Spectral Sparse Representation for Clustering: Evolved from PCA, K-means, Laplacian Eigenmap, and Ratio Cut

Zhenfang Hu*, Gang Pan*, Yueming Wang†, and Zhaohui Wu*

*College of Computer Science and Technology, Zhejiang University, China, zhenfhu@gmail.com, gpan@zju.edu.cn, zjuwuzh@gmail.com
†Qiushi Academy for Advanced Studies, Zhejiang University, China, ymingwang@zju.edu.cn

March 26, 2014

Abstract
Dimensionality reduction methods, e.g., PCA and Laplacian eigenmap (LE), and cluster analysis methods, e.g., K-means and ratio cut (Rcut), are two kinds of widely-used unsupervised data analysis tools. The former concerns high representation accuracy, while the latter semantics. Some preliminary relations between these methods have been established in the literature, but they are not yet integrated into a unified framework. In this paper, we show that under an ideal condition, the four methods: PCA, K-means, LE, and Rcut, are unified together; and when the ideal condition is relaxed, the unification evolves to a new sparse representation method, called spectral sparse representation (SSR). It achieves the same representation accuracy as PCA/LE, and is able to reveal the cluster structure of data as K-means/Rcut. SSR is inherently related to cluster analysis, and the sparse codes can be directly used to do clustering. An efficient algorithm NSCrt is developed to solve the sparse codes of SSR. It is observed that NSCrt is able to effectively recover the underlying solutions. As a direct application of SSR, a new clustering algorithm Scut is devised. It reaches the start-of-the-art performance. Compared with K-means based clustering methods, Scut does not depend on initialization and avoids getting trapped in local minima; and the solutions are comparable to the optimal ones of K-means run many times. Extensive experiments using data sets of different nature demonstrate the properties and strengths of SSR, NSCrt, and Scut.

Keywords: sparse representation, dimensionality reduction, cluster analysis, PCA, K-means, spectral clustering, Laplacian eigenmap.

1 Introduction
As the rise of information age, we are overwhelmed by the large amount of data generated day by day, e.g., images, videos, speeches, text, financial data, biomedical data, and so on. But the information contained in these data is usually not explicit in their original forms. Thus, the task of automatic analysis becomes urgent; and this calls for advance in methodology. In this paper, we focus on unsupervised learning methods, whose input data do not include any target values. We will explore the intrinsic structure of data by representing them in the other forms. The methods include dimensionality reduction methods, cluster analysis methods, and sparse representation methods. We will unify some representative methods of the first two kinds of methods, thus establish a link between dimensionality reduction and cluster analysis; and then based on the unification we develop a new sparse representation method, which is inherently related to dimensionality reduction and cluster analysis.

1.1 Dimensionality Reduction Methods and Cluster Analysis Methods
Dimensionality reduction methods and cluster analysis methods are two kinds of traditional data analysis methods that have found wide applications:
• Dimensionality reduction methods. For example, principal component analysis (PCA) [25], linear discriminant analysis (LDA) [40], kernel PCA [40], ISOMAP [43], LLE [37], Laplacian eigenmap (LE) [2], and locality preserving projections (LPP) [23]. They aim at representing high dimensional data by efficient low dimensional codes with high accuracy. The codes will preserve the relationship of original data as much as possible, e.g. distance between data points. They are widely applied, since many data we encountered are of high dimensions but whose intrinsic dimensions are much lower.

• Cluster analysis methods. For example, centroid-based K-means clustering [29] and its distribution-based version: clustering via Gaussian mixture models (GMM) [4], connectivity-based hierarchical clustering [22], density-based DBSCAN [19], and graph-based spectral clustering [44, 11] including ratio cut (Rcut) [8], normalized cut (Ncut) [42, 48, 33]. They try to partition the originally unorganized set of data points into disjoint groups such that similar data points become in the same group and dissimilar data points are separated into different groups. In this way, the cluster structure of data is revealed. They can also be seen as representing the original data most sparsely, since each data point is represented by only one group.

The dimensionality reduction methods are concerned with accuracy, while the cluster analysis methods are concerned with semantic. Nevertheless, both of them can be seen as representation methods.

Within each kind of the above methods, according to the form of input data they work with, there are two types of methods too. One works with original data, e.g. PCA, K-means; the other works with similarity matrix of data, e.g. LE, spectral clustering. Since usually the similarity matrix is constructed using some kernel function [44, 41], we can call the latter type kernel methods.

Among the various methods of dimensionality reduction and cluster analysis, PCA, K-means, LE, and spectral clustering are the four representative ones: they are elementary, have principled mathematical formulations, and are effective when applied in practice. In this paper, we will focus on these four methods; and among spectral clustering, we put emphasis on Rcut. These methods appear distinct at first sight. Some are dimensionality reduction methods; some are cluster analysis methods; some work with original data; some work with similarity matrix. However, they are closely related. Some pair-wise connections have been found in the literature.

1.2 Sparse Representation Methods

Sparse representation methods (SR) represent data by a dictionary and sparse codes. In existing SRs, the dictionary is generally over-complete, i.e. the number of dictionary columns (called atoms) is larger than the dimension of data. The codes are called sparse when there are only a few nonzero entries. In the past several years, signal processing, computer vision and pattern recognition communities have witnessed the great success of various SR models [6, 17, 45, 38]. We mention some representative work.

• In signal processing, the compressed sensing theory [15, 7,6] states that if a signal is sparse under some basis, then far fewer measurements than the Shannon theorem indicates are required to reconstruct the signal.

• In computer vision, [34] learnt an over-complete dictionary from natural images based on $\ell_1$ norm optimization. It was found surprisingly that the atoms of the dictionary is similar to the receptive fields in primary visual cortex. The KSVD algorithm [1] learnt a sparse representation similarly. But it is based on

11The LE we refer to hereafter is different from the original one [2]. The definition will be given in later section. We believe the original LE may be better called normalized LE for a reason that will be clear later.
ℓ₀ norm optimization. Taking advantage of the reconstruction power of SR, it has achieved state-of-the-art performance on a series of image processing problems [17], e.g. image compression, denoising, deblurring, inpainting, and super resolution.

- In pattern recognition, sparse codes are frequently used as features for classification, e.g. face recognition [46], image classification [47, 5]. [21] applied kernel trick and developed a kernel SR which extends the work of [46] and [47]. Comparing with the popular applications of SR on classification, the applications on clustering are relatively few. Some known work include [36] and sparse subspace clustering (SSC) [18].

Generally, except SSC, existing SRs are not directly related to dimensionality reduction and cluster analysis. Comparing with the popular applications on classification, the applications on clustering are relatively few.

1.3 Our Work

In this paper, we deepen and complete the relations of PCA, K-means, LE, and Rcut so that they are unified together. And, we propose a new SR called spectral sparse representation (SSR) which evolves from the unification of the four methods. Thus, SSR is directly related to dimensionality reduction and cluster analysis.

The idea of the unification and SSR can be briefly described as follows. The low dimensional codes obtained by dimensionality reduction methods PCA and LE are the leading eigenvectors of some matrices (data matrix in PCA, Laplacian matrix in LE). The cluster analysis methods K-means and Rcut use the same matrices as PCA and LE respectively. When an ideal condition is met, the indicator vectors corresponding to the underlying clusters in K-means and Rcut become the leading eigenvectors of those matrices, so PCA, K-means, LE, and Rcut are unified. When the ideal condition is met nearly, the leading eigenvectors become noisy indicator vectors, which are sparse and still contain some cluster information of the data, so the unification evolves to SSR.

We begin the unification by establishing the bilateral conversions between PCA and LE; K-means and Rcut. In effect, we convert the objective of one method into the form of the other. It turns out that PCA and K-means are equivalently working with a similarity matrix built by the Gram matrix of data, i.e. linear kernel matrix. So they can be converted to the forms of kernel methods; and roughly we can say that PCA and K-means are linear LE and linear Rcut respectively. Conversely, the similarity matrix used by LE and Rcut can be converted to a Gram matrix of some virtual data. So the objectives of LE and Rcut can be written into the forms of PCA and K-means respectively. Naturally, our theory includes two versions, so does SSR below: one works with original data, called original-data version; the other works with similarity matrix, called kernel version. The former one is in fact a special case of the latter one, i.e. linear kernel version.

To complete the unification, we bridge the link between Rcut and LE under an ideal graph condition. This is done through spectral graph theory [9, 32, 31], as [2] did. The solution of Rcut is a set of indicator vectors corresponding to the best partition, and that of LE is a set of eigenvectors. These two sets of vectors span the same subspace, and they are equivalent in the sense of a rotation transform. In brief, under the condition, the indicator vectors become the leading eigenvectors of PCA and LE. Based on the above results, consequently, the link between PCA and K-means is automatically built. Thus under the ideal graph condition, PCA, K-means, LE, and Rcut are unified together.

The unification evolves to SSR when the ideal condition is relaxed, i.e. in a noisy case. In this case, the leading eigenvectors of PCA and LE span the same subspace as the noisy versions of original indicator vectors. We call the noisy indicator vectors “sparse codes”, since every code vector is usually dominated by one entry; and the “noise” indeed quantitatively reflects the overlapping status of clusters. We develop an algorithm NSCrt to find a rotation matrix, by which the eigenvectors turn into noisy indicator vectors. Finally, as an application of SSR, a clustering algorithm sparse cut (Scut) is devised, which determines the cluster membership of each data point by simply checking the maximal entry of its code vector.

The contributions of the paper are:

1. PCA, K-means, LE, and Rcut are unified under an ideal graph condition. The following three consequences are highlighted. First, it is found that PCA and K-means are linear LE and Rcut respectively, which work

2We clarify that the “unification” do not mean that PCA working with original data is equivalent to LE working with general similarity matrix, so is the case of K-means and Rcut. In addition, it is different to the “unified view”, e.g. [3, 10], which usually discovers the general objective function shared by a set of methods. We investigate the equivalence relations on the solution level, as well as the condition when they hold.

3
with similarity matrix built by linear kernel. Second, through the introduction of spectral graph theory from Rcut, the exact equivalence of PCA and K-means is established, together with a condition when it holds. Third, the clustering scheme of applying K-means on the normalized principal components of data is found to be a linear Rcut algorithm.

2. A new sparse representation method SSR is proposed. It has the following four characteristics. First, it achieves the same representation accuracy as the dimensionality reduction methods PCA/LE. Second, it also reveals cluster structure as the cluster analysis methods K-means/Rcut. But, in contrast to the hard clustering nature of K-means/Rcut, SSR is soft and descriptive: it reveals the clusters that emerge and also describes the overlapping status of them. Nevertheless, the sparse codes of SSR can be directly used to do clustering. Third, rather than imposed explicitly, the sparsity in SSR is implicitly determined by the data structure: if the clusters overlap less, the codes become sparser. Fourth, SSR has two versions, one linear version which is under-complete, and one kernel version which is more powerful.

3. An efficient algorithm NSCrt is proposed to solve the sparse codes, which has a linear computational complexity about data size. Empirically, it is found that it can effectively recover the underlying solutions.

4. A clustering algorithm Scut is proposed, which performs clustering by checking the maximal entry of each sparse code-vector. Owning to the good performance of NSCrt, Scut generally outperforms K-means based methods which depend on initialization and are easily trapped in local minima; the solutions obtained by Scut are comparable to the optimal ones of K-means that are picked over many trials.

The paper is arranged as follows. Section 2 elaborates some related work. Section 3 reviews PCA, K-means, Rcut, and LE, and introduces the most appropriate forms of their objectives for later theory. The ideal graph condition is introduced in Section 3.3. Section 4 establishes the bilateral conversions between PCA and LE; K-means and Rcut. Section 5 presents the equivalence relation of LE and Rcut, and unifies the four methods together. A summary of the main results of the whole unification is provided at the end of this section. It will pave the way for SSR. Section 6 proposes SSR, NSCrt, and Scut. Section 7 shows experimental results. The paper is concluded with discussions in Section 8 where we make comparisons between related work and our work, including a detailed account of the difference of over-complete SRs and SSR.

**Notations.** They are listed in Table 1. The symbol $H$ is also used to denote noisy normalized indicator matrix, i.e. sparse codes.

### 2 Related Work

We will elaborate some related work that have been briefly introduced in the previous section, as well as some clustering methods that are close to our Scut.
2.1 Pair-wise Relations of PCA, K-means, LE, and Spectral Clustering

Concerning the unification part, some pair-wise relations among the methods are found in the literature: normalized LE and Ncut; PCA and K-means; spectral clustering and kernel K-means.

Normalized LE and Ncut [2]: their objectives can be written into similar forms except that spectral clustering additionally requires the variable to be an indicator matrix for the purpose of clustering. The solution of normalized LE is a set of generalized eigenvectors, while that of Ncut is indicator vectors. When a condition is met, which is in fact the ideal graph condition in this paper, the indicator vectors become the leading generalized eigenvectors; so the two methods are equivalent. When the condition is nearly met, the generalized eigenvectors are a rotation of some noisy indicator vectors. Thus, usually clustering is done by postprocessing the generalized eigenvectors, e.g. applying K-means on rows of these generalized eigenvectors. But, there is a straightforward counterpart LE and Rcut, which has been overlooked. In this paper, we will focus on LE and Rcut rather than Normalized LE and Ncut.

PCA and K-means [13]: their objectives can be written into similar forms except that K-means requires the variable to be an indicator matrix. PCA is thus seen as a relaxation of K-means; then clustering may be done by applying K-means on the normalized principal components of PCA, i.e. some leading eigenvectors. It is easy to see that this pair shares surprising features with the first pair. But this analogy may be ignored, to our knowledge. In the absence of spectral graph theory, the condition under which the relaxation and the clustering scheme work well has not yet been uncovered. In this paper, we will catch the analogy by converting PCA and K-means to LE and Rcut respectively, and then establish the exact equivalence relation.

Spectral clustering and kernel K-means [11]: the trace minimization or maximization form of spectral clustering can be converted to the trace maximization form of (weighted) kernel K-means, so spectral clustering can be solved by (weighted) kernel K-means. And an efficient multilevel algorithm Graclus [12] was developed, which is applicable to large-scale problem. But, on the one hand the conversion stops at kernel K-means and does not go further to the dictionary-based sparse representation. In this paper, it will be shown that the dictionary form can enrich our understanding of spectral clustering. On the other hand, the conversion from K-means to Rcut is ignored[3].

We will supplement this conversion and show that this conversion will lead to a linkage between dimensionality reduction and cluster analysis, as the first paragraph stated.

In summary, the relations remain pair-wise and not complete yet. They have not been integrated into a unified framework.

2.2 Over-complete SRs

Concerning SR, existing methods are quite different from our SSR. The representative work include compressed sensing theory in signal processing community, sparse and redundant dictionary learning in computer vision community and the applications of them in pattern recognition community. Generally, they are over-complete.

In signal processing, the compressed sensing theory [15, 7, 6] states that if a signal is sparse under some basis, then far fewer measurements than the Shannon theorem indicates are required to reconstruct the signal. The over-complete dictionary is designed rather than learnt from samples. It should satisfy good mutual coherence property, i.e. the atoms of dictionary are not close to each other. Surprisingly, random Gaussian matrix suffices. If the signal is intrinsically sparse enough, then the sparse codes are guaranteed to be solved exactly by a greedy algorithm orthogonal matching pursuit (OMP), or by the $\ell_1$ norm based convex optimization basis pursuit (BP). Thus, the signal can be exactly reconstructed. The compressed sensing theory is concerned with signal compression and reconstruction, but this paper and the SSR will deal with the semantic aspect of signal. Nevertheless, this line of work together with the celebrated work [34] triggered the research enthusiasm on SR in computer vision and pattern recognition fields.

In computer vision, [34] learnt an over-complete dictionary from natural images based on $\ell_1$ norm optimization. It was found surprisingly that the atoms of the dictionary are similar to the receptive fields in primary visual cortex. The KSVD algorithm [1] learnt a sparse representation similarly. But it is based on $\ell_0$ norm optimization. Taking advantage of the reconstruction power of SR, i.e. the product of dictionary and sparse codes, it has achieved state-of-the-art performance on a series of image processing problems [17], e.g. image compression, denoising, deblurring, inpainting, and super resolution. These two SRs are closest to SSR in this paper, especially KSVD. The model and optimization process of KSVD are generalizations of those of K-means [1]. But, it is still not certain

---

[1] In the rigorous sense of this paper, the conversion from weighted K-means to spectral clustering is infeasible.
whether or how it is related to cluster analysis. The over-completeness prevents it from the reach of spectral graph theory, as will be detailed in Section 8.2.

In pattern recognition, after the SRs are solved, the sparse codes are frequently used as features for classification, e.g. face recognition [46], image classification [47,5]. Usually, state-of-the-art performances are reached. [21] applied kernel trick and developed a kernel SR which extends the work of [46] and [47]. But the kernel trick is applied on the dictionary rather than on the data. Since the dictionary may be unknown beforehand, the optimization becomes tricky. On the other hand, the applications on clustering are not as popular. [36] achieves clustering via alternatively partitioning the data and learning a sparse representation for each cluster. But the method depends on a sophisticated initialization scheme that involves spectral clustering. Sparse subspace clustering (SSC) [18] deals with data that lie in a union of independent low-dimensional linear/affine subspaces, with each subspace containing a cluster. First the sparse codes of each data point are solved with respect to the dictionary composed by the remaining data. Then based on these codes, a sparse similarity matrix is established. Finally spectral clustering is applied. SSC is well-found and can handle noise, outliers as well as missing data. But it is limited to clusters lie in independent subspaces.

