

CACTUS—Clustering Categorical Data Using Summaries

Venkatesh Ganti* Johannes Gehrke† Raghu Ramakrishnan‡
Department of Computer Sciences, University of Wisconsin-Madison
{vganti, johannes, raghu}@cs.wisc.edu

Abstract

Clustering is an important data mining problem. Most of the earlier work on clustering focussed on numeric attributes which have a natural ordering on their attribute values. Recently, clustering data with categorical attributes, whose attribute values do not have a natural ordering, has received some attention. However, previous algorithms do not give a formal description of the clusters they discover and some of them assume that the user post-processes the output of the algorithm to identify the final clusters.

In this paper, we introduce a novel formalization of a cluster for categorical attributes by generalizing a definition of a cluster for numerical attributes. We then describe a very fast summarization-based algorithm called CACTUS that discovers exactly such clusters in the data. CACTUS has two important characteristics. First, the algorithm requires only two scans of the dataset, and hence is very fast and scalable. Our experiments on a variety of datasets show that CACTUS outperforms previous work by a factor of 3 to 10. Second, CACTUS can find clusters in subsets of all attributes and can thus perform a subspace clustering of the data. This feature is important if clusters do not span all attributes, a likely scenario if the number of attributes is very large. In a thorough experimental evaluation, we study the performance of CACTUS on real and synthetic datasets.

1 Introduction

Clustering is an important data mining problem. The goal of clustering, in general, is to discover dense and sparse regions in a dataset. Most previous work in clustering focussed on numerical data whose inherent geometric properties can be exploited to naturally define distance functions between points. However, many datasets also consist of categorical

attributes¹ on which distance functions are not naturally defined. Recently, the problem of clustering categorical data started receiving interest [GKR98, GRS99].

As an example, consider the MUSHROOM dataset in the popular UCI Machine Learning repository [CBM98]. Each tuple in the dataset describes a sample of gilled mushrooms using twenty two categorical attributes. For instance, the *cap color* attribute can take values from the domain {*brown, buff, cinnamon, gray, green, pink, purple, red, white, yellow*}. It is hard to reason that one color is “like” or “unlike” another color in a way similar to real numbers.

An important characteristic of categorical domains is that they typically have a small number of attribute values. For example, the largest domain for a categorical attribute of any dataset in the UCI Machine Learning repository consists of 100 attribute values (for an attribute of the *Pendigits* dataset). Categorical attributes with large domain sizes typically do not contain information that may be useful for grouping tuples into classes. For instance, the *CustomerId* attribute in the TPC-D database benchmark [Cou95] may consist of millions of values; given that a record (or a set of records) takes a certain *CustomerId* value (or a set of values), we cannot infer any information that is useful for classifying the records. Therefore, it is different from the age or geographical location attributes which can be used to group customers based on their age or location or both. Typically, relations contain 10 to 50 attributes; hence, even though the size of each categorical domain is small, the cross product of all their domains and hence the relation itself can be very large.

In this paper, we introduce a fast summarization-based algorithm called CACTUS² for clustering categorical data. CACTUS exploits the small domain sizes of categorical attributes. The central idea in CACTUS is that summary information constructed from the dataset is sufficient for discovering well-defined clusters. The properties that the summary information typically fits into main memory, and that it can be constructed efficiently—typically in a single scan of the dataset—result in significant performance improvements:

¹ Attributes whose domain is totally ordered are called *numeric*, whereas attributes whose domain is not ordered are called *categorical*.

² Categorical ClusTering Using Summaries

*Supported by a Microsoft Graduate Fellowship.

†Supported by an IBM Graduate Fellowship.

‡This research was supported by Grant 2053 from the IBM corporation.

a factor of 3 to 10 times over one of the previous algorithms. Our main contributions in this paper are:

1. We formalize the concept of a cluster over categorical attributes (Section 3).
2. We introduce a fast summarization-based algorithm CACTUS for clustering categorical data (Section 4).
3. We then extend CACTUS to discover clusters in subspaces, especially useful when the data consists of a large number of attributes (Section 5).
4. In an extensive experimental study, we evaluate CACTUS and compare it with earlier work on synthetic and real datasets (Section 6).

