New Approaches for Clustering High Dimensional Data

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ABSTRACT

JINZE LIU: New Approaches for Clustering High Dimensional Data. (Under the direction of Wei Wang.)

Clustering is one of the most effective methods for analyzing datasets that contain a large number of objects with numerous attributes. Clustering seeks to identify groups, or clusters, of similar objects. In low dimensional space, the similarity between objects is often evaluated by summing the difference across all of their attributes. High dimensional data, however, may contain irrelevant attributes which mask the existence of clusters. The discovery of groups of objects that are highly similar within some subsets of relevant attributes becomes an important but challenging task. My thesis focuses on various models and algorithms for this task.

We first present a flexible clustering model, namely OP-Cluster (Order Preserving Cluster). Under this model, two objects are similar on a subset of attributes if the values of these two objects induce the same relative ordering of these attributes. OP-Clustering algorithm has demonstrated to be useful to identify co-regulated genes in gene expression data. We also propose a semi-supervised approach to discover biologically meaningful OP-Clusters by incorporating existing gene function classifications into the clustering process. This semi-supervised algorithm yields only OP-clusters that are significantly enriched by genes from specific functional categories.

Real datasets are often noisy. We propose a noise-tolerant clustering algorithm for mining frequently occuring itemsets. This algorithm is called approximate frequent itemsets (AFI). Both the theoretical and experimental results demonstrate that our AFI mining algorithm has higher recoverability of real clusters than any other existing itemset mining approaches.

Pair-wise dissimilarities are often derived from original data to reduce the complexities of high dimensional data. Traditional clustering algorithms taking pair-wise dissimilarities as input often generate disjoint clusters from pair-wise dissimilarities. It is well known that the classification model represented by disjoint clusters is inconsistent with many real classifications, such gene function classifications. We develop a

Poclustering algorithm, which generates overlapping clusters from pair-wise dissimilarities. We prove that by allowing overlapping clusters, Poclustering fully preserves the information of any dissimilarity matrices while traditional partitioning algorithms may cause significant information loss.

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Chapter 1

Introduction

Clustering is one of the most effective methods for analyzing datasets that contain a large number of objects with numerous attributes. Clustering seeks to identify groups, or *clusters*, of similar objects. Traditionally, a cluster is defined as a subset of objects that take similar values at each attribute. A more general notion of cluster is a subset of objects which are more similar to each other than they are to the objects in other clusters.

Clustering results are frequently determined by dissimilarities between pairs of objects. If the objects with d attributes are viewed as points in a d-dimensional Euclidean space, distances can be adopted as a dissimilarity measure. A variety of alternative dissimilarity measures have been created to capture pair-wise relationships in different applications. These pair-wise dissimilarity measures are often a summary of the dissimilarities across all the attributes.

Traditional clustering algorithms have been successfully applied to *low-dimensional data*, such as geographical data or spatial data, where the number of attributes is typically small. While objects in some datasets can be naturally described by 3 or fewer attributes, researchers often collect as many attributes as possible to avoid missing anything important. As a result, many datasets contain objects with tens of or even hundreds of attributes. We call such objects *high dimensional data*.

Clustering can be naturally extended to analyze high dimensional data, which results in groups of objects that are similar to each other along *all* the attributes. However, unlike low dimensional data where each of the attributes is considered equally informative, not all the attributes are typically relevant in characterizing a cluster. Dissimilarities computed along all attributes including those irrelevant ones can be arbitrarily high, which, in turn, prohibits the true clusters from being discovered. Hence, the discovery of groups of objects that are highly similar within some relevant subset

of attributes (thus eliminating irrelevant attributes) becomes an important but challenging task. My thesis focuses on various models and algorithms for this task.

In this chapter, we first describe high dimensional data and depict the challenges encountered in the analysis of high-dimensional data. We then discuss the state of the art in clustering approaches that aim to tackle these challenges. We conclude with a discussion of the thesis contribution.

1.1 High Dimensional Data

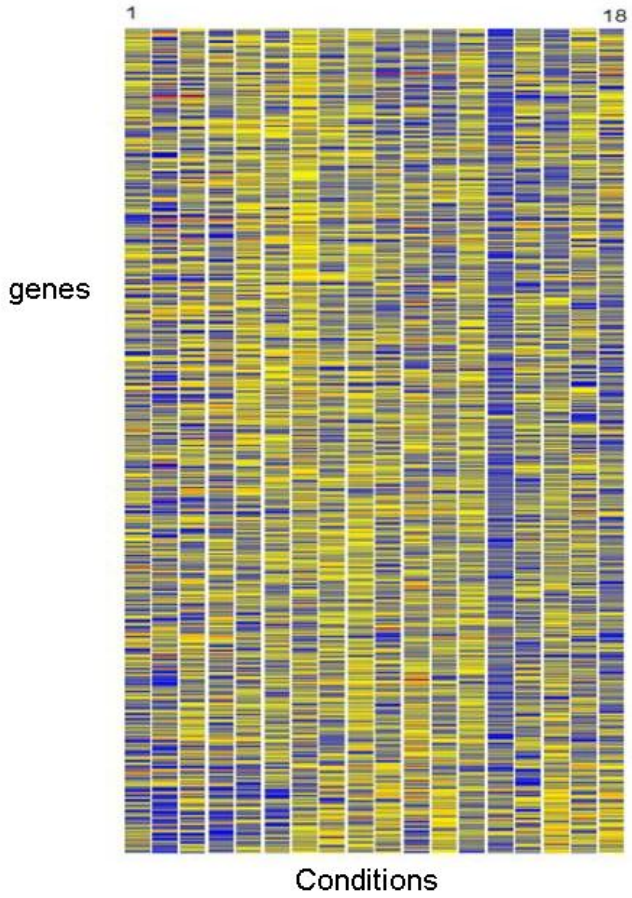


Figure 1.1: An example of gene expression data matrix with 3447 genes and 18 conditions. The expression levels are mapped to a heatmap, where red corresponds to high expression level and blue corresponds to low expression level

Recent technology advances have made data collection easy and fast, resulting in large datasets that record values of hundreds of attributes for millions of objects.

TrID	Itemlist
1	cheese
2	diaper, babyfood, beer
3	diaper, babyfood, milk
4	babyfood, milk, beer, juice, cheese, flower
5	diaper, milk, beer, juice, cheese
6	diaper, babyfood, milk, beer, juice, cheese, lamb meat
7	milk, beer, juice, cheese
8	milk
9	paper
...	...

(A) An example of transactional database.

	p	d	b	m	r	j	c	l	f	
1							1			...
2		1	1		1					...
3		1	1	1						...
4			1	1	1	1	1		1	...
5		1		1	1	1	1			...
6		1	1	1	1	1	1	1		...
7				1	1	1	1			...
8				1						...
9	1									...
	...	...	...	...	...	...	...	...	...	...

paper diaper babyfood milk beer juice cheese lamb flower

(B) A binary format of the transactional database in (A).

Figure 1.2: An example of transactional database and its binary format

Many high dimensional datasets arise in biological applications. One typical example is gene expression profiles generated by microarray technology. With a single array, it is possible to measure the expression levels for thousands of genes of an organism. The experiments can be repeated under different conditions. These conditions may correspond to different time points or different environmental conditions. The measurements may come from different organs, from cancerous or healthy tissues, or even from different individuals. Usually, gene expression data is arranged in a data matrix, where each gene corresponds to a row and each experimental condition corresponds to a column. Each element of this matrix is typically a real number representing the expression level of a gene under a specific condition, usually expressed as the logarithm of the relative abundance of the mRNA of the gene under the specific condition. The gene expression data can be visualized by mapping the expression values to a heatmap, as shown in Figure 1.1.

Market-basket data collected in commercial applications provides another example of high dimensional data. This type of database records the purchases made by customers. A market-basket database can be viewed as a binary matrix in which each row represents a customer's transaction and each column represents an item available for purchase in the market. In a transaction, entries are marked with '1' if the corresponding items were purchased. Market-basket data is collected to understand the purchasing behaviors of customers (see Figure 1.2).

In summary, the datasets addressed by this thesis are all high dimensional data, where the number of attributes of an object is on the order of tens or even hundreds.

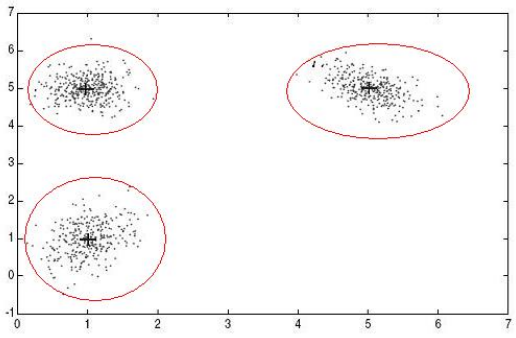


Figure 1.3: An example of k-means Clustering of points in 2D space. $k = 3$ and $+$ marks the centroid of a cluster

1.2 The Challenge

High-dimensional data requires greater computational power. However, a much bigger challenge is introduced by the high dimensionality itself, where the underlying associations between objects and attributes are not always strong and noise is often prevalent. Hence, the effectiveness of any approach to accurately identify salient clusters becomes a real concern. The rest of this section details the challenges faced in high dimensional data.

1.2.1 The curse of dimensionality

One immediate problem faced in high dimensional data analysis is *the curse of dimensionality*, that is, as the number of dimensions in a dataset increases, evaluating distance across all attributes become increasingly meaningless.

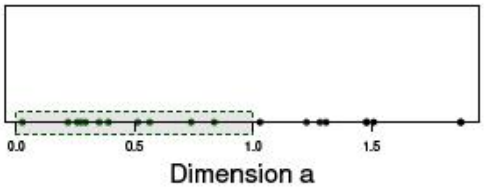
When we consider each object as a point in Euclidean space, it has been observed (Parsons et al., 2004) that the points in high dimensional space are more spread out than in a lower dimensional space. In the very extreme case with very high dimensions, all points are almost equidistant from each other. In this case, the traditional definition of clusters as a set of points that are closer to each other than to the rest of points does not easily apply. Clustering approaches become ineffective to analyze the data.

The phenomena of *the curse of the dimensionality* is illustrated by the following example. A high dimensional space can be created by repeatedly adding additional dimensions starting from an initial low dimensional space as shown in Figure 1.4 (Parsons et al., 2004). Initially, there exists a set of closely located points in one dimensional space. As the set of points expands to a new space by adding additional dimension, they are more spread out and finding a meaningful cluster gets harder.

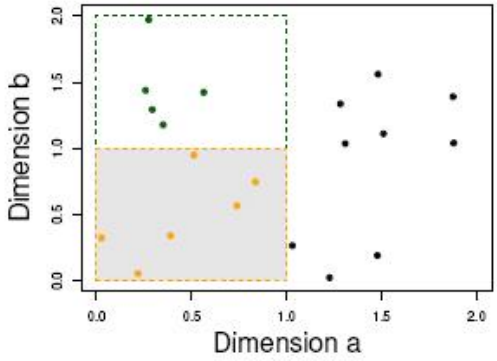
As a result, when the set of attributes in a dataset becomes larger and more varied, clustering of objects considering across all dimensions becomes problematic.

1.2.2 Dissimilarity Measures

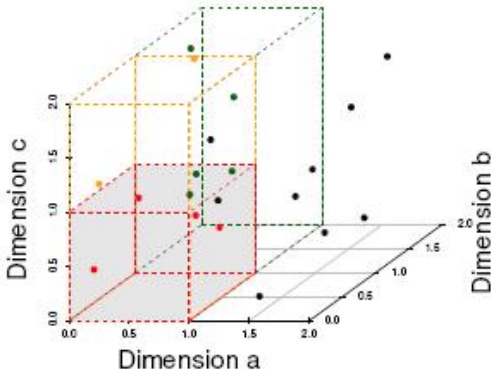
When the objects are viewed as points in high dimensional space, the dissimilarity between objects is often determined based on spatial distance functions. Well-known distance functions include Euclidean distance, Manhattan distance, and cosine distance. These criteria often generate clusters that tend to minimize the variance of objects in each attribute.



(a) 11 Objects in One Unit Bin



(b) 6 Objects in One Unit Bin



(c) 4 Objects in One Unit Bin

Figure 1.4: As the dimensionality goes higher,points in the space are more spread out.

However, these distance functions are not always sufficient for capturing the correlations among objects. In the case of gene expression analysis, it may be more useful to identify more complex relations between the genes and the conditions regardless of their spatial distances. For example, we may be interested in finding a subset of genes that are either consistently increasing or consistently decreasing across a subset of conditions without taking into account their actual expression values; or we may be interested in identifying a subset of conditions that always have the positive or negative effect on a subset of genes. Strong correlations may exist between two objects even if they are far apart in distance.

1.2.3 Multi-Clusters Membership

Clustering is also referred to as an unsupervised learning of classification structure, where each cluster corresponds to a learned classification category. Most existing clustering algorithms require clusters to be flat or hierarchial partitions. Therefore, one object is not allowed to belong to multiple clusters (at the same level).

However, high dimensional data provides much richer information regarding each object than low dimensional data. An object might be similar to a subset of objects under one subset of attributes but also similar to a different subset of objects under another set of attributes. Therefore, an object may be a member of multiple clusters. However, multi-cluster membership is prohibited by traditional clustering algorithms which typically generate disjoint clusters.

1.2.4 Noise Tolerance

Datasets collected in real applications often include error or noise. In a transaction database, noise can arise from both recording errors of the inventories and the vagaries of human behavior. Items expected to be purchased together by a customer might not appear together in a particular transaction because an item is out of stock or because it is overstocked by the customer. Microarray data is likewise subject to measurement noise, stemming from the underlying experimental technology and the stochastic nature of the biological systems.

In general, the noise present in real applications undermines the ultimate goal of traditional clustering algorithms: recovering consistent clusters amongst the set of attributes considered. As a matter of fact, the presence of noise often breaks the real underlying clusters into small fragments. Applying existing algorithms recovers these

fragments while missing the real underlying clusters. The problem is worsened in high dimensional data, where the number of errors increases linearly with dimensionality.

Noise-tolerance in clustering is very important to understand the real cluster structures in the datasets. However, distinguishing noise from accurate and relevant values is hard, consequently, searching for noise-tolerant clusters is even harder since many large potential clusters need to be considered in order to identify the real clusters.

1.2.5 Applicability to Biological Applications

Clustering has been one of the popular approaches for gene expression analysis. The feasibility for applying clustering to gene expression analysis is supported by the hypothesis that genes participating in the same cellular process often exhibit similar behavior in their expression profiles. Unfortunately, traditional clustering algorithms do not suit the needs of gene expression data analysis well, due to a variety of biological complications. First, an interesting cellular process may be active only in a subset of the conditions. Genes co-regulated under these conditions may act independently and show random expression profiles under other conditions. Computing dissimilarities by evaluating all conditions, as adopted by traditional clustering approaches, may mask the high similarity exhibited by genes under a subset of conditions, which in turn, prohibits the discovery of genes that participate in the cellular process. Secondly, a gene may have multiple functions. It may be involved in multiple biological pathways or in no pathways at all. However, the classification model underlying most of the traditional clustering algorithms forces one gene to be a member of exactly one cluster. This classification model itself is too restrictive to represent the more complicated classification model underlying gene functions. A desirable clustering algorithm applicable to gene expression analysis should have the following characteristics.

- A cluster of genes should be defined with respect to a subset of relevant conditions.
- Overlapping should be allowed between two clusters, i.e, a gene/condition is allowed to belong to more than one cluster or to no cluster at all.

1.3 State Of the Art

The state of the art methods for clustering high dimensional data can be divided into the following two categories: dimensionality reduction and subspace clustering.

1.3.1 Dimensionality Reduction

Dimensionality reduction techniques include both *feature transformation* and *feature selection*. Two representative examples of feature transformation techniques include principal component analysis (PCA) and multi-dimensional scaling (MDS). The goal of PCA and MDS is to find the minimum set of dimensions that capture the most variance in a dataset. More precisely, PCA is based on computing the low dimensional representation of a high dimensional data set that most faithfully preserves its covariance structure. MDS is based on computing the low dimensional representation of a high dimensional data set that most faithfully preserves dissimilarities between different objects. Though based on a somewhat different geometric intuitions, the two approaches generate similar results. The dimensionality reduction techniques are not ideal for clustering since they are not able to eliminate irrelevant attributes that mask the clusters. In addition, the new features derived from either PCA or MDS are linear combinations of the original features. They are not straightforward to interpret in real applications, especially when each of them carries independent meanings.

As suggested by its name, feature selection methods attempt to select a proper subset of features that best satisfies a relevant function or evaluation criterion. The results of feature selection make it possible to reduce storage, to reduce the noise generated by irrelevant features and to eliminate useless features. While feature selection methods find the most important features (subspaces), they may fail to discover multiple independent subspaces, which contain significant clusters.

1.3.2 Subspace Clustering

Subspace clustering algorithms take the concept of feature selection one step further by selecting relevant subspaces for each cluster independently. These algorithms attempt to find the clusters and their subspaces simultaneously. Subspace clustering is also called biclustering or co-clustering since the algorithm clusters objects and attributes at the same time.

One branch of subspace clustering algorithm divides both the set of objects and the set of attributes into disjoint partitions, where the partitions maximize global objective functions(Dhillon et al., 2003; Chakrabarti et al., 2004). Even though a globally optimal partition may be reached, the local properties of a single cluster generated by partition-based clustering is hard to characterize. In addition, since each object belongs to exactly one cluster and so does each attribute, partition-based subspace clustering does not fit

the needs of certain applications where an object and/or an attribute may belong to multiple clusters or to no cluster at all.

The other branch of subspace clustering algorithms, eliminates the restriction of partition-based algorithms by looking for clusters satisfying given criteria. These criteria define the properties of desired clusters. These clustering algorithms are also called pattern-based algorithms. Unlike partition-based algorithms that search for the best global partitions, pattern-based algorithms do not restrict one object to a single cluster. Instead, pattern-based algorithms guarantees that any clusters they generate must satisfy the cluster pattern criteria.

Pattern-based algorithms can be different from each other based on the type of patterns they are looking for. One of the natural patterns is a set of objects (points) closely located together in high dimensional space. The algorithms to search for this type of clusters has been extensively studied in (Agrawal et al., 1998; Cheng et al., 1999; Nagesh et al., 1999; Aggarwal et al., 1999; Aggarwal and Yu, 2000). Subspace clustering based on spatial distance is limited in its ability to find clusters with high correlations. In biological applications, genes that are far apart from each other may still exhibit consistent up and down regulations under a subset of conditions, which are called co-regulation patterns. Recently, clustering algorithm such as residue-based biclustering (Cheng and Church, 2000), Order preserving biclustering (Ben-Dor et al., 2002) and the search of shifting and scaling patterns (Wang et al., 2002) were developed to look for specific co-regulation patterns.

Not all the algorithms above generate the complete set of patterns. Some take a greedy approach of finding one maximal pattern at a time, as in (Cheng and Church, 2000; Ben-Dor et al., 2002). These algorithms often carry a polynomial time complexity with regard to the number of objects and the number of attributes for searching one cluster. Such algorithms may not identify a globally optimal solution and they may miss many important subspace clusters as well.

The exhaustive approach is adopted by a number of subspace clustering algorithms (Wang et al., 2002; Agrawal et al., 1998; Cheng et al., 1999). Rather than identifying one or a subset of clusters at a time, the exhaustive approach finds the complete set of subspace clusters satisfying the pattern criteria. My thesis work follows the line of the pattern-based exhaustive subspace clustering algorithms.

1.4 Thesis statement and contributions

Thesis Statement: Techniques developed in this work identify clusters in subspaces of high dimensional data with different criteria for similarity and in the presence of noise. The clusters found using these techniques are relevant to important application domains. The performance of these clustering techniques scales to large datasets.

The goals of this research are studying new clustering models to analyze high dimensional data, deriving algorithms based on these models and subsequently performing detailed experiments to demonstrate the efficiency and effectiveness of these algorithms on different domains.

Each of the clustering algorithms proposed in this thesis tackle a combination of two or more of the independent challenges arising from high dimensional data. In order to minimize the effect of the irrelevant features on clustering, we design algorithms that conduct clustering and the relevant subspace selection simultaneously. We also refine clustering criteria to incorporate similarity measurements in order to reveal hidden patterns arising from biological data or noisy data. In addition, we go beyond the disjoint clustering approach by allowing overlap between clusters, which has been demonstrated to be necessary for real biological applications.

The contributions of this thesis are:

- We propose a flexible clustering model, namely OP-Cluster (Order Preserving Cluster). Under this model, two objects are similar on a subset of dimensions if the values of these two objects induce the same relative ordering of these dimensions. Such a cluster arises when the expression levels of (coregulated) genes rise or fall together in response to a sequence of environment stimuli. Hence, the discovery of OP-Cluster may prove useful for revealing significant gene regulatory networks.

- We propose a semi-supervised approach to discover biologically meaningful OP-Clusters. Our approach incorporates existing gene function classifications, such as Gene Ontology, into the clustering process, yielding only OP-clusters that are significantly enriched with genes from a particular functional categories.

- We propose a noise-tolerant itemset model, which we call approximate frequent itemsets (AFI). The AFI model extends traditional exact frequent itemset model by tolerating a controlled fraction of errors in each item and each supporting transaction. Both the theoretical and experimental results demonstrate that the AFI criterion is well suited to the recovery of real clusters in the presence of noise.

- We propose a general approach for postprocessing subspace clusters (AFIs). A direct consequence of subspace clustering and itemset mining is an overwhelmingly large set of overlapping clusters, which hinders the interpretability of clustering results. To reveal the true underlying clusters, we propose several similarity measurements for subspaces clusters and adopt multi-dimensional scaling to allow the exploration and analysis of subspace clusters.

- We study the space of partially ordered sets that are derivable from pair-wise dissimilarity-based clustering methods. We prove that the set of PoClusters, generated by Poclustering of dissimilarity data, has one-to-one correspondence with the set of all dissimilarity matrices. We present the necessary and sufficient conditions to determine whether the information a given poset may be coded lossless by a dissimilarity matrix. An optimal incremental algorithm and a heuristic clustering algorithm to derive Poclusters are developed.

Chapter 2

Background

This chapter focuses on the current state of the art clustering algorithms. Each section in this chapter will cover one of the clustering approaches.

2.1 Terms and Notations

Here is the notation used in the rest of the thesis. We will be working with a $n \times m$ matrix D, where each element D_{ij} is a real or binary value. The set of rows in D corresponds to a set of objects denoted by O and the set of columns corresponds to the set of attributes (conditions) denoted by A.

In the view of the space, A refers to the set of m-dimensional attributes, i.e., $\{a_1, a_2, ..., a_m\}$. They are bounded and totally ordered. $\mathcal{S}$ denotes the full space of A, which is $a_1 \times a_2 \times \ldots \times a_m$, a m-dimensional numerical space. Each object i in O is represented by m-dimensional vector where $v_i = < v_{i1}, v_{i2}, \ldots, v_{id} >$. The jth component of v_i is drawn from domain a_j.

In gene expression data, each object is a gene, and each attribute may represent an experimental condition or tissue sample. An entry in the matrix D_ij represents the expression level of a gene i under condition j.

In transactional database, each row of D corresponds to a transaction i and each column of j corresponds to an item a. The i, j-th element of D, denoted $D(i, j)$, is 1 if transaction o contains item a, and 0 otherwise.

Given the data matrix D, as defined above, we define a row cluster as a subset of rows that exhibit similar behavior across the set of all columns.

This means that a row cluster $C = (I, A)$ is a subset of rows defined over the set of all columns A (the full space) , where $I \subseteq O$. Similarly, a column cluster is a subset of columns that exhibit similar behavior across the set of all rows. A column cluster

$C = (O, J)$ is a subset of columns (a subspace) defined over the set of all rows O, where $J \subseteq A$.

A subspace cluster (bicluster) is a subset of rows that exhibit similar behavior across a subset of columns, and vice versa. The bicluster $C = (I, J)$ is thus a subset of rows and a subset of columns where $I \subseteq O$ and $J \subseteq A$.

We frequently refer to objects as rows and attributes as columns.

2.2 Overview of Clustering

The main objective of clustering is to find high quality clusters within a reasonable time. However, different approaches to clustering often define clusters in different ways. Traditionally clustering techniques are broadly divided into hierarchical and partitioning methods. Partitioning methods can be further divided into distribution-based, density-based and grid-based methods. In this section, we review the existing clustering approaches following this taxonomy.

2.2.1 Hierarchical Clustering

Hierarchical clustering (Karypis et al., 1999; Guha et al., 1998; Guha et al., 2000) builds a cluster hierarchy or, in other words, a tree of clusters, often represented in a dendrogram. Such an approach allows exploring data on different levels of granularity. Hierarchical clustering can be further categorized into agglomerative and divisive methods based on how it is constructed. An agglomerative clustering starts with one-point (singleton) clusters and recursively merges two or more of the most appropriate clusters. A divisive clustering starts with one cluster of all data points and recursively splits the most appropriate cluster. The process continues until a stopping criterion is achieved. In hierarchical clustering, the regular object-by-attribute data representation is sometimes of secondary importance. Instead, hierarchical clustering deals with the $N \times N$ dissimilarities between each pair of objects. Therefore, hierarchical clustering provides the ease of handling many forms of dissimilarity or distance measures.

Hierarchical clustering proceeds iteratively with merging or splitting until the stopping criterion is achieved. To merge or split clusters of points rather than individual points, the distance between individual points has to be generalized to the distance between clusters. Such derived proximity measure is called a linkage metric. The type of the linkage metric used significantly affects hierarchical algorithms, since it reflects

the particular concept of closeness and connectivity. Major inter-cluster linkage metrics include single link, average link and complete link. The underlying dissimilarity measure is computed for every pair of points with one point in the first set and another point in the second set. A specific operation such as minimum (single link) and average (average link), or maximum (complete link) is applied to pair-wise dissimilarity measures. These methods carry $O(N^3)$ time complexity and are called graph methods. Linkages defined by geometric method use the distance between any pair of cluster representations rather than points in the cluster. A cluster is represented by its central point. It results in centroid, median and minimum variance linkage metrics.

Hierarchical clustering provides flexibility regarding the level of granularity. The method has been used to construct a numerical taxonomy in biological application. In addition, they handle any form of dissimilarity measures.

2.2.2 Clustering by Partitioning

Data partitioning algorithms systematically divide data into subsets. One approach to data partitioning is to take a conceptual point of view that identifies the cluster with a certain probabilistic model whose unknown parameters have to be found. In the probabilistic model, data is considered to be a sample drawn from a mixture model of several probability distributions. The goal of the clustering is to maximize the overall likelihood of the training data coming from the learned mixture model. Expectation-Maximization (EM) method is often used to search for a local optimal solution that maximizes the objective function. K-means and K-Medoids are representatives of methods which starts with the objective function depending on the partition. While both algorithm iteratively search for the best k partitions, K-means represents each cluster by the cluster centroid and K-Medoids represents each cluster by one of its points, namely, its medoid. In K-means algorithm, the sum of discrepancies between a point and its centroid, expressed through appropriate distance metric, is used as the objective function. The basic K-means algorithm is similar to the EM algorithm and consists of two iteration steps. The first step reassigns all the points to their nearest centroids and the second step recomputes centroids of newly classified groups. Iterations continue until a stopping criterion is achieved.

Another type of data partitioning algorithm is based on density(Ester et al., 1996; Ankerst et al., 1999). The implementation of density-based methods requires concepts of density, connectivity and boundary. The *density-based* algorithms are often applied

to spatial data clustering, based on the hypothesis that a set of points in the metric space can be divided into a set of connected components. A cluster is often defined as a connected dense component. It grows in any direction that dense region leads. The property guarantees that density-based clustering can be applied to find clusters with arbitrary shapes. DBScan (Ester et al., 1996), GDBScan (Sander et al., 1998) and Optics (Ankerst et al., 1999) are representative density-based clustering algorithms

The *grid-based* algorithms adopt space partitioning with multi-rectangular segments (Wang et al., 1997; Sheikholeslami et al., 1998). A grid is superimposed on the space. A segment(also cube, cell, region), is a direct Cartesian product of individual attribute sub-ranges(contiguous in the case of numerical attributes). Data partitioning(clustering) is induced by points' membership in segments resulted from space partitioning. A cluster includes all points within the set of connected dense cells. Sting (Wang et al., 1997) and WaveCluster (Sheikholeslami et al., 1998) are the representatives of grid-based algorithms. CLIQUE (Agrawal et al., 1998) is also a grid-based algorithm, we will discuss it in detail in the section of Subspace Clustering.

2.3 Overview of Dimensionality Reduction

Dimensionality reduction is often a preprocessing step before clustering. There are two primary types of techniques dimensionality reduction. *Feature transformation* attempts to describe the overall variance of a high dimensional dataset using fewest possible set of dimensions, while *feature selection* tries to select the most relevant dimensions that best differentiate groups of objects.

Principal component analysis(PCA) and singular value decomposition(SVD) are two important techniques used in feature transformation. Both the two techniques preserve pair-wise dissimilarities (distances) between objects. In this way, they summarize the dataset by creating linear combinations of the original attributes. Feature transformation allows a clustering algorithm to use a few of the newly created features and ignores features that are attributed to noise. A few clustering methods have incorporated the use of such transformations to identify important features and iteratively improve their clustering (Hinneburg and Keim, 1999). Although PCA transforms the original space into a different low-dimensional space, it preserves the original dissimilarities. Hence, it does not help clustering. Also, they are not able to identify irrelevant features, which makes it impossible to discover clusters masked by meaningless features. Last but not least, the newly obtained features, which are the linear combination of the

original attributes, are not easy to interpret. Therefore, the successful application of feature transformations for clustering purposes often assume that most of the features are relevant to the clustering task, but many are highly redundant.

Feature selection attempts to identify a small subset of features that are most relevant for clustering. Feature selection involves searching through various feature subsets and evaluating each of these subsets using some criterion (Blum and Langley, 1997; Liu and Motoda, 1998; Yu and Liu, 2003). The most popular search strategies are greedy sequential searches through the feature space. Subsequently, clustering of all the data points has to be performed on the selected feature space. This approach hinders the discovery of clusters which exist in subspaces formed by different subsets of features.

2.4 Overview of Subspace Clustering

2.4.1 Grid-based Subspace Clustering

The subspace clustering problem finds clusters in the subspaces of the high dimensional space. Formally, a subspace cluster $C = (I, J)$ consists of a set of objects I and a subset of attributes J where $I \subseteq O$ and $J \subseteq A$, such that the data points in I have a high similarity in the subspace J. A naive approach to subspace clustering might be to search through all possible subspaces and use cluster validation techniques to determine the subspaces with the best clusters. This is not feasible because the number of subspaces is generally intractable.

Existing subspace clustering algorithm often assume a metric space, such as Euclidean space. Therefore, many clustering algorithms are grid-based. One of the pioneering subspace clustering is CLIQUE (Agrawal et al., 1998), which was followed by ENCLUS (Cheng et al., 1999), MAFIA (Nagesh et al., 1999) and so on. All of these algorithms adopt a bottom-up search method, which takes advantage of the downward closure property of density to reduce the search space, using an Apriori style approach.

To approximate the density of the data points, CLIQUE partitions the data space using a uniform grid and count the data points that lie inside each cell of the grids. This is accomplished by partitioning each dimension into the same number of equal length intervals. This means that each unit has the same volume, and therefore the number of points inside it can be used to approximate the density of the unit. Formally, the data space $\mathcal{S}$ is partitioned into non-overlapping rectangular units. The units are obtained by partitioning every dimension into ξ intervals of equal length, which is an

input parameter.

The algorithm first creates a histogram for each dimension and select those bins with densities above a given threshold. The downward closure property of density means that if there are dense units in k dimensions, there are dense units in all $(k-1)$ dimensional projections. Candidate subspaces in two dimensions can then be formed using only those dimensions which contained dense units, dramatically reducing the search space. The algorithm proceeds until there are no more dense units found. Adjacent dense units are then combined to form clusters.

Each unit u is the intersection of one interval from each attribute. It has the form $\{u_1, \ldots, u_d\}$ where $u_i = [l_i, h_i)$ is a right open interval in the partitioning of A_i. We similarity define units in all subspaces of the original d-dimensional space. Given a projection of the data set V into $A_{t1} \times A_{t2} \times \ldots \times A_{tk}$, where $k < d$ and $t_i < t_j$ if $i < j$, a unit in the subspace is defined as the intersection of an interval from each of the k attributes. A point $v =< v_1, \ldots, v_d >$ is contained in a unit $u =< u_1, \ldots, u_d >$ if $l_i \leq v_i < h_i$ for all u_i. The selectivity of a unit u is defined to be the fraction of total data points contained in the unit. Given a selectivity threshold τ, we call a unit u is dense if selectivity(u) is greater than τ. A cluster is a maximal set of connected dense units in k-dimensions. Units are connected by sharing a common face.

Two k-dimensional units u_1, u_2 are connected if they have a common face or if there exists another k-dimensional unit u_3 such that u_1 is connected to u_3 and u_2 is connected to u_3. Units $u_1 = \{r_{t_1}, \ldots, r_{t_k}\}$ and $u_2 = \{r'_{t_1}, \ldots, r'_{t_k}\}$ have a common face if there are $k-1$ dimensions, assume dimensions $A_{t_1}, \ldots, A_{t_{k-1}}$, such as $r_{t_j} = r'_{t_j}$, and either $h_{t_k} = l'_{t_k}$ or $l_{t_k} = h'_{t_k}$.

Given a k-dimensional space S, and a set of data points $\mathcal{V}$, the algorithm to find all clusters as defined above has the following steps.

1. Partition the k-dimensional space into ξ^k equal length units.

2. Identify the dense units. This can be done by scanning all the data points in $\mathcal{V}$ once. For each of the data points, increase the counter corresponding to the units it lies in. Go through all the units again, determine the set of dense units D by density threshold τ.

3. Identify the clusters. Given the set of dense units identified in the previous step, the clusters can be identified by finding all the connected dense units.

The first two steps in identifying clusters in a specific subspace are straightforward.

Therefore, we will discuss the third step which is the identification of clusters given the set of dense units D. A depth first search algorithm can be used to find the connected dense units. We start with one of the dense units in D, assign it to the first cluster number, and apply the same procedure to all the dense units it is connected to. Then, if there are still some dense units left in D, but have not yet been visited, we find one and repeat the procedure.

2.4.2 Projection-based Subspace Clustering

The projection-based algorithms generate clusters that are partitions of the dataset. These partitions best classify the set of points that are embedded in lower dimensional subspaces given some objective functions. Instead of projecting all the points into the same subspace, the algorithm allows each cluster to have a different subspace with variable dimensionality.

(Aggarwal and Yu, 2000) uses hierarchical clustering to compute projective clusters in different subspaces. Given the number of clusters k, their algorithm initially computes a large number of clusters of a given dimension d. It then hierarchically merges the closest clusters (as defined by some criteria) while decreasing the dimensionality of the clusters by a constant factor. After a number of such merges, the number of remaining clusters is k, and the dimensionality of each cluster has been reduced to the required dimensionality d. Though each cluster is associated with a different subspace, the algorithm requires the dimension of each cluster to be the same, and more importantly, it must be specified by the user. An attempt to overcome the shortcomings of the above approach, proposed by (M. Procopiuc and Murali, 2002), is to use an iterative method to extract the best projective cluster: the algorithm finds the best projective cluster from the remaining points by guessing points belonging to the optimal cluster (via random sampling), and then computes the best dimensions associated with the cluster. The algorithm has the advantage that it allows each cluster to have a different number of dimensions. Furthermore, the algorithm computes the best dimensionality automatically. A major disadvantage of the algorithm is that it is restricted to finding only clusters in orthogonal subspaces.

2.4.3 Bipartitioning-based Subspace Clustering

Co-clustering is a branch of subspace clustering methods that usually generates partitions along both rows and columns simultaneously, which is the reminiscent of the

k-means algorithms.

One of the pioneering co-clustering algorithms based on information theory was proposed by Dhillon *et.al.* in (Dhillon et al., 2003). Taking the numbers of row and column clusters as input, the co-clustering algorithm maximizes an objective function of the mutual information between row and column clusters. In each iteration, the row clusters are adjusted to maximize the mutual information between row and column clusters followed by adjusting the column clusters in a similar fashion. The algorithm continues until there is no significant improvement in mutual information. In (Dhillon, 2001), a co-clustering algorithm based on bipartite spectral graph partitioning was developed. The co-clustering is performed by singular value decomposition. A *k-means* algorithm is then applied on the calculated singular vectors to form k clusters, for some given k. Long et al. proposed another co-clustering based on block value decomposition (Long et al., 2005),. It factorizes the data matrix into three components: row-coefficient matrix, column-coefficient matrix, and block value matrix, by iterative computation based on multiplicative updating rules. The final co-cluster is established according to the decomposed matrices. The clustering scheme of fully crossed association proposed in (Chakrabarti et al., 2004) adopts a data compression technique and does not require any input parameters. Because they favor lossy compression, their algorithms usually terminates with considerably more number of rows (columns) clusters than the actual number of clusters in real data, and it is sensitive to noise . Although they use a similar splitting procedure in order to approach the optimal number of clusters, the clusters are formed by reassignment of each individual rows and columns, which is similar to the reassignment step in *k-means* clustering rather than hierarchical clustering.

2.4.4 Pattern-based Subspace Clustering

The first algorithm proposed in this category finds interesting patterns carried by a subset of genes under a subset of conditions by Cheng et al. (Cheng and Church, 2000). Instead of a subspace cluster, they call it a bicluster. The biclustering algorithm tries to measure the coherence of the genes and the conditions in a sub-matrix of a DNA array. Yang et al (Yang et al., 2002) proposed a move-based algorithm to find biclusters in a more efficient way. However, as pointed out in (Wang et al., 2002), the bicluster model has two drawbacks: (1) A bicluster may contain outliers. (2) It requires the number of clusters as an input parameter. Recently, $\delta-$pcluster was introduced by Wang et al (Wang et al., 2002) to cluster objects exhibiting shifting patterns in a data

set efficiently. Let I be a subset of objects in the database O and let J be a subset of attributes ($J \subseteq A$). The pair (I, J) specifies a sub-matrix. Given $x, y \in I$, and $a, b \in J$, $pScore$ of the 2×2 matrix is defined as:

$$pScore\left(\begin{bmatrix} d_{xa} & d_{xb} \\ d_{ya} & d_{yb} \end{bmatrix}\right) = |(d_{xa} - d_{xb}) - (d_{ya} - d_{yb})| \tag{2.1}$$

(I, J) forms a pCluster if, for any 2×2 submatrix X in $(\mathcal{O}, \mathcal{T})$, the $pScore$ is less than some threshold δ^p.