In summary, while SSR evolves from the dimensionality reduction and cluster analysis backgrounds, and one version of it is under-complete, most of existing SRs stem from the signal compression background and are over-complete. While the applications of existing SRs on classification are popular, the applications on clustering are few.

2.3 Clustering Methods Close to Scut

Concerning the application of SSR on clustering, there are some close work to Scut. Scut consists of three steps: compute some leading eigenvectors, employ NSCrt to recover the noisy indicator vectors (sparse codes) from these eigenvectors via rotation, and recover the discrete indicator vectors by selecting the maximal entries in the noisy indicator vectors. Some spectral clustering methods follow similar paradigm: first the eigenvectors are solved, then some post-processing techniques are employed to recover the discrete indicator vectors. Besides the most simple post-processing technique, K-means, as classical spectral clusterings use [44], there are some other attempts have been made.

The closest one to Scut is the work of [50], with the main difference be the solution scheme of rotation matrix. Assume the eigenvectors are arranged column wise. They tried to find a rotation matrix through which rows of the eigenvectors best align with the canonical coordinate system. This is in fact attempting to recover the noisy indicator vectors. And then as Scut, non-maximum suppression was applied to finish clustering. [50] solved the rotation matrix by gradient descent scheme under a different cost function. But the computational cost of this scheme is high when the number of cluster is somewhat large.

[48] found rotation matrix too, but they did not aim at recovering the noisy indicator vectors. Rather, they directly solved the discrete indicator vectors from some transformed eigenvectors. In detail, first rows of the eigenvectors were normalized to be unit length, and then they found a rotation matrix and a set of discrete indicator vectors such that after the rotation the discrete indicator vectors approximate the normalized eigenvectors.

Somewhat different to spectral clustering, [49] found a set of soft indicator vectors different to the noisy indicator vectors. Then non-maximum suppression was applied to finish clustering. The soft indicator vectors were solved by nonnegative factorization of a transformed similarity matrix. In contrast, the orthogonal eigenvectors of spectral clustering can be seen as solved by factorization of some other transformed similarity matrices. For a set of vectors, except indicator vectors, nonnegativity and orthogonality do not coexist. [49] kept the nonnegativity and dropped the orthogonality, while [50] and Scut keep the orthogonality and sacrifice the nonnegativity.

In summary, there are very close work to Scut, but the solution schemes of rotation matrix are quite different. Another difference of these work to Scut is that they focus on clustering task itself: the task is not under the background of sparse representation of data.

3 Reviews: PCA, K-means, Rcut, and LE

We will introduce classical formulations for these methods, as well as the most appropriate forms for the unification. The most appropriate forms of PCA and K-means are the dictionary representation forms, and those of Rcut and LE are the trace optimization forms. Along with them, some important properties and interpretations are elaborated. Besides, the important ideal graph condition will be introduced in Section 3.3.
3.1 PCA

Given mean-removed data matrix \( A \in \mathbb{R}^{p \times n} \), i.e. \( A1 = 0 \), PCA \(^3\) approximates the data by representing them in another basis, called loadings \( Q = [Q_1, \ldots, Q_r] \in \mathbb{R}^{p \times r} \) (\( r \ll p \)): \( A_i \approx Q Y_i, \forall i \), where \( Y_i \in \mathbb{R}^r \) are the low dimensional codes called principal components. The loadings are computed sequentially by maximizing the scaled covariance matrix \( C = AA^T \):

\[
\max_{Q_i} Q_i^T C Q_i, \text{ s.t. } \|Q_i\|_2 = 1, Q_i^T Q_j = 0, \forall 1 \leq j < i. \tag{1}
\]

Let \( A = U \Sigma V \) be the compact SVD \(^4\) where \( \Sigma \in \mathbb{R}^{m \times n} \), and \( m \) is the rank of \( A \). Then \( C = U \Sigma^2 U^T, Q^* = U_{1:r}, \) and \( Y^* = Q^T A = \Sigma_{1:r} V_{1:r} \).

PCA can also be derived from the well-known Eckart-Young Theorem \(^5\), which is in a dictionary representation form:

**Theorem 1. (Eckart-Young Theorem)** \(^5\) Let \( A = U \Sigma V \) be the compact SVD. A particular solution of the rank \( r \) (\( r \leq \text{rank}(A) \)) approximation of \( A \)

\[
\min_{D,X} \|A - DX\|_F^2, \text{ s.t. } XX^T = I, \tag{2}
\]

where \( D \in \mathbb{R}^{p \times r} \) and \( X \in \mathbb{R}^{r \times n} \), is provided by

\[
X^* = V_{1:r}, \quad D^* = AX^T = U_{1:r} \Sigma_{1:r}. \tag{3}
\]

In fact, for any rotation matrix \( R \in \mathbb{R}^{r \times r}, R^T R = I \), \( RX^* \) and \( D^* R^T \) also constitutes a solution. It is easy to see that if we impose normality on \( D \) rather than on \( X \), we get \( D^* = U_{1:r}, \) i.e. loadings of PCA, and \( X^* = \Sigma_{1:r} V_{1:r}, \) i.e. principal components of PCA. Henceforth, we view \((2)\) as the main formulation of PCA.

The formulation \((2)\) has the following interpretations: each sample in \( A \) is approximated by a dictionary representation, e.g. \( A_i \approx DX_i \), namely a linear combination of atoms (columns) of dictionary \( D \) using the code \( X_i \). When orthonormality is imposed on \( X \), the optimal dictionary comes from linear combinations of samples, \( D^* = AX^T \). Then \( A_i \approx AX^T X_i^*, \) i.e. \( A_i \) can be approximated by a linear combination of the whole data set with weight vector \( X^* X_i^T \). So the Gram matrix of codes \( X^* X^T \) encodes linear data relationship within rank \( r \) limitation.

3.2 K-means

Given data matrix \( A \in \mathbb{R}^{p \times n} \) \(^6\) K-means \(^2\) \(^\[13\]\) aims to partition the data into \( K \) clusters by minimizing the within-cluster variance:

\[
\min_{C_1, \ldots, C_K, D} \sum_{k=1}^K \sum_{A_i \in C_k} \|A_i - D_k\|_2^2, \tag{4}
\]

where \( C_k \) is the \( k \)th cluster, \( D = [D_1, \ldots, D_K] \in \mathbb{R}^{p \times K} \) are the \( K \) cluster centers. The global optimal solution is hard to obtain. After initializing \( D \), K-means finds a local solution via alternating two steps: given \( D \), assign each sample to the nearest cluster center; given the partition, update \( D_k \) by the mean of its members.

Using the indicator matrix notation, the original objective can be written in a dictionary representation form similar to \((2)\) \^[13]:

\[
\min_{D,F} \sum_{i=1}^n \|A_i - DF_i\|_2^2 = \|A - DF\|_F^2, \text{ s.t. } F \in \mathcal{F}. \tag{5}
\]

It can be solved alternatively. Given \( D \), solving \( F_i \) corresponds to the nearest-center search; given \( F \), it becomes a linear regression problem, and \( D^* = AF^\dagger = AF^T (FF^T)^{-1}. \) Since \( FF^T \) is a diagonal matrix of the cluster sizes, atoms of \( D^* \) are the averages of cluster members. Hence, the solution process is exactly identical to that of traditional K-means.

---

\(^3\) For SVD of data, by default we use the compact form, and assume a descending order of singular values.

\(^4\) It holds for general matrix not necessarily mean-removed.

\(^5\) K-means is translation invariant, we may assume \( A \) is mean-removed.
Substituting $D^* = AF^\dagger$ into the above objective, we obtain $\min_F \| A - AF^T (FF^T)^{-1} F \|^2_F$, s.t. $F \in \mathcal{F}$. Using the normalized indicator notation instead, it is equivalent to

$$\min_X \| A - AX^T X \|^2_F, \text{ s.t. } X \in \mathcal{H},$$

(6)

and

$$\min_{D,X} \| A - DX \|^2_F, \text{ s.t. } X \in \mathcal{H},$$

(7)

with $D^* = AX^*T$.

The formulation (7) has the following interpretations: $A_i \approx DX_i$. Since $\| X_i \|_0 = 1$, it only allows to use one atom to represent $A_i$, and so the representation error is large compared with PCA. Since $XX^T = I$, $D^* = AX^T$ which implies $D^*_k = AX^T_k$, i.e. a weighted average of cluster members. And $A_i \approx AX^*T X_i$. Note that $X^T X^*$ takes the form of $[\frac{1}{n_k}, \ldots, \frac{1}{n_k}, 0, \ldots, 0]^T$ for instance, and $1^T (X^*T X^*) = 1$, so $A_i$ is approximated by the mean of cluster members, i.e. the cluster center. And the Gram matrix of codes $X^*T X^*$ reflects the cluster structure of data.

### 3.3 Ratio Cut (Rcut)

Rcut [844] is also a clustering algorithm, but it works with a similarity (or weight) matrix $W \in \mathbb{R}^{n \times n}$, where $W_{ij} = W_{ji} \geq 0$ measures the similarity between data $A_i$ and $A_j$. It seeks a partition via minimizing the one-versus-versing weights (normalized by cluster size):

$$\min_{C_1, \ldots, C_K} \sum_{k=1}^K \frac{g(C_k, \bar{C}_k)}{n_k}.$$  

(8)

$C_k$ is the $k$th cluster, and $\bar{C}_k$ the complement; $g(C_k, \bar{C}_k) = \sum_{i \in C_k} \sum_{j \in \bar{C}_k} w_{ij}$; $n_k$ the size of $C_k$.

The objective can be expressed more explicitly by the indicator notation and a graph Laplacian matrix $L = S - W$, where $S$ is a diagonal degree matrix with $i$th element $s_i = \sum_{j=1}^n W_{ij}$. Before that, we introduce some well-known properties of the Laplacian matrix [3231] and the important ideal graph condition.

$$\forall f \in \mathbb{R}^n, \ f^T L f = \sum_{i<j} (f_i - f_j)^2 W_{ij} \geq 0.$$  

(9)

So

1. $L$ is positive semi-definite.
2. When $f$ is an indicator vector for $C_k$, $f^T L f = g(C_k, \bar{C}_k)$.
3. $\text{null}(L) \neq \phi$. Vector $1 \in \mathbb{R}^n$ is always an eigenvector of eigenvalue 0. Besides, $1^T \in \text{span}(F), \forall F \in \mathcal{F}$; $1^T \in \text{span}(X)$ and $X^T X 1 = 1, \forall X \in \mathcal{H}$.
4. The multiplicity of eigenvalue 0 equals the number of connected components of the graph, and the $K$ indicator vectors of the partition span the eigenspace of eigenvalue 0. Especially, it holds under the ideal graph condition, as defined below. This fundamental fact will play a key role in the unification.

**Definition 2. (Ideal graph condition)** Targeting for $K$ clusters, if there happens to be exactly $K$ connected components in the graph of similarity matrix, then the graph (or similarity matrix) is called ideal (with respect to $K$ clusters). Especially, the between-cluster weights are zero: $W_{ij} = 0$ if $A_i \in C_l, A_j \in C_m, l \neq m$. If members in the same cluster are arranged consecutively, the similarity matrix would emerge $K$ diagonal blocks, and there are no sub diagonal blocks in each block.  

\(^{4}\text{It is the separability condition used routinely in the spectral clustering literature [4433], where it is often informally called “ideal case”. We define it formally and precisely.}\)
In practice, for $K$ clusters, the similarity matrix is often not exactly ideal, but near to it, which means there are $K$ weakly connected components. In this case, we call the ideal graph condition is met well or nearly. And in this case, the between-cluster weights are weak, and if members in the same cluster are arranged consecutively, the similarity matrix would emerge $K$ noisy diagonal blocks. Besides, according to matrix perturbation theory [14,14]: 1) the $K$ smallest eigenvalues are close to 0, with the smallest one still be 0; 2) the eigenspace is spanned by $K$ noisy indicator vectors which do not deviate much from those in the ideal case; 3) the eigenvectors $V$ are a rotation of the $K$ noisy indicator vectors $H$, i.e. $V = RH$, for some unitary matrix $R$.

Back to $Rcut$, now using indicator notation and Laplacian matrix,

$$\min_{C_1,...,C_K} \sum_{k=1}^{K} \frac{g(C_k, \hat{C}_k)}{n_k}$$

$$= \min_{F} \sum_{k=1}^{K} \frac{F_k L F_k^T}{F_k F_k^T}, \text{ s.t. } F \in \mathcal{F}$$

$$= \min_{X} \sum_{k=1}^{K} X_k L X_k^T, \text{ s.t. } X_k = (F_k F_k^T)^{-1/2} F_k$$

$$= \min_{X} tr\{X L X^T\}, \text{ s.t. } X \in \mathcal{H}.$$  \hfill (10)

Generally, the objective is hard to solve due to the discrete nature of $X$. Instead, it is relaxed to

$$\min_{X} tr\{X L X^T\}, \text{ s.t. } X X^T = I,$$  \hfill (11)

where discrete constraint is ignored. By the well-known Ky Fan theorem [20], the solution set consists of all the rotations of the $K$ smallest eigenvectors of $L$.

1) When the graph is ideal, the corresponding indicator matrix $X^*$ will be the smallest eigenvectors thus it constitutes a solution. Note $X^* \in \mathbb{R}^K$ is the indicator vector for the $i$th data: there is only one nonzero entry, e.g. $x_{i, i}$; and the index of it signals the cluster membership. All members of a cluster share the same pattern; and the indicator vectors of two data belonging to different clusters is orthogonal. So clustering is trivial. But, any rotation of $X^*$ spans the same null space and constitutes an optimal solution too. In numerical computation, we may get $\hat{X} = RX^*$, for some rotation matrix $R \in \mathbb{R}^{K \times K}$. So the indicator structure is destroyed. However, members of a cluster still share the same pattern; and the orthogonality is preserved. Traditionally, the clustering task is finished by applying $K$-means on the columns of $\hat{X}$.

2) When the graph is near ideal, according to matrix perturbation theory, the eigenvectors do not deviate much from the ideal ones, so the main structure of indicator matrix is preserved. But it becomes somewhat noisy. In this case, some post-processing algorithm like $K$-means is more necessary.

### 3.4 Laplacian Eigenmap (LE)

LE is a dimensionality reduction algorithm that works with similarity matrix $W$ [2]. It finds low dimensional codes $X_i \in \mathbb{R}^t$ for the $i$th data:

$$\min_X \frac{1}{2} \sum_{i,j} \|X_i - X_j\|^2 W_{ij} = tr\{X L X^T\}, \text{ s.t. } X X^T = I,$$  \hfill (12)

where $X_i$ is the $i$th column of $X$, $L = S - W$ is the Laplacian matrix of $W$. The left-hand side can be read as: if a data pair is close originally, i.e. $W_{ij}$ large, their codes should be close too, i.e. $\|X_i - X_j\|^2$ small. The constraint $X X^T = I$ is to avoid trivial solution. In this way, the data relationship embodied by $W$ is approximately preserved by the codes. Considering [9], it is not hard to see the equivalence of the left-hand side to the right-hand side. Note that it takes exactly the form of (11). However, the task here focuses on representation rather than clustering. It does not care whether the data has cluster structure or not.

\*The original version imposes $X S X^T = I$, whose counterpart in spectral clustering is $Ncut$ [12,2]. However, the simplified version here, whose counterpart in spectral clustering is $Rcut$, makes the connection to other methods more straightforward.
Any rotation of the \( r \) smallest eigenvectors of \( L \) is a qualified solution. Let \( L = V^T A V \) be the full spectral decomposition\(^a\) with \( V_1 = \frac{1}{\sqrt{n}} 1^T \) the smallest eigenvector. For the purpose of dimensionality reduction, the constant \( V_1 \) is often omitted. One can either restrict \( X 1 = 0 \) to obtain \( r \) dimensional codes \( X^* = V_{2:r+1} \), or restrict \( X = \left[ \sqrt{n} 1^T \over X \right] \) to obtain \( r - 1 \) dimensional codes \( \tilde{X}^* = V_{2:r} \).

4 Bilateral Conversions: PCA \( \leftrightarrow \) LE, K-means \( \leftrightarrow \) Rcut

We begin the unification by establishing the bilateral conversions between PCA and LE; K-means and Rcut. We will convert the objective of one method into the form of the other. It will turn out that PCA and K-means are equivalently working on a similarity matrix defined by the Gram matrix using linear kernel function. So they can be converted to the forms of kernel methods LE and Rcut respectively. Or we can say that the objectives of PCA and K-means are special cases of those of LE and Rcut respectively, which use linear kernel. Conversely, the similarity matrix used by LE and Rcut can be converted to a Gram matrix of some virtual data. So the objectives of LE and Rcut can be written into the forms of PCA and K-means respectively.