2 Related Work

In this section, we discuss previous work on clustering categorical data. The EM (Expectation-Maximization) algorithm is a popular iterative clustering technique [DLR77, CS96]. Starting with an initial clustering model (a mixture model) for the data, it iteratively refines the model to fit the data better. After an indeterminate number of iterations, it terminates at a locally optimal solution. The EM algorithm assumes that the entire data fits into main memory and hence is not scalable. We now discuss two previous scalable algorithms STIRR and ROCK for clustering categorical data.

Gibson et al. introduce STIRR, an iterative algorithm based on non-linear dynamical systems [GKR98]. They represent each attribute value as a weighted vertex in a graph. Multiple copies $b_1, \dots, b_m$, called *basins*, of this set of weighted vertices are maintained; the weights on any given vertex may differ across basins. b_1 is called the *principal* basin; $b_2, \dots, b_m$ are called *non-principal* basins. Starting with a set of weights on all vertices (in all basins), the system is “iterated” until a fixed point is reached. Gibson et al. argue that when the fixed point is reached, the weights in one or more of the basins $b_2, \dots, b_m$ isolate two groups of attribute values on each attribute: the first with large positive weights and the second with small negative weights, and that these groups correspond intuitively to projections of clusters on the attribute. However, the automatic identification of such sets of closely related attribute values from their weights requires a non-trivial post-processing step; such a post-processing step was not addressed in their work. Moreover, the post-processing step will also determine what “clusters” are output. Also, as we show in Section 3.2, certain classes of clusters are not discovered by STIRR.

Guha et al. introduce ROCK, an adaptation of an agglomerative hierarchical clustering algorithm, which heuristically optimizes a criterion function defined in terms of the number of “links” between tuples [GRS99]. Informally, the number of links between two tuples is the number of common neighbors³

³Given a *similarity function*, two tuples in the dataset are said to be *neighbors* if the similarity between them is greater than a certain threshold.

they have in the dataset. Starting with each tuple in its own cluster, they repeatedly merge the two closest clusters till the required number (say, K) of clusters remain. Since the complexity of the algorithm is *cubic* in the number of tuples in the dataset, they cluster a sample randomly drawn from the dataset, and then partition the entire dataset based on the clusters from the sample. Beyond that the set of all “clusters” together may optimize a criterion function, the set of tuples in each individual cluster is not characterized.

3 Definitions

In this section, we formally define the concept of a cluster over categorical attributes, and other concepts used in the remainder of the paper. We then compare the class of clusters allowed by our definition with those discovered by STIRR.

3.1 Cluster Definition

Intuitively, a cluster on a set of numeric attributes identifies a “dense region” in the attribute space. That is, the region consists of a significantly larger number of tuples than expected. We generalize this intuitive notion for the class of hyper-rectangular clusters to the categorical domain.⁴

As an illustrative example, the region $[1, 2] \times [2, 4] \times [3, 5]$ may correspond to a cluster in the 3-d space spanned by three numeric attributes. In general, the class of rectangular regions can be expressed as the cross product of intervals. Since domains of categorical attributes are not ordered, the concept of an interval does not exist. However, a straightforward generalization of the concept of an interval to the categorical domain is a *set* of attribute values. Consequently, the generalization of rectangular regions in the numeric domain to categorical domain is the cross product of sets of attribute values. We call such regions *interval regions*.

Intuitively, a cluster consists of a significantly larger number of tuples than the number expected if all attributes were independent. In addition, a cluster also extends to as large a region as possible. We now formalize this notion for categorical domains by first defining the notion of a tuple *belonging* to a region, and then the *support* of a region, which is the number of tuples in the dataset that belong to the region.

Definition 3.1 Let $A_1, \dots, A_n$ be a set of categorical attributes with domains $\mathcal{D}_1, \dots, \mathcal{D}_n$, respectively. Let the dataset D be a set of tuples where each tuple t : $t \in \mathcal{D}_1 \times \dots \times \mathcal{D}_n$. We call $S = S_1 \times \dots \times S_n$ an *interval region* if for all $i \in \{1, \dots, n\}$, $S_i \subseteq \mathcal{D}_i$. Let $a_i \in \mathcal{D}_i$ and $a_j \in \mathcal{D}_j$, $i \neq j$. The *support* $\sigma_D(a_i, a_j)$ of the attribute value pair (a_i, a_j) with respect to D is defined as follows:

$$\sigma_D(a_i, a_j) \stackrel{\text{def}}{=} |\{t \in D : t.A_i = a_i \text{ and } t.A_j = a_j\}|$$

⁴Classes of clusters that correspond to arbitrarily shaped regions in the numeric domain cannot be generalized as cleanly to the categorical domain because the categorical attributes do not have a natural ordering imposed on their domains. Therefore, we only consider the class of hyper-rectangular regions.

