Document Clustering Using Locality Preserving Indexing

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Abstract

We propose a novel document clustering method, which aims to cluster the documents into different semantic classes. The document space is generally of high dimensionality, and clustering in such a high dimensional space is often infeasible due to the curse of dimensionality. By using Locality Preserving Indexing (LPI), the documents can be projected into a lower dimensional semantic space in which the documents related to the same semantics are close to each other. Different from previous document clustering methods based on Latent Semantic Indexing (LSI) or Non-negative Matrix Factorization (NMF), our method tries to discover both the geometric and discriminating structures of the document space. Theoretical analysis of our method shows that LPI is an unsupervised approximation of the supervised Linear Discriminant Analysis (LDA) method which give the intuitive motivation of our method. Extensive experimental evaluations are performed on Reuters-21578 and TDT2 data sets.

Keywords

Document Clustering, Locality Preserving Indexing, Dimensionality Reduction, Semantics

1 INTRODUCTION

Document clustering is one of the most crucial techniques to organize the documents in an unsupervised manner. It received a lot of attentions in recent years [18][28][27][17][24].

Many clustering methods have been proposed, such as k-means [20], naïve Bayes or Gaussian mixture model [16][1][18], single-link [16] and DBSCAN [11]. From different perspectives, these clustering methods can be classified into agglomerative or divisive, hard or fuzzy, deterministic or stochastic. The typical data clustering tasks are directly performed in the data space. However, the document space is always of very high dimensionality, ranging from several hundreds to thousands. Due to the consideration of the *curse of dimensionality*, it is desirable to first project the documents into a lower dimensional subspace in which the semantic structure of the document space becomes clear. In the low dimensional semantic space, the traditional clustering algorithms can be then applied. To this end, spectral clustering [23][21], clustering using LSI [29] and clustering based on non-negative matrix factorization [28][27] are most well-known techniques.

Some recently work on spectral clustering shows its capability to handle highly non-linear data (the data space has high curvature at every local area). Also, its strong connections to differential geometry make it capable of discovering the manifold structure of the document space. The spectral clustering usually cluster the data points using the top eigenvectors of *graph Laplacian*, which is defined on the affinity matrix of data points. From the graph partitioning perspective, the spectral clustering tries to find the best cut of the graph so that the predefined criterion function can be optimized. Many criterion functions, such as the ratio cut [4], average association [23], normalized cut [23], and min-max cut [8] have been proposed along with the corresponding eigen-problem for finding their optimal solutions. From the perspective of dimensionality reduction, spectral clustering embeds the data points into a low dimensional space where the traditional clustering algorithm (e.g., k-means) is then applied. One major drawback of these spectral clustering algorithms might be that they use the non-linear embedding (dimensionality reduction) which is only defined on "training" data. They have to use all the data points to learn the embedding. When the data set is very large, to learn such an embedding is computational expensive, which restricts the application of spectral clustering on large data set.

Latent Semantic Indexing (LSI) [7] is one of the most popular linear document indexing methods which produces low dimensional representations. LSI aims to find the best subspace approximation to the original document space in the sense of minimizing the *global* reconstruction error. In other words, LSI seeks to uncover the most representative features rather the most discriminative features for document representation. Therefore, LSI might not be optimal in discriminating documents with different semantics which is the ultimate goal of clustering.

Recently, Xu et al. applied the Non-negative Matrix Factorization (NMF) algorithm for document clustering [28][27]. They model each cluster as a linear combination of the data points, and each data point as a linear combination of the clusters. And they compute the linear coefficients by minimizing the *global* reconstruction error of the data points using Non-negative Matrix Factorization. Thus, NMF method still focuses on the global geometrical structure of document space. Moreover, the iterative update method for solving NMF problem is computational expensive.

In this paper, we propose a novel document clustering algorithm by using Locality Preserving Indexing (LPI). Different from LSI which aims to discover the global Euclidean structure, LPI aims to discover the *local* geometrical structure. LPI can have more discriminating power. Thus, the documents related to the same semantics are close to each other in the low dimensional representation space. Also, LPI is derived by finding the optimal linear approximations to the eigenfunctions of the Laplace Beltrami operator on the document manifold. Laplace Beltrami operator takes the second order derivatives of the functions on the manifolds. It evaluates the smoothness of the functions. Therefore, it can discover the non-linear manifold structure to some extent. Some theoretical justifications can be traced back to [15][14]. The original LPI is not optimal in the sense of computation in that the obtained basis functions might contain a trivial solution. The trivial solution contains no information and thus useless for document indexing. A modified LPI is proposed to obtain better document representations. In this low dimensional space, we then apply traditional clustering algorithms such as k-means to cluster the documents into semantically different classes.

The rest of this paper is organized as follows: In Section 2, we give a brief review of LSI and LPI. Section 3 introduces our proposed document clustering algorithm. Some theoretical analysis is provided in Section 4. The experimental results are shown in Section 5. Finally, we give concluding remarks and future work in Section 6.

2 A BRIEF REVIEW OF LSI AND LPI

LSI is one of the most popular algorithms for document indexing. It is fundamentally based on SVD (Singular Value Decomposition). Given a set of documents $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^m$, they can be represented as a term-document matrix $X = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n]$. Suppose the rank of X is r, LSI decomposes the X using SVD as follows:

$$X = U\Sigma V^T,$$

where $\Sigma = diag(\sigma_1, \cdots, \sigma_r)$ and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$ are the singular values of X, $U = [\mathbf{a}_1, \cdots, \mathbf{a}_r]$ and $\mathbf{a}_i$ is called left singular vector, $V = [\mathbf{v}_1, \cdots, \mathbf{v}_r]$ and $\mathbf{v}_i$ is called right singular vector. LSI use the first k vectors in U as the transformation matrix to embed the original documents into a k dimensional subspace. It can be easily checked that the column vectors of U are the eigenvectors of XX^T. The basic idea of LSI is to extract the most representative features and at the same time the reconstruction error can be minimized. Let $\mathbf{a}$ be the transformation vector. The objective function of LSI can be stated below:

$$\begin{aligned} \mathbf{a}_{opt} &= \arg\min_{\mathbf{a}} \|X - \mathbf{a}\mathbf{a}^T X\|^2 \\ &= \arg\max_{\mathbf{a}} \mathbf{a}^T X X^T \mathbf{a}, \end{aligned}$$

with the constraint

$$\mathbf{a}^T\mathbf{a} = 1.$$

Since XX^T is symmetric, the basis functions of LSI are orthogonal. It would be important to note that XX^T becomes the data covariance matrix if the data points have a zero mean, i.e., $X\mathbf{e} = \mathbf{0}$ where $\mathbf{e} = [1, \cdots, 1]^T$. In such a case, LSI is identical to Principal Component Analysis [10]. More details on theoretical interpretations of LSI using SVD can refer to [2][9][22].

Different from LSI which aims to extract the most representative features, LPI aims to extract the most discriminative features. Given a similarity matrix S, LPI can be obtained by solving the following minimization problem:

$$\begin{aligned}\mathbf{a}_{opt} &= \arg\min_{\mathbf{a}} \sum_{i=1}^{m}\sum_{j=1}^{m}\left(\mathbf{a}^T\mathbf{x}_i - \mathbf{a}^T\mathbf{x}_j\right)^2 S_{ij} \\ &= \arg\min_{\mathbf{a}} \mathbf{a}^T X L X^T \mathbf{a},\end{aligned}$$

with the constraint

$$\mathbf{a}^T X D X^T \mathbf{a} = 1,$$

where $L = D - S$ is the *graph Laplacian* [5] and $D_{ii} = \sum_j S_{ij}$. D_{ii} measures the local density around $\mathbf{x}_i$. LPI constructs the similarity matrix S as:

$$S_{ij} = \begin{cases} \mathbf{x}_i^T\mathbf{x}_j, & \text{if } \mathbf{x}_i \text{ is among the } p \text{ nearest neighbors of } \mathbf{x}_j \\ & \text{or } \mathbf{x}_j \text{ is among the } p \text{ nearest neighbors of } \mathbf{x}_i \\ 0, & \text{otherwise.} \end{cases}$$

Thus, the objective function in LPI incurs a heavy penalty if neighboring points $\mathbf{x}_i$ and $\mathbf{x}_j$ are mapped far apart. Therefore, minimizing it is an attempt to ensure that if $\mathbf{x}_i$ and $\mathbf{x}_j$ are “close” then y_i $(= \mathbf{a}^T\mathbf{x}_i)$ and y_j $(= \mathbf{a}^T\mathbf{x}_j)$ are close as well [14]. Finally, the basis functions of LPI are the eigenvectors associated with the smallest eigenvalues of the following generalized eigen-problem:

$$XLX^T\mathbf{a} = \lambda XDX^T\mathbf{a}.$$

3 THE PROPOSED METHOD

In this section, we describe our clustering algorithm which can be thought of as a combination of subspace learning and k-means. We begin with the motivations of our work.

3.1 Motivation

In this section, we will provide some motivations about the reasoning of LPI follow by a traditional clustering algorithm like k-means.