Ben-Dor, Chor, Karp, and Yakhini(2002) introduced a model, namely OPSM(order preserving submatrix) (Ben-Dor et al., 2002), to discover a subset of genes identically ordered among a subset of the conditions. Unlike the bicluster and pCluster model, it focused on the coherence of the relative ordering of the conditions rather than the coherence of the actual expression levels. These types of patterns can be expected when considering data from nominally identical exposure to environmental effects, data from drug treatment, data representing some temporal progression, etc. For example, in expression data that comes from a population of patients, it is reasonable to expect that each individual is in a particular stage of the disease. There is a set of genes that are co-expressed with this progression and we therefore expect the data to contain a set of genes and a set of patients such that the genes are identically ordered on this set of patients.

The OPSM problem has been shown to be NP-hard. The algorithm designed in the paper, grows its partial model iteratively. The partial model is scored by measuring the expected number of planted(valid) rows associted with it. The larger the row support, the better the score. Given any $n * m$ matrix and the number of columns s included in the resulted OPSM, the algorithm starts from building the partial model with $s = 2$, chooses l of them with the best scores. For each of them, it tries all the $m-2$ extensions and choose the best l of them. This process continues until the partial models have a size s. The model with the best score is selected as the OPSM.

Pattern-based subspace clustering is shown be relevant to biological applications, especially the analysis of gene expression data.

Chapter 3

Order Preserving Subspace Clustering

In this chapter, we introduce a deterministic algorithm to search for OP-Cluster(Order Preserving Cluster). Under this model, two objects are similar in a subset of dimensions if the values of two objects induce the same ordering of those dimensions. Such a cluster arises when the expression levels of a group of genes rise or fall synchronously in response to a sequence of stimuli. OP-Cluster may prove useful in revealing significant gene regulatory networks. In addition, E-commerce application can also benefit from this model to identify customer groups that have consistent behaviors within a set of activities(purchasing, browsing, etc).

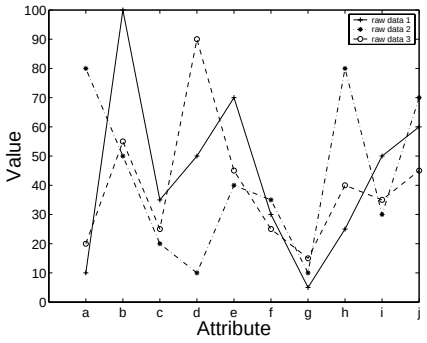
The OP-Clustering adopts a more reflexible yet powerful model that improves previous work on δ-cluster and δ-pCluster, which are designed to capture either shifting patterns or scaling patterns. Our experiments on several real biological data sets demonstrate its effectiveness and efficiency in detecting co-regulated patterns.

3.1 Introduction

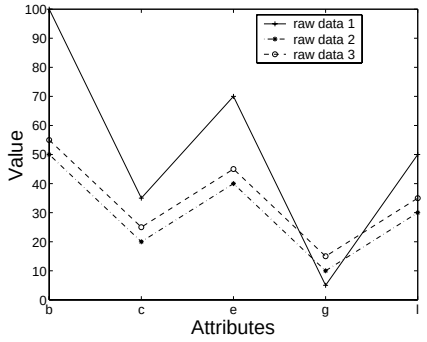
We introduce a flexible clustering model, OP-Cluster, which is able to capture the general tendency of objects across a subset of dimensions in high dimensional space.

Figure 3.1 a) shows a set of 3 objects with 10 columns (attributes). In this raw data, no pattern is obvious. However, if we pick the set of columns $\{b, c, e, g, l\}$ as in Figure 3.1 b) for the 3 objects, we can observe the following trend: *The rank among these columns based on the matrix entry values is the same for all the three objects.* If we rearrange the columns in ascending order of their ranks: $< g, c, l, e, b >$, such as in Figure 3.1 c), the increasing pattern can be seen more clearly.

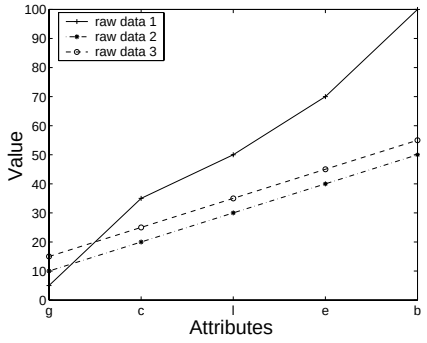
Discovery of clusters in data sets based on tendency along a subset of dimensions is of great importance because of its potential for actionable insights in a variety of



a) Raw Data



b) A OP-cluster



c) Rearranged by Rank

Figure 3.1: An Example of OP-cluster

applications such as microarray analysis and E-commerce applications.

- *DNA microarray analysis.* Microarrays are one of the latest breakthroughs in experimental molecular biology. They provide a powerful tool by which the expression patterns of thousands of genes can be monitored simultaneously and they have already produced huge amount of valuable data. Analysis of such data is becoming one of the major bottlenecks in the utilization of the technology. The gene expression data are organized as matrices where rows represent genes, columns represent various samples such as tissues or experimental conditions, and numbers in each cell characterize the expression level of the particular gene in the particular sample. Investigators have shown that more often than not, if several genes contribute to a disease, it is possible to identify a subset of conditions, under which these genes show a coherent tendency. Since a gene's expression level may vary substantially due to environment, the direction of movement (up or down) in response to condition change is often considered more credible than its actual value. Discovering clusters of genes sharing a common tendency is essential in revealing the significant connections in gene regulatory networks(Cheng et al., 1999)

- *E-commerce.* Recommendation systems and targeted marketing are important applications in the E-commerce area. In these applications, sets of customers/clients with similar behavior need to be identified so that we can predict customers' interest and make proper recommendation for future marketing. The following is an example. Three viewers rate four movies ("DareDevil", "The hours", "Chicago", "Lord of rings, the two towers") as (1,4,7,10), (5,6,7,8) and (3,4,9,10), where 1 is the lowest and 10 is the highest. Although the reviews given by each viewer differ in both their values and their scales it is clear that they have coherent affinities. In this case, the relative order of the ratings play a more important role than the absolute values. In the future, if the first and second viewers rate two movies as (2,6) and (4,5), respectively, we may have certain confidence that the third viewer may also favor the second movie over the first.

This observation motivated us to design a model to characterize the general tendency and develop an algorithm to discover clusters of objects that preserve coherent tendencies. To achieve this goal, we need to tackle two major challenges.

- *Large number of potential rankings.* If we have m attributes, there are $m!$ different permutations of (subsets of) attributes. Each permutation corresponds to one

unique ranking for this set of attributes. And each unique ranking corresponds to a subset of object. Moreover, the ranking of the subsets of the N attributes might be shared by a larger set of objects, which in turn, generates more clusters with less columns but more rows. So totally, the number of potential candidates for OP-Clusters is $\sum_{1 \leq i \leq n} \binom{m}{i}$

Data sets used in DNA array analysis or collaborative filtering can have hundreds of attributes. This results in a huge number of candidates of various lengths, posing a significant challenge to the pattern discovery.

- *Massive Cluster Size.* Compared with δ-pCluster, which has a more restrictive similarity function, the clusters under our model tend to be much larger along both attributes and objects. As a result, scalability with respect to the size of the largest cluster (rather than the volume of the data) becomes very important

Our contributions include:

- A new clustering model, namely OP-Cluster, to capture general tendencies exhibited by the objects. The OP-Cluster model is a generalization of existing subspace clustering models. It has a wide variety of applications, including DNA array analysis and collaborative filtering, where tendency along a set of attributes carries significant meaning.

- An efficient and effective tree structure OPC-Tree for mining OP-Cluster. Compared with one of fastest sequential pattern mining algorithms, prefixSpan(modified to serve our purpose), the OPC-Tree based algorithm performs more efficiently, especially when the data is pattern-rich.

The remainder of the chapter is organized as follows. Section 3.2 discusses related work. Section 3.3 defines the model proposed. Section 3.4 presents the two algorithms in detail. An extensive performance study is reported in Section 3.5. Section 3.6 concludes the paper.

3.2 Related Work

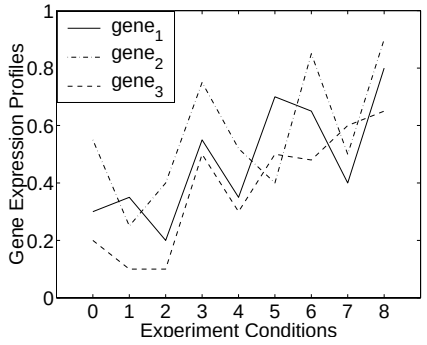
3.2.1 Subspace Clustering

Our proposed is closely related to pattern-based subspace clustering. Cheng and Church (Cheng and Church, 2000) are among the pioneers to introduce the pattern-based

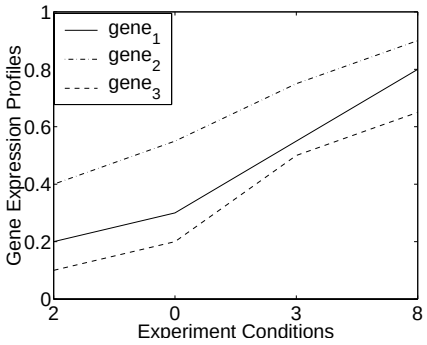
clustering. Their biclusters are based on uniformity criteria, and a greedy algorithm is developed to discover them. However, the algorithm is limited to find only one largest cluster at a time. The submatrix of the cluster is then replaced by random noise in order to find the second largest clusters. The introduced noise may prohibit the discovery of the potentially overlapping clusters. The efficiency of the algorithm is further improved by simultaneously finding multiple clusters in (Yang et al., 2003). δ-pCluster was introduced by Wang et al (Wang et al., 2002) to cluster objects exhibiting shifting or scaling patterns in a data set in a very efficient way. However, in many applications, only allowing shifting or scaling patterns is restrictive. To include more objects within a cluster, the threshold has to be relaxed. This, in turn, can result with inconsistency within a cluster.

Ben-Dor et.al. introduced the model of OPSM (order preserving submatrix) (Ben-Dor et al., 2002) to discover a subset of genes identically ordered among a subset of conditions. It focuses on the coherence of the relative order of the conditions rather than the coherence of actual expression levels. For example, in the gene expression data of patients with the same disease, the genes interfering with the progression of this disease shall behave similarly in terms of relative expression levels on this set of patients. These types of pattern can be observed in data from nominally identical exposure to environmental effects, data from drug treatment, and data representing some temporal progression, etc. The OPSM problem was proven to be NP-hard in (Ben-Dor et al., 2002). A stochastic model was developed to discover the best row supported submatrix given a fixed size of conditions. However, one major drawback of the pioneer work is the strict order of conditions enforced by the OPSM model. Secondly, only one cluster can be found at a time and it is heuristic, which means it might not be either the largest or maximal. And the quality of the resulted cluster is very sensitive to the given parameters and the initial selection of starting points. Secondly, OPSM algorithm favors clusters with a large row support, which as a result, can obstruct the discovery of small but significant clusters.

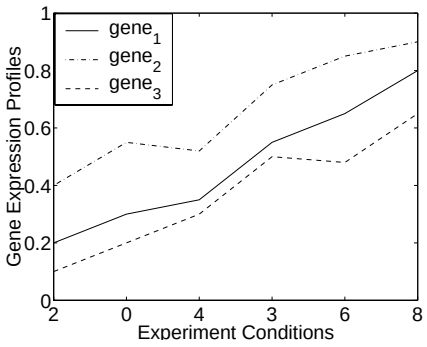
In our work, we generalize the OPSM model by relaxing the strict ordering between values with small difference. Based on the new model, we propose a deterministic subspace clustering algorithm, namely OPC-Tree, which can capture all the general tendencies exhibited by a subset of objects along a subset of dimensions in one run.



a) Raw Gene Expression Matrix



b) Largest OPSM



c) Largest OP-Cluster

Figure 3.2: Comparison of clusters discovered by OPSM and OP-Clustering

3.2.2 Sequential Pattern Mining

The algorithm we developed is also related to sequential pattern mining. Since it was first introduced in (Agrawal and Srikant, 1995), sequential pattern mining has been studied extensively. Conventional sequential pattern mining finds frequent subsequences in the database based on exact match. There are two classes of algorithms: bread-first algorithms and depth-first algorithms. Breadth-first search methods (e.g., GSP (Srikant and Agrawal, 1996) and SPADE (Zaki, 2001)) employ the Apriori principle (Agrawal and Srikant, 1995) and conduct level-by-level candidate-generation-and-

tests. Alternatively, depth-first search methods (e.g., PrefixSpan (Pei et al., 2001) and SPAM (Ayres et al., 2002)) grow long patterns from short ones by constructing projected databases.

We are faced with a similar but more complicated problem than sequential pattern mining. Rows in matrix will be treated as a sequence to find sequential patterns. However, in order to finally determine OP-Cluster, the ID associated with each sequence has to be kept during the mining process. A depth-first traversal of the tree is carried out to generate frequent subsequences by recursively concatenating legible suffixes with the existing frequent prefixes.

3.3 Model

In this section, we define the OP-Cluster model for mining objects that exhibit tendency on a set of attributes.

3.3.1 Definitions and Problem Statement

Definition 3.3.1 *Let o be an object in the database, $\langle d_{o1}, d_{o2}, ..., d_{om} \rangle$ be the attribute values in a non-decreasing order, m be the number of attributes and δ be the user specified threshold. We say that object o is* **similar** *on attributes i, $i+1$, ..., $i+j$, $(0 < i \leq m,\ 0 < j \leq m)$, if*

$$(d_{o(i+j)} - d_{oi}) < \mathcal{G}(\delta, d_{oi}) \tag{3.1}$$

we call the set of attributes $\langle i, i+1, ..., i+j \rangle$ a **similar group**. *Attribute d_{oi} is called a* **pivot point**.

The grouping function $\mathcal{G}(\delta, d_{oi})$ return a difference threshold based on δ and may or may not be related to d_{oi}.

The intuition behind this definition is that, if the difference between the values of two attributes is not significant, we regard them to be "equivalent" and group them together. There are multiple ways to define the grouping function $\mathcal{G}(\delta, d_{oi})$. One way is to define it as the average difference between every pair of attributes whose values are closest.

$$\mathcal{G}(\delta) = \delta \times \sum_{0<j\leq m} (d_{o_j+1} - d_{oj}) \tag{3.2}$$

This definition is independent of d_{oj} and is usually used when each attribute has a finite domain and its value is uniformly distributed. The previous example on movie rating belongs to this case. When the value of each attribute follows a skewed distribution, Equation 3.3 is a better choice. The gene expression data often belongs to this scenario. For the sake of simplicity in explanation, we assume Equation 3.3 in the remainder of this paper, unless otherwise specified.

$$\mathcal{G}(\delta, d_{oj}) = \delta \times d_{oj}. \tag{3.3}$$

For example, suppose a reviewer's rates of five movies (A, B, C, D, E) as (1, 4, 4.5, 8, 10). If $\delta = 0.2$, 4 and 4.5 are considered equivalent. The rating are divided into four groups $\{\{1\}, \{4, 4.5\}, \{8\}, \{10\}\}$.

Definition 3.3.2 *Let o be an object in the database, and* (g_{o1}) $(g_{o2})...(g_{ok})$ *be a sequence of similar groups of o by Equation 3.1 and in non-descending order of their values. o shows an 'UP' pattern on an ordered list of attributes* $a_1, a_2, ..., a_j$ *if* $a_1, a_2, ..., a_j$ *is a subsequence of* $(g_{o1})(g_{o2})...(g_{ok})$

In the above example, $(1, 4, 4.5, 8, 10)$ is the rating for movies (A, B, C, D, E). After we apply the group similarity, we are able to transform the original rating to the sequence $A(BC)DE$. $ABDE$, AE, and $(BC)E$ show 'UP' patterns.

Definition 3.3.3 *let I be a subset of objects in the database,* $I \subseteq O$. *Let J be a subset of attributes* $\mathcal{A}$. *(I, J) forms a OP-Cluster if there exists a permutation of attributes in* $\mathcal{J}$, *on which every object in I shows the same "UP" pattern.*

Suppose we have two movie ratings o_1 and o_2 for movies (A, B, C, D, E). The ratings are (1, 4, 4.5, 8, 10) and (2, 5, 7, 4.5, 9), respectively. According to Definition 3.3.3, the corresponding sequence of groups for o_1 is $A(BC)DE$, and for o_2 is $A(DB)CE$. Since $ABCE$ is a common subsequence of them, we say that o_1 and o_2 form a OP-Cluster on the attributes sets of $ABCE$.

Lemma 3.3.1 *Let* $(\mathcal{O}^p, \mathcal{T}^p)$ *be a δ-pCluster, where* δ^p *is the user defined threshold for δ-pCluster.* $(\mathcal{O}^p, \mathcal{T}^p)$ *is also identified as a OP-Cluster if the value difference between any two attributes of an object is at least* $\frac{\delta^p}{2}$.

Proof 3.3.1 *Given any two objects x and y* ($x, y \subseteq \mathcal{O}^p$), *we first sort attribute values of x for all attributes in* $\mathcal{T}^p$ *in non-descending order. Without loss of generality, assume*

that we have two attributes a and b ($a, b \subseteq \mathcal{T}^p$) where $d_{xa} < d_{xb}$. If $d_{ya} > d_{yb}$ and any two attributes of an object differ in value by at least $\frac{\delta^p}{2}$, we have

$$(d_{xa} - d_{xb}) < -\frac{\delta^p}{2}; (d_{ya} - d_{yb}) \geq \frac{\delta^p}{2}; \tag{3.4}$$

The absolute difference between them, which is pScore defined in δ-pCluster, is

$$|(d_{xa} - d_{xb}) - (d_{ya} - d_{yb})| > \delta^p. \tag{3.5}$$

However, because $x, y \subseteq \mathcal{O}^p$ and $a, b \subseteq \mathcal{T}^p$, $(\mathcal{O}^p, \mathcal{T}^p)$ forms a δ-pCluster. We should have

$$|(d_{xa} - d_{xb}) - (d_{ya} - d_{yb})| < \delta^p. \tag{3.6}$$

This gives a contradiction between Equations 3.5 and 3.6. Therefore, our hypothesis of $d_{ya} > d_{yb}$ is incorrect. So, we have $d_{ya} \leq d_{yb}$ when $d_{xa} < d_{xb}$, and hence ($\{x, y\}$, $\{a, b\}$) forms a OP-Cluster.

Similarly, we can prove that any two objects $\subseteq \mathcal{O}^p$ and any two attributes $\subseteq \mathcal{T}^p$ can form a OP-Cluster. Thus, for any two objects, they form a OP-Cluster on all attributes $\subseteq \mathcal{T}^p$. Since there is only one unique order of attributes $\subseteq \mathcal{T}^p$ such that all objects $\subseteq \mathcal{O}^p$ show the 'up' pattern. We conclude that $(\mathcal{O}^p, \mathcal{T}^p)$ is also a OP-Cluster.

In above discussion, we assume that the threshold of group similarity is set to 0. In this case, if the difference between any two attributes of an object is smaller than the threshold $\frac{\delta^p}{2}$, it will be included in δ-pCluster, but it will not be able to present in OP-Cluster. To accommodate this in OP-Cluster, we can set $\delta = \frac{\delta^p}{2}$. Then, any δ-pCluster will be included in a OP-Cluster.

Lemma 3.3.2 *Given a matrix with size $n \times m$, the probability of finding a submatrix with size $nc \times nr$ is*

$$p(nc, nr) = \frac{m!}{nc!} \sum_{i=nr}^{n} \begin{pmatrix} n \\ i \end{pmatrix} (\frac{1}{nc!})^i (1 - \frac{1}{nc!})^{n-i} \tag{3.7}$$

The above probability originally discussed in (Ben-Dor et al., 2002)measures the significance of a submatrix with size ($nc \times nr$). Hence, given the size of the cluster, we will be able to determine the significance of cluster. This can be used during the postprocessing in order to select the most significant clusters.

Problem Statement Given a cluster threshold δ, a minimal number of columns nc, and a minimal number of rows nr, the goal is to find all (maximum) submatrices $(\mathcal{O}, \mathcal{T})$ such that $(\mathcal{O}, \mathcal{T})$ is a OP-Cluster according to Definition 3.3.3, and $|\mathcal{O}| \geq nr$, $|\mathcal{T}| \geq nc$.

3.4 Algorithm

In this section, we present our algorithm to generate OP-Clusters, which consists of two steps: (1) preprocess the data into sequences of similarity groups; (2) mine frequent subsequences and the sets of rows containing them.

The second step in our algorithm is similar to sequential pattern mining in that frequent patterns needed to be discovered. However, they also differ from each other since OP-clustering needs the identification of original sequences(rows) which each frequent pattern is embedded in.

We propose a novel compact structure OPC-Tree to organize the sequences and to guide the pattern generation. We also modified and optimized the fastest sequential pattern mining prefixSpan in (Liu and Wang, 2003) to discover OP-Clusters. Compared with prefixSpan, the structure of OPC-Tree is more compact. Sequences sharing the same prefixes will be sharing the same paths in the tree. For those sequences, further mining down the prefix can be done simultaneously instead of one-by-one as in prefixSpan. In addition, single path subtrees in OPC-Tree will not be examined further. Only the closed pattern is considered in this time since we would like the maximum OP-cluster. The prefixSpan algorithm is not able to look forward and takes advantage of this.

3.4.1 Preprocessing

To preprocess the data, first, we sort all the row values in non-decreasing order for each row. Secondly, each sorted row is organized into a sequence of similarity groups based on the similarity threshold. The resulted sequences are taken as input to the second step — mining OP-Cluster. Let's take a look at the raw data in Table 4.2 a). If the threshold δ for group similarity is set to be 0.1, for the row 1, the sorted order of attributes is $[228 : d, 284 : b, 4108 : c, 4392 : a]$. a and c can be grouped together since $4392 - 4108 < 4108 \times 0.1$. By processing the rest of rows similarly, the sequences are generated as shown in Table 4.2 b). Attributes in "()" are in the same similarity

group. Since order in the same groups does not matter, without loss of generality, they will be arranged in the alphabetical order.

(Equation 3.3).

rID	a	b	c	d
1	4392	284	4108	228
2	401	281	120	298
3	401	292	109	238
4	280	318	37	215
5	2857	285	2576	226
6	48	290	224	228

a) Raw Data Matrix

rID	sequence
1	$db(ac)$
2	$c(bd)a$
3	$cdba$
4	$cdab$
5	$dbca$
6	$a(cd)b$

b) Sequences after Preprocessing

Table 3.1: Example Data Set

3.4.2 OPC-Tree

In the above section, each row in the matrix has been converted into a sequence of column labels. The goal in the next step is to discover all the frequent subsequence in the given sequences. This problem seems to be a sequential pattern mining problem, however,it differs from a conventional sequential pattern mining problem in two respects. First, the set of rows associated with each frequent subsequence has to be recorded in order to determine the rows involved in a OP-Cluster. Conventional sequential mining algorithms only the number of appearance of frequent subsequences. To discover the set of rows associated with them, one possible approach is to scan database to collect the related rows. However, this method is very time consuming and is not scalable to the size of the database. Secondly, our data sets is special. For example, the appearance frequency of each item(column) is the same since each item appears only once in each sequence. As a result, no pruning happens in the first round of operation in either apriori-based or projection-based algorithm. Based on the characteristics of our algorithms, we develop the following algorithm.

Our algorithm uses a compact tree structure to store the crucial information used in mining OP-Clusters. Meanwhile, sequences sharing the same prefixes are grouped together. As a result, further operations along the shared prefixes by a set of rows are only performed once. Pruning techniques can also be applied easily in the OPC-Tree structure. To make the algorithm more scalable to the number of columns, an improve-

ment over OPC-Tree by collapsing nodes in a single paths will be further illustrated in the OPC-Tree.

Before we define OPC-Tree formally, we first give the following example.

Example 3.4.1 *For the sequences in Table 4.2 b), with* $nc = 3, nr = 3$*, the OPC-Tree algorithm performs in the following steps.*

Step 1: *Create root -1 and insert all the sequences into the tree.* This is showed in Figure 3.3 (1). Notice that same prefix falls on same branch of the tree. The sequence ID is stored in the leaves. The current root is -1 and the current depth is 0.

Step 2: *For each child of the root, insert suffixes in its subtree to the root's child that has a matching label.* In Figure 3.3 (2), c is a child of the root -1. In this subtree, the suffix subtree starting at d (for sequence $3, 4$) is inserted into the root -1's child d. Each insertion is illustrated by a dotted line connecting the two involved nodes, with the arrow pointing to the *destination node* in Figure 3.3. The sequence IDs associated with the suffixes are combined with existing IDs in the destination node. In the case where a suffix is too short to satisfy *current depth + length of the suffix* $>$ *nc*, the suffix will not be inserted. For example, ba in sequence 3 is also a suffix, it is not to be inserted because the *depth 0 + length of* $ba < nc$.

Step3: *Prune current root's children.* If the number of rows falling in a subtree is smaller than nr, the subtree will be deleted since no further development can generate a cluster with more than nr rows. For example, subtree leading from $-1b$ in Figure 3.3 (2) is deleted in Figure 3.3 (3) since there are only two sequences falling in this subtree.

Step4: *Repeat Step2-Step5 for the root's first child recursively until there is no child node left.* For example, c is the first child of root-1. Therefore, the same procedure in step2 is applied to c first. The suffixes of c's subtree d, such as ba and ab are inserted into c's subtree b and a respectively. Since there was less than three sequences fall on c's subtrees a and b, the branches $-1ca-$ and $-1cb-$ are deleted. Following the same procedure, we develop c's only subtree $-1cd-$, which is shown in Figure 3.3(4).

Step5: *Repeat Step2-Step5 for the root's next siblings recursively.* For example, after finishing $-1c-$'s subtree development, the next subtree to develop is $-1c-$'s sibling $-1d-$. $-1db$'s suffix ac is inserted to subtree $-1da$. However, both subtrees are deleted because they do not have sufficient support count.

Definition 3.4.1 *OPC-tree (Order Preserving Clustering tree). An OPC-Tree is a tree structure defined below.*

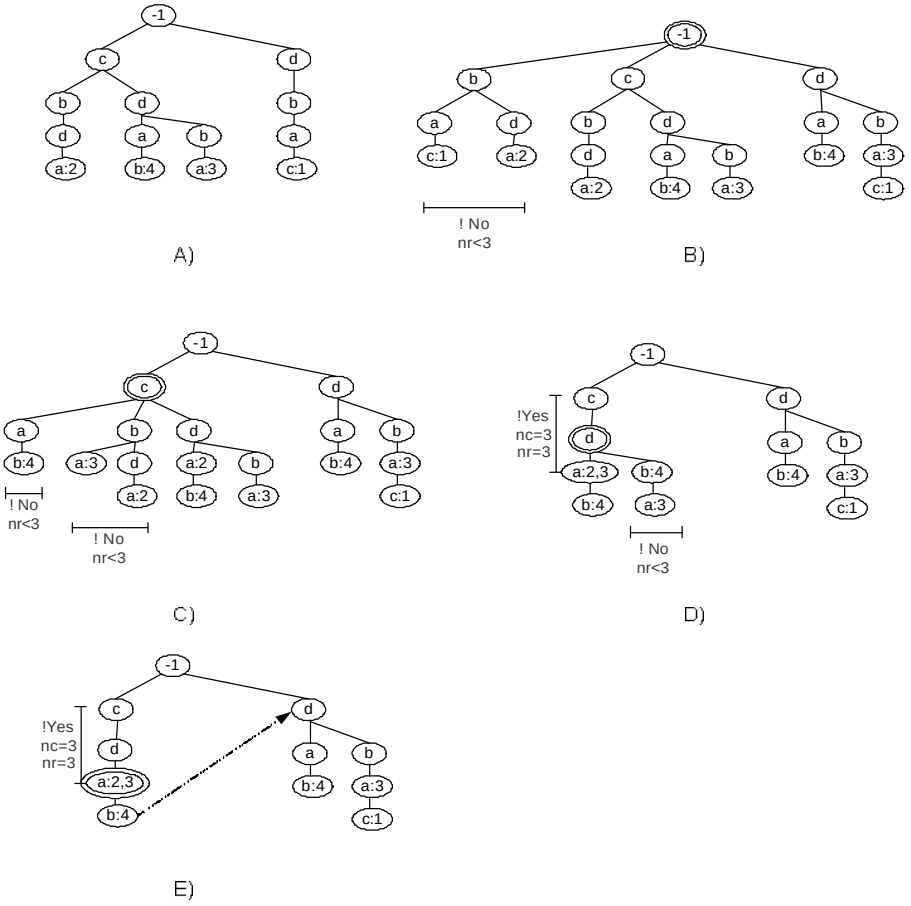


Figure 3.3: OPC-Tree for Table 4.2. The label in the oval shape represents the column. The number following ':' represents the row ID. The node with double oval means active node in the depth first traveral. '!No' means the must-be-pruned subtree. 'Yes' means a valid subtree. A) . Initiate the tree with all the rows B). Insert the suffix of -1's subtrees to -1's subtrees. C). Prune the subtree ($nr < 3$), Insertion. D). Identify the first E). Finish growing the -1's first subtree-1a, the next is -1d.

1. It consists of one root labeled as "-1", a set of subtrees as the children of the root;
2. Each node in the subtrees consists of four entries: entry value, a link to its first children node, a link to its nearest sibling node, and a link list of all the rows that share the same path leading from root to this node, but do not have longer subsequences passing this node. In other words, the sequence IDs are only recorded at the nodes which marked the end of a subsequence.

Algorithm 1 $OPC - Tree(S, nr, nc)$ newline**Input**: S: The sequence set from preprocessing of original Matrix,nr: minimal number of rows, nc: minimal number of columns.
Output: All the subsequence with frequency count$\geq nr$ and length $\geq nc$.
Main program to develop the tree. Create the root of an OPC-Tree, T, and label it as "-1".

---

for each sequence s in $\mathcal{S}$ **do**
  insertSequence(s, T)
  growTree(T)
end for

Algorithm 2 insertSequence(s, T)
Input:$s[i..n]$: the sequence to be inserted, T: the root of OPC-Tree
Output:T: tree with the path corresponding to s
Insert a sequence into the root of a tree

---

if $i = n$ **then**
  insert the ID of s into N's IDlist
  return
else
  if T has a child N such that $N.value = s[i].value$ **then**
    $insertSequence(s[i+1..n]); N)$;
  else
    create a new node N.
    if T's first child $\neq \emptyset$ **then**
      the last sibling's next sibling $\leftarrow N$.
    else
      T's first child $\leftarrow N$.
    end if
    $insertSequence(s[i+1..n]); N)$
  end if
end if
return

Algorithm 3 growTree(T, nc, nr, $depth$)
Input: T: the root of the initiated tree, nc and nr
Output: OP-Clusterexisted in T
Grow patterns based on original T

```
if T = ∅ then
  return;
end if
T_child ←T's first child;
for each sub-tree subT of T do
  insertSubTree(subT, T)
end for
pruneTreeNode(T);
growTree(T_child, nc, nr, depth + 1);
growTree(T's next sibling, nc, nr, depth);
return.
```

Analysis of OPC-Tree construction Only one scan of the entire data matrix is needed to construct an OPC-Tree. For each row, we sort it into a sequence of similarity groups. Then we insert the sequences into the OPC-Tree. As a result, rows with the same prefixes share the same paths from root. To save memory, only the row number associated with each path is recorded at the node corresponding to the end of the sequence. To find the OP-Cluster using the OPC-Tree, subsequences are developed by adding suffixes of each sub-tree as the tree's children, via a pre-order traversal of the OPC-Tree.

Lemma 3.4.1 *Given a matrix M, a similarity grouping threshold, the initiated OPC-Tree contains all the information of matrix M.*

Rationale: Based on the OPC-Tree construction process, each row in the matrix is mapped onto one path in the OPC-Tree. The row IDs and the order of the columns are completely stored in the initiated OPC-Tree.

Mining OP-Cluster Using OPC-Tree

Lemma 3.4.2 *The developed OPC-Tree on a set of sequences contains all subsequences hidden in the initial OPC-Tree.*

Rationale: Given any sequence $S = x_1x_2x_3x_4 \dots x_n$, we want to show that all subsequences of S will be found in a path starting from root. Through the initiation of

OPC-Tree, we know that S will exist in the OPC-Tree. Then given any subsequence $SS = x_i x_j \dots x_s, (i \geq 1, s \leq n)$, we can obtain SS by the following steps. First, at node x_i, if $i = 1$, then insert suffix $x_i x_{i+1} \dots x_n$. Now in the subtree of x_i, we can find node x_j because it will be along the path $x_i x_{i+1} \dots x_n$ that is inserted in the first step. Similarly, we insert the suffix $x_j \dots x_n$ starting from x_j. Now we get the path $x_i x_j x_{j+1} \dots x_n$. By repeating the same procedure, a suffix starting with x_s is inserted. We get the path $x_i x_j \dots x_s$. Since we insert all the suffixes in the OPC-Tree, the OPC-Tree contains all the subsequences presented in the original OPC-Tree.

Rows in a OP-Cluster share the same set of columns, which share the same path in the OPC-Tree. We can conclude that the OPC-Tree contains all the clusters. This leads to the following lemma.

Lemma 3.4.3 *The developed OPC-Tree on a set of sequences contains all potential OP-Clusters. The columns in these clusters are on the paths leading from the root to any tree node with depth no less than nc and row support count in its subtree no less than nr .*

Pruning OPC-Tree

Without any pruning, the whole OPC-Tree fits well into memory when we have a small matrix (15 columns by 3000 rows). However, for large matrices, some pruning strategies must be employed to minimize the size of the OPC-Tree. There are two useful pruning techniques. One strategy is to prune the suffixes with the to-be subsequence shorter than *nc*; the other is to prune the subtrees where the row support count is below *nr*.

Lemma 3.4.4 *For a node N in OPC-Tree with depth d, and for a suffix S with length l in its sub-tree, if $d + l < nc$ (the minimum columns required for a cluster), this suffix S will not be useful in forming any OP-Cluster cluster.*

Rationale: The length of the path L generates by combining the path from root to N and S is $d + l$. Based on Lemma 3.4.3, L will not form any cluster. Therefore, suffix S need not be inserted. In our implementation, we check depth of the node at which the end of the suffix is inserted. If the depth is smaller than *nc*, the row IDs recorded in this node will be deleted.

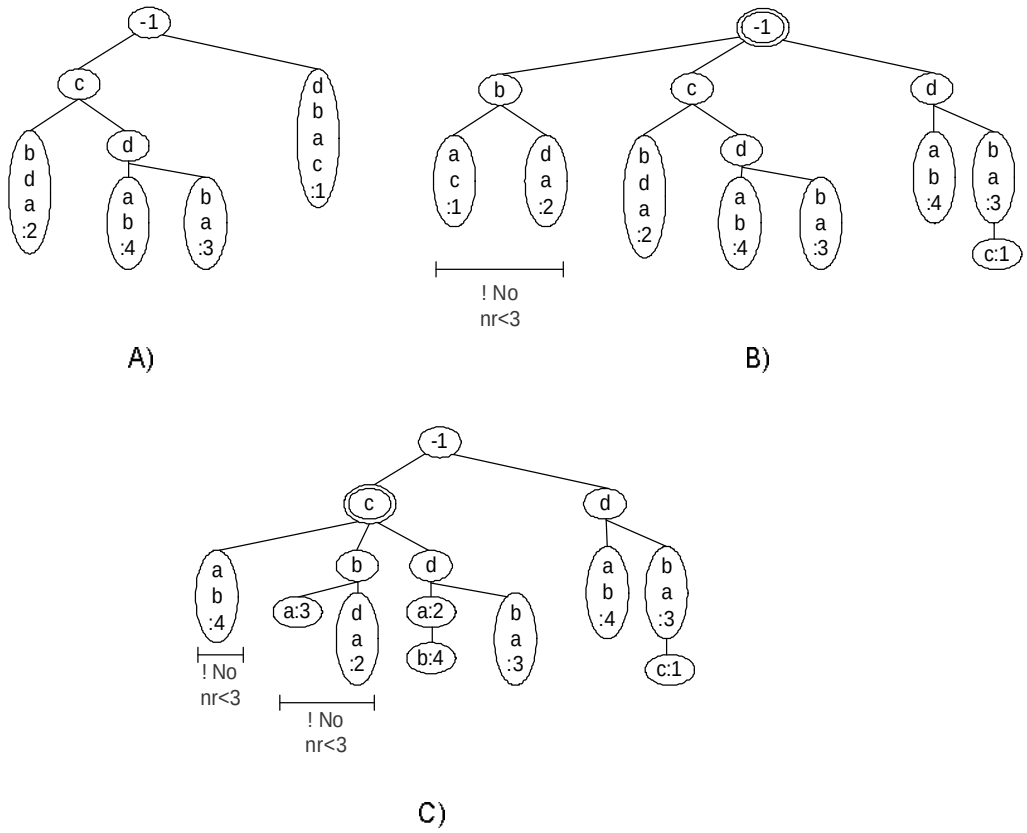


Figure 3.4: Collapsing OPC-Tree for Table 4.2. Sequences in the large vertical oval means collapsed nodes

3.4.3 Improvement with Collapsing Node

The major cost of OPC-Tree development is to concatenate suffix trees to existing prefixes. To minimize the memory footprint, we introduc a more compact OP-Cluster structure, in which single-path tree can collapse into one node.

Figure 3.4 shows the procedure to construct collapsed OP-Cluster structure for the same problem as in Example 3.4.1. All collapsed nodes are denoted by rectangles. There are two scenarios when collapsed node needs to be split.

- *The collapsed node will split if a new branch has to be inserted in the middle of path.* For example, in Figure 3.4, sequence 1 (*dbac*) is collapsed into one node when the tree is initiated. In the development of depth 2, since the subsequence *dab* in sequence 4 will be inserted into path *dbac*, and the only common prefix they have is *d*, a new branch *ab* has to be added in *d*'s sub-tree. The original node which contains *dbac* will split into two nodes which contain *d* and *bac* respectively. *bac* will become a sub-tree of *d*.

- *The collapsed node will split if the inserted branch is a contiguous portion of the single path in the collapsed node.* For example, in Figure 3.4, when the subsequence *dba* in sequence 3 is inserted into *dbac* of sequence 1, *dba* is a portion of *dbac*, *dbac* is split into two parts *dba* and *c*. The number 3 is stored at the end of *dba* to record sequence ID correctly.

