Improved Spectral Clustering via Embedded Label Propagation

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Abstract

Spectral clustering is a key research topic in the field of machine learning and data mining. Most of the existing spectral clustering algorithms are built upon Gaussian Laplacian matrices, which are sensitive to parameters. We propose a novel parameter-free, distance-consistent Locally Linear Embedding (LLE). The proposed distance-consistent LLE promises that edges between closer data points have greater weight. Furthermore, we propose a novel improved spectral clustering via embedded label propagation. Our algorithm is built upon two advancements of the state of the art: 1) label propagation, which propagates a node's labels to neighboring nodes according to their proximity; and 2) manifold learning, which has been widely used in its capacity to leverage the manifold structure of data points. First we perform standard spectral clustering on original data and assign each cluster to \( k \)-nearest data points. Next, we propagate labels through dense, unlabeled data regions. Extensive experiments with various datasets validate the superiority of the proposed algorithm compared to current state-of-the-art spectral algorithms.

Introduction

Data clustering is a fundamental research topic that is widely used for many applications in the fields of artificial intelligence, statistics and the social sciences. The purpose of clustering is to partition the original data points into various groups so that data points within the same cluster are dense while those in different clusters are far apart. Among various implementations of clustering, \( k \)-means is one of the most popular in reality because of its simplicity and effectiveness. The general procedure of traditional \( k \)-means (TKM) is to randomly initialize \( c \) clustering centers, assign each data point to its nearest cluster and compute a new clustering center. Current researchers claim the curse of dimensionality may deteriorate the performance of TKM. A straight-forward solution to this problem is to project original datasets to a low-dimensional subspace by dimensionality reduction, i.e., PCA, before performing TKM. Discriminative analysis has proven effective in enhancing clustering performance. Discriminative k-means (DKM) and discriminative \( k \)-means (DKM) has gradually attracted increasing research attention for its capacity to mine intrinsic data geometric structures, which facilitates partitioning data with more complicated structures.

On a further note, spectral clustering (SC) has gradually attracted increasing research attention for its capacity to mine intrinsic data geometric structures, which facilitates partitioning data with more complicated structures. The basic idea of SC is to find a cluster assignment of data points by adopting a spectrum of the similarity matrix that leverages the nonlinear and low-dimensional manifold structure of original data. Inspired by the benefits of spectral clustering, different variants of the SC method have been proposed to demonstrate its effectiveness. For example, local learning-based clustering (LLC) utilizes a kernel regression model for label prediction based on the assumption that the class label of a data point can be determined by its neighbors. Similarly, self-tuning SC is able to tune parameters automatically in an unsupervised scenario. Normalized cuts are capable of balancing the volume of clusters for the usage of data density information.

Label propagation has been shown effective in propagating labels through the dataset along high density areas defined by unlabeled data in a low-dimensional manifold structure of original data. Inspired by the benefits inherent to label propagation, we intend to introduce label propagation into the field of spectral clustering.
Our proposed spectral clustering algorithm therefore combines the strengths of spectral clustering and label propagation. The main process of our algorithm is shown in Fig. 1. We first perform standard spectral clustering on our original dataset and obtain $c$ clusters. Then, we select $k$ data points that are respectively close to each cluster center and form label matrix $Y$. By way of manifold learning, we propagate labels through dense unlabeled data regions. We call the proposed method improved Spectral Clustering via embedded Label Propagation (SCLP).

The main contributions of this paper can be summarized as follows:

1. To the best of our knowledge, this is the first time spectral clustering and embedded label propagation have been incorporated into a single framework. We propagate the labels obtained by spectral clustering to other unlabeled data points.

2. We integrate the advantage of manifold learning, which is capable of leveraging manifold structure among data points, into the proposed framework.

3. A novel distance-consistent Locally Linear Embedding is proposed herein as well. Unlike a traditional Guassian graph approach, the proposed graph is parameter-free.

4. Extensive experiments on seven real-world datasets demonstrate that the proposed spectral clustering framework (SCLP) outperforms state-of-the-art clustering algorithms.