Generally, the document space is of high dimensionality, typically ranging from several thousands to tens of thousands. Learning in such a high dimensional space is extremely difficult due to the *curse of dimensionality.* Thus, document clustering necessitates some form of dimensionality reduction. One of the basic assumptions behind data clustering is that, if two data points are close to each other in the high dimensional space, they tend to be grouped into the same cluster. Therefore, the optimal document indexing method should be able to discover the local geometrical structure of the document space. To this end, the LPI algorithm is of particular interest. LSI is optimal in the sense of reconstruction. It respects the global Euclidean structure while fails to discover the intrinsic geometrical structure especially when the document space is non-linear, see [14] for details.

Another consideration is due to the discriminating power. One can expect that the documents should be projected into the subspace in which the documents with different semantics can be well separated while the documents with common semantics can be clustered. As indicated in [14], LPI is an optimal unsupervised approximation to the Linear Discriminant Analysis algorithm which is supervised. Therefore, LPI can have more discriminant power than LSI. There are some other linear subspace learning algorithms such as informed projection [6] and Linear Dependent Dimensionality Reduction [25]. However, none of them has shown discriminating power.

Finally, it would be interesting to note that LPI is fundamentally based on manifold theory [14][15]. LPI tries to find a linear approximation to the eigenfunctions of the Laplace Beltrami operator on the compact Riemannian manifold, see [15] for details. Therefore, LPI is capable of discovering the nonlinear structure of the document space to some extent.

3.2 Clustering Based on Locality Preserving Indexing

Given a set of documents $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n \in \mathbb{R}^m$. Suppose $\mathbf{x}_i$ has been normalized to 1, thus the dot product of two document vectors is exactly the cosine similarity of the two documents. Our clustering algorithm is performed as follows:

1. **Constructing the adjacency graph**: Let G denote a graph with n nodes. The i-th node corresponds to the document $\mathbf{x}_i$. We put an edge between nodes i and j if $\mathbf{x}_i$ and $\mathbf{x}_j$ are "close", i.e. $\mathbf{x}_i$ is among p nearest neighbors of $\mathbf{x}_j$ or $\mathbf{x}_j$ is among p nearest neighbors of $\mathbf{x}_i$. Some fast p nearest neighbor search algorithms can be used here to improve the overall speed [12][30].

2. **Choosing the weights**: If nodes i and j are connected, put

$$S_{ij} = \mathbf{x}_i^T \mathbf{x}_j.$$

   Otherwise, put $S_{ij} = 0$. The weight matrix S of graph G models the local structure of the document space. We define D as a diagonal matrix whose entries are column (or row, since S is symmetric) sums of S, i.e., $D_{ii} = \sum_j S_{ji}$. We also define $L = D - S$, which is called the Laplacian matrix in spectral graph theory [5].

3. **Data Preprocessing and SVD Projection**: We remove the weighted mean of $\mathbf{x}$ from each $\mathbf{x}$

$$\hat{\mathbf{x}} = \mathbf{x} - \bar{\mathbf{x}}, \quad \bar{\mathbf{x}} = \frac{1}{(\sum_i D_{ii})} \left(\sum_i \mathbf{x}_i D_{ii} \right),$$

   and project the document vector into the SVD subspace by throwing away those *zero* singular values.

$$\widehat{X} = U \Sigma V^T,$$

   where $\widehat{X} = [\hat{\mathbf{x}}_1, \cdots, \hat{\mathbf{x}}_n]$. We denote the transformation matrix of SVD by W_{SVD}, i.e., $W_{SVD} = U$. After SVD projection, the document vector $\hat{\mathbf{x}}$ becomes $\tilde{\mathbf{x}}$:

$$\tilde{\mathbf{x}} = W_{SVD}^T \hat{\mathbf{x}}.$$

   After this step, the term-document matrix X becomes $\widetilde{X} = [\tilde{\mathbf{x}}_1, \cdots, \tilde{\mathbf{x}}_n]$.

4. **LPI Projection**: Compute the eigenvectors and eigenvalues for the generalized eigenproblem:

$$\widetilde{X} L \widetilde{X}^T \mathbf{a} = \lambda \widetilde{X} D \widetilde{X}^T \mathbf{a}. \quad (1)$$

Let $W_{LPI} = [\mathbf{a}_1, \cdots, \mathbf{a}_k]$ be the solutions of Eq. (1), ordered according to their eigenvalues, $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k$. Thus, the embedding is as follows:

$$\mathbf{x} \rightarrow \mathbf{y} = W^T \hat{\mathbf{x}},$$

$$W = W_{SVD} W_{LPI}, \quad \text{and} \quad \hat{\mathbf{x}} = \mathbf{x} - \frac{1}{(\sum_i D_{ii})} \left(\sum_i \mathbf{x}_i D_{ii} \right),$$

where $\mathbf{y}$ is a k-dimensional representation of the document $\mathbf{x}$. W is the transformation matrix.

5. **Clustering in the Lower Dimensional Semantic Space**: Now we get lower dimensional representations of the original documents. In the reduced semantic space, those documents belonging to the same underlying class are close to one another. The traditional clustering methods (we choose k-means in this paper) can be applied in the reduced semantic space. The connection between LPI and LDA motivates us to use $k-1$ eigenvectors where k is the number of clusters [14][10].

3.3 Computational Analysis

In this section, we provide a computational analysis of our algorithm. One of the major modifications over the original LPI [14] lies in the third step of our algorithm. In the new algorithm, we remove the weighted mean of the document vectors and use SVD to ensure that the term-document matrix $\widetilde{X}$ is of full rank in row.

Making the matrix $\widetilde{X}$ of full rank in row can guarantee that the matrix $\widetilde{X} D \widetilde{X}^T$ is positive definite, which is necessary in solving the generalized eigen-problem (Eq. (1)) in the fourth step [13].

In the following, we discuss why it is necessary to remove the weighted mean from the original document vectors. We first analyze the properties of the eigenvector of the eigen-problem (Eq. (1)). Let $\mathbf{1} = [1, 1, \cdots, 1]^T$. We have the following theorem.

Theorem 1 *If there exists $\boldsymbol{a}_0$ which satisfies $\widetilde{X}^T \boldsymbol{a}_0 = \boldsymbol{1}$ (in other words, the vector **1** in the* *space spanned by the column vectors of* $\widetilde{X}^T$*),* $\mathbf{a}_0$ *is the eigenvector of Eq. (1) with respect to eigenvalue 0.*

Proof

$$
\begin{aligned}
\widetilde{X}L\widetilde{X}^T\mathbf{a}_0 &= \widetilde{X}(D-S)\mathbf{1} = \widetilde{X}(D\mathbf{1}-S\mathbf{1}) \\
&= \widetilde{X}\mathbf{0} = \mathbf{0} = 0\widetilde{X}D\widetilde{X}^T\mathbf{a}_0.
\end{aligned}
$$

Therefore, $\mathbf{a}_0$ is the eigenvector of Eq. (1) with respect to eigenvalue 0. $\blacksquare$

Since the matrices $\widetilde{X}L\widetilde{X}^T$ and $\widetilde{X}D\widetilde{X}^T$ are both positive semi-definite, the eigenvalues of Eq. (1) are no less than zero. Therefore, $\mathbf{a}_0$ will be the first eigenvector. However, it is clearly of no use for document representation since all the document vectors collapse into a single point along this direction.

The LPI eigen-problem (Eq. (1)) can be written as the Rayleigh Quotient format [13]:

$$
\mathbf{a}_0 = \arg\min_{\mathbf{a}} \frac{\mathbf{a}^T\widetilde{X}L\widetilde{X}^T\mathbf{a}}{\mathbf{a}^T\widetilde{X}D\widetilde{X}^T\mathbf{a}}, \quad \text{and} \quad \mathbf{a}_i = \arg\min_{\mathbf{a}_i^T\widetilde{X}D\widetilde{X}^T\mathbf{a}_j=0,\ 0\le j<i} \frac{\mathbf{a}^T\widetilde{X}L\widetilde{X}^T\mathbf{a}}{\mathbf{a}^T\widetilde{X}D\widetilde{X}^T\mathbf{a}}.
$$

If $\mathbf{1}$ is in the space spanned by the column vectors of $\widetilde{X}^T$, the eigenvectors of LPI eigen-problem (Eq. (1)) have the following property:

$$
\widetilde{X}^T\mathbf{a}_0 = \mathbf{1} \quad \text{and} \quad \mathbf{a}_i^T\widetilde{X}D\mathbf{1} = 0,\ i>0. \tag{2}
$$

Now let us consider the data preprocessing step of our algorithm. We can show that, after removing the weighted mean of document vectors, for any vector $\mathbf{a}$, $\mathbf{a}^T\widetilde{X}D\mathbf{1} = 0$.

$$
\begin{aligned}
\mathbf{a}^T\widetilde{X}D\mathbf{1} &= \mathbf{a}^T W_{SVD}^T\hat{X}D\mathbf{1} = \mathbf{a}^T W_{SVD}^T[\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \cdots, \hat{\mathbf{x}}_n]D\mathbf{1} \\
&= \mathbf{a}^T W_{SVD}^T(\sum_i \hat{\mathbf{x}}_i D_{ii}) = \mathbf{a}^T W_{SVD}^T(\sum_i \mathbf{x}D_{ii} - \sum_i \bar{\mathbf{x}}D_{ii}) \\
&= \mathbf{a}^T W_{SVD}^T(\sum_i \mathbf{x}D_{ii} - \bar{\mathbf{x}}\sum_i D_{ii}) \\
&= \mathbf{a}^T W_{SVD}^T\mathbf{0} = \mathbf{0}.
\end{aligned}
$$

Thus the preprocessing step of our algorithm can guarantee that the solutions of Eq. (1) will not contain the trivial eigenvector as described above and all the eigenvectors will satisfy the second part of Eq. (2).