Compared with the original OPC-Tree, the collapsed OPC-Tree occupies less space and takes much less time. For example, at depth 0, the original tree needs 15 nodes, while the collapsed tree only needs 5. At depth 1, the original tree needs 21 nodes, but collapsed one needs only 12. In addition, with collapsed OPC-Tree, inserting suffix of single-path tree is avoided.

The single-path is compacted into one collapsed node already. The OP-Cluster can be identified immediately.

3.4.4 Addition Feature: δ-pCluster

According to Lemma 3.3.1, δ-pCluster can be a special case of OP-Cluster if $\delta \geq \frac{\delta^p}{2}$. Therefore, our algorithm for mining OP-Cluster can also be used to find δ-pCluster. Some experiments along this direction is presented in Section 6.7.

3.4.5 Additional Feature: Extension of Grouping Technique

Based on Definition 3.3.1, We can generate different similarity groups if we start from different pivot attributes. For example, If we have an object with four attributes $[A, B, C, D]$. The values for the attributes are $[0.5, 1, 1.5, 2]$. With the similarity threshold as $\delta = 100\%$. We can group them either as $(AB)(CD)$ or as $A(BCD)$. Now have objects 2 and 3 with attribute values $[1, 2, 4, 5]$ and $[9, 4, 5, 6]$, respectively. Their corresponding group sequences are $(AB)(CD)$ and $(BCD)A$. If we set $nc = 3$ and $nr = 2$, the cluster we can get is $(AB)(CD)$ if we group object 1 as $(AB)(CD)$. However, if we use $A(BCD)$, the cluster will be (BCD). And both are valid clusters. To find them, we propose an alternative grouping approach. We put all (possibly overlapping) similar groups in one sequence. For example, in the above example, object 1 becomes $A(AB)(BCD)(CD)$. Then, we can find all sequential patterns of these three objects, which are $(AB)(CD)$ and (BCD). Since we introduce some redundancy, when one attribute appears more than once in a final cluster, we remove all duplicates.

3.5 Experiments

We experimented with our OP-Cluster algorithm on two real data sets. The algorithm was implemented in C and executed on a Linux machine with a 700 MHz CPU and 2G main memory. We also implemented the optimized prefixSpan algorithm for comparison. The following tests are organized into three categories. First, we studied the sensitivity of OP-Cluster to various parameters. Secondly, we evaluated the performance of OPC-Tree and compared it with the prefixSpan algorithm. To conclude, we show two promising patterns found in the drug activity data set.

3.5.1 Data Sets

We experimented with our OP-Cluster algorithm on two real data sets.

Gene Expression Data

Gene expression data are generated by DNA chips and other microarray techniques. The yeast microarray contains expression levels of 2,884 genes under 17 conditions (Spellman et al., 1998). The data set is presented as a matrix. Each row corresponds to a gene and each column represents a condition under which the gene is developed. Each entry

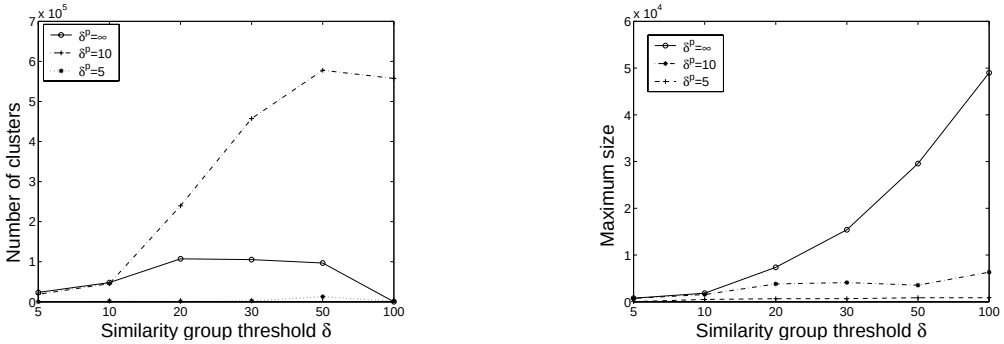
represents the relative abundance of the mRNA of a gene under a specific condition. The entry value, derived by scaling and logarithm from the original relative abundance, is in the range of 0 and 600. Biologists are interested in finding subsets of genes exhibiting similar up-regulation or down-regulation under a subset of conditions (Cheng and Church, 2000).

Drug Activity Data

Drug activity data is also a matrix with 10000 rows and 30 columns. Each row corresponds to a chemical compound and each column represents a descriptor/feature of the compound. The value of each entry varies from 0 to 1000.

3.5.2 Model Sensitivity Analysis

In this section, we evaluate how the similarity threshold δ and δ^p influences the number of clusters and their sizes. We use the yeast data set in this set of experiments. The minimum number of rows is set to be 30 and the minimum number of columns is 10. We vary δ^p from ∞ to 5. Figure 3.5 (a) shows the number the clusters generated and (b) presents the maximum cluster size.

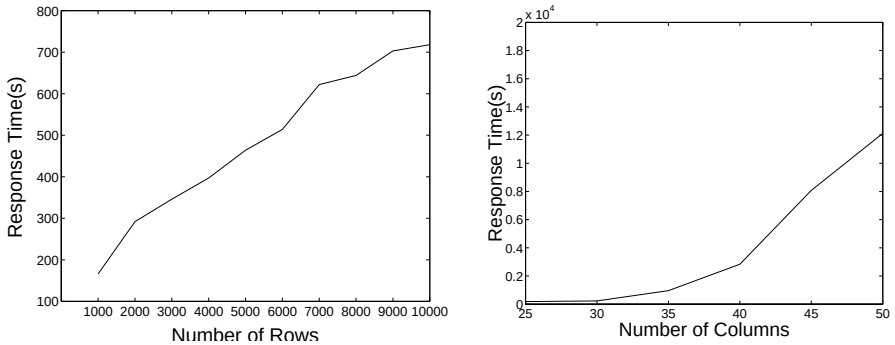


(a) Total number of clusters as a function of similarity threshold

(b) Size(#column×#rows) as a function of similarity threshold

Figure 3.5: Performance Study: cluster number and cluster size V.S.similarity threshold

OP-Clusters are generated when δ^p is infinity. As δ increases, the total number of clusters begins to increase, which implies that more columns are grouped together and that more rows are sharing the same subsequences. However, when the similarity threshold is larger than 100%, the total number of clusters decreases. This is because the overlapped clusters generated by small δ begin to merge into bigger clusters when



(a) Scalability with respect to number of rows

(b) Scalability with respect to number of columns

Figure 3.6: Performance Study: Response time V.S. number of columns and number of rows

delta increases. Since long subsequence of columns have a higher chance to fall on a single path, smaller enclosed subsequences are not counted. Thus, the total number of clusters decreases. Figure 3.5(b) shows that the maximum size of the OP-Cluster increases dramatically in this case.

As δ^p decreases, large clusters tends to split into smaller ones and the total number of clusters increases. The size of each cluster becomes smaller. When more clusters with size smaller than $nc \times nr$ are eliminated, the total number of clusters restricted by δ^p drops below the number of OP-Clusters.

3.5.3 Scalability

We evaluate the performance of the OP-Cluster algorithm as we increase the number of objects and the number of columns in the data set. The response time of the OPC-Tree is determined by the size of the tree. Figure 3.6 shows the response time of the drug activity data set. The columns and the rows of the matrix carry the same significance in the OP-Cluster model, which is symmetrically defined in Formula 3.1. Although the algorithm is not entirely symmetric in the sense that it chooses to project column-pairs first, the curves in Figure 3.6 demonstrate similar trends.

For experiments in Figure 3.6(a), the number of columns is 30. The minimal number of columns of the embedded OP-Cluster is 9, and the minimal number of rows is set to $0.01N$, where N is the number of rows of the drug activity data. The mining algorithm is invoked with $\delta = 0.2$, $nc = 9$, and $nr = 0.01N$. Data sets used in Figure 3.6(b) are taken from the drug activity data with the number of rows fixed as 1000. The mining

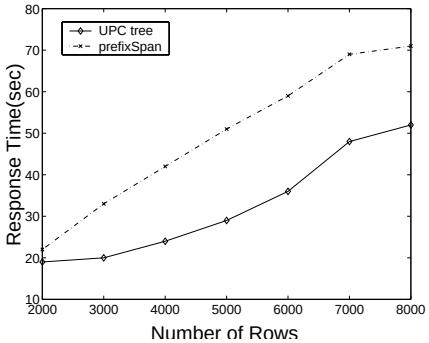


Figure 3.7: Performance comparison of prefixSpan and UPC-tree

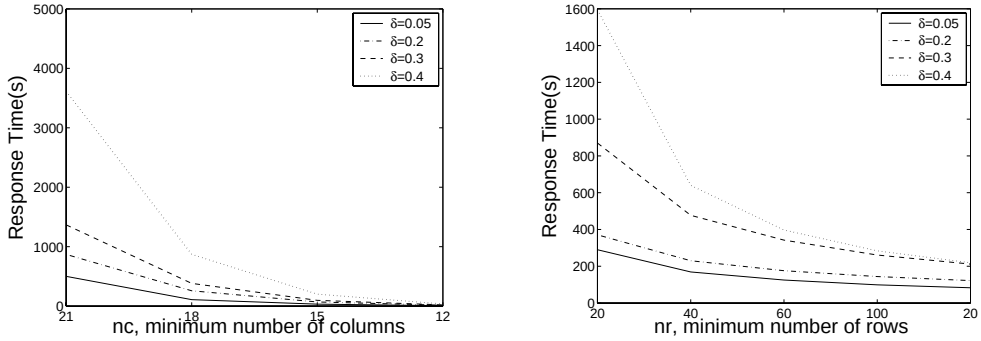
algorithm is invoked with $\delta = 0.2$, $nc = 0.66C$, and $nr = 30$.

Figure 3.7 presents the performance comparison between the prefixSpan algorithm and the OPC-Tree algorithm. In this experiment, we used drug activity data to see the performance with different number of rows. The parameter setting for this set of experiment is the following: $nc = 9$, $nr = 0.01N$, $\delta = 0.2$. The number of columns is set to be 20. We observe that the OPC-Tree algorithm constantly outperforms the prefixSpan algorithm and the advantage becomes more substantial with larger datasets.

Next, we studied the impact of the parameters (δ, nc, and nr) towards the running time. The results are shown in Figure 3.8. The size of matrix is 27×3776. When nc and nr are fixed, the running time prolongs when the similarity threshold increases. This is because the size of the clusters increase as we relax the similarity threshold. Therefore, the OPC-Tree has to spend more time to construct a deeper tree. When similarity threshold is fixed, it takes longer time to construct the OPC-Tree as nc decreases. This is showed in Figure 3.8. According to the pruning techniques we discuss in Lemma 3.4.4, a fewer number of subsequences can be eliminated when using smaller nc. As a result, a larger tree is constructed, which consumes more time. A similar effect can be observed with respect to nr from Figure 3.8(b).

3.5.4 Results from Real Data

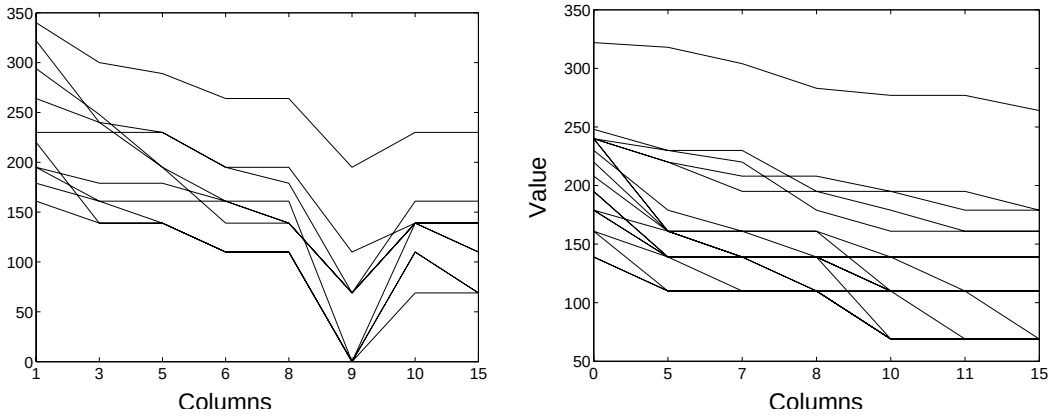
We applied the OP-Cluster algorithm to the datasets. With parameter $\delta = 10$, Some interesting clusters are reported in both of the data sets. As showed in Figure 3.9, the two patterns generated from yeast dataset (Cheng and Church, 2000) present the coherent tendency along the columns on the Y axis. In Figure 3.9(a), if we rearrange the columns as 15, 10, 9, 8, 6, 5, 3, 1, we will see the 'up' pattern embedded in it. Figure 3.9 (b) shows another interesting cluster which present with a 'down' tendency



(a) Response time varying similarity threshold and nc

(b) Response time varying similarity threshold and nr

Figure 3.8: Performance Study: Response time V.S. similarity threshold , nc and nr



(a) Cluster #1

(b) Cluster #2

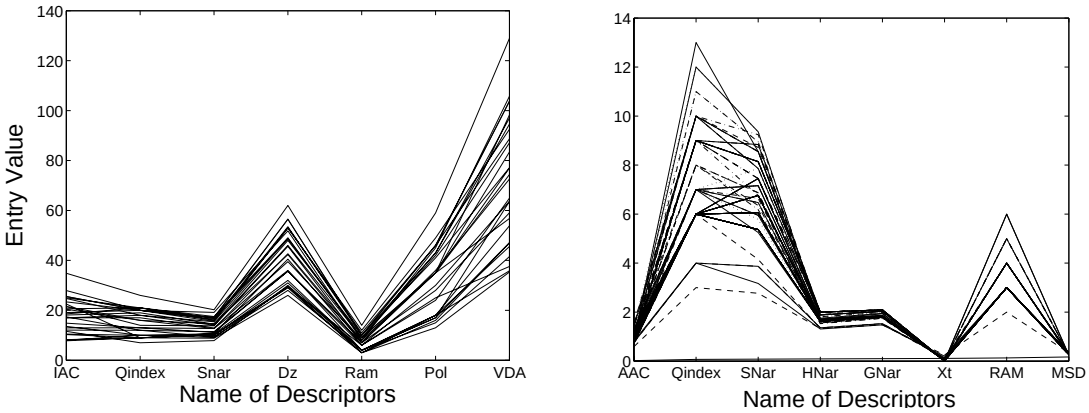
Figure 3.9: Cluster Analysis: Two examples OPC-Tree in yeast data

itself. Another pair of patterns are showed in Figure 3.10. They present a series of consistent patterns under a subset of features. It is also interesting to notice that, the patterns includes all of three Nars, which is SNar, GNar and HNar.

Besides this, in both of the figures, we observe that the curves with sharper slopes are discovered with 'up' pattern, while it can never be discovered by the traditional distance measure nor other pattern-based models.

3.6 Conclusions

In this chapter, we proposed a new model called OP-Cluster to capture the consistent tendency clusters exhibited by a subset of dimensions in high dimensional space. In many applications including collaborative filtering and DNA array analysis, although



(a) Cluster #1 (b) Cluster #2

Figure 3.10: Cluster Analysis: Two examples OPC-Tree in drug activity data

the distance (e.g., measured by Euclidean distance or cosine distance) among the objects may not be close, they can still manifest consistent 'up' pattern over a permutation of a subset of dimensions. To address this issue, we introduce a new model called OP-Cluster to model tendency among a set of objects. We proposed a compact tree structure, namely OPC-Tree, and devised a depth-first algorithm that can efficiently and effectively discover all OP-Clusters with a user-specified minimum size.

Chapter 4

Ontology Driven Subspace Clustering

This chapter introduces a semi-supervised subspace clustering framework by directly incorporating partial domain knowledge into clustering process. The algorithm yields a set of subspace clusters with strong classification implication. During the clustering process, ontology information is utilized to efficiently prune the exponential search space of the subspace clustering algorithms. Meanwhile, the algorithm generates automatical interpretation of the clustering result by mapping the natural hierarchical organized subspace clusters with significant categorical enrichment onto the ontology hierarchy. Our experiments on a set of gene expression data using gene ontology demonstrate that our pruning technique driven by ontology significantly improve the clustering performance with minimal degradation of the cluster quality. Meanwhile, many hierarchical organizations of gene clusters corresponding to a sub-hierarchies in gene ontology were also successfully captured.

4.1 Introduction

Clustering analysis is purely syntactical in the sense that it does not take advantage of the existing knowledge in the learning process. Eventually, the most challenging problem is how to approach the matters of *interpretability*, i.e. why the objects in a cluster should be clustered together. In many applications, people may have significant amount of knowledge on the data set, which are usually utilized to measure the significance of a cluster. Traditionally, this knowledge is only used during the postprocessing step for validation of the clustering results. The following are some examples.

- Gene Expression Profiles. The gene expression profile is represented as a matrix where each row is a gene and each column is a condition while the corresponding

entry records the expression level of the given gene under the given condition. A large number of gene expression profile analysis tools have been developed (Wang et al., 2002; Yang et al., 2002; Liu and Wang, 2003). However, all these work ignore one fact that there exists an extensive amount knowledge of the genes. For instance, gene ontology (GO) (ash,) has been developed to categorize the relationship among genes. The Gene Ontology(GO) has become a well accepted standard in organizing the classification categories for genes. The relationships, such as 'part of' and 'overlapping', between any two function groups can be very sophisticated. Until now, no clustering algorithm can generate the clusters among which the relationships can similarly model the GO hierarchy. The failure in resembling the relationships may limit the quality of gene function prediction. Meanwhile, the existing classification of genes are not taken advantage by any clustering algorithm in order to improve the clustering quality and interpretability. Therefore, GO can be utilized to not only speed up the clustering process, but also produce more biologically meaningful results.

- Customer Preference Profiles. In a user preference data set, each user (customer) may rank a set of goods. In reality, various goods are not independent of each other. For instance, VCR, DVD players, and VCD players are very similar while they are quite different from clothing and sports equipments. This type of knowledge could be utilized for analyzing the customer preferences.

It would be very beneficial (in both execution time and clustering results) if these knowledge could be utilized. In this paper, we assume that the domain knowledge is captured in an ontology. The reason that we choose ontology to represent the domain knowledge is following. (1) This model is flexible yet powerful to capture the various degrees of relationship among objects (or attributes). (2) It is used in real applications. For example, in the bioinformatics community, the GO Consortium was formed to converge the efforts to make the controlled vocabulary of various genomic databases about diverse species in such a way that it can show the essential features shared by all the organisms (ash,).

We propose a hierarchical framework to directly incorporate the ontology knowledge into subspace clustering process. Our particular interest lies in searching subspace clusters that can be well explained by its ontology categories. However, is there a natural correspondence between the hierarchy of subspace clusters and the hierarchy of ontology? To answer this question, we give the following example.

Example 4.1.1 *Table 4.1 presents a subset of zoo data in UCI KDD repository.*

animals	head	breathe	milk	legs	size	meat
squirrel	1	1	1	4	0	1
puma	1	1	1	4	1	0
dove	1	1	0	2	0	1
flamingo	1	1	0	2	1	1
perch	1	0	0	0	0	1
shark	1	0	1	0	1	0

Table 4.1: A database for a subset of zoo animals

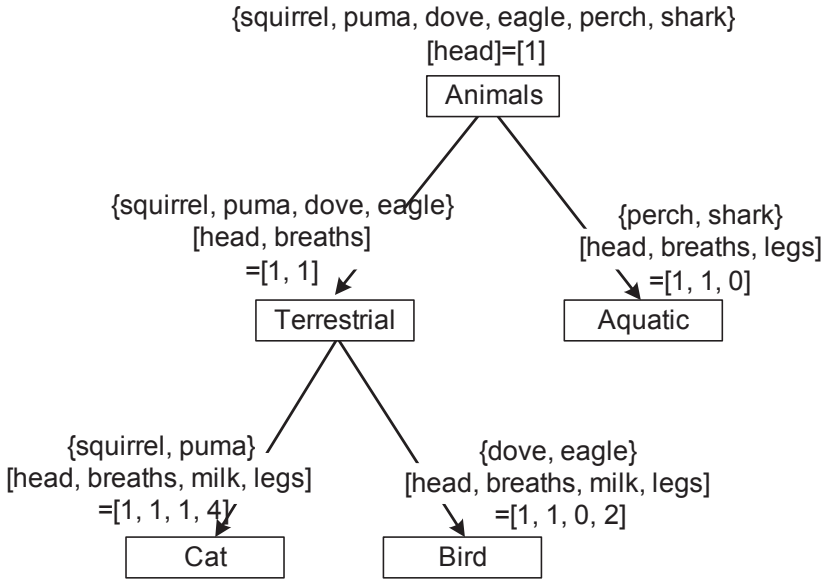


Figure 4.1: An animal ontology and subspace clusters corresponding to each category

A possible ontology for this small database is shown in Figure 7.5. Based on the ontology and the number of attributes shared by the animals at each ontology level, we observe that the higher level the category is in the hierarchy, the less attributes the objects in that category may share. For example, in each of "cat" and "bird" categories, the set of attributes$\{head, breaths, legs, milk\}$ are shared among the animals respectively, while the "terrestrial" category which includes both "cat" and "bird" only share the attributes $\{head, breaths\}$.

The ontology can not only be used to guide the clustering process, but also can be used to validate the clustering results. If a cluster contains terms very far apart on the ontology hierarchy, then the cluster may not be very meaningful in that domain. According to this example, we may have the following observations of ontology:

- The traditional clustering algorithm might generate the irrelevant clustering result for classification since some irrelevant attributes might distance the objects that should be in the same category from each other. For example, while "puma" and "squirrel" are both related to the same category along the attribute set $\{head, breaths, legs, milk\}$, including the other two attributes "size" and "meat" may enlarge the distance between them. Therefore, good clustering result for the a category may only be located in a subset of attributes.

- Given an ontology hierarchy, it is intuitive that the objects in the higher level of the category might share less attribute sets than the objects in the lower level of the hierarchy, as is the case with the animal ontology in Example 4.1.1.

Based on the above observation, given a database with a set of objects featuring a set of attributes, it will be interesting to find out which subset of objects can be clustered together over which subset attributes that can be classified into the same category located in the ontology hierarchy. We also want to find out for each category, which subset of attributes might contribute to the split of the object sets into more detailed classification.

We create a general framework for ontology-driven subspace clustering. This framework can be most beneficial for the hierarchically organized subspace clustering algorithm and ontology hierarchy, i.e., it is independent of the clustering algorithms and ontology application domain. To demonstrate the usefulness of this framework, we choose TP-cluster algorithm (Liu and Wang, 2003) and the gene ontology as two representatives of exhaustive subspace clustering and ontology respectively. Both of them have been proven useful in clustering gene expression profiles and gene function annotation.

Contribution

- We formally define an ontology hierarchy. Based on this, we use a substructure of the ontology hierarchy to interpret the categorical meaning of a cluster.

- We build a framework to incorporate domain knowledge (represented as ontology) into subspace clustering. This novel clustering algorithm automatically generates meaningful clusters (with respect to the ontology) while improving the performance.

- We design a new model to assess the objects' distribution of each ontology category in a cluster. Based on this, we developed a ontology-based pruning technique to minimize the redundancy in the subspace clusters.

- Our experiment results demonstrate that the ontology paths are well corresponded to certain local structure of hierarchically organized subspace clusters. Meanwhile, the performance of ontology-driven subspace clustering algorithm has great improvement with minimum loss of clustering quality.

The remainder of this chapter is organized as follows. Section 4.3 defines the model proposed in the paper. Section 4.4 presents the algorithm in detail. An extensive performance study is reported in Section 4.5. Section 4.6 concludes the paper and discusses some future work.

4.2 Ontology Framework

The ontology essentially defines a hierarchy (or DAG) as illustrated in Figure 7.5 where each node corresponds to a *lexion* which is the category term. In addition, each term classified a set of objects and the set of objects in a descendent term is always part of the set of objects in its ancestor.

Definition 4.2.1 *An ontology is a sign system* $\mathcal{O}:=(\mathcal{L}, \mathcal{H}, \mathcal{R})$*, which consists of*

- *A lexicon: The lexicon* $\mathcal{L}$ *contains a set of natural language terms.*

- *A hierarchy* $\mathcal{H}$*: Terms in* $\mathcal{L}$ *are taxonomically related by the directed , acyclic, transitive, reflexive relation* $\mathcal{H}$*. (*$\mathcal{H} \subset \mathcal{L} \times \mathcal{L}$*);*

A top term $\mathcal{R} \in \mathcal{L}$*. For all* $l \in \mathcal{L}$*, it holds:* $\mathcal{H}(l, \mathcal{R})$*.*

One example of the ontology in Bioinformatics application is Gene Ontology. GO Consortium was formed to integrate the efforts to make the controlled vocabulary of various genomic databases about diverse species in such a way that it can show the

essential features shared by all the organisms (ash,). GO has three ontology files corresponding to its three categories, namely molecular function, biological process and cellular component. An acyclic directed graph can be obtained for each category with GO terms as nodes. The recognition of the GO hierarchical system as a diagraph with top-down directions makes us easily catch the structure of the ontology. Figure 4.2 presents a screen shot of the top levels of the gene ontology. At the first level, genes are divided into three categories, i.e., Molecular Function(MF), Cellular Component(CC) and Biological Process(BP).

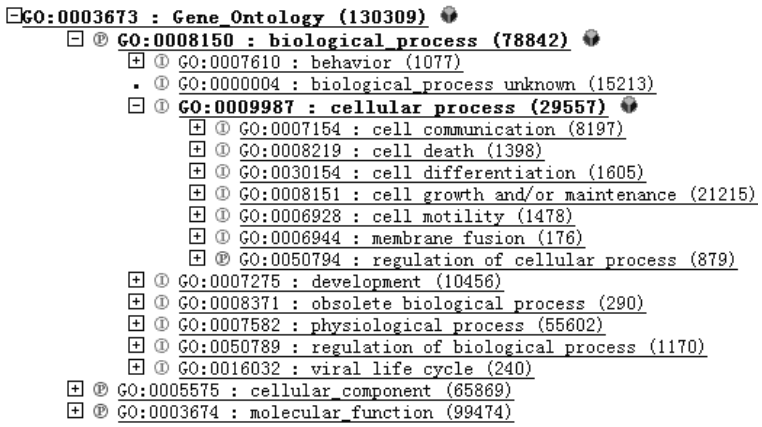


Figure 4.2: Schema of GO annotation terms.

Formally, GO hierarchy is naturally described as a directed acyclic graph (DAG). $GO =< \mathcal{V}, \mathcal{E} >$, where $\mathcal{V}$ is a set of gene function description (GO terms) and $\mathcal{E}$ is a binary relation on $\mathcal{V}$ such that genes with functions described by v_j are a subset of genes with functions described by v_i, denoted $v_j \preceq v_i$, if and only if there exists a path $(v_i, v_{i+1}\ , ..., v_{j-1}, v_j)$ such that $(v_{m-1}, v_m) \in \mathcal{E}$ for $m = i+1, i+2, ..., j-1, j$. The relationship between the children terms and the parent term is also called "part of" or "specific", which means that all the genes annotated as the children GO terms will also be included as part of the genes annotated as the parent GO term.

Nevertheless, to fit GO in our model, we will transform the original digraph of GO into our desired form, an ordered tree that is a directed tree with an order defined for siblings. Note that the same GO term may occur several times (in different lines) in an ontology file. From a biological viewpoint, these occurrences should be considered

distinct because the important thing is not the term itself, but rather the location of the term in the hierarchy (i.e., the path from the root to the term).

Let $\mathcal{D}$ be the universe of the objects and let $a : \mathcal{D} \rightarrow \mathcal{V}^{|\mathcal{V}|}$ be a classification annotating each object with a set of classification category at the most specific level of the classification. Given a set of categories $\mathcal{G} = v_1, v_2, ..., v_t$, an object is called a *known gene* if there exist a category v, $v \in \mathcal{G}$, such that the set of object-category pairs $\{(x, v) \, | x \in \mathcal{D}$ and $u \in a(x)$ and $u \preceq v$ and $v \in \mathcal{G}\}$ is not empty. Otherwise, the object will be denoted as an *unknown* . In Gene Ontology, the set of objects corresponds to the set of genes and the set of categories corresponds to the set of gene function terms. Unknown genes are either the genes without annotation or genes with annotations not inside the scope of the given GO term set $\mathcal{G}$.

4.3 TP-Cluster Model and Ontology Interpretation

We are interested in the TP-Clusters, in which the subset of objects in I exhibits a coherent tendency on the subset of attributes J of $\mathcal{A}$.

gID	a	b	c	d	*sequence*
1	4002	284	4108	228	*dbac*
2	401	281	120	298	*cbda*
3	401	292	109	238	*cdba*
4	280	318	37	215	*cdab*

Table 4.2: Example Data Set.

Definition 4.3.1 *Let I be a subset of objects in the database $\mathcal{D}$, $I \subseteq \mathcal{O}$. Let J be a subset of attributes, $J \subseteq \mathcal{A}$. Let $\mathcal{R}$: $\mathcal{T} \times \mathcal{O} \times 2^{|\mathcal{A}|} \rightarrow int$ be the function that assigns the rank of an object i's attribute j to be r, if the value of the object i under attributes j is the r^{th} lowest value among that under all the conditions in $\mathcal{T}$. ($\mathcal{O}$, $\mathcal{T}$) forms a* **TP-Cluster (Tendency Preserving Cluster)**, *if $\forall$ i, j ($i, j \in I$), $\forall$ a ($a \in J$), $\mathcal{R}(i, a, J) = \mathcal{R}(j, a, J)$ and $\forall$ k ($k \in \mathcal{O} - \mathcal{I}$), $\forall l (l \in I)$, $\exists b$ ($b \in J$), $\mathcal{R}(k, b, J) \neq \mathcal{R}(l, b, J)$.*

Definition 4.3.1 first defines the rank function. Based on the rank function, the TP-Cluster is defined as a subset of objects which have the same ranks under a subset of attributes. Meanwhile, each TP-Cluster is defined as a maximal cluster in that adding any additional object in the database will violate the rank coherence with the cluster.

For example, in Table 4.2, we say that the gene set $\{2, 3\}$ forms a cluster along the subset of conditions $\{a, c, d\}$, since the ranks of the three conditions for both genes are the same, i.e. (3, 1, 2).

Next,we show that each TP-Cluster can be mapped onto an ordered sequence of condition labels by choosing a consistent order of the conditions in any of the TP-Clusters, such as monotonically increasing or decreasing.

Definition 4.3.2 *Given a TP-Cluster $\mathcal{C}$ with object set $\mathcal{O}$ and condition set $\mathcal{T}$, We call a sequence of conditions S representing $\mathcal{C}$ in a monotonically increasing order, if S=$\pi(\mathcal{T})$, where function π places each condition a in $\mathcal{T}$ at the position $\mathcal{R}(a)$ in sequence S.*

For example, for cluster $\{2, 3\}\times\{a, c, d\}$ in Table 4.2, the sequence of conditions that represents the monotonically increasing order is *cda*. For condition c, its rank is 1 and the position in the sequence is 1. It is also the increasing order of the sequence of conditions

Definition 4.3.3 *Given two TP-Cluster $\mathcal{C}_1$ and $\mathcal{C}_2$ with condition set $\mathcal{T}_1$ and $\mathcal{T}_2$ respectively, we call $\mathcal{C}_1$ is the ancestor of $\mathcal{C}_2$ if $\pi(\mathcal{T}_1)$ is a prefix of sequence $\pi(\mathcal{T}_2)$.*

For example in Table 4.2, the sequence representing cluster $\mathcal{C}_1$=$\{2, 3\}\times\{a, c, d\}$ is *cda*. The sequence representing cluster $\mathcal{C}_2$=$\{2, 3, 4\}\times\{c, d\}$ is *cd*. Since *cd* is the prefix of *cda*, we call $\mathcal{C}_2$ is the ancestor cluster of $\mathcal{C}_1$.

Based on the mapping from TP-Cluster to the sequences, we are able to organize the TP-Clusters into a prefix tree. We will introduce an algorithm which builds the HTP-clustering tree in a very compact fashion in the Section 4.4.

The following Lemma present the 'part-of' relationships of the TP-Clusters.

Lemma 4.3.1 *Let $\mathcal{C}$ and $\mathcal{C}'$ be two TP-Clusters in the database $\mathcal{D}$. Let I and I be the object sets of $\mathcal{C}$ and $\mathcal{C}'$ respectively, if $\mathcal{C}'$ is the ancestor of $\mathcal{C}$, then $I \subseteq I'$.*

Proof 4.3.1 *Since $\mathcal{C}'$ is ancestor of $\mathcal{C}$, $\pi(J')$ must be a prefix of $\pi(J)$, based on Definition 4.3.3. $\forall i(i \in I)$, i supports πJ. Thus, g must support any prefix of πJ. Therefore, i supports $\pi(J')$, $i \in I'$. Since $\forall i, i \in I$ implies $i \in I'$, we have $I \subseteq I'$.*

Obviously, cluster $\mathcal{C}_1$ and $\mathcal{C}_2$ follows this property. $\mathcal{C}_2$ is the ancestor of $\mathcal{C}_1$ and $\{2, 3, 4\}\supseteq\{2, 3\}$.

4.3.1 The HTP-clustering tree

In this section, we will introduce the HTP-clustering tree.

The ODTP-clustering is generally analogous to a prefix tree of a predefined set of sequences. However, it is also different because of its unique interpretation of each node and the parent-child relationship. Each node in HTP-clustering tree represents a unique TP-Cluster.The root node corresponds to the null space. The nodes at level m correspond to m dimensional TP-Cluster. The TP-Cluster at a node is related to its immediate parent by being part of cluster. Each TP-Cluster other than the null root is 1-dimensional extension of its parent cluster. In order to elucidate HTP-clustering tree we give a maximal TP-Cluster tree of three conditions in Figure 4.3, where each TP-Cluster is represented by a sequence. We call it 'maximal' since there does not exist another TP-Cluster that may not be included in the lattice given the condition set. The figure contains a three-level tree structure which corresponds to 1-, 2- and 3-dimensional TP-Clusters. Each node u in the HTP-clustering tree is represented by the path from the root of the TP-Cluster leading to u. For example, the TP-Cluster with two conditions $\{b, c\}$ ordered increasingly as (bc) will be put at the node $-(\emptyset)bc$. The gene set associated with each node in the HTP-clustering tree is not shown in the figure.

Definition 4.3.4 *The HTP-clustering tree is a hierarchical arrangement of TP-Clusters with the following properties: 1) The tree is rooted at level 0 with* $\emptyset$*. (2) Each node at level* m *corresponds to a* m*-dimensional TP-Cluster represented by a length-*m *sequence. 2) Each node at level* $(m+1)$ *is a 1-dimensional extension of its immediate ancestor, which corresponds to a length* $(m+1)$ *sequence.*

The problem we are interested here is the hierarchical relationship among TP-Clusters. Investigating the relationships among TP-Clusters may help us with the prediction of the behavior of higher dimensional clusters based on the lower dimensional ones.

4.3.2 Annotation of a Cluster

In this subsection, we present the annotation of a cluster given an ontology. We first introduce the P-value to assess the significance of a particular category within a cluster.

The hypergeometric distribution is used to model the probability of observing at least k objects from a cluster of g objects by chance in a category containing f objects

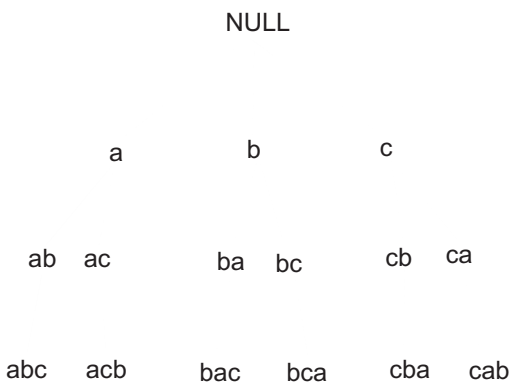


Figure 4.3: The maximal hierarchy of the TP-Clusters given a condition space $\mathcal{A}=\{a, b, c\}$.

from a total set of n genes. The P-value is given by $P = 1 - \sum_{i=0}^{k} \frac{\binom{f}{i}\binom{n-f}{g-i}}{\binom{n}{g}}$. The test measures whether a cluster is enriched with genes from a particular category to a greater extent than that would be expected by chance. For example, if the majority of genes in a cluster appear from one category, then it is unlikely that this happens by chance and the category's P-value would be close to 0. Adopting the Bonferroni correction for multiple independent hypotheses, $\frac{0.01}{Na}$ is used as the threshold θ_p, to measure the significance of the P-value.

To annotate a cluster, the P-value of each category present in the cluster will be computed first. Given a cut-off P-value threshold, categories which have relatively large P-value will be dropped without further consideration. The result is a set of significant categories $\mathcal{V}=\{v_1, v_2, ..., v_t\}$. There are two naive ways to annotate the clusters with the set of the significant categories $\mathcal{V}$. One method is to keep all the significant categories as annotation candidates. The disadvantage of this one is that it will be hard to determine the object categories when being assigned to too many functionalities. The other way is to annotate a cluster with the category that has the least P-value. Choosing the most significant category to represent the cluster is reasonable. However, it may discard some important information, such as the significance of the subcategories of the most significant category.

In our method, we adopt a middle way between the two methods. We use an appropriate subtree in the ontology to represent the cluster annotation. The subtree is rooted at the node of the most significant category and includes all the significant categories that are located in the root's subtree. The annotation is formally defined as

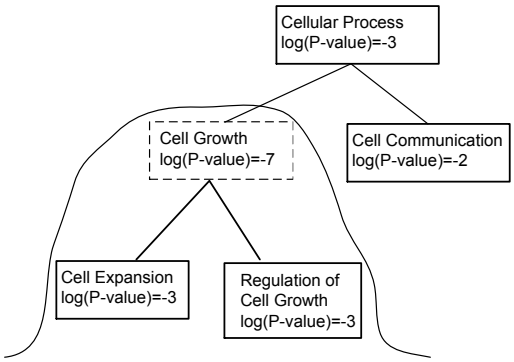


Figure 4.4: An example of OST representing a Cluster. The two values in each node represent the function category and its P-value.

the Ontology SubTree(OST) in Definition 4.3.5

Definition 4.3.5 *Given a cluster $\mathcal{C}$, and its significant function categories $\mathcal{V} = \{v_1, v_2, ...v_t\}$, Ontology SubTree(OST) representing a cluster is defined as a tree $\mathcal{H}$. The root of $\mathcal{H}$ is the category v_r, $0 < r \leq t$, where $P(v_r, \mathcal{C}) = \min_{0<i\leq t}(P(v_i, \mathcal{C}))$. The descendants of $\mathcal{H}$ are the set of the categories which are the immediate descendants of v_r in the ontology.*

First, with the level-wise structure of ontology, a gene that is classified into a certain category will always be a member in its ancestor's category. Therefore, the OST is rooted at most significant category to ignore the less detailed ancestor function categories.