In the following four subsections, firstly the main results are stated, then detailed derivations follow.

4.1 PCA \( \rightarrow \) LE

To our knowledge, this conversion is not yet established in the literature.

**Theorem 3. (PCA \( \rightarrow \) LE) PCA is a special LE that uses linear kernel. The objective of PCA**

\[
\min_{D,X} \|A - DX\|_F^2, \text{ s.t. } XX^T = I, \tag{13}
\]

where \( A 1 = 0, X \in \mathbb{R}^{r \times n}, r \leq \text{rank}(A) \), can be converted to the form of LE

\[
\min_{X} \text{tr} \{ \tilde{X} L \tilde{X}^T \}, \text{ s.t. } \tilde{X} = \left[ \sqrt{n} 1^T \over X \right], \tilde{X} \tilde{X}^T = I, \tag{14}
\]

where \( L \) is the Laplacian matrix of a similarity matrix defined by \( W = \tilde{A}^T \tilde{A} \). \( \tilde{A} = \left[ \sqrt{n} 1^T \over A \right] \) is called augmented data, where \( \beta = -\min_{i,j} (A^T A)_{i,j} \) so that \( W_{i,j} \geq 0 \). \( W \) is in fact a kernel matrix built by the linear kernel function \( \phi(A_j, A_j) = A_j^T A_j + \beta \). Solutions of \( X \) in (13) and (14) are equal. Let the SVD of \( A \) be \( A = U \Sigma V \), one common solution is \( V_{1:r} \).

**Objective conversion:** When we substitute \( D = AX^T \) into (2), only one variable is left:

\[
\min_{X} \|A - AX^T X\|_F^2, \text{ s.t. } XX^T = I. \tag{15}
\]

Since \( X^T X \) is a projection matrix, it means to find a \( r \) dimensional subspace spanned by the rows of \( X \) so that after projecting rows of \( A \) onto it, the reconstructions \( AX^T X \) are closest to their original ones, i.e. the lengths are best preserved. By Pythagorean theorem \( \|A - AX^T X\|_F^2 = \|A\|_F^2 - \|AX^T X\|_F^2 = \text{tr}\{A^T A\} - \text{tr}\{X A^T AX^T\} \).

So (15) becomes

\[
\max_{X} \text{tr}\{X A^T AX^T\}, \text{ s.t. } XX^T = I. \tag{16}
\]

This is equivalent to \( \min_{X} \text{tr}\{X (-A^T A)X^T\} \). In this form, PCA is close to LE. Define the similarity matrix to be \( W = A^T A \), which is in fact built by linear kernel. Since \( A 1 = 0, S = \text{diag}(W 1) = 0 \). So \( -A^T A \) is a Laplacian matrix\(^b\) except that \( W \) may not be nonnegative. Now we tackle this problem so as to turn PCA

---

\(^a\)For spectral decomposition of Laplacian matrix, by default we use the full form that includes all zero eigenvalues, and assume an ascending order of eigenvalues.

\(^b\)Applying kernel trick on the Gram matrix \( A^T A \) we get kernel PCA [40].

\(^c\)Applying kernel trick on \( L = \text{diag}(A^T A) - A^T A \), we get traditional LE [12].
In the above conversions, firstly we pad products of all data-pairs become nonnegative. Let \( X \in \mathbb{R}^{n \times m} \) be the augmented data matrix \( = \beta \) since of the augmented data \( \beta \in \mathbb{R}^{m \times m} \).

And then the Eckart-Young Theorem, \( X^\ast \) must be orthogonal to 1. So we can restrict \( X1 = 0 \). Then (16) is equivalent to

\[
\min_X -\text{tr}\{X(\beta 11^T + A^T A)X^T\} - \left( \frac{1}{\sqrt{n}} 1 \right)^T (\beta 11^T + A^T A) \left( \frac{1}{\sqrt{n}} 1 \right) \quad \text{s.t.} \quad X^T X = I, \quad X1 = 0
\]

\[
\min_X -\text{tr}\{\tilde{X}(\beta 11^T + A^T A)\tilde{X}^T\} \quad \text{s.t.} \quad \tilde{X} = \begin{bmatrix} \frac{1}{\sqrt{n}} 1^T \\ X \end{bmatrix}, \quad \tilde{X} \tilde{X}^T = I
\]

(17)

In the above conversions, firstly we pad \( A^T A \) uniformly with \( \beta \geq 0 \) in order to make \( A^T A \) nonnegative, e.g. choose \( \beta = -\min_{ij} (A^T A)_{ij} \). Secondly we augment \( X \) to be \( \tilde{X} \); next we turn the padded Gram matrix into Gram matrix of the augmented data \( \tilde{A} \). The padding trick can be interpreted as translating \( A \) along a new dimension so that inner products of all data-pairs become nonnegative.

Since \( S = \text{diag}(A^T A) = \beta n I \) and \( \tilde{X} \tilde{X}^T = I \), finally we can turn (17) into a problem about Laplacian matrix \( L = \beta n I - \tilde{A}^T \tilde{A} \):

\[
\min_X \text{tr}\{\tilde{X} L \tilde{X}^T\} \quad \text{s.t.} \quad \tilde{X} = \begin{bmatrix} \frac{1}{\sqrt{n}} 1^T \\ X \end{bmatrix}, \quad \tilde{X} \tilde{X}^T = I,
\]

(18)

which is a form of LE using linear kernel.

**Solution equivalence:** If the SVD of \( A \) is \( A = U \Sigma V \), then

\[
\tilde{A} = \tilde{U} \Sigma \tilde{V} = \begin{bmatrix} 1 \\ U \end{bmatrix} \begin{bmatrix} \sqrt{\beta} I \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ V \end{bmatrix}.
\]

(19)

And then

\[
L = \beta n I - \tilde{A}^T \tilde{A} = \tilde{V}(\beta n I - \Sigma^2) \tilde{V} = \begin{bmatrix} \frac{1}{\sqrt{n}} 1 \\ V \end{bmatrix} \begin{bmatrix} \sqrt{\beta} I \\ 0 \end{bmatrix} \begin{bmatrix} \beta n I - \Sigma^2 \\ \sqrt{n} 1 \end{bmatrix},
\]

(20)

since \( L \) is positive semi-definite we know that \( \beta n - \sigma_i^2 \geq 0 \). Therefore, \( X^\ast = \tilde{V}_{1:r} \), i.e. the solution of linear LE is still equivalent to that of original PCA (3).

### 4.2 K-means \( \rightarrow \) Rcut

To our knowledge, this conversion is not yet established in the literature.

**Theorem 4. (K-means \( \rightarrow \) Rcut)** Concerning objectives, K-means is a special Rcut that uses linear kernel. The objective of K-means

\[
\min_{D,X} \|A - DX\|_F^2, \quad \text{s.t.} \quad X \in \mathcal{H},
\]

(21)

can be converted to the form of Rcut

\[
\min_X \text{tr}\{XLXT\}, \quad \text{s.t.} \quad X \in \mathcal{H},
\]

(22)

where \( L \) is the Laplacian matrix defined as in Theorem 3. The solutions of \( X \) in (21) and (22) are equal. But, the algorithmic results may be different. Let \( A = U \Sigma V \) be the SVD, where \( \Sigma \in \mathbb{R}^{m \times m} \). Assume \( K \leq m + 1 \). Then K-means algorithm equivalently works with the full principal components \( \Sigma V \), while Rcut algorithm applies K-means algorithm on the leading \( K - 1 \) principal components with singular values ignored, i.e. \( V_{1:K-1} \), which we call normalized principal components.

**Objective conversion:** Since \( X^T X \) is a projection matrix, following the same reasoning as above of (16), (6) is equivalent to

\[
\max_X \text{tr}\{XA^T AX^T\}, \quad \text{s.t.} \quad X \in \mathcal{H}.
\]

(23)

\[\text{Since } A1 = 0, \text{ we are sure } \min_{ij} (A^T A)_{ij} \leq 0.\]
It is close to Rcut, but we are faced with the similar situation as \(^{16}\). Again we apply the padding trick to make the Gram matrix \(A^TA\) become nonnegative similarity matrix. Since \(\operatorname{tr}\{X11^TX\} = n\), (23) is equivalent to
\[
\min_X \operatorname{tr}\{X(\beta nI - (\beta 11^T + A^TA))X^T\}
= \min_X \operatorname{tr}\{X(\beta nI - \tilde{A}^T\tilde{A})X^T\}, \text{ where } \tilde{A} = \left[\sqrt{\beta}1^T\right]_A
\]
where \(\beta = -\min_{ij} (A^TA)_{ij}\). This is exactly the form of Rcut that uses linear kernel.

**Relation of algorithmic results:** Let \(A = U\Sigma V\) be the SVD, where \(\Sigma \in \mathbb{R}^{m \times n}\). Assume \(K \leq m + 1\). Then on the one hand, \(\|A(I - X^TX)\|_F^2 = \|\Sigma V(I - X^TX)\|_F^2\), i.e. K-means is rotation invariant. On the other hand, since \(1^T \in \text{span}(X)\) and by (19) \(V_{1:K} = [1 \sqrt{\lambda_1} \ldots 1 \sqrt{\lambda_K}]^T\), \(\|V_{1:K}(I - X^TX)\|_F^2 = \|V_{1:K}(I - \frac{1}{\sqrt{n}}1\sqrt{n}1^T)(I - X^TX)\|_F^2\), i.e. K-means is translation invariant. Now the contrast between K-means and Rcut in the sense of algorithm is apparent. K-means algorithm equivalently works with the full principal components of \(A\), i.e. \(\Sigma V\), while by (11) and (20) Rcut algorithm equivalently applies K-means on the first \(K - 1\) principal components with singular values ignored, i.e. \(V_{1:K-1}\).

When the graph is ideal (Definition 2), ignoring the singular values makes no difference, since they are all equal. However, in practice, this condition can hardly be met well, which essentially requires that after translating along a new dimension different clusters become near orthogonal. So the indicator structure embedded in the principal components may deviate much from the ideal one; and the singular values diverge. In this case, from the perspective of dimensionality reduction, another choice of clustering is to follow PCA exactly and apply K-means on the exact principal components. The arguments are: 1) the singular value weights its singular vector\(^{12}\) principal components are the best rank \(K\) approximation to the data according to the Eckart-Young Theorem.

### 4.3 LE → PCA

The conversion from LE to kernel PCA is implied by the work \(^{11}\) which studies relation between spectral clustering and kernel K-means. But the conversion does not go further to the dictionary representation form of PCA.

**Theorem 5. (LE → PCA)** The objective of LE
\[
\min_X \operatorname{tr}\{XLX^T\}, \text{ s.t. } X = \left[\frac{1}{\sqrt{n}}1^T\right], \quad XX^T = I,
\]
where \(X \in \mathbb{R}^{r \times n}\), can be converted to the form of dictionary representation
\[
\min_{D,X} \|\tilde{A} - DX\|_F^2, \text{ s.t. } X = \left[\frac{1}{\sqrt{n}}1^T\right], \quad XX^T = I,
\]
and further to PCA
\[
\min_{D,X} \|\tilde{A} - D\tilde{X}\|_F^2, \text{ s.t. } \tilde{X}\tilde{X}^T = I,
\]
where \(\tilde{A}\) and \(\bar{A}\) are defined as: Let \(L = V^T\Lambda V\) be the spectral decomposition, and \(V_1 = 1\sqrt{n}1^T\), \(\lambda_n\) the largest eigenvalue. Then we call \(\tilde{A} = (\lambda_n I - \Lambda)\hat{X}\) the virtual data; and \(\bar{A} = \tilde{A}(I - \frac{1}{\sqrt{n}}1\sqrt{n}1^T)\) is the mean-removed version. Their solutions of \(\tilde{X}\) are equal, one of which is \(V_{2:r}\).

**Objective conversion:** We will turn the trace minimization in (12) into dictionary representation (2). Let the spectral decomposition of \(L\) be \(L = V^T\Lambda V\), and \(V_1 = 1\sqrt{n}1^T\), \(\lambda_n\) the largest eigenvalue. We define virtual data \(\tilde{A} = (\lambda_n I - \Lambda)\hat{X}\). Then \(\lambda_n I - L = V^T(\lambda_n I - \Lambda) V = \tilde{A}^T\tilde{A}\). So
\[
\min_X \operatorname{tr}\{XLX^T\} \Leftrightarrow \max_X \operatorname{tr}\{X(\lambda_n I - L)X^T\} = \max_X \operatorname{tr}\{X\tilde{A}^T\tilde{A}X^T\}, \text{ s.t. } XX^T = I.
\]

\(^{13}\)Likewise, applying kernel trick on \(L = \text{diag}(A^TA1) - A^TA\) we get traditional Rcut.

\(^{14}\)The weighting is impossible in the original Rcut formulation, since the “weights” include zero.
Define virtual data

The conversion from Rcut to kernel K-means is established by the work [11]. But the conversion does not go further to the dictionary representation form of K-means; and the difference of algorithmic results between them is not discussed.

Further, (28) is equivalent to

$$\min_{X} \| \bar{A} - \bar{A}X^TX \|_F^2, \ s.t. \ XX^T = I, \quad (29)$$

and

$$\min_{D,X} \| \bar{A} - DX \|_F^2, \ s.t. \ XX^T = I, \quad (30)$$

with $D^* = \bar{A}X^{*T}$. Under this context, that is the reason we call $\bar{A}$ the virtual data.

There remains minor difference to PCA: $\bar{A}$ is not mean-removed. But, as stated in Section 3.4 we can restrict $X = \left[ \frac{1}{\sqrt{n}}1^T \right]$ . Then (29) is equivalent to

$$\min_{X} \| \bar{A}(I - \frac{1}{\sqrt{n}}1\frac{1}{\sqrt{n}}1^T)(I - \bar{X}^T\bar{X}) \|_F^2 = \min_{X} \| \bar{A} - \bar{A}\bar{X}^T\bar{X} \|_F^2, \ s.t. \ \bar{X}^T = I, \quad (31)$$

where $\bar{A} = \bar{A}(I - \frac{1}{\sqrt{n}}1\frac{1}{\sqrt{n}}1^T)$ is the mean-removed version of $\bar{A}$. The equivalence of (31) to PCA is apparent.

**Solution equivalence:** Since $\lambda_n I - L = V^T(\lambda_n I - \Lambda)V$, the magnitudes of eigenvalues of $\lambda_n I - L$ are reversed. Especially, the eigenvalue 0 associated with eigenvector 1 becomes largest $\lambda_n$. But $\lambda_n I - L$ remains positive semi-definite, and the eigenvectors remain the same. Note that the SVD of $\bar{A}$ is trivial $\bar{A} = I(\lambda_n I - \Lambda)^{\frac{1}{2}}V$. So the smallest eigenvectors of $L$ are the largest singular vectors of $\bar{A}$. And thus the solution of LE, $V_{1,r}$, is identical to those of (29) and (30) by the Eckart-Young Theorem. Finally, the SVD of $\bar{A}$ is $\bar{A} = I(\lambda_n I - \Lambda_{2,n})^{\frac{1}{2}}V_{2,n}$. So ignoring the constant $V_1$, the solution of LE is the same to that of PCA, $V_{2,r}$.

### 4.4 Rcut $\rightarrow$ K-means

The conversion from Rcut to kernel K-means is established by the work [11]. But the conversion does not go further to the dictionary representation form of K-means; and the difference of algorithmic results between them is not discussed.

**Theorem 6. (Rcut $\rightarrow$ K-means)** The objective of Rcut

$$\min_{X} \text{tr} \{XLL^TX\}, \ s.t. \ X \in \mathcal{H}, \quad (32)$$

can be converted to the form of K-means

$$\min_{D,X} \| \bar{A} - DX \|_F^2, \ s.t. \ X \in \mathcal{H}, \quad (33)$$

where $\bar{A}$ is defined as in Theorem 5. The solutions of $X$ in (32) and (33) are equal. However, the algorithmic results may be different. Rcut algorithm relaxes (32) to (11) and applies K-means algorithm on the leading $K$ normalized principal components of $\bar{A}$, while K-means algorithm works with the full principal components, which in fact faithfully follows (32).

**Objective conversion:** The conversion follows the same lines from (28) to (30), except that additional constraint $X \in \mathcal{H}$ is added. For completeness, we present them here. Let $L = V^T\Lambda V$, $\lambda_n$ the largest eigenvalue. Define virtual data $\bar{A} = (\lambda_n I - \Lambda)^kV$. Then (10) is equivalent to

$$\min_{X} \| \bar{A} - \bar{A}X^TX \|_F^2, \ s.t. \ X \in \mathcal{H}, \quad (34)$$

and

$$\min_{D,X} \| \bar{A} - DX \|_F^2, \ s.t. \ X \in \mathcal{H}, \quad (35)$$

with $D^* = \bar{A}X^{*T}$.

**Relation of algorithmic results:** The relation is similar to that in Section 4.2 K-means algorithm works with $\bar{A}$ which faithfully follows the original objective (10), while Rcut algorithm relaxes (10) to (11) and applies K-means algorithm on the leading $K$ normalized principal components of $\bar{A}$. But unlike Section 4.2 the ideal graph condition can be met well here. And when the data set is moderately large, the smallest eigenvalues of $L$ are about the same (zero) compared with the largest eigenvalue. So the largest singular values of $\bar{A}$ do not differ much; and the choice of applying K-means on the exact principal components dose not make much sense.

