Graph-cut based Constrained Clustering by Grouping Relational Labels

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Abstract— **This paper proposes a novel constrained clustering method that is based on a graph-cut problem formalized by SDP (Semi-Definite Programming). Our SDP approach has the advantage of convenient constraint utilization compared with conventional spectral clustering methods. The algorithm starts from a single cluster of a whole dataset and repeatedly selects the largest cluster, which it then divides into two clusters by swapping rows and columns of a relational label matrix obtained by solving the maximum graph-cut problem. This swapping procedure is effective because we can create clusters without any computationally heavy matrix decomposition process to obtain a cluster label for each data. The results of experiments using datasets from the ODP and WebKB corpus demonstrated that our method outperformed other conventional and the state of the art clustering methods in many cases. In particular, we discuss the difference between our approach and another similar one that uses the same SDP formalization as ours. Since the number of constraints used in the experiments is relatively small and can be practical for human feedback, we consider our clustering provides a promising basic method to interactive Web clustering.**

I. Introduction

Clustering has long been one of the most essential and popular techniques in data mining [1]. It is used not only for visualization of huge data sets but also for image segmentation [2], medical applications, recommendation systems, and so on.

Constrained clustering is a semi-supervised learning approach that utilizes pre-given knowledge about data pairs to improve normal clustering accuracy [3], [4]. The knowledge used is generally of two simple types: a constraint about data pairs that must be in the same cluster, and a constraint about data pairs that must be in a different cluster. These are usually called *must-link* and *cannot-link*, respectively.

Recent research about distance metric learning interprets the constraint information as the distance or kernel value of data pairs and tries to produce a new distance measure or kernel matrix for a whole dataset to ensure the distance of must-link is small and the distance of cannot-link is large [5], [6], [7]. In this research, we do not interpret the constraint as a distance or kernel value but rather as a relational label that indicates whether data pairs should be in the same cluster or not. Our objective is to predict the correct label for each data pair (not for each individual piece of data) by using sample labels converted from pre-given constraint information according to the framework of the transductive learning.

Our method is based on the graph-cut problem. Although graph-cut based clustering (e.g., spectral clustering) is a well known approach and many methods have been proposed so far [8], [9], their solutions are mostly based on the graph spectrum obtained by eigen decomposition, which requires complicated processes to add in the constraint information. Our approach is to solve it as a semi-definite programming (SDP) problem. The advantage of SDP is that we can naturally incorporate constraints without any complicated processing and do not need any specific objective functions (e.g., normalized cut) to avoid a trivial solution (as is the case with many other spectral clustering methods).

In terms of formalization, our problem is the same as Li's [10] or Hoi's [11], although the introduction is completely different. The most critical difference is the interpretation of the SDP solution. They interpret the solution as a kernel matrix and use it for multi-class clustering, while we interpret it as a label matrix (as described above) and use it for two-class clustering. As we will show in the experiments, our two-class clustering approach performs better than the multi-class clustering approach. Our approach is based on the divide and conquer algorithm. It starts from a single cluster of a complete dataset and repeatedly selects the largest cluster, which it then divides into two clusters until we get the target numbers of clusters. In each iteration, we obtain relational labels for all data pairs from the solution of the SDP problem. We then use the label matrix to create clusters by swapping rows and columns to reduce the clusters' label distribution entropies. This swapping procedure is very effective because we can create clusters without any computationally heavy matrix decomposition processing.

In summary, we propose a constrained clustering method that has the following features.

- Clustering is performed based on the relational labels of all data pairs that are obtained by solving a graph-cut problem formalized by semi-definite programming. Our SDP approach has the advantage convenient constraint utilization compared with conventional spectral clustering methods.
- The interpretation of the obtained matrix is different from Li and Hoi's approaches, although the problem

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formalization is similar. They use the matrix as a kernel matrix for one-time multi-class clustering, while we use it as binary label matrix for divide and conquer-based two-class clustering.

These advantages make constrained clustering more efficient, especially in the case of small number of constraints such as interactive web clustering like [12].