Secondly, although the children of v are not as significant as v in cluster $\mathcal{C}$, it is still possible that later split of the cluster may signify the coherence of the children categories of v. Thus, we keep these function categories for further clustering.

Figure 4.4 show an OST that annotates a cluster. To determine the OST representing this cluster, we first find out the location of most significant function groups, which in this case, is cell growth,with $log(P - value)$=-7. We then discard its parent category of cellular process, and siblings, cell communication, which has less P-value. The resulting OST is the subtree rooted at cell growth.

Definition 4.3.6 *Given a cluster $\mathcal{C}$, we call $\mathcal{C}$ is functionally enriched if there exists an OST representing the cluster, given a P-value threshold θ_p.*

Definition 4.3.7 defines the $\prec$ relationship between two OSTs.

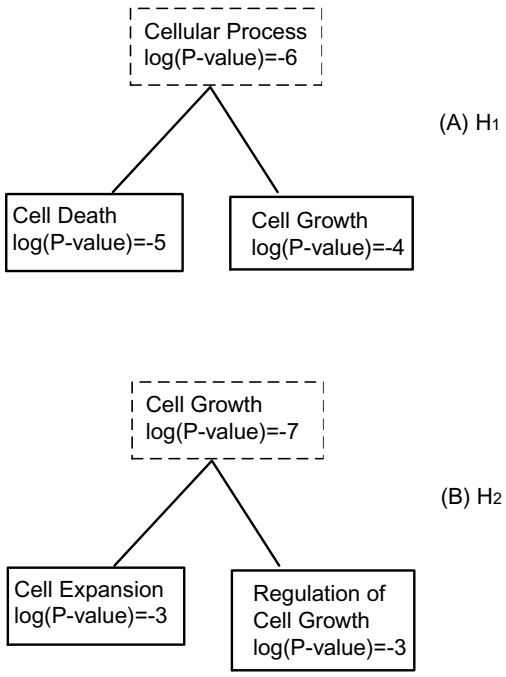


Figure 4.5: An example of two OSTs $\mathcal{H}_1$ and $\mathcal{H}_2$, $\mathcal{H}_2 \prec \mathcal{H}_1$.

Definition 4.3.7 *Given two OSTs $\mathcal{H}_1$ and $\mathcal{H}_2$, we call $\mathcal{H}_1 \prec \mathcal{H}_2$ if the root node of $\mathcal{H}_1$ appears in the nodes of $\mathcal{H}_2$.*

For example, Figure 4.5 contains two clusters' OSTs, we call $\mathcal{H}_2 \prec \mathcal{H}_1$ since we can find the root node cellular growth of $\mathcal{H}_2$ in $\mathcal{H}_1$'s subtree.

4.3.3 Mapping the HTP-clustering tree onto Ontology

In this section, we define the relationship between HTP-clustering tree and ontology. The children and parent relationship in GO hierarchy is "part-of" and "more specific". Or, in other words, the genes in the children node should be more similar and consistent. Here we assume that in the GO hierarchy, the genes assigned to one category stay close in a larger subset of conditions than the genes assigned to its parent category, which is exactly the relationship of child and parent node in HTP-clustering tree. In this way, we unite the two hierarchy together.

Next, we use the child and parent relationship of gene ontology to evaluate against the child and parent relationship in the HTP-clustering tree.

Definition 4.3.8 *Let $\mathcal{C}$ be a TP-Cluster and $\mathcal{C}'$ be one of $\mathcal{C}$'s descendants. Let $\mathcal{H}$ be $\mathcal{C}$'s OST, and let $\mathcal{H}'$ be $\mathcal{C}'$'s OST, $\mathcal{C}'$ is a biological descendent of $\mathcal{C}$ if $\mathcal{H}' \prec \mathcal{H}$.*

If the cluster $\mathcal{C}_1$ represented by $\mathcal{H}_1$ in Figure 4.5 is immediate ancestor of the cluster $\mathcal{C}_2$ represented by $\mathcal{H}_2$, we call $\mathcal{C}_2$ is the biological descendent of $\mathcal{C}_1$ if $\mathcal{C}_1$ is its ancestor.

Problem Statement Let $\mathcal{D}$ be a database with a set of objects $\mathcal{O}$ and condition set $\mathcal{A}$. Given a threshold θ_p for cluster enrichment, our goal is to extract a biologically relevant hierarchy of enriched TP-Clusters.

4.4 Construction of Ontology Relevant HTP-clustering tree

4.4.1 Construction of HTP-clustering tree

In this section, we show the HTP-clustering tree can be constructed by suffix concatenation in conjunction with extracting only biologically relevant TP-Clusters. The inputs to the HTP-clustering tree construction algorithm include the database $\mathcal{D}$, the GO ontology, and function enrichment threshold θ_p. The HTP-clustering tree is constructed hierarchically in a top-down fashion, along which the dataset $\mathcal{D}$ is partitioned. The HTP-clustering tree construction uses a depth-first pre-order traversal algorithm in order to build the tree structure. We prefer the depth-first order to the breadth-first order because we can minimize the amount of storage needed for each level to develop clusters in the next level. The depth-first traversal is also correct because for each node, the construction of its subtree will be relatively independent of the construction of its siblings.

The HTP-clustering tree construction process can be summarized in two steps:

1. We first preprocess the data. Each row in the data matrix will be converted to an ordered sequence of column labels based on rank in Definition 4.3.1. Those sequences will be the inputs to the next steps. An initial prefix tree containing the sequence of every gene in the database will be constructed.

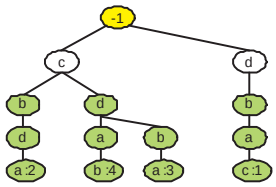
2. The initial prefix tree will be recursively visited and developed in the depth-first order to reveal all frequent subsequences, which represent TP-Clusters. The ontology information of the genes in the database will be fed into the HTP-clustering tree at the root level. Ontology-based pruning will be performed upon the visit at each node.

We focus on the second step which is more challenging and important during the whole mining process. The data structure representing the HTP-clustering tree is defined below.

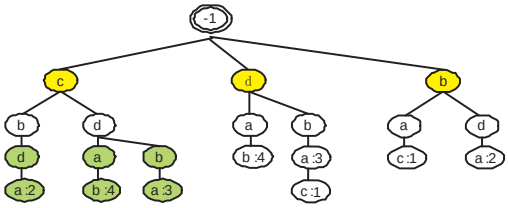
1. It consists of one root labeled as "-1" and a set of subtrees as the children of the root;

2. Each node in the subtrees has four entries: entry value, a link to its first child node, a link to its next sibling node, and the list of gene IDs, each of which has a suffix corresponds to the path from the root to this node. In other words, the gene IDs are only recorded at the node that marks the end of a common subsequence.

We use the dataset in Table 4.2 in the following example to illustrate the suffix concatenation step during the tree construction process.



(A) Initial tree



(B) First suffix concatenations at level 1

Figure 4.6: The illustration of suffix tree concatenation.

Example 4.4.1 *For sequences in Table 4.2, the initial prefix tree representing the whole database is presented in Figure 4.6 (A) and the suffix concatenation upon visiting the first node "-1" is illustrated in Figure 4.6 (B).*

Let's denote the node currently being visited to be the active node. Given an active node in the HTP-clustering tree construction process, for example, the "-1"(NULL) node in Figure 4.6 (B), the suffixes to be inserted to "-1"'s subtree are those inside the rectangle box shown in Figure 4.6 (A). The concatenation of the suffixes to the current active node is done by merging the suffix tree of the active node with the

corresponding subtree one level below the active node. For example, suffix tree "-1cd" in (A) is merged with "-1d". The generated subtree is shown as the "-1d" subtree in (B). (B) is the subsequent tree after the visit of the node "-1". The same procedure will be applied recursively in the depth-first order to construct the HTP-clustering tree. For example, after the first node visit at the root "-1", the next node to be visited will be "-1c", the suffix inside the rectangle box in Figure 4.6(B) will be the next set of suffixes to be inserted. The TP-Cluster algorithm without biological assessment is presented in Algorithm 4.

Algorithm 4 g

rowTree(H, *depth*)
Input: H: the root of the initial tree,
Output: TP-Cluster existed in H
Grow patterns on the initial TP-Cluster H

```
if tree H = ∅ then
  return
end if
H_child = H's first child;
for each sub-tree subH of H do
  insertSubTree(subH, H);
end for
growTree(H_child,depth + 1);
growTree(H's next sibling,depth);
```

The correctness of HTP-clustering tree construction is proved in Lemma 4.4.1.

Lemma 4.4.1 *Given a database $\mathcal{D}$, the HTP-clustering tree contains all the TP-Clusters embedded in the database.*

Rationale: According to Definition 4.3.2, each TP-Cluster corresponds to a unique sequence of the conditions. Therefore, the proof of the Lemma is equivalent to the the proof that the HTP-clustering tree contains all the frequent subsequences of the set of sequences representing rows in the database. Given any subsequence S', we want to prove that all the sequences containing S' will be projected onto the path corresponds to S'. Given any sequence $S = x_1x_2x_3x_4 \dots x_n$, we want to show that all subsequences of S can be found in a path starting from the root. S is inserted into the tree during the initiation procedure. Then given any subsequence $SS = x_ix_j \dots x_s, (1 \leq i, s \leq n)$, we can obtain SS by the following steps. First, at node x_i, insert suffix $x_ix_{i+1} \dots x_n$. Now in the subtree of x_i, node x_j can be found because it should be along the path

$x_i x_{i+1} \ldots x_n$ that is inserted in the first step. Similarly, we insert the suffix $x_j \ldots x_n$. As a result, we get the path $x_i x_j x_{j+1} \ldots x_n$. By repeating the same procedure until we insert the suffix starting with x_s, we get the path $x_i x_j \ldots x_s$. Since the path representing a subsequence is unique, all the sequences contain S' will fall on the node corresponds to S'. The HTP-clustering tree contains all the subsequences, or, in other words, TP-Clusters.

4.4.2 Ontology Based Pruning Techniques

Several pruning techniques based on the ontology are discussed here. The first pruning technique we will discuss is the functional distribution pruning. For any cluster $\mathcal{C}$, we expect that there exists at least one function category in $\mathcal{C}$ that is statistically significant. Given a cluster $\mathcal{C}$ and the distribution of categories, we use the following Lemma for early detection of the potential appearance of significant function categories.

Lemma 4.4.2 *Let $\mathcal{C}$ be a cluster, let $\mathcal{V}$=$\{v_1, v_2, ..., v_t\}$ be a set of function categories and let S be a counter vector in which s_i records the number of objects appearing in $\mathcal{C}$ in category v_i. Let the minimum number of objects required in a cluster to be nr and let θ_p to be P-value threshold. $\forall v_i$, $v_i \in \mathcal{V}$, Let $\mathcal{C}_i$' be a cluster with size nr and contains $\min(s_i, nr)$ objects in category v_i. If $\forall$ i, $P(s_i, \mathcal{C}_i') > \theta_p$, then $\mathcal{C}$ will not become an enriched cluster.*

Proof 4.4.1 *$\forall v_i, v_i \in \mathcal{V}$, we have $P(s_i, \mathcal{C}_i') < P(s_i, \mathcal{C})$ based on the property of P-value, i.e, the P-value increases as the number of objects in the same cluster increases. According to the condition in the Lemma, we have $\theta_p < \mathcal{C}_i' < P(s_i, \mathcal{C})$. This implies that $\forall v_i, v_i \in \mathcal{V}$, $\mathcal{C}_i') < P(s_i, \mathcal{C})$. Therefore, according to Definition 4.3.6, $\mathcal{C}$ is not enriched by a particular category.*

The second technique is to use OST extracted in a parent cluster to guide the selection of its descendent clusters, by favoring biological children clusters defined in Definition 4.3.8. Our criterion are based on the assumption that, the TP-Clusters in the higher dimensional space will be enriched in the more specific categories.

Criterion 4.4.1 *Let $\mathcal{C}$ and $\mathcal{C}'$ be two clusters and $\mathcal{C}$ is the parent of $\mathcal{C}'$ in the TP-Cluster hierarchy. We say the development of $\mathcal{C}'$ is not eligible if $OST_{\mathcal{C}'} < OST_{\mathcal{C}}$.*

Combining the two pruning techniques, we apply the following procedure at each node of the traversal.

1. Evaluate the prediction potential of the cluster corresponding to this node. If it has no potential become a functionally enriched clusters= based on Lemma 4.4.1, stop further development of this node and its descendants, then go to the next node in the order of the traversal. If it is not, go to step 2.

2. Extract OST of the cluster. If OST is not biologically eligible according to Criteria 4.4.1 stop further development of this node and its descendants. Go to the next node in the order of the traversal.

We present the algorithm of extracting the biologically relevant TP-Clusters by ODTP-clustering tree in Algorithm 5. Its major differences from the pure tree construction algorithm is the recursively feeding and pruning of OST structure and cluster evaluation and pruning based on the significance of OST.

Algorithm 5 growTree(H, nc, nr, $depth$, $parentOST$)
Input: H: the root of the initial tree,
Output: TP-Cluster existed in H, original OST
Grow patterns on the initial TP-Cluster H

```
if H = emptyset then
  return;
end if
H_child = H's first child;
for each sub-tree subH of H do
  insertSubTree(subH, H);
end for
curOST= extractOST(H);
if curOST is not empty then
  if curOST≺parentOST then
    growTree(H_child, nc, nr, depth + 1, curOST);
  else
    growTree(H_sib, nc, nr, depth + 1, parentOST);
  end if
else
  potential = evalFunction(H, parentOST)
  if potential = good then
    growTree(H_child, nc, nr, depth + 1, curOST);
  else
    growTree(H_sib, nc, nr, depth, parentOST);
  end if
end if
```

Analysis of HTP-clustering tree and ODTP-clustering tree construction For both HTP-clustering tree and ODTP-clustering tree, only one scan of the entire data matrix is needed during the construction. Each row is converted into a sequence of column labels. The sequences are then inserted into the prefix tree. In the initial tree structure, sequences with the same prefix naturally fall onto the same path from the root to the node corresponding to the end of prefix. To save memory, the row IDs associated with each path are only recorded at the node marking the end of the longest common prefix shared by these sequences.

Both the time and space complexity of the two algorithms are determined by the potential size of TP-Clusters. In the worst case scenario, given a gene expression matrix $n \times m$, the size of tree is $\sum_{s=1}^{m} s!\binom{m}{s}$. However, since we use the depth-first traversal of the tree and the part of tree that has been traversed will not be needed for future mining, they can be deleted and the space can be reused. At level $i, i \neq 0$, we only need to keep $m - i + 1$ nodes. Therefore, the maximal space to be allocated during the running time will be limited to $O(n \sum_{i=1}^{m} m - i + 1) = O(n * m^2)$.

ODTP-clustering tree will be more space and time efficient than HTP-clustering tree in that it uses Ontology information to prune the exponential search space of HTP-clustering tree construction. The effective of the pruning is largely determined by the percentage of objects with the same categorization can be clustered together.

4.5 Evaluation

In this section, we use a real dataset to evaluate our algorithm. The dataset is the yeast cell cycle data from Spellman *et al.*(Spellman et al., 1998). Our experiments demonstrate the usefulness of ODTP-clustering algorithm in clustering biologically related genes with effective pruning techniques based on gene ontology. The results are evaluated against the mapping between gene ontology and HTP-clustering tree. The algorithm was implemented in C and executed on a Linux machine with a 700 MHz CPU and 2G main memory.

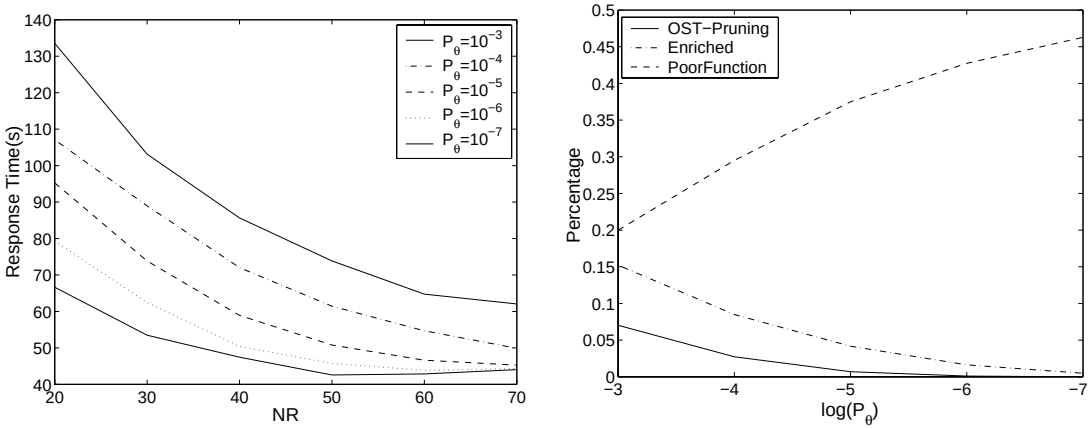
The HTP-clustering algorithm is tested on the yeast cell cycle data of Spellman et al.(1998). The study monitored the expression levels of 6,218 S. cerevisiae putative gene transcripts (genes) measured at 10-minute intervals over two cell cycles (160 minutes) with 18 time points. Spellman *et al.* identified 799 genes that are cell cycle regulated. We used the expression levels of the 799 genes across 18 time points as the original input matrix. The HTP-clustering procedure groups together genes on the basis of

their common expression tendency across a subset of time points.

To assess the classification capability of the clusters, we map gene ontology information to each gene to evaluate whether the cluster has significant enrichment of one or more function groups. The ontology of the 799 yeast genes is downloaded from gene ontology consortium (ash,) in Feb, 2004. We use functions from the three categories: molecular function, cell component and biological process. We extract categories between ontology level 2 and level 5 with a family size of at least 5. The discovered TP-Clusters in each level of the hierarchy are evaluated for enrichment with any of those function categories.

Types	#Known genes	#Categories (> 5)	#Anno per gene
MF	370	16	0.77
CC	616	48	3.4
BP	538	38	5.72

Table 4.3: Statistics for the three categories.

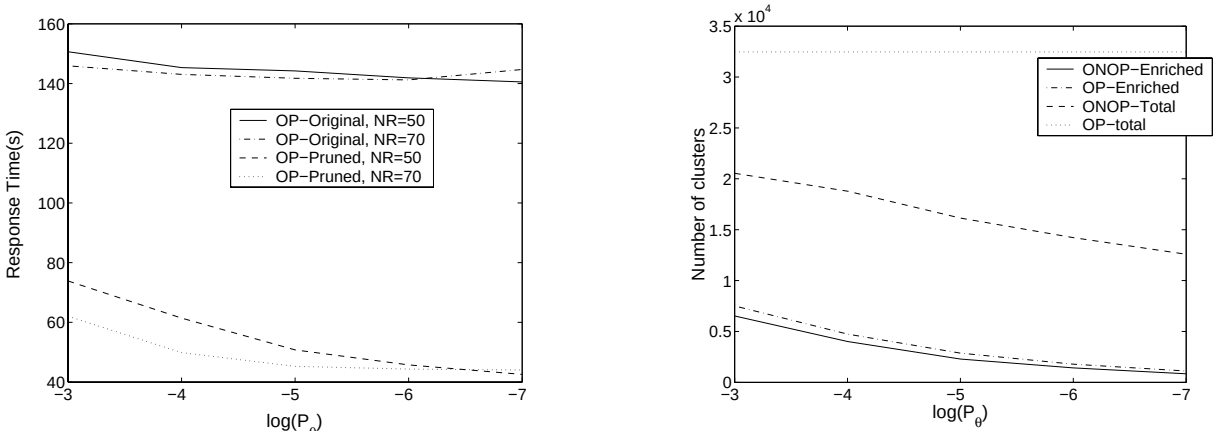


a) Response Time b) The distribution of the clusters

Figure 4.7: The performance of the ODTP-clustering varying nr and θ_p.

4.5.1 Performance Evaluation

The first set of experiment was done using the ODTP-clustering algorithm and cellular component ontology to evaluate the performance under various parameters nr and θ_p. As shown in Figure 4.7 a), the response time of the ODTP-clustering algorithm



a) The comparison of response time b) The comparison of enriched clusters and total clusters

Figure 4.8: The comparison between ODTP-clustering and HTP-clustering.

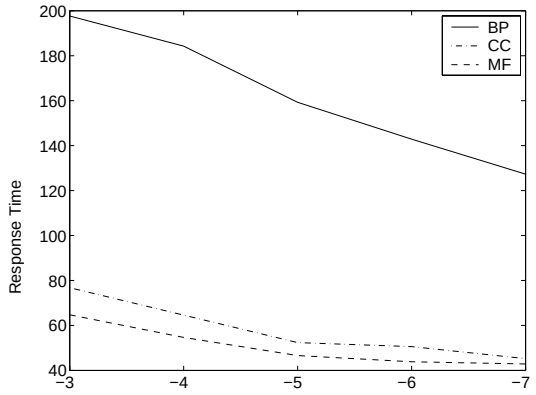


Figure 4.9: The comparison of performance of ODTP-clustering among three categories.

decreases as the significance threshold decreases and as the minimum number of rows increases. Using the cluster functional prediction function, high significance threshold allows early drop of cluster with poor functional implication. The nr which is related to the cluster size help to prune some clusters because of the size limitation. More early pruning enables shorter response time. The application of the same algorithm to other two categories exhibits the same trend when varying nr and θ_p.

Figure 4.7 b) presents the distribution of the generated clusters in three categories: poor functional cluster, enriched cluster, and cluster deleted based on Criterion 4.4.1. The percentage of not enriched cluster increases significantly as θ_p decreases. It also explains the performance gain of ODTP-clustering at the same time. Also the percentage of clusters that have been pruned according to criterion 4.4.1 drops significantly compared to percentage of number of enriched clusters as the significance threshold

decreases. This may also indicate that the more significance the enrichment of the clusters, the more confident that its OST leads to the right direction of selecting the biologically appropriate subset of conditions.

The second set of experiment in Figure 4.8 a) is a comparison between ODTP-clustering algorithm and the original clustering algorithm. For each algorithm, we have done two tests with different setting of nr. We can observe significant and consistent improvement of ODTP-clustering algorithm over HTP-clustering tree especially when θ_p is relatively low. The performance of HTP-clustering can be as short as 1/4 of that in the original algorithm with appropriate P-value.

Figure 4.8 b) compares the number of enriched clusters and the total number of clusters. Clearly, the total number of original TP-Clusters remains the same without ontology based pruning. On the other hand, the total number of clusters using ODTP-clustering is much smaller than TP-Clusters while the number of enriched TP-Clusters generated by ODTP-clustering almost stays the same as the number of enriched TP-Clusters. Overall, ODTP-clustering improves the performance with minimum loss of categorically enriched clusters.

Figure 4.9 gives the comparison of response time of applying the three different ontology files. The input parameter for the algorithm is nr=50. We can observe a clear trend that biological process ontology consistently spends more time than the rest. The reason behind this can be explained by the data in Table 4.3. The average number of categories that a gene might have is 5.7, which is much higher than that of either cellular component or molecular function. With less categories but more gene annotations, the distribution of function groups in a cluster has higher probability to be more concentrated in one or more function groups rather than evenly distributed in any of them. As a result, less functional clusters might be pruned, and hence, the response time is longer. In addition, this may also be coincident with the hypotheses that similar gene expression profile may indicate a function relation in biological process (bro,). As a result, more time will be taken for generating more enriched significant clusters compared with the rest two branches in the ontology.

Overall, our experiment shows that ontology-based pruning is effective in reducing the search space of subspace clustering. In addition, the response time of our algorithm is determined by the two input parameters and the distribution of genes in each category in the ontology.

4.5.2 Mapping between GO and the HTP-clustering tree

In this section, we present a generic example of hierarchically organized clusters that map to a hierarchical substructure of GO.

In Figure 4.10, (A) presents a three-level hierarchy of TP-Clusters, while (B) shows the corresponding OSTs. The gene ontology summarizing the relationships among all the function categories appearing in (B) is "Necleoside → DNA metabolism → DNA repair".

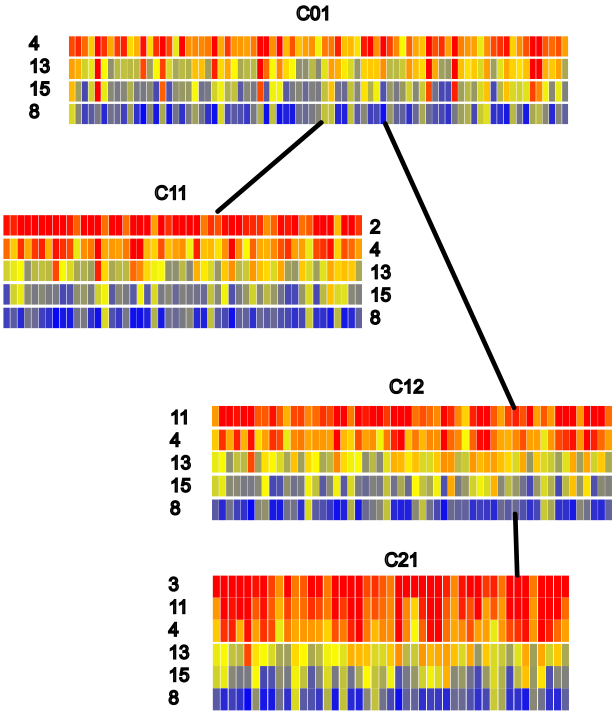
The root cluster C_{01} in (A) is the largest cluster with 71 genes. However, it has the least number of conditions shared by all genes in its cluster, i.e. $(4, 15, 13, 8)$. Its OST shown at the top of the hierarchy in (B) is rooted at the category, Necleoside. As we go down the hierarchy of clusters in (A), we observe cluster with smaller number of genes but larger number of consistent conditions. In addition, the OSTs tend to exist in the subtree of the OST in its parent cluster. For example, the root cluster C_{01} is split into two smaller overlapping clusters C_{11} and C_{12} featuring enriched function "DNA metabolism", which is a subcategories of *necleoside*. $OST_{C_{11}}$ and $OST_{C_{12}}$ suggest that the two clusters in level one have more significant grouping at a deeper level in GO hierarchy than cluster C_{01}. The further clustering of cluster C_{12} in a six dimensional space again signifies the function group in a even deeper level, i.e. "DNA repair".

This example illustrates the connection between the ontology hierarchy and subspace clustering hierarchy. In addition, only a subset of conditions matter for a ontology category. Also, the deeper the level an ontology category is in, the more the conditions under which the genes in that category can be close.

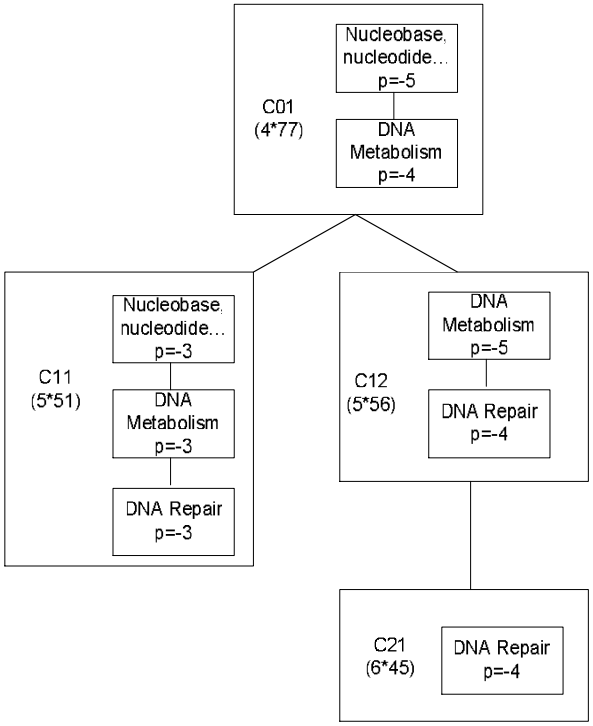
4.6 Conclusions and Future Work

Clustering on gene expression data has been used for gene function annotation based on the hypothesis that similar expression profiles indicate a function relation during the biological process. However, traditional clustering algorithm is weak in modeling the hierarchy of GO based on the fact that traditional algorithm cannot generate overlapping clusters and a hierarchy of clusters in various sizes. To overcome these problems, we propose to use hierarchically arranged biclusters to model the hierarchy of GO. We present a biclustering algorithm guided by GO which efficiently and effectively extracts the biological relevant gene clusters. Our experiment on yeast gene expression data demonstrates the effectiveness of ontology-based pruning. Our future work will be

using the generated bicluster hierarchy for efficient and effective classification for the unknown genes.



(A) Expression profiles of the TP-Cluster subtrees



(B) Corresponding *OST*s of clusters in (A)

Figure 4.10: An example of mapping from a hierarchy of TP-Clusters to their *OST*s. For each cluster in (A), the rows correspond to conditions while the columns correspond to the genes.

Chapter 5

Noise-Tolerant Subspace Clustering

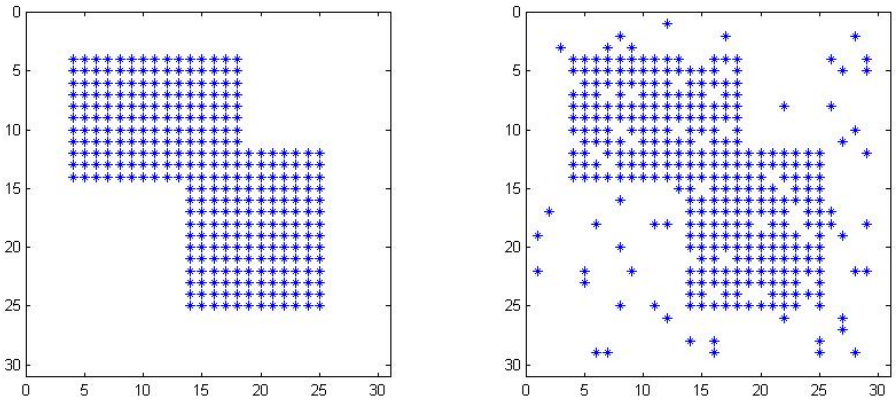
Subspace clustering has originally evolved from searching submatrices of interests in binary data matrix, which is called **frequent itemset mining**. Frequent itemset mining discovers all 1s submatrics in binary data. The well-known apriori property to efficiently enumerate itemsets has also influenced the development of the subspace enumeration techniques in major subspace clustering algorithm. Besides, the itemset mining is a popular and important first step in the analysis of data arising in a broad range of applications. The application of traditional "exact" model for frequent itemsets are mostly market basket analysis. It looks for an all 1s submatrics which corresponds to a subset of transactions(objects) and a subset of items(attributes) and requires that every item occur in each supporting transaction.

However, real data is typically subject to noise and measurement error. To date, the effect of noise on exact frequent pattern mining as well as subspace clustering algorithms have been addressed primarily through simulation studies, and there has been limited attention to the development of noise tolerant algorithms. In this chapter. we study the mining of frequent itemset mining in the presence of noise, which we call approximate frequent itemsets (AFI). The AFI model tolerates a controlled fraction of errors in each item and each supporting transaction. Motivating this model are theoretical results (and a supporting simulation study presented here) which state that, in the presence of even low levels of noise, large frequent itemsets are broken into fragments of logarithmic size; thus the itemsets cannot be recovered by a routine application of frequent itemset mining. By contrast, we provide theoretical results showing that the AFI criterion is well suited to recovery of block structures subject to noise.

The mining of AFIs is rather challenging since the traditional apriori property does not hold any more. We developed and implemented an algorithm to mine AFIs that generalizes the level-wise enumeration of frequent itemsets by allowing noise. We pro-

pose the noise-tolerant support threshold, a relaxed version of support, which varies with the length of the itemsets and the noise threshold. We exhibit an Apriori property that permits the pruning of an itemset if any of its sub-itemset is not sufficiently supported. Several experiments presented demonstrate that the AFI algorithm enables better recoverability of frequent patterns under noisy conditions than existing frequent itemset mining approaches. Noise-tolerant support pruning also renders an order of magnitude performance gain over existing methods.

5.1 Introduction



Embedded Pattern(X) Observed Pattern(Y)

Figure 5.1: Patterns with and without noise.

Relational databases are ubiquitous, cataloging everything from market-basket data to gene-expression data. One common representation for relational databases is a binary matrix. Rows in the matrix correspond to objects, while columns represent various attributes of the objects. The binary value of each matrix entry then indicates the presence (1) or absence (0) of an attribute for a given object. For example, in a market-basket database, rows represent transactions, columns represent product items, and a binary entry indicates whether an item is contained in a given transaction (Agrawal and Srikant, 1995). Frequent itemset mining (Agrawal and Srikant, 1995) is a key technique for the analysis of such data.

In the binary representation, a *frequent itemset* corresponds to a sub-matrix of 1s containing a sufficiently large set of rows (transactions). Although frequent itemset mining was originally developed to discover association rules, its broader application

provides the basis for subspace clustering and for building classifiers. In these applications the ultimate goal is to discover interesting associations between object and attribute sets, rather than associations among attributes alone. One important experimental application of frequent itemset mining is the exploration of gene expression data, where the joint discovery of both the set of conditions that significantly effect gene regulation and the set of co-regulated genes is of great interest.

In real data applications a "1" can be accidentally recorded as "0" and vice versa. In a *transaction database*, the noise can arise from both accidents of the market and the vagaries of human behavior. Items expected to be purchased together by a customer might not appear together in a particular transaction either because one item is out of stock or because it has been overstocked by the customer. *Microarray data* is likewise subject to measurement noise, stemming from the underlying experimental technology and the stochastic nature of the studied biological behavior. In addition, uncertainty involved in choosing the proper thresholds when imputing discrete observations from the continuous gene expression values can introduce error. Figure 5.1 illustrates how pattern in the data – although perceptible – is obscured by noise. While frequent itemsets and the algorithms that generate them have been well studied, the difficulties that arise from noise have not been adequately addressed.

In general, the noise present in real applications undermines the ultimate goal of traditional frequent itemset algorithms: recovering itemsets that appear without error in a sufficient fraction of transactions. In fact, as we discuss below, when noise is present, classical frequent itemset algorithms discover multiple small fragments of the true itemset, but miss the true itemset itself. The problem is worse for the most interesting, longer itemsets as they are more vulnerable to noise.

5.1.1 Fragmentation of Patterns by Noise

In order to analyze the potential effects of noise on frequent pattern mining, Sun and Nobel (Sun and Nobel, 2005) considered a simple statistical model for the observed binary data matrix $\mathbf{Y}$. Formally,

$$\mathbf{Y} \;=\; \mathbf{X} \oplus \mathbf{Z}, \tag{5.1}$$

where $\mathbf{Y}$, $\mathbf{X}$ and $\mathbf{Z}$ are $m \times n$ binary matrices and $\oplus$ is the entry-wise exclusive-or operation (modulo 2 sum). The matrix $\mathbf{X}$ contains the unobserved "true" data values of interest, in the absence of noise, and $\mathbf{Z}$ is a binary noise matrix whose entries $z_{i,j}$

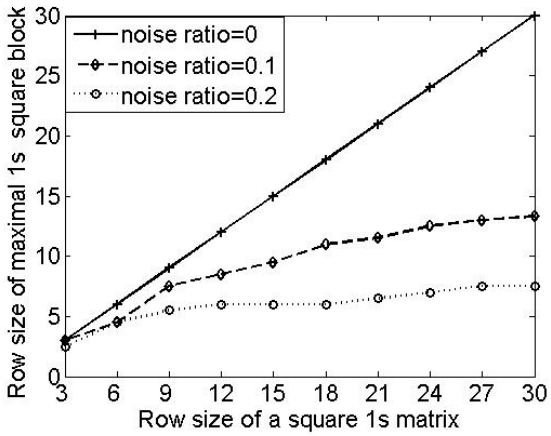


Figure 5.2: When noise is present, the observed size of the largest square sub-matrix of 1's increases far more slowly than the size of the initial square matrix of 1's. (Note: noise ratio refers to the value of p).

are independent Bernoulli random variables with $P(z_{i,j} = 1) = p = 1 - P(z_{i,j} = 0)$ for some $p \in (0, 1/2)$. In this case we will write $\mathbf{Z} \sim \text{Bern}(p)$. An example is shown in Figure 5.1. The statistical model (5.1) is equivalent to the standard communication model, widely studied in information theory, in which the values of $\mathbf{X}$ are observed after being passed through a binary symmetric channel. It is the binary version of the standard additive noise model in statistics inference.

Suppose for the moment that $m = n$, and let $M(\mathbf{Y})$ be the largest k such that $\mathbf{Y}$ contains a $k \times k$ submatrix of 1s, or equivalently, the largest k such that $\mathbf{Y}$ contains k transactions having k common items. The following proposition is proposed in (Sun and Nobel, 2005). It extends the earlier result on the clique number of random graphs to binary random matrices.

Proposition 1 *With probability 1,* $M(\mathbf{Y}) \leq 2\log_a n - 2\log_a \log_a n$ *when* n *is sufficiently large, regardless of the structure of* $\mathbf{X}$. *Here* $a = (1-p)^{-1}$.

Proposition 1 shows that, even for small noise levels $p > 0$, large blocks of 1s or other structures in the true matrix $\mathbf{X}$ leave behind only fragments of logarithmic size in $\mathbf{Y}$. Thus no exact frequent itemset mining algorithm will be able to recover such underlying structure directly from $\mathbf{Y}$.

To demonstrate this effect, we added noise to a square matrix of 1s. Each entry of the initial matrix was changed to 0 with some probability p, independently from entry to entry. We applied standard frequent itemset mining to the corrupted matrix, and

applied this process to matrices of different sizes. Figure 5.2 plots the size of the largest recovered square sub-matrix of 1s against the size of the original matrix, for different values of p (corresponding to different levels of data corruption). In the presence of noise, only a fraction of the initial block of 1s was recovered, and this fraction diminished with an increase in the size of the original matrix. Furthermore, the number of unique itemsets reported increased exponentially with both corruption level and original block size (see the spurious itemsets curve shown in Figure 5.9 in the experiment section).

