013; Feng et al., 2014; Ji et al., 2014; Vidal and Favaro, 2014; Ji et al., 2015; You et al., 2016a] have proved especially successful. The main idea is that each point can be expressed by a linear combination of points from the same subspace. This property is used to learn a quadratic-size coefficient matrix from which cluster labels can be extracted in a post-processing step using spectral clustering. The quadratic number of parameters prevents these methods from scaling beyond small datasets and makes them transductive and thus

[https://github.com/buschju/sscn](https://github.com/buschju/sscn)

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Figure 1: Data flow within our model. Square boxes denote tensors, rectangular boxes denote functions, and dashed lines indicate parameter sharing.

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where we take advantage of the observation that points from independent clusters will have orthogonal

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where the \( i \)-th column of the \( N \times N \) coefficient matrix \( C \) contains the coefficients for expressing

Given the learned coefficient matrix, cluster assignments can be extracted in a post-processing step by applying spectral clustering to the subspace affinity matrix \( A = |C| + |C|^T \). The unique solution to this problem can be expressed in closed-form as the solution \( C^* \) of the linear system

\[
(I + \lambda X^T X) C = \lambda X^T X
\]

Let \( r := \text{rank}(X) = \dim \left( \bigoplus_{i=1}^K S_i \right) \) denote the rank of \( X \). In a noise-free setting, if the subspaces are independent, i.e., if \( r = \sum_{i=1}^K \dim(S_i) \), then \( C^* \) is guaranteed to be block-diagonal with \( C^*_{ij} = 0 \) if \( x_i \) and \( x_j \) originate from different subspaces [Vidal et al. 2008]. The corresponding solution is called subspace-preserving.

The central idea of our approach is to view subspace clustering from a metric learning perspective. To this end, we employ a siamese neural network [Bromley et al. 1994] consisting of two identical branches with shared weights and mirrored parameter updates which is optimized such that dot-products in latent space correspond to self-expression coefficients:

**Definition 2** (Siamese Dense Subspace Clustering).

\[
\min_{\theta_h} \frac{1}{2} \| Q \|_F^2 + \lambda \| X - XQ \|_F^2 \quad \text{s.t.} \quad Q = HT H, \quad H = h(X; \theta_h)
\]

where \( Q \in \mathbb{R}^{N \times N} \) contains the self-expression coefficients corresponding to dot-products of the embeddings \( H \in \mathbb{R}^{d_H \times N} \) computed by the embedding function \( h \). Note that weight sharing leads to symmetric coefficient matrices. Even though the reduction of parameters compared to (1) is quadratic, we can show that this model is able to recover the exact solution to the original subspace clustering problem, even when \( h \) consists of only a single linear layer with a sufficient number of neurons. Note that (2) is convex in this case.

**Theorem 1.** Let \( h(X) = WX \), \( W \in \mathbb{R}^{d_H \times d_X} \), \( d_H \geq r \), then (2) attains its global minimum at \( W^* = R \sqrt{\lambda \left( I - \lambda \left( \Sigma_r^{-2} + \lambda I \right)^{-1} \right)} U_r^T \) where \( X = U_r \Sigma_r V_r^T \) is the reduced SVD of \( X \) and \( R \in \text{St}(d_H, r) \) is an arbitrary orthonormal matrix. The unique optimal coefficient matrix \( Q^* \) of (2) corresponds to the unique solution of (1).

Above, \( \text{St}(n, p) = \{ X \in \mathbb{R}^{n \times p} \mid X^T X = I \} \) for \( n \geq p \) denotes the Stiefel manifold which is composed of all \( n \times p \) orthonormal matrices. Since (2) leads to a well-studied optimal solution, it can be analyzed directly within existing theory. In particular, it is guaranteed that under the independence assumption and in a noise-free setting, (2) yields a subspace-preserving solution. Also note that we don’t need to know the exact rank of \( X \); it is sufficient to have an upper bound. Since \( r \leq \sum_{i=1}^K \dim(S_i) \), we can simply estimate the number of clusters \( K \) and the maximum cluster dimension \( q \) and set \( d_H = Kq \) and \( R \in \text{St}(d_H, d_H) \).