The rest of the paper is organized as follows. First we explain the standard maximum graph cut problem and its solution by semi-definite programming relaxation in Section II. Next, we describe our clustering algorithm, which is based on the approximate solution of the SDP. We describe the entire clustering procedure including binarizing and swapping of the solution matrix in Section III. Section IV shows the results of experiments performed using datasets from the ODP and WebKB corpus. We discuss our methods in Section V, and finally we conclude our work in Section VI.

II. Constrained Graph Cut Problem

Graph-cut formalization is a powerful clustering approach that many algorithms have adopted. In this section, we first formalize the maximum cut problem and then introduce a solution by semi-definite programming.

A. Maximum Cut Problem

The objective of the problem is to divide a graph into two parts as its cut amount reaches the maximum. More formally, consider a graph $G = (V, E)$, where V is a set of vertices and E is a set of edges. The problem is to find partitioning (V_1, V_2) such as $V_1 \cup V_2 = V$ and $V_1 \cap V_2 = \phi$ and a maximum cut amount of $\sum_{i \in V_1, j \in V_2} w_{ij}$. Here, w_{ij} is the weight of an edge between data $i \in V_1$ and data $j \in V_2$. We decide on a "maximum" cut when w_{ij} is defined by some distance (e.g., Euclid distance). In contrast, if w_{ij} is defined by some similarity (e.g., Gauss kernel), the "minimum" cut is appropriate.

By introducing a cluster label variable u_i for each vertex, we can formalize the maximum cut problem as follows.

Maximum Cut Problem

$$\begin{aligned} \text{maximize} \quad & \frac{1}{4} \sum_{i \in V_1} \sum_{j \in V_2} w_{ij}(1 - u_i u_j) \\ \text{subject to} \quad & u_k^2 = 1 \quad (k \in V) \\ & u_k = \begin{cases} +1 & (k \in V_1) \\ -1 & (k \in V_2) \end{cases} \end{aligned}$$

According to the standard method of spectral clustering or segmentation by the random walk model, we can solve this problem with the method of Lagrange multipliers. The u_i labels are obtained as eigen vectors corresponding to the second largest eigen value.

Our aim is to incorporate given constraints into the above problem and find a method to solve constrained maximum cut problems. While there are constrained versions of spectral clustering methods, we adopt a different approach, solution by semi-definite programming (SDP), which is practically easier to use because it can handle constraints intrinsically.

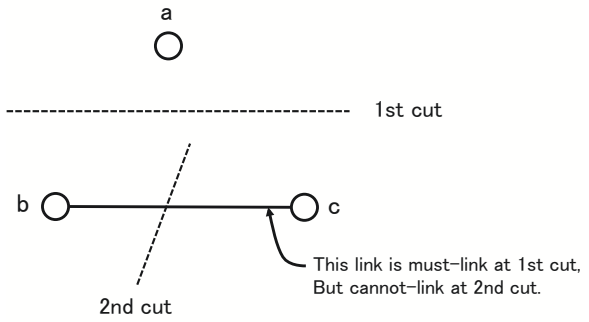


Figure 1. Cannot-link is not applicable in divide and conquer approach

B. Formalization by SDP

Semi-definite programming is a kind of convex optimization that is used to relax several optimization problems such as combinatorial optimization, 0-1 integer programming, and non-convex quadratic programming. Since the maximum cut problem is an example of 0-1 integer programming, SDP can also relax it.

For the standard formalization of SDP, we transform the above objective function into a matrix representation with a weight matrix W and a matrix X whose element is the product of u_i and u_j.