A tuple $t = \langle t.A_1, \dots, t.A_n \rangle \in D$ is said to *belong* to the region S if for all $i \in \{1, \dots, n\}$, $t.A_i \in S_i$. The *support* $\sigma_D(S)$ of S is the number of tuples in D that belong to S .

If all attributes $A_1, \dots, A_n$ are independent and the attribute values in each attribute are equally likely (henceforth referred to as the *attribute-independence assumption*) then the *expected support* $E[\sigma_D(S)]$ of a region $S = S_1 \times \dots \times S_n$ is $|D| \cdot \frac{|S_1| \times \dots \times |S_n|}{|\mathcal{D}_1| \times \dots \times |\mathcal{D}_n|}$. As before, the expected support of (a_i, a_j) $E[\sigma_D(a_i, a_j)]$ is $|D| \cdot \frac{1}{|\mathcal{D}_i| \times |\mathcal{D}_j|}$. Since the dataset D is understood from the context, we write $\sigma(S)$ instead of $\sigma_D(S)$, and $\sigma(a_i, a_j)$ instead of $\sigma_D(a_i, a_j)$. Finally, we note that the attribute independence assumption can be modified to take any prior information into account; e.g., the marginal probabilities of attribute values.

Intuitively, $\sigma(a_i, a_j)$ captures the co-occurrence, and hence the similarity, of attribute values a_i and a_j . Values a_i and a_j are said to be *strongly connected* if their co-occurrence ($\sigma(a_i, a_j)$) is significantly higher (by some factor α) than the value expected under the attribute-independence.⁵ We now define σ^* to formalize this intuition, and then give a formal definition of a cluster.

Definition 3.2 Let $a_i \in \mathcal{D}_i$, $a_j \in \mathcal{D}_j$, and $\alpha > 1$. The attribute values a_i and a_j are *strongly connected* with respect to D if $\sigma_D(a_i, a_j) > \alpha \cdot \frac{|D|}{|\mathcal{D}_i| \cdot |\mathcal{D}_j|}$. The function $\sigma_D^*(a_i, a_j)$ is defined as follows:

$$\sigma_D^*(a_i, a_j) \stackrel{\text{def}}{=} \begin{cases} \sigma_D(a_i, a_j), & \text{if } a_i \text{ and } a_j \text{ are} \\ & \text{strongly connected} \\ 0, & \text{otherwise} \end{cases}$$

Let $S_i \subseteq \mathcal{D}_i$ and $S_j \subseteq \mathcal{D}_j$, $i \neq j$, be two sets of attribute values. An element $a_i \in S_i$ is strongly connected with S_j if, for all $x \in S_j$, a_i and x are strongly connected. S_i and S_j are said to be strongly connected if each $a_i \in S_i$ is strongly connected with S_j and each $a_j \in S_j$ is strongly connected with S_i .

Definition 3.3 For $i = 1, \dots, n$, let $C_i \subseteq \mathcal{D}_i$, $|C_i| > 1$, and $\alpha > 1$. Then $C = \langle C_1, \dots, C_n \rangle$ is a *cluster* over $\{A_1, \dots, A_n\}$ if the following three conditions are satisfied. (1) For all $i, j \in \{1, \dots, n\}$, $i \neq j$, C_i and C_j are strongly connected. (2) For all $i, j \in \{1, \dots, n\}$, $i \neq j$, there exists no $C'_i \supset C_i$ such that for all $j \neq i$, C'_i and C_j are strongly connected. (3) The support $\sigma_D(C)$ of C is at least α times the expected support of C under the attribute-independence assumption.

We call C_i the *cluster-projection* of C on A_i . C is called a *sub-cluster* if it satisfies conditions (1) and (3). A cluster C over a subset of all attributes $S \subset \{A_1, \dots, A_n\}$ is called a *subspace cluster* on S ; if $|S| = k$ then C is called a *k-cluster*.