---

15In precise, it holds when $r$ is greater or equal than the dimension of null space of $L$ so that $1$ is a component of the solution.

16Though any value larger than $\lambda_n$ meets our purpose, we have chosen the minimal one.
5 Unification of PCA, K-means, LE, and Rcut

In Section 4, the equivalence of PCA and LE; K-means and Rcut have been established. Now, under an ideal graph condition (Definition 2), we will establish the equivalence of LE and Rcut. Then the equivalence of PCA and K-means is automatically established. And the four methods are unified together. The main results of the whole unification are summarized at the end of this section. Roughly speaking, the dimensionality reduction methods, PCA and LE, and the cluster analysis methods, K-means and Rcut, can be unified when the graph is ideal, in which case the indicator vectors become leading singular vectors. In this case, the solutions of these two kinds of methods are equivalent in the sense of a rotation transform.

Given a data set $A \in \mathbb{R}^{p \times n}$, assumed mean-removed, we have two choices: one is to work with original $A$; the other is to work with similarity matrix constructed from $A$. So the unification has two versions: an original-data version and a kernel version. Nevertheless, both of the conditions of the two versions are based on similarity matrices. That of the later one is usually built by the K-Nearest Neighbor (KNN) graph or the $\varepsilon$-neighborhood graph with Gaussian kernel [44]. That of the former one is defined by outer product of data matrix $W = A^T A$, where $A = [\sqrt{n} 1, A^T]^T$. This similarity matrix is in fact built by the linear kernel $\phi(A_i, A_j) = A_i^T A_j + \beta$. And as shown earlier, PCA and K-means are special cases of LE and Rcut respectively, which work with the above linear kernel matrix. Thus in fact, the original-data version is a linear kernel version; and the two versions can be integrated into one general kernel version, which works with similarity matrix that can be built by linear kernel, nonlinear kernel, or any other general nonnegative similarity measure. But to make things clear, we decide to distinguish the two versions.

We now go into details. First by the spectral graph theory [9,32,31], and as elaborated much in Section 3.3 under the ideal graph condition, the indicator vectors become leading eigenvectors of the Laplacian matrix, so the equivalence of LE and Rcut is manifest. And there is a counterpart in the prior work [2], i.e. normalized LE and Ncut.

Theorem 7. (Rcut & LE) Under the ideal graph condition, i.e. Definition 2 if the solution of LE (25) is $X^*$, and that of Rcut (32) is $H$, and $r = K$, then they are related by a rotation transform:

$$X^* = RH,$$

where $R \in \mathbb{R}^{K \times K}$, $R^T R = I$.

Then we have the original-data version of unification. It says that the solutions of PCA/LE and K-means/Rcut are equivalent in the sense of a rotation transform.

Theorem 8. (Unification: original-data version) Working with original data, by Theorem 7 if the solutions of PCA (13) and LE (14) are $X^* = V_{1,K-1}$ and $\tilde{X}^* = \begin{bmatrix} \sqrt{n} 1^T \\ V_{1,K-1} \end{bmatrix}$ respectively, $K \leq \text{rank}(A) + 1$; and by Theorem 4 if the normalized indicator solutions of K-means (27) and Rcut (22) are $H \in \mathbb{R}^{K \times n}$, then under the ideal graph condition, by Theorem 7 they are related by:

$$\begin{bmatrix} \frac{1}{\sqrt{n}} 1^T \\ V_{1,K-1} \end{bmatrix} = RH,$$

for some rotation matrix $R \in \mathbb{R}^{K \times K}$, $R^T R = I$.

Note that this theorem establishes the exact equivalence of PCA and K-means, together with a condition when it holds. It also suggests that, as an alternative to K-means, when $K \leq \text{rank}(A) + 1$, we can do clustering by Rcut algorithm: apply some clustering algorithm, e.g. K-means, on the normalized principal components $V_{1,K-1}$. But, as argued in Section 4.2, the ideal condition may hardly be met even approximately, so we can not expect this linear Rcut algorithm would produce better performance except may be efficiency.

Finally, we have the kernel version of unification. It also says that the solutions of LE/PCA and Rcut/K-means are equivalent in the sense of a rotation transform.

Theorem 9. (Unification: kernel version) Working with similarity matrix, by Theorem 5 if the solutions of LE (25) and PCA (27) are $X^* = \begin{bmatrix} \frac{1}{\sqrt{n}} 1^T \\ V_{2,K} \end{bmatrix}$ and $\tilde{X}^* = V_{2,K}$ respectively; and by Theorem 6 if the normalized indicator
solutions of $\text{Rcut}$ (32) and $\text{K-means}$ (33) are $H \in \mathbb{R}^{K \times n}$, then under the ideal graph condition, by Theorem 2 they are related by:

$$\begin{bmatrix} \frac{1}{\sqrt{n}}1^T \\ V_{2:K} \end{bmatrix} = RH,$$

for some rotation matrix $R \in \mathbb{R}^{K \times K}$, $R^TR = I$.

For convenience, we summarize the main results of the whole unification in the followings. They will pave the way for SSR.

5.1 Kernel version: similarity matrix as input

LE finds dimension-reduced code $X_i \in \mathbb{R}^r$ for data $A_i \in \mathbb{R}^p$, $r \ll p$:

$$\min_{X \in \mathbb{R}^{r \times n}} \frac{1}{2} \sum_{i,j} \|X_i - X_j\|^2 W_{ij} = \text{tr}\{XLXT\}, \ s.t. \ XXT = I,$$

$L = \text{diag}(W1) - W$ is a Laplacian matrix. Let $L = V^TAV$ with $\lambda_1 = 0$, $V_1 = \frac{1}{\sqrt{n}}1^T$ and $\lambda_n$ the largest eigenvalue, a solution is $V_{1:r}$. To remove the redundant constant $V_1$, a restriction $X1 = 0$ or $X = [\frac{1}{\sqrt{n}}1 \ X^T]^T$ is usually added. Next, define virtual data $\tilde{A} = (\lambda_n I - \Lambda)^{\frac{1}{2}}V$, then (39) is equivalent to a dictionary representation form

$$\min_{D \in \mathbb{R}^{n \times r}, X \in \mathbb{R}^{r \times n}} \|\tilde{A} - DX\|^2_F, \ s.t. \ XXT = I,$$

By the Eckart-Young Theorem, a solution is $X^* = V_{1:r}$, $D^* = \tilde{A}X^{\dagger T}$. Though conversion to the exact PCA is possible, (40) is the right form for SSR, so we stop. Under the ideal graph condition (Definition 2), by spectral graph theory, LE is equivalent to Rcut in the sense of a rotation transform:

$$\min_{D \in \mathbb{R}^{n \times r}, X \in \mathbb{R}^{r \times n}} \|\tilde{A} - DX\|^2_F, \ s.t. \ X \in \mathcal{H}.$$

If the solution is $H$, then there exists some rotation matrix $R \in \mathbb{R}^{r \times r}$, $R^TR = I$, such that $V_{1:r} = RH$. (41) can be further converted to a form of K-means with solution $H$ unchanged

$$\min_{D \in \mathbb{R}^{n \times r}, X \in \mathbb{R}^{r \times n}} \|\tilde{A} - DX\|^2_F, \ s.t. \ X \in \mathcal{H}.$$

$D^* = \tilde{A}X^{\dagger T}$. It is equivalent to an original form $\min_{D,F} \|\tilde{A} - DF\|^2_F$, s.t., $F \in \mathcal{F}$, with $D^* = \tilde{A}F^{\dagger T}(F^*F^{\dagger T})^{-1}$. When solving $D,F$ alternatively, the process is traditional K-means algorithm.

5.2 Original-data version: original data as input

Given mean-removed data $A \in \mathbb{R}^{p \times n}$, and $r \leq \text{rank}(A)$, PCA can be written in a dictionary representation form

$$\min_{D \in \mathbb{R}^{p \times r}, X \in \mathbb{R}^{r \times n}} \|A - DX\|^2_F, \ s.t. \ XXT = I.$$

Let $A = U\Sigma V$ be the compact SVD. A solution is $X^* = V_{1:r}$, $D^* = AX^{\dagger T} = U_{1:r}V_{1:r}$. $X^*$ are the normalized principal components; $D^*$ are the scaled loadings. Since $A1 = 0$, $V1 = 0$. We can restrict $X1 = 0$, then (43) is equivalent to a LE that uses linear kernel:

$$\min_{X \in \mathbb{R}^{r \times n}} \text{tr}\{X^T\}, \ s.t. \ X = \begin{bmatrix} \frac{1}{\sqrt{n}}1^T \\ V_{2:K} \end{bmatrix}, \ XXT = I.$$

$L = \text{diag}(W1) - W$ is a Laplacian matrix of the similarity matrix $W$ defined by $W = \tilde{A}^T\tilde{A}$. $\tilde{A} = \begin{bmatrix} \sqrt{n}1^T \\ U \end{bmatrix}$ is the augmented data; $\beta = -\min_{ij} (A^TA)_{ij}$ so that $W_{ij} \geq 0$. If $A = U\Sigma V$, then

$$\tilde{A} = U\Sigma V = \begin{bmatrix} 1 \\ U \end{bmatrix} \begin{bmatrix} \sqrt{n} \Sigma \\ \sqrt{n} V \end{bmatrix}.$$
So the SVD of $\tilde{A}$ is also an augmented version. And then
\[ L = \beta n I - \tilde{A}^T \tilde{A} = \tilde{V}^T (\beta n I - \tilde{\Sigma}^2) \tilde{V} = \begin{bmatrix} \frac{1}{\sqrt{n}} & V^T \end{bmatrix} \begin{bmatrix} 0 & \beta n I - \Sigma^2 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{n}} & V \end{bmatrix}. \] (46)

Since $L$ is positive semi-definite, $\beta n - \sigma^2 \geq 0$. One solution of (44) is $X^* = V_{1:r}$, the same to that of PCA. Next, under the ideal graph condition (Definition 2), the linear LE (44) is equivalent to a linear Rcut
\[ \min_{\tilde{X} \in \mathbb{R}^{(r+1) \times n}} tr\{ \tilde{X} L \tilde{X}^T \}, \text{ s.t. } \tilde{X} \in \mathcal{H}, \] (47)
in the sense of a rotation transform. Let the solution be $H$, then there exists some rotation matrix $R$ such that
\[ \begin{bmatrix} \frac{1}{\sqrt{n}} & 1 \end{bmatrix} = RH. \] (47) is equivalent to K-means, with solution $H$ unchanged:
\[ \min_{D \in \mathbb{R}^{p \times (r+1)}, \tilde{X} \in \mathbb{R}^{(r+1) \times n}} \| A - D \tilde{X} \|_F^2, \text{ s.t. } \tilde{X} \in \mathcal{H}. \] (48)

---

**Algorithm 1** NSCrt for solving sparse codes

**Input:**
- row-wise orthonormal eigenvectors $X \in \mathbb{R}^{r \times n}$, threshold $\lambda \in (0, 1)$

**Output:**
- sparse codes $H \in \mathbb{R}^{r \times n}$ and its truncated version $\bar{H}$, rotation matrix $R \in \mathbb{R}^{r \times r}$

1: Initialize $R$: $R \leftarrow I$
2: repeat
3: Rotation: $H \leftarrow R^T X$
4: Truncation: $\forall i, j, H_{ij} \leftarrow H_{ij}$ if $H_{ij} \geq \lambda$ and $\bar{H}_{ij} \leftarrow 0$ otherwise
5: Update $R$: compute SVD $X \bar{H}^T = U \Sigma V$, then $R \leftarrow UV$
6: until convergence

---

**Algorithm 2** SSR of kernel version (SSRk)

**Input:**
- similarity matrix $W \in \mathbb{R}^{n \times n}$, code dimension $r$, threshold $\lambda$

**Output:**
- sparse codes: $H \in \mathbb{R}^{r \times n}$, rotation matrix $R \in \mathbb{R}^{r \times r}$

1: Compute Laplacian matrix: $L \leftarrow diag(W1) - W$
2: Compute the $r$ smallest eigenvectors of $L$: $V \in \mathbb{R}^{r \times n}$
3: Solve sparse codes: $\{H, R\} \leftarrow$ NSCrt($V, \lambda$)

---

**Algorithm 3** SSR of original-data version (SSRo)

**Input:**
- mean-removed data set $A \in \mathbb{R}^{p \times n}$, code dimension $r$ ($r \leq rank(A) + 1$), threshold $\lambda$

**Output:**
- sparse codes: $H \in \mathbb{R}^{r \times n}$, rotation matrix $R \in \mathbb{R}^{r \times r}$

1: Compute rank $r - 1$ SVD of $A$: $A = U \Sigma V$
2: Solve sparse codes: $\{H, R\} \leftarrow$ NSCrt($[\frac{1}{\sqrt{n}}1, V^T]^T, \lambda$)

---

6 Spectral Sparse Representation

Under the ideal graph condition (Definition 2), PCA, K-means, LE, and Rcut are unified. When this condition is met well but may not exactly, it leads to spectral sparse representation.
PCA and LE can be roughly expressed as

\[
\min_{D, X} \| A - DX \|^2_F, \quad \text{s.t.} \quad XX^T = I,
\]

where \( A \) is either transformed from the original data matrix or factored from the Laplacian matrix. K-means and Rcut additionally impose indicator constraint on \( X \). For the above objective, the leading eigenvectors of \( A \) are a solution of \( X \). But any rotation of these eigenvectors constitutes a solution. When the graph is ideal, some rotation of the eigenvectors turns into indicator vectors. So PCA, K-means, LE, and Rcut are unified. When the graph is near ideal, the rotation of eigenvectors can only lead to noisy indicator vectors. When \( A \) is represented by these noisy indicator vectors, which we call sparse codes, that is spectral sparse representation.

In this case, according to matrix perturbation theory, the eigenvectors do not deviate much from those in the ideal case, so the main structure of indicator matrix is preserved but becomes somewhat noisy [14, 44]. We call the perturbed indicator matrix sparse codes, since each column of it corresponds to a data point and is usually dominated by a single entry. We give a measure of the sparsity as follows. For a vector \( x \in \mathbb{R}^n \),

\[
\text{sparsity}(x) = \|x\|_2 \|x\|_1.
\]

\( 1/\sqrt{n} \leq \text{sparsity}(x) \leq 1 \). It achieve the minimum when the magnitude of the entries are uniform. The indicator matrix is the most sparse in that there is exactly one nonzero entry in each column. In this case, the sparsity achieves maximum 1.

SSR is a new kind of representation method. It represents data in a dimensionally reduced way while achieving the best representation accuracy as PCA/LE. Meanwhile the codes are sparse and approximate to the optimal indicator matrix of K-means/Rcut, so the underlying cluster structure is revealed. However, in contrast to the hard clustering nature of K-means/Rcut, SSR is a soft and descriptive one. It describes the emergence of clusters as well as the overlapping status of them. Overall, SSR lies in the intermediate of the two kinds of methods and combines merits of both sides.

Before going into details, we give a qualitative interpretation of the cluster information embedded in the sparse codes \( \mathbf{H} \). Roughly speaking, the values in the code vector suggest the probabilities that the data point belongs to different clusters. Assume a point \( A_m \) lies on the overlapping region of two clusters \( C_1 \) and \( C_2 \). To minimize \( \frac{1}{2} \sum_{i,j} \| X_i - X_j \|^2 W_{ij} \), s.t. \( XX^T = I \), \( H_m \) should be close to both \( [1/\sqrt{n_1}, 0]^T \) and \( [0, 1/\sqrt{n_2}]^T \), where \( n_i \) is the size of \( C_i \). So there is a positive value in each row. But their magnitudes are less than \( 1/\sqrt{n_1} \) and \( 1/\sqrt{n_2} \) respectively. Then in order to meet the orthogonality constraint, small negative values must appear on the zero entries. When the overlap becomes heavy, the largest value in each row would be paired with a larger negative value in the opposite row. The two points corresponding to the largest values must be the most far apart, since the distance of their indicator vectors is the largest. In all, for \( H_r \), if there is only one positive entry, then the index of it indicates its cluster membership. If there are several positive entries, then it is an overlapping point of some corresponding clusters. Further, if the cluster sizes are similar, then the larger the value is, the closer the point is to the corresponding cluster.

As before, SSR has two versions: original-data version (SSRo) and kernel version (SSRk). We will introduce SSRk first, since it will be shown that this version is more practical.