4 THEORETICAL ANALYSIS

In this section we give the theoretical analysis of our algorithm. First, we will discuss the relationship between LPI, LSI and LDA. We will show that the key difference between them is the different ways to construct the adjacency graph. The adjacency graph construction in LPI gives a best approximation to LDA which is supervised. Second, our clustering algorithm has intrinsic connections to spectral clustering and manifold learning. This makes it clear that our algorithm is capable of dealing with complex data.

4.1 Relationship Between LPI and LSI

LPI is essentially obtained from a graph model. The graph structure represents the geometrical structure of the document space. In our algorithm, a p-nearest neighbor graph is constructed to discover the *local* manifold structure. Intuitively, LPI with a complete graph should discover the *global* structure. In this subsection, we present a theoretical analysis on the relationship between LPI and LSI. Specifically, we show that LPI with a complete graph is similar to LSI.

As shown in Section 2, LSI tries to solve the maximum eigenvalue problem:

$$XX^T\mathbf{a} = \lambda\mathbf{a}.$$

In LPI, recall that the weight on an edge linking $\mathbf{x}_i$ and $\mathbf{x}_j$ is set to their inner product $\mathbf{x}_i^T\mathbf{x}_j$. Thus, the affinity matrix S of the complete graph can be written as X^TX. Since we first apply SVD to remove the components corresponding to the zero singular value, the matrix XX^T is of full rank. The generalized minimum eigenvalue problem of LPI can be written as follows:

$$\begin{aligned}
& XLX^T\mathbf{a} = \lambda XDX^T\mathbf{a} \\
\Rightarrow\quad & X(D-S)X^T\mathbf{a} = \lambda XDX^T\mathbf{a} \\
\Rightarrow\quad & XSX^T\mathbf{a} = (1-\lambda)XDX^T\mathbf{a} \\
\Rightarrow\quad & XX^TXX^T\mathbf{a} = (1-\lambda)XDX^T\mathbf{a}. \qquad (3)
\end{aligned}$$

If we assume the diagonal matrix D is close to the identity matrix, $XDX^T \approx XX^T$, the *minimum* eigenvalues of Eq. (3) correspond to the *maximum* eigenvalues of the following equation:

$$XX^TXX^T\mathbf{a} = \lambda XX^T\mathbf{a}.$$

Since XX^T is of full rank, we get:

$$XX^T\mathbf{a} = \lambda\mathbf{a},$$

which is just the eigenvalue problem of LSI. The above analysis shows that LPI with a complete graph is actually similar to LSI. Both of them discover the global structure. The only difference is that there is a diagonal matrix D in LPI which reflects the importance of the different document vectors. In LSI, every document vector is treated equally important. In LPI, the weight of document $\mathbf{x}_i$ is D_{ii}. We define $\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i$ as the center vector of these document vectors. In complete graph situation, we have

$$\begin{aligned} D_{ii} &= \sum_{j=1}^{n} S_{ij} = \sum_{j=1}^{n}(X^TX)_{ij} = \sum_{j=1}^{n}\mathbf{x}_i^T\mathbf{x}_j \\ &= \mathbf{x}_i^T\sum_{j=1}^{n}\mathbf{x}_j = n\mathbf{x}_i^T\bar{\mathbf{x}} = \delta\mathbf{x}_i^T\frac{\bar{\mathbf{x}}}{||\bar{\mathbf{x}}||}, \end{aligned}$$

where $\delta = n||\bar{\mathbf{x}}||$ is a constant. Note that all the $\mathbf{x}_i$'s are normalized to 1. Thus they are distributed on a unit hypersphere. $\bar{\mathbf{x}}/||\bar{\mathbf{x}}||$ is also on this unit hypersphere. Thus, D_{ii} evaluates the cosine of the angle between vectors $\mathbf{x}_i$ and $\bar{\mathbf{x}}$. In other words, D_{ii} evaluates the cosine similarity between document $\mathbf{x}_i$ and the center. The closer to the center the document is, the larger weight it has. Some previous studies [28] show that such D will improve the performance and our experiments will also show this.

4.2 Relationship Between LPI and LDA

In supervised mode, the label information is available, so we can apply Linear Discriminant Analysis (LDA) to reduce the document space to a low dimensional space in which the documents of different classes are far from each other and at the same time the documents of the same class are close to each other. LDA is optimal in the sense of discrimination.

Suppose the data points belong to k classes. LDA can be obtained by solving the following maximization problem:

$$\mathbf{a}_{opt} = \arg\max_{\mathbf{a}} \frac{|\mathbf{a}^T S_b \mathbf{a}|}{|\mathbf{a}^T S_w \mathbf{a}|},$$

$$S_b = \sum_{i=1}^{k} n_i \left(\mathbf{m}^i - \mathbf{m}\right)\left(\mathbf{m}^i - \mathbf{m}\right)^T, \text{ and}$$

$$S_w = \sum_{i=1}^{k} \left(\sum_{j=1}^{n_i} \left(\mathbf{x}_j^i - \mathbf{m}^i\right)\left(\mathbf{x}_j^i - \mathbf{m}^i\right)^T \right).$$

This leads to the following generalized maximum eigenvalue problem:

$$S_b \mathbf{a} = \lambda S_w \mathbf{a}, \tag{4}$$

where $\mathbf{m}$ is the total sample mean vector, n_i is the number of samples in the i^{th} class, $\mathbf{m}^i$ is the average vector of the i^{th} class, and $\mathbf{x}_j^i$ is the j^{th} sample in the i^{th} class. We call S_w the *within-class scatter matrix* and S_b the *between-class scatter matrix*.

We define:

$$W_{ij} = \begin{cases} \frac{1}{n_l}, & \text{if } \mathbf{x}_i \text{ and } \mathbf{x}_j \text{ both belong to the } l^{th} \text{ class;} \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

and

$$D_{ij} = \begin{cases} \sum_j W_{ij}, & \text{if } i = j \\ 0, & \text{if } i \neq j. \end{cases}$$

It is easy to check that the row sum of W is 1, therefore the diagonal matrix D is exactly the identity matrix I.

$$L = D - W = I - W.$$

With some algebraic steps [14], we can show that: if the sample mean is zero, the eigen-problem of Eq. (4) is equivalent to

$$XLX^T\mathbf{a} = \lambda XX^T\mathbf{a}. \tag{6}$$

This analysis tells us that if the affinity matrix S in LPI is defined as the W in Eq. (5), the result of LPI will be identical to the LDA.

In clustering scenario, the label information is not available. Therefore, the matrix W is unknown. However, based on the assumption that neighboring points probably belong to the same underlying class, the affinity matrix S in our LPI algorithm gives an optimal approximation to the similarity matrix W in Eq. (5). Even though the label information is not available, we can still discover the discriminating structure to some extent by using LPI. Thus, in the subspace obtained by LPI, those data points belonging to the same underlying class are close to one another. Note that, an upper bound of the number of non-zero eigenvalues of LDA is $k-1$ where k is the number of classes, please see [10] for details. This motivates us to use $k-1$ eigenvectors in LPI for clustering the documents into k categories.

4.3 The Construction of Affinity Matrix S

The previous two sections show that the key difference among LSI, LPI and LDA is the construction of affinity matrix (the weighted matrix of graph). The LSI tries to discover the global structure (with the complete weighted graph). The LPI tries to discover the local geometrical structure of the document space (with a p-nearest neighbor graph). The LDA is performed in supervised mode, thus the graph can be constructed to reflect the label information. From this point of view, the LPI can be performed in either supervised, unsupervised or semi-supervised manner. The label information can be used to guide the construction of affinity matrix S.

The construction of the affinity matrix is also very important in spectral clustering [23][21] and spectral embedding [3]. It includes two steps: constructing the graph and setting the weight. In our algorithm, we construct a p-nearest neighbor graph and choose the dot product (cosine similarity) as the weight. There are also some other choices as discussed below.

In the step of graph construction, we put an edge between nodes i and j if $\mathbf{x}_i$ and $\mathbf{x}_j$ are "close". There are two variations:

1. ***p*-nearest neighbors**: Nodes i and j are connected by an edge if $\mathbf{x}_i$ is among p nearest

neighbors of $\mathbf{x}_j$ or $\mathbf{x}_j$ is among p nearest neighbors of $\mathbf{x}_i$. The advantage of this method is that it is simpler to choose connected edges, which tends to lead to connected graphs. However, the edges so chosen are less geometrically intuitive.

2. ϵ **neighbors**: Nodes i and j are connected by an edge if $||\mathbf{x}_i - \mathbf{x}_j||^2 < \epsilon$. The advantage of this method is that it is geometrically motivated, and the relationship is naturally symmetric. However, the method often leads to graphs with several disconnected components, and it is difficult to choose ϵ.

In the step of setting the weight, there are several choices:

1. **0-1 weighting**: $S_{ij} = 1$ if and only if nodes i and j are connected by an edge. This is the simplest weighting method and is very easy to compute.

2. **Gaussian kernel weighting**: If nodes i and j are connected, put

   $$S_{ij} = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{t}}.$$

   The Gaussian kernel weighting is also called heat kernel weighting. It has intrinsic connection to the Laplace Beltrami operator on differentiable functions on a manifold [3].

