Constrained Sparse Subspace Clustering with Side-Information

Chun-Guang Li, Junjian Zhang, and Jun Guo
School of Information and Communication Engineering
Beijing University of Posts and Telecommunications, Beijing 100876, P.R. China
Email: \{lichuanguang; zhjj; guojun\}@bupt.edu.cn

Abstract—Subspace clustering refers to the problem of segmenting high dimensional data drawn from a union of subspaces into the respective subspaces. In some applications, partial side-information to indicate “must-link” or “cannot-link” in clustering is available. This leads to the task of subspace clustering with side-information. However, in prior work the supervision value of the side-information for subspace clustering has not been fully exploited. To this end, in this paper, we present an enhanced approach for constrained subspace clustering with side-information, termed Constrained Sparse Subspace Clustering plus (CSSC+), in which the side-information is used not only in the stage of learning an affinity matrix but also in the stage of spectral clustering. Moreover, we propose to estimate clustering accuracy based on the partial side-information and theoretically justify the connection to the ground-truth clustering accuracy in terms of the Rand index. We conduct experiments on three cancer gene expression datasets to validate the effectiveness of our proposals.

I. INTRODUCTION

High dimensional data in many applications can be considered as samples drawn from a union of multiple low-dimensional subspaces. Assigning data points into their own subspaces and then recovering the underlying low-dimensional structure of the data refer to a well-known problem – subspace clustering [1]. It has found important applications in motion segmentation [2], genes expression profiles clustering [3], hybrid system identification [4], matrix completion [5], etc.

A. Prior Work

Over the past decade, a large number of algorithms have been developed, e.g., K-plane [6], Generalized Principal Component Analysis (GPCA) [7], Spectral Curvature Clustering (SCC) [8], Sparse Subspace Clustering (SSC) [9], [10], [11], Low Rank Representation (LRR) [12], [13], Least Square Regression (LSR) [14], [15], Correlation Adaptive Subspace Segmentation (CASS) [16], Latent SSC [17], Low-Rank Sparse Subspace Clustering (LRSSC) [18], Structured SSC [19], [20], [21], and Elastic-net Subspace Clustering (EnSC) [22].

Among the existing work, self-expression [9] based algorithms, e.g., SSC, LRR, LSR, EnSC, gain the most attention. Roughly speaking, different algorithms differ in using different regularization in the self-expressiveness model. For example, SSC [3] makes use of the $\ell_1$ norm on the coefficients vector, LRR [12] adopts the nuclear norm on the coefficients matrix, LSR [14] uses Frobenius norm on the coefficients matrix, LRSSC [18] uses a mixture of the $\ell_1$ norm and the nuclear norm on the coefficients matrix, and EnSC [22] takes a mixture of the $\ell_1$ and the $\ell_2$ norm on the coefficients vector. On the other hand, different error models have also been used to yield robustness, e.g., the $\ell_2$ norm is used to account for the Gaussian noise in data, the $\ell_1$ norm used in SSC to account for the outlying entries in data, the $\ell_{2,1}$ norm used in LRR to account the column-wise corruptions in data, and the mixture of Gaussian model [23] and the correntropy [24] are used to model complicated corruptions.

The subspace clustering methods mentioned above are purely unsupervised. In some applications, partial supervision information is available. For example, in the task of clustering genes in DNA microarray data [25], [26], there often exists prior knowledge about the relationships between some subset of genes or genes expression profiles [27], [28], [29], [30]. Gene expression data of different cancer subtypes are usually lying on multiple clusters [31] and each cluster can be well approximated by a low-dimensional subspace [3]. [32]. If some pairs of genes expression profiles are known to have the same (or different) subtypes, then it would be helpful to use this knowledge in subspace clustering. Such prior knowledge essentially provides partial side-information to indicate “must-link” or “cannot-link” constraints in clustering, which leads to the task of subspace clustering with side-information.

The side-information is important because it provides partial supervision for clustering. Previous work has demonstrated that incorporating side-information in the self-expressiveness model could bring performance improvements. For sample, in [33], some “must-links” are encoded into a binary weights matrix to encourage nonzero self-expressive coefficients in the corresponding positions; in [20], both “must-link” and “cannot-link” in side-information are encoded into a weights matrix to encourage or penalize the self-expressiveness coefficients in the corresponding positions. While encoding side-information into a weights matrix used in self-expressiveness model could improve the induced affinity, the supervision value of the side-information has not been fully exploited because, encoding pairwise constraints as weights to improve the affinity does not imply that the final clustering must satisfy the constraints. Besides, there is still a reminding issue in prior work on how to select a proper model parameter (e.g., $\lambda$).
B. Our Contributions

In this paper, we present an enhanced approach for constrained subspace clustering with side-information, termed Constrained Sparse Subspace Clustering plus (CSSC+), in which the side-information is used not only in the stage of learning an affinity matrix but also in the stage of spectral clustering. In the stage of learning an affinity matrix, each data point is expressed as a linear combination of all other data points, in which the connections to those data points having “must-link” are inhibited and the connections to those data points having “cannot-link” are encouraged. In the stage of spectral clustering, the “must-link” constraints and the “cannot-link” constraints in side-information are both taken into account into the procedure of clustering. Moreover, we propose to estimate clustering accuracy based on the available side-information and theoretically justify the connection to the ground-truth clustering accuracy in terms of the Rand index. Experiments conducted on three cancer gene expression datasets demonstrate the effectiveness of our proposals.