The failure of classical frequent itemset mining to detect simple patterns in the presence of random errors compromises the ability of these algorithms to detect associations, cluster items, or build classifiers when such errors are present. Noise is ubiquitous in real data: it presents new challenges for algorithm development, and its consequences should not ignored. In this paper, we focus on noise-tolerant frequent itemset mining of the binary matrix representation of databases.

5.1.2 Approximate Frequent Itemset Models

The formal setting of our problem is as follows. The available data take the form of an $n \times m$ binary matrix D. Each row of D corresponds to a transaction i and each column of D corresponds to an item j. The i, j-th element of D, denoted $D(i, j)$, is 1 if transaction i contains item j, and 0 otherwise. Let $O = \{i_1, i_2, \ldots, i_n\}$ and $A = \{j_1, j_2, \ldots, j_m\}$ be the set of transactions and items associated with D, respectively. An itemset is called *frequent*, if the fraction of transactions supporting it exceeds a given threshold, $minsup \in (0, 1]$.

One natural algorithmic approach for handling errors is to relax the requirement that a sub-matrix determined by the frequent itemset consists entirely of 1s, and allow it instead to contain a large fraction of 1s (and a small fraction of 0s), *e.g.*, the "presence" signal (Chakrabarti et al., 2004; Yang et al., 2001). This requirement is evidently a necessary condition, but it is not sufficient to define a sub-matrix of interest. To see why this is the case, consider the matrix shown in Figure 5.3.

The matrix in Figure 5.3 contains 3 sub-matrices $\{A, B, C\}$. The fraction of 1s in each sub-matrix is the same, namely 75%, however, the 1s are distributed quite differently in each. In sub-matrix A, each row and column contains 75% 1s, but in sub-matrix B and C the 1s are concentrated in the dense sub-matrix $B \cap C$. Both column g and row 7 are in a sense free riders on $B \cap C$. Clearly, neither sub-matrix B nor C should be used for association rule mining or classification purposes: in sub-matrix

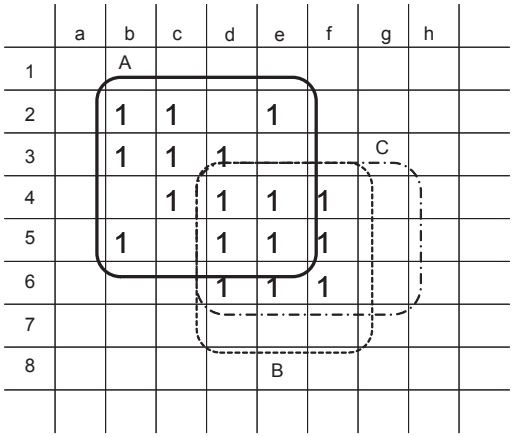


Figure 5.3: A binary matrix with three weak AFI(0.25) They can be more specifically classified as, A: AFI(0.25, 0.25); B: AFI(*, 0.25); C: AFI(0.25, *).

B row 7 does not support any item in the itemset, and in sub-matrix C item g is not supported by any transaction. It is possible to generate many more sub-matrices like B and C by combining any of the remaining columns and rows with $B \cap C$ to form a sub-matrices with densities of at least 75%.

Besides requiring a large fraction of 1s in a sub-matrix of interest, we advocate imposing two other conditions. First, for a given itemset, a *supporting transaction* should contain most of the items. Second, to be included in an itemset, an *associated item* has to appear in most of the supporting transactions. In the binary matrix representation, this means that the fraction of 0s in each row and each column of the sub-matrix representing the *approximate itemset* has to fall below a user-defined threshold. The threshold may differ for rows versus columns, and is denoted by ϵ_r and ϵ_c, respectively. If the approximate itemset has sufficiently many rows, it is judged to be an *approximate frequent itemset* (AFI).

Definition 5.1.1 *Let D be as above, and let $\epsilon_r, \epsilon_c \in [0,1]$. An itemset $J \subseteq A$ is an approximate frequent itemset AFI(ϵ_r, ϵ_c), if there exists a set of transactions $I \subseteq O$ with $|I| \geq |O| \cdot minsup$ such that the following two conditions hold:*

$$1.\ \forall i \in I, \frac{1}{|J|} \sum_{j \in J} D(i,j) \geq (1 - \epsilon_r);$$

$$2.\ \forall j \in J, \frac{1}{|I|} \sum_{i \in I} D(i,j) \geq (1 - \epsilon_c);$$

Let AFI(ϵ_r, ϵ_c) denote the collection of all AFI sub-matrices of D. Classical or

exact frequent itemsets (EFI) are a special case of AFI, where both noise thresholds ϵ_r and ϵ_c are set to zero. In cases where the noise in either the rows or the columns is not restricted, AFI$(\epsilon_r, *)$ or AFI$(*, \epsilon_c)$ is used to denote the corresponding families. The noise threshold replaced by "$*$" means that no constraint is employed for the corresponding parameter, or the noise threshold is 1, i.e., $\epsilon = 1$. We also define the sub-matrices that satisfy the global noise constraint as *weak* AFIs in Definition 5.1.2.

Definition 5.1.2 *Let D be as above, and let $\epsilon \in [0, 1]$. An itemset $J \subseteq A$ is a weak AFI(ϵ) if there exists a set of transactions $I \subseteq O$ with $|I| \geq |O| \cdot minsup$ such that the following condition holds:*

$$\frac{1}{|I||J|} \sum_{i \in I} \sum_{j \in J} D(i, j) \geq 1 - \epsilon \tag{5.2}$$

According to our definition, the three sub-matrices in Figure 5.3 are weak AFIs. However, only sub-matrix A constitutes a valid AFI$(0.25, 0.25)$. B and C do not satisfy the constraints of AFI$(0.25, 0.25)$, but they are valid AFI$(*, 0.25)$ and AFI$(0.25, *)$ respectively.

Note that an AFI(ϵ_r, ϵ_c) also qualifies as both an AFI$(\epsilon_r, *)$ and an AFI$(*, \epsilon_c)$. The relationships among the various criteria are summarized in the Venn diagram of Figure 5.4. The differences in the sizes of the families and the maximum lengths of itemsets contained in each leads to substantial differences in the computational costs for the algorithms that search for them. This will be further elaborated upon in the experimental sections.

In this work we proceed from the premise that, while the exact frequent itemset criterion is too restrictive, simple application of the weak AFI, AFI$(\epsilon_r, *)$ and AFI$(*, \epsilon_c)$ criteria allows poor approximations to frequent itemsets.

Yang *et.al.* (Yang et al., 2001) have developed models equivalent to the weak AFI and AFI$(\epsilon_r, *)$, but use the terms weak ETI and strong ETI, respectively, instead. For ease in comparing the competing criteria, we adopt their terminology for the remainder of this paper.

5.1.3 Challenges and Contributions

Accommodating the refined noise criteria creates substantial algorithmic challenges not posed by exact frequent itemset mining. First and foremost, the AFI criterion distin-

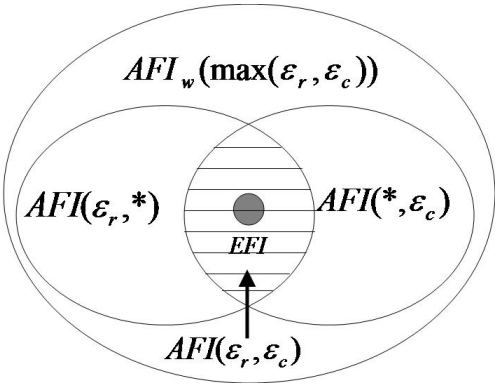


Figure 5.4: Relationships of various AFI criteria.

guishes itself from traditional exact frequent itemsets as it violates the anti-monotone (Apriori) property. An exact itemset cannot be frequent if any of its sub-itemsets fails to be frequent. However, a sub-itemset of an AFI need not be an AFI. For example, given $minsup = 4$ and $\epsilon_r = \epsilon_c = 25\%$, sub-matrix A in Figure 5.3 is a valid AFI, but none of its sub-itemsets have sufficient support to be an AFI. The *minsup* can no longer be employed as a pruning threshold for itemset. No accurate pruning threshold has ever been found in any of existing work on noise-tolerant itemset mining. As a result, algorithms, such as ETI mining, have to rely on heuristics to prune the search space. These heuristics do not guarantee the completeness of the search. Another algorithm to discover dense itemsets (Sepp and Mannila, 2004) enforces the constraint that all sub-itemsets of a dense itemset must be frequent. Since this algorithm requires minsup support for all sub-itemsets, it can fail to identify larger itemsets that have sufficient support.

Noise-tolerance also affects the way in which supporting transactions are maintained in the algorithm. With exact frequent itemset mining, a transaction supporting an itemset also supports its sub-itemsets. This property is fundamental to any depth-first approach. This property, however, does not hold for AFI: one cannot derive the support set of an AFI from the common support sets of its sub-patterns, as is done in exact frequent itemset mining. (Examination of sub-matrix A in Figure 5.3 makes this clear.) To solve this problem, the algorithms proposed in(Yang et al., 2001; Sepp and Mannila, 2004) require repeated scans of the entire database to identify the support for each itemset. The exponential number of potential itemsets makes this very expensive.

In this paper, we investigate the noise-tolerant property of approximate frequent itemsets that provides both the algorithmic basis for itemset generation, and the po-

tential for pruning based on an AFI's support. The property is a generalization of Apriori under noisy conditions and includes the Apriori property as a special case when noise is absent. By incorporating noise-tolerant attributes, we designed an efficient and effective approach for mining the complete set of approximate frequent itemsets.

5.1.4 Outline

The rest of the chapter is organized as follows. Section 5.2 outlines related work in the area of noise-tolerant itemset mining. Section 5.3 contains a theoretical analysis showing how the AFI criterion can be used to recover block structures in the presence of noise, a problem for which standard frequent pattern mining fails. Section 5.4 presents the algorithm and two pruning strategies. Assessment of the AFI algorithm on synthetic and real data sets and an examination of its scalability are presented in Section 5.5. Section 5.6 concludes the paper.

5.2 Background and Related Work

In the standard frequent itemset problem (Agrawal and Srikant, 1995), the goal is to enumerate all the frequent itemsets in D; there is no allowance for noise. This corresponds to our AFI definition when $\epsilon_r = \epsilon_c = 0$.

Noise-tolerant itemsets were first discussed by in (Yang et al., 2001), who proposed two error tolerant models, termed weak error-tolerant itemsets (ETI)(equivalent to weak AFI) and strong ETI (equivalent to AFI($\epsilon, *$)). As noted in the discussion of Figure 5.3, the ETI models do not preclude columns of zeros. Although this problem is identified by Yang *et al.* (Yang et al., 2001), it is not resolved in their paper. In addition, without an efficient pruning technique the authors had to employ a variety of heuristics and sampling techniques instead. In (Sepp and Mannila, 2004) the authors seek weak ETIs by constraining the subsets of ETIs to also be weak ETIs. This constraint may not only miss valid itemsets of interest, but also generates irrelevant itemsets, such as cluster (B) in Figure 5.3.

Other lines of work to find itemsets tolerating noise are (Steinbach et al., 2004). These approaches admit only a fixed number of 0s in the itemsets. In contrast to our AFI model, the fraction of noise can not vary with the size of a submatrix defining an itemset, and therefore, is not guaranteed to be bounded relative to the size of the result. The support envelope technique (Steinbach et al., 2004) identifies regions of the

data matrix where each transaction contains at least a given number of items and each item appears in at least a given number of transactions. The support envelope is a tool for exploring and visualizing high-level itemset structures in a data matrix. The paper defines a symmetric error tolerant itemset model (Symmetric ETI). It is similar to AFI but restricts the fraction of errors allowed to be the same for columns and rows. Also, no additional properties or algorithms for the symmetric ETI are developed by the authors.

5.3 Recovery of Block Structures in Noise

In this section we present some theoretical support for the AFI model in the context of a simple recovery problem for matrices with noise. Proposition 1 of Section 5.1.1 shows that exact frequent itemset mining cannot directly recover blocks of 1s and other structures in the presence of noise. The weak ETI (weak AFI), ETI (AFI(ϵ_r, *)) and AFI model address this problem by allowing zeros in their target sub-matrices. One means of validating and comparing these criteria is to see if they are able to recover simple structures in cases where exact frequent pattern mining fails. To this end, we show how the AFI model can be applied to the simple problem of recovering a sub-matrix of 1s set against a background of zeros when noise is present. (A complete analysis can be found in (Sun and Nobel, 2005)). For simplicity, we only consider square matrices and sub-matrices. However, analogous results hold for rectangular matrices and sub-matrices.

Let $\mathbf{X}$ be an $n \times n$ binary matrix that consists of an $l \times l$ sub-matrix C^* of 1s, with all other entries equal to 0. (Note that the rows and columns of C^* need not be contiguous.) Suppose that we observe $\mathbf{Y} = \mathbf{X} \oplus \mathbf{Z}$, where $\mathbf{Z} \sim \text{Bern}(p)$, with $0 < p < 1/2$, and wish to accurately recover C^*. Let p_0 be any number such that $p < p_0 < 1/2$, and let $\tau = 1 - p_0$ be an associated error threshold. If C is a sub-matrix of $\mathbf{X}$, let $C \in \text{AFI}_\tau(\mathbf{X})$ denote the fact that every row and column of C has at least $100\,\tau\%$ 1s.

In order to recover C^*, we identify the largest square AFI in the observed matrix $\mathbf{Y}$ having an error threshold τ. More precisely, let $\mathcal{C}$ be the family of all square sub-matrices C of $\mathbf{X}$ such that $C \in \text{AFI}_\tau(\mathbf{X})$, and define

$$\hat{C} \;=\; \text{argmax}_{C \in \mathcal{C}} |C|$$

to be any maximal sized sub-matrix in $\mathcal{C}$. Note that $\hat{C}$ depends only on the observed matrix $\mathbf{Y}$. Let

$$\text{SetClu} \;=\; |\hat{C} \cap C^*|/|\hat{C} \cup C^*|$$

measure the overlap between the estimated index set $\hat{C}$ and the true index set C^*. Then $0 \leq \text{SetClu} \leq 1$, and values of SetClu close to one indicate better overlap. A sketch of proof of the following theorem can be found in the appendix.

Theorem 1 *Let $\hat{C}$ be the estimate of C^* based on the family $AFI_\tau(\mathbf{X})$ as described above. Let $\delta = p - p_0 > 0$. When n is sufficiently large, for any $0 < \alpha < 1$ and l satisfying $l > 16\alpha^{-1}(\log_b n + 2)$,*

$$P\left(\textit{SetClu} \leq \frac{1-\alpha}{1+\alpha}\right) \;\leq\; \Delta_1(l) \,+\, \Delta_2(\alpha, l). \tag{5.3}$$

Here $\Delta_1(l) = 2e^{-3\,\delta^2\, l/8p}$, $\Delta_2(\alpha, l) = 2n^{-\frac{1}{4}\alpha l + 4\log_b n}$, and the log base $b = \exp\{3(1 - 2\,p_0)^2/8p\}$.

The following is an example illustrating Theorem 1. Let X be a $n \times n$ binary matrix with $n = 800$ and let C^* be a $l \times l$ submatrix of X with $l = 400$. Suppose the noise level $p = 0.1$ and suppose the user specified noise level $p_0 = 0.15$. When $\alpha = \frac{1}{4}$, since $l > 16\alpha^{-1}(\log_b n + 2) = 360.1$, it follows Theorem 1 that $P\left(\text{SetClu} \leq \frac{3}{5}\right) \leq 2(e^{-3.75} + 800^{-10.448}) = 0.047$, i.e. the probability that the overlap of the recovered AFI and C* will be less than 0.6 is small (less than 5%).

The conditions of Theorem 1 require that the noise level $p < 1/2$ and that the user-specified parameter p_0 satisfy $p < p_0 < 1/2$. Thus, in advance, one only needs to know an upper bound on the noise level p. A similar recovery result can be established for the weak ETI model. However, the proof is considerably more complicated, and more importantly, the recovery method requires exact knowledge of the noise level p. It appears that the same restriction is necessary for recovery with the ETI model as well. In the context of the simple recovery problem, the two-way restriction of the AFI model has direct advantages over the weak-ETI model.

Here we illustrate the essential ideas behind the proof of Theorem 1. Note that the entries of $\mathbf{Y}$ in C^* are i.i.d. Bernoulli$(1-p)$ random variables. Consequently, the sum of each row and each column of C^* has a Binomial$(l,1-p)$ distribution. Using this fact and the condition that $1 - p_0 < 1 - p$, it can be shown that the probability that any row or column of C^* has average density less than $1 - p_0$ is very small. This implies

that $C^* \in \text{AFI}_\tau(X)$ with high probability. Since $\hat{C}$ is the maximal sized sub-matrix in $\text{AFI}_\tau(X)$, it follows that $|\hat{C}|$ is greater than or equal to $|C^*|$ with high probability. Now, we want to show that $\hat{C}$ can not be too large either, and that it can only contain a small proportion of entries outside C^*. When $\hat{C}$ is much larger than C^*, it must contain a large number of rows (or columns) whose entries are from outside C^*. The definition of $\hat{C}$ via the AFI criterion implies that each such row (column) has density greater than τ. Moreover, the rows (columns) will necessarily contain a large rectangular region with entries from outside C^*, and this region should also have density greater than τ. But as the entries of $\mathbf{Y}$ outside C^* are i.i.d. Bernoulli(p), the probability of finding a rectangular region as above is very small.

Theorem 1 can readily be applied to the asymptotic recovery of structure in a sequential framework. Suppose that $\{\mathbf{X}_n : n \geq 1\}$ is a sequence of square binary matrices, where $\mathbf{X}_n$ is $n \times n$ and consists of an $l_n \times l_n$ sub-matrix C_n^* of 1s with all other entries equal to 0. For each n we observe $\mathbf{Y}_n = \mathbf{X}_n \oplus \mathbf{Z}_n$, where $Z_n \sim$Bern(p), and wish to recover C_n^*. Let SetClu_n measure the overlap between C_n^* and the estimate $\hat{C}_n$ produced by the AFI recovery method above. The following corollary of Theorem 1 shows that, under suitable conditions on l_n, $\hat{C}_n$ provides asymptotically consistent estimates of C_n^*. The proof can be found in the appendix.

Corollary 1 *If* $l_n > 16\psi(n)(\log_b n + 2)$ *where* $\psi(n) \to \infty$ *as* $n \to \infty$, *then with probability one*

$$\mathit{SetClu}_n \leq \frac{1 - \psi(n)^{-1}}{1 + \psi(n)^{-1}}$$

when n is sufficiently large.

5.4 AFI Mining Algorithm

Mining approximate frequent itemsets poses a number of new algorithmic challenges beyond those faced when mining exact itemsets. The foremost difficulty is that noise-tolerant itemset mining cannot employ the anti-monotone property that has led to the success of frequent itemset mining. The development of an efficient algorithm for finding AFIs calls for new itemset generation strategies to limit the search space. We present a noise-tolerant Apriori property in Section 5.4.1. In addition, the AFI criteria allow the number of errors to increase with the size of the itemset. It is therefore critical to take account of the additional errors in an itemset as its dimensionality increases while collecting the supporting transactions. Solving this problem is the key to AFI

mining, and is addressed in subsection 5.4.1. The AFI mining algorithm adapts the methods of level-wise breadth-first frequent itemset mining to this new setting, and takes advantage of our new techniques to generate noise-tolerant approximate frequent itemsets.

5.4.1 Mining AFIs

The algorithm's enumeration of the AFI differs from the existing work of weak ETI algorithm(Yang et al., 2001) in the following aspects: First, even though the Apriori property doesn't hold for any type of AFI(except those that allow no noise), we have developed a noise-tolerant Apriori property (Theorem 5.4.1) and apply it to prune and generate candidate itemsets. Secondly, by taking different approaches in extending the itemsets, we are able to collect the support of an noise-tolerant itemset based on the support set in the sub-itemsets.

Noise-Tolerant Support Pruning

The anti-monotone property of exact frequent itemsets is the key to minimizing exponential searches in frequent itemset mining. In particular, the anti-monotone property ensures that a $(k+1)$ exact itemset can be pruned if any one of its k sub-itemsets is not frequent. However, this property is no longer true for any variation of AFI. Instead, in this paper, we derive a noise-tolerant support to serve as the Apriori pruning threshold. The noise-tolerant support is determined by the size of the itemset and the noise thresholds. This support threshold leads to substantial performance gain for our algorithm.

Theorem 5.4.1 *Given a support threshold minsup, if a length $(k+1)$-itemset J' is an AFI(ϵ_r, ϵ_c), then for any of its k item subset $J \subseteq J'$, the number of transactions containing no more than ϵ_r fraction of noise in J is at least*

$$n \cdot minsup \cdot \left(-\frac{k\epsilon_c}{\lfloor k\epsilon_r \rfloor + 1} \right) \tag{5.4}$$

Proof: By assumption, there exists a set of transactions I' such that $|I'| \geq n \cdot minsup$ and $I' \times J' \in \text{AFI}(\epsilon_r, \epsilon_c)$ Let J be a k item subset of J' with support set I. Thus each $i \in I$ contains at most $k\epsilon_r$ zeros on J.

Let $num_0(C)$ be a function that returns the number of 0s in any submatrix C of D. Since the transactions in $I' \setminus I$ do not support J, each such transaction contains more than $k\epsilon_r$ zeros on J. It follows that

$$\begin{aligned} num_0((I' \setminus I) \times J) &\geq |I' \setminus I| \cdot (\lfloor k\epsilon_r \rfloor + 1) \\ &\geq (|I'| - |I|) \cdot (\lfloor k\epsilon_r \rfloor + 1) \end{aligned}$$

As $I' \times J'$ is an AFI, each item in J contains at most $\epsilon_c|I'|$ zeros on J'. Therefore,

$$num_0(I' \times J) \leq k \cdot |I'| \cdot \epsilon_c.$$

Combining the last two inequalities gives

$$\begin{aligned} (|I'| - |I|) \cdot &(\lfloor k\epsilon_r \rfloor + 1) \\ &\leq num_0((I' \setminus I) \times J) \\ &\leq num_0(I' \times J) \\ &\leq k \cdot |I'| \cdot \epsilon_c \end{aligned} \tag{5.5}$$

where the second inequality follows from the fact that $I' \setminus I \subseteq J'$. Expressing the last inequality in terms of $|I|$ yields

$$\begin{aligned} |I| &\geq |I'| \left(1 - \frac{k\epsilon_c}{\lfloor k\epsilon_r \rfloor + 1}\right) \\ &\geq n \cdot minsup \cdot \left(1 - \frac{k\epsilon_c}{\lfloor k\epsilon_r \rfloor + 1}\right) \end{aligned} \tag{5.6}$$

Based on the bound of Theorem 5.4.1 we make the following definition.

Definition 5.4.1 *Given ϵ_c, ϵ_r and minsup, the* **noise-tolerant pruning support** *for a length-k itemset is,*

$$minsup^k = minsup \cdot \left(1 - \frac{k\epsilon_c}{\lfloor k\epsilon_r \rfloor + 1}\right)_+ \tag{5.7}$$

Here $(a)_+ = \max\{a, 0\}$.

The noise-tolerant support threshold is used as the basis of a pruning strategy for AFI mining. The strategy removes supersets of a given AFI$(\epsilon_r, *)$ I from further

consideration when the number of transactions which contain less than ϵ_r fraction of errors in I is less than $n \cdot minsup^k$. In the special case that $\epsilon_r = \epsilon_c = 0$, $minsup^k = minsup$, which is consistent with the anti-monotone property of exact frequent itemsets. The support threshold decreases as ϵ_c increases and as ϵ_r decreases. In the former case, a less stringent column constraint is applied to a block with fixed row constraints, and conversely in the case of decreasing ϵ_r. In particular, the support threshold is equal to 0 when $k \cdot \epsilon_c > \lceil k \cdot \epsilon_r \rceil$. Therefore, no pruning can be applied at all.

0/1 Extensions

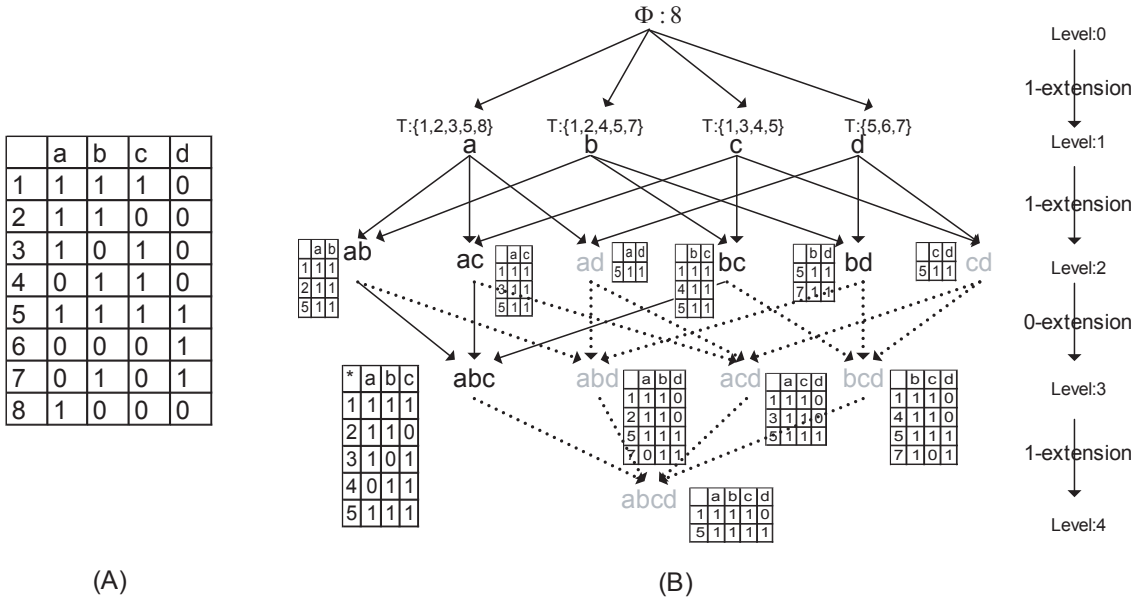
Starting with singleton itemsets, the AFI algorithm generates $(k+1)$-itemsets from k-itemsets in a sequential fashion. The number of 0s allowed in the itemset grows with the length of the itemset in a discrete manner. If $\lfloor (k+1)\epsilon_r \rfloor > \lfloor k\epsilon_r \rfloor$, then transactions supporting the $(k+1)$-itemset are permitted one more zero than transactions supporting k-itemsets. When $\lfloor (k+1)\epsilon_r \rfloor = \lfloor k\epsilon_r \rfloor$, no additional zeros are allowed. For example, if $\epsilon_r = 0.25$, additional zeros are permitted in transactions when extending itemsets of length $3, 7, 11$ and so on. Whether the maximal number of zeros will increase in a $(k+1)$ itemset makes a difference in deriving its set of supporting transactions. Intuitively, if an additional zero is allowed at level $(k+1)$, any transaction supporting a k itemset should also support its $(k+1)$ superset. On the other hand, when the maximum number of zeros allowed in an itemset stay the same at level $(k+1)$, a transaction that does not support k itemset will not have enough 1s to support its $(k+1)$ superset. These two properties are formally addressed in Lemma 5.4.2 and Lemma 5.4.3 as 1-Extension and 0-Extension respectively.

Lemma 5.4.2 *(1-Extension) If* $\lfloor k \cdot \epsilon_r \rfloor = \lfloor (k+1) \cdot \epsilon_r \rfloor$ *then any transaction that does not support a* k*-itemset will not support its* $(k+1)$ *item superset.*

The Lemma is based on the fact that if no additional noise is allowed when generating a $(k+1)$ itemset, a transaction that does not support a k-itemset will not support its $(k+1)$ superset since the number of 1s it contains is always smaller than or equal or $\frac{\lfloor k*\epsilon \rfloor - 1 + 1}{k+1} < \epsilon$. Thus if $\lfloor k \cdot \epsilon_r \rfloor = \lfloor (k+1) \cdot \epsilon_r \rfloor$ then the transaction set of a $(k+1)$ itemset I is the *intersection* of the transaction sets of its length k subsets. This is called a *1-extension.*

Lemma 5.4.3 *(0-Extension) If* $\lfloor k \cdot \epsilon_r \rfloor + 1 = \lfloor (k+1) \cdot \epsilon_r \rfloor$ *then any transaction supporting a* k*-itemset also supports its (k+1) supersets.*

The procedure of 0-extension illustrates how noise can be incorporated into a frequent itemset. If additional noise is allowed for a $(k+1)$ itemset relative to a k itemset, it is intuitive that a transaction that supports a k-itemset will also support its $(k+1)$-item supersets, no matter whether the $(k+1)^{th}$ entry is 1 or 0. To utilize this property, if $\lfloor k \cdot \epsilon_r \rfloor + 1 = \lfloor (k+1) \cdot \epsilon_r \rfloor$, the transaction set of a $(k+1)$ itemset I is the *union* of the transaction sets of its length k subsets. This is called a *0-extension*.



	a	b	c	d
1	1	1	1	0
2	1	1	0	0
3	1	0	1	0
4	0	1	1	0
5	1	1	1	1
6	0	0	0	1
7	0	1	0	1
8	1	0	0	0

Figure 5.5: (A) Sample database; (B) Level wise mining of AFI in database (A). See Section 5.4.2 for more details. Only black colored itemsets will be generated by AFI, while every itemset including the grey-colored itemsets will have to be generated to mine ETIs.

0-extension and 1-extension suggest two basic steps to be taken for efficient maintenance of the supporting transactions. They allow the algorithm to obtain the support transactions of an itemset from its item subsets while avoiding the repeated scan of databases that plagues the algorithms proposed by (Yang et al., 2001; Sepp and Mannila, 2004). In the next section, we illustrate through an example the use of the two techniques together with noise-tolerant support-based pruning method.

5.4.2 An Example

In this section we present a simple example in which the data matrix D of Figure 5.5 is used to illustrate the AFI algorithm. Let $\epsilon_r = \epsilon_c = 1/3$ and let $minsup = 0.5$. The number of transactions in the database, n, equals 8. We wish to find the complete set of AFIs in D. In this case, the algorithm proceeds as follows.

Step 1: $k = 1, minsup^1 = 0.5$. The database is scanned once and the support of each singleton item is recorded.

Step 2: $k = 2, minsup^2 = 0.5 * 1/3$. As $\lfloor k \cdot \epsilon_r \rfloor = \lfloor (k-1) \cdot \epsilon_r \rfloor$, no additional 0's are allowed and a 1-extension is performed. In particular, the transaction set of the itemset ab is obtained by intersecting the transaction set of a, equal to $\{1, 2, 3, 5, 8\}$, with that of b, equal to $\{1, 2, 4, 5, 7\}$; the result is $\{1, 2, 5\}$. Since the number of transactions supporting ad and cd is equal to 1. Therefore, their supports are below the support threshold $minsup^2$, any AFI that contains them can be pruned. These itemsets are colored gray in Figure 5.5.

Step 3: $k = 3, minsup^3 = 0.5 * 2/3$. In this case, $\lfloor k \cdot \epsilon_r \rfloor = \lfloor (k-1) \cdot \epsilon_r) \rfloor + 1$. Thus one additional 0 is allowed in 3-itemsets, and a 0-extension (union of transaction sets) is performed. For example, a transaction supports itemset abc if it supports any of $\{ab, ac, bc\}$; the transaction set of abc is the union of the transaction sets for $\{ab, ac, bc\}$, which is $\{1, 2, 5\} \cup \{1, 3, 5\} \cup \{1, 4, 5\} = \{1, 2, 3, 4, 5\}$.

Step 4: $k = 4, minsup^4 = 0.5 * 1/3$. Because of support constraint $minsup$, i.e, 0.5, $\{a, b, c, d\}$ cannot be a valid AFI. No further extension of the current itemset is possible since all of the search space is covered.

Step 5: The candidate AFIs are $\{b, d\}$ and $\{a, b, c\}$. The first does not satisfy the $minsup$ size constraint. The second is readily shown to be a valid AFI, and constitutes the output of the algorithm.

5.4.3 Global Pruning

In order for an individual item i to appear in an AFI, its overall support must exceed $minsup \cdot n \cdot (1 - \epsilon_c)$. During the level-wise generation of AFI$(\epsilon_r, *)$, the total number of transactions under consideration in a given level will decrease or remain the same, and the number of transactions supporting an individual item will have the same property. If the support of item i among the transactions at level k drops below $minsup \cdot n \cdot (1 - \epsilon_c)$, then i can not appear in any AFI generated at levels $k' \geq k$. In particular, any itemset containing i can be eliminated from consideration. To illustrate, in the example presented in Figure 5.5 the number of transactions supporting an itemset should not be below 4. In addition, the number of supporting transactions for an individual item has to be above $\lceil 4 \cdot (1 - \epsilon_c) \rceil = \lceil 4(1 - 1/3) \rceil = 3$. The set of transactions remaining at level 2 is $T = \{1, 2, 3, 5, 7\}$; the number of transactions in T supporting item d is 2, which is less than 3, so any itemset in level $k \geq 2$ containing d can be eliminated from

Algorithm 6 A

FI Mining
Input: D, ϵ_r, ϵ_c, $minsup$
Output: The sets of approximate frequent itemsets

```
for i = 1 : m do
   T(i)=genSupport(D, i);
end for
k = 1;
L_1=∪_{i>0}^{m}{i};
repeat
   k := k+1;
   L_k := GenCandidateItemset(L_{k-1}, minsup^{k-1})
   if (⌊k · ε_r⌋ = ⌊(k + 1) ∗ ε_r⌋) then
      T(L_k) := 1-Extension(I, L_{k-1});
   else
      T(L_k) := 0-Extension(I, L_{k-1});
   end if
   AFI_p := AFI_p ∪ L_k;
until L_k is ∅
AFI :=filter(AFI_p, minsup, ε_c)
return AFI
```

consideration.

5.4.4 Identification of AFI

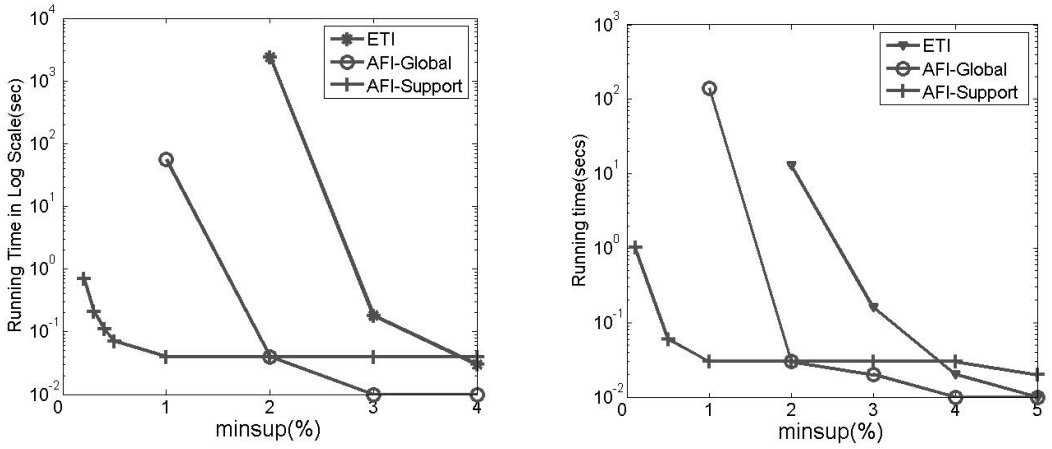
The AFI algorithm so far generates a superset of approximate frequent itemsets. The postprocessing of this subset can be done separately from the level-wise generation since it will neither benefit nor prohibit the traversing of the search space. The verification of whether an AFI$(\epsilon_r, *)$ is an AFI can be easily done by simply checking the percentage of 0's in each candidate itemset. Finding a maximal AFI in an AFI$(\epsilon_r, *)$ is more difficult. In (Liu et al., 2005), we describe a heuristic algorithm for this problem that scales linearly with respect to $|T|+|I|$, where I is an itemset supported by a transaction set T. The algorithm works by removing transactions having a large number of zeros, beginning with those whose zeros are aligned with low density items. Due to space limitations, a complete description of this algorithm is omitted.

5.5 Experiments

We performed four experiments to assess the performance of AFI. The first explored the scalability of the AFI mining algorithm and the effectiveness of the pruning methods. The second experiment used synthetic data to compare the results of AFI mining to exact frequent itemset mining and ETI. Finally, we applied AFI to a zoology data set with known underlying patterns.

5.5.1 Scalability

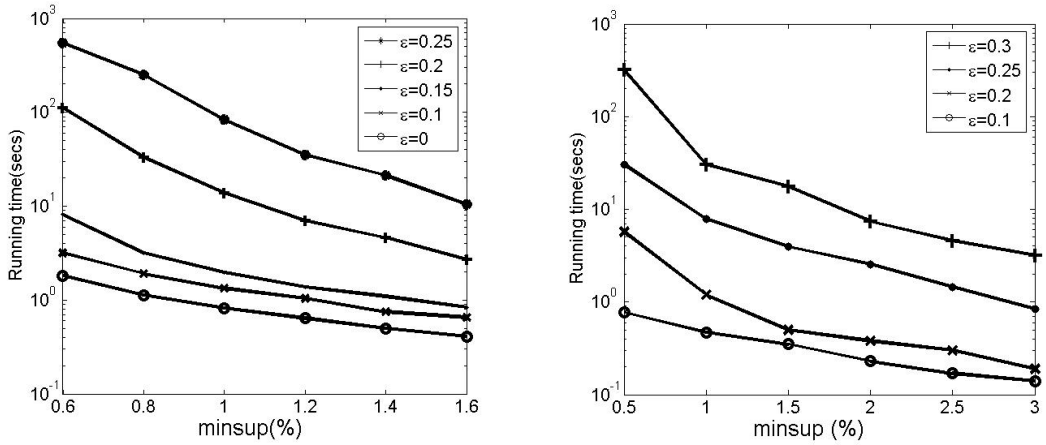
Two data sets were employed to measure scalability. The first, T10KI100, was generated by the IBM synthetic data set generator. It contains 10K transactions and 100 items, with an average of 10 items per transaction. The second data set was the chess data set, which is available from the UCI machine learning repository(D.J. Newman and Merz, 1998). It contains 28K transactions and 65 items with at least one third nonzero elements per transaction. We built the exhaustive level-wise algorithm presented in (Yang et al., 2001) to discover the complete set of strong ETIs. The experiments were run on a 2GHz PC with 2G memory.