6.1 Kernel Version (SSRk): Similarity Matrix as Input

For convenience, we repeat some important formulations. Let \( L = V^T \Lambda V \), where \( V_1 = \frac{\mathbf{1}}{\sqrt{n}} \), \( \lambda_1 = 0 \) and \( \lambda_n \) is the largest eigenvalue. Define virtual data \( \hat{A} = (\lambda_1 \mathbf{I} - \Lambda)^{1/2} V \). LE is equivalent to

\[
\min_{D \in \mathbb{R}^{n \times r}, X \in \mathbb{R}^{r \times n}} \| \hat{A} - DX \|^2_F, \quad \text{s.t.} \quad XX^T = I.
\]

One solution is \( X^* = V_{1:r} \). Then we have

**Theorem 10. (SSRk) When the graph is near ideal, there is a sparse representation**

\[
\hat{A} \approx \hat{D} H = \hat{A}(H^T H).
\]

**The approximation accuracy is optimal in the Frobenius-norm sense.** \( H \) is the sparse codes, i.e. noisy indicator matrix, which satisfies

\[
X^* = V_{1:r} = RH,
\]
for some rotation matrix $R$. $\hat{D}$ is a dictionary that defined as

$$
\hat{D} = \hat{A}H^T = \hat{A}V_{1,r}^T R = \left[ (\lambda_n I - \Lambda_{1,r})^\frac{1}{2} R \right] \approx \left[ \lambda_n^\frac{1}{2} R \right].
$$

(54)

The approximation holds, since $\Lambda_{1,r} \approx 0$. It implies atoms of $\hat{D}$ are near-orthogonal and have similar lengths. And $D^T \hat{D} = R^T (\lambda_n I - \Lambda_{1,r}) R \approx \lambda_n I$, so the mutual coherence of $\hat{D}$ is about zero. The Gram matrix of codes $H^T H \in \mathbb{R}^{n \times n}$ reflects the linear relationship of data, which has property

$$
1^T H^T H = 1^T V_{1,r}^T V_{1,r} = 1^T,
$$

(55)
i.e. the sum of each weight vector is one.

We now detail. If the ideal normalized indicator matrix is $H^*$, then $Y = RH^*$ are also the ideal eigenvectors of $L$, where $R$ is a rotation matrix so that $Y_1 = \frac{1}{\sqrt{n}} 1^T$. According to matrix perturbation theory, the solution $V_{1,r}$ of (51) is a perturbed version of $Y$, i.e. $X^* = V_{1,r} = RH^* + E$, where $E$ is some noise. Then we have the relationship (53), where $H = H^* + R^T E$ is the noisy indicator matrix.

It is easy to see that if $D^* = AX^{*T}$ and $X^*$ is a solution of (51), then $D = D^* R = \hat{A}X^{*T} R = \hat{A}H^T$ and $H$ is also a solution. So we obtain SSRk (52). The approximation accuracy is optimal in the Frobenius-norm sense, as indicated by the Eckart-Young Theorem.

This SSR has the following interpretations (it would be better to compare with those of PCA and K-means in Section 3.1 and Section 3.2 respectively):

1. $\tilde{A}_i \approx \hat{D}H_i$, i.e. $\tilde{A}_i$ is approximated by a linear combination of a few (usually one) atoms of dictionary $\hat{D}$.

2. $\hat{D}_k = \hat{A}H_{k}^T$ implies $\hat{D}_k$ comes mainly from the linear combination of samples which the cluster $C_k$ relates to. So $\hat{D}_k$ can be seen as a normalized cluster center. But compared with K-means, firstly, the weights are not uniform. They distribute according to the relevance; and they are signed. The relevance is proportional to the value; and the magnitude of the negative weight is close to zero. Secondly, the dictionary is incoherent, a desirable property in compressive sensing [6]. Since $\hat{D} = \hat{A}X^{*T} R = [(\lambda_n I - \Lambda_{1,r})^\frac{1}{2} R]^T 0^T]^T$, and the smallest eigenvalues of $L$ are about the same (zero) in contrast to the largest $\lambda_n$ when the data set is moderately large, $\hat{D}$ is near-orthogonal, as (54) shown. And the mutual coherence [6]

$$
\mu(\hat{D}) = \max_{i \neq j} |\hat{D}_i^T \hat{D}_j|/(\|\hat{D}_i\|_2 \cdot \|\hat{D}_j\|_2),
$$

(56)
is about zero.

3. $\tilde{A}_i \approx \hat{A}(H^T H_i)$ implies $\tilde{A}_i$ can be represented by a linear combination of relevance samples. Note that since $V_{1,r}$ is orthogonal and $V_1 = \frac{1}{\sqrt{n}} 1^T$, we get (55), i.e. the sum of weights, including negative values, is always 1. This coincides with K-means.

4. There is another representation form that is analogous to the un-normalized indicator representation form of K-means: $\tilde{A}_i \approx \hat{D}_U H_i$, where $\hat{D}_U = \hat{A}S_{H}^{-\frac{1}{2}}$, $H_U = S_H H$, and $S_H = diag(H1)$. $H_U$ is the analogy of un-normalized indicator matrix, since $1^T (H_U)^{-1}_i = 1$ as can be verified by (55). $\hat{D}_U$ are the proper cluster centers, since $\hat{D}_U = \hat{A}(H^T S_{H}^{-\frac{1}{2}})$ and $1^T H^T S_{H}^{-\frac{1}{2}} = 1^T$.

6.2 Original-data Version (SSRo): Original Data as Input

After turning PCA (43) to LE (44), we turn it back to the dictionary representation form:

$$
\min_{D \in \mathbb{R}^{(r+1) \times n}, X \in \mathbb{R}^{(r-1) \times n}} \| \hat{A} - D \hat{X} \|_F^2, \ s.t. \hat{X} = \left[ \frac{1}{\sqrt{n}} 1^T \right], \hat{X} \hat{X}^T = I,
$$

(57)

where for convenience we have replaced $r$ with $r - 1$. From the SVD of $\hat{A}$ (45), one solution is $\hat{X}^* = \tilde{V}_{1,r} = \begin{bmatrix} \frac{1}{\sqrt{n}} 1^T \\ V_{1,r-1} \end{bmatrix}$. Then we have

18
Theorem 11. (SSRo) When the graph is near ideal, there is a sparse representation
\[
A \approx \hat{D}H = A(H^TH).
\] (58)
The approximation accuracy is optimal in the Frobenius-norm sense. \(H \in \mathbb{R}^{r \times n} (r \leq \text{rank}(A) + 1)\) is the sparse codes, i.e. noisy indicator matrix, which satisfies
\[
\tilde{X}^* = \left[\frac{1}{\sqrt{n}} \mathbf{1}^T \right] V_{1:r-1} = RH,
\] (59)
for some rotation matrix \(R, \hat{D} \in \mathbb{R}^{p \times r}\) is a dictionary defined as
\[
\hat{D} = AH^T = A[\frac{1}{\sqrt{n}} \mathbf{1}, V_{1:r-1}]R = U_{r-1} \Sigma_{r-1} R_{2:r},
\] (60)
The Gram matrix of codes \(H^TH \in \mathbb{R}^{n \times n}\) reflects the linear relationship of data, which has property \(X^TH^TH = 1^T V_{1:r}^T V_{1:r} = 1^T\), i.e. the sum of each weight vector is one.

Following similar reasoning of SSRK, we have \(59\). First there is a sparse representation of the augmented data: \(\hat{A} \approx \hat{D}H = \hat{A}H^T.\) By the SVD of \(\hat{A}\) \(45\) and \(59\), \(\hat{D} = \hat{A}H^T = \left[\frac{1}{\sqrt{n}} \mathbf{1} \right] V_{1:r-1} \Sigma_{1:r-1} R_{2:r}\).

Next, we reduce \(57\) to a form that involves only the original data. Substituting \(D = \hat{A}X^T\) into \(57\), note that the first row of \(\hat{A}X^T\) is always \(\sqrt{n}1^T\), which is equal to the first row of \(\hat{A}\). So essentially we can remove this artificial component:
\[
\min_{D,X} \| A - DX \|_F^2, s.t. \hat{X} = \left[\frac{1}{\sqrt{n}} \mathbf{1}^T \right] X, \hat{X}X^T = I.
\] (61)
where the dimension of \(D\) is reduced accordingly. The solution of (sparse) codes remain unchanged. So we have a sparse representation of the original data \(58\). And it is easy to see that \(60\) holds.

The main difference of \(61\) to PCA \(45\) is that \(61\) augments \(X\) by a constant component \(\frac{1}{\sqrt{n}} \mathbf{1}\). But they are equivalent, since \(A1 = 0\) and \(\|A(I - \tilde{X}^* X^*)\|_F^2 = \|A(I - \frac{1}{\sqrt{n}} \mathbf{1} \frac{1}{\sqrt{n}} \mathbf{1}^T)(I - X^* X^*)\|_F^2 = \|A(I - X^* X^*)\|_F^2\). However, without the redundant \(\frac{1}{\sqrt{n}} \mathbf{1}\), sparse codes can not be recovered through rotating \(V_{1:r-1}\) only. So PCA do not explicitly reveal cluster structure.

The interpretations to the sparse representations of augmented data and original data are both similar to that of SSRK, except that the dictionaries are usually not near-orthogonal. This is because the singular values are not uniform. In practice they decay exponentially. The more fundamental reason underlying this phenomenon is that, as argued before, the ideal graph condition can hardly be met well in practice, which essentially requires that after translating along a new dimension different clusters become near orthogonal. So we recommend the kernel version. Nevertheless, this linear version still constitutes an indispensable part of the theory.

### 6.3 NSCrt: to Solve Sparse Codes

To make SSR practical, we have to find the rotation matrix \(R\) in \(53\) and \(59\). Here, we employ a modified version of an algorithm called SPCArt \(24\) to accomplish this task. SPCArt is a sparse PCA algorithm designed to solve sparse loadings. It finds a sparse loading matrix so that after some rotation it matches the loading matrix of original PCA. By replacing loadings with normalized principal components, we see that it meets our need. Considering our sparse codes is noisy indicator matrix, the dominant values of which are nonnegative, we additionally impose nonnegative constraint. This algorithm is called NSCrt (nonnegative sparse coding via rotation and truncation).

Given a row-wise orthonormal matrix \(X \in \mathbb{R}^{n \times n}\), the objective is
\[
\min_{R \in \mathbb{R}^{r \times r}, \tilde{H} \in \mathbb{R}^{r \times n}} \| X - RH \|_F^2 + \lambda^2 \| \tilde{H} \|_0, \ s.t. \ R^T R = I, \ \tilde{H}_{ij} \geq 0,
\] (62)
where \(R\) is a rotation matrix, \(\tilde{H}\) is sparse codes, \(\| \tilde{H} \|_0\) counts the number of nonzero entries of \(\tilde{H}\), \(\lambda\) is some small threshold in \((0, 1)\).
Originally, SPCArt solves the problem by alternatively optimizing $R$ and $\bar{H}$. When initializing $R = I$, the solution process results into operations of alternatively rotating and truncating PCA loadings. It will be found that NSCrt follows similarly. Fixing $R$, (62) becomes

$$\min_{\bar{H}} \|R^T X - \bar{H}\|_F^2 + \lambda^2 \|\bar{H}\|_0, \text{s.t.}, \bar{H}_{ij} \geq 0.$$  \hspace{1cm} (63)

Denote $H = R^T X$. $H$ is a rotation of $X$, so it is still orthonormal and spans the same subspace as $X$. It is not hard to see that $\hat{H}^*_{ij} = H_{ij}$ if $H_{ij} \geq \lambda$ and $\hat{H}^*_{ij} = 0$ otherwise, i.e. it is obtained by truncating small values of $H$ below $\lambda$. Fixing $\hat{H}$, (62) becomes a Procrustes problem

$$\min_{R} \|X \hat{H}^T - R\|_F^2, \text{s.t.} R^T R = I.$$ \hspace{1cm} (64)

Let $X \hat{H}^T = U \Sigma V$ be the SVD, then $R^* = UV$.

For our purpose, after convergence, $H = R^T X$ rather than $\hat{H}$ is what we need. On the one hand, $H$ is sparse in the sense of SSR. This is because truncating small values of it, it becomes sparse in the $\ell_0$ norm sense, i.e. $\hat{H}$, which indicates that $H$ is dominated by a few entries. On the other hand, according to (53) and (59), in SSR, $H = R^T X^*$ and $\hat{H} = R^T \tilde{X}^*$. So the $H$ defined here coincides with the forms of them. Nevertheless, $\hat{H}$ can be seen as a noise-reduced version of $H$. The NSCrt algorithm is presented in Algorithm 1 (SSRk and SSRo are in Algorithm 2 and Algorithm 3 respectively). The time complexity of it is $O(n r^2)$, which scales linearly with data size. It is efficient if $r$ is not too large.

According to the performance-guarantee analysis in SPCArt, we may choose $\lambda$ around $1/\sqrt{n}$. In our case, we found $\lambda = 0.6/\sqrt{n}$ consistently performs well.

**Algorithm 4 Clustering via Scut**

**Input:**

- sparse codes $H \in \mathbb{R}^{r \times n}$ output by SSR, each column for a sample

**Output:**

- cluster labels $c \in \mathbb{N}^{1 \times n}$

1: $c_i \leftarrow \arg\max_{k=1, \ldots, r} H_{ki}$, $i = 1, \ldots, n$

**6.4 Sparse Cut (Scut): an Application of SSR on Clustering**

We propose a clustering scheme called sparse cut (shown in Algorithm 4): after solving the sparse codes $H$ via NSCrt for either SSRk or SSRo, we can make an application on clustering. Since the sparse codes $H$ is a noisy version of the normalized indicator matrix, a natural clustering scheme is to check the maximal entry in each column of $H$ and assign the cluster label as the index of it:

$$c_i \leftarrow \arg\max_k H_{ki}, \ 1 \leq i \leq n.$$ \hspace{1cm} (65)

In SSRk, Scut has a more concrete interpretation. As shown in Theorem 10, atoms of $\hat{D}$ are near-orthogonal cluster centers with similar lengths. In this case, Scut can be interpreted as assigning the cluster label according to
the least included angle or distance between cluster center and virtual data. It can be proved that

$$\argmax_k \cos \theta(\hat{D}_k, \hat{A}_i)$$

$$= \argmax_k \frac{\hat{D}_k^T \hat{A}_i}{\|\hat{D}_k\|_2 \cdot \|\hat{A}_i\|_2}$$

$$\approx \argmax_k \hat{D}_k^T \hat{A}_i$$

$$\approx \argmax_k [\lambda_n^2 R_k^T, 0](\lambda_n I - \Lambda)^{1/2}V_i$$

$$= \argmax_k \lambda_n R_k^T (\lambda_n I - \Lambda_1, r)^{1/2}(V_{1, r})_i$$

$$\approx \argmax_k \lambda_n R_k^T R H_i$$

$$= \argmax_k H_{ki}.$$ (66)

And since \(\argmin_k \|\hat{A}_i - \hat{D}_k\|_2^2 = \|\hat{A}_i\|_2^2 + \|\hat{D}_k\|_2^2 - 2\hat{D}_k^T \hat{A}_i \approx \argmax_k \hat{D}_k^T \hat{A}_i\), it is also in the sense of the least distance between cluster center and virtual data.

7 Experiments

We conduct the following six parts of experiments. 1) We first test the ability of NSCrt in recovering rotation matrix, since both versions of SSR are practical and Scut is feasible only if NSCrt can find the correct rotation matrix, which uniquely determines the sparse codes of SSR. 2) We demonstrate how the sparse codes reveal cluster structure of data, for both SSRk and SSRo. 3) We make a comparison between the original-data version and kernel version, including how well the ideal graph condition is met and its influence on clustering. 4) We investigate the relation between the ideal graph condition, the sparsity of SSR, and the clustering accuracy of Scut. 5) We test the performance of kernel Scut, i.e. Scut of kernel version, on clustering, and compare it with some popular clustering algorithms. 6) We compare over-complete SRs with SSR on clustering performance.

| data set | description | #classes | size | #samples in each class |
|----------|-------------|----------|------|-----------------------|
| G1,G2,G3 | three artificial Gaussian data with more and more heavy overlaps, shown in Figure 2 | 3 | 2×150 | 50,50,50 |
| onion | an artificial data of unbalanced classes, shown in Figure 4 | 3 | 2×75 | 5,20,50 |
| iris | Fisher’s iris flower data set | 3 | 3×150 | 50,50,50 |
| wdbc | breast cancer Wisconsin (diagnostic) data set | 2 | 30×569 | 212,357 |
| Isolat | spoken (English) letter recognition data set, subset of the first set, excluding classes “c,d,e,g,k,n,s” | 19 | 617×1140 | each 60 |
| USPS3, USPS8, USPS10 | three subsets of the United States Postal Service (USPS) handwritten digit database. USPS3: “0”,“2”, USPS8: no “5”, “9”, since “3” and “5”, “4” and “9”, “7” and “9” heavily overlap, USPS10: “0”,“9” | 3,8,10 | 256×2930, 256×6091, 256×7291 | 1194,1005,731,658,656,665,645,542,644 |
| 4News | four groups of 20 Newsgroups documents: {2,9,10,15}. tf.idf feature | 4 | 26214×2372 | 389,398,397,394 |
| TDT2 | the largest 30 categories of Nist Topic Detection and Tracking corpus | 30 | 36771×9394 | 1844,1828,1222,811,…,52 |
| polb | a relation network of books about US Politics (“liberal”, “conservative”, or “neutral”), edges represent copurchasing of books by the same buyers | 3 | 105×105 | 43,49,13 |

The data sets we used, with ground-truths of class labels provided, are listed in Table 2. The data sets come from various domains and are of diverse nature. G1, G2, and G3 are with overlaps more and more heavy. Onion
and TDT2 have highly unbalanced classes. USPS10 and TDT2 are relatively large data sets. 4News and TDT2 are high dimensional data sets of $p > n$. Isolet and TDT2 have relatively large number of classes. Polib is a network data. These data sets are chosen for the reason that their underlying clusters are nearly in good accord with the class labels assigned by man. So we can access the performance of algorithms with these class labels.