Paper Outline. The remainder of the paper is organized as follows. Section II gives a review on self-expressiveness based subspace clustering. Section III presents our proposal—CSSC+. Section IV describes clustering quality estimation based on partial side-information. Section V shows experiments and Section VI concludes the paper.

II. FROM SPACe CLUSTeRING TO CONSTRAINTeD SPACe CLUSTeRING WITH SIDE-INFORMATION

This section will briefly review methods for subspace clustering and constrained subspace clustering with side-information.

A. Subspace Clustering

State-of-the-art subspace clustering methods, e.g., SSC [10], LRR [13], LSR [14], EnSC [22], are usually based on self-expressiveness model. These approaches can be summarized into a unified optimization problem as follows:

$$\min_{C,E} \|C\|_C + \lambda \|E\|_E \quad \text{s.t. } X = XC + E, \quad \text{diag}(C) = 0,$$

where $\| \cdot \|_C$ and $\| \cdot \|_E$ are two properly chosen norms, $\lambda > 0$ is a tradeoff parameter, and $\text{diag}(C) = 0$ is optionally used to rule out the trivial solution. Different approaches employ different regularization terms $\|C\|_C$ and/or $\|E\|_E$.

Once the optimal representation matrix $C$ is obtained, spectral clustering [24] can be applied on the induced affinity matrix $A$ where $A = \frac{1}{2}(|C| + |C^\top|)$. Let $Q = [q_1, \ldots, q_n]$ be an $N \times n$ indicator matrix where $q_{ij} = 1$ if the $i$-th column of $X$ lies in subspace $S_j$ and $q_{ij} = 0$ otherwise. Spectral clustering can be formulated as follows:

$$\min_{Q} \text{trace}(Q^\top LQ) \quad \text{s.t. } Q \in \mathbb{Q},$$

where $L = D - A$, $D$ is a diagonal matrix with $D_{ij} = \sum_{i} A_{ij}$, and $\mathbb{Q}$ is the set of all valid segmentation matrices with $n$ groups.

B. Structured Subspace Clustering

Note that the objective function [2] of spectral clustering measures the cost of cutting the affinity graph into $n$ parts, and also measures the discrepancy between the coefficient matrix and the segmentation matrix, because

$$\text{trace}(Q^\top LQ) = \sum_{i,j} C_{ij} \frac{1}{2} \|q^{(i)} - q^{(j)}\|_2^2 = \|C\|_{Q},$$

where $\|C\|_{Q}$ is called subspace structured norm of representation matrix $C$ with respect to segmentation matrix $Q$ [19].

By noticing of the connection between the representation matrix $C$ and the segmentation matrix $Q$, it is natural to integrate problem [11] and [2] into a joint optimization problem

$$\min_{C,E,Q} \|C\|_C + \alpha \|C\|_Q + \lambda \|E\|_E$$

s.t. $X = XC + E, \quad \text{diag}(C) = 0, \quad Q \in \mathbb{Q},$

where $\alpha > 0$ is a tradeoff parameter. This is called structured subspace clustering [20]. Then, if the $\ell_1$ norm is used for $\|C\|_C$, problem [3] turns out to be:

$$\min_{C,E,Q} \|C\|_1 + \alpha \|C\|_Q + \lambda \|E\|_E$$

s.t. $X = XC + E, \quad \text{diag}(C) = 0, \quad Q \in \mathbb{Q},$

which is called Structured Sparse Subspace Clustering (S$^3$C) [20].

The algorithms mentioned above are unsupervised. When some side-information is available, there is a desire to incorporate the partial supervision information to facilitate subspace clustering.

C. Constrained Subspace Clustering with Side-Information

Recently, an approach, called Constrained Structured Sparse Subspace Clustering (CSSC$^+$) [20] is proposed, in which the side-information is encoded into weights matrix $\Psi$ to modify the $\ell_1$ norm of $C$ (i.e., $\|C \odot \Psi\|_1$), where the operator $\odot$ is the element-wise product and the elements of weights matrix $\Psi$ are defined by:

$$\Psi_{ij} = \begin{cases} e^{-1}, & \text{if } i \text{ and } j \text{ have a "must-link"}, \\ e^{+1}, & \text{if } i \text{ and } j \text{ have a "cannot-link"}, \\ e^{0}, & \text{if there is no side-information}. \end{cases}$$

Then, the available side-information is incorporated into the optimization problem [5] as follows:

$$\min_{C,E,Q} \|C \odot \Psi\|_1 + \alpha \|C\|_Q + \lambda \|E\|_E$$

s.t. $X = XC + E, \quad \text{diag}(C) = 0, \quad Q \in \mathbb{Q},$

Encoding the side-information into a weighting matrix $\Psi$ is able to penalize or encourage the coefficients when having “cannot-link” or “must-link”, which thus is helpful to yield an improved coefficients matrix. However, it is not guaranteed that the constraints in side-information could be automatically satisfied in clustering. Besides, it is in principle unclear how to determine the model parameters, e.g., $\lambda$ and $\alpha$ in [7]. If a set of improper tradeoff parameters are used, the clustering
results might dramatically degenerate (see, e.g., Fig.1(b)). To tackle these deficiencies, in this paper, we propose an enhanced approach for subspace clustering with side-information, in which the side-information is used not only to weight the self-expressiveness model, but also to conduct spectral clustering and parameters selection.

III. CONstrained SPARSE SUBSPACE CLUSTERING with SIDE- INFORMATION

This section will present an enhance approach for subspace clustering with side-information.

A. Constrained Sparse Self-Expressiveness Model

In SSC, each data point is expressed as a sparse linear combination of all other data points. To take into account the side-information, we impose the constraints into the self-expressiveness model, such that the connections to those data points having “cannot-link” are inhibited and the connections to those data points having “must-link” are encouraged. To be specific, as in CS³ [20], we solve for $C$ and $E$ by solving a weighted sparse representation problem as follows

$$\min_{C,E} \| C \odot \Psi \|_1 + \lambda \| E \|_E$$

s.t. $X = XC + E$, $\text{diag}(C) = 0$, (8)

where $\Psi$ is a weights matrix which encodes the available side-information as in [6].

We term problem (8) as Constrained Sparse Subspace Clustering (CSSC). This problem can be solved using the Alternating Direction Method of Multipliers (ADMM) [35], [36], [37]. For the details of the derivation of algorithm to solve problem (8), we refer the readers to [20].

B. Spectral Clustering with Constraints

Given coefficients matrix $C$, we define the data affinity matrix $A$ via $A = \frac{1}{2}([C] + [C^T])$. When partial side-information is available, we impose the constraints into spectral clustering and thus solve spectral clustering with constraints as follows:

$$\min_{Q} \text{trace}(Q^T L Q) \text{ s.t. } Q \in \tilde{Q},$$

where $L$ is the graph Laplacian of the data affinity matrix $A$ and $\tilde{Q} \subseteq Q$ is the set of all feasible segmentation matrices $Q$ which satisfy the pairwise constraints encoded in $\Psi$.

To solve problem (9), we relax the constraint $Q \in \tilde{Q}$ to the constraint $Q^T D Q = I$ and perform spectral embedding at first, i.e., solving

$$\min_{Q \in \mathbb{R}^{N \times n}} \text{trace}(Q^T L Q) \text{ s.t. } Q^T D Q = I,$$

to find $Q \in \mathbb{R}^{N\times n}$. Then, we quantize $Q$ into the set of feasible segmentation matrices $\tilde{Q}$ by applying a constrained $k$-means algorithm [38].

We call the two-step approach—first solving the coefficient matrix $C$ via problem (8) and then finding the segmentation matrix $Q$ via problem (9) as Constrained Sparse Subspace Clustering plus (CSSC+).

Remark 1. In CS³C [20], instead of searching for a segmentation matrix $Q \in \mathbb{Q}$, we can also search for $Q \in \tilde{Q}$, which thus turns problem (7) into the following:

$$\min_{C,E,Q} \| C \odot \Psi \|_1 + \alpha \| C \|_Q + \lambda \| E \|_E$$

s.t. $X = XC + E$, $\text{diag}(C) = 0$, $Q \in \tilde{Q}$. (11)

We call problem (11) as Constrained Structured Sparse Subspace Clustering plus (CSSC+). It can be solved by solving subproblems (8) and (9) alternatingly.

IV. PERFORMANCE EVALUATION AND ESTIMATION WITH SIDE-INFORMATION

This section will present a general method to perform parameter (or model) selection for subspace clustering with side-information.

A. Clustering Error with Respect to Groundtruth Label

When the groundtruth label of each data point is available, the quality of clustering can be evaluated by clustering error (ERR), which is defined as

$$\text{ERR}(a, \hat{a}) = 1 - \max_{\pi} \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{\{\pi(a_i) = a_{\hat{i}}\}},$$

where $a, \hat{a} \in \{1, \cdots, n\}^N$ are the original and estimated assignments of the columns in $X$ to $n$ subspaces, and the maximum is taken with respect to all permutations

$$\pi : \{1, \cdots, n\}^N \rightarrow \{1, \cdots, n\}^N.$$

While ERR is a valid measure to compare the partitions of the data with respect to the groundtruth labels, it is not a valid measure to evaluate the partitions of the data with respect to the pairwise side-information (or partial pairwise side-information).

To evaluate the accuracy of clustering with respect to pairwise side-information, we introduce a measure to compare two data partitions, which is called Rand index [39].

B. Rand Index based on Complete Pairwise Side-Information

Denote $\Theta$ as a subspace structure matrix of the obtained clustering where $\Theta_{ij} = 0$ if data points $i$ and $j$ belong to the same cluster and $\Theta_{ij} = 1$ otherwise.

Definition 1. The Rand index, denoted as $\mu$, is defined as

$$\mu = 1 - \frac{1}{N^2 - N} \| \Theta - \Theta^* \|_1,$$

where $\Theta$ and $\Theta^*$ are the subspace structure matrices of the currently returned clustering and the ground-truth clustering, respectively.

When the pairwise ground-truth information $\Theta^*$ is available, the Rand index is easy to compute. We have that $0 \leq \mu \leq 1$. If the currently returned clustering is perfect, then $\Theta = \Theta^*$ and thus $\mu = 1$; otherwise $\mu < 1$.3

1We assume that the constraints in the given side-information are correct and consistent. Thus, there exists a segmentation matrix $Q$ which satisfies all the constraints.
Since that subspace clustering is an unsupervised task, complete ground-truth knowledge (e.g., $\Theta_*$) of the data is unknown. Without complete ground-truth knowledge, there is no means to provide a criterion which directly links to the clustering accuracy with theoretical guarantee. Nevertheless, in the setting of clustering with side-information, the side-information is able to provide partial observations of the pairwise ground-truth knowledge. By using the partial observations, there is a hope to define a clustering accuracy estimator, which directly links to the Rand index with theoretical justification.

C. Rand Index Estimator based on Partial Side-Information

**Definition 2.** The Rand Index Estimator (RIE), denoted by $\hat{\mu}$, is defined as

$$\hat{\mu} = 1 - \frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} |\Theta_{i,j} - \Phi_{i,j}^*|,$$

where $\Theta$ is the subspace structure matrix of the currently returned clustering. $\Omega$ is the index set of the given pairwise constraints in $\Phi^*$ in which $\Phi_{i,j}^* = 0$ if the paired data points $(i, j)$ have a “must-link” and $\Phi_{i,j}^* = 1$ if they have a “cannot-link”.

It is clear that $0 \leq \hat{\mu} \leq 1$, where $\hat{\mu} = 1$ if the clustering result indicated by $\Theta$ is feasible with respect to the constraints in $\Phi^*$, and $\hat{\mu} < 1$ otherwise.

**Theorem IV.1.** Assume that the given constraints in set $\Omega$ are sampled independently at random with probability $p$ from a population of $N(N-1)$ constraints. Then, we have that

$$|\hat{\mu} - \mu| < \frac{2}{pN(N-1)-1},$$

holds with probability at least $1 - 4e^{-2N(N-1)}$, where $\mu$ is the Rand index defined in (14) and $\hat{\mu}$ is the Rand index estimator defined in (15).

**Proof.** Let $\{Z_{i,j}\}_{1 \leq i \leq N, 1 \leq j \leq N, i \neq j}$ be $M$ independent identically distributed Bernoulli random variables, where $P(Z_{i,j} = 1) = p$, $\Omega = \{(i, j) : Z_{i,j} = 1\}$, and $M = N(N-1)$. Denote $Y_{i,j} = Z_{i,j}\Delta_{i,j}$ where $\Delta_{i,j} = |\Theta_{i,j} - \Phi_{i,j}^*| \in \{0, 1\}$, then $Y_{i,j} \in \{0, 1\}$ is also a random variable.

Let $\rho := \frac{1}{M} \sum_{i,j} \Delta_{i,j}$ and $\hat{\rho} := \frac{1}{M} \sum_{i,j \in \Omega} Z_{i,j} \Delta_{i,j}$, then we have $\rho = 1 - \mu$, $\hat{\rho} = 1 - \hat{\mu}$. Moreover, we have

$$E[\sum_{i,j} Y_{i,j}] = E[\sum_{i,j} Z_{i,j}\Delta_{i,j}],$$

$$= \sum_{i,j} E[Z_{i,j}]\Delta_{i,j},$$

$$= p \sum_{i,j} \Delta_{i,j},$$

and

$$E[\sum_{i,j} Z_{i,j}] = \sum_{i,j} E[Z_{i,j}] = pM,$$

where $E[\cdot]$ is the expectation of a random variable.

By applying Hoeffding’s inequality [40] to $M$ independent random variables $\{Y_{i,j}\}_{i \neq j}$ and $\{Z_{i,j}\}_{i \neq j}$, separately, we have

$$P(\left| \sum_{i,j} Y_{i,j} - pM\rho \right| > \epsilon) < 2e^{-2\epsilon^2M},$$

and

$$P(\left| \sum_{i,j} Z_{i,j} - pM\rho \right| > \epsilon) < 2e^{-2\epsilon^2M}.$$

Then, with probability at least $1 - 4e^{-2\epsilon^2M}$, we have

$$pM\rho - \epsilon \leq \sum_{i,j} Y_{i,j} \leq pM\rho + \epsilon,$$

and

$$pM - \epsilon \leq \sum_{i,j} Z_{i,j} \leq pM + \epsilon.$$

By combining (24) and (25), we bound $\hat{\rho}$ as follows:

$$\frac{pM\rho - \epsilon}{pM + \epsilon} \leq \hat{\rho} \leq \frac{pM\rho + \epsilon}{pM - \epsilon}.$$

i.e.,

$$\frac{-2\epsilon}{pM + \epsilon} \leq \hat{\rho} - \rho \leq \frac{2\epsilon}{pM - \epsilon}.$$

So, we have

$$|\hat{\rho} - \rho| \leq \frac{2\epsilon}{pM - \epsilon},$$

holds with probability at least $1 - 4e^{-2\epsilon^2M}$.

Note that $M = N(N-1)$, $\hat{\rho} - \rho = \mu - \hat{\mu}$, and by taking $\epsilon = 1$, then we have that:

$$|\hat{\mu} - \mu| < \frac{2}{pN(N-1)-1},$$

holds with probability at least $1 - 4e^{-2N(N-1)}$. This completes the proof.

Fig. 1. The Rand index estimator (RIE) and the clustering error (ERR) for CSK/C on dataset Novartis BPLC with 5% side-information. (This figure is best viewed in color.)

**Remark 2.** If the available side-information is sampled at random and sufficient, the Rand index estimator could provide a good estimation for the Rand index, which connects to the true clustering accuracy. Nevertheless, in case of that the side-information is neither sufficient nor sampled at random, the Rand index estimator might fail to give an acceptable estimation for the Rand index.
D. Parameter Selection via the Rand Index Estimator

When the side-information are sufficient and sampled at random, we use the Rand index estimator \( \hat{\mu} \) to estimate the Rand index. As an interesting application, we employ the Rand index estimator \( \hat{\mu} \) to select the proper parameters\(^2\) e.g., \( \alpha \) and \( \lambda \) in (7), \( \alpha \) in (8). More specifically, we conduct experiments with the parameters varying in a range, record the Rand index estimator \( \hat{\mu} \) as a function of the parameters, and then pick up the parameters which associate to the peak value of the Rand index estimator.

An example of parameters selection with the Rand index estimator is shown in Fig. 1 where panel (a) shows the Rand index estimator of CS\(^3\)C as a function of the parameters \( \lambda_0 \) and \( \alpha \), and panel (b) shows the corresponding clustering error. The coordinates of the brightest region in panel (a) indicate the potentially proper parameters. As verified by experiments, the corresponding dark blue region in panel (b) did yield the lowest clustering error.

V. EXPERIMENTS

This section will evaluate the effectiveness of our proposals for subspace clustering with side-information.

We consider three publicly available benchmark cancer datasets\(^3\), St. Jude leukemia [41], Lung Cancer [42], and Novartis BPLC [43]. For clarity, we list the summary information of the three datasets in Table I. To prepare the side-information, following the protocol used in [20], we sample uniformly at random a proportion \( p \) of entries from the ground-truth subspace structure matrix \( \Theta^* \), where \( p = 1\% \) and \( 5\% \).

A. Performance Evaluation on Subspace Clustering with Side-Information

To evaluate the performance of using side-information, we choose three popular spectral clustering based methods: SSC [10], LRR [12, 32], LSR [14], and a PCA based subspace clustering method, Predictive Subspace Clustering (PSC) [3]. Moreover, we conduct experiments to compare the following approaches: CS\(^3\)C [20], SSC+, LRR+, LSR+, and CS\(^3\)C+, where the appendix “+” means using the \( k \)-means with constraints in spectral clustering. Note that if the percentage of given side-information is 0%, then CS\(^3\)C and CSSC reduce to S\(^3\)C and SSC, respectively.

The average clustering error (ERR) with standard deviation is recorded over 20 trials. Experimental results are presented in Table II. The results of PSC are directly cited from [3]. The parameter \( \lambda \) used in each baseline method is listed in Table III, where the parameter \( \lambda \) used in the family of SSC, including CS\(^3\)C, CSSC, CSSC+, and CS\(^3\)C+, is kept the same as in SSC by default.\(^4\) We observe that:

- When the side-information is relatively sufficient, e.g., \( p = 5\% \), the clustering errors of all methods with side-information are significantly reduced, compared to the counterpart method without side-information. This hints the importance of incorporating the constraints to clustering.
- When the side-information is relatively not sufficient, e.g., \( p = 1\% \), the clustering errors of SSC+, CSSC+, and CS\(^3\)C+ are still notably reduced compared to SSC, CSSC, and CS\(^3\)C; however, the clustering errors of LRR+, LSR1+, and LSR2+ are exceptionally increased, respectively, in most cases. This suggests that the effect of imposing constraints in clustering depends on the quality of the affinity matrix.
- Compared to SSC, both CSSC and CSSC+ reduce the clustering errors notably. Comparing to CSSC, CSSC+ reduces the clustering error more significantly. It is similar for CS\(^3\)C and CS\(^3\)C+. This confirms the superiority of incorporating the constraints into not only the self-expressiveness model but also the process of clustering.

B. Parameter Selection via Rand Index Estimator

To demonstrate the feasibility of using the Rand index estimator to guide parameters selection, we conduct experiments on dataset Novartis BPLC with CS\(^3\)C by varying parameters \( \lambda \) and \( \alpha \), where \( \alpha \in \{0.05, 0.1, 0.2, \ldots , 0.9, 1.0, 1.2, 1.5, 2.0\} \) and \( \lambda \) is set by

\[
\lambda = \frac{\lambda_0}{\max_{i,j \neq j} \{x_i^T x_j\}} = \frac{\lambda_0}{\max_{i,j \neq j} \{x_i^T x_j\}}
\]

with \( \lambda_0 \in \{2, 3, 4, 5, 6, 7, 8, 9, 10\} \). The clustering error (ERR) and the Rand index estimator (RIE) under all combination of parameters are recorded. We show ERR and RIE in Fig. I panels (a) and (b), respectively, as a function of parameters \( \alpha \) and \( \lambda_0 \). As could be observed that, the change patterns of the two panels are consistently correlated. This confirms the feasibility of using the Rand index estimator to conduct parameters selection in CS\(^3\)C.

Moreover, we also conduct experiments for CSSC and CSSC+ on all three datasets. We show the clustering accuracy (1 - ERR), the Rand index (RI), and the Rand index estimator (RIE) under all combination of parameters are recorded. We show ERR and RIE in Fig. I panels (a) and (b), respectively, as a function of parameters \( \alpha \) and \( \lambda_0 \). As could be observed that, the change patterns of the two panels are consistently correlated. This confirms the feasibility of using the Rand index estimator to conduct parameters selection in CS\(^3\)C.

For CS\(^3\)C, once an exceptionally worse clustering result occurs, we use the Rand index estimator to tune the parameters \( \alpha \) and \( \lambda \). The parameter \( \alpha \) in CS\(^3\)C and CS\(^3\)C+ is kept the same.

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\(^2\)It is also possible to use the Rand index estimator to determine the number of subspaces when it is unknown.

\(^3\)http://www.broadinstitute.org/cgi-bin/cancer/datasets.cgi

\(^4\)For CS\(^3\)C, one uses the Rand index estimator to tune the parameters \( \alpha \) and \( \lambda \). The parameter \( \alpha \) in CS\(^3\)C and CS\(^3\)C+ is kept the same.
TABLE II

Average clustering error (ERR %) with standard derivation (STD) on three cancer data sets under different proportions of side-information. The best results are in bold font.

| Data sets Side-info. | St. Jude leukemia 0% | 1% | 5% | Lung Cancer 0% | 1% | 5% | Novartis BPLC 0% | 1% | 5% |
|---------------------|----------------------|----|----|----------------|----|----|-----------------|----|----|
| PSC (1) [3]         | 3.10 ± 0.16          | -  | -  | 7.80 ± 4.16    | -  | -  | 4.60 ± 0.97     | -  | -  |
| LRR (12)            | 11.11 ± 1.11         | -  | -  | 5.08 ± 2.33    | -  | -  | 14.60 ± 3.14    | -  | -  |
| LRR+ [14]           | 11.11 ± 18.0 ± 3.87  | -  | -  | 6.73 ± 3.02    | 1.55 ± 1.88  | -  | 14.60 ± 13.01   | 4.76 ± 1.75  | -  |
| LSR2+ [14]          | 9.27 ± 2.80          | -  | -  | 4.57 ± 7.77    | -  | -  | 7.77 ± 1.80     | 3.59 ± 1.94  | -  |
| LSR2+ [14]          | 9.27 ± 15.52 ± 2.97  | -  | -  | 10.23 ± 3.01   | 3.50 ± 3.01  | -  | 6.80 ± 12.0 ± 2.50 | -  | -  |
| LSR2+ [14]          | 9.68 ± 15.08 ± 1.80  | 9.82 ± 1.95  | -  | 4.57 ± 3.02    | 3.38 ± 3.03  | 7.77 ± 18.0 ± 1.90 | 3.59 ± 1.94  | -  |
| SSC (19)            | 3.23 ± 7.77          | -  | -  | 5.08 ± 7.77    | -  | -  | 2.91 ± 1.80     | -  | -  |
| SSC (19)            | 3.23 ± 2.80 ± 0.29   | 1.03 ± 0.69  | -  | 4.80 ± 1.41    | 1.45 ± 2.02  | -  | 2.91 ± 1.55 ± 1.11 | 0.24 ± 0.53  | -  |
| SSC (19)            | 3.23 ± 3.02 ± 0.95   | 0.56 ± 0.50  | -  | 3.02 ± 0.99    | 1.04 ± 1.22  | 2.91 ± 2.82 ± 0.43 | 2.52 ± 1.11  | -  |
| SSC (19)            | 3.23 ± 2.82 ± 0.34   | 1.33 ± 0.40  | -  | 4.06 ± 1.41    | 1.31 ± 0.48  | 2.91 ± 2.7 ± 0.48 | 2.33 ± 1.02  | -  |
| CSS²+ (20)          | 2.42 ± 3.02 ± 5.4    | 1.33 ± 0.40  | -  | 4.06 ± 1.37    | 0.84 ± 0.98  | 2.91 ± 1.6 ± 0.96 | 0.34 ± 0.65  | -  |

that the Rand index estimator is of practical value to conduct parameter selection, especially for CSSC+.

VI. CONCLUSION

We have presented an enhanced framework to perform constrained subspace clustering with side-information, in which the constraints in side-information are used not only in the stage of learning the affinity matrix but also in the stage of spectral clustering. Moreover, we have proposed an Rand index estimator based on partial side-information for estimating the clustering accuracy with theoretical guarantee and used it to conduct parameters selection. Experiments on three cancer gene expression datasets have validated the effectiveness of our proposals.

The Rand index estimator is a general measure for estimating the clustering accuracy with partial pairwise side-information, not limited to subspace clustering. More comprehensive evaluations on the performance of constrained subspace clustering with side-information, model selection with the Rand index estimator, and more active way to exploit the partial supervision of side-information will be our future work.

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REFERENCES

[1] R. Vidal, “Subspace clustering,” IEEE Signal Processing Magazine, vol. 28, no. 3, pp. 52–68, March 2011.
[2] S. Rao, R. Tron, R. Vidal, and Y. Ma, “Motion segmentation in the presence of outlying, incomplete, or corrupted trajectories,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 32, no. 10, pp. 1832–1845, 2010.
[3] B. McMWilliams and G. Montana, “Subspace clustering of high dimensional data: a predictive approach,” Data Mining and Knowledge Discovery, vol. 28, no. 3, pp. 736–772, 2014.
[4] L. Bako, “Identification of switched linear systems via sparse optimization,” Automatica, vol. 47, no. 4, pp. 668–677, 2011.
[5] C.-G. Li and R. Vidal, “A structured sparse plus structured low-rank framework for subspace clustering and completion,” IEEE Transactions on Signal Processing, vol. 64, no. 24, pp. 6557–6570, 2016.
[6] P. S. Bradley and O. L. Mangasarian, “k-plane clustering,” Journal of Global Optimization, vol. 16, no. 1, pp. 23–32, 2000.
[7] R. Vidal, Y. Ma, and S. Sastry, “Generalized Principal Component Analysis (GPCA),” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 27, no. 12, pp. 1–15, 2005.
[8] G. Chen and G. Lerman, “Spectral curvature clustering (SSC),” International Journal of Computer Vision, vol. 81, no. 3, pp. 317–330, 2009.
[9] C.-G. Li and R. Vidal, “Structured sparse plus structured low-rank representation,” in IEEE Conference on Computer Vision and Pattern Recognition, 2016, pp. 3918–3927.
[10] C. You, D. Robinson, and R. Vidal, “Scalable sparse subspace clustering by orthogonal matching pursuit,” in IEEE Conference on Computer Vision and Pattern Recognition, 2009, pp. 2790–2797.
[11] C. You, D. Robinson, and R. Vidal, “Sparse subspace clustering: theory, algorithms, and applications,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 35, no. 11, pp. 2765–2781, 2013.
[12] C.-G. Li, M. Min, Z.-Q. Zhao, L. Zhu, D.-S. Huang, and S. Yan, “Robust subspace segmentation by trace lasso,” in European Conference on Computer Vision, 2013, pp. 1345–1352.
[13] C.-G. Li, Z. Lin, S. Yan, J. Sun, and Y. Ma, “Robust recovery of subspace structures by low-rank representation,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 35, no. 1, pp. 171–184, Jan 2013.
[14] C.-G. Li, H. Lin, Z.-Q. Zhao, L. Zhu, D.-S. Huang, and S. Yan, “Robust and efficient subspace segmentation via least squares regression,” in European Conference on Computer Vision, 2012, pp. 347–360.
[15] X. Peng, Z. Yu, Z. Yi, and H. Tang, “Constructing the l2-graph for robust subspace learning and subspace clustering,” IEEE Transactions on Cybernetics, vol. 47, no. 4, pp. 1053–1066, 2017.
[16] C. Lu, Z. Lin, and S. Yan, “Correlation adaptive subspace segmentation by trace lasso,” in IEEE International Conference on Computer Vision, 2013, pp. 1345–1352.
[17] V. M. Patel, H. V. Nguyen, and R. Vidal, “Latent space sparse subspace clustering,” in IEEE International Conference on Computer Vision, 2013, pp. 225–232.
[18] Y.-X. Wang, H. Xu, and C. Leng, “Probable subspace clustering: When LRR meets SSC,” in Neural Information Processing Systems, 2013.

TABLE III

Parameter λ or λ0 used in each method on each dataset.

| Methods | LRR (λ) | LSR1 (λ) | LSR2 (λ) | SSC (λ0) |
|---------|---------|----------|----------|----------|
| St. Jude leukemia | 1.4 ± 0.12 | 0.13 ± 0.5 | 0.18 ± 0.8 | 4 ± 2.3 |
| Lung Cancer | 0.5 ± 0.8 | 0.13 ± 0.5 | 0.18 ± 0.8 | 4 ± 2.3 |
| Novartis BPLC | 1 ± 0.5 | 1 ± 0.5 | 1 ± 0.5 | 5 ± 2.5 |
Cancer (middle row) and Novartis BPLC (bottom row), where the percentage in bracket is the proportion of the available side-information.

C.-G. Li, C. You, and R. Vidal, “Structured sparse subspace clustering: A joint affinity learning and subspace clustering framework,” IEEE Transactions on Image Processing, vol. 26, no. 6, pp. 2988–3001, 2017.

J. Zhang, C.-G. Li, H. Zhang, and J. Guo, “Low-rank and structured sparse subspace clustering,” in IEEE International Conference on Visual Communication and Image Processing (VCIP), Nov. 2016.

C. You, C.-G. Li, D. Robinson, and R. Vidal, “Oracle based active set algorithm for scalable elastic net subspace clustering,” in Proceedings of IEEE International Conference on Computer Vision and Pattern Recognition, 2016, pp. 3928–3937.

B. Li, Y. Zhang, Z. Lin, and H. Lu, “Subspace clustering by mixture of gaussian regression,” in IEEE Conference on Computer Vision and Pattern Recognition, 2015, pp. 2094–2102.

R. He, L. Wang, Z. Sun, Y. Zhang, and B. Li, “Information theoretic subspace clustering,” IEEE Transactions on Neural Networks and Learning Systems, vol. 27, no. 12, pp. 2643–2655, 2016.

D. Lockhart and E. Winzeler, “Genomics, gene expression, and dna arrays,” Nature, vol. 405, pp. 827–836, 2000.

M. Schena, D. Shalon, R. Davis, and P. Brown, “Quantitative monitoring of gene expression patterns with a complementary dna microarray,” Science, vol. 270, pp. 467–470, 1995.

Z. Fang, J. Yang, Y. Li, Q. Luo, L. Liu, and et al., “Knowledge guided analysis of microarray data,” Journal of Biomedical Informatics, vol. 39, no. 4, pp. 401–411, 2006.

P. Chopra, J. Kang, J. Yang, H. Cho, H. Kim, and M. Lee, “Microarray data mining using landmark gene-guided clustering,” BMC Bioinformatics, vol. 9, no. 1, p. 92, 2008.

D. Huang and W. Pan, “Incorporating biological knowledge into distance-based clustering analysis of microarray gene expression data,” Bioinformatics, vol. 22, no. 10, pp. 1259–1268, 2006.

E. Bair, “Semi-supervised clustering methods,” Wiley Interdisciplinary Reviews: Computational Statistics, vol. 5, no. 5, pp. 349–361, 2013.

U. Alon, N. Barkai, D. Notterman, K. Gish, S. Ybarra, D. Mack, and A. Levine, “Broad patterns of gene expression revealed by clustering analysis of tumor and normal colon tissues probed by oligonucleotide arrays,” Proceedings of the National Academy of Sciences of the United States of America, vol. 96, no. 12, pp. 6745–6750, 1999.

Y. Cui, C.-H. Zheng, and J. Yang, “Identifying subspace gene clusters from microarray data using low-rank representation,” Plos ONE, vol. 8, no. 3, p. e59377, 2013.

D. Wang, Q. Yin, R. He, L. Wang, and T. Tan, “Semi-supervised subspace segmentation,” in IEEE International Conference on Image Processing, 2014, pp. 2854–2858.

U. von Luxburg, “A tutorial on spectral clustering,” Statistics and Computing, vol. 17, no. 4, pp. 395–416, 2007.

Z. Lin, M. Chen, L. Wu, and Y. Ma, “The augmented Lagrange multiplier method for exact recovery of corrupted low-rank matrices,” arXiv:1009.5055v2, 2011.

Z. Lin, R. Liu, and Z. Su, “Linearized alternating direction method with adaptive penalty for low rank representation,” in Neural Information Processing Systems, 2011.

S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein, “Distributed optimization and statistical learning via the alternating direction method of multipliers,” Foundations and Trends in Machine Learning, vol. 3, no. 1, pp. 1–122, 2010.

K. Wagstaff, C. Cardie, S. Rogers, and S. Schrödl, “Constrained k-means clustering with background knowledge,” in ICDM, 2001, pp. 577–584.

W. Rand, “Objective criteria for the evaluation of clustering methods,”
[40] W. Hoeffding, “Probability inequalities for sums of bounded random variables,” *Journal of the American Statistical Association*, vol. 58, no. 301, pp. 13–30, 1963.

[41] E. J. Yeoh, M. E. Ross, S. A. Shurtleff, and et al., “Classification, subtype discovery, and prediction of outcome in pediatric acute lymphoblastic leukemia by gene expression profiling,” *Cancer Cell*, vol. 1, pp. 133–143, 2002.

[42] A. Bhattacharjee, W. Richards, J. Staunton, and et al., “Classification of human lung carcinomas by mrna expression profiling reveals distinct adenocarcinomas sub-classes,” *Proceedings of the National Academy of Sciences of the United States of America*, vol. 98, no. 24, pp. 13,790–13,795, 2001.

[43] A. I. Su, M. P. Cooke, K. A. Ching, and et al., “Large-scale analysis of the human and mouse transcriptomes,” *Proceedings of the National Academy of Sciences of the United States of America*, vol. 99, no. 7, pp. 4447–4465, 2002.

[44] C.-G. Li, Z. Lin, H. Zhang, and J. Guo, “Learning semi-supervised representation towards a unified optimization framework for semi-supervised learning,” in *Proceedings of IEEE International Conference on Computer Vision*, 2015, pp. 2767–2775.