(A) T10KI100 (B)Chess

Figure 5.6: Comparison between AFI and ETI

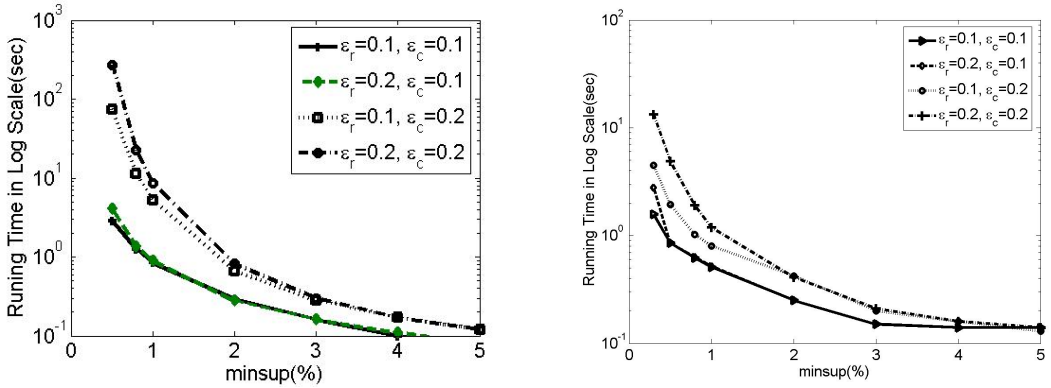
Figure 5.6 presents the run-time performance for both data sets, with $\epsilon_r = \epsilon_c = 20\%$. All algorithms performed well when *minsup* was 5% or higher; however, ETI was not able to compete when *minsup* dropped below 2%. In contrast to AFI, ETI lacks an effective pruning strategy; therefore, a much larger set of candidate itemsets



(A) T10KI100 (B)Chess

Figure 5.7: The running time of AFI with noise-tolerant support pruning varying *minsup* and ϵ. $\epsilon = \epsilon_c = \epsilon_r$.

may be generated in order to build the complete set of ETIs. In addition, because the noise criterion of ETI is less stringent, the maximum length of an ETI can be much larger than that of an AFI. This leads to an exponentially larger number of candidate itemsets. Both shortfalls explain why AFI can outperform ETI by such a large margin. AFI mining with downward pruning appears to be superior to global support pruning, especially when the minimum support is low. The AFI algorithm employing both pruning strategies was also tested, although not shown in the Figure; the performance was almost the same as AFI using only the support pruning property.



(A) T10KI100 (B)Chess

Figure 5.8: The running time of AFI with noise-tolerant support pruning as *minsup* varies. $\epsilon_c \neq \epsilon_r$.

We tested the scalability of our algorithm as the noise threshold and minimum sup-

port varied. The result is shown in Figure 5.7. To reduce the parameter space, the transaction-wise threshold ϵ_r was set equal to the item-wise noise threshold ϵ_c in this set of experiments. Figure 5.7 shows that running time increases with increases in noise tolerance, as expected. Here the algorithm is essentially looking for approximate frequent itemsets with higher-dimensionality. Allowing more noise in an itemset results in larger approximate frequent itemsets; consequently, more candidate itemsets have to be explored, and computation increases exponentially with respect to the dimensionality of the itemsets. Nevertheless, even with a very high error rate of 30%, our algorithm proves competent in finding the complete sets of AFI in a reasonable time.

Figure 5.8 shows how different transaction-wise and item-wise noise thresholds can affect performance. Relatively speaking, reducing the item-wise error constraint leads to a greater reduction in running time than reducing the transaction-wise error constraint, as the former leads to higher levels of pruning according to Theorem 5.4.1.

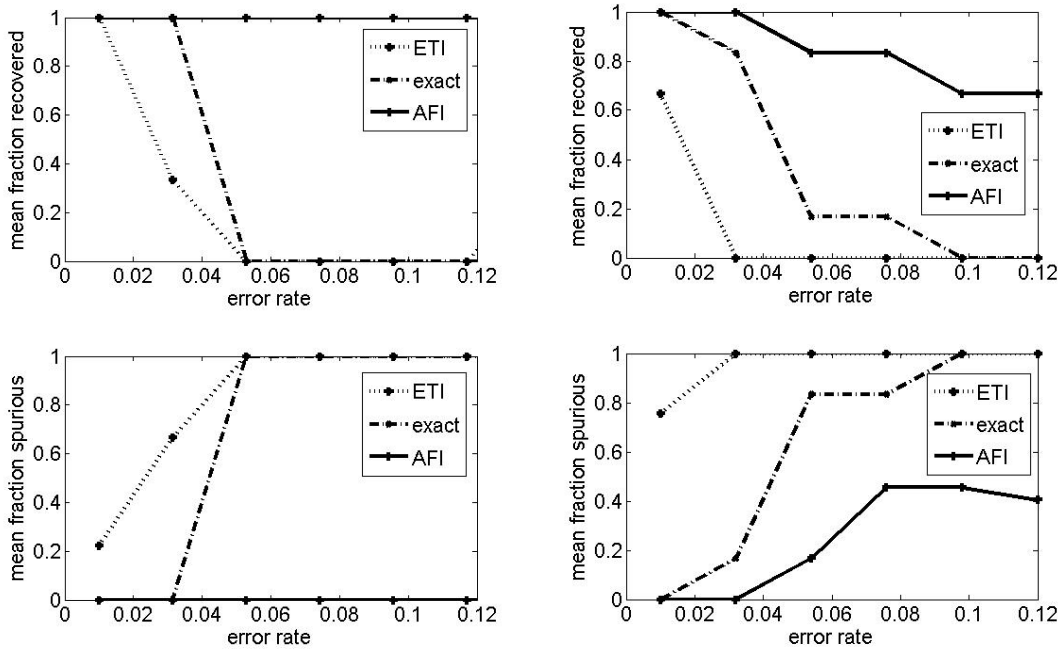
5.5.2 Quality Testing with Synthetic Data

In addition to run-time performance we also tested the quality of the results produced by AFI. To do so we created data with an embedded pattern and then overlaid random errors. By knowing the true patterns, we were able to assess the quality of the various results. To each synthetic data set created, an exact method (ETI with $\epsilon_c = 0$), ETI and AFI were each applied.

To evaluate the performance of an algorithm on a given data set, we employed two measures that jointly describe quality: "recoverability" and "spuriousness." Recoverability is the fraction of the embedded patterns recovered by an algorithm, while spuriousness is the fraction of the mined results that fail to correspond to any planted cluster. A truly useful data mining algorithm should achieve high recoverability with little spuriousness to dilute the results. A detailed description of the two measures is given in (Liu et al., 2005). Multiple data sets were created and analyzed to explore the relationship between increasing noise levels and the quality of the result. Noise was introduced by bit-flipping each entry of the full matrix with a probability equal to p. The probability p was varied over different runs from 0.01 to 0.2. The number of pattern blocks embedded also varied, but the results were consistent across this parameter. Here we present results when 1 or 3 blocks were embedded in the data matrix (Figure 5.9(A) and (B), respectively).

In both cases, the exact method performed poorly as noise increased. Beyond $p =$

0.05 the original pattern could not be recovered, and all of the discovered patterns were spurious. In contrast, the error-tolerant algorithms, ETI and AFI, were much better at recovering the embedded matrices at the higher error rates. However, the ETI algorithm reported many more spurious results than AFI. Although it may discover the embedded patterns, ETI also reports many additional patterns that are not of interest, often including irrelevant columns. The AFI algorithm consistently demonstrated higher recoverability of the embedded pattern while maintaining a lower level of spuriousness.



(A) Single Cluster (B) Multiple Clusters

Figure 5.9: Algorithm quality versus noise level.

5.5.3 Zoo Data Set

We also applied AFI to a database downloaded from the UCI Machine Learning Repository(D.J. Newman and Merz, 1998). The Zoo Database contains 101 instances and 18 attributes (animal name, 15 boolean attributes, 2 numerics). The boolean attributes are *hair*, *feathers*, *eggs*, *milk*, *airborne*, *aquatic*, *predator*, *toothed*, *backbone*, *breathes*, *venomous*, *fins*, *tail*, *domestic* and *catsize*. The numeric attributes are *legs* and *type*, where the *type* attribute appears to be the class attribute. All the instances are classified into 7 classes (*mammals, birds, fish*, etc.).

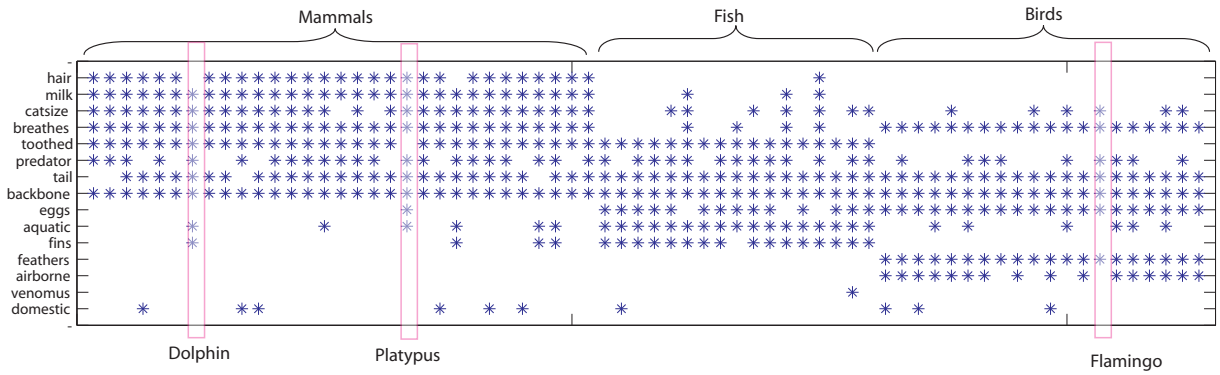


Figure 5.10: Three AFI blocks discovered in the zoo dataset. * indicates the presence of a feature.

One task could be to discover the common features of a set of animals in the same class. For example, mammals produce milk, are covered in hair, are toothed, and grow tails. However, not every mammal exhibits these common features: platypuses lack teeth and dolphins are hairless. If such exceptions are not tolerated, it is hard to find the complete set of features that characterizes a class.

For testing purposes, we adopted the 7 classes into which the instances were already categorized as the true underlying pattern. Then we examined how well the competing frequent itemset mining methods recovered these classes. We focused on the 4 classes with at least 5 instances and where each class had least 3 commonly shared features.

The exact method, ETI(ϵ_r), and AFI(ϵ_r, ϵ_c) were each applied to the dataset. When we required a perfect match between the output of a method and the true pattern, only AFI was able to recover 3 out of the 4 classes. Here "perfect match" refers to a step in the evaluation of the output, not the criteria for adding a transaction to the support of an itemset. When the criteria for a match was relaxed to 85% overlap, then AFI recovered the fourth class: bugs. Figure 7.5 displays the sets of animals and their common features identified by AFI.

Neither the exact method nor ETI were able to recover a single class under the perfect match evaluation criterion. Exact frequent itemset mining generated subsets of the animals in each class and then found subsets of their common features. The instance *flamingo* presented a typical problem: in this data set *flamingo* lacks the *airborne* attribute – perhaps because the zoo clipped their wings. Thus flamingo cannot be included in the class *bird* with the common feature *airborne*.

Although such "errors" as clipped wings are accommodated by ETI, sometimes the type of tolerance featured by ETI identified irrelevant items. It identified *fin* and

domestic as common features for *mammals*, which is not generally true. Because only the row-wise constraint was applied, the set of features discovered was not reliable.

5.6 Conclusion

In this chapter we have outlined an algorithm for mining approximate frequent itemsets from noisy data. The AFI model places two criteria on the fraction of noise in both the rows and columns, and so ensures a relatively reasonable distribution of the error in any patterns found. Our work generalizes the classical level-wise frequent itemset mining based on the Apriori-property into a new algorithm where the Apriori-property does not hold and noise has to be incorporated. Our work generates not only more reasonable and useful itemsets than classical frequent itemset mining and existing noise-tolerant frequent itemset mining, but it is computationally more efficient as well. We are currently investigating depth-first methods for approximate frequent itemset mining.

5.7 Appendix

The detailed proofs of the following Lemma 1 and Lemma 2 can be found in (Sun and Nobel, 2005). We only state them here.

Lemma 1 *Under the conditions of Theorem 1,*

$$P\left(|\hat{C}| \leq l^2\right) \leq \Delta_1(l). \tag{5.8}$$

Lemma 2 *For any sufficiently large n, let $\mathcal{A} = \{C : \ C \in \mathcal{C}_n$ such that $|C| > \frac{l^2}{2}$ and $\frac{|C \cap C^{*c}|}{|C|} \geq \alpha\}$. Let $A = \{\mathcal{A} \neq \emptyset\}$. If $l \geq 16\alpha^{-1}(\log_b n + 2)$, then*

$$P(A) \leq \Delta_2(\alpha, l)$$

Proof of Theorem 1: Let E be the event that $\{\text{SetClu} \leq \frac{1-\alpha}{1+\alpha}\}$. It is clear that E can be expressed as the union of two disjoint events E_1 and E_2, where

$$E_1 = \{|\hat{C}| \leq |C^*|\} \cap E$$

and

$$E_2 = \{|\hat{C}| > |C^*|\} \cap E$$

On the other hand, by the definition of SetClu, inequality SetClu $\leq \frac{1-\alpha}{1+\alpha}$ can be rewritten equivalently as

$$1 + \frac{|\hat{C} \cap C^{*c}|}{|\hat{C} \cap C^*|} + \frac{|\hat{C}^c \cap C^*|}{|\hat{C} \cap C^*|} \geq \frac{1+\alpha}{1-\alpha}.$$

Moreover, when $|\hat{C}| > |C^*|$, one can verified the trivial fact that $|\hat{C} \cap C^{*c}| > |\hat{C}^c \cap C^*|$, which also implies that

$$1 + \frac{|\hat{C} \cap C^{*c}|}{|\hat{C} \cap C^*|} + \frac{|\hat{C}^c \cap C^*|}{|\hat{C} \cap C|} \leq 1 + 2\frac{|\hat{C} \cap C^{*c}|}{|\hat{C} \cap C^*|}.$$

Furthermore, one can verified that $E_2 \subset E_2'$, where

$$E_2' = \{|\hat{C}| > |C^*|\} \cap \left\{1 + 2\frac{|\hat{C} \cap C^*|}{|\hat{C} \cap C^*|} \geq \frac{1+\alpha}{1-\alpha}\right\}.$$

Therefore, it suffices to bound $P(E)$ by $P(E_1)$ and $P(E_2')$ separately.

Immediately, one can bound $P(E_1)$ by $\Delta_1(l)$ via Lemma 1. It remains to bound $P(E_2')$. Notice that inequality

$$1 + 2\frac{|\hat{C} \cap C^{*c}|}{|\hat{C} \cap C^*|} \geq \frac{1+\alpha}{1-\alpha} \text{ implies } \frac{|\hat{C} \cap C^{*c}|}{|\hat{C}|} \geq \alpha.$$

Therefore, by Lemma 2, one can bound $P(E_2')$ by

$$P(E_2') \leq P\left(E_2' \,\middle|\, |\hat{C}| \geq l^2\right) \leq \Delta_2(\alpha, l),$$

where the first inequality holds because the unconditional probability is always less or equal to the conditional probability. Consequently, we have

$$P\left(\text{SetClu} \leq \frac{1-\alpha}{1+\alpha}\right) \leq \Delta_1(l) + \Delta_2(\alpha, l).$$

Proof of Corollary 1: Theorem 1 implies that if we can bound both $\Delta_1(l_n)$ and $\Delta_2(\psi(n)^{-1}, l_n)$ by $2n^{-2}$ for any sufficiently large n, then Borel -Cantelli Lemma can be applied to establish the almost sure convergency.

When n is sufficiently large, the condition $l_n > 16\psi(n)(\log_b n + 2)$ and $\psi(n) \to n$, implies $l_n > 2(\frac{3}{4}(p - p_0)^2 \log_b e)^{-1} \log_b n$. By plugging this lower bound of l_n into $\Delta_1(l_n)$, one can get $\Delta_1(l_n) < 2n^{-2}$. Meanwhile, by plugging the condition that $l_n >$

$16\psi(n)(\log_b n + 2)$ into $\Delta_2(\psi(n)^{-1}, l_n)$, one can get $\Delta_2(\psi^{-1}(n), l_n) < 2n^{-2}$.

Chapter 6

Clustering Dissimilarity Data into Partially Ordered Set

In this chapter, we present a clustering method which clusters the objects based on dissimilarity data. Instead of requiring disjoint clusters as in traditional dissimilarity-based clustering, we allow overlapping between clusters that have no strict subset or superset relationships. We extend clustering from the space of hierarchy to the space of partially ordered sets(posets). We study the set of posets that are derivable from pair-wise dissimilarity-based clustering methods.

Only special types of dissimilarity matrices can be exactly preserved by existing clustering methods (For example, there is a one-to-one correspondence between ultrametric matrices and cluster hierarchies). We prove that the set of PoClusters, generated by Poclustering of dissimilarity data, has the one-to-one correspondence with the set of all dissimilarity matrices. We present the necessary and sufficient conditions to determine whether a given poset can be recovered by PoClustering of a dissimilarity matrix. An algorithm to derive a dissimilarity ranking from a PoCluster is also presented. Since the optimal PoClustering approach is NP-complete, we also introduce a polynomial time approximation algorithm, and show it to be both efficient and effective by experiments.

Different from previous chapters, the algorithm proposed in this chapter does not explore subspace. It tries to cluster objects given their dissimilarities. It also derives relative dissimilarities based on classification ontology.

6.1 Introduction

Categorizations are natural ways to organize a set of objects. The structure of categorization ranges from hierarchies(taxonomies), where subclasses are disjoint partitions of

their parent class, to ontologies, which allow overlapping subclasses as well as multiple parents. Clustering pair-wise dissimilarity data into hierarchies has been studied extensively. The problem is referred to as numerical taxonomy(N. Ailon, 2005). Numerical taxonomies are useful in a number of applications, such as estimating evolutionary branching processes in biology. Since strict taxonomies form disjoint partitions, these structures are insufficient for capturing categorizations with richer relationships, such as ontologies.

In this paper, we consider the problem of automatically constructing *numerical ontologies* by clustering dissimilarities between object pairs from a given set. Numerical ontologies provide a more general categorization approach than taxonomies, and their added categorization power may benefit applications in multiple disciplines. For example, in animal classification, while aquatic animals and mammals are two reasonably different classes, a dolphin can be classified as both an aquatic animal and a mammal. Such relationships cannot be represented in a hierarchy. In biology, a gene may have multiple functions. Building a gene hierarchy from observed pairwise dissimilarities limits each gene to one specific function. The hierarchical structure does not parallel existing gene function classifications, such as Gene Ontology(ash,), where gene subclasses may overlap or belong to multiple parents.

Before proceeding, we clarify the specific classification notion assumed in this paper. We consider the most general classification system, which is a partially ordered set(ash,), or poset. A poset contains the sets(clusters) of objects as the elements, ordered according to their subset relationships. Since a given poset can be constructed from any combination of subsets taken from the set's power set, it has a maximal cardinality of $2^{2^{|\mathcal{N}|}}$, where $\mathcal{N}$ is the object set. The set of hierarchies, for example, is a special subset of the set of posets.

It has been proven(N. Ailon, 2005) that the information of any given ultrametric dissimilarity matrix corresponds to a unique hierarchy. A dissimilarity D is ultrametric, if for any three objects A, B and C in the set, $D(A, C) \leq \max(D(A, B), D(B, C))$. The correspondence means that the same dissimilarity matrix can be recovered from the hierarchy. For example, Figure 6.1 (a.1) shows an ultrametric dissimilarity matrix. A hierarchy shown in (a.2) is constructed from it by hierarchical clustering with a complete linkage criterion. The pair-wise dissimilarity between any pair of objects shown in (a.1) can be recovered by assigning it the minimum diameter of the clusters containing the pair. On the other hand, the dissimilarity matrix shown in (b.1) is not an ultrametric dissimilarity matrix, because for objects A, B and C,

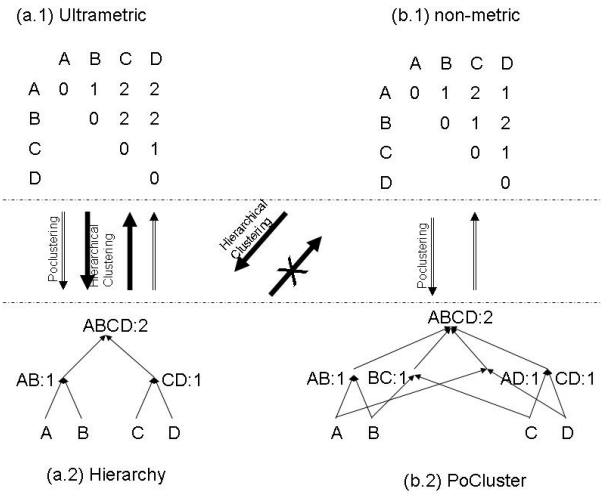


Figure 6.1: (a.1) An ultrametric dissimilarity matrix; (a.2) Hierarchy constructed from (a.1) by either hierarchical clustering or PoClustering; (b.1) A non-metric dissimilarity matrix. (b.2) PoCluster constructed from (b.1) by PoClustering. Note: (a.1) can be derived from the hierarchy in (a.2) by assigning each pair the minimum diameter of the sets containing it; (b.2) can be used to derive dissimilarities of (b.1) in the same way; Applying hierarchical clustering to (b.1) can also construct the hierarchy in (a.2), but (b.1) cannot be derived from (a.2)

$D(A, C) > \max(D(A, B), D(B, C))$. Applying the same clustering algorithm to this dissimilarity matrix generates the same hierarchy shown in (a.2). But the dissimilarities in (b.1) cannot be derived from the hierarchy, which corresponds to the ultrametric dissimilarities in (a.1). Therefore, building a hierarchy from a dissimilarity matrix that does not satisfy the ultrametric property potentially loses information. The problem of interest in this paper is *whether there exists a clustering approach that preserves the information of any given dissimilarity data?*

In this chapter, we study PoClustering. A *PoCluster* is a collection of *clique clusters* arrived at by smoothly varying the threshold from 0 to the maximum pair-wise dissimilarity in the set. It adopts a definition of the cluster as a maximal clique from graph theory. A *clique cluster* is a maximal subset of objects whose maximum pair-wise dissimilarity does not exceed a given threshold. An example of PoCluster is shown in Figure 6.1 (b.2), which is generated from dissimilarity matrix (b.1) by PoClustering. PoClusters differ from hierarchies by incorporating all clique clusters rather than only disjoint clusters. As a result, it allows overlaps between clusters that are not strict subsets, as shown in Figure 6.1 (b.2). In addition, it preserves the information provided in the dissimilarity data. The dissimilarity matrix shown in Figure 6.1 (b.1), which could not be recovered from the hierarchy in (a.2), can be derived from the PoCluster in (b.2).

In this paper, we formally prove that, there exists a one-to-one correspondence between the set of PoClusters and the set of dissimilarity matrices. The set of PoClusters is, therefore, the most general notion of clustering that can be derived from dissimilarities alone. In addition, we prove that the set of PoClusters contains all possible pyramidal and hierarchical clusters as subsets.

Based on these theoretical results, we further investigate two practical issues. First, given an arbitrary poset, can it be derived from any dissimilarity matrix? If it can, how can we establish the pair-wise dissimilarities when given a poset structure? The answer to this question is important in order to derive the pair-wise categorical dissimilarities between objects when given a classification structure such as a taxonomy or an ontology. For example, biologists are interested in obtaining gene-gene categorical similarities based on their classification in gene ontology. Another example is to derive word similarity given the structure of wordnet(Budanitsky, 2001). In this paper, we provide an algorithm which identifies whether a poset structure can be generated by PoClustering and derives relative pair-wise dissimilarities from the given structure if possible.

We develop two versions of the PoClustering algorithm. The optimal PoClustering algorithm is an exact algorithm. The algorithm by itself is incremental and more efficient than the naive approach. Nevertheless, the PoClustering problem is NP-complete. In this paper, we present a greedy approximation algorithm for PoClustering which replaces maximum clique finding by solving a minimum edge clique cover problem. Our experiments on both synthetic and real data show the effectiveness and efficiency of this approximation algorithm in comparison to the conventional hierarchical and pyramidal clustering algorithms.

The remainder of this paper is organized as follows. Section 6.2 addresses related work in clustering, automated taxonomy construction, and dissimilarity measures appropriate for ontologies. Section 6.3 presents the preliminary definitions of PoClusters, followed by Section 6.5 which examines their properties and the relationships with existing clustering algorithms. Section 6.6 provides an approximation algorithm for constructing PoClusters from dissimilarity data. A performance study is reported in Section 6.7. Section 6.8 concludes the paper and discusses future work.

6.2 Related Work

Many clustering algorithms take a dissimilarity matrix as input. However, relatively few investigations have been conducted to establish the relationship between the dissimilarity matrix input and the clustering results. In this section, we review previous studies on clustering algorithms that have known relationships to special classes of dissimilarity matrices.

6.2.1 Hierarchial and Pyramidal Clustering

Both hierarchical(Berkhin, 2002; JAIN and Dubes, 1988) and pyramidal clustering (Bertrand and Janowitz, 2002; Diday, 1986) generate clusters that have bijections to special sub-classes of dissimilarity matrices.

Hierarchical clustering(Berkhin, 2002; JAIN and Dubes, 1988) refers to the formation of a nested disjoint partition of data objects. It is often represented by a *dendrogram*, that is, a tree with the objects at its leaves and a root corresponding to the universal set (of all objects). The heights of the internal nodes represent the maximum dissimilarities between the descendant leaves. It has been proven that a bijection exists between hierarchical clustering and the set of *ultrametric*(Diday, 1986) dissimilarity matrices which satisfy the *ultrametric triangle inequality*, i.e., for any set of three objects $\{a, b, c\}$, $D(a, c) \leq max\{D(a, b), D(b, c)\}$. An equivalent statement of the ultrametric condition is that there exists a linear order of all objects such that their dissimilarities are the distances between them.

Pyramidal clustering(Bertrand and Janowitz, 2002; Diday, 1986) allows for a more general model than hierarchical clustering. A child cluster may have up to two parent clusters. Two clusters may overlap by sharing a common child cluster. The structure can be represented by a directed acyclic graph. It is known that a bijection exists between pyramidal clustering and the set of dissimilarity matrices that are Robinson matrices. A matrix is a *Robinson matrix* if there exists an ordering among all objects such that the dissimilarities in the rows and columns do not decrease when moving horizontally or vertically away from the main diagonal (see Figure 6.4 for an example). An ultrametric matrix is a special case of Robinson matrix and hierarchical clustering is a special case of pyramidal clustering. Note that a dissimilarity matrix may not always be a Robinson matrix, and in such cases, neither hierarchical clustering nor pyramidal clustering is able to generate clustering from which the original dissimilarity matrix can be re-derived. That is, no bijection exists.

We prove in this paper, that PoClustering preserves the bijection between PoCluster and a given dissimilarity matrix. It also includes both hierarchical clustering and pyramidal clustering as special cases.

6.2.2 Dissimilarity Derived from Ontology Structure

Relative pair-wise dissimilarities between objects can easily beh derived from a hierarchy and pyramidal structure. Obtaining pair-wise dissimilarities from ontologies is more challenging. Heuristic methods have been proposed. One representative example is categorical similarity, which was introduced to measure the similarity between two concepts in the WordNet(Budanitsky, 2001). Similar measures have been applied to determine the categorical dissimilarity between pairs of genes from Gene Ontology(Sevilla et al., 2005; ash,).

The *information content* of a term c measures the probability of encountering this term given a structure with M nodes, where $p(c) = 1 - frequency(c)/|M|$. The higher the frequency of a given term, the lower its information content. Guided by the intuition that the similarity between a pair of concepts may be assessed by "the extent to which they share information", Resnik defined the dissimilarity between two concepts as the information content of their lowest super-ordinate, that is, $sim(c1, c2) = -\log p(lso(c1, c2))$. Jiang and Conrath's(Budanitsky, 2001) also proposed a dissimilarity measure which uses the notion of information content, but in the form of the conditional probability of encountering an instance of a child-term give an instance of a parent-term. Thus, the information content of the two nodes as well as that of their most specific lowest common ancestor, plays a part. $dis(c1, c2) = 2\log p(lso(c1, c2)) - (\log(p(c1)) + \log(p(c1)))$. A similarity approach was presented by Lin(Linde et al., 1980) in a different way: $dis(c1, c2) = 1 - \frac{2\log p(lso(c1,c2))}{(\log(p(c1))+\log(p(c1)))}$. Leacock and Chodorow proposes another similarity measure that relies on the length $len(c1, c2)$ of the shortest path between two concepts. However, they limit their attention to special links and scale the path length by the overall depth D of the taxonomy: $dis(c_1, c_2) = \frac{-log(len(c_1,c_2))}{2D}$. It is unclear how the clusters derived from these dissimilarities relate to the original ontology. In Section 6.7, we compare our dissimilarity measure to each of these in terms of their ability to recover the original ontology.

6.3 Preliminaries

6.4 Model

In the following discussion, we assume a universal set of objects denoted by $\mathcal{N}$. A *pair* in $\mathcal{N}$ refers to an object pair $\{x, y\}$, where $x, y \in \mathcal{N}$. Given a set $S \subseteq \mathcal{N}$, the set of pairs in S is denoted by $S \times S$ or S^2.

A *dissimilarity matrix* describes the pair-wise relationships between objects. It is a mapping D from $(\mathcal{N} \times \mathcal{N})$ to a real nonnegative value. A dissimilarity matrix has the following two properties (1) reflectivity: $\forall x,\ D(x, x) = 0$; (2) symmetry: $\forall x, y$, $D(x, y) = D(y, x)$. A dissimilarity matrix can be directly mapped to an undirected weighted graph $G = \langle V, E, W \rangle$, where each node in V corresponds to an object in $\mathcal{N}$, and each edge $e = \langle x, y \rangle$ with weight w depicts the dissimilarity $D(x, y)$ between the two objects it connects. We denote the graph implied by the dissimilarity D as $G(D)$.

Example: Figure 6.2 (B) shows a dissimilarity matrix of object set $\{A, B, C, D, E\}$. It satisfies both reflectivity(0 diagonal) and symmetry. This dissimilarity matrix can be mapped to the undirected weighted graph in Figure 6.3 ($d = 4$). Each node in graph corresponds to an object, each edge corresponds to a pair and the weight of the edge is the dissimilarity between the pairs of objects.

A clique is a fully connected subgraph in an undirected graph.The *diameter* of a clique is the maximum edge weight within the clique. A *clique cluster* is defined as a maximal clique with a diameter d. A diameter indicates the level of dissimilarity of the set of objects in the clique cluster.

Definition 6.4.1 *(Clique Cluster). Let $G(D)$ be an undirected weighted graph of a dissimilarity matrix D. A clique cluster $C = \langle S, d \rangle$ is a maximal clique S with diameter d in graph $G(D)$.*

When there are multiple cliques within the graph with the same diameter d, we denote this set of clique clusters as $\text{cliqueset}_\delta(d)$.

Example: Given the dissimilarity matrix shown in Figure 6.2(B), $ABCD$ forms a clique with maximum edge weight 2, as shown in Figure 6.3. Therefore, $ABCD$ is a clique cluster with diameter 2. So is BCE. We denote them as $\text{cliqueset}_\delta(2) = \{ABCD, BCE\}$.

PoCluster

The notion of clique cluster is not new. The intermediate clusters generated by hierarchical clustering using a complete linkage criterion is similar to clique clusters in spirit, since they both look for a cluster with minimum diameter. However, when two clusters are merged in hierarchical clustering, the relationship(linkage) between two clusters to be merged solely depends on the maximum or minimum dissimilarity between a pair of objects within two clusters. This oversimplified similarity measure ignores many pair-wise relationships between objects in the two clusters. To best explore and preserve the information carried by a dissimilarity matrix, in this paper, we present PoCluster. PoCluster reveals clique clusters with all possible diameters present in the dissimilarity matrix. The non-disjoint feature allows us to explore richer and deeper relationships among objects. We formally define PoCluster in Definition 6.4.2.

Definition 6.4.2 *(PoCluster) Let D be a dissimilarity matrix, a PoCluster P of D is defined as*

$$P = \bigcup_{\forall d \in W(D)} cliqueset_{\delta}(d). \tag{6.1}$$

which is the collection of clique clusters of all possible diameters in diameter set $W(D)$.

Example: The dissimilarity matrix in Figure 6.2(B) consists of 4 possible diameters, they are $\{1, 2, 3, 4\}$. For each diameter, we map them into an undirected graph, namely, diameter graph, where there exists an edge between two nodes only if their dissimilarities are smaller than or equal to the diameter. For each graph, there exists a set of cliques in it. For example, in Figure 6.3, when $d = 1$, there are four 2-cliques in the graph. The set of the clique clusters generated in each of the diameter graph is shown as poClusters in Figure 6.2(A).

Now, we examine the properties of PoClusters. Similar to hierarchical clustering, PoCluster also includes the set $\mathcal{N}$ containing all the objects. This set has the maximum dissimilarity in D as its diameter. PoCluster does not ignore dissimilarity measures as hierarchical clusters do since each pair-wise dissimilarity is covered by at least one clique cluster whose diameter equals to the pair-wise dissimilarity. In addition, the maximal clique cluster insures that if one cluster is a subset of the other, one's diameter will be strictly lower than the other. This property generates a partial order of the clusters in the PoCluster as shown in Figure 6.2(A).

d	$\text{cliqueset}_\delta(d)$
d=1	AC, BD, CD, BE
d=2	$ABCD, BCE$
d=3	$ABCE$
d=4	$ABCDE$

Table 6.1: PoCluster generated based on dissimilarity matrix in Figure 6.2(B).

Property 6.4.1 *Let D be a dissimilarity matrix of object set N, Let P be a PoCluster of dissimilarity matrix D, P has the following properties.*

1. $N \in P$
2. $\forall C_1, C_2 \in P$, *if* $C_1 \subset C_2$, *then* $diam(C_1) < diam(C_2)$
3. $\forall x, y \in N$, *there exists a cluster* $C \in P$, *such that* $\{x, y\} \subseteq C$ *and* $diam(C) = D(x, y)$;
4. $\forall x \in N$, $\{x\} \in P$.

Next, we further examine the properties of PoCluster with regard to dissimilarity matrices. Although it is possible to run classical hierarchal clustering or pyramidal clustering on any dissimilarity matrix, this mapping is not, in general, invertible. However, PoClustering goes beyond them by generating a PoCluster, which provides a one-to-one correspondence with the input dissimilarity matrix. This property is presented and proven in Theorem 6.4.1.

Theorem 6.4.1 *There exists a bijection between the set of PoClusters $\mathcal{P}$ and the set of dissimilarity matrices $\mathcal{D}$.*

Proof 6.4.1 *According to Cantor-Bernstein-Schroeder theorem(Fraenkel, 1953), if there exist injective functions $\psi : \mathcal{D} \mapsto \mathcal{P}$ and $\xi : \mathcal{P} \mapsto \mathcal{D}$, there exists a bijection function between $\mathcal{D}$ and $\mathcal{P}$.*

In order to prove $\psi : \mathcal{D} \mapsto \mathcal{P}$ is an injection, we prove that $\forall D_1, D_2 \in \mathcal{D}$, if $D_1 \neq D_2$, then $\psi(D_1) \neq \psi(D_2)$. Since $D_1 \neq D_2$, there exists a pair (x, y), such that $D_1(x, y) \neq D_2(x, y)$. Let's assume $D_1(x, y) < D_2(x, y)$. In $\psi(D_1)$, according to the PoCluster definition, there exists a clique cluster S with diameter $D_1(x, y)$, $S \in cliqueset_\delta(D_1(x, y))$, such that (x, y) is contained in S. However, In $\psi(D_2)$, since

$D_2(x,y) > D_1(x,y)$, (x,y) does not appear in any cliques with diameter smaller than $D_2(x,y)$. Therefore, $\psi(D_1) \neq \psi(D_2)$.

In order to prove $\xi : \mathcal{P} \mapsto \mathcal{D}$ is also an injection, we prove that $\forall P_1, P_2 \in \mathcal{P}$, if $P_1 \neq P_2$, then $\xi(P_1) \neq \xi(P_2)$. Let $D_1 = \xi(P_1)$ and $D_2 = \xi(P_2)$. Assume there exists a cluster C with diameter d in P_1 that does not exist in P_2. The following scenarios may happen i)There exists a cluster C_2 in P_2, such that the set of objects contained in C_2 is the same as those in C. However, $diam(C) \neq diam(C_2)$. Therefore, if $diam(C) > diam(C_2)$, then Let (x_1, x_2) be the pair with the maximum dissimilarity $diam(C)$, then $D_1(x_1,x_2) > diam(C_2) > D_2(x_1,x_2)$. Similar case can be proven for $diam(C) < diam(C_2)$

ii) There does not exist a cluster C_2 in P_2 containing the same set of the objects. Assume C_2 be the minimum cluster in P_2 with minimum diameter, such that $C_1 \subset C_2$. Therefore. It is trivial to prove $D_1 \neq D_2$ if $diam(C_1) \geq diam(C_2)$. Now we prove that $D_1 \neq D_2$ under the condition that $diam(C_1) < diam(C_2)$. Let X be the set of objects contained in C_1, let d be the maximum diameter of X by D_2. If $d = diam(C_2)$, then the pairs whose dissimilarity in D_2 equals to d will have a smaller distance in D_1. If $d < diam(C_2)$, then according to the PoCluster property, there exists a set C_2' in P_2, such that $X \subseteq C_2'$ and $diam(C_2') == d$, which contradicts with the assumption.