The matching between the clustering result and the ground-truth is established by the Hungarian algorithm [26]. Clustering performance is measured by four criteria: accuracy (percentage of total correctly classified points), normalized mutual information (NMI), rand index (RI), and time cost.

Similarity matrices of the kernel version are built by 4NN graph (4News use 9NN) [43] and Gaussian kernel $\phi(A_i, A_j) = \exp\{-0.5\|A_i - A_j\|^2/v\}$ with $v$ [24]. For NSCrt, we set $\lambda = 0.6/\sqrt{n}$, 200 maximal iterations, and convergence condition $\|R(t) - R(t-1)\| F/\sqrt{r} \leq 0.01$. Usually, we observed it converges within a dozen iterations. The algorithms are implemented using MATLAB. They are run on a PC of 2.93GHz duo core, 2GB memory.

![Figure 1: Accuracy of NSCrt in recovering rotation matrix, and comparison with some other algorithms. The horizontal axis corresponds to increasing noise levels. (a)-(c) uniform cluster-sizes. (d) exponential cluster-sizes. ZP is absent in (c), since it is too slow to run.](source_url)

7.1 Accuracy of NSCrt in Recovering Rotation Matrix

SSR is practical and Scut is feasible only if we can find the right rotation matrix, so we test the accuracy of NSCrt in recovering the rotation matrix first. Randomly generated rotation matrices and sparse codes are used for the test. The performance is compared with some other algorithms: $\ell_0$ norm based SPCArt [24] (Section 6.3), ZP [50] (Section 2.3), $\ell_0$ norm based KSVD [1] (Section 2.2) and an $\ell_1$ norm based dictionary learning algorithm.

We first randomly generate a rotation matrix $R \in \mathbb{R}^{r \times r}$, design a normalized indicator matrix $\tilde{H}^* \in \mathbb{R}^{r \times 1024}$, and generate Gaussian noise $E$. Then we synthesize data $X$ via $X \leftarrow R(H^* + E)$, where $H^* + E$ simulates the sparse codes. We input $X$ into the algorithms and test their accuracies in recovering $R[\tilde{H}]$. The accuracy is measured by the mean of cosines between the estimated rotation $\hat{R}$ and $R$: $1/r \sum_{k=1}^{r} |\hat{R}^T_k R_k|$, where the matching of columns is established by the Hungarian algorithm [25]. Four cases of code-dimension $r$ are tested: 2, 16, 128, and 9. The first three cases correspond to uniform cluster-sizes: each row of $H^*$ has the same number of nonzeros $n_k = n/r$, $1 \leq k \leq r$, with entry value $1/\sqrt{\pi n_k}$. The last case corresponds to exponential cluster-sizes: the $k$th row, $k < 9$, has $n_k = 2^k$ nonzero entries with value $1/\sqrt{\pi n_k}$; the last row has $n_9 = n - \sum_{k=1}^{8} n_k$ nonzero entries with value $1/\sqrt{\pi 9}$. Note that the smallest cluster has only 2 samples, while the largest one has 514 samples. So the cluster sizes are highly unbalanced. Within each case, the algorithms are tested under increasing Gaussian noise levels $\sigma = a/\max_k (\sqrt{n_k})$.

The mean accuracies over 20 runs are shown in Figure I. We see that NSCrt outperforms the others, except mainly in the case $a = 1/8$, $r = 128$. The improvement is most significant when the cluster sizes are unbalanced, where the margin is more than 20%. Besides, NSCrt frequently obtains mean accuracies above 98%, which indicates the standard deviations are very small. So the performance of NSCrt is stable. Note that though NSCrt
intends to find local solutions, in moderate noise cases, it recovers the underlying solutions with high accuracies. The accuracy of ZP is not good when the number of cluster is somewhat large and the computational cost is higher than NSCrt.

![Figure 2: Gaussian data of different overlaps. Black dots are points misclassified by kernel Scut.](image)

![Figure 3: Row vectors of sparse codes of Gaussian data. They reveal the clusters and the overlaps of these clusters. Within each subfigure, top: eigenvectors $V \in \mathbb{R}^{3 \times 150}$ (each color plots a vector); middle: sparse codes $H = R^T V$ obtained by NSCrt; bottom: truncated sparse codes $\bar{H}$. Within each cluster $C_k$, columns of these vectors are rearranged in descending order according to the entry value of $H_k$.](image)

### 7.2 Cluster Structure Revealed by Sparse Codes

We demonstrate how the sparse codes reveal cluster structure from three perspectives: row perspective, column perspective, and Gram matrix perspective. The Gaussian data G1, G2, G3, and onion data are taken as examples. We show both SSRk and SSRo.

Row vectors of sparse codes reveal the clusters as well as the overlaps of these clusters. They are plotted in Figure 3 and Figure 5. In Figure 3, the cross sections of these vectors become larger and larger from (a) to (c), faithfully reflecting the overlapping status; samples in these cross sections will be misclassified by Scut; they are the black dots in Figure 2 and Figure 4.

Column vectors of sparse codes make the cluster structure more prominent, compared with the original data. For G2, they are plotted in Figure 6. In contrast to the codes of K-means, the sparse codes are soft; they describe
Figure 4: Onion data: artificial data of unbalanced classes.

Figure 5: Row vectors of sparse codes of onion data. The interpretation is similar to that in Figure 4.

Figure 6: Sparse code-vector of each sample of Gaussian data G2, i.e. column vectors of sparse codes $H \in \mathbb{R}^{3 \times 150}$. Left: intrinsic 2D manifold, i.e. $V_{2:3}$; middle: $H$; right: truncated sparse codes $\bar{H}$. For SSRk, the sparse codes make the cluster structure prominent compared with the original data in Figure 2(b).

7.3 Original-data Version v.s. Kernel Version

We compare how well the ideal graph condition is met for the two versions, and investigate its influence on clustering.

First, a clearer block-diagonal structure of the similarity matrix indicates the condition is met better. Similarity matrices on some representative data sets are shown in Figure 7. We see that so long as the data has clear clusters, the similarity matrix of kernel version will meet the ideal graph condition well. But that of the original-data version does not necessarily be so. In Figure 7(a)-(c), the condition is satisfied from well to badly by the original-data...
Figure 7: Gram matrices of Gaussian data G2. Yellow shows negative value; red implies larger magnitude. In each subfigure, from left to right: similarity matrix/Gram matrix $W$, $H^T H$, $\bar{H}^T \bar{H}$. Data is rearranged as Figure 2. The weights in each column of $H^T H$ distribute according to the relevance of the corresponding sample to all samples; and they are signed. $H^T H$ makes the main relation more clear.

(a) SSRk
(b) SSRo

Figure 8: Original-data version vs. kernel version: a comparison of the similarity matrices. In each subfigure, left: original-data version; right: kernel version. A clearer block-diagonal structure indicates the ideal graph condition is met better. $\rho$’s are shown in parentheses.

(a) G2 (-, 0.59)
(b) USPS3 (0.02, 0.61)
(c) iris (0.01, 0.63)
(d) onion (-, 0.39)
(e) wdbc (0.13, 0.68)
(f) USPS8 (0.01, 0.05)

version, as can be expected from the data distributions of these data sets (see Figure 2(b) and Figure 9).

Next, we investigate the condition quantitatively. To this end, we propose a $\rho$ value, measuring how well the ideal graph condition is met. The $\rho$ value of a similarity matrix $W \in \mathbb{R}^{n \times n}$ for $1 \leq K < n$ clusters is defined as

$$\rho = \frac{\lambda_{K+1} - \lambda_{K}}{\lambda_{K+1}},$$

(67)

where $\lambda_i$ is the $i$th smallest eigenvalue of the Laplacian matrix of $W$. If $\lambda_{K+1} = 0$, $\rho$ is defined to be 0. We have the following theorem:

**Theorem 12.** $0 \leq \rho \leq 1$, and $\rho = 1$ if and only if the ideal graph condition is met.

**Proof.** When the ideal graph condition is met, according to the properties of Laplacian matrix in Section 3.3, $\lambda_K = 0$, and by assumption, $\lambda_{K+1} \neq 0$, so $\rho = 1$. Conversely, if $\rho = 1$, then $\lambda_{K+1} \neq 0$ and $\lambda_1 = \cdots = \lambda_K = 0$, which means the graph has $K$ connected components. So the ideal graph condition is met.

When the graph is near ideal, according to matrix perturbation theory [14, 44], $\lambda_K$ is perturbed from 0 but still close to it, so $\rho$ is close to 1. In other words, the better the condition is met, the higher $\rho$ is.

A comparison of the $\rho$ values between the original-data version and kernel version over all data sets are shown in Table 3. It is clear that generally the kernel version meets the condition better than the original-data version.

Finally, we compare the performance of some clustering methods of the two versions. The results are shown in Table 4. The results on TDT2 and polb are absent, since the original-data version fails to run on them. Concerning accuracy, there is no significant difference between the methods within original-data version. The kernel version

22The $\rho$ values of the original-data version on the artificial data sets are unable to compute, since the ranks of the Laplacian matrices, which are limited by the dimensions of the data, are smaller than the numbers of classes.
Table 3: Original-data version v.s. kernel version: $\rho$ values ($0 \leq \rho \leq 1$) of the similarity matrices. A higher value indicates the ideal graph condition is met better.

|                | G1 | G2 | G3 | onion | iris | wdbc | Isolet | USPS3 | USPS8 | USPS10 | 4News | TDT2 | polb |
|----------------|----|----|----|-------|------|------|--------|-------|-------|--------|-------|------|------|
| $\rho$ (%)     | 100.0 | 59.4 | 58.4 | 39.4 | 63.2 | 67.7 | 16.8 | 60.5 | 5.1 | 6.8 | 1.9 | 4.7 | 45.0 |

generally performs better, since it meets the ideal graph condition better. The contrasts are most apparent on onion, iris, and wdbc, as implied by Figure 8. But on G2 and G3, the original-data version seems to meet the condition well, as Figure 8(a) shows, so the contrasts are reversed. Concerning time cost, K-PC and Rcuto are more efficient than K-means; the cost of kernel version on USPS10 are larger than that of original-data version, which is mainly contributed by the construction of similarity matrix.

Figure 10: The relation between $\rho$, sparsity of SSR, and clustering accuracy of Scut (kernel version) on a set of random Gaussian data with more and more heavy overlaps, just like G1, G2, and G3. The curve and bar show the mean and standard derivation over 50 trials respectively. A clear proportional relation appears.

7.4 The Relation between $\rho$, Sparsity of SSR, and Clustering Accuracy

The sparsity of SSR is the mean sparsity of codes (defined in (50)) of all samples. In principal, the three quantities are proportionally related: $\rho$ is a measure of how well the ideal graph condition is met; and the condition itself reflects how well the data is separable, which is directly related to clustering accuracy. When the condition is met better, the noise in the indicator vectors, i.e. sparse codes, is less, which means the codes are sparser. We validate the relation by a set of Gaussian data with more and more heavy overlaps (the centers of the Gaussian are pulled closer and closer), just like G1, G2, and G3. The result is shown in Figure 10. A clear proportional relation appears.

7.5 Clustering via Kernel Scut

Since the above section has shown the kernel version is superior to the original-data version on clustering, now we focus on kernel Scut. We compare it with some popular clustering algorithms using four criteria.
Table 4: Original-data version v.s. kernel version: performance of clustering methods. K-PC: K-means applied on principal components \(\Sigma_{1,K-1}^1\). Rcuto: K-means applied on \(V_1:K-1\). Rcuto: Scut of SSRo. Rcuto and Scut refer to kernel versions by default. For random algorithms, mean / standard deviation of accuracy over 20 trials are shown. The mean of time cost for the two largest data sets USPS10 and 4News are shown at the end. The time cost of K-PC, Rcuto, and Scuto is eigen-computation + K-means or NScrt; that of Rcut and Scut is similarity-matrix construction + eigen-computation + K-means or NScrt.

|                | original-data version | kernel version |
|----------------|-----------------------|----------------|
|                | kmeans | K-PC | Rcuto | Scuto | kmeans | K-PC | Rcuto | Scuto |
| G1             | 91.0 / 18.5 | 93.5 / 15.9 | 97.6 / 10.6 | 100.0     | 91.4 / 17.6 | 100.0 |
| G2             | 95.3 / 0.0  | 95.3 / 0.0  | 96.0 / 0.0  | 95.3      | 90.8 / 8.3  | 92.7  |
| G3             | 82.7 / 0.0  | 82.7 / 0.0  | 82.7 / 0.0  | 83.3      | 82.0 / 0.0  | 82.0  |
| Onion          | 61.7 / 6.9  | 62.5 / 7.2  | 62.6 / 5.3  | 61.3      | 90.5 / 6.6  | 90.7  |
| USPS3          | 81.5 / 13.9 | 80.8 / 13.9 | 77.3 / 7.0  | 80.0      | 87.4 / 9.1  | 95.3  |
| USPS8          | 65.8 / 4.0  | 65.8 / 4.0  | 65.8 / 4.0  | 65.8      | 66.6 / 8.8  | 66.4  |
| USPS10         | 100.0       | 100.0       | 100.0       | 100.0     | 100.0       | 100.0 |
| Isolet         | 82.7 / 0.0  | 82.7 / 0.0  | 82.7 / 0.0  | 82.7      | 82.7 / 0.0  | 82.7  |
| Onion          | 61.7 / 6.9  | 62.5 / 7.2  | 62.6 / 5.3  | 61.3      | 90.5 / 6.6  | 90.7  |
| USPS3          | 81.5 / 13.9 | 80.8 / 13.9 | 77.3 / 7.0  | 80.0      | 87.4 / 9.1  | 95.3  |
| USPS8          | 65.8 / 4.0  | 65.8 / 4.0  | 65.8 / 4.0  | 65.8      | 66.6 / 8.8  | 66.4  |
| USPS10         | 100.0       | 100.0       | 100.0       | 100.0     | 100.0       | 100.0 |
| 4News          | 82.7 / 0.0  | 82.7 / 0.0  | 82.7 / 0.0  | 82.7      | 82.7 / 0.0  | 82.7  |
| mean           | 80.9 / 5.8  | 79.5 / 5.2  | 78.8 / 4.1  | 79.6      | 84.2 / 7.9  | 89.4  |

The results of accuracy, NIM, and RI are shown in Table 5. According to the mean scores of the three criteria, overall, Scut performs best. Comparing with the others, the performance of Scut is stable, either in the sense of no random initialization or in the sense of performance across data sets of different nature. Although the scores of Rcuto are very good, they are the best ones taken over 20 trials; the mean scores are much worse, and the variances are large, as shown in Table 4. Graclus does best on quite a few data sets, however occasionally it performs poorly on some well-separable data sets. ZP is the most close method to Scut, clearly it does worse than Scut.

The time cost on the three largest data sets, USPS10, 4News, and TDT2, are shown in Table 6. Scut is efficient. GMM and Kmeans are the slowest. Graclus which is designed to improve the computational cost of traditional spectral clustering methods, e.g. Ncut, Rcuto, and NJW, avoids the computation of eigenvectors. It achieves the best efficiency. On the data sets we test, which are of sizes up to 10,000 scale, the total time cost of those methods working with similarity matrix is dominated by the construction of similarity matrix. So, the cost of Scut is still close to Graclus. Table 6 highlights the cost of the main ingredients of methods, i.e. post-processing of eigenvectors. On the largest data set TDT2, the timing is most accurate. In this set, the cost of Scut is significantly lower than the others.

We conclude that Scut is stable and it reaches the state-of-the-art performance.

7.6 Over-complete SRs v.s. SSR on clustering

SSR is inherently related to cluster analysis, while existing over-complete SRs may not be so. Although KSVD, one representative method of over-complete SR, is generalized from K-means [1], there is still no an explicit relation to cluster analysis. It is of interest to compare KSVD with SSR on clustering performance. On the other hand, sparse subspace clustering (SSC) [18] is the main sparse-representation-based clustering method in existing SRs. Although SSC deals with clusters that lie in independent low-dimensional subspaces, we let it participate in the comparison.

First, for KSVD, we learn a dictionary and codes with the same sizes as SSRo, and apply the same clustering strategy as Scut, i.e. checking the maximal entry of each code-vector. The maximal \(\ell_0\) norm is set to be \([\lfloor r/3\rfloor]\), where \(r\) is the dimension of codes (the number of clusters). For SSC, independent affine subspaces is assumed, since the results are better. The results are shown in Table 7. The result of KSVD on TDT2 is absent, because KSVD is too slow to run. KSVD depends on random initialization, it is repeated 20 times. Since there is no proper

---

23 Codes of Graclus, Ncut, and ZP are downloaded from the Internet. For 4News and TDT2 since \(p > n\), GMM can not run. Kmeans is implemented by MATLAB and it fails to run on TDT2.
Table 5: Clustering results of kernel Scut and other algorithms. Graclus: [12]; Ncut: [42]; ZP: [50]; GMM-V: Gaussian mixture model based clustering, applied on $V_{1,r}$ of Laplacian matrix; Kmeans, GMM: K-means and GMM on original data; NJW: [33]. Random algorithms (from GMM-V to Rcut) are tried 20 times; the score when the objective function obtains the best value over 20 trials is shown. The final row is the average score taken over all data sets.