3. **Polynomial kernel weighting**: If nodes i and j are connected, put

   $$S_{ij} = (\mathbf{x}_i^T \mathbf{x}_j + 1)^d.$$

   The parameter d in the equation indicates the degree of the polynomial kernel. Order d polynomial kernel can discover non-linear structure with polynomial basis functions of order d.

4. **Dot-product weighting**:If nodes i and j are connected, put

   $$S_{ij} = \mathbf{x}_i^T \mathbf{x}_j.$$

   Note that if $\mathbf{x}$ is normalized to 1, the dot product of two vectors is equivalent to the cosine similarity of the two vectors. The dot-product weighting can discover the linear Euclidean structure of the document space.

We will compare the different weighting choices in our experiments section.

4.4 Relationship Between Clustering Using LPI and Spectral Clustering

The spectral clustering algorithm [23][26][21] can be thought of as a combination of spectral dimensionality reduction [3] and a traditional clustering method, such as k-means.

Spectral dimensionality reduction or spectral embedding is the key part of spectral clustering. In this step, a weighted graph S is first constructed as described in Section 4.3. We define D as a diagonal matrix whose entries are column (or row, since S is symmetric) sums of S, $D_{ii} = \sum_j S_{ji}$. We also define $L = D - S$. All the spectral clustering methods can be reduced to an eigen-problem. The different methods have different eigen-problems.

1. Normalized cut [23] and Min-Max cut [8] have the following *minimum* eigenvalue problem:

$$L\mathbf{y} = \lambda D\mathbf{y}. \tag{7}$$

2. Ng's method [21] has the following *maximum* eigenvalue problem:

$$D^{-1/2}SD^{-1/2}\mathbf{y} = \lambda\mathbf{y}. \tag{8}$$

3. Average association [23] and Ratio cut [4] have the following *minimum* eigenvalue problem:

$$L\mathbf{y} = \lambda\mathbf{y}. \tag{9}$$

Let $\mathbf{z} = D^{1/2}\mathbf{y}$, with some mathematical deduction of Eq. (7), we have:

$$\begin{aligned}
& L\mathbf{y} = \lambda D\mathbf{y} \\
\Rightarrow\ & (D - S)\mathbf{y} = \lambda D\mathbf{y} \\
\Rightarrow\ & S\mathbf{y} = (1 - \lambda)D\mathbf{y} \\
\Rightarrow\ & SD^{-1/2}D^{1/2}\mathbf{y} = (1 - \lambda)D^{1/2}D^{1/2}\mathbf{y} \\
\Rightarrow\ & SD^{-1/2}\mathbf{z} = (1 - \lambda)D^{1/2}\mathbf{z} \\
\Rightarrow\ & D^{-1/2}SD^{-1/2}\mathbf{z} = (1 - \lambda)\mathbf{z}.
\end{aligned}$$

Thus the *maximum* eigenvalue problem (8) has direct connection to the *minimum* eigenvalue problem (7). Let $\mathbf{y}$ be the eigenvector of Eq. (7) with eigenvalue λ, then $D^{1/2}\mathbf{y}$ is the eigenvector of Eq. (8) with eigenvalue $1 - \lambda$. In the following discussion, we only consider the minimum eigenvalue problem Eq. (7). After the spectral embedding step, the eigenvector $\mathbf{y}$ will be the low dimensional representation of original data points.

Recall the eigen-problem in LPI:

$$XLX^T\mathbf{a} = \lambda XDX^T\mathbf{a}. \tag{10}$$

The eigenvector $\mathbf{a}$ will be the mapping function and $X^T\mathbf{a}$ will be the low dimensional representation of original data points. The LPI imposes a constraint on Eq. (7) that $\mathbf{y}$ should be the linear combination of the column vectors of X^T [15].

The dimensionality reduction method in traditional spectral clustering is non-linear, and the embedding result is only defined on “training” data points. The dimensionality reduction method in our clustering algorithm is linear and the mapping function $\mathbf{a}$ can be applied to the unseen data which provide us more flexibility. When the data set is very large, to learn such an embedding is computational expensive. Since the LPI is linear and defined everywhere, we can use part of the data to learn such an embedding. Our experiments will show this.

It is interesting to see in which condition, the LPI result will be identical to the result of spectral dimensionality reduction in traditional spectral clustering. In this case, our clustering algorithm will be identical to the traditional spectral clustering [3].

Theorem 2 *If X is a full rank square matrix, the embedding result of LPI ($X^T\boldsymbol{a}$ in Eq. (10)) is identical to embedding result in spectral clustering ($\boldsymbol{y}$ in Eq. (7)) if the S is the same.*

Proof Let $\mathbf{y} = X^T\mathbf{a}$. Eq. (10) can be rewritten as follows:

$$XL\mathbf{y} = \lambda XD\mathbf{y}.$$

Since X is a full rank square matrix, the inverse of X always exists. Thus the above equation can be changed to

$$X^{-1}XL\mathbf{y} = \lambda X^{-1}XD\mathbf{y}.$$

Finally, we get

$$L\mathbf{y} = \lambda D\mathbf{y}.$$

Thus we have proved the embedding result of LPI ($X^T\mathbf{a}$ in Eq. (10)) is identical to embedding result of spectral clustering ($\mathbf{y}$ in Eq. (7)). ∎

In our algorithm, we use SVD projection in our data preprocessing step to remove those components corresponding to the zero singular value. If the rank of original term-document matrix X equals to the number of documents, the X will be a full rank square matrix after SVD projection. In document clustering, the number of terms is often larger than the number of documents, thus if all the document vector $\mathbf{x}$ are linearly independent, the X will be a full rank square matrix after SVD projection.

5 EXPERIMENTAL RESULTS

In this section, several experiments were performed to show the effectiveness of our proposed algorithm. Two standard document collections were used in our experiments: Reuters-21578 and TDT2. We compared our proposed algorithm with clustering based on LSI, spectral clustering method, and Non-negative Matrix Factorization clustering method [28].

Table 1: 30 semantic categories from Reuters-21578 used in our experiments

category	**num of doc**	**category**	**num of doc**	**category**	**num of doc**
earn	3713	money-supply	87	iron-steel	37
acq	2055	gnp	63	ipi	36
crude	321	cpi	60	nat-gas	33
trade	298	cocoa	53	veg-oil	30
money-fx	245	alum	45	tin	27
interest	197	grain	45	cotton	24
ship	142	copper	44	bop	23
sugar	114	jobs	42	wpi	20
coffee	110	reserves	38	pet-chem	19
gold	90	rubber	38	livestock	18

Table 2: 30 semantic categories from TDT2 used in our experiments

category	**num of doc**	**category**	**num of doc**	**category**	**num of doc**
20001	1844	20048	160	20096	76
20015	1828	20033	145	20021	74
20002	1222	20039	141	20026	72
20013	811	20086	140	20008	71
20070	441	20032	131	20056	66
20044	407	20047	123	20037	65
20076	272	20019	123	20065	63
20071	238	20077	120	20005	58
20012	226	20018	104	20074	56
20023	167	20087	98	20009	52

5.1 Data Corpora

Reuters-21578 corpus[1] contains 21578 documents in 135 categories. In our experiments, we discarded those documents with multiple category labels, and selected the largest 30 categories. It left us with 8067 documents in 30 categories as described in Table 1.

The TDT2 corpus[2] consists of data collected during the first half of 1998 and taken from six sources, including two newswires (APW, NYT), two radio programs (VOA, PRI) and two television programs (CNN, ABC). It consists of 11201 on-topic documents which are

[1] Reuters-21578 corpus is at http://www.daviddlewis.com/resources/testcollections/reuters21578/

[2] Nist Topic Detection and Tracking corpus is at http://www.nist.gov/speech/tests/tdt/tdt98/index.html

classified into 96 semantic categories. In this dataset, we also removed those documents appearing in two or more categories and use the largest 30 categories thus leaving us with 9394 documents in 30 categories as described in Table 2.

Each document is represented as a term-frequency vector. We simply removed the stop words, and no further preprocessing was done. Each document vector is normalized to 1, and the Euclidean distance is used as the distance measure.