6.4.1 Relationships with Hierarchy and Pyramid

Hierarchical and pyramidal clusterings are known to have one-to-one correspondences with ultrametric and Robinson matrices respectively. In addition, hierarchical clustering is a special case of the pyramidal clustering as shown in (Diday, 1986). We answer a similar question in this section, i.e., *Does PoCluster recover the same hierarchy or pyramid as pyramidal clustering given an ultrametric or a Robinson matrix?*

Lemma 6.4.2 *The set of pyramids is included in the set of PoCluster.*

Proof 6.4.2 *(Sketch of proof) As shown in paper(Diday, 1986), there exists a bijection between a pyramid and a Robinson matrix. A matrix is a Robinson matrix if there exists an ordering θ of the objects, such that the rows and columns are in non-decreasing order as they are moving away from the diagonal. Any given pyramid cluster is an interval of such an ordering. Now let $\{x_1, x_2, ..., x_n\}$ be an ordered list of objects according to θ. Let D be the Robinson dissimilarity matrix shown in Figure 6.4. Let P be a PoCluster. For any entry $\{x_i, x_j\}$ in a Robinson matrix D, the sub-triangle below $\{x_i, x_j\}$ above*

the main diagonal corresponding to the rows $\langle x_i, ..., x_j \rangle$ *and the columns* $\langle x_i, ..., x_j \rangle$ *will contain lesser dissimilarity values than* $D(x_i, x_j)$*, therefore,* $\{x_i, ..., x_j\}$ *will be a cluster in* P*, which is an interval of* θ*. Therefore, starting from the entries from the upper right corner, then recursively traversing the two lower sub-triangles* $\langle x_i, ..., x_{j-1} \rangle$ *and* $\langle x_{i+1}, ..., x_j \rangle$ *returns the whole pyramid, which is also a PoCluster.*

6.5 PoCluster Derivable Ontology

In practice, a classification taxonomy can be an arbitrary collection of sets, referred to as *poset*, where neither the diameters of the clusters nor the pair-wise dissimilarities between objects are available. In this section, we address a particular subset of posets. A poset is *PoCluster derivable* if applying PoClustering to a dissimilarity matrix generates the same set of clusters. A *PoCluster derivable* poset can be considered as a PoCluster of which the diameter information is unknown. Therefore, each PoCluster derivable poset corresponds to a infinite collection of PoClustersthat contain the same clusters but with different diameters.

However, not every poset is PoClusterderivable. For example, let Q represent a set of object sets, $Q \in 2^{2^{\mathcal{N}}}$. A poset Q containing 4 clusters, i.e. $\{AB, AC, BC, ABC\}$, is not PoCluster derivable. Set $\{ABC\}$ must have the same diameter of at least one of two element subsets, $\{AB\}$, $\{AC\}$, or $\{BC\}$. Therefore, the two elements subset with the same diameter as ABC cannot be a cluster in a PoCluster since it is not maximal.

Since each PoCluster corresponds to a unique dissimilarity matrix, it is possible to derive dissimilarities or relative dissimilarities between objects in the *PoCluster derivable* set.

In this section, we are particularly interested in *how to determine whether an arbitrary poset is PoCluster derivable and if it is, how the elements in the poset can be used to derive the ranking of dissimilarity entries.*

Definition 6.5.1 *Let* Q *be a set over the sets of objects in* $\mathcal{N}$*, i.e. ,* $Q \in 2^{2^{\mathcal{N}}}$*. We say* Q *is* **PoCluster derivable** *if there exists a PoCluster* P *of some dissimilarity matrix* D*, such that* Q *is the set of clusters in* P *obtained by ignoring the cluster diameters.*

In the following, we examine both necessary and sufficient conditions to identify Q as a PoCluster derivable set.

We define $\langle q_1, q_2, ..., q_m \rangle$ as a *partition* of the elements(clusters) in Q as follows. Each element of Q (i.e. a subset of objects) appears in exactly one group q_i of the partition.

We denote $edges(q_i)$ as all pairs of objects drawn from group q_i. The partition has the properties that each group q_i is a subset of the elements in Q, the union of all the groups is the universal set in Q, $\cup_{i>0}^{m} q_i = Q$, and for any pair of groups $(i,j), i \neq j$, $q_i \cap q_j = \emptyset$.

Theorem 6.5.1 *Q is PoCluster derivable, if and only if there exists an ordered partition of sets in Q, $\langle q_1, q_2, ..., q_m \rangle$, such that $\forall t, 1 < t \leq m$*

$$q_t = cliqueset_e(\bigcup_{0<i\leq t} edges(q_i)) \setminus cliqueset_e(\bigcup_{0<j<t} edges(q_j)). \tag{6.2}$$

Proof 6.5.1 *First, we prove its sufficiency: Assume there exists an ordered partition of the poset $\langle q_1, q_2, ..., q_m \rangle$. We assign dissimilarity d(x,y) between two objects as the following:*

$$\begin{cases} d(x,y) = 1, & \text{if } e(x,y) \in edges(q_1); \\ d(x,y) = t, & \text{if } e(x,y) \in edges(q_t) \setminus \cup_{0<i<t} edges(q_i). \end{cases} \tag{6.3}$$

To prove Q is a PoCluster derivable, we prove that the sets in Q is equivalent to the sets generated by $\psi(D)$.

$$\begin{aligned} P &= \cup_{0<t\leq m} cliqueset_\delta(d \leq t) && (6.4)\\ &= \cup_{0<t\leq m} cliqueset_e(\cup_{0<j\leq t} edges(q_j)) && (6.5)\\ &= cliqueset_e(edges(q_1)) \cup \\ &\quad \cup_{1<t\leq m}(cliqueset_e(\cup_{1<i\leq t} edges(q_i)) \setminus \\ &\quad cliqueset_e(\cup_{1<j\leq(t-1)} edges(q_j))) && (6.6)\\ \Rightarrow S(P) &= \cup_{0<i\leq t} q_i \end{aligned}$$

We next prove it is a necessary condition. If Q is PoCluster derivable, we want to prove that the condition is true. Let D be the dissimilarity, which has the bijection with Q, such that $Q = S(p(D))$. Assume that $\langle d_1, d_2, ..., d_m \rangle$ is the dissimilarity coefficient in D with increasing order. We can group the clusters according to the rank of the dissimilarities. Let $q_1 = cliqueset_\delta(d_1)$. $\forall 1 < t \leq m$, let q_t be the maximal clique with diameter d_t, which does not occur in q_{t-1}, such that $q_t = cliqueset_\delta(d_t) - cliqueset_\delta(d_{t-1}) = cliqueset_e(\cup_{0<i\leq t} edges(q_i)) \setminus cliqueset_e(\cup_{0<j<t} edges(q_t))$.

Groups	Rank1(good)	Rank2(bad)
q_0	A, B, C, D, E	A, B, C, D, E
q_1	AC, BD, CD, BE	AC, BD, CD, BE
q_2	$ABCD, BCE$	$ABCE, BCE$
q_3	$ABCE$	$ABCD$
q_4	$ABCDE$	$ABCDE$

Table 6.2: Two ranking of sets in the PoCluster shown in Figure 6.2(d).

Intuitively, the condition of Q being PoClusterderivable implies the following procedure. Assume $\langle q_1, q_2, ..., q_m \rangle$ is an ordered partition of the elements in Q. We start from a graph G consisting of the objects in $\mathcal{N}$ but with no edges. At each iteration t, we incrementally add the edges in q_t into G and recover the set of cliques in current graph G. Q is PoCluster derivable if and only if the newly created set of cliques in each step t equals q_t, which is the set of all the cliques in current graph ,cliqueset$_e$($\bigcup_{0<i\leq t}$ edges(q_i)), minus the set of cliques already discovered in previous graph, cliqueset$_e$($\bigcup_{0<j<t}$ edges(q_j)).

Now given an ordered partition of the poset $\langle q_1, q_2, ..., q_m \rangle$, we may assign the relative rank of dissimilarity d(x,y) between two objects as the following:

$$\begin{cases} d(x,y) = 1, & \text{if } e(x,y) \in \text{edges}(q_1); \\ d(x,y) = t, & \text{if } e(x,y) \in \text{edges}(q_t) \setminus \cup_{0<i<t} \text{edges}(q_i). \end{cases} \tag{6.7}$$

Example: Table 6.2 shows two possible rankings of sets in poset Figure 6.2(d) . Rank1 satisfies the condition while Rank2 does not. According to Rank2, cliqueset$_e$(edges(q_1)$\cup$ edges(q_2)) \cliqueset$_e$(edges(q_1)) generates cluster $\{BCD\}$, which does not appear in q_2.

Theorem 6.5.1 presents a necessary and sufficient condition to identify an arbitrary collection of sets as a PoCluster. The condition implicitly presents an approach to assign the rank of dissimilarities given a PoCluster as shown in Equation 6.7. Therefore, how to rank the sets in a collection of sets is crucial to assigning the ranking of dissimilarities. The next section addresses this question.

6.5.1 The Implication of PoCluster on Dissimilarities

In this section, we examine how to establish the ranking of pair-wise dissimilarities between objects given a PoCluster whose diameter information is unknown. For example, researchers are interested in those subsets of genes that are more closely related than others, based on the structure of Gene Ontology. We provide an approach to derive an

appropriate dissimilarity assignment between pairs in a PoCluster derivable clusters.

According to Theorem 6.5.1, in order to derive a dissimilarity rank of pairs as in Equation 6.7, it is necessary to partition the set of clusters into ordered subgroups. One of the basic principles for ranking sets is based on their subset relationships. In this section, we further study the PoCluster properties to infer the set ranking.

Let S be a cluster in PoCluster P, and e be a pair in $S \times S$. We say S is the *minimum cluster* containing e if e is not contained in any subset of S. We denote $\overline{S}$ as the sets of pairs for which S is a minimum cluster. The remaining pairs, which are contained in at least one of S's subsets, are denoted as $\underline{S}$. The minimum cluster for a pair is important since its diameter determines the pair's dissimilarity. In addition, a pair might exist in multiple sets, therefore, it is possible that there exists multiple minimum clusters containing this pair. Given e as a pair, we denote the set of minimum clusters containing e as e^*.

Example: According to the PoCluster from Figure 6.2 (d), set $ABCE$ is the minimum cluster containing the pair (A, E). Therefore, $(A, E)^* = \{ABCE\}$, and $(A, B)^* = \{ABCE, ABCD\}$. In addition, $\overline{ABCE} = \{(A, E), (A, B)\}$, and $\underline{ABCE} = \{(A, C), (B, C), (B, E), (C, E)\}$.

Corollary 6.5.1 *Let P be a PoCluster and D be its corresponding, yet unknown, dissimilarity matrix. For any set S in P,*

1. $|\overline{S}| \neq \emptyset$;
2. *Let $e \in \underline{S}$, $diam(S) > D(e)$.*
3. *Let $e \in \overline{S}$, $diam(S) \geq D(e)$.*
4. *Let $e \in \overline{S}$, $diam(S) = D(e)$, if there only exists one minimal cluster containing $e (|e^*| = 1)$ or e is the only edge that S is a minimum cluster ($|\overline{S}| = 1$).*

Corollary 6.5.1 presents three relationships between the distance of pairs in a set S and the set's diameter. First, a set has to be a minimum cluster of a pair, i.e.,$|\overline{S}| \neq \emptyset$, or it conflicts with property 2. Properties 2 and 3 provide order constraints between any element within a set and the diameter of the set; property 4 identifies a way to assign a pair-wise dissimilarity as the diameter of the set. We denote these pairs in a set as *diameter determinant pairs*.

The following two corollaries determine the relative order between the diameters of two clusters based on a shared edge following corollary 6.5.1. These two corollaries are used in Algorithm 7 that follows.

Corollary 6.5.2 *Let P be a PoCluster and D be its corresponding dissimilarity matrix, then for any two clusters S_1 and S_2 in P, if one of S_1's diameter determinant pair e also belongs to $\underline{S_2}$, then $diam(S_1) < diam(S_2)$;*

Corollary 6.5.3 *Let P be a PoCluster and D be its corresponding dissimilarity matrix. Let S be a cluster in P. If any pair e, $e \in \overline{S}$, belongs to a cluster with diameter less than δ, then $diam(S) < \delta$.*

6.5.2 Algorithm of Deriving Dissimilarities

In this section, we present an algorithm to identify whether an input poset is a PoCluster derivable set. It also derives a relative ranking of pair-wise dissimilarities simultaneously.

The algorithm proceeds in a top-down fashion and the diameter is reduced in each step. In each step, the algorithm first identifies the maximum set of independent object sets. By independent, we mean that the sets are not subsets of another. It then removes those clusters from current maximum independent sets that have lower diameters. The remaining sets are then assigned the current diameter and are removed from the current pool of sets. The process repeats until all sets are assigned diameters, or the collection of sets is invalidated as PoCluster.

Function getMaxTopSets first extracts the maximum independent sets within the current poset P^t, denoted by $\top$. This step follows the basic property of PoCluster, which states that a superset of a set has a larger diameter.

Next, function removeLowerRankSet removes any sets that have lesser diameter than one of the sets in current $\top$. One criterion is based on Corollary 6.5.2. If one determinant pair of a set S_1 appears as lower ranked pair in another set S_2 of current $\top$, then S_1 is removed. The second criterion is based on Corollary 6.5.3. If for any top ranked pair e in a set S_1, $e \in \overline{S_1}$, there exists a set S_2 in $\top$, such that e is lower ranked $e \in \underline{S_2}$, then set S_1 from the top will be moved to the lower ranked sets.

Finally, we check whether the rank of the set violates Theorem 6.5.1, in the function checkCliques. If this is violated, the solution is to find a superset containing these additional sets and put it into the bottom. If no such superset exists, then the poset is

not a PoCluster. However, this step requires the process to find all clique sets, which has NP-complete complexity. Therefore, in practice, this step is usually approximated. Of course, degenerate cases might arise due to the approximation and the recovered dissimilarity might not be exactly faithful to the poset.

If all checks are passed, then we assign those pairs contained solely in the top part $\top$ dissimilarities equal to the current diameter δ. Failure of any of the above steps invalidates the poset as a PoCluster. The procedure continues by reducing the diameter and removing the top from the remaining poset. It stops when the current pool is either empty or unchanged between successive iterations. If the pool remains unchanged, the poset is not PoCluster derivable set.

Algorithm 7 RankPoset: Deriving dissimilarity from poset
Input: P: A poset
Output: D: Dissimilarity matrix derived from P

$t \leftarrow 1$; $P^t \leftarrow P$; $P_0 \leftarrow \emptyset$
$\text{diam}^t \leftarrow \frac{1}{2}|N| * (|N| - 1)$;
while $(P^t \neq P^{t-1})\&(P^t \neq \emptyset)$ **do**
  $\top = \text{getMaxTopSet}(P^t)$;
  $\top = \text{removeLowerRankSet}(P^t, \top)$;
  $\top = \text{cliqueCheck}(P^t, \top)$;
  $D(e) \leftarrow \text{diam}, \forall e$, where $e \in P^t \setminus \top$
  $t \leftarrow t + 1$;$P^t \leftarrow P^{t-1} - \top$; $\text{diam}^t \leftarrow \text{diam}^{t-1}$;
end while
return D.

Example 6.5.1 *The following steps can be taken in order to derive the dissimilarity matrix of PoCluster in Figure 6.2 (d).*

1. Starting from the maximal set $ABCDE$ when $t = 1$, the diameter can be set to 10, since all the sets are its children. $g'_1 = ABCDE$ will be removed from the poset, and the program will continue to the next iteration $t = 2$.

2. Next, the maximal independent sets include $ABCD$ and $ABCE$. And $E_{low} = \{BC, BD, BE, AC, CD, CE\}$. Since no maximal pairs appear in E_{low}, therefore, no set is removed. So both $ABCD$ and $ABCE$ are inserted in $\top_1$. Then, we compute the $\text{cliqueset}_e(E_{low})$ and check whether it results in any additional sets. The completeness check finds the additional set BCD in the $\text{cliqueset}_e E_{low}$, therefore, a superset of BCD will have to be removed from $\top_2$, which would be $ABCD$, (i.e., $g'_2 = ABCE$).

3. Among the rest of poset, the maximal independent sets includes $ABCD$ and BCE. None of them has determinant pairs. The current $E_{low} = \{BC, CD, AC, BE\}$. And cliqueset$_e(E_{low})$ contains all the sets in the $ABCD$ and BCE's children, so completeness check is passed. Therefore, $ABCD$ and BCE both can be placed in g'_3.

4. The rest of sets are maximal and serve as determinant pairs for themselves. Therefore, they are assigned to g'_4.

5. The order of groups are reversed and rearranged in the increasing order of the diameter. The final result appears in Table 6.2.

6.6 PoClustering Algorithm

Given a dissimilarity matrix D, the corresponding PoCluster P (i.e., $P = \{\text{cliqueset}_\delta(d)|\forall d \in W(D)\}$) can be found by repeating a simple procedure. In the naive algorithm, one needs only to find all cliques in a subgraph of $G(D)$ that includes only those edges corresponding to the pair-wise dissimilarities less than or equal to a threshold d as the threshold varies from the smallest to the largest dissimilarity in D.

An incremental and exact PoClustering algorithm was proposed by (J. Liu and Prins, 2006). The algorithm only computes clique clusters that are affected by the introduction of new edges. The algorithm maintains a pool of all clusters in the previous graph. Given the next graph with more edges, the pool of cliques can be updated as follows: First, all the cliques in the pool that share a vertex with the new edges are found. Second, if a clique in the pool can be extended by adding one or more of the new edges, the extended clique is added to the pool, and the cliques that are subgraphs of the new clique are removed. The parent-child relationships can be established between new cliques and removed cliques.

Though more efficient, the exact algorithm still bears the NP-Complete complexity of the PoClustering problem because of the search of clique clusters. In addition, the number of clique clusters in a undirected graph with n nodes is $o(3^{1/3*n})$. Most real classifications are *polynomial* posets, which means the number of clusters in the poset is polynomial with respect to the number of objects. In this section, we present a heuristic algorithm for the construction of approximate PoClusters. This approach addresses both the NP-completeness of finding all cliques and the huge number of clique clusters generated.

Instead of searching for all clique clusters in a graph, we approximate them with a minimum set of cliques that covers all the edges in the graph, i.e, a minimum edge clique cover(ECC). The minimum number of clique clusters covering all edges are a subset of all clique clusters.

Definition 6.6.1 *Given a graph* $G =< V, E >$*, an* **edge clique cover***(ECC)* R *of* G *is defined as a set of maximal cliques induced by* G*, such that for any* $e \in E$*, there exists a maximal clique* $c \in R$*, where* e *is an edge in* c*.*

Graph G^t in Figure 6.5 contains a figure with 6 nodes. There are five maximal cliques in the graph, i.e., {1234, 1256, 2467, 1246, 2567}. However, all edges can be covered with a minimum of 4 maximal cliques. One option of minimum edge clique covers is {1234, 1256, 2467,2567} since the edges of the omitted clique 1246 are covered by the four cliques.

Algorithm 8 $R_{new} = \text{gen\_ECC}(G, R, e)$
Input: G: graph; R: an edge clique cover does not cover e, $e = \{x, y\}$: a new edge
Output: R_{new}: a new clique cover covering $E(G) \cup \{e\}$

1: $c_{x,y} \leftarrow \max\{c_1 \cap c_2 | c_1 \in \pi(x), c_2 \in \pi(y)\}$.
2: $c_{new} \leftarrow \{c \cup \{x, y\}\}$
3: $k \leftarrow \text{argmin}_k\{(c_1, c_2, ..., c_k)\ covers\ E(G) \cup \{e\}\}$
4: return $R_{new} \leftarrow c_1, c_2, ..., c_k$

Next, we describe an incremental greedy algorithm to approximate the minimum edge clique cover in order to construct the poset. The algorithm, given in Algorithm 8, is similar to the original algorithm proposed in (J. Liu and Prins, 2006) in detecting the new cliques. The difference is that at each step, it only keeps a minimum number of cliques that covers all the edges. Given an input clique cover from time t and an inserted edge $\{x, y\}$. The algorithm first goes through each clique in the clique cover that is connected with one of the edges, let's say, x, and let $\pi(x)$ be all the maximal cliques containing x. The algorithm then looks for the maximum sets of points in $\pi(x)$ that are also connected to y. The subgraph, though complete, might not be maximal. The algorithm then extends it into a maximal clique by calling the function maxclique. In the end, the algorithm goes through the current list of cliques sequentially, and removes redundant cliques whose edges have already been covered.

The total number of clique covers in the graph is bounded by the number of edges since, at most, only one clique will be added into the cover, at each step an edge is inserted into the graph. In practice, the number is considerably smaller than that.

The number of outer loop iterations of the algorithm are determined by the number of edges, which is $O(n^2)$. For a new clique, the greedy algorithm goes through the cliques in the existing clique cover, and find the maximal clique cover. Assume the number of cliques in the cover is k, creating a maximal clique takes $O(kn)$. Checking the coverage of edges by the cliques also takes $o(kn^2)$ time.

6.7 Experiments

We have experimented with both synthetic and real datasets comparing hierarchical clustering(Hierarchy), pyramidal clustering(Pyramid), and edge clique cover(ECC). We do not present the results of the exact algorithm because of its prohibitively long running time.

6.7.1 Evaluation Criteria

The *match* score is used to measure the approximation of the recovered poset to the original poset. We take each poset as a set of sets. Given two PoClusters P_1 and P_2, the match score of P_2 to P_1 is computed as:

$$match(P_1, P_2) = mean_{s_1 \in P_1}(max_{s_2 \in P_2}(\frac{|s_1 \cap s_2|}{|s_1 \cup s_2|})) \tag{6.8}$$

For each set in P_1, only the best match in P_2 is taken account of by Jaccard coefficient. The overall match score is determined by the mean match score of the whole sets.

6.7.2 Synthetic Data

We created a synthetic poset generator that is controlled by three parameters. They are the number of objects of the universal set N, the total number of clusters (sets), and the overlap probability between clusters. The overlap probability follows a normal distribution with a user-specified mean value and a default standard deviation of $\sqrt{(0.2)}$. It defines the likelihood that an element in a parent cluster appears in more than one child cluster. The synthetic generator of the poset then works as follows: starting from the root node of the poset with n objects, the program recursively generates the child sets that respect the overlap probability distribution. For each parent set, whether an object should appear in multiple child sets is determined by coin-flipping with overlap

probability $p_{overlap}$. After the poset is generated, we computed the rank and assigned the pair-wise distances based on the algorithm presented in Section 6.5.2. We then take the distance matrix as the input to the three clustering algorithms.

We first examined how the overlap probability affects the performance. In this setting, the total number of objects in N is set to 500, and the maximum number of clusters in P is 200. Figure 6.6(A) shows that overlap probability affects match score of all three algorithms. Starting from 0 overlap, all of the three algorithms have almost 100% match score. However, ECC does a much better job than the other two. The reason is that the number of overlapping clusters increases as the overlap probability increases. The match score drops significantly for hierarchical and pyramidal clustering because of their inability to allow arbitrary overlaps between clusters. Figure 6.6(B) and (C) show the total number of clusters generated and the running time comparison. Both hierarchical clustering and pyramidal clustering have shorter running time than ECC. It is due to the fact that both algorithms fail to recover most clusters in the original poset. This can be observed from Figure 6.6(B) where, among the three algorithms, ECC is the only one that is able to recover most clusters in the original poset (its number of clusters is shown as the top curve in Figure 6.6(B)) .

Our second experiment demonstrated how the number of objects affects the performance. The overlap probability is set to 0.2 and maximum number of clusters is 120. The results are shown in Figure 6.6 (D), (E), and (F). The match score is close to 1 for ECC but drops below 0.5 for the other two algorithms. Again, the difference in the running time (Figure 6.6 (F)) between ECC and others is because both hierarchical clustering and pyramidal clustering recover only a small fraction of the sets(clusters) in the original poset (the top curve shown in Figure 6.6 (E)).

In the last experiment, we fixed the number of objects to 500 and the overlap probability to 0.2, and varied the number of clusters in the poset. The result are shown in Figure 6.6 (G) and (H). A side effect of increasing the number of clusters defined on a fixed set of objects is an increase in the degree of overlap. Therefore, the match scores of hierarchical clustering and pyramidal clustering fall as the number of clusters increases, whereas ECC maintains a high match score. As shown in Figure 6.6 (H), ECC is able to recover almost all clusters in the original poset. However, pyramidal clustering and hierarchical clustering generate considerably fewer clusters.

6.7.3 Gene Ontology

Our next experiment compares the quality of the three clustering algorithms given a real ontology categorization. We also compare our method for deriving dissimilarities with the previous approaches reviewed in Section 6.2.

We used 2884 genes, which are the most active and co-regulated in the yeast cell cycle data selected by Tavazoie *et al.* (1999)(Tavazoie et al., 1999). This set of genes has been frequently studied. Therefore, we expect most of them to have comprehensive annotations and classifications. We consider three GO files: biological process (BP), cellular component (CC), and molecular function (MF), from the Gene Ontology databases. We extracted all GO categories that contain at least two genes from the identified set and removed duplicate categories. The remaining GO categories are used to generate dissimilarity matrices as the input to the clustering algorithms. Table 6.3 presents size and overlap statistics of our data. The statistics of the three GO files are shown in Table 6.3.

GO files	# Known genes	# Terms	Max level	Mean Overlap
BP	1313	2631	18	37%
CC	1316	1142	14	22%
MF	1309	624	17	31%

Table 6.3: Statistics for the three GO files. MF: Molecular Function, CC: Cellular Component; BP: Biological Process

The result of applying the three algorithms is consistent with that of the synthetic data. ECC performs the best in recovering Gene Ontologies. In this case, two additional measurements are used to evaluate the relationships between a reconstructed poset(P) and GO files(go). Besides the match score, we also look at recovery rate and accuracy. The recovery rate is the percentage of GO categories recovered; the accuracy is the percentage of the discovered clusters that actually appear in GO categories. The two measurements provide more information about those clusters. As shown in Table 6.5, more than 50% and even closer to 79%(MF) of the categories cannot be properly discovered by hierarchical and pyramidal clustering. Meanwhile, according to the third column in the same table, over 96% of the discovered clusters by ECC are actual matches to the GO categories. In comparison, the spuriousness clusters in

pyramidal clustering and hierarchical clustering exceeds 50%, which is unacceptable for real applications.

Similarity	BP	CC	MF
RankPoset	0.8473	0.8976	0.8031
Resnik	0.7917	0.8601	0.7761
LC	0.5466	0.7268	0.6724

Table 6.4: Reconstructed poset match score to original GO based on various similarity measures

	match score			recovery rate			accuracy		
Algo	BP	CC	MF	BP	CC	MF	BP	CC	MF
ECC	0.8299	0.8976	0.8831	0.7813	0.8953	0.8273	0.9352	0.9534	0.9932
Pyra.	0.5367	0.4923	0.6735	0.3931	0.4704	0.4651	0.4504	0.6345	0.6023
Hier.	0.4577	0.4260	0.5262	0.2779	0.4392	0.4175	0.3733	0.5702	0.4645

Table 6.5: Reconstructed poset match score to original GO by the three algorithms. *go* represents the GO file and P is the reconstructed poset

We also compared the three different (dis)similarity measures including the RankPoset, which we developed in Section 6.5.2, Resnik, and Leacock and Chodorow (LC) (Budanitsky, 2001). We computed three dissimilarity matrices, one by each method. We then applied ECC algorithm to each of them. The matching score is shown in Table 6.4. Our RankPoset generates a slightly better result than Resnik, while both are substantially better than LC.

6.8 Conclusions

PoClustering can be used for automatic construction ontologies based on the pairwise relationships between objects. PoClustering represents a one-to-one correspondence between all possible dissimilarity matrices and a subset of posets, which we call the PoClusters. The clustering approach preserves all of the information in a dissimilarity matrix, and we have shown algorithms in both directions — constructing a PoCluster from dissimilarities, and assigning meaningful dissimilarity values to any given PoCluster .

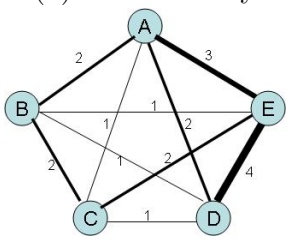
PoClusters are a generalization of both hierarchical clustering and pyramid clustering. PoClusters provide both homogeneity within a cluster, as measured by the cluster's diameter as well as separation between clusters. They are also able to handle overlaps in a meaningful way.

The formal definition of PoClusters is primarily of theoretical interest, since the problem of computing them exactly is likely to be intractable for large problems. To address this shortcoming we have introduced a polynomially bounded approximation algorithm to automatically generate classification hierarchies. Classification hierarchies are useful for automatically generating categorizations, taxonomies, and ontologies in a wide range of applications.

Alternatively, our mapping from PoCluster to dissimilarity provides a meaningful pairwise dissimilarity measure between objects in taxonomies. At the very least, the resulting dissimilarity matrix, when coupled with our new clustering algorithm, is capable of exactly reconstructing a hierarchical set of clusters identical to the original categories, both in terms of the subsets generated and their parentage.

	A	B	C	D	E
A	0	2	1	2	3
B		0	2	1	1
C			0	1	2
D				0	4
E					0

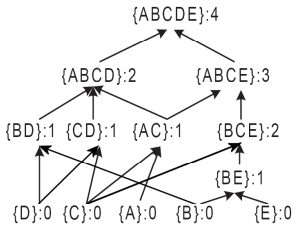
(a) Dissimilarity



(b) Weighted graph

d	$\text{cliqueset}_\delta(d)$
d=0	A, B, C, D, E
d=1	AC, BD, CD, BE
d=2	$ABCD, BCE$
d=3	$ABCE$
d=4	$ABCDE$

(c) Clique Clusters



(d) PoCluster.

Figure 6.2: A running example. (a) shows a dissimilarity matrix of 5 objects {A, B, C, D, E}; (b) shows an undirected weighted graph implied by (c); Table (c) contains the list of clique clusters with all diameters; (d) shows a PoCluster which contains 13 clusters and their subset relationships (Each cluster in the PoCluster represents a clique cluster with its diameter in (c). The PoCluster is organized in DAG with subset relationship between the nodes. There is a directed path from node S_1 to S_2 if $S_1 \subset S_2$). Note: Applying PoClustering algorithm can construct PoCluster shown in (d) given dissimilarity matrix (a). Applying Algorithm in Section 6.5.2 can derive the dissimilarities in (a) from PoCluster in (d).

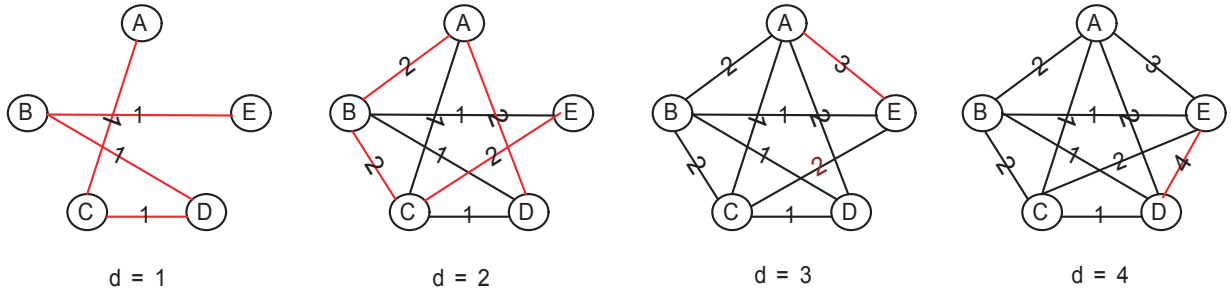


Figure 6.3: Four directed weighted graphs corresponding to the dissimilarity matrix in Figure 6.2 (B) with maximum edge weight $\{d = 1, 2, 3, 4\}$.

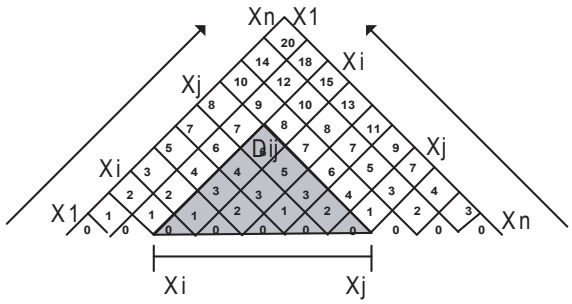


Figure 6.4: A structure of Robinson matrix. There exists a linear ordering of the objects, such that the dissimilarity never decreases as they move away from diagonal along both row and column.

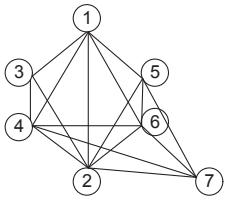


Figure 6.5: An example graph with nodes {1,2,3,4,5,6,7}. All the cliques in the graph are {1234, 1256, 2467, 1246, 2567}; The Minimum ECC is {1234, 1256, 2467, 2567}.

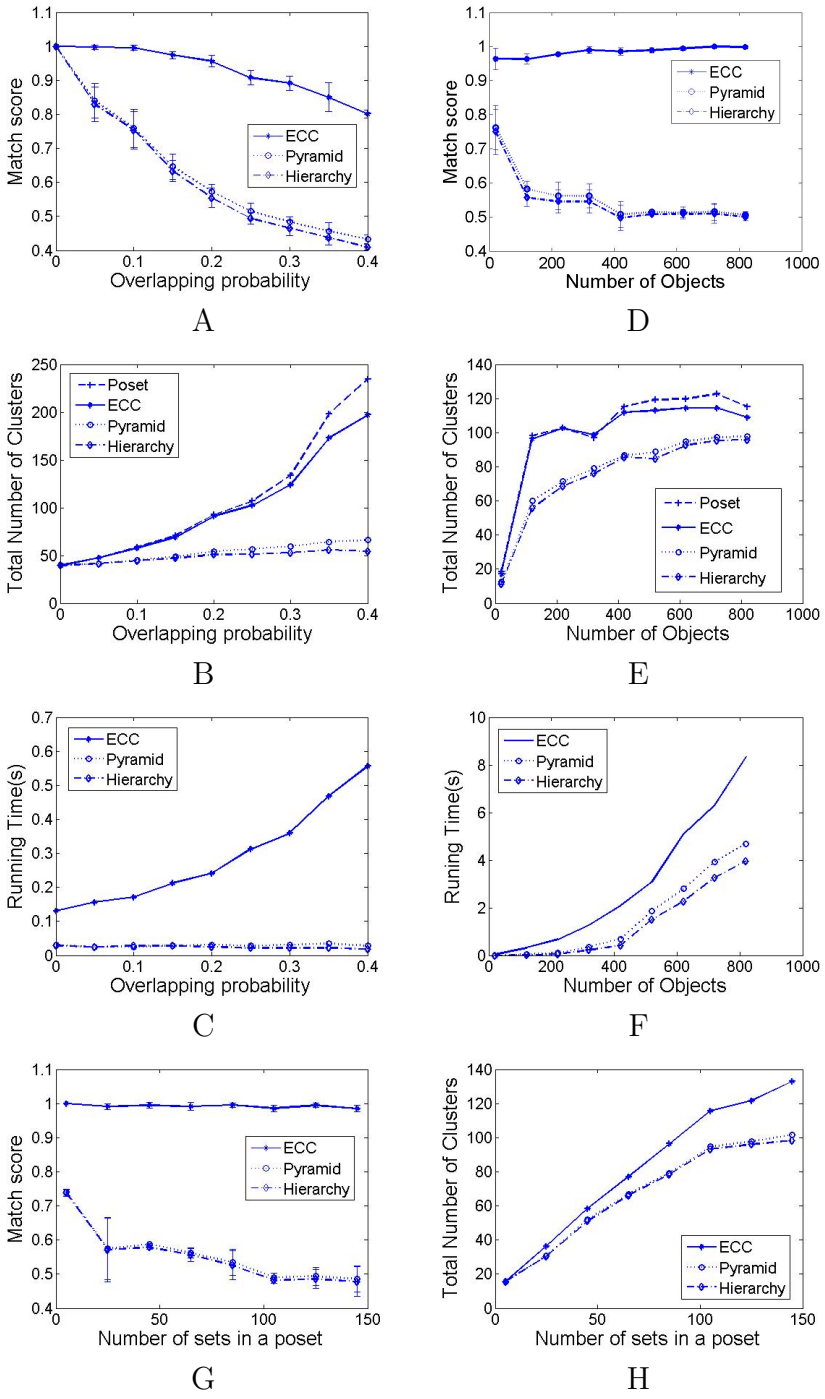


Figure 6.6: Experimentation on synthetic data

Chapter 7

Visualization Framework to Summarize and Explore Clusters

Subspace clustering has proven itself as a useful data-mining tool for finding significant relationships within high-dimensional data. However, exploring the potentially exponential number of identified subspace clusters is unwieldy and presents it own data mining challenges. Inspecting subspace clusters for meaningful relationships is like searching for a needle in a haystack.

In this chapter, we build a visualization framework to aid the analysis of the entire set of subspace clusters mined from a given dataset. We develop measures to establish pairwise dissimilarities between subspace clusters. These measures incorporate notions of coverage between the subspace clusters, as well as how similar the exhibited patterns of the pair are. Dissimilarity measures are requisite for our visualization and clustering analysis (i.e. clusters of subspace clusters). We present our experience with the visualization framework on two real datasets.

7.1 Introduction

Subspace clustering (Agrawal et al., 1998; Yang et al., 2002; Ben-Dor et al., 2002) is an effective method for finding meaningful homogeneous groups within lower-dimensional subspaces of high-dimensional data. It has been widely used in bioinformatics applications, such as gene expression analysis (Ben-Dor et al., 2002; Cheng and Church, 2000). However, the usefulness of subspace clustering algorithms are often overshadowed by the multitudes of results they generate. The lack of efficient interpretation tools often keeps domain experts from making sense of the results. The motivation for our work is to organize and summarize the results of subspace clustering. We achieve this by constructing an analogy of a subspace cluster as a point in an abstract data space, where various relationships between points (subspace

clusters) are analogous to proximity. We then employ a visualization interface to explore relationships between and filter subspace clusters.

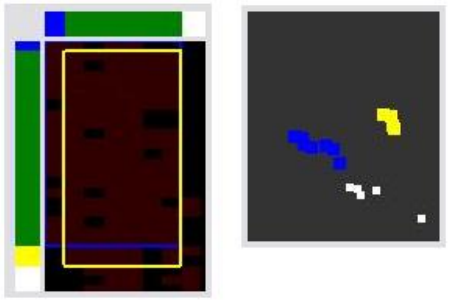


Figure 7.1: Left: A visualization of the overlap between the yellow and blue sets of subspace clusters as shown in the image on the right. The intersection of the two sets of subspace clusters is shown in green. There are over 10 subspace clusters in each set. Right: The 3D point-cloud view of subspace clusters.

A subspace cluster can be thought as a combination of a binary selection pattern with an analog pattern imposed on it. In the binary matrix, a submatrix of 1s indicates the presence of the item-feature pair within the submatrix. Correlations between the signals superimposed on this submatrix validate it as a subspace cluster. Random noise can exclude an item or feature out of the subspace cluster, which is equivalent of turning the corresponding entry into 0.

Subspace clustering algorithms often generate thousands, or even tens of thousands of clusters. However, many of the discovered relationships within a subspace cluster are either trivial or highly redundant relative to others. Researchers tend to address the problems of excessive and mundane subspace clusters by varying thresholds, which indeed reduce the number of outputs and increase pattern variations, but at a cost of masking potentially significant results.

Subspace clusters are frequently highly *overlapped*, due to the overlapping nature of subspaces and the well known A-priori property. We show an example of this in Figure 7.1. Figure 7.1 shows 2 sets of clusters, colored blue and yellow, which are highly overlapped. The colorbars to the left and top of the left panel indicate which rows and columns, respectively, belong to which subspace cluster. Their intersection is shown in green (mixing blue and yellow makes green). The dominance of the green in the colorbar indicates a high level of overlap, and is one aspect of our visualization tool. If a set of items does not form a subspace cluster in subspace S, then this set of items, and any subset of them, won't form a cluster in any superspace of S.

Moreover, the generated subspace clusters are often fragments of logarithmic size with respect to original subspace clusters according to our previous study in (Jinze Liu and Prins,

2006).

These characteristics present tremendous challenges for applying subspace clustering methods and understanding their results. We propose an abstract mapping of subspace clustering results to a geometric analogy, and employ visualization methods to address these challenges. Our approach requires meaningful pairwise metrics to compare relationships between subspace clusters, scalable visualization techniques, and tools for exploring the results. We make the following contributions:

- We define and justify a set of useful pair-wise relationships between subspace clusters. These relationships include notions of coverage similarity and pattern similarity.
- We develop a geometric analogy where the subspace clusters generated from any given algorithm are treated as point and the relationships between them are treated as distances. This allows us to find patterns, and in fact, *cluster* subspace clusters into similar groups.
- We build a visualization framework to support our geometric analogy. This allows us to visualize and interact with the points, and their clusters. Our visualization tool makes the abstract notations of our model concrete. Our visualization is further enabled by a scalable algorithm that we have developed, fastMDS, for supporting the interactive display of large subspace-cluster datasets.

7.2 Related Work

Visualizing the results of clustering algorithms can provide many insights about the data, as well as the clustering algorithm itself. For instance, a visualization may help in verifying the accuracy of a clustering algorithm, as well as give a user some intuition for what parameters to use and further experiments to try. Thus, there are many different ways to visualize a clustering solution.

7.2.1 Cluster and Subspace Cluster Visualization

Cluster visualization methods have been studied for years to assist the interpretation of clustering results. However, previous cluster visualizations have often been limited to full dimensional clustering, such as hierarchical clustering(Seo and Shneiderman, 2002) and K-means clustering(Spence, 2001). In full dimension clustering, the difference among the clusters are only in the object sets. To visualize them, people often project them onto a low dimensional space and color them according to class labels. As for hierarchical clustering, the tree structured dendrogram is often used as the visualization tool.

While there has been much work on visualizing traditional full space clusters, there has been relatively little work done on visualizing subspace clusters. The visualization of subspace clusters has been complicated by their overlapping nature. As a result it is difficult to visualize the objects using just cluster labels in low dimensional space without ambiguity. Therefore, in current literature on subspace clustering, people often plot the pattern or the sets of objects in each subspace cluster separately. For example, each gene expression cluster generated by Cheng *et.al.*(Cheng and Church, 2000) is shown as a line graph, where the line plots a gene's expression value under the set of conditions in the subspace cluster. In addition, a cluster of data objects can also be projected onto pairs of features and plotted as points in 2D. If points are separated by certain features, peaks are exhibited in density plots of the data in those dimensions(Parsons et al., 2004).

7.2.2 Postprocessing of Subspace Clusters

The postprocessing of large amounts of clusters has been used recently in identifying representatives of frequent itemsets. The work by Afrati *et.al.*(Afra-ti et al., 2004) finds the top-k itemset that can cover the whole border of the frequent itemset. Yan *et.al.*(Yan et al., 2005) improves it by taking the statistical support of each itemset into account.

The compression of subspace clusters is a more general problem than that of frequent itemset in the following aspects: first, subspace clusters have pattern associated with them. Finding representative sets that are both faithful and noise tolerant with respect to the original pattern is a challenging problem. While frequent itemsets only take into account the set of items, a subspace cluster considers either sets of rows or columns, or both, depending on the application.

7.3 Model

We consider the set of subspace clusters that is output from subspace clustering algorithms. First, we give a general definition of subspace clusters. We then define two measures of dissimilarities between a pair of subspace clusters based on their coverage and pattern consistency. Neither of the dissimilarity measures alone can perfectly represent the relationships between two subspace clusters. Therefore, we also propose a linear combination of two measures of dissimilarity.

7.3.1 Subspace Cluster

A subspace cluster is a subset of objects, which exhibits consistent patterns along a subset of conditions. Assume M is an n by m matrix which contains a set of objects(rows) $I_0 =$

$\{i_1, i_2, ..., i_n\}$ and a set of attributes(columns) $J_0 = \{j_1, j_2, ..., j_m\}$. Each entry value $M_{i,j}$ represent the value of the object i under attribute j.

A subspace cluster P in M is depicted by a tuple $\langle I, J, P\rangle$. I is a subset of objects, $I \in I_0$ and J is a subset of attributes $J \in J_0$(so-called subspace). P is the consistency measure of the set of objects in I in subspace J.

In this paper, we focus on *maximal subspace clusters*. By maximal, we mean that adding any additional row or column from the rest of matrix will violate the consistency measure of the cluster. Since non-maximal subspace clusters are easy to filter out, in the rest of discussion, we only consider the maximal subspace clusters.

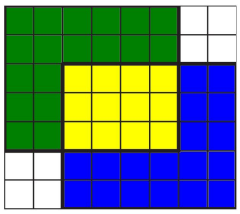


Figure 7.2: The relationships between two overlapping clusters. The green and blue rectangles represent two separate subspace clusters. The yellow region is the intersection of two. The whole region including green, blue, yellow and white is the merged (or unioned) cluster of the two clusters.

7.3.2 Coverage Dissimilarity

One relevant way to measure dissimilarities between subspace clusters is to measure the diversity of set of objects and the set of attributes they contain. One well known measure that serves this purpose is the Jaccard distance.

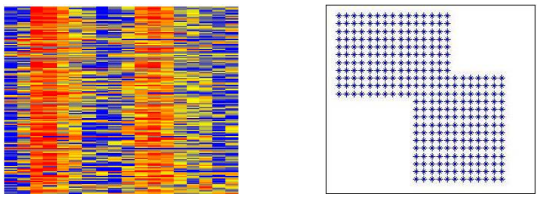
Definition 7.3.1 *Given two subspace clusters $C_1 = \langle I_1, J_1\rangle$ and $C_2 = \langle I_2, J_2\rangle$, the coverage dissimilarity between C_1 and C_2 is defined as*

$$cDis(C_1, C_2) = 1 - \frac{|I_1 \cap I_2| \times |J_1 \cap J_2|}{|I_1 \cup I_2| \times |J_1 \cup J_2|} \tag{7.1}$$

Figure 7.2 shows how two clusters can overlap. The green area is the coverage of cluster 1 ($I_1 \times J_1$) and the blue area is the coverage of cluster 2 ($I_2 \times J_2$). The intersection of cluster 1 and cluster 2 is shown in the the yellow area $(I_1 \cap I_2) \times (J_1 \cap J_2)$. And $(I_1 \cup I_2) \times (J_1 \cup J_2)$ is the merged area.The coverage dissimilarity is computed as the percentage of uncommon area in the merged area versus the merged area.

7.3.3 Pattern Dissimilarity

Coherent patterns are important criteria for subspace clusters. The consistency measure of subspace clusters varies according to different applications. The following two subsections introduce two types of patterns studied recently(Wang et al., 2002; Agrawal et al., 1998; **?**). Though we propose two different pattern dissimilarities between two clusters according to their consistency measures, they both capture similar notions which is the degree of pattern degradation if two clusters are merged.



(A) A $\delta-$pCluster (B) An itemset cluster

Figure 7.3: Example of two subspace clusters. (A) is the heatmap of a $\delta-$pCluster; (B) is an itemset cluster, where each * represents a 1 entry.

δ-pCluster

δ-pCluster(Wang et al., 2002) is a subspace clustering algorithm which captures the set of objects that vary consistently together. This type of pattern is useful for discovering gene co-regulation networks from gene expression data. The consistency measure of the subspace cluster is often related to whether a group of objects consistently go up and go down.

Definition 7.3.2 *Let $C = \langle I, J, P_\delta \rangle$ be a δ-pCluster. The consistency measure P_δ is defined as*

$$|(d_{xa} - d_{xb}) - (d_{ya} - d_{yb})| \leq \delta \tag{7.2}$$

$\forall x, y \in I$, $\forall a, b \in J$, $\forall \delta \geq 0$

Equation 7.2 computes the so called p-score for any 2 x 2 submatrix in the cluster. The p-score is the consistency measure of $\delta-$pCluster. Intuitively, the lower the p-score, the lower the difference between the variation of rows under two conditions, and the higher the consistency between two rows within the two columns.

Intuitively, the distance measure presented in Equation 7.2 represents the average consistency measure between the means of the two subspace clusters. $dis_\delta(C_1, C_2) = 0$, if $C_1 = C_2$ or if they have exactly the same mean vector within their submatrices. In addition, dis_δ is

symmetric, since $dis_\delta(C_1, C_2)$=$dis_\delta(C_2, C_1)$.

$$\begin{aligned} & dis_\delta(C_1, C_2) \\ = & \frac{1}{\frac{1}{2}|\check{J}||\check{J}-1|} \sum_{j_1, j_2 \in \check{J}}^{j_1<j_2} |(d_{I_1 j_1} - d_{I_2 j_1}) - (d_{I_1 j_2} - d_{I_2 j_2})| \end{aligned} \tag{7.3}$$

where $\check{J}$ is union of J_1 and J_2, and

$$d_{Ij} = \frac{1}{|I|} \sum_{i \in I} d_{ij} \tag{7.4}$$

Itemset Cluster

Frequent itemset mining can be considered a special branch of subspace clustering methods. It looks for an itemset that is contained in a sufficient number of objects. In binary representation, a "1" entry corresponds to the presence of an item in the objects and a "0" corresponds to the absence. A frequent itemset corresponds to a submatrix of all 1s, as shown in Figure 7.3(B).

Definition 7.3.3 *(Itemset Cluster) The submatrix $I \times J$ is a itemset cluster if $\forall\ i \in I$, $\forall\ j \in J$, $M_{i,j} = 1$ and $\frac{|I|}{|I_0| \leq \delta}$, where δ is the minimum support threshold, $0 \leq \delta \leq 1$.*

The pattern degradation due to merging two subspace clusters can be often measured by the difference of the fraction of 1s in each of the union columns.

$$\begin{aligned} & dis_{item}(C_1, C_2) \\ = & \frac{1}{|\check{J}|} \sum_{j \in \check{J}} |d_{Ij_1} - d_{Ij_2}| \end{aligned} \tag{7.5}$$

where d_{iJ} is defined the same as Equation 7.4

It so happens that the mean of the itemset cluster is the same as the probability of seeing a 1 entry in that column. The mean of the itemset clusters can be taken as a distribution vector, and either the KL divergence or Jensen-Shannon divergence (Yan et al., 2005) can be used to measure the pattern dissimilarity between the two clusters. This method is the same as the approach taken by Yan *et.al.*(Yan et al., 2005).

7.3.4 Blending of Dissimilarities

Neither coverage dissimilarity nor pattern dissimilarity alone are perfect. They capture different aspects of dissimilarity between subspace clusters. Sometimes mixtures of the two may

reveal better separation of the clusters than either can alone. We allow different combinations of dissimilarity measures to be used by assigning different weights to the coverage and pattern dissimilarities.

7.3.5 View of A Set of Subspace Clusters

Given a set of closely related subspace clusters, we define two types of simplifications to describe them. One is a summary of the data, which contains the union of the rows and columns of all subspace clusters in the set. In addition, we find a representative subspace cluster, defined as the medioid of the set of clusters. The medioid has the property of minimizing the sum of the dissimilarity from it to any of the subspace clusters in the set of subspace clusters.

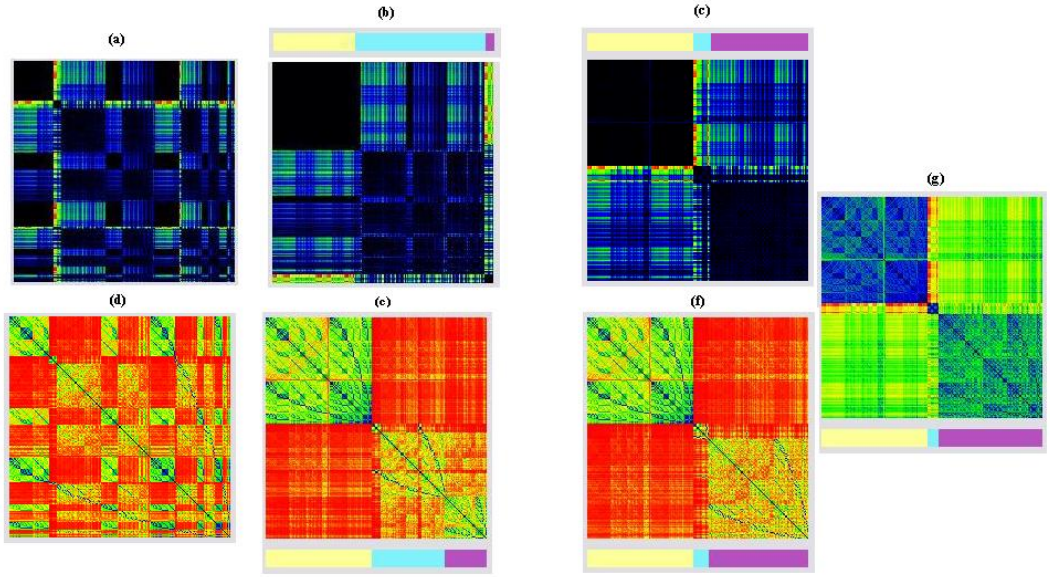


Figure 7.4: The top row of matrices (a),(b),(c) represent pattern dissimilarity. The bottom row (d),(e),(f) represents coverage dissimilarity. (a) The original pattern dissimilarity matrix; (b) Permuted pattern dissimilarity matrix, based on the clustering of subspace clusters by pattern dissimilarity alone; (c) Permuted pattern dissimilarity matrix based on the clustering by a 50/50 blend of both pattern and coverage dissimilarity; (d) The original coverage dissimilarity matrix; (e) Permuted coverage dissimilarity matrix, based on clustering subspace clusters on just coverage dissimilarity; (f) Permuted coverage dissimilarity matrix based on a 50/50 blend of both pattern and coverage dissimilarity; (g) Blended Matrix of both pattern dissimilarity and coverage dissimilarity, permuted to show clustering

7.4 Methods

Although the visualization of dissimilarity matrices, provides useful insights, it is not natural enough for human to identify possible relationships, such as clusters within the sets of SSC. In addition, it is not sufficient for the visualization of the evolution of clusters in response to changes in parameters. Therefore, we employ classical multidimensional scaling(MDS) to derive a 3D point-cloud view of the clusters that treats the dissimilarity matrices as the Euclidean distance between points. This visualization provides a spatial representation of the clusters in a low dimensional setting suitable for direct viewing. Under this view, it is possible to see potential clusters of SSCs as well as track the evolution of existing clusters under reweighing. However, the difficulty with MDS is that it does not scale well to large datasets, usually less than 1000 data points. However, typical subspace clustering generates more than 10,000 subspace clusters, which makes visualization far from interactive.Our high-speed MDS approximation is based on partitioning the dissimilarity matrix into submatrices along the diagonal.

7.4.1 MDS and fastMDS

Multidimensional scaling (MDS) is a well-known statistical method for mapping pairwise relationships to coordinates. The coordinates that MDS generates are an optimal linear fit to the given dissimilarities between points, in a least squares sense, assuming the distance used is metric. An MDS solution is unique down to a rigid-body transformation, with a possible reflection. MDS takes as input a matrix containing pairwise dissimilarities between all n data objects.

The objective of MDS is to find coordinates for each point that preserve the given pairwise dissimilarities as faithfully as possible. There are two stages in computing classical MDS. The first is to convert the input matrix D into a matrix of dot products, or a Gram matrix B. This is done by multiplying D^2 on both sides with a "centering matrix" H, which subtracts out the row and column average of each entry and adds back the overall matrix average.

$$B = \frac{-HD^2H}{2} \tag{7.6}$$

Where $h_{ij} = d_{ij} - d_{iI}, d_{iJ}, d_{IJ}$.

Since B is symmetric, it can be eigen decomposed into USU^T , where U is a matrix of eigenvectors and S is a diagonal matrix containing the corresponding eigenvalues. MDS derives its lower-dimensional coordinates by taking successive rows from Q

$$Q = \sqrt{S}U^T, \text{ where } B = USU^T \tag{7.7}$$

Due to the eigendecomposition method used in Equation 7.4.1, standard MDS method has a complexity of $O(n^3)$, which does not scale well to the large dataset.

7.4.2 fastMDS

Our FastMDS approach is based on the observation that a submatrix along the diagonal of a dissimilarity matrix is itself a dissimilarity matrix. Therefore, our method tries to minimize the time complexities by applying MDS on a linear number of small submatrix with size l to obtain the results.

We partition D along the diagonal into $\frac{p=n}{l}$ submatrices $D_1, D_2, ..., D_p$, each of size l by l. We also obtain a submatrix, D_{Align} by sampling at least s samples from each submatrix in $D_1, D_2, ..., D_p$. In principle, s should be at least 1 + the estimated dimensionality of the dataset. In practice, we oversample by a factor of 2 or more, to ensure that we capture the data's inherent dimensionality.

We compute the MDS solution for each submatrix D_i and D_{Align} to get coordinates for the sampled points. We now have two MDS solutions for each of the sampled points; one from performing MDS on D_i, i.e., Q_i and one from performing MDS on D_{Align}, i.e, Q_{align}. The next step is to compute an affine mapping A_i between the coordinates of samples in Q_i, denoted as Q_i^s and corresponding samples in Q_{align}, denoted as Q_i^s. This is a linear least squares problem:

$$A_i = \text{argmin}_{A_i} \|A_i Q_i^S - Q_{align}^S\|; \tag{7.8}$$

$$Q_i = A_i Q_i, \quad \forall i, 0 < i \leq \frac{n}{l}. \tag{7.9}$$

Solving for A_i gives us a mapping between D_i and D_{align}. We apply the same affine transformation A_i to all the points in D_i to get the coordinates for all points.

In case when the alignment matrix D_{align} is too big to run the stand MDS efficiently, we recursively apply the above process to the alignment until an optimal size of alignment matrix is reached.

Time Complexity The overall time complexity of fastMDS is

$$T(n) = \begin{cases} \frac{n}{l} MDS(l) + T(\frac{ns}{l}) + Z(n), & n > l \\ MDS(n), & n \leq l. \end{cases} \tag{7.10}$$

The sampling size s is constant with respect to n, therefore, we treat operations related to it as a constant-time operation, such as computing the affine map A_i between the s sample points in D_i and D_{align}. Z is a function that applies A_i to a matrix of size D_i, which is in the order of $o(n)$.

The following is the overall complexity of fastMDS algorithm.

$$T(n) = \sum_{k=\text{argmin}_{n(\frac{s}{l})^k \leq l}} \frac{n}{l}(\frac{s}{l})^{k-1} mds(l) \\ \sum_{k=\text{argmin}_{n(\frac{s}{l})^k \leq l}} \frac{n}{l}(\frac{s}{l})^{k-1} O(l^3) \tag{7.11}$$

7.4.3 Visualization of Clustering

Though clustering is a data analysis tool, it is closely coupled with visualization in the following aspects. First, clusters of SSCs are reflected in both the dissimilarity view and the point cloud view. Second, the user can explore the size and the representative SSCs in each cluster. Most important of all, user will be able to determine the actual number of clusters according to clusters of points in the point-cloud view or histogram of linkage distance. Lastly, user can supervise and guide the clustering process. For example, user may select the set of SSCs, since they believe they belong to the same cluster, or they want to force to divide a cluster into multiple parts since they believe there should be more than one clusters mixed together.

In our paper, we follow the path of traditional hierarchical clustering. We start by taking each SSC as a separate cluster, whose representative PPM is the single SSC it contains and so is the coverage. The pair-wise wDisbetween any two clusters based on its coverage and representative PPM is computed. The following is the process of creating a new cluster. First, two clusters of minimum wDisare merged into a new cluster. Next, the coverage and the representative PPM of the newly created cluster are computed. In addition, the pair-wise distance between the new cluster and the rest of clusters is computed as well. The above process is repeated until there is only one cluster left.

Our hierarchical clustering not only provides dendrogram of subspace clusters, the mean pattern obtained in each cluster provides a representative of subspace clusters in the clusters. Most important of all, the linkage distance between two clusters during the merging process reflects the stableness of the merged clusters. If the linkage distance is extremely high, which means that the clusters are essentially different. Putting all linkage distances in a histogram may help us determine the threshold of linkage distance for the identification of true clusters.

However, hierarchical clustering carries a $o(n^2 log(n))$ complexity. When size of data exceeds 5000, hierarchical clustering becomes rather slow and does not fit into the interactive visualization framework. To speed up this process, we can build the hierarchical clustering on top of K-means clustering since it has a much lower complexity. K, the number of clusters input for k-Means will be set at a reasonable number to minimize error while still provide good compression of the data. The mean pattern will then be computed for each k-Means

clusters. Those representative mean pattern will become the input of the further hierarchical clustering.

7.5 Experiments

We demonstrate our visualization techniques on two real datasets. The first dataset is a zoo dataset (D.J. Newman and Merz, 1998). The Zoo Database contains 101 instances and 18 attributes (animal name, 15 boolean attributes, 2 numerics). The attributes are hair, feathers, eggs, milk, airborne, aquatic, predator, toothed, backbone, breathes, venomous, fins, tail, domestic and catsize. And the numeric attributes are legs and type, where the type attribute appears to be the class attribute. All the instances are classified into 7 classes. We consider this as a binary dataset and applied itemset mining on it. Though small, the set of subspace clusters may generate over 600 subspace clusters. And it is hard to find useful classification information from the 600 clusters. In addition, those clusters exhibits other characteristics of subspace clusters, such as overlap and incompleteness(No perfect classification of any cluster).

The second dataset is a yeast gene expression dataset. It contains 2884 genes and 17 conditions. These genes were selected according to Spellman *et.al.*(Spellman et al., 1998) The range of the gene expression value are between 0 and 600. One of the objectivity of two datasets of this data is to find the co-regulated genes under a subset rather than the whole sets of conditions. We apply the $\delta-$pCluster to the dataset. By varying the p-score threshold and minimum number of genes within a cluster, the maximum number of clusters easily exceeds 5000.

7.5.1 Results on Zoo Dataset.

We use around 600 subspace clusters generated from the Zoo dataset. The following discussion is based on Figure 7.4. We compute both the coverage dissimilarity (a) and pattern dissimilarity (d). We then cluster the subspace clusters based on each of their dissimilarity into three clusters. The rows and columns of the dissimilarity matrix are permuted so that rows and columns that are in the same cluster are adjacent. The cluster manifests itself as darker blocks along the diagonal as shown in both (b) and (e). Figure (b) and (e) don't show the same clustering results because they represent different dissimilarity measures. We then combine the two dissimilarity measure by assigning them similar weights. The mixture of the dissimilarity measure is shown in Figure (g). Clustering is also applied to the dissimilarity measure. By grouping the rows and columns based on the clustering results, we also see the strong clustering signal in (c) and (f). Note that (c) and (f) is a permutation of coverage dissimilarity and pattern dissimilarity respectively and they are clustered according to

the clustering of dissimilarity matrix (g). Compared with (b) and (c), the clustering of the mixture of dissimilarity show much clearer separation than (c) or (f).

We then model the subspace clusters as points the 3D space as shown in Figure 7.5. Interestingly, the clusters are well separated into three clusters. Applying hierarchical clustering onto them confirms this. The dissimilarity of subspace clusters and the distance approximated by MDS in the 3D space are largely consistent.

Our tool found the 3 representatives medoid for each of the clusters. We view the representative of each cluster and its summary, which is the union of row and column sets of the cluster of subspace clusters. The relationship between representatives and the summary are shown in the three side panel of Figure 7.5.

By examining the features(shown in the side panel) and the animals(not shown because of the space) found in the clusters, the three clusters represent three main categories of the animal clusters. Our visualization apparently simplifies the process of going through the 600 subspace clusters while finally getting lost.

7.5.2 Results on Gene Expression Dataset

We also apply our visualization techniques on gene expression data. In this experiment we will show how our tool can help to visualize and explore two sets of clusters.

The 3D plots of the subspace clusters are shown both in Figure 7.6(a) and Figure 7.6(b). In Figure 7.6(a), we compare two sets of subspace clusters that are far away in 3D space. The relationships of the two clusters in the original matrix are shown in the side panel. According to the figure, the two sets do not intersect much. The gene expression of the representative cluster is also shown on the bar graph in the side panel. Apparently, the two sets of subspace clusters are not similar with regard to the pattern either. These results are echoed with the distances shown in the 3D plot.

In figure 7.6(b), we compare two sets of subspace clusters that are side-by-side and close to each other. Interestingly, the two sets of clusters shared the same set of columns, while the yellow clusters seems to include more rows than the rest. But if we examine their representative patterns shown on the top of the data matrix, they are very similar. This figure might suggest that the two sets of clusters might be very close and can be merged into one. This merging help us to discover new clusters, which would never be reveals by the result of subspace clustering results alone.

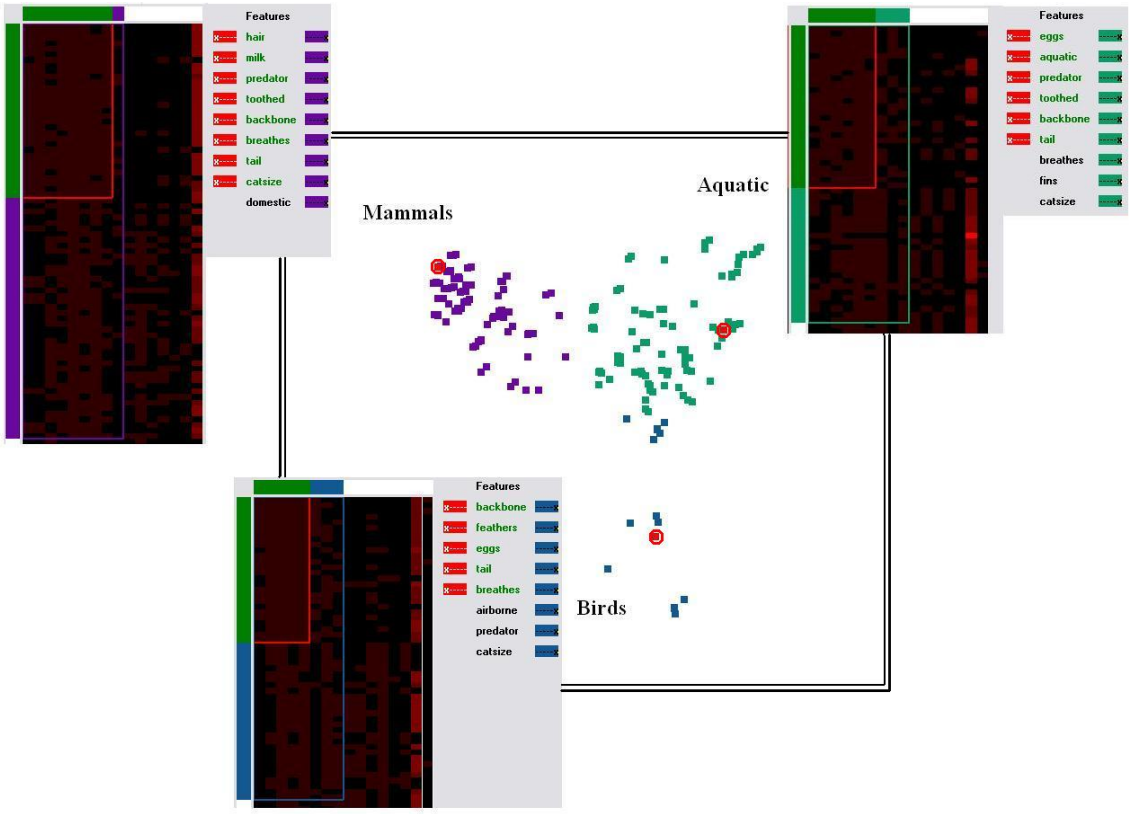


Figure 7.5: Results of the Zoo dataset. Middle: The 3D point-cloud view of subspace clusters by applying MDS on the combined dissimilarity of coverage and pattern dissimilarities. Each different color represent a cluster. The red points circled in red in each cluster refers to the subspace cluster that is the representative of the cluster containing it. The three clusters can be easily classified into Mammals, Aquatic, and Birds. Side panels: the relationships and summary between the representative cluster and the rest of the cluster. The red colored rectangle corresponds to the representative cluster, which is a large fraction of the summary of the set of subspace clusters.

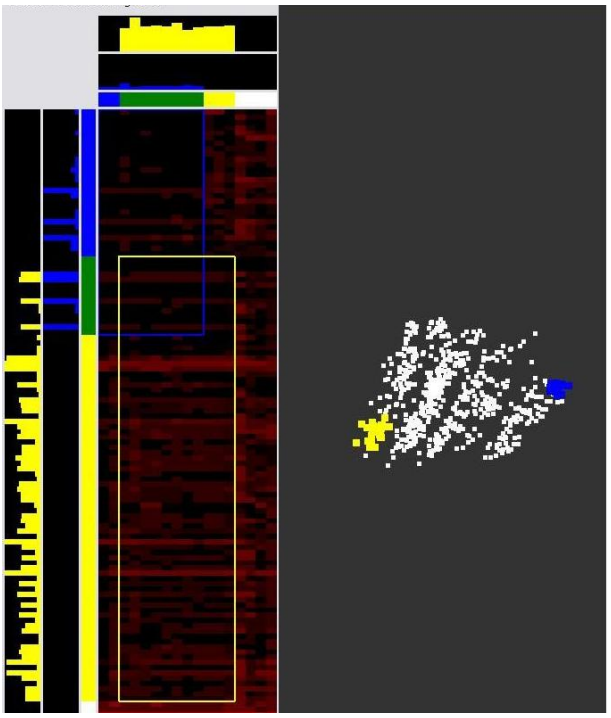
7.6 Conclusion

We have presented a tool for exploring the results of subspace clustering algorithms. At its foundation are dissimilarity measures that relate both the coverage and the pattern similarities between any pair of subspace clusters. These dissimilarities can be directly visualized to expose patterns between sets of subset clusters. These visualizations are even more effective when the subspace clusters are themselves clustered. The application of Multidimensional Scaling to the dissimilarity matrices permits the creation of a geometric analogy for the dataset, in which every subspace cluster is a point, and the distances between points reflect the dissimilarities.

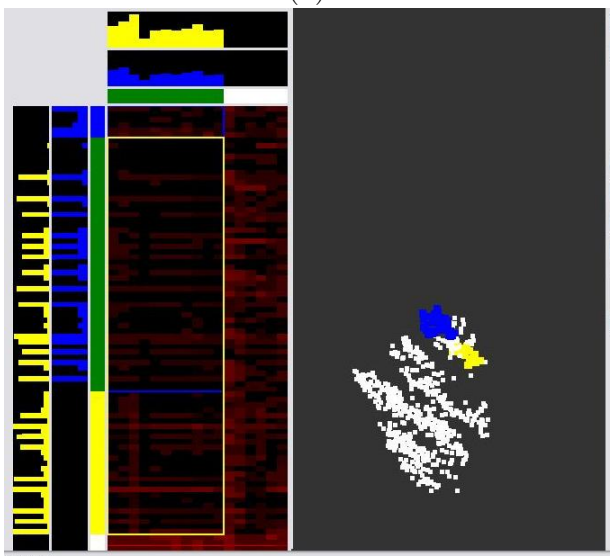
Our visualization framework aids in the analysis of the large sets of subspace clusters mined from a given dataset. It encourages the use of large cluster sets, instead of smaller clusters, and thus retains pattern sensitivity.

By clustering subspace clusters it is possible to define summarizations over the whole dataset. It is possible to extract an intrinsic medoid representing the entirety of a cluster of subspace clusters. We can also aggregate subspaces with similar patterns, while retaining interesting or distinct subspaces which would have, in all likelihood, been masked if one is restricted to tuning the clustering parameters.

We imagine that there are even more visualization possibilities for subspace clusters. MDS provides a valuable tool with rich possibilities for additional enhancements.



(a)



(b)

Figure 7.6: Result of Gene expression. Right: The 3D point cloud view of subspace clusters. (a) Left Panel: the relationships between two distant sets of subspace clusters in the original matrix. Their dissimilarity relationships are shown in the point cloud view. (b) Left panel: the relationships of two similar sets of subspace clusters in the original data matrix. The two selected clusters are shown in the two sets of points in the point cloud view. Note: The blue histograms on top of the data matrix are gene expression patterns of the representative subspace cluster in the set.

Chapter 8

Conclusion and Future Work

Clustering real-world data sets is often hampered by the so-called curse of dimensionality: many real-world datasets consist of a very high dimensional feature space. In general, most traditional algorithms fail to generate meaningful results because of the inherent sparsity of the data space. Clusters are embedded in subspaces since some features of the original space may be irrelevant. In my thesis, I developed subspace clustering techniques which identify clusters in subspaces of high dimensional data.

One of the algorithms, OP-Clustering, is designed to reveal salient subspace clusters where the objects in a cluster rise and fall coherently within its subspace. The definition of OP-Clusters goes beyond traditional notion of clusters where the dissimilarity are often measured by distance or correlation. Objects in an OP-Cluster exhibit consistent tendency while still far apart from each other in distance. The definition can be more robust in the analysis of gene expression data, where a subset of genes are expressed in different amounts under different environmental conditions while maintaining the same variation of expression values along a subset of conditions. OP-Clustering has been effectively applied to the analysis of gene expression data, such as breast cancer datasets and yeast datasets. Subspace clusters containing genes that are expressed differently between two types of breast cancers have been identified. In the analysis yeast datasets, genes which perform similar biological functions are also revealed in many OP-Clusters.

Noise is ubiquitous in datasets collected in real applications. The noise tolerant AFI algorithms were developed in my thesis identify hidden itemsets that are obscured by noise in binary matrices. Both the theoretical and experimental results demonstrate that the AFI criterion is well suited to the recovery of block structures subject to noise in binary dataset. The model of AFI only handles noise in a binary matrix. Noise in continuous data, such as gene expression is more prevalent. Like the effect of noise in binary data, an error in continuous data can easily knock either a row or a column out of a underlying subspace clustering. As a result, the observed subspace clusters are often small segments of underlying patterns. Therefore, it is important to tolerate noise in order to find the hidden subspace

clusters in high precision. One possible method to approach the problem is to consider the subspace clusters in continuous space as a pattern embedded in a binary submatrix, where the 1 entry within the submatrix identifies whether the corresponding row and column share the pattern. Therefore, we might be able to extend AFI on binary data matrix to noise-tolerant subspace clustering in continuous datasets.

In bioinformatics applications, a small subset genes, metabolites, and proteins have already been well studied by biologists. This knowledge can be easily obtained from a number of databases, such as Gene ontology and protein-protein interaction network databases. This knowledge is often ignored by unsupervised learning. On the other hand, it is not sufficient to constitute a perfect training set for supervised learning. Semi-supervised learning is a recent branch of data mining that resides midway between supervised learning and unsupervised learning. Annotated genes, however, are often difficult, expensive or time consuming to obtain, as they require the efforts of experienced human annotators. Meanwhile, unlabeled data may be relatively easy to collect, but they are inherently less useful. In order to take advantage of existing knowledge, while still being faithful to empirical datasets, a semi-supervised version of OP-Clustering has been developed in the thesis. The semi-supervised OP-Clustering incorporates partially known gene function annotation into the clustering of all genes. It directly generates biologically relevant OP-Clusters while avoiding the spurious clusters. The approach improves not only the quality of the results but the efficiency of the algorithms four fold. Semi-supervised learning addresses this problem by using large amounts of unlabeled data together with a small number of annotated instances, to build better predictive models.

Clustering a single type of data has led to a variety of research problems as addressed in my thesis. However, data in real world is not independent. Instead, multiple datasets regarding the same set of objects can be collected from different platforms or regarding different aspects. Given a set of patients, doctors may be a number of datasets that may be useful in order to identify specific disease markers. These datasets include but are not limited to , patients clinical data, genotype data(DNA), gene expression data, and proteomics data. Observations that are supported by multiple experimental datasets are likely to lead to new insights that might not be as readily available from analyzing one type of data in isolation. For instance, experimental datasets often contain errors arising from imperfections in the applied technology. Thus, some of the findings of methods that analyze a single type of data may be erroneous. Combining additional data types might increase our confidence in such predicted interactions. For example, if evidence from a gene expression dataset indicated that two genes have similar expression profiles, and the protein byproducts also indicate correlations, this association is unlikely to be a coincidence. If we assume that noise across different datasets are largely independent, then the probability of errors in results that are supported by two different datasets is dramatically reduced. Integrating heterogeneous data

has been an active research area in data mining. We may find patterns in each individual type of data, and then find common patterns that are supported by multiple datasets, or alternatively we may find patterns that are only apparent when all data are incorporated into a single large dataset. Such comparative analyses are easily automated. Patterns are often evaluated by their association to some disease or medical condition in a statistical sense. The presence of statistically significant patterns is important, and might lead to new discoveries. Several questions should be answered for this approach. First, given a pattern, how do we evaluate its significance in each type of data, and how do we define the pattern similarity across different data types? Secondly, how do we evaluate the confidence level of patterns from multiple data types? In other words, do we trust each piece of data equivalently, or do we place more emphasis on one over the others? Lastly, the statistical significance of a pattern is determined by the prevalence of the pattern, the confidence level of each dataset, and the popularity of the patterns among all data types. As a result, patterns discovered by this approach will serve as excellent starting points for generating testable hypotheses.

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