(a) accuracy

|          | Graclus | Ncut | ZP | GMM-V | GMM | Kmeans | NJW | Rcut | Scut |
|----------|---------|------|----|-------|-----|--------|-----|------|------|
| G1       | 100.0   | 100.0| 100.0| 100.0| 100.0| 100.0  | 100.0 | 100.0| 100.0 |
| G2       | 76.4    | 78.5 | 75.5 | 78.5 | 83.9 | 80.9   | 75.5 | 75.5 | 75.5 |
| onion    | 94.6    | 88.4 | 88.4 | 77.9 | 74.4 | 64.6   | 68.4 | 71.4 | 68.4 |
| iris     | 75.0    | 75.0 | 75.6 | 72.2 | 68.4 | 75.8   | 77.8 | 77.8 | 84.6 |
| wdbc     | 49.4    | 35.2 | 49.0 | 42.5 | 37.1 | 46.7   | 39.2 | 49.9 | 49.4 |
| Islet1   | 79.3    | 88.0 | 82.0 | 93.6 | 62.7 | 84.8   | 87.8 | 87.8 | 83.9 |
| USPS1    | 97.2    | 95.8 | 95.8 | 95.7 | 84.6 | 80.0   | 95.8 | 95.4 | 95.8 |
| USPS10   | 85.8    | 86.9 | 86.8 | 83.7 | 58.7 | 90.5   | 85.6 | 87.2 | 86.2 |
| TDT2     | 81.0    | 80.1 | 77.0 | 79.0 | 41.0 | 64.0   | 78.6 | 78.6 | 78.4 |
| mailbooks | 85.3   | 85.2 | 85.2 | 85.7 | 84.8 | 85.1   | 85.5 | 85.5 | 82.4 |
| mean     | 73.8    | 71.2 | 75.8 | 70.9 | 63.1 | 70.8   | 75.3 | 75.7 | 77.4 |

(b) NMI

|          | Graclus | Ncut | ZP | GMM-V | GMM | Kmeans | NJW | Rcut | Scut |
|----------|---------|------|----|-------|-----|--------|-----|------|------|
| G1       | 100.0   | 100.0| 100.0| 100.0| 100.0| 100.0  | 100.0| 100.0| 100.0 |
| G2       | 76.4    | 78.5 | 75.5 | 78.5 | 83.9 | 80.9   | 75.5 | 75.5 | 75.5 |
| onion    | 94.6    | 88.4 | 88.4 | 77.9 | 74.4 | 64.6   | 68.4 | 71.4 | 68.4 |
| iris     | 75.0    | 75.0 | 75.6 | 72.2 | 68.4 | 75.8   | 77.8 | 77.8 | 84.6 |
| wdbc     | 49.4    | 35.2 | 49.0 | 42.5 | 37.1 | 46.7   | 39.2 | 49.9 | 49.4 |
| Islet1   | 79.3    | 88.0 | 82.0 | 93.6 | 62.7 | 84.8   | 87.8 | 87.8 | 83.9 |
| USPS1    | 97.2    | 95.8 | 95.8 | 95.7 | 84.6 | 80.0   | 95.8 | 95.4 | 95.8 |
| USPS10   | 85.8    | 86.9 | 86.8 | 83.7 | 58.7 | 90.5   | 85.6 | 87.2 | 86.2 |
| TDT2     | 81.0    | 80.1 | 77.0 | 79.0 | 41.0 | 64.0   | 78.6 | 78.6 | 78.4 |
| mailbooks | 85.3   | 85.2 | 85.2 | 85.7 | 84.8 | 85.1   | 85.5 | 85.5 | 82.4 |
| mean     | 73.8    | 71.2 | 75.8 | 70.9 | 63.1 | 70.8   | 75.3 | 75.7 | 77.4 |

(c) RI

|          | Graclus | Ncut | ZP | GMM-V | GMM | Kmeans | NJW | Rcut | Scut |
|----------|---------|------|----|-------|-----|--------|-----|------|------|
| G1       | 100.0   | 100.0| 100.0| 100.0| 100.0| 100.0  | 100.0| 100.0| 100.0 |
| G2       | 90.8    | 91.6 | 90.8 | 91.6 | 94.8 | 94.0   | 90.8 | 90.8 | 90.8 |
| onion    | 81.7    | 79.0 | 79.0 | 78.6 | 56.4 | 79.7   | 79.0 | 79.2 | 79.6 |
| iris     | 66.7    | 85.3 | 85.3 | 63.8 | 88.7 | 64.1   | 85.3 | 86.5 | 85.3 |
| wdbc     | 79.5    | 63.3 | 79.2 | 72.4 | 74.5 | 75.0   | 70.3 | 80.3 | 79.5 |
| Islet1   | 96.7    | 97.5 | 95.6 | 96.2 | 91.1 | 97.3   | 97.4 | 97.2 | 97.5 |
| USPS1    | 99.4    | 75.9 | 99.0 | 88.9 | 95.0 | 90.8   | 99.0 | 98.9 | 99.0 |
| USPS10   | 94.6    | 93.5 | 92.9 | 94.6 | 78.8 | 91.7   | 93.3 | 93.2 | 93.2 |
| TDT2     | 95.7    | 96.2 | 95.8 | 83.6 | -    | 92.5   | 96.2 | 95.9 | 96.1 |
| mailbooks | 85.6   | 85.1 | 85.0 | 81.4 | -    | -      | 83.1 | 86.0 | 83.0 |
| mean     | 82.4    | 87.0 | 90.5 | 87.2 | 84.2 | 87.7   | 90.2 | 91.5 | 91.7 |
Table 6: Time cost on the three largest data sets, USPS10 (256 × 7291, 10 classes), 4News (26214 × 2372, 4 classes), and TDT2 (36771 × 9394, 30 classes). For random algorithms, the average cost is shown. The total time cost includes the construction of similarity matrix, computation of eigenvectors, and post-processing of eigenvectors.

(a) total time cost

|        | Graclus | Scut  | ZP    | GMM-V | GMM  | Kmeans | NJW  | Rcut | Scut |
|--------|---------|-------|-------|-------|------|--------|------|------|------|
| USPS10 | 7.5     | 8.2   | 12.0  | 11.0  | 101.0| 8.7    | 7.9  | 8.0  |      |
| 4News  | 1.1     | 1.1   | 1.5   | 1.5   | -    | 584.7  | 1.1  | 1.4  | 1.5  |
| TDT2   | 17.7    | 19.7  | 187.8 | 22.8  | 22.7 | 19.3   |      |      |      |

(b) time cost excluding the construction of similarity matrix

|        | Graclus | Scut  | ZP    | GMM-V | GMM  | Kmeans | NJW  | Rcut | Scut |
|--------|---------|-------|-------|-------|------|--------|------|------|------|
| USPS10 | 0.1     | 0.8   | 4.6   | 3.6   | 101.0| 8.7    | 0.4  | 0.5  | 0.5  |
| 4News  | <0.1    | 0.1   | 0.4   | 0.4   | -    | 584.7  | 0.1  | 0.4  | 0.4  |
| TDT2   | 0.3     | 2.3   | 10.0  | 29.7  | -    | -      | 5.3  | 3.3  | 1.9  |

(c) time cost excluding the construction of similarity matrix and computation of eigenvectors, i.e., time cost of post-processing, problem size #classes × #samples

|        | Graclus | Scut  | ZP    | GMM-V | GMM  | Kmeans | NJW  | Rcut | Scut |
|--------|---------|-------|-------|-------|------|--------|------|------|------|
| USPS10 | 4.20    | 3.13  | 0.08  | 0.10  | 0.12 |        |      |      |      |
| 4News  | 0.05    | 0.06  | 0.01  | 0.01  | 0.05 |        |      |      |      |
| TDT2   | 168.80  | 28.10 | 2.66  | 3.69  | 0.34 |        |      |      |      |

Table 7: KSVD and SSC v.s. SSRo on clustering. KSVD has the same size of dictionary and codes as SSR, and non-maximum suppression is applied to do clustering. The mean accuracy of KSVD over 20 trials is shown. SSC assumes independent affine subspaces.

|        | G1    | G2    | G3    | onion | iris | wdbc | Isolet | USPS3 | USPS8 | USPS10 | 4News |
|--------|-------|-------|-------|-------|------|------|--------|-------|-------|--------|-------|
| KSVD   | 91.3  | 71.8  | 51.3  | 52.1  | 48.7 | 53.8 | 54.4   | 67.5  | 56.1  | 48.6   | 74.3  |
| SSC    | 100.0 | 66.7  | 53.3  | 60.0  | 78.0 | 87.3 | 78.8   | 59.0  |       |        |
| Scut   | 100.0 | 95.3  | 83.3  | 61.3  | 78.0 | 87.5 | 85.0   | 72.6  | 76.3  | 64.9   | 94.9  |

criterion to pick the optimal choice, the mean accuracy is shown. Many results of SSC are absent, since SSC runs out of memory. Also, SSC is slow, e.g. on Isolet it takes more than 10 minutes while Scut takes less than 1 second totally. Generally, Scut outperforms KSVD and SSC on these data sets.

Second, a traditional over-complete KSVD is learnt and clustering is performed by applying K-means on the codes. The number of atoms is set to be $m = 2p$, where $p$ is the dimension of codes; the maximal $\ell_0$ norm is set to be $\min(8, \lceil m/3 \rceil)$. The results comparing with kernel Scut are shown in Table 8. The results on 4News and TDT2 are absent, since KSVD fails to run on them. KSVD still performs worse than Scut.

Finally, to investigate the reason of the inferior performance of KSVD against SSR, we want to see how well the cluster structure of data is enhanced by the sparse codes. To this end, we compare the ratio of within-class distance of sparse codes with that of original data. The ratio of within-class distance is commonly used in the objective of linear discriminative analysis. For data $H$, it is defined as $SW/SF = \sum_{k=1}^{K} \sum_{H_i \in C_k} ||H_i - D_k||_2^2 / \sum_{j=1}^{n} ||H_j - d||_2^2$, where $D_k$ is the mean of class $C_k$, and $d$ is the mean of the whole set. This ratio is between 0 and 1. A smaller value implies the data is better separable. Corresponding to Table 8, the ratios of original data, sparse codes of KSVD, and sparse codes of SSRk are shown in Figure 11. We see that the ratios of SSR are generally smaller than those of original data, which means SSR enhances the cluster structure of data. But, those of KSVD are significantly larger, so the codes of KSVD are dispersed, which may not good for clustering.

8 Discussions

We will make some technical discussions about the relation of our work to [13], over-complete SRs, and subspace clustering. Besides, the relation between kernel PCA and SSR is discussed. We conclude with some future work.
Table 8: KSVD+Kmeans v.s. kernel Scut. The optimal accuracy with respect to objective function of K-means over 20 trials is shown.

|                | G1  | G2  | G3  | onion | iris | wdbc | Isolet | USPS3 | USPS8 | USPS10 |
|----------------|-----|-----|-----|-------|------|------|--------|-------|-------|--------|
| KSVD accuracy  | 91.3| 93.3| 74.7| 58.7  | 82.0 | 67.0 | 23.9   | 43.1  | 19.7  | 17.5   |
| Scut accuracy  | 100.0| 92.7| 82.0| 90.7  | 95.3 | 88.4 | 82.0   | 99.2  | 91.0  | 66.4   |

Figure 11: Ratios of within-class distance of original data, sparse codes of KSVD, and sparse codes of SSRk. U3 is shorthand for USPS3.

8.1 Relation between [13] and Our Unified Framework

The pioneering work [13] had discovered that PCA is a relaxation of K-means, whose reasoning may be described as: starting from (6) with notation $X$ replaced by $H$, and defining $X \sim \left[\frac{1}{\sqrt{m}}, \tilde{X}^T_{1:K-1}\right]^T \sim RH$, it gets to (15); then the constraint between $X$ and $H$ is relaxed; finally it arrives at the form similar to (31) which is PCA. By the relaxation relation, it was proposed that clustering may be done by applying K-means on the normalized principal components $V_{1:K-1}$, which is in line with Rcut of the original-data version. The reasoning does not depend on the conversion to Rcut/LE. In this paper, we establish the link between PCA and K-means together with LE and Rcut. The conversion to Rcut has introduced the spectral graph theory which facilitates the analysis. Especially, on the one hand, it gives an ideal graph condition to establish the exact equivalence of PCA and K-means. On the other hand, it tells that in practice the condition is hardly met, so the relation (37) may not accurate, and the linear Rcut may not promise better performance.

8.2 Relation between Over-complete SRs and SSRo

We focus on two classical over-complete SRs: [34] and [11], and compare them with SSRo. We will show that the common point of them is to find a sparse basis so that the basis covers the row space of data matrix as much as possible. The main differences are: 1) SSRo is under-complete (so is the sparse basis of it), while traditional SRs are over-complete (so are the sparse basis of them). 2) SSR is derived from spectral clustering, so it is inherently related to cluster analysis, and its major application is on clustering; while over-complete SRs are designed as data representation models, and one of their main applications is on classification. 3) The sparsity of SSR emerges naturally according to the cluster structure of data, while the sparsity of over-complete SRs are imposed by the designers. Nevertheless, due to SSR is under-complete, the dimension of codes, i.e. the number of clusters it can handle, is limited by the dimension of data, while over-complete SRs can cross this limitation. From this perspective, as sparse representation models, they complement each other.

The dictionary and sparse codes of usual over-complete SRs are solved alternatively, where the sparse coding step may employ some sophisticated algorithms e.g. OMP. The sparse codes of SSR are solved via rotating the normalized principal components so that they become sparse. This SSR is under-complete. The sparse codes of SSR are in fact noisy indicator vectors, since the normalized principal components are the leading eigenvectors of a Laplacian matrix. So SSR is related to spectral clustering. However, the usual over-complete SRs do not possess this close tie. In SSR, the sparse codes can be directly used to do clustering (since they are noisy indicator vectors): trivally checking the maximal entry. But this non-maximum suppression strategy may not work for over-complete SRs.
We now detail. \cite{34} had proposed an $\ell_1$-norm based over-complete SR
\begin{equation}
\min_{D \in \mathbb{R}^{p \times r}, H \in \mathbb{R}^{r \times n}} \|A - DH\|_F^2 + \lambda \|H_i\|_1, \quad 1 \leq i \leq n,
\end{equation}
while \cite{1} had proposed an $\ell_0$-norm based over-complete SR
\begin{equation}
\min_{D \in \mathbb{R}^{p \times r}, H \in \mathbb{R}^{r \times n}} \|A - DH\|_F^2, \quad \text{s.t.} \quad \|H_i\|_0 \leq L, \quad 1 \leq i \leq n.
\end{equation}
In both case, $p \ll r$, i.e. over-complete, and $r < n$. \cite{69} is called KSVD, which is generalized from K-means. Local solutions of both objectives can be solved by alternatively optimizing $D$ and $H$, much like K-means. The simplest update of $D$ is $D = AH^\dagger = AH^T(HH^T)^{-1}$. The sparse coding step of (68) can be solved by e.g. SLEP \cite{28}, while that of KSVD is solved by OMP \cite{35}. Note these SRs are designed as data representation models and the sparsities are imposed.

SSR does not have an explicit objective; and the sparsity emerges implicitly. If we have to write a corresponding objective, it may be expressed as
\begin{equation}
\min_{D, H} \|A - DH\|_F^2, \quad \text{s.t.} \quad HH^T = I, \quad H \text{ sparse}.
\end{equation}
When substituting $D = AH^\dagger$ into the objectives, all of them reduce to
\begin{equation}
\min_H \|A - AH^T(HH^T)^{-1}H\|_F^2, \quad \text{s.t.} \quad H \text{ sparse},
\end{equation}
for some sparse constraint on $H$. Since $H^T(HH^T)^{-1}H$ is a projection matrix built by the row-wise basis $H$, the above objective can be interpreted as: to find a sparse basis so that it covers the row space of data as much as possible. This is the common point of the three SRs.