We now extend our notion of similarity to attribute value pairs on the same attribute. Let $a_1, a_2 \in \mathcal{D}_i$ and $x \in \mathcal{D}_j$. If (a_1, x) and (a_2, x) are strongly connected then (a_1, a_2) are “similar” to each other with respect to A_j . The level of similarity is the number of such distinct attribute values $x \in \mathcal{D}_j$. We now formalize this intuition.

Definition 3.4 Let $a_1, a_2 \in \mathcal{D}_i$. The *similarity* $\gamma^j(a_1, a_2)$ between a_1 and a_2 with respect to A_j ($j \neq i$) is defined as follows.

$$\gamma^j(a_1, a_2) \stackrel{\text{def}}{=} |\{x \in \mathcal{D}_j : \sigma^*(a_1, x) > 0 \text{ and } \sigma^*(a_2, x) > 0\}|$$

Below, we define the summary information which we need later to describe the CACTUS algorithm. The summary information is of two types: (1) *inter-attribute* summaries and (2) *intra-attribute* summaries. The inter-attribute summaries consist of all strongly connected attribute value pairs where each pair has attribute values from different attributes; the intra-attribute summaries consist of similarities between attribute values of the same attribute.

Definition 3.5 Let $A_1, \dots, A_n$ be a set of categorical attributes with domains $\mathcal{D}_1, \dots, \mathcal{D}_n$ respectively, and let D be a dataset. The *inter-attribute summary* Σ_{IJ} is defined as: $\Sigma_{IJ} \stackrel{\text{def}}{=} \{\Sigma_{ij} : i, j \in \{1, \dots, n\}, i \neq j\}$ where $\Sigma_{ij} \stackrel{\text{def}}{=}$

$$\{(a_i, a_j, \sigma_D^*(a_i, a_j)) : a_i \in \mathcal{D}_i, a_j \in \mathcal{D}_j, \text{ and } \sigma_D^*(a_i, a_j) > 0\}$$

The *intra-attribute summary* Σ_{II} is defined as:

$$\Sigma_{II} \stackrel{\text{def}}{=} \{\Sigma_{ii}^j : i, j \in \{1, \dots, n\} \text{ and } i \neq j\} \text{ where } \Sigma_{ii}^j \stackrel{\text{def}}{=}$$

$$\{(a_{i1}, a_{i2}, \gamma^j(a_{i1}, a_{i2})) : a_{i1}, a_{i2} \in \mathcal{D}_i, \text{ and } \gamma^j(a_{i1}, a_{i2}) > 0\}$$

3.2 Discussion

We now compare the class of clusters allowed by our definition with the clusters discovered by STIRR. For the comparison, we generate test data using the data generator developed by Gibson et al. for evaluating STIRR [GKR98]. We consider three datasets shown in Figures 1, 2, and 3. Each dataset consists of 100000 tuples. DS1 and DS2 have two attributes, DS3 has three attributes where each attribute consists of 100 attribute values. These tuples are distributed over all attribute values on each attribute according to the attribute-independence assumption. We control the location and the size of clusters in each dataset by distributing an additional number of tuples (5% of the total number in the dataset) in regions designated to be clusters thus increasing their supports above the expected value under the attribute-independence assumption. In Figures 1, 2, and 3, the cluster-projection of each cluster is shown within an ellipse. The boundaries of the cluster-projections (ellipses) of a cluster are connected by lines of the same type (e.g., solid, dashed etc.).

⁵Because a deviation of 2 or 3 times the expected value is usually considered significant [BD76], typical values of α are between 2 and 3.

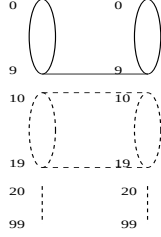


Figure 1: DS1

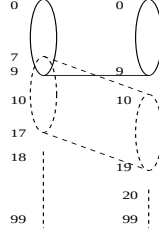


Figure 2: DS2

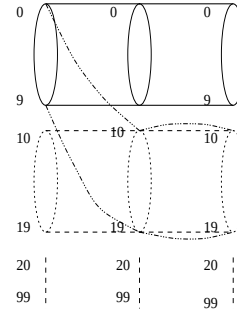


Figