Sparse Subspace Clustering with Entropy-Norm

Liang Bai 1  Jiye Liang 1

Abstract
In this paper, we provide an explicit theoretical connection between Sparse subspace clustering (SSC) and spectral clustering (SC) from the perspective of learning a data similarity matrix. We show that spectral clustering with Gaussian kernel can be viewed as sparse subspace clustering with entropy-norm (SSC+E). Compared to SSC, SSC+E can obtain an analytical, symmetrical, nonnegative and nonlinearly-representational similarity matrix. Besides, SSC+E makes use of Gaussian kernel to compute the sparse similarity matrix of objects, which can avoid the complex computation of the sparse optimization program of SSC. Finally, we provide the experimental analysis to compare the efficiency and effectiveness of sparse subspace clustering and spectral clustering on ten benchmark data sets. The theoretical and experimental analysis can well help users for the selection of high-dimensional data clustering algorithms.

1. Introduction
Clustering is an important problem in statistical multivariate analysis, data mining and machine learning (Han & Kamber, 2001). The goal of clustering is to group a set of objects into clusters so that the objects in the same cluster are highly similar but remarkably dissimilar with objects in other clusters (Jain, 2008). To tackle this problem, various types of clustering algorithms have been developed in the literature (e.g., (Aggarwal & Reddy, 2014) and references therein), including partitional, hierarchical, density-based, grid-based clustering, etc.

Recently, increasing attention has been paid to clustering high-dimensional data which is ubiquitous in real-world data mining applications, such as image processing, text analysis, and bioinformatics et al. Sparsity is an accompanying phenomenon of high-dimensional data, which leads to “curse of dimensionality”, i.e., all pairs of points tend to be almost equidistant from one another. It is a special challenge for clustering high-dimensional data. In order to solve this problem, lots of clustering algorithms have been developed in the literature (e.g., (Parsons et al., 2004; Elhamifar & Vidal, 2013) and references therein). Among them, spectral clustering and sparse subspace clustering are two state-of-the-art methods to effectively separate the high-dimensional data in accordance with the underlying subspace. Spectral clustering (Shi & Malik, 2000; Ng et al., 2001) is a representative of graph-based clustering, which first converts a data set into a graph or a data similarity matrix and then uses a graph cutting method to identify clusters. However, the clustering results of the spectral clustering are sensitive to the converted graph. In the classical spectral clustering algorithm, the graph is often constructed by kernel functions (Dhillon et al., 2007) or k-nearest neighbors (KNN) (Zhu et al., 2014). Besides, some scholars developed graph-learning methods to obtain a high-quality graph from the data set. For example, Nie et al. proposed a clustering algorithm with adaptive neighbors (Nie et al., 2014), which learns the data similarity matrix by assigning the adaptive and optimal neighbors for each data point based on the local connectivity.

Sparse subspace clustering can also be seen as a special spectral clustering. It makes use of self representation of the data to construct the sparse similarity graph and apply spectral clustering on such graph to obtain the final clustering result. In (Elhamifar & Vidal, 2009), Elhamifar and Vidal presented the SSC algorithm with $L_1$-norm in detail. Furthermore, several variants of SSC have been proposed to find out the sparse representation of the data under different assumptions. Wang and Xu proposed noisy SSC to handle noisy data that lie close to disjoint or overlapping subspaces (Wang & Xu, 2016). Yang et al. proposed SSC with $L_0$-norm (Yang et al., 2016). Liu et al. proposed a low rank representation of all data jointly by using the structured sparsity loss (Liu et al., 2013). Hu et al. investigated theoretically the grouping effect for self-representation based approaches and presented a smooth representation.
Although scholars have provided lots of studies on spectral clustering and sparse subspace clustering, the relation between them is rarely discussed. Therefore, in this paper, we provide an explicit theoretical connection between them. We propose a sparse subspace clustering model with entropy-norm. In this optimization model, we transform a sparse subspace clustering problem into an optimization problem of learning a sparse similarity matrix and uses the Entropy-norm as the regularization term. We derive its optimal solution which is equivalent to Gaussian kernel as follows.

\[ w_{ij} = \exp \left( -\frac{||x_i - x_j||^2}{\gamma} \right), \]  

where \( \gamma \) is a kernel parameter. Besides, we know that \( \hat{W} = D^{-1/2}WD^{-1/2} \) is the normalized similarity matrix of \( W \). In this case, the spectral clustering becomes the normalized spectral clustering. The spectral clustering problem is the standard trace minimization problem which is solved by the matrix \( H \) which contains the first \( k \) eigenvectors of \( L \) as rows.

The formulation of sparse subspace clustering is

\[ \min_Z F = L(X, XZ) + \lambda \Omega(Z), \]

where \( \lambda > 0 \) is the tradeoff factor, \( L(X, XZ) \) is a loss function which wishes \( X = XZ \) and \( \Omega(.) \) is a regularization term which is used to sparsify \( Z \). If \( X = XZ \) is required and \( \Omega(Z) = ||Z||_1 \), the optimization problem is the classical SSC problem, i.e.,

\[ \min_Z ||Z||_1, \text{s.t.}, X = XZ, diag(Z) = 0. \]

In the noisy SSC algorithm which allows some tolerance for inexact representation, the optimization problem is defined as

\[ \min_Z ||X - XZ||_F^2 + \lambda ||Z||_1, \text{s.t.}, diag(Z) = 0. \]

Besides, in order to make the data lie in a union of subspaces, the constraint \( 1^T Z = 1^T \) is added to the sparse subspace problem (Elhamifar & Vidal, 2013).

The optimization problem of SSC and noisy SSC can be solved efficiently using convex programming tools. With the reconstruction coefficient matrix \( Z \), the sparse similarity matrix of objects is computed by

\[ W = |Z| + |Z^T|. \]
subspace clustering is very expensive, which is not suitable for large-scale data. Furthermore, we can see from Eq.(6) that the SSC algorithm explicitly converts the similarity matrix $Z$ into a symmetrical and nonnegative matrix $W$. This conversation may bring some misleading information. For example, we should think that the lower the value of $z_{ij}$ is, the more the dissimilarity between $x_i$ and $x_j$ is. However, if $z_{ij}$ is negative, the lower $z_{ij}$ is, the higher $|z_{ij}|$ is. In this case, the similarity between $x_i$ and $x_j$ are thought to be high. Thus, the similarity matrix $W$ obtained based on the conversation is not necessarily effective. Besides, $Z$ or $W$ obtained by the SSC algorithm is not an analytical solution. This indicates that we cannot observe the explicit similarity relation between objects from $Z$ and $W$, which prevents users from understanding the similarity. Compared to SSC, the similarity matrix by using Gaussian kernel function in the spectral clustering is analytical, symmetrical and nonnegative. Although we can see the difference between the two algorithms, there is the lack of their theoretical connection. This is the motivation of our work.

3. Sparse Subspace Clustering with Entropy-Norm

In this section, we analyze the theoretical connection between spectral clustering and sparse subspace clustering from the perspective of learning the data similarity matrix $W$. In the analysis, we first transform a sparse subspace clustering problem into an optimization problem of learning a sparse similarity matrix. Furthermore, we use the Entropy-norm as the regularization term and derives its optimal solution to show the relation between spectral clustering and sparse subspace clustering. In the following, we provide the theoretical analysis in detail.

According to the definition of $W$ in the sparse subspace clustering, we can conclude that if $Z$ is a symmetrical and nonnegative matrix, $W$ is equivalent to $Z$. In this case, the minimization problem $F$ can be converted as follows:

$$
\min_Z F, \text{ s.t., } Z = Z^T, Z \geq 0, \text{diag}(Z) = 0. \tag{7}
$$

According to Eq.(7), we can see that the sparse subspace clustering problem can be viewed as learning a similarity matrix. However, we know that the SSC algorithm cannot guarantee the optimization solution $Z$ is symmetric and nonnegative. Some scholars enforce the symmetric positive semi-definite (PSD) constraint on $Z$ to explicitly obtain a symmetric PSD matrix, such as (Ni et al., 2010). However, it is very complex for the optimization program of SSC to obtain a symmetric and nonnegative $Z$.

Therefore, we select information entropy as the regularization term of the objective function $F$ and propose a sparse subspace clustering with entropy-norm to solve this problem. The objective function $F$ is re-defined as

$$
F = \mathcal{L}(X, X Z) + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} z_{ij} \ln z_{ij}, \tag{8}
$$

While using the Lagrangian multiplier to directly minimize $F$, we can obtain

$$
\frac{\partial F}{\partial z_{ij}} = \frac{\partial \mathcal{L}}{\partial z_{ij}} + \lambda (\ln z_{ij} + 1) = 0
\Rightarrow z_{ij} = \beta \exp \left( -\frac{f_{ij}}{\lambda} \right) \tag{9}
$$

where $\beta = \exp(-1)$ and $f_{ij} = \frac{\partial \mathcal{L}}{\partial z_{ij}}$. According to Eq.(9), we can see that $Z$ is nonnegative, and if $f_{ij} = f_{ji}$ for $1 \leq i, j \leq n$, then $Z$ is symmetric, i.e., $z_{ij} = z_{ji}$.

Furthermore, we add the constraint $1^T Z = 1^T$ to the optimization problem. While using the Lagrangian multiplier to minimize $F$ with the constraint, we can obtain

$$
\min_Z F = \mathcal{L}(X, X Z) + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} z_{ij} \ln z_{ij}
+ \alpha \sum_{i=1}^{n} \left( \sum_{h \neq i}^{n} z_{ih} - 1 \right)
\Rightarrow \frac{\partial F}{\partial z_{ij}} = \frac{\partial \mathcal{L}}{\partial z_{ij}} + \lambda (\ln z_{ij} + 1) + \alpha = 0 \tag{10}
\Rightarrow \exp \left( -\frac{\lambda + \alpha}{\lambda} \right) = \frac{1}{2} \sum_{h \neq i}^{n} \exp \left( -\frac{f_{ih}}{\lambda} \right)
\Rightarrow z_{ij} = \frac{\exp \left( -\frac{f_{ij}}{\lambda} \right)}{\sum_{h \neq i}^{n} \exp \left( -\frac{f_{ih}}{\lambda} \right)}.\tag{11}
$$

However, in Eq.(10), if $f_{ij} = f_{ji}$, we can not guarantee $z_{ij}$ is equal to $z_{ji}$. In order to improve this problem, we relax the constraint $1^T Z = 1^T$ and replace it with a new constraint $\sum_{h \neq i}^{n} z_{ih} + \sum_{h \neq j}^{n} z_{hj} = 2$, for $1 \leq i \neq j \leq n$. It notes that the sum of any row and column of $Z$ is 2. While using the Lagrangian multiplier to minimize $F$ with the new constraint, we can obtain

$$
\min_Z F = \mathcal{L}(X, X Z) + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} z_{ij} \ln z_{ij}
+ \alpha \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \sum_{h \neq i}^{n} z_{ih} + \sum_{h \neq j}^{n} z_{hj} - 2 \right)
\Rightarrow z_{ij} = \frac{2 \exp \left( -\frac{f_{ij}}{\lambda} \right)}{\sum_{h \neq i}^{n} \exp \left( -\frac{f_{ih}}{\lambda} \right) + \sum_{h \neq j}^{n} \exp \left( -\frac{f_{hj}}{\lambda} \right)}.\tag{11}
$$
We can conclude that if $f_{ij} = f_{ji}$ in Eq. (11), $z_{ij} = z_{ji}$ for $1 \leq i, j \leq n$. We can also observe that the representations of $z_{ij}$ in Eqs. (9) and (11) are similar to Gaussian kernel.

According to Eqs. (9) and (11), we can see that we need to compute $f_{ij}$ to obtain $z_{ij}$ for $1 \leq i, j \leq n$. In order to easily compute $f_{ij}$, we wish it is irrelevant with $z_{ij}$. Therefore, we first assume $L(X, XZ)$ is a linear function with $z_{ij}$, i.e.,

$$L(X, XZ) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} z_{ij} + b_{ij}. \quad (12)$$

In this case, $f_{ij} = \frac{\partial L}{\partial z_{ij}} = a_{ij}$. We can see that this assumption reduces the computational complexity of $z_{ij}$ and $f_{ij}$. According to Eq. (12), we also see that it is a key issue for computing $f_{ij}$ to define $a_{ij}$.

Based on the self-representation constraint $X = XZ$, we have

$$x_i = \sum_{j=1, j \neq i}^{n} z_{ij} x_j, \quad (13)$$

for $1 \leq i \leq n$. According to Eq. (13), we can see that $z_{ij}$ should reflect the similarity between $x_i$ and $x_j$. The more similar they are, the higher the value of $z_{ij}$ should be. In order to make $z_{ij}$ reflect the similarity, we assume $a_{ij}$ is a distance metric between $x_i$ and $x_j$, i.e., $a_{ij} = d(x_i, x_j)$. According to the symmetry of the distance metric, we have $a_{ij} = a_{ji}$. Next, we discuss how to use the constraint $X = XZ$ to define $d(x_i, x_j)$.

For object $x_i$ ($1 \leq i \leq n$), we have the following relation

$$x_i = \sum_{j=1, j \neq i}^{n} z_{ij} x_j \Rightarrow x_i^T x_i = \sum_{j=1, j \neq i}^{n} z_{ij} x_j^T x_j. \quad (14)$$

Based on the constraint $I^T Z = I^T$, we have

$$\left( \sum_{j=1}^{n} z_{jj} + \sum_{j=1}^{n} z_{ij} \right) x_i^T x_i = 2 \sum_{j=1, j \neq i}^{n} z_{ij} x_j^T x_j. \quad (15)$$

Therefore, the constraint $x_i - \sum_{j=1, j \neq i}^{n} z_{ij} x_j = 0$ is transformed into

$$\left( \sum_{j=1}^{n} z_{jj} + \sum_{j=1}^{n} z_{ij} \right) x_i^T x_i - 2 \sum_{j=1, j \neq i}^{n} z_{ij} x_j^T x_j = 0. \quad (16)$$

Furthermore, we have

$$\sum_{i=1}^{n} \left( \sum_{j=1}^{n} z_{jj} + \sum_{j=1}^{n} z_{ij} \right) x_i^T x_i - 2 \sum_{j=1, j \neq i}^{n} z_{ij} x_j^T x_j = \sum_{i=1}^{n} \sum_{j=1}^{n} ||x_i - x_j||^2 z_{ij}. \quad (17)$$

Based on Eq. (17), the objective function $F$ of the optimization problem can be rewritten as

$$Q = \sum_{i=1}^{n} \sum_{j=1}^{n} ||x_i - x_j||^2 z_{ij} + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} z_{ij} \ln z_{ij}. \quad (18)$$

In this case, $d(x_i, x_j)$ is defined as Euclidean distance. According to Eq. (9), $d(x_i, x_j)$ is Euclidean distance, $Z$ in Eq. (9) is equivalent to Gaussian kernel, i.e.,

$$z_{ij} = \exp \left( -\frac{||x_i - x_j||^2}{\lambda} \right). \quad (19)$$

According to Eq. (19), the spectral clustering with Gaussian kernel can be viewed as a sparse subspace clustering with entropy-norm.

Furthermore, if we use $d(x_i, x_j)$, instead of $f_{ij}$ in Eq. (10), $Z$ is defined by

$$z_{ij} = \frac{2 \sum_{h \neq i} \exp \left( -\frac{||x_i - x_h||^2}{\lambda} \right)}{\sum_{h \neq i} \exp \left( -\frac{||x_i - x_h||^2}{\lambda} \right) + \sum_{h \neq j} \exp \left( -\frac{||x_j - x_h||^2}{\lambda} \right)}. \quad (20)$$

In this case, we have the following relation

$$Z \leq D^{-1/2} W D^{-1/2}. \quad (21)$$

Eq. (21) illustrates that $Z$ is a lower bound of the normalized Gaussian kernel and used to approximate it. According to the above analysis, we can see the relation between Gaussian kernel and sparse subspace clustering.

Furthermore, we discuss the selection of the regularization term on the objective function $Q$. If we define the regularization term $\Omega(Z) = ||Z||_2$, the objective function $Q$ becomes

$$\sum_{i=1}^{n} \sum_{j=1}^{n} ||x_i - x_j||^2 z_{ij} + \lambda ||Z||_2. \quad (22)$$

In this case, the optimization problem $Q$ is equivalent to that of Clustering with Adaptive Neighbors (Nie et al., 2014) which is proposed by Nie et al.. The authors improved the spectral clustering and used the optimization model to learn the data similarity matrix. The optimal solution $Z$ is computed by

$$z_{ij} = 1 - \frac{||x_i - x_j||^2}{2\lambda} + \eta_i. \quad (23)$$

where $\eta_i = \frac{\sum_{i=1}^{n} ||x_i - x_h||^2 + 1}{n}$. Since each $\eta_i$ may be different, the non-negativeness of $Z$ depends on $\eta_i$. Besides, we can see that the similarity $z_{ij}$ reflects a linear relation with the distance $||x_i - x_h||^2$ in the case that $L_2$ norm is used as the regularizer.
If the regularization term $\Omega(Z) = \|Z\|_1$, the optimal solution $Z$ is computed by

$$z_{ij} = \begin{cases} 1, & j = \arg \min_{t=1} \|x_i - x_t\|^2, \\ 0, & \text{otherwise}. \end{cases} \quad (24)$$

In this case, the solution is trivial, since only its nearest object can be used to represent it. According to Eqs.(23) and (24), we can see the advantages of the entropy-norm, compared to other norms.

According to the above theoretical analysis, we can get the following conclusions:

- From the perspective of learning a data similarity matrix, the spectral clustering with Gaussian kernel can be viewed as a sparse subspace clustering with entropy-norm (SSC+E);
- Compared to SSC, SSC+E can directly compute the data similarity matrix by Gaussian kernel, which can reduce the computational cost.
- SSC+E can be used to obtain an analytical, nonnegative, symmetrical, and nonlinear representation of a data set.

However, it is worth noting that the proposed theoretical connection is not to prove and show that spectral clustering with Gaussian kernel is better than sparse subspace clustering, but to help users to understand the solution of the SSC algorithm by Gaussian kernel. Besides, although the theoretical connection is built based on some constraints, we still think that it is very valuable to provide a guidance for users to select and understand different algorithms.

### 4. Experiment Analysis

In the experiments, we analyze and compare the effectiveness and efficiency of the sparse subspace clustering algorithm (SSC) (Elhamifar & Vidal, 2009), the spectral clustering with adaptive neighbors (CAN) (Nie et al., 2014), and the spectral clustering with Gaussian kernel (SSC+E) (Ng et al., 2001). Differently from SSC and CAN which compute a data similarity matrix by the optimization methods, SSC+E uses Gaussian kernel to compute the similarity matrix. The codes of these algorithms have been publicly shared by their authors.

The experiments are conducted on an Intel i9-7940X CPU@3.10HZ and 128G RAM. We carry out these algorithms on 10 benchmark data sets (Bache & Lichman; Cai) which are described in Table 1. It is worth noting that we did not select large-scale data sets to test these algorithms in our experiments. The main reason is that the computational cost of the SSC algorithm is very high. For example, it needs more than 60 hours on the data set Landsat Satellite which includes 6,435 points. Furthermore, we employ two widely-used external indices (Aggarwal & Reddy, 2014), i.e., the normalized mutual information (NMI) and the adjusted rand index (ARI), to measure the similarity between a clustering result and the true partition on a data set. If the clustering result is close to the true partition, then its NMI and ARI values are high.

Before the comparisons, we need to set some parameters for these algorithms as follows. We set the number of clusters $k$ is equal to its true number of classes on each of the given data sets. For the parameter $\lambda$, we test each algorithm with different $\lambda$ values which are selected in the set $\{\lambda_1 = \frac{\delta}{5}, \lambda_2 = \frac{\delta}{3}, \lambda_3 = \frac{\delta}{2}, \lambda_4 = \frac{\delta}{3}, \lambda_5 = \frac{\delta}{5}, \lambda_6 = \delta\}$, where $\delta$ is the covariance of a data set. Besides, the SSC and CAN algorithms need to set the number of the nearest neighbors $K$. We set $K$ to 10 in our experiments.

We first compare the effectiveness of the three algorithms with different $\lambda$ values on these benchmark data sets. The comparison results are shown in Fig.1. According to the figures, we see that the performance of the SSC+E algorithm is superior to SSC and CAN on these tested data sets, except Heart Statlog.

Furthermore, we compare the efficiency of the three algorithms with different $\lambda$ values on these benchmark data sets. The comparison results are shown in Table 2. According to the table, we see that the SSC algorithm need very expensive computational costs, compared to SSC+E and CAN. We also can observe that the clustering speed of the SSC+E algorithm is slightly faster than CAN on these tested data sets. The main reason is that the SSC+E algorithm does not need learn the sparse representation but directly compute it by Gaussian kernel. According to the above analysis, we can conclude that the SSC+E algorithm can better balance the effectiveness and efficiency of obtaining a high-quality clustering results, compared to the SSC and CAN algorithms.

<table>
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<th>n</th>
<th>m</th>
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</tr>
<tr>
<td>Wine</td>
<td>178</td>
<td>13</td>
<td>3</td>
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<td>Heart Statlog</td>
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**Table 1. Description of data sets:** Number of Data Objects (n), Number of Dimensions (m), Number of Clusters (k).
Figure 1. Clustering accuracies of different algorithms.
Table 2. Clustering speeds (seconds) of different algorithms

<table>
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<td>0.534</td>
<td>0.547</td>
<td>0.563</td>
<td>0.563</td>
<td>0.578</td>
</tr>
<tr>
<td>Isolet</td>
<td>SSC</td>
<td>56079.227</td>
<td>55180.180</td>
<td>54446.940</td>
<td>64799.694</td>
<td>72375.284</td>
</tr>
<tr>
<td></td>
<td>SSC+E</td>
<td>0.657</td>
<td>0.703</td>
<td>0.657</td>
<td>0.734</td>
<td>0.766</td>
</tr>
<tr>
<td>Handwritten Digits</td>
<td>SSC</td>
<td>13990.391</td>
<td>13495.460</td>
<td>13250.659</td>
<td>12951.093</td>
<td>12793.112</td>
</tr>
<tr>
<td></td>
<td>CAN</td>
<td>216.325</td>
<td>154.261</td>
<td>148.512</td>
<td>148.73</td>
<td>140.842</td>
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<tr>
<td></td>
<td>SSC+E</td>
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<td>3.577</td>
<td>3.702</td>
<td>3.625</td>
<td>3.843</td>
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<tr>
<td>Landsat Satellite</td>
<td>SSC</td>
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<td>14463.630</td>
<td>14510.508</td>
<td>15019.646</td>
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<tr>
<td></td>
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<td>265.11</td>
<td>317.706</td>
<td>204.983</td>
<td>318.269</td>
<td>315.863</td>
</tr>
</tbody>
</table>
|                 | SSC+E     | 4.467          | 4.374          | 4.452          | 4.562          | 4.452          | 4.545          

It should be noted that due to the fact that the number of the tested data sets is very limited, we can not conclude that the effectiveness of the data similarity matrices by Gaussian kernel are better than SSC and CAN. However, our experimental results only illustrate that spectral clustering with Gaussian kernel is still a good choice to rapidly obtain a good sparse representation for a data set, although it had been easily proposed.

5. Conclusions

In this paper, we have analyzed the theoretical connection between spectral clustering and sparse subspace clustering from the perspective of learning the data similarity matrix. We have shown that the spectral clustering with Gaussian kernel can be viewed as a sparse subspace clustering with entropy-norm, which is called SSC+E. We have analyzed the advantages and disadvantages of SSC+E and SSC. Compared to SSC, the SSC+E algorithm can rapidly obtain a sparse, analytical, symmetrical, nonnegative and nonlinerly-representational similarity matrix. Finally, we have compared the efficiency and effectiveness of sparse subspace clustering and spectral clustering on ten benchmark data sets. The experimental results show that the spectral clustering with Gaussian kernel is still a good choice to rapidly obtain a high-quality clustering results.

Acknowledgement

The authors are very grateful to the editors and reviewers for their valuable comments and suggestions. This work is supported by the National Natural Science Foundation of China (Nos. 61876103, 61773247, 61976128), the Technology Research Development Projects of Shanxi (No. 201901D211192) and the 1331 Engineering Project of Shanxi Province, China.
References