But, there are striking differences. First, for the first two SRs, the number of basis vectors is larger than that of row vectors of $A$, so they are over-complete, and zero reconstruction error may be obtained; for SSR, since $r \leq \text{rank}(A) + 1 \leq p + 1$, usually it is under-complete. Second, the solution schemes are distinct. Over-complete SRs solve the problems via alternatively optimizing $D$ and $H$, while SSR first solves the normalized principal components of $A$, and then employs NSCrt to solve $H$ via rotating these principal components. In this way, the reconstruction error of SSR is minimal within rank-$r$ constraint.\footnote{Note that, NSCrt shares similar objective and optimization strategy with over-complete SRs. However, the target of NSCrt is orthonormal eigenvectors, and the dictionary is a rotation matrix, which is complete. By virtue of the special properties of them, NSCrt exhibits good performance, parts of which have been analyzed by \cite{24}.}

The normalized principal components are one-one corresponding to the eigenvectors of a Laplacian matrix, which is built from the Gram matrix of data. Since the leading eigenvectors of the Laplacian matrix are rotated noisy indicator vectors, the sparse codes of SSR are in fact these noisy indicator vectors. So SSR is related to spectral clustering. Besides, when the clusters of data overlap less, the codes become sparser, and vice versa. Thus the sparsity is implicitly determined by the structure of data. However, the number of normalized principal components is limited by the dimension of data, so is the eigenvectors of the Laplacian matrix. The over-completeness prevents over-complete SRs from the reach of spectral graph theory: an over-complete basis goes beyond the whole set of principal components.

Nevertheless, the dimension of codes of SSR, i.e. the number of clusters it can handle, is limited by the dimension of data, while over-complete SRs can cross this limitation. From this perspective, as sparse representation models, they complement each other.

### 8.3 Relation between Subspace Clustering and SSRs

Subspace clustering refers to a series of clustering work dealing with data that lie in a union of independent and low-dimensional linear/affine subspaces. It is pioneered by sparse subspace clustering (SSC) \cite{18}. Later an important variant LRR (low-rank representation) \cite{27} was proposed.

We will show that under the ideal graph condition and a low-dimensional assumption, SSC, LRR, and SSR are closely related. All of them obtain a sparse/low-rank code matrix to represent the data matrix with respect to a dictionary composed of the data matrix itself. Then a similarity matrix is built using the code matrix, and spectral
clustering is employed to finish clustering. Since under the condition the code matrix is “block-diagonal”, it makes clustering become easy. The code matrix of SSC is sparse, that of LRR is low-rank, while that of SSR has lowest rank. The representations of SSC and LRR are exact, while that of SSR is approximate.

The ideal graph condition for SSRo requires that the clusters are orthogonal as the end of Section 4.2 mentioned. This is a special case of the independent-subspaces assumption made by SSC and LRR, which requires that the clusters lie in independent linear/affine subspaces. If further each subspace is low-dimensional as SSC and LRR assume, it is interesting to investigate their relations. We describe SSC first, and then LRR, and finally SSR and their relations.

SSC first solves the sparse codes separately for each sample with respect to the dictionary composed of the remaining samples:

$$\min_{y_i} \|y_i\|_1, \text{ s.t. } A_i = A_{-i}y_i,$$

(72)

where $A_{-i}$ is the data matrix with the $i$th sample removed. Under the condition, in general case, [28] proved that the nonzero entries of $y_i^\ast$ correspond to the samples in the same subspace (cluster) as $A_i$. After all codes are solved, the data can be represented as

$$A = AZ_{SSC},$$

where the $i$th column of $Z_{SSC}$ is $y_i$ with the $i$th entry inserted by a zero, i.e. $\text{diag}(Z_{SSC}) = 0$. If the samples in the same cluster are arranged consecutively, $Z_{SSC}$ would be block-diagonal. Next a similarity matrix $W$ is heuristically defined as $W \approx |Z_{SSC}| + |Z_{SSC}|^T$ and spectral clustering is employed to finish clustering.

LRR is similar to SSC. It seeks a low-rank representation of the data:

$$\min_{Z_{LRR}} \|Z_{LRR}\|_*, \text{ s.t. } A = AZ_{LRR},$$

where $\|\cdot\|_*$ is the nuclear norm. Under the condition, [27] proved that $Z_{LRR}$ is block-diagonal too. The remaining steps follow SSC.

Recall SSRo [58]:

$$A \approx A(H^TH)'.$$

Defining $Z_{SSR} \doteq H^TH$, we obtain a representation similar to SSC and LRR. But the following steps can be omit. First $Z_{SSR}$ is positive and symmetry and thus can be directly defined as a similarity matrix. Second, it can be shown that the eigenvectors of the Laplacian matrix are just $H$.

We see that they all obtain a sparse/low-rank code matrix to represent the data matrix with respect to the dictionary composed of the data matrix itself. But there are some differences: SSC is sparse and usually full rank, and the representation is exact; LRR is low-rank and exact; SSR has the lowest rank but is approximate. More precise, let $V$ be the full normalized principal components of data. Under the condition $V^TV$ is block-diagonal too. The general solutions of $A = AZ$ are \{$V^TV + V^TVx, \forall x \in \mathbb{R}^n$\}, where $V$ is the complement basis of $V$. SSC finds the most sparse solution among this solution space and thus usually is full rank. The representations of SSC and LRR are exact, while that of SSR is approximate.

### 8.4 Relation between Kernel PCA and SSR

We point out that kernel PCA [40] is inherently related to cluster analysis, and can be incorporated into SSR. The underlying reason is very simple: PCA constitutes a part of SSR; and kernel PCA can be seen as a normal PCA, with original data replaced by high-dimensional features.

It can be shown that there is a sparse representation for kernel PCA similar to that of PCA (see [59]):

$$\begin{bmatrix} 1^T \\ \bar{V}_{1:r-1}^T \end{bmatrix} = RH,$$

where $V_{1:r-1}$ are the eigenvectors of kernel PCA. It means that the eigenvectors of kernel PCA are rotated

---

25In this section, we talk about the augmented data rather than the original data.

26We can convert SSR and LRR to the zero-diagonal form as SSC. $A = AZ + AZ_{di}$, where $Z_{di}$ is the diagonal of $Z$ and $\bar{Z}$ the remaining. Then $A = AZ(I - Z_{di})^{-1}, \bar{Z}(I - Z_{di})^{-1}$ is still block-diagonal with zero diagonal.

27Of course, if we deem block-diagonal matrix as sparse, all of them are sparse. 

32
noisy indicator vectors. So kernel PCA is inherently related to cluster analysis. And this explains why the principal components of kernel PCA, when projected to two dimensions for visualization, frequently exhibits a triangle shape (see e.g. [39], and compare with the leftmost figures in Figure 6).

To detail, assume the original data $A$ is not mean-removed, and a kernel matrix $G$ is used by kernel PCA and LE. Then PCA, kernel PCA, and LE can be seen as working with the following three similarity matrices respectively:

$\mathbf{W}_{\text{PCA}} \triangleq \beta \mathbf{1}^T \mathbf{1} + \mathbf{A}^T \overline{\mathbf{A}}$, $\mathbf{W}_{\text{KPCA}} \triangleq \beta' \mathbf{1}^T + G_{\text{KPCA}}$, and $\mathbf{W}_{\text{LE}} \triangleq G$, where $\overline{\mathbf{A}} \triangleq \mathbf{A}(\mathbf{I} - \frac{1}{n} \mathbf{1} \mathbf{1}^T)$, $G_{\text{KPCA}} \triangleq (\mathbf{I} - \frac{1}{n} \mathbf{1} \mathbf{1}^T)G(\mathbf{I} - \frac{1}{n} \mathbf{1} \mathbf{1}^T)$, and $\beta$, $\beta'$ ensure the nonnegativity of the corresponding similarity matrices. By the correspondence between $\overline{\mathbf{A}}^T \mathbf{A}$ and $G_{\text{KPCA}}$, the relation introduced at the beginning is established.

To what extent does the noisy indicator vectors embedded in kernel PCA reveal cluster structure? Or how the clustering performance will be when those vectors are fed into Scut? They can be answered by investigating the ideal graph condition. Generally, following the analysis of the original-data version, we expect the similarity matrix used by kernel PCA meets the condition better than that of PCA while worse than that of LE. Our experiments validated this, though not shown in the paper. Finally, we mention that a significant drawback of kernel PCA is that it demands a large storage when dealing with large data sets, since the kernel matrix is dense.

8.5 Future Work

To make SSR fully useful, we have to be able to solve sparse codes for the out-of-sample data. We leave it to subsequent work. Two open questions have not been answered: 1) the theoretical analysis of the ability of NSCrt in recovering underlying noisy indicator matrix. 2) the performance analysis of the optimality of solution obtained by Scut.

Acknowledgment

We would like to acknowledge support for this project from the National 973 Program (2013CB329500), and the Program for New Century Excellent Talents in University (NCET-13-0521).

References

[1] Michal Aharon, Michael Elad, and Alfred Bruckstein. K-svd: An algorithm for designing overcomplete dictionaries for sparse representation. *Signal Processing, IEEE Transactions on*, 54(11):4311–4322, 2006.

[2] Mikhail Belkin and Partha Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Computation*, 15(6):1373–1396, 2003.

[3] Yoshua Bengio, Olivier Delalleau, Nicolas Le Roux, Jean-François Paiement, Pascal Vincent, and Marie Ouimet. Learning eigenfunctions links spectral embedding and kernel pca. *Neural Computation*, 16(10):2197–2219, 2004.

[4] Christopher M Bishop. *Pattern recognition and machine learning*, volume 1. springer New York, 2006.

[5] Y-L Boureau, Francis Bach, Yann LeCun, and Jean Ponce. Learning mid-level features for recognition. In *Computer Vision and Pattern Recognition (CVPR), 2010 IEEE Conference on*, pages 2559–2566. IEEE, 2010.

[6] Alfred M Bruckstein, David L Donoho, and Michael Elad. From sparse solutions of systems of equations to sparse modeling of signals and images. *SIAM review*, 51(1):34–81, 2009.

[7] Emmanuel J Candès and Michael B Wakin. An introduction to compressive sampling. *Signal Processing Magazine, IEEE*, 25(2):21–30, 2008.

[8] Pak K Chan, Martine DF Schlag, and Jason Y Zien. Spectral k-way ratio-cut partitioning and clustering. *Computer-Aided Design of Integrated Circuits and Systems, IEEE Transactions on*, 13(9):1088–1096, 1994.

[9] Fan RK Chung. *Spectral Graph Theory*, volume 92. Amer Mathematical Society, 1997.
[10] Fernando De la Torre. A least-squares framework for component analysis. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 34(6):1041–1055, 2012.

[11] Inderjit Dhillon, Yuqianguan, and Brian Kulis. A unified view of kernel k-means, spectral clustering and graph cuts. *Technical Report No. UTCS TR-04-25*, 2005.

[12] Inderjit S Dhillon, Yuqiang Guan, and Brian Kulis. Weighted graph cuts without eigenvectors a multilevel approach. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 29(11):1944–1957, 2007.

[13] Chris Ding and Xiaofeng He. K-means clustering via principal component analysis. In *Proceedings of the twenty-first international conference on Machine learning*, page 29. ACM, 2004.

[14] Chris HQ Ding, Xiaofeng He, and Hongyuan Zha. A spectral method to separate disconnected and nearly-disconnected web graph components. In *Proceedings of the seventh international conference on Knowledge discovery and data mining (SIGKDD)*, pages 275–280. ACM, 2001.

[15] David Leigh Donoho. Compressed sensing. *Information Theory, IEEE Transactions on*, 52(4):1289–1306, 2006.

[16] C. Eckart and G. Young. The approximation of one matrix by another of lower rank. *Psychometrika*, 1(3):211–218, 1936.

[17] Michael Elad, Mario AT Figueiredo, and Yi Ma. On the role of sparse and redundant representations in image processing. *Proceedings of the IEEE*, 98(6):972–982, 2010.

[18] Ehsan Elhamifar and Rene Vidal. Sparse subspace clustering: Algorithm, theory, and applications. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 35(11):2765–2781, 2013.

[19] Martin Ester, Hans-Peter Kriegel, Jörg Sander, and Xiaowei Xu. A density-based algorithm for discovering clusters in large spatial databases with noise. In *Proceedings of the Second International Conference on Knowledge Discovery and Data Mining (KDD-96)*, volume 96, pages 226–231. AAAI Press, 1996.

[20] K. Fan. A generalization of tychonoff’s fixed point theorem. *Mathematische Annalen*, 142(3):305–310, 1961.

[21] Shenghua Gao, Ivor Wai-Hung Tsang, and Liang-Tien Chia. Kernel sparse representation for image classification and face recognition. In *Proceedings of the 11th European conference on Computer Vision: Part IV*, pages 1–14, 2010.

[22] Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin. The elements of statistical learning: data mining, inference and prediction. *The Mathematical Intelligencer*, 27(2):83–85, 2005.

[23] Xiaofei He and Partha Niyogi. Locality preserving projections. In *Advances in Neural Information Processing Systems 16: Proceedings of the 2003 Conference*, volume 16, page 153. MIT Press, 2004.

[24] Zhenfang Hu, Gang Pan, Yue Ming Wang, and Zhaohui Wu. Sparse principal component analysis via rotation and truncation. *arXiv preprint arXiv:1403.1430*, 2014.

[25] Ian T Jolliffe. *Principal component analysis*, volume 487. Springer-Verlag New York, 1986.

[26] Harold W Kuhn. The hungarian method for the assignment problem. *Naval research logistics quarterly*, 2(1-2):83–97, 1955.

[27] Guangcan Liu, Zhouchen Lin, Shuicheng Yan, Ju Sun, Yong Yu, and Yi Ma. Robust recovery of subspace structures by low-rank representation. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 35(1):171–184, 2013.

[28] J. Liu, S. Ji, and J. Ye. *SLEP: Sparse Learning with Efficient Projections*. Arizona State University, 2009.

[29] James MacQueen et al. Some methods for classification and analysis of multivariate observations. In *Proceedings of the fifth Berkeley symposium on mathematical statistics and probability*, volume 1, page 14. California, USA, 1967.
[30] Aleix M. Martinez and Avinash C. Kak. Pca versus lda. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 23(2):228–233, 2001.

[31] Bojan Mohar. *Some applications of Laplace eigenvalues of graphs*. Springer, 1997.

[32] Bojan Mohar and Y Alavi. The laplacian spectrum of graphs. *Graph theory, combinatorics, and applications*, 2:871–898, 1991.

[33] Andrew Y Ng, Michael I Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. *Advances in neural information processing systems*, 2:849–856, 2002.

[34] Bruno A Olshausen et al. Emergence of simple-cell receptive field properties by learning a sparse code for natural images. *Nature*, 381(6583):607–609, 1996.

[35] Yagyensh Chandra Pati, Ramin Rezaifar, and PS Krishnaprasad. Orthogonal matching pursuit: Recursive function approximation with applications to wavelet decomposition. In *Proceedings of the 27 th Annual Asilomar Conference on Signals, Systems, and Computers*, pages 40–44. IEEE, 1993.

[36] Ignacio Ramirez, Pablo Sprechmann, and Guillermo Sapiro. Classification and clustering via dictionary learning with structured incoherence and shared features. In *Computer Vision and Pattern Recognition (CVPR), 2010 IEEE Conference on*, pages 3501–3508. IEEE, 2010.

[37] Sam T Roweis and Lawrence K Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500):2323–2326, 2000.

[38] Ron Rubinstein, Alfred M Bruckstein, and Michael Elad. Dictionaries for sparse representation modeling. *Proceedings of the IEEE*, 98(6):1045–1057, 2010.

[39] Lawrence K Saul, Kilian Q Weinberger, Jihun H Ham, Fei Sha, and Daniel D Lee. Spectral methods for dimensionality reduction. *Semisupervised learning*, pages 293–308, 2006.

[40] Bernhard Schölkopf, Alexander Smola, and Klaus-Robert Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10(5):1299–1319, 1998.

[41] John Shawe-Taylor and Nello Cristianini. *Kernel methods for pattern analysis*. Cambridge university press, 2004.

[42] Jianbo Shi and Jitendra Malik. Normalized cuts and image segmentation. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 22(8):888–905, 2000.

[43] Joshua B Tenenbaum, Vin De Silva, and John C Langford. A global geometric framework for nonlinear dimensionality reduction. *Science*, 290(5500):2319–2323, 2000.

[44] Ulrike Von Luxburg. A tutorial on spectral clustering. *Statistics and Computing*, 17(4):395–416, 2007.

[45] John Wright, Yi Ma, Julien Mairal, Guillermo Sapiro, Thomas S Huang, and Shuicheng Yan. Sparse representation for computer vision and pattern recognition. *Proceedings of the IEEE*, 98(6):1031–1044, 2010.

[46] John Wright, Allen Y Yang, Arvind Ganesh, S Shankar Sastry, and Yi Ma. Robust face recognition via sparse representation. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 31(2):210–227, 2009.

[47] Jianchao Yang, Kai Yu, Yihong Gong, and Thomas Huang. Linear spatial pyramid matching using sparse coding for image classification. In *Computer Vision and Pattern Recognition (CVPR), 2009 IEEE Conference on*, pages 1794–1801. IEEE, 2009.

[48] Stella X Yu and Jianbo Shi. Multiclass spectral clustering. In *Computer Vision, 2003 IEEE International Conference on*, pages 313–319. IEEE, 2003.

[49] Ron Zass and Amnon Shashua. A unifying approach to hard and probabilistic clustering. In *Computer Vision, 2005 IEEE International Conference on*, volume 1, pages 294–301. IEEE, 2005.

[50] Lihi Zelnik-Manor and Pietro Perona. Self-tuning spectral clustering. In *Advances in neural information processing systems*, pages 1601–1608, 2004.