Since we can choose \( R \) arbitrarily from \( \text{St}(d_H, d_H) \) and still obtain the same optimal coefficient matrix \( Q^* \), we are able to optimize \( R \) on the Stiefel manifold w.r.t. to a cluster assignment objective where we take advantage of the observation that points from independent clusters will have orthogonal embeddings in \( H \). To this end, we compute rotated embeddings \( \tilde{H} = RH \) and then classify points by assigning them to their closest subspace w.r.t. orthogonal projection distance and applying the sofmin function:

\[
y_{ij} = \exp \left( - ||h_i - S_j h_{ij}||_2^2 / \sum_{k=1}^K \exp \left( - ||h_i - S_k h_{ij}||_2^2 / ||h_i||_2^2 \right) \right)
\]

The subspaces are fixed a-priori to be axis-aligned and don’t need to be optimized. The matrix \( R \) is optimized such that classifications agree with self-expression affinities. For now, we compute the coefficient matrix of the training set using our trained model and then apply the same post-processing as in [Ji et al. 2017b] to obtain pseudo-labels which are used to train the classifier using cross-entropy loss and the Cayley-Adam algorithm [Li et al. 2020]. In future work, we plan to employ a triplet-loss [Hermans
We can see that our model provides competitive performance while drastically reducing the required number of model parameters and GPU-memory. Even large amounts of out-of-sample data can be clustered reliably without any memory overhead. All hyper-parameter values and complete code for reproducing the reported results are provided in our public code repository. In future work we plan to train our model end-to-end using a triplet-loss and additional feedback from the classifier to the encoder and self-expression module. We further plan to evaluate on more datasets, with different architectural choices and against more baselines.

Table 1: Results on the MNIST dataset. Upper part: Transductive clustering of the 10,000 test images. Lower part: Inductive clustering of the 60,000 out-of-sample training images using our previously trained model. Note that our model did not see these images during training and that DSC-Net does not support clustering out-of-sample data and would require more than 4.9B parameters and 39GB of GPU-memory to cluster the whole dataset. All results are aggregated over 10 independent runs with different random initializations. For better comparability, all models use the same pre-trained encoder and self-expression module. We further plan to evaluate on more datasets, with different settings for both models wherever possible. For SSCN, we model bias as motivated above and train with a batch-size of 1000. The results are summarized in Figure 1.

To account for non-linearity, we can simply add an auto-encoder to our model with the task of mapping the original data into a $d_{z}$-dim. latent space in which the subspace assumption, and additionally the independence assumption, can be better satisfied. This non-linear transformation is learned together with the rest of the model. We formalize our complete model in Definition 3.

**Definition 3** (Siamese Subspace Clustering Network (SSCN)),

\[
\min_{\theta_e, \theta_s, \theta_d, R} \frac{1}{2} \|Q\|_F^2 + \frac{\lambda_1}{2} \|Z - ZQ\|_F^2 + \frac{\lambda_2}{2} \|X - \hat{X}\|_F^2 + \lambda_3 L_{clf}(R; X)
\]

s.t. \(Q = H^T H, \quad H = h(Z; \theta_h), \quad Z = enc(X; \theta_e), \quad \hat{X} = dec(ZQ; \theta_d)\)

Above, $Z \in \mathbb{R}^{d_{z} \times N}$ are non-linear embeddings of the input $X$ computed by the encoder function $enc$. After self-expression in latent space, $X$ is reconstructed as $\hat{X} \in \mathbb{R}^{d_{x} \times N}$ using $dec$, a decoder function matching $enc$. The reconstruction loss ensures that the learned embeddings are actually compatible with the original data and prevents trivial solutions. Note that training with the full data batch $X$ would lead to materialization of the full $N \times N$ coefficient matrix $Q$. This is not an issue for our model, however, since it can be trained with mini-batches and thus scale to large datasets. The only requirements are that batches need to be sampled uniformly at random and that the batch-size needs to be sufficiently large so that we sample enough instances from each class on average and thus obtain a representative sample. An illustration of the data flow is provided in Figure 1.

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