After revisiting related work on Locally Linear Embedding and spectral clustering in Section 2, we detail our SCLP algorithm in Section 3. Extensive experiments are given in Section 4 and Section 5 concludes this paper.
In this section, we illustrate the detailed framework of our modified to Local Learning Clustering (LLC).

According to (Dhillon, Guan, and Kulis 2004), the overall function of spectral clustering can be defined as follows:

$$\min_F \text{Tr}(F^T R)$$

s.t. $F = Y (Y^T Y)^{-1/2}$, \quad (4)

where $\text{Tr}(\cdot)$ denotes the trace operator and $L$ is a graph Laplacian matrix computed in accordance with local data structure. Among different strategies, a common way to compute the weight matrix is thus:

$$a_{ij} = \begin{cases} \exp(-\frac{\|x_i - x_j\|^2}{\delta}), & \text{if } x_i \text{ and } x_j \text{ are } k \text{ nearest neighbours}. \\ 0, & \text{otherwise} \end{cases} \quad (5)$$

where $A_k(x_j)$ denotes $k$ nearest neighbors of $x_j$ and $\delta$ is utilized to control the spread of neighbors. The Laplacian graph is then computed by $L = D - W$, where $D$ is a diagonal matrix with its diagonal elements as $D_{ii} = \sum_j A_{ij}$.

By replacing $L$ in Eq. (4) by the normalized Laplacian matrix $L_n$,

$$L_n = D^{-1/2} LD^{-1/2} = I - D^{-1/2} AD^{-1/2} \quad (6)$$

the objective function becomes the well-known SC algorithm normalized cut (Shi and Malik 2000). In the same manner, if we replace $L$ in Eq. (4) with $L_t$, which is a Laplacian matrix obtained by local learning (Wu and Schlkopf 2006), the objective function is then modified to Local Learning Clustering (LLC).

The Proposed Framework

In this section, we illustrate the detailed framework of our algorithm.

We aim to cluster the dataset into $c$ clusters. Suppose $X \in \mathbb{R}^{d \times n}$ indicates the dataset; $d$ is the dimension of data points and $n$ is the total number of data points.

Distance-Consistent Similarity Learning

Following the work in (Karasuyama and Mamitsuka 2013), we propose leveraging manifold regularization built upon the Laplacian graph for label propagation. To begin, we first present a novel distance-consistent Local Linear Embedding (LLE).

Intuitively, we expect close data points to have similar labels. We create a graph in which all data points are considered nodes. If $x_i$ ($x_j$) is in $k$-Nearest-Neighbor of $x_j$ ($x_i$), then the two nodes are connected. The edge between them is weighted so that the closer the nodes are in Euclidean distance, the larger the weight $a_{ij}$. Because we have $\sum_j a_{ij} = 1$, the objective function of LLE in Eq. (1) can be safely rewritten as follows:

$$\min_A \sum_{i=1}^n \|x_i - \sum_{j=1}^k x_j a_{ij}\|^2_2, \quad (7)$$

By way of simple mathematical deduction, we can rewrite the above objective function in this manner:

$$\min_A \sum_{i=1}^n \|x_i - x_{i1}, \ldots, x_i - x_{ik}\|_2^2 \quad (8)$$

$\Rightarrow \min_A \sum_{i=1}^n Tr(a_i^T [x_i - x_{i1}, \ldots, x_i - x_{ik}]^T [x_i - x_{i1}, \ldots, x_i - x_{ik}]a_i) \quad (9)$

For simplicity’s sake, we assign all the non-diagonal elements of $[x_i - x_{i1}, \ldots, x_i - x_{ik}]^T [x_i - x_{i1}, \ldots, x_i - x_{ik}]$ to zero. The above objective function is equivalent to the following:

$$\min_A \sum_{i=1}^n \sum_{j=1}^k \|x_i - x_{ij}\|^2_2 a_{ij}^2 \quad (10)$$

s.t. $\sum_{j=1}^k a_{ij} = 1$, $a_{ij} \geq 0$

From the above function, we can observe that the proposed distance-consistent LLE suggests that the edge between closer nodes has a greater weight.

The Lagrangian function of problem of Eq. (10) can be written as

$$\sum_{j=1}^k \|x_i - x_{ij}\|^2_2 a_{ij}^2 - \gamma (\sum_{j=1}^k a_{ij} - 1), \quad (11)$$

where $\gamma$ is a Lagrange multiplier. By setting the derivative of Eq. (11) w.r.t. $a_{ij}$ to zero, we have

$$a_{ij} = \frac{\gamma}{2\|x_i - x_{ij}\|^2_2}. \quad (12)$$

By substituting the resultant $a_{ij}$ in Eq. (12) into the constraint $\sum_{j=1}^k a_{ij} = 1$, we arrive at

$$\gamma = \frac{1}{\sum_{j=1}^k \|x_i - x_{ij}\|^2_2}. \quad (13)$$

By integrating Eq. (12) and Eq. (13), we obtain the final solution for $a_{ij}$.

By denoting $D$ as a diagonal matrix with its diagonal $d_i = \sum_j a_{ij}$, the graph Laplacian can be calculated as

$$L = D - A. \quad (14)$$

Refined Spectral Clustering

After initially clustering the dataset into $c$ clusters through traditional spectral clustering, we select $k$ data points per cluster, which are nearest to each clustering center, and mark them as labeled data points. The remaining points are marked as unlabeled data points. Note that we assume these $k$ data points are grouped into the proper clusters. Hence, we obtain the label matrix $Y \in \mathbb{R}^{n \times c}$ and diagonal selection matrix $U \in \mathbb{R}^{n \times n}$, where $U_{ij} = 1$ if $X_i$ is labeled, and $X_j$ belongs to the $j$-th cluster. $Y_{i,j} = 0$ otherwise. $U_{ii} = \infty$ if
which is defined as:

\[ \text{Eq. (17)} \]

We have a problem in the following steps. By setting the derivative of \( f \) w.r.t. \( X \), to zero, we have

\[ \begin{align*}
\min_{F} & \quad \text{Tr}(F^T L F) + \text{Tr}((F - Y)^T U (F - Y)) \\
& + \alpha \|X^T W - F\|_F^2 + \beta \|W\|_2,1
\end{align*} \]

where \( \text{Tr}(\cdot) \) denotes the trace operator. The purpose of this definition is to keep the predicted labels \( F \) consistent with the ground truth labels \( Y \).

We further incorporate a regularization term into the objective function to correlate the features with the predicted labels. Consequently, the objective function arrives at

\[ \begin{align*}
\min_{F} & \quad \text{Tr}(F^T L F) + \text{Tr}((F - Y)^T U (F - Y)) \\
& + \alpha \|X^T W - F\|_F^2 + \beta \|W\|_2,1
\end{align*} \]

where \( \| \cdot \|_F \) denotes the Frobenius norm of a matrix.

Since the least square loss function is very sensitive to outliers, we employ \( l_{2,1} \)-norm on the regularization term to handle this issue. Hence, we can rewrite the objective function as follows:

\[ \begin{align*}
\min_{F} & \quad \text{Tr}(F^T L F) + \text{Tr}((F - Y)^T U (F - Y)) \\
& + \alpha \|X^T W - F\|_F^2 + \beta \|W\|_2,1
\end{align*} \]

It is worth noting that the proposed framework can be readily applied to out-of-sample clustering. By calculating \( X^T W \), we obtain the label predictor matrix for outside samples.

**Optimization**

The proposed function involves the \( l_{2,1} \)-norm, which is difficult to solve in a closed form. We propose to solve this problem in the following steps. By setting the derivative of Eq. (17) w.r.t. \( W \) to zero, we have

\[ W = \alpha (\alpha X X^T + \beta D)^{-1} X F, \]

where \( I \) is an identity matrix and \( D \) is a diagonal matrix which is defined as:

\[ D = \begin{bmatrix} \frac{1}{2 \|w^1\|_2} & \cdots & \frac{1}{2 \|w^c\|_2} \end{bmatrix}. \]

Letting \( H \) represent \( (\alpha X X^T + \beta D)^{-1} \), the objective becomes

\[ \begin{align*}
\min_{F} & \quad \text{Tr}(F^T L F) + \text{Tr}((F - Y)^T U (F - Y)) \\
& + \alpha \|X^T H X F - F\|_F^2 + \beta \|X^T H X F\|_F^2
\end{align*} \]

By denoting \( P \) as \( P = \alpha X^T H X - I \), the objective becomes

\[ \begin{align*}
\min_{F} & \quad \text{Tr}(F^T L F) + \text{Tr}((F - Y)^T U (F - Y)) \\
& + \alpha \|P F\|_F^2 + \beta \|\alpha X^T H X F\|_F^2
\end{align*} \]

By setting the derivative of Eq. (21) w.r.t. \( F \) to zero, we have

\[ F = (L + \alpha P P + \alpha^2 X^T H H X)^{-1} U Y \]

Based on the above mathematical deduction, we propose an efficient iterative algorithm to optimize the objective function Eq. (17), which is summarized in Algorithm 1.

**Algorithm 1:** Optimization Algorithm for SCLP

**Data:** Data \( X \in \mathbb{R}^{d \times n} \)

- The number of clusters \( c \)
- Parameters \( \alpha \) and \( \beta \)

**Result:** The cluster indicator matrix \( F \)

1. Construct the Laplacian matrix \( L \) according to Eq. (14);
2. Compute the selecting matrix \( U \in \mathbb{R}^{n \times n} \);
3. Cluster data \( X \) into \( c \) clusters through Spectral Clustering;
4. Pick out \( n_L \) data points that are close to each cluster center and construct \( Y \);
5. repeat
6. Compute \( D \) according to

\[ D = \begin{bmatrix} \frac{1}{2 \|w^1\|_2} & \cdots & \frac{1}{2 \|w^c\|_2} \end{bmatrix}. \]

7. Compute \( H \) according to \( H = (\alpha X X^T + \beta D)^{-1} \);
8. Compute \( P \) according to \( P = \alpha X^T H X - I \);
9. Compute \( F \) according to

\[ F = (L + \alpha P P + \alpha^2 X^T H H X)^{-1} (U * Y) \]

10. until Convergence;
11. Return \( F \)

**Experiments**

In this section, we conduct extensive experiments to validate the proposed SCLP’s performance and compare it with related state-of-the-art spectral clustering algorithms, following a study of parameter sensitivity.

**Dataset Description**

We use seven trademark datasets to validate the performance of the proposed algorithm. The USPS dataset has 9298 gray-scale handwritten digital images with an image size of 256 scanned from envelovers with the U.S. Post service. The Yale-B dataset (Georghiades, Belhumeur, and Kriegman 2001)
Matrix Size Dataset Size Class #
LUNG 3312 203 4
PALM 256 2000 100
MSRA50 1024 1799 12
FRGC 1296 5658 275
AR 768 840 120
YaleB 1024 2414 38
USPS 256 9298 10

Table 1: DATASET DETAILS

consists of 2414 near frontal images from 38 persons under different illuminations. The AR dataset (Martinez and Benavente 1998) has 840 images with a dimension of 768. The FRGC dataset (Phillips et al. 2005) was collected at the University of Notre Dame and contains 50,000 images. All the images were taken across 13 different poses, under 43 different illumination conditions and with four different expressions per person. The MSRA50 dataset (He et al. 2004) consists of 1799 images and 12 classes. The PALM dataset consists 700 right-hand images, seven samples per person across 100 users, taken via digital camera. The images are resized to the same dimension of 100 × 100. The human lung carcinomas (LUNG) dataset (Singh et al. 2002) contains 203 samples and 3312 genes.

Experiment Setup

We compare the proposed SCLP with traditional k-means (TKM) (Ye, Zhao, and Wu 2007), Local Learning Clustering (LLC) (Wu and Scholkopf 2006), Non-negative Normalized Cut (NNC) (Shi and Malik 2000), Spectral Clustering (SC), LLC (Wu and Scholkopf 2006), CLGR (Wang, Zhang, and Li 2009) and Spectral Embedding Clustering (SEC) (Nie et al. 2009).

The size of neighborhood k is set to 5 for all spectral clustering algorithms. For the parameter, δ, in NNC, we perform a self-tuning algorithm (Zelnik-Manor and Perona 2004) to determine the best parameter. For parameters in DKM, LLC, CLGR and SEC, we tune them in the range of {10^{-6}, 10^{-4}, 10^{-2}, 10^{0}, 10^{2}, 10^{4}, 10^{6}} and report the best results. Note that the results of all clustering algorithms vary based on initialization. To reduce the influence of statistical variation, we repeat each clustering 50 times with random initialization and report the results according to the best objective function values. For SCLP, we select 2 data points per cluster nearest to the clustering center.

Evaluation Metrics

Following related clustering studies, we utilize clustering accuracy (ACC) and normalized mutual information (NMI) as our experiments’ evaluation metrics.

Let $q_i$ represent the clustering label result from a clustering algorithm; $p_i$ represent the corresponding ground truth label of arbitrary data point $x_i$. From there, $ACC$ is defined as follows:

$$ACC = \frac{\sum_{i=1}^{n} \delta(p_i, \text{map}(q_i))}{n},$$  

where $\delta(x, y) = 1$ if $x = y$ and $\delta(x, y) = 0$ otherwise. $\text{map}(q_i)$ is the best mapping function that permutes clustering labels to match the ground truth labels using the Kuhn-Munkres algorithm. A larger ACC indicates a better clustering performance.

For any two arbitrary variables $P$ and $Q$, NMI is defined as follows (Strehl and Ghosh 2003)

$$NMI = \frac{I(P, Q)}{\sqrt{H(P)H(Q)}},$$

where $I(P, Q)$ computes mutual information between $P$ and $Q$, and $H(P)$ and $H(Q)$ are the entropies of $P$ and $Q$. Let $t_l$ represent the number of data points in the cluster $C_l (1 \leq l \leq c)$ generated by a clustering algorithm and $\bar{t}_h$ represent the number of data points from the $h$-th ground truth class. The NMI metric is then computed as follows (Strehl and Ghosh 2003)

$$NMI = \frac{\sum_{l=1}^{c} \sum_{h=1}^{n} t_l \log \frac{t_l}{n} / \bar{t}_h \log \frac{\bar{t}_h}{n}}{\sqrt{\sum_{l=1}^{c} t_l \log \frac{t_l}{n} / \left(\sum_{h=1}^{n} \bar{t}_h \log \frac{\bar{t}_h}{n}\right)}}$$

where $t_{l,h}$ is the number of data samples that lies in the intersection between $C_l$ and $h$th ground truth class. Similarly, a larger NMI indicates a better clustering performance.

Experimental Results

We show the clustering results of different algorithms in terms of ACC and NMI over seven benchmark datasets in Tables 2 and 3. Based on the results of our experiment, we can make the following observations:

1. When comparing the k-means based algorithms (i.e., TKM and DKM), DKM generally outperforms TKM because discriminative dimension reduction is integrated into a single framework. Thus each cluster is more identifiable and facilitates clustering performance. We can therefore safely conclude that discriminative information is beneficial for clustering.

2. SC outperforms LLC on the YaleB and USPS datasets, while LLC outperforms SC on all those remaining. That is, CLGR achieves better performance on all datasets than both algorithms combined.

3. SEC obtains the second-best performance over the seven datasets, which indicates that linearity regularization can also facilitate clustering performance. Similar to our algorithm, SEC is capable of dealing with out-of-sample data.

4. The proposed algorithm SCLP generally outperforms the compared clustering algorithms on the seven benchmark datasets, which demonstrates that manifold regularization-based label propagation is beneficial for spectral clustering.
Table 2: Performance Comparison (ACC %) of KM, DKM, NNC, SC, LLC, CLGR, SEC and SCLP. The proposed algorithm, SCLP, generally outperforms the compared algorithms, which indicates that manifold regularization-based label propagation is beneficial for spectral clustering.

|       | KM   | DKM | NNC   | SC    | LLC  | CLGR | SEC   | SCLP |
|-------|------|-----|-------|-------|------|------|-------|------|
| LUNG  | 82.8 | 84.1 | 83.2  | 83.4  | 85.2 | 85.7 | 87.8  | 91.6 |
| PALM  | 73.4 | 73.9 | 73.8  | 74.3  | 74.8 | 76.3 | 77.8  | 79.3 |
| MSRA50| 52.9 | 63.4 | 55.3  | 58.1  | 65.8 | 67.3 | 69.8  | 71.7 |
| FRGC  | 32.0 | 40.3 | 34.6  | 36.1  | 36.6 | 38.9 | 42.4  | 46.1 |
| AR    | 37.4 | 43.8 | 40.5  | 42.6  | 47.8 | 48.2 | 60.1  | 61.9 |
| YaleB | 13.6 | 37.2 | 36.5  | 35.2  | 32.8 | 37.3 | 46.3  | 48.4 |
| USPS  | 66.5 | 71.2 | 67.8  | 65.3  | 64.6 | 65.8 | 70.6  | 75.1 |

Table 3: Performance Comparison (NMI %) of KM, DKM, NNC, SC, LLC, CLGR, SEC and SCLP. The proposed algorithm, SCLP, generally outperforms the compared algorithms, which indicates that manifold regularization-based label propagation is beneficial for spectral clustering.

|       | KM   | DKM | NNC   | SC    | LLC  | CLGR | SEC   | SCLP |
|-------|------|-----|-------|-------|------|------|-------|------|
| LUNG  | 59.1 | 60.4 | 60.0  | 63.8  | 64.9 | 68.2 | 73.3  | 73.3 |
| PALM  | 81.8 | 83.4 | 82.1  | 85.6  | 87.2 | 87.5 | 89.3  | 91.4 |
| MSRA50| 61.7 | 63.4 | 62.5  | 62.8  | 69.4 | 68.5 | 70.9  | 73.3 |
| FRGC  | 66.3 | 68.5 | 67.8  | 66.7  | 68.9 | 69.2 | 71.2  | 73.9 |
| AR    | 69.3 | 73.8 | 72.1  | 73.7  | 74.2 | 74.6 | 75.3  | 77.4 |
| YaleB | 17.3 | 37.2 | 36.5  | 35.2  | 32.8 | 37.3 | 67.6  | 67.1 |
| USPS  | 60.2 | 62.4 | 61.8  | 63.2  | 63.9 | 65.2 | 69.6  | 74.4 |

Parameter Sensitivity

In this section, we study performance variance w.r.t. on the regularization parameters $\alpha$ and $\beta$.

We use the MSRA50 dataset for these experiments. Fig. 2 shows how clustering performance varies w.r.t. different combinations of $\alpha$ and $\beta$. We can see that better performance occurs when $\alpha$ and $\beta$ are comparable.

**Conclusion**

In this paper, we have proposed a novel improved spectral clustering algorithm SCLP. Most of the existing spectral clustering algorithms are based on Gaussian matrices or LLE, each of which are extremely sensitive to parameters. Moreover, the parameters are difficult to tune. We have therefore presented a novel distance-consistent LLE that is parameter-free. The distance-consistent LLE can promise that the edge between closer data points has a greater weight. Utilizing this distance-consistent LLE, we have proposed an improved means of spectral clustering via label propagation. The proposed algorithm takes advantage of label propagation and manifold learning. With label propagation, we can propagate the labels obtained through spectral clustering to other unlabeled data points. By adopting manifold learning, we leverage the manifold structure among data points. Note that our framework can also be readily applied to out-of-sample data. Finally, we have evaluated the clustering performance of the proposed algorithm over seven datasets. The experimental results demonstrate that the proposed algorithm consistently outperforms other algorithms to which it is compared.
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