5.2 Evaluation Metric

The clustering performance is evaluated by comparing the obtained label of each document with that provided by the document corpus. Two metrics, the accuracy (AC) and the normalized mutual information metric ($\overline{MI}$), are used to measure the clustering performance [28]. Given a document $\mathbf{x}_i$, let r_i and s_i be the obtained cluster label and the label provided by the corpus, respectively. The AC is defined as follows:

$$AC = \frac{\sum_{i=1}^{n} \delta(s_i, map(r_i))}{n},$$

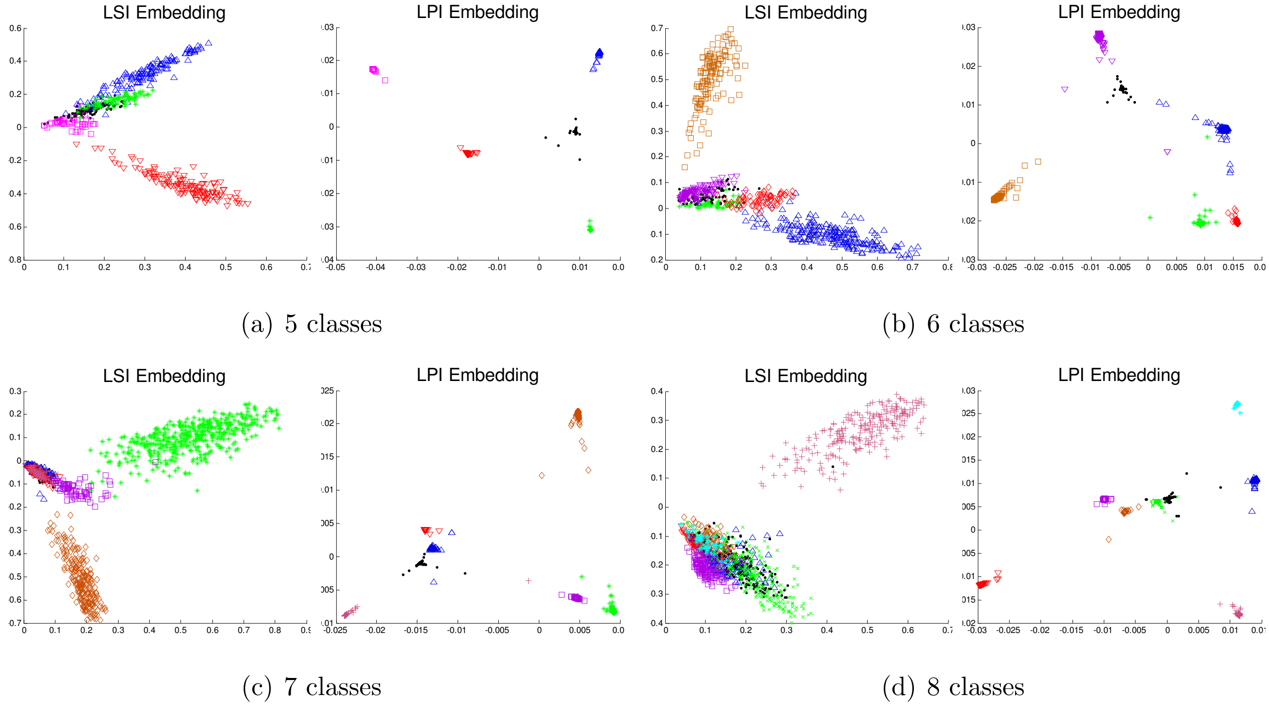
where n is the total number of documents, $\delta(x, y)$ is the delta function that equals one if $x = y$ and equals zero otherwise, and map(r_i) is the permutation mapping function that maps each cluster label r_i to the equivalent label from the data corpus. The best mapping can be found by using the Kuhn-Munkres algorithm [19].

Let C denote the set of clusters obtained from the ground truth and C' obtained from our algorithm. Their mutual information metric $MI(C, C')$ is defined as follows:

$$MI(C, C') = \sum_{c_i \in C, c'_j \in C'} p(c_i, c'_j) \cdot log_2 \frac{p(c_i, c'_j)}{p(c_i) \cdot p(c'_j)},$$

where $p(c_i)$ and $p(c'_j)$ are the probabilities that a document arbitrarily selected from the corpus belongs to the clusters c_i and c'_j, respectively, and $p(c_i, c'_j)$ is the joint probability that the arbitrarily selected document belongs to the clusters c_i as well as c'_j at the same time. In our experiments, we use the normalized mutual information $\overline{MI}$ as follows:

$$\overline{MI}(C, C') = \frac{MI(C, C')}{\max(H(C), H(C'))},$$



(a) 5 classes

(b) 6 classes

(c) 7 classes

(d) 8 classes

Figure 1: 2D Embedding results of LSI and LPI on the TDT2 corpus. The dimensions of document vectors are reduced to 2 using LSI and LPI. Each color (shape) represents a topic. As can be seen, LPI is more powerful than LSI as to separating the documents with different semantics.

where $H(C)$ and $H(C')$ are the entropies of C and C', respectively. It is easy to check that $\overline{MI}(C, C')$ ranges from 0 to 1. $\overline{MI} = 1$ if the two sets of clusters are identical, and $\overline{MI} = 0$ if the two sets are independent.

5.3 LPI Embedding vs. LSI Embedding

Our theoretical analysis shows that LPI is able to map the documents related to the same semantics as close to each other as possible. This motivates us to perform traditional clustering in the LPI subspace rather than directly in the original space. In this subsection, we first present some embedding results by using LPI and LSI.

Fig. (1) shows the 2-D embedding results on the TDT2 corpus. The experiments were conducted on 5, 6, 7 and 8 classes, respectively. The parameter p was set to 15 in LPI. As can be seen, LPI is more powerful than LSI as to separating the documents with different semantics.

5.4 Clustering Results

To demonstrate how our method improves the performance of document clustering, we compared five methods on two data sets: Reuters-21578 and TDT2. These five methods are listed below:

- k-means on original term-document matrix (Kmeans),which is treated as our baseline
- k-means after LSI (LSI),
- k-means after LPI (LPI),
- Spectral Clustering (k-means after Laplacian Eigenmaps, or LE), and
- Non-negative Matrix Factorization based clustering (NMF-NCW, [28]).

Note that, the two methods LPI and LE need to construct a graph on the documents. In the following experiments, we used the same graph for these two methods, and the parameter p was set to 15. The weighted Non-negative Matrix Factorization-based document clustering algorithm (NMF-NCW, [28]) is a recently proposed algorithm, which has shown to be very effective in document clustering. Please see [28] for details.

Tables 3 and 4 showed the experimental results on the TDT2 and the Reuters corpus, respectively. The evaluations were conducted with different number of clusters, ranging from 2 to 10. For each given cluster number k, 50 tests were conducted on different randomly chosen clusters, and the average performance was computed over these 50 tests. For each test, k-means algorithm was applied 10 times with different start points, and the best result in terms of the objective function of k-means was recorded.

After LSI, LPI or Laplacian Eigenmaps, how to determine the dimensions of the subspace is still an open problem. In k cluster situation, we choose the first $k-1$ dimensions in LPI

Table 3: Performance comparisons on TDT2 corpus

	Accuracy						
k	Kmeans	LSI(best)	LSI	LPI(best)	LPI	LE	NMF-NCW
2	0.989	0.992	0.977	0.998	0.998	0.998	0.985
3	0.974	0.985	0.944	0.996	0.996	0.996	0.953
4	0.959	0.970	0.894	0.996	0.996	0.996	0.964
5	0.948	0.961	0.914	0.993	0.993	0.993	0.980
6	0.945	0.954	0.879	0.993	0.992	0.992	0.932
7	0.883	0.903	0.849	0.990	0.988	0.987	0.921
8	0.874	0.890	0.829	0.989	0.987	0.988	0.908
9	0.852	0.870	0.810	0.987	0.983	0.984	0.895
10	0.835	0.850	0.786	0.982	0.979	0.978	0.898
ave.	0.918	0.931	0.876	0.992	0.990	0.990	0.937
	Mutual Information						
k	Kmeans	LSI(best)	LSI	LPI(best)	LPI	LE	NMF-NCW
2	0.962	0.965	0.925	0.981	0.981	0.981	0.939
3	0.946	0.962	0.894	0.977	0.976	0.976	0.924
4	0.932	0.942	0.856	0.979	0.979	0.979	0.951
5	0.935	0.942	0.892	0.975	0.973	0.973	0.965
6	0.936	0.939	0.878	0.975	0.974	0.974	0.923
7	0.884	0.892	0.849	0.969	0.968	0.966	0.915
8	0.889	0.895	0.841	0.970	0.967	0.967	0.911
9	0.875	0.878	0.831	0.970	0.966	0.967	0.905
10	0.865	0.869	0.813	0.962	0.959	0.958	0.897
ave.	0.914	0.920	0.864	0.973	0.971	0.97	0.926

based on our previous analysis. For Laplacian Eigenmaps, since the first eigenvector is **1**, we use the following $k-1$ dimensions. Note that, in typical spectral clustering, the dimension of subspace are set to the number of clusters [21] which is the same with our selection in spirit (since [21] does not remove the first **1** eigenvector). For LSI, we choose the k dimensions for comparison. Besides such determined dimension, for LSI and LPI, we also compute their best performance on different dimensions in each test. We iterate all the dimensions for the best clustering performance and average all the 50 best results. In real situation, it might not be possible to iterate all the dimensions to get the best performance.