$$\begin{aligned} \sum_{i \in V_1} \sum_{j \in V_2} w_{ij}(1 - u_i u_j) &= (diag(W\mathbf{e}) - W) \bullet X \\ &= L \bullet X \end{aligned}$$

$$X = \mathbf{u}^T \mathbf{u}$$

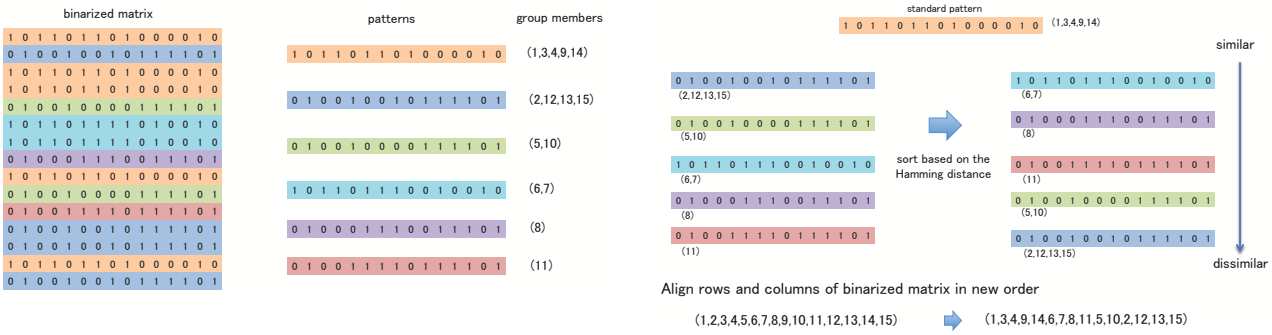
$$\mathbf{u} = (u_1, u_2, ..., u_n), \quad n = |V|$$

L is the graph Laplacian matrix and $\mathbf{e}$ is a vector whose elements are all one. As a final step, we add *must-link* constraints to formalize the constrained maximum cut problem as follows.

Maximum Cut Problem with SDP Relaxation

$$\begin{aligned} \text{maximize} \quad & L \bullet X \\ \text{subject to} \quad & E_{ii} \bullet X = 1, \quad (i = 1 \sim n) \\ & E_{ij} \bullet X = 1, \quad (i, j) \in M \\ & X \succeq O \end{aligned}$$

E_{ij} is an $n \times n$ matrix in which only the (i, j) element is 1, and all others are 0. M is a set of *must-link*.



(a) Grouping patterns

(b) Sort pattern groups

Figure 2. Clustering process using label matrix

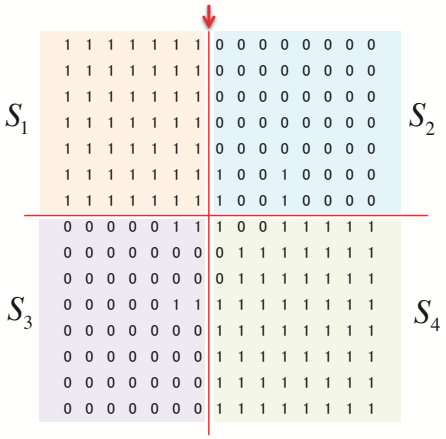


Figure 3. Clustering Boundary

Although available constraints are not limited to must-link, meaning we can also use *cannot-link*, it is very difficult to select applicable cannot-links during multi-class clustering because the partitioning order determined in the graph cut process is usually unpredictable in advance. Figure 1 gives an idea of the difficulty of using cannot-link. There are three data in the figure - a, b, c - and cannot-link is applicable only at the second cut. It cannot be used at the first cut because b and c are in the same cluster at that time.

There are several freely available SDP solvers that we can use to obtain an approximate solution $\tilde{X}$. Although we need to decompose $\tilde{X}$ to obtain partitioning label **u**, we found a way to complete partitioning by using only $\tilde{X}$. We explain this method in the next section.

III. Clustering through Swapping Rows and Columns in a Label Matrix

In this section, we describe a concrete partitioning procedure using matrix $\tilde{X}$, which is given as the SDP solution, and then an entire clustering with an iterative dual-partitioning process.

As described in the previous section, we solve the maximum cut problem with relaxed SDP, so the elements

Algorithm 1 Constrained Iterative Graph Cut Clustering

```
Input: D_0      // Dataset
       W        // Weight Matrix
       M        // Must-Link Set
       K        // Number to be Clustered
Output: C = {D_1, D_2, ..., D_K}    // K clusters

Let C = D_0
for i = 1 to K-1 do
    Select the largest cluster D_t^max
    Extract a subset of must-link constraints M_t^sub related to D_t^max
    Input D_t^max and M_t^sub to SDP solver and get divided clusters {D_t^1, D_t^2}
    Subtract D_t^max from C
    Add {D_t^1, D_t^2} to C
end for
```

of $\tilde{X}$ are assigned a real value ranging from -1 to 1. We therefore decided on a different approach in which we first binarize $\tilde{X}$ with 0-1 values, then swap rows and columns to maximize the evaluation measure, and finally determine the partitioning border.

The concrete procedures are as follows.

1) Each element of $\tilde{X}$ is binarized as follows.

$$\tilde{X}_{ij} = \begin{cases} 1, & \text{if } \tilde{X}_{ij} \geq 0 \\ 0, & \text{if } \tilde{X}_{ij} < 0 \end{cases}$$

The value does not matter because we treat 0 and 1 as a character in the following steps.

2) For each row, treat the column's value as a character (0 or 1) and make a string (or pattern) by concatenating each character in the original order. Next, make groups of the same string (select a representative of each kind of string). Figure 2(a) illustrates this procedure.

3) Determine the most frequent string s_0, and calculate the Hamiltonian distance between s_0 and the other strings. Next, align other strings in descending order of the Hamming distance. String s_1 is the most

TABLE I.
DIRECTORIES USED IN ODP CORPUS

No.	Directory	#data
1	Anomalies and Alternative Science	47
2	Science in Society	45
3	Environment/Water Resources	42
4	Astronomy	24
5	Technology/Structural Engineering	24
6	Agriculture	19
7	Biology/Genetics	16
8	Social Sciences/Linguistics	15
9	Physics	15
10	Earth Sciences	11
11	Math	10
12	Chemistry	6

TABLE II.
DATASETS IN ODP CORPUS

Dataset	#data	#cluster
odp_odd	154	6
odp_even	120	6
odp_small	92	7
odp_all	274	12

similar to s_0. Figure 2(b) illustrates this procedure.

4) Determine the partitioning boundary according to the following measure.

$$F(i,j) = \sum_{k=1}^{4} -p^{S_i}\log(p^{S_i}) - (1-p^{S_i})\log(1-p^{S_i})$$

(i,j) represents the partitioning boundary. If we partition the above aligned matrix in the boundary between i's row and j's row (i.e., also in the boundary of i's column and j's column), there are four partitioned areas in the matrix. p_0^k and p_1^k are the probabilities of 0 and 1, respectively, that appears in the area k. Thus, $F(i,j)$ is the sum of the entropy in four areas when partitioned between ith and jth row (and column). The more clearly partitioned, $F(i,j)$ becomes lower.

5) Determine the boundary at the lowest $F(i,j)$.

This is a heuristic method because the original problem is a combinatorial one and practically intractable. There is no guarantee for obtaining global optimum. However, experimentally it works well, as described in the next section.

We describe an entire procedure of our clustering algorithm in **Algorithm 1**.

IV. EXPERIMENTS

A. Datasets

We evaluated our proposed method on two Web page corpora. One is a ODP corpus, a set of web pages extracted from the Open Directory Project (ODP)[1] by ourselves. We selected 12 subdirectories from the the "Science" top directory, and downloaded top pages of the Web sites listed in each directory. We removed tags and stopwords from the pages, and stemmed each word. The summary of each directory is listed in Table I.

We treated each directory as a target cluster, and made four datasets using those clusters. One is a dataset (odp_all) using all the directories in the corpus. The other two (odp_odd and odp_even) are half size of odp_all. The directories of odp_odd and odp_even are selected from the odd and even number ones in Table I, respectively. The final one (odp_small) is a set of small directories (No.6∼12) that include under 20 data. We summarize about datasets in Table II.

We also used the WebKB corpus [2]. This corpus consists of seven datasets, and each one has fixed five clusters named "Cornel", "Texas", "Washington", "Wisconsin" and "misc", respectively. Since the last "misc" cluster consists of Web pages from miscellaneous universities and lacks unity, we removed it from each dataset. We also removed department dataset because it has only one page for each cluster. The datasets are summarized in Table III. We applied the same preprocessing as ODP corpus and evaluated each method on all the datasets.

TABLE III.
WEBKB CORPUS

Dataset	#data	#cluster
student	558	4
faculty	153	4
staff	46	4
course	244	4
project	86	4
other	3033	4

B. Compared methods

We compared our proposed method with other three methods. The notation and brief introduction of each method is listed below.

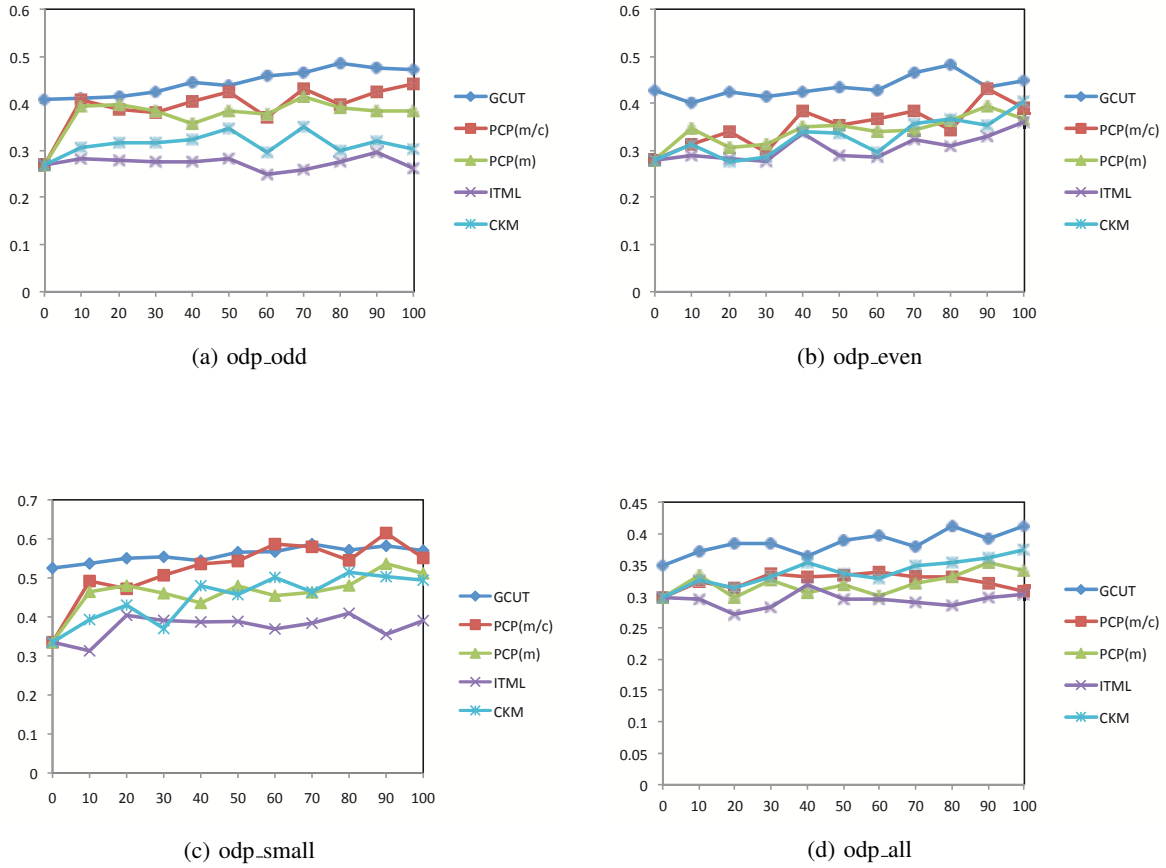
GCUT This is our proposed method. We calculated the Euclid distance for the weight of the graph edge, which is indicated as w_{ij} in the maximum graph cut problem in Section II. We used the SDPT3 package [3] to solve SDP. The default parameters are used for each run.

PCP PCP is one of the state of the art distance metric learning methods proposed by Li [10]. It learns a kernel matrix using the same SDP formulation with ours. The difference between two methods lies in the usage of the solution matrix. PCP uses it as a kernel matrix for kernel k-means while ours uses it for iterative graph cut. The weight of the graph edge and the parameters for SDPT3 are the same with GCUT. Since this method can use both must/cannot-link constraints, we conducted two trials. One is the trial using only must-link constraints, the other uses both must/cannot-link constraints. the

[1] http://www.dmoz.org/

[2] http://www.cs.cmu.edu/afs/cs.cmu.edu/project/theo-20/www/data/

[3] http://www.math.nus.edu.sg/ mattohkc/sdpt3.html



(a) odp_odd (b) odp_even

(c) odp_small (d) odp_all

Figure 4. Results of ODP corpus (horizontal axis is the number of constraints and vertical axis is NMI)

former is denoted by PCP(m) and the latter is PCP(m/c).

ITML ITML is an another distance metric learning method proposed by Jain [13]. It learns a transform matrix to calculate desired distance. Since this method follows online learning process, we tuned its learning parameter η by selecting the best value from 0.1 to 1.0 with 0.1 steps. Clustering is done by normal k-means with learned Euclid distance. Since cannot-link on this method showed terrible performance deterioration, we applied only must-link for it.

CKM CKM is the constrained k-means clustering algorithm (called COP-Kmeans) proposed by Wagstaff [14]. Since cannot-link often caused deadlock and stopped all the algorithm procedure, we applied must-link only as well as ITML.

C. Other settings

We use normalized mutual information (NMI) to measure the clustering accuracy. NMI is calculated by the following formula.

$$\mathrm{NMI}(C,T) = \frac{I(C,T)}{\sqrt{H(C)H(T)}}$$

where C is the set of clusters returned by each algorithm and T is the set of true clusters. $I(C,T)$ is the mutual information between C and T, and $H(C)$ and $H(T)$ are the entropies.

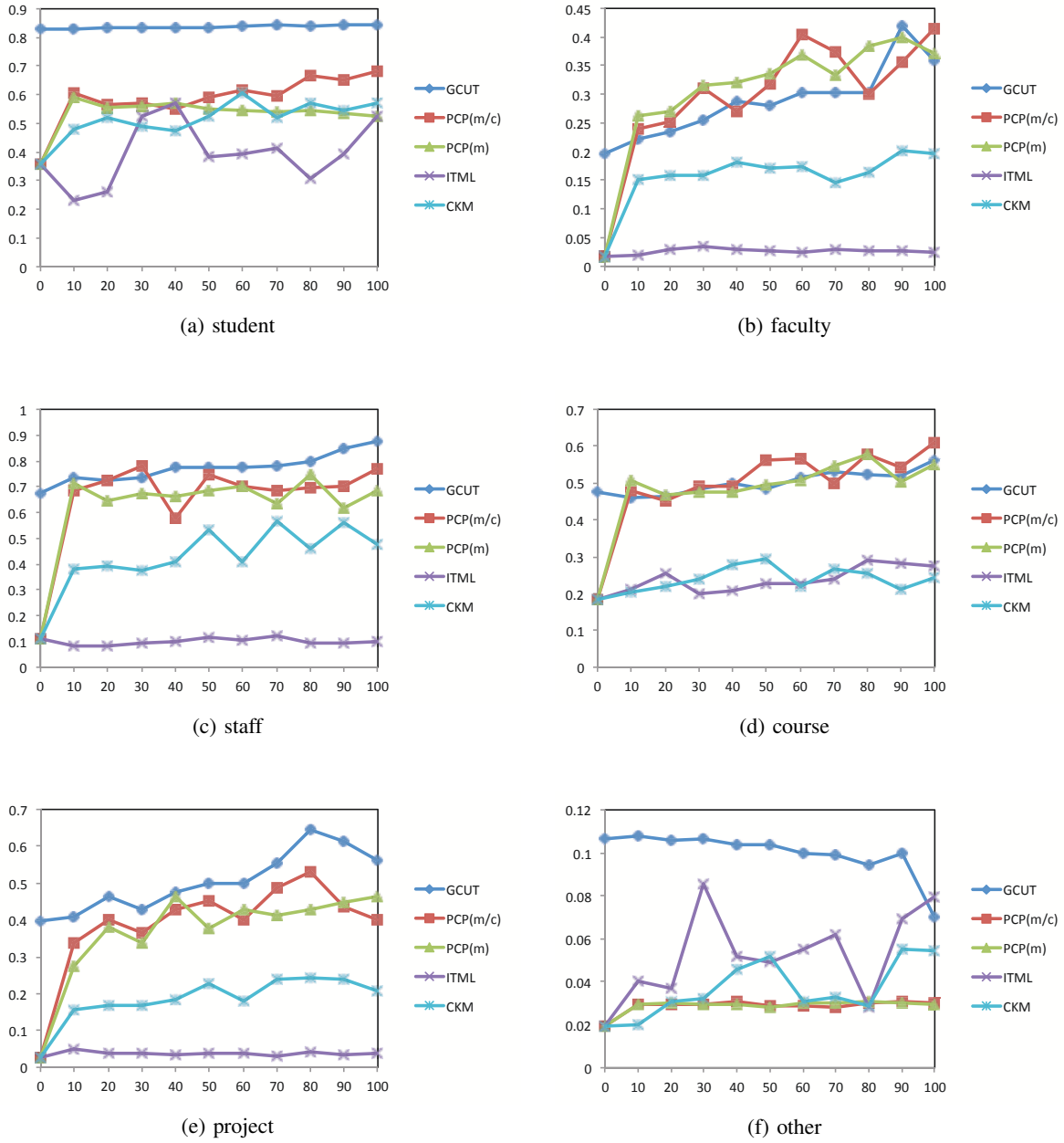
Constraints are selected randomly. We changed the number of constrains from 0 to 100 with 10 steps. For each number of constraints, we selected 10 different sets of constraints and used the same sets for each method. The NMI is calculated as the average value of those 10 sets.

D. Results

Figure 4 is the results of the ODP corpus. The horizontal axis is the number of constraints and the vertical axis is the value of normalized mutual information (NMI).

In this corpus, GCUT outperformed other methods in all the datasets, especially at the points where the number of constraints is small.

PCP(m/c) showed comparable or slightly better performance at some points in the odp_odd, the odp_even and



(a) student (b) faculty

(c) staff (d) course

(e) project (f) other

Figure 5. Results of the WebKB corpus (horizontal axis is the number of constraints and vertical axis is NMI)

odp_small datasets though it remained the second best or worse in other points. PCP(m) is slightly worse than PCP. CKM outperformed other methods without GCUT in the odp_all dataset. ITML did not show the good results in this corpus.

Figure 5 shows the results of the WebKB corpus. The meaning of the horizontal and vertical axis is the same as the ODP corpus. In this corpus, GCUT indicated the best results in four datasets. The results in the other two datasets is comparable and slightly worse than the other methods. GCUT showed clearly better performance especially in the student and "other" datasets whose number of data is relatively larger than others. The performance of all methods in "other" dataset is low because the topic of this dataset is diverse and does not have unity as a cluster. GCUT also showed better performance than other methods in the staff and project datasets whose number of data is relatively small. In those datasets, performance gap between GCUT and others widened as the number of constraints increased. PCP showed comparable and slightly better performance in the course and faculty datasets. We did not observe significant difference between PCP(m/c) and PCP(m) in this corpus. The performance of CKM and ITML remained worse than GCUT and PCP in all the datasets.

The performance of GCUT as well as all the other

methods does not grow monotonically and sometimes drops despite the increase of constraints. This is because the effectiveness of constraints are generally quite uneven. Some sets of constraints may work better for some methods. On the other hand some sets may bring negative effect (e.g. because of must-link constraints related outliers).

V. Discussions

Our proposed clustering method (GCUT) repeatedly divides the largest cluster into two sub-clusters until the given number of clusters is obtained. This procedure delivers a good property compared to a one-time multi-class clustering approach represented by PCP as shown in the experiments. The results indicate that we can obtain more accurate clusters if we interpret the SDP problem described in Section II as a constrained graph cut problem and use its solution for iterative two-class clustering.

As described in Section I, our method uses the same SDP formulation as PCP. However the purpose, derivation and interpretation of the solution for our method is different from PCP. In this section, we explain a brief introduction of PCP and clarify the difference from our method, and then discuss the cause of the experimental results in the previous section.

PCP is a method to produce a kernel matrix of a dataset by projecting original feature vectors to a higher dimensional space. Constraints are used as desired inner product values for some selected data pairs in the projected feature space. In order to propagate the effect of the constraints to other data pairs, Li et al. formulated an optimization problem according to a well-known regularization in spectral graph theory.

Optimization Problem derived in PCP

$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\sum_{i,j=1}^{n} w_{i,j}\left|\left|\frac{\phi(\mathbf{x}_i)}{\sqrt{d_{ii}}}-\frac{\phi(\mathbf{x}_j)}{\sqrt{d_{jj}}}\right|\right|_F^2 \\
\text{subject to} \quad & <\phi(\mathbf{x}_i),\phi(\mathbf{x}_i)>_F = 1 \quad i=1,2,...,n \\
& <\phi(\mathbf{x}_i),\phi(\mathbf{x}_j)>_F = 1 \quad {}^{\forall}(\mathbf{x}_i,\mathbf{x}_j)\in M \\
& <\phi(\mathbf{x}_i),\phi(\mathbf{x}_j)>_F = 0 \quad {}^{\forall}(\mathbf{x}_i,\mathbf{x}_j)\in C
\end{aligned}
$$

Here, $\phi(\mathbf{x}_i)$ is a feature vector in the projected space, w_{ij} is an initial similarity between data i and j, d_{ii} is $\sum_k w_{ik}$, and $<\cdot,\cdot>_F$ indicates inner product calculation in the projected space. The objective function of the above problem can be finally transformed into the formula $L\bullet X$ that is the same one as described in Section II.

In this way, GCUT and PCP solve the same SDP problem except for the use of cannot-link. However their derivations of the problem are different from each other like following.

1) PCP places the SDP problem as a basis to define a proximity measure in a dataset. Thus it solves a SDP problem only once for a clustering trial. The proximity measure is actually got as a kernel matrix.
2) The SDP problem in GCUT is a constrained graph cut clustering problem itself. Thus it iterates to solve SDP $k-1$ times. k is a target number of clusters.

Though the reason for the performance increase of GCUT compared with PCP superficially seems to be multiple SDP executions, it is more important that the derivations of the SDP problem in both methods are different. GCUT derives from a constrained graph cut problem while PCP derives from a problem to define a desired proximity measure.

VI. Conclusions

In this paper, we proposed a constrained clustering method that is based on a graph-cut problem formalized by semi-definite programming and deterministic iterative two-class partitioning approach. While graph-cut based clustering is a particularly promising way to improve conventional techniques like k-means method, few methods have been proposed, which can naturally incorporate constraint like must-link.

Our method has the advantages of more convenient constraint incorporation compared to other graph-cut based method such as spectral clustering and can utilize SDP's solution matrix more appropriately compared with other SDP-based methods. Since our method adopts deterministic clustering approach unlike k-means using random seeds, the performance is stable and robust to outliers. These advantages were clearly demonstrated through experiments using many datasets from two Web corpus. Results showed that our proposed clustering method constantly outperformed conventional methods in many cases and utilized constraints effectively.

A few problems still remain in this work. First, we need to investigate how the constraint quality influences the clustering. This is an active learning problem and in the future we aim to develop a new active-learning technique by utilizing the properties of our clustering methods. Second, we need to develop a constraint propagation method to improve clustering accuracy even if the number of constraint is small. There are already various propagation methods in place [15], but we need something more powerful to improve the effectiveness of very small constraints.

The advantages of our proposed clustering is efficiency, especially in the case of small number of constraints. Thus we are planning to apply this clustering method to interactive (Web) clustering with GUI [12].

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