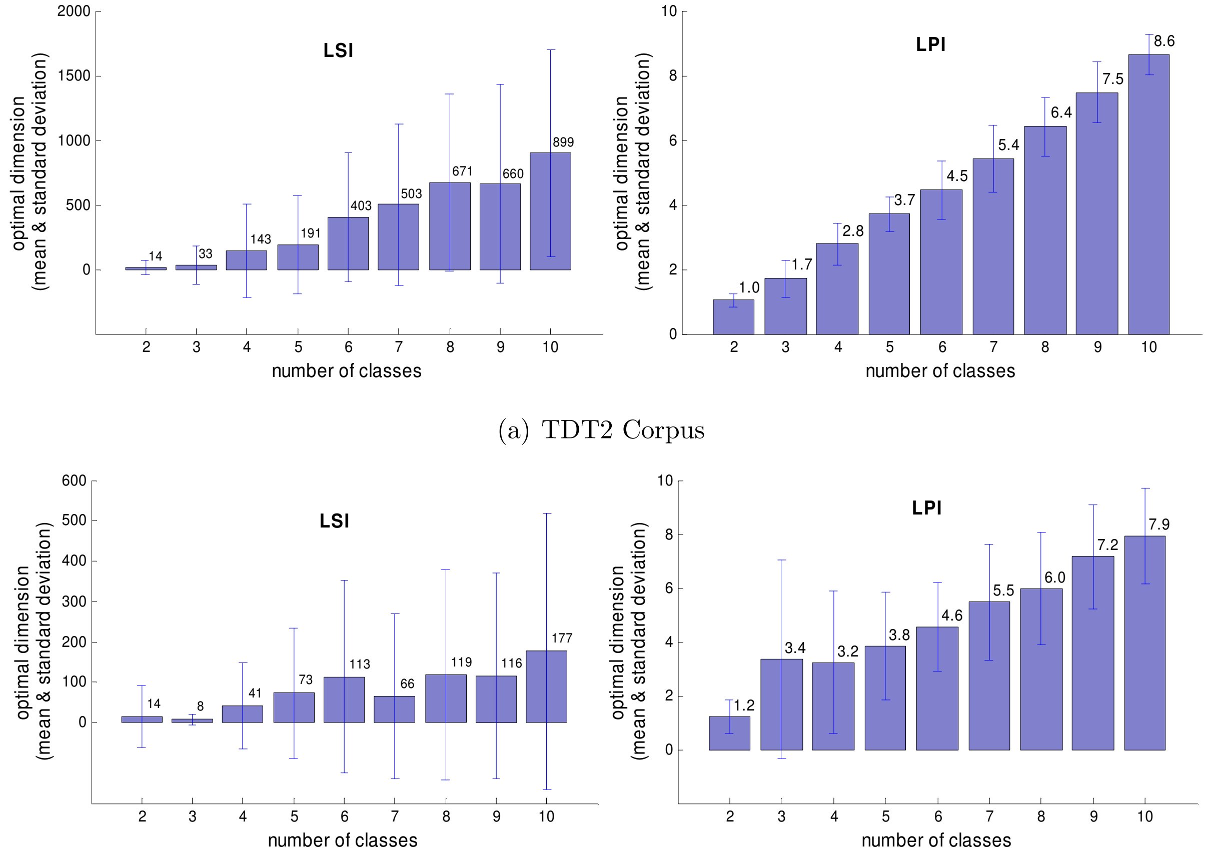
Table 4: Performance comparisons on Reuters corpus

	Accuracy						
k	Kmeans	LSI(best)	LSI	LPI(best)	LPI	LE	NMF-NCW
2	0.871	0.913	0.864	0.963	0.923	0.923	0.925
3	0.775	0.815	0.768	0.884	0.816	0.816	0.807
4	0.732	0.773	0.715	0.843	0.793	0.793	0.787
5	0.671	0.704	0.654	0.780	0.737	0.737	0.735
6	0.655	0.683	0.642	0.760	0.719	0.719	0.722
7	0.623	0.651	0.610	0.724	0.694	0.694	0.689
8	0.582	0.617	0.572	0.693	0.650	0.650	0.662
9	0.553	0.587	0.549	0.661	0.625	0.625	0.623
10	0.545	0.573	0.540	0.646	0.615	0.615	0.616
ave.	0.667	0.702	0.657	0.773	0.730	0.730	0.730

	Mutual Information						
k	Kmeans	LSI(best)	LSI	LPI(best)	LPI	LE	NMF-NCW
2	0.600	0.666	0.569	0.793	0.697	0.697	0.705
3	0.567	0.594	0.536	0.660	0.601	0.601	0.600
4	0.598	0.621	0.573	0.671	0.635	0.635	0.634
5	0.563	0.567	0.538	0.633	0.603	0.603	0.587
6	0.579	0.587	0.552	0.636	0.615	0.615	0.603
7	0.573	0.572	0.547	0.629	0.617	0.617	0.600
8	0.556	0.557	0.530	0.615	0.587	0.587	0.583
9	0.549	0.545	0.532	0.605	0.586	0.586	0.560
10	0.552	0.549	0.528	0.607	0.586	0.586	0.561
ave.	0.571	0.584	0.545	0.650	0.614	0.614	0.604

In Tables 3 and 4, LSI, LPI and LE indicate this determined dimension while “LSI (best)” and “LPI (best)” are the best performance. Fig. (2) shows the optimal dimensions with different numbers of clusters by using LPI and LSI. The optimal dimension in LSI is much higher than LPI. Also, the variance of the dimensions obtained by using LSI is much higher than that obtained by using LPI. For LPI, the optimal number is nearly $k-1$, where k is the number of clusters. This figure showed that LPI is more powerful than LSI in finding the intrinsic dimensionality of the document space. Thus LPI is very suitable for clustering.

The experimental results showed that LSI seems not promising in dimension reduction for clustering because the k-means on the LSI subspace is even worse than k-means on the



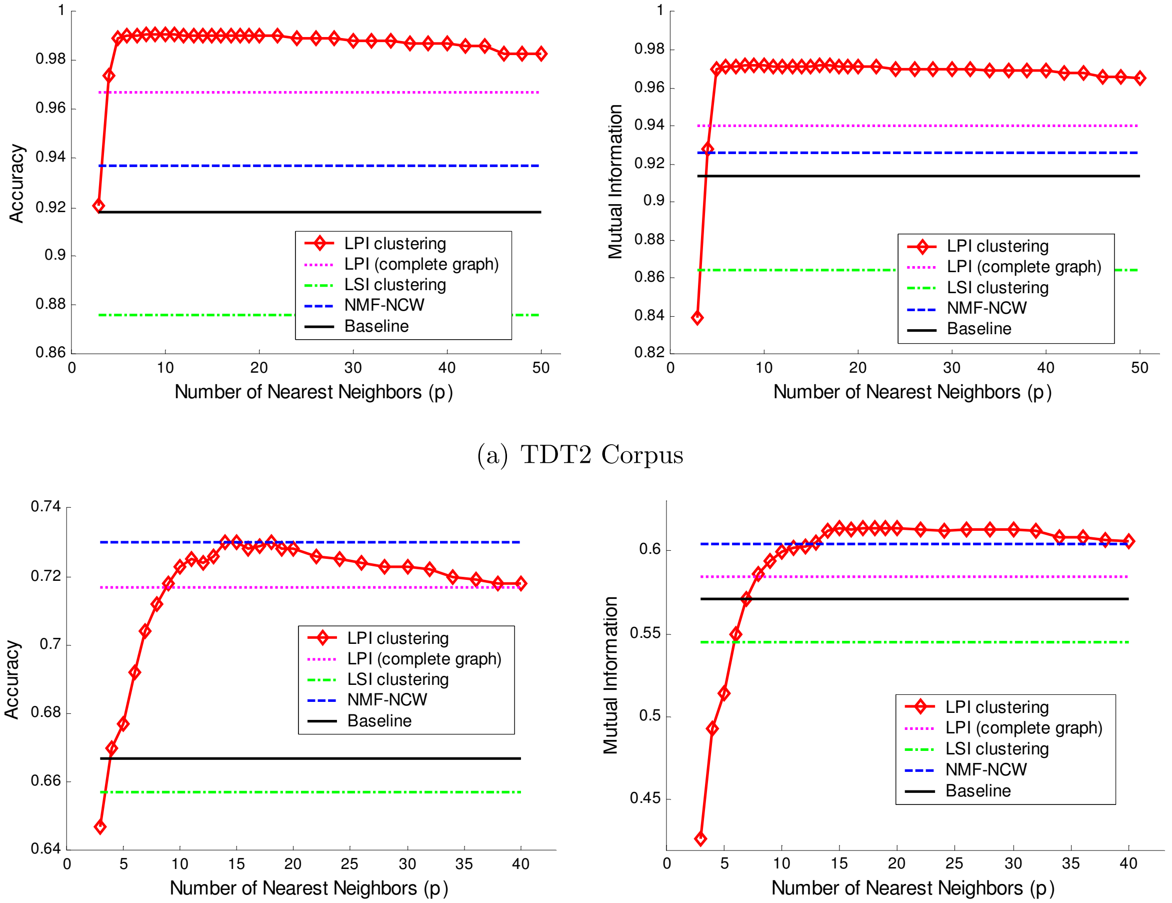
(a) TDT2 Corpus

(b) Reuters Corpus

Figure 2: Optimal dimension with different number of classes. Each bar shows the average of 50 test runs, the error bar indicates the standard deviation.

original document space. As can be seen, LPI performed much better than LSI. We also see that the result of Laplacian Eigenmaps is nearly identical to the result of LPI. Actually in our experiments, for 312 of 450 (50 × 9) tests on Reuters corpus and 430 of 450 (50 × 9) tests on TDT2 corpus, the X is full rank square matrix, thus the results of clustering using LPI are identical to those of clustering using Laplacian Eigenmaps.

In [28], Xu et al. compared the NFM-NCW method with the spectral clustering method. In their comparison, they construct the affinity matrix in spectral clustering as a complete graph. While in our LSI and LE methods, the p-nearest neighbor graphs which put more focus on the local geometric document structure were used. More experiments on the different graph construction will be given in the next sub-section.



(a) TDT2 Corpus

(b) Reuters Corpus

Figure 3: Graph model - Local vs. Global

5.5 Clustering Performance on Different Graph Model

The construction of the adjacency graph is one of the key points in our algorithm. Also, it is the key difference among LSI, LPI and LDA. In this subsection, we test our algorithm under different adjacency graph constructions to see how the different graph structures will affect the clustering performance.

5.5.1 Local vs. Global

In LPI clustering, one needs to set the number of nearest neighbors, i.e., the value of p, which defines the "locality". As we examined in Section 4.1, LPI approximates LSI when p tends to be infinite (complete graph). In Fig. (3), we show the relationship between the clustering performance and the value of p. Here, the clustering performance is the average over 2∼10 classes. The value of p varies from 3 to 40. As can be seen, the performance of LPI clustering reaches its peak when p is 6 in TDT2 corpus and 15 in Reuters21578 corpus. As p increases, the performance decreases. This experiment shows that the local structure is more important than the global structure as to discovering the semantic structure of the document space.

In Fig. (3), we can also find that, even performed under complete graph, clustering after LPI is better than clustering after LSI. Our theoretical analysis in Section 4.1 shows that the only difference between LPI with complete graph and LSI is that LPI has the D matrix. Xu et al. [28] show a similar result that D can really improve the clustering result.

5.5.2 Gaussian vs. Polynomial vs. 0-1

Our algorithm uses the dot-product weighting in constructing the nearest neighbor graph. We can also use other kind of weighting methods as described in Section 4.3. In this experiment, we examine the LPI clustering performance under different weighting choices.

We compare four kinds of weighting method.

1. 0-1 weighting,
2. Gaussian kernel weighting, where the parameter t is set as 1,
3. dot-product weighting, and
4. polynomial kernel weighting with degrees 2 and 5.

The clustering results are shown in Table 5. We can see that LPI-based clustering is insensitive to the weighting function. Even the simplest one (0-1 weighting) can achieve the similar results. This tells us that the local document structure (p-neighbor graph) is essential in LPI-based clustering whereas the specific weighting values in the connected edges are not so influential.

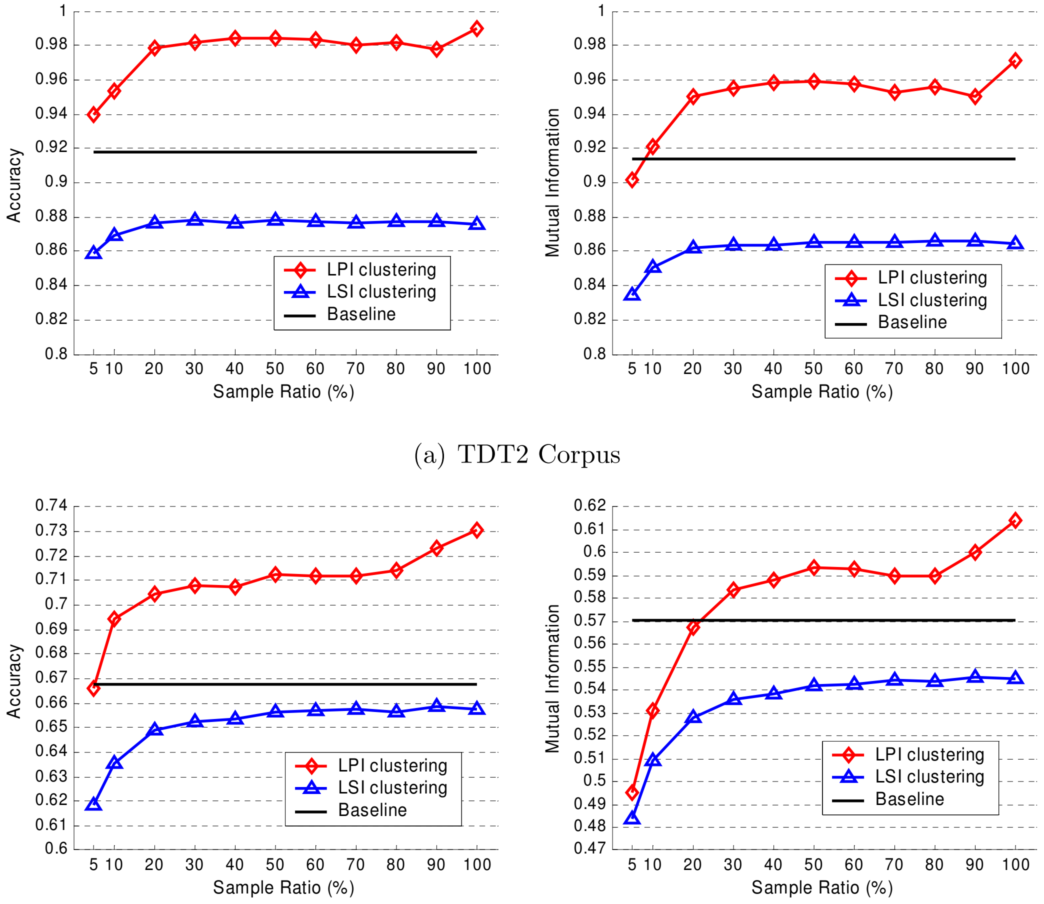
Table 5: Comparison using different weighting functions

TDT2 Corpus										
	Accuracy					Mutual Information				
k	0-1	Gaussian	DotProd	Poly2	Poly5	0-1	Gaussian	DotProd	Poly2	Poly5
2	0.998	0.998	0.998	0.998	0.998	0.982	0.983	0.982	0.982	0.981
3	0.997	0.997	0.997	0.997	0.997	0.981	0.981	0.980	0.981	0.981
4	0.996	0.995	0.995	0.996	0.995	0.979	0.977	0.976	0.978	0.976
5	0.994	0.994	0.994	0.994	0.994	0.977	0.976	0.976	0.976	0.977
6	0.993	0.993	0.993	0.992	0.993	0.975	0.975	0.974	0.974	0.974
7	0.990	0.990	0.989	0.989	0.990	0.970	0.969	0.968	0.968	0.969
8	0.989	0.986	0.986	0.988	0.988	0.968	0.965	0.965	0.967	0.966
9	0.983	0.986	0.985	0.985	0.985	0.964	0.968	0.966	0.966	0.966
10	0.974	0.974	0.973	0.974	0.974	0.954	0.954	0.954	0.953	0.953
ave.	0.990	0.990	0.990	0.990	0.990	0.972	0.972	0.971	0.972	0.971

Reuters Corpus										
	Accuracy					Mutual Information				
k	0-1	Gaussian	DotProd	Poly2	Poly5	0-1	Gaussian	DotProd	Poly2	Poly5
2	0.928	0.924	0.923	0.923	0.922	0.715	0.703	0.697	0.697	0.693
3	0.821	0.815	0.816	0.814	0.812	0.613	0.604	0.601	0.607	0.599
4	0.809	0.791	0.793	0.796	0.790	0.644	0.631	0.635	0.636	0.625
5	0.735	0.733	0.737	0.733	0.732	0.604	0.603	0.603	0.603	0.600
6	0.716	0.713	0.719	0.715	0.715	0.616	0.613	0.615	0.613	0.609
7	0.697	0.698	0.694	0.700	0.695	0.624	0.618	0.617	0.621	0.617
8	0.649	0.650	0.650	0.647	0.649	0.587	0.585	0.587	0.584	0.588
9	0.617	0.619	0.625	0.617	0.632	0.579	0.582	0.586	0.580	0.590
10	0.611	0.613	0.615	0.612	0.612	0.583	0.584	0.586	0.584	0.584
ave.	0.731	0.728	0.730	0.728	0.729	0.618	0.614	0.614	0.614	0.612

5.6 Generalization Capability

Both LSI and LPI try to learn an optimal embedding function in the dataset. In real applications, some new data might be registered into the dataset. The performance on the new data can reflect the generalization capability of the algorithms. This generalization capability is very important for the clustering methods performed on the reduced dimensional space. In these clustering algorithms, learning the low dimensional representation is time consuming and scales with the number of data points. LSI and LPI are linear, and their mapping functions are defined everywhere. Thus in large dataset situation, LSI and LPI



(a) TDT2 Corpus

(b) Reuters Corpus

Figure 4: Generalization capability of LSI and LPI

can choose part of the data to learn such mapping function and map all the data points to the low dimensional space which can speed up the whole process. It is hard for the spectral clustering to adopt such technique, since traditional spectral clustering use non-linear embedding methods which is only defined on "training" samples.

To compare the generalization capability of LSI and LPI, we designed the following experiment: In each test in the previous experiment, we only chose part of the data to learn the embedding function, embedded the whole data set, and then performed clustering in the subspace. The size of the training set ranged from 5% to 90% of the data set. For each case, 10 times of random selection were performed to minimize the impact of occasionality.

The average accuracy (averaged over 2∼10 classes) and normalized mutual information (averaged over 2∼10 classes) are shown in Fig. (4). It is clear that the performance improves with the number of training samples. Both LSI and LPI have good generalization capability, however, the performance of LSI is always below the baseline which makes LSI less practical. For LPI, it achieved similar performance to that using all the samples when only 30% of training samples were used. This makes it practical for clustering large sets of documents.

5.7 Discussions

We summarize the experiments below:

1. In document clustering, dimension reduction can make significant improvement (the best performances obtained by both LSI and LPI are better than the baseline). However, in the real world, one cannot test all the possibilities to find the optimal dimensionality. Therefore, LSI is less practical since it is hard to estimate the optimal dimensionality. In contrast to LSI, clustering after LPI might be a better choice. It is easy for LPI to estimate the optimal dimension, and the performance is always better than baseline.

2. In dimension reduction for clustering, the local geometric structure is more important than the global structure. Based on the assumption that neighboring points probably belong to the same underlying class, the p-nearest graph in our LPI algorithm gives an optimal approximation to the labeled similarity matrix W in Eq. (5). Thus even in unsupervised mode, LPI has discriminating power to some extent which provides a better low dimensional representation for clustering.

3. In document clustering, clustering after LPI is a good linear approximation to spectral clustering. The experiments on generalization capability showed that LPI clustering might be more applicable than spectral clustering in that LPI is linear and is defined everywhere rather than just on the training data points.

6 CONCLUSIONS

A novel document clustering algorithm based on Locality Preserving Indexing is proposed in this paper. Based on the analysis of the computational properties of LPI, we presented the modified LPI algorithm for document clustering. Analysis on the relationship among LSI, LPI and LDA indicates that the affinity graph is the key to distinguish these algorithms. The p-nearest neighbor graph makes LPI approximate to LDA which is supervised. A complete graph makes LPI similar to LSI. Extensive experiments on Reuters-21578 and TDT2 showed that our algorithm performed much better than the LSI-based clustering algorithm and close to the traditional spectral clustering algorithm. Moreover, the linearity of LPI makes our clustering algorithm more applicable than spectral clustering when the data set is large.

Several questions remain to be investigated in our future work:

1. In this paper, we gave some empirical estimation on the dimensionality using LPI. However, it lacks of strong theoretical foundation. How to estimate the dimensionality in theory remains to be investigated. Also, it remains unclear how to estimate the number of topics hidden in the document set. These two problems seem to be two sides of a coin in that the dimensionality can be inferred from the number of topics as suggested in our experiments.

2. As shown in Section 4, LPI provides an optimal approximation to LDA which is supervised. Specifically, we approximate the graph defined in Eq. (5) by a p-nearest neighbor graph. The more accurate the approximation is, the more discriminating power our algorithm has. However, it is unclear if there exists a better approximation and how to obtain it.

3. Clustering is inherently an unsupervised learning process. In all of our experiments, the data points are unlabelled. However, sometimes a small set of labeled data points might be available. In such a case, the unsupervised learning becomes semi-unsupervised (or, semi-supervised) learning. Thus, the optimal projection can be obtained by preserving

locality as well as separating the data points with different labels. It is unclear how to obtain such constrained LPI, though it seems to be promising.

References

[1] L. Baker and A. McCallum. Distributional clustering of words for text classification. In *Proc. 1998 Int. Conf. on Research and Development in Information Retrieval (SIGIR'98)*, pages 96–103, Melbourne, Australia, Aug. 1998.

[2] B. T. Bartell, G. W. Cottrell, and R. K. Belew. Latent semantic indexing is an optimal special case of multidimensional scaling. In *Proc. 1992 Int. Conf. on Research and Development in Information Retrieval (SIGIR'92)*, pages 161–167, Copenhagen, Denmark, June 1992.

[3] M. Belkin and P. Niyogi. Laplacian eigenmaps and spectral techniques for embedding and clustering. In *Advances in Neural Information Processing Systems 14*, pages 585–591. MIT Press, Cambridge, MA, 2001.

[4] P. K. Chan, D. F. Schlag, and J. Y. Zien. Spectral k-way ratio-cut partitioning and clustering. *IEEE Trans. Computer-Aided Design*, 13:1088–1096, 1994.

[5] Fan R. K. Chung. *Spectral Graph Theory*, volume 92 of *Regional Conference Series in Mathematics*. AMS, 1997.

[6] David Cohn. Informed projections. In *Advances in Neural Information Processing Systems 15*, pages 849–856. MIT Press, Cambridge, MA, 2002.

[7] S. C. Deerwester, S. T. Dumais, T. K. Landauer, G. W. Furnas, and R. A. harshman. Indexing by latent semantic analysis. *Journal of the American Society of Information Science*, 41(6):391–407, 1990.

[8] C. Ding, X. He, H. Zha, M. Gu, and H. D. Simon. A min-max cut algorithm for graph partitioning and data clustering. In *Proc. 2001 Int. Conf. Data Mining (ICDM'01)*, pages 107–114, San Jose, CA, Nov. 2001.

[9] C. H. Ding. A similarity-based probability model for latent semantic indexing. In *Proc. 1999 Int. Conf. on Research and Development in Information Retrieval (SIGIR'99)*, pages 58–65, Berkeley, CA, Aug. 1999.

[10] R. O. Duda, P. E. Hart, and D. G. Stork. *Pattern Classification*. Wiley-Interscience, Hoboken, NJ, 2nd edition, 2000.

[11] M. Ester, H.-P. Kriegel, J. Sander, and X. Xu. A density-based algorithm for discovering clusters in large spatial databases with noise. In *Proc. 1996 Int. Conf. Knowledge Discovery and Data Mining (KDD'96)*, pages 226–231, Portland, Oregon, Aug. 1996.

[12] K. Funkunaga and P. Navendra. A branch and bound algorithm for computing k-nearest neighbors. *IEEE Trans. Computers*, 24(7):750–753, 1975.

[13] G. H. Golub and C. F. Van Loan. *Matrix computations*. Johns Hopkins University Press, 3rd edition, 1996.

[14] Xiaofei He, Deng Cai, Haifeng Liu, and Wei-Ying Ma. Locality preserving indexing for document representation. In *Proc. 2004 Int. Conf. on Research and Development in Information Retrieval (SIGIR'04)*, pages 96–103, Sheffield, UK, July 2004.

[15] Xiaofei He and Partha Niyogi. Locality preserving projections. In *Advances in Neural Information Processing Systems 16*. MIT Press, Cambridge, MA, 2003.

[16] A. K. Jain and R. C. Dubes. *Algorithms for Clustering Data*. Prentice-Hall, Inc., Upper Saddle River, NJ, 1988.

[17] Tao Li, Sheng Ma, and Mitsunori Ogihara. Document clustering via adaptive subspace iteration. In *Proc. 2004 Int. Conf. on Research and Development in Information Retrieval (SIGIR'04)*, pages 218–225, Sheffield, UK, July 2004.

[18] Xin Liu, Yihong Gong, Wei Xu, and Shenghuo Zhu. Document clustering with cluster refinement and model selection capabilities. In *Proc. 2002 Int. Conf. on Research and Development in Information Retrieval (SIGIR'02)*, pages 191–198, Tampere, Finland, Aug. 2002.

[19] L. Lovasz and M. Plummer. *Matching Theory.* Akadémiai Kiadó, North Holland, Budapest, 1986.

[20] J. Mcqueen. Some methods for classification and analysis of multivariate observations. In *Proc. 5th Berkeley Symp. Mathematical Statistics and Probability*, pages 281–297, Berkeley, CA, 1967.

[21] Andrew Y. Ng, Michael Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. In *Advances in Neural Information Processing Systems 14*, pages 849–856. MIT Press, Cambridge, MA, 2001.

[22] C.H. Papadimitriou, P. Raghavan, H. Tamaki, and S. Vempala. Latent semantic indexing: a probabilistic analysis. In *Proc. 17th ACM Symp. Principles of Database Systems*, Seattle, WA, June 1998.

[23] J. Shi and J. Malik. Normalized cuts and image segmentation. *IEEE Trans. on PAMI*, 22(8):888–905, 2000.

[24] Stefan Siersdorfer and Sergej Sizov. Restrictive clustering and metaclustering for self-organizing document collections. In *Proc. 2004 Int. Conf. on Research and Development in Information Retrieval (SIGIR'04)*, pages 226–233, Sheffield, UK, July 2004.

[25] Nathan Srebro and Tommi Jaakkola. Linear dependent dimensionality reduction. In *Advances in Neural Information Processing Systems 16.* MIT Press, Cambridge, MA, 2003.

[26] Yair Weiss. Segmentation using eigenvectors: A unifying view. In *Proc. Int. Conf. Computer Vision (ICCV'99)*, pages 975–982, Kerkyra, Greece, Sept. 1999.

[27] Wei Xu and Yihong Gong. Document clustering by concept factorization. In *Proc. 2004 Int. Conf. on Research and Development in Information Retrieval (SIGIR'04)*, pages 202–209, Sheffield, UK, July 2004.

[28] Wei Xu, Xin Liu, and Yihong Gong. Document clustering based on non-negative matrix factorization. In *Proc. 2003 Int. Conf. on Research and Development in Information Retrieval (SIGIR'03)*, pages 267–273, Toronto, Canada, Aug. 2003.

[29] H. Zha, C. Ding, M. Gu, X. He, , and H. Simon. Spectral relaxation for k-means clustering. In *Advances in Neural Information Processing Systems 14*, pages 1057–1064. MIT Press, Cambridge, MA, 2001.

[30] Bin Zhang and Sargur N. Srihari. A fast algorithm for finding k-nearest neighbors with non-metric dissimilarity. In *Proc. 8th Int. Workshop on Frontiers in Handwriting Recognition (IWFHR-8)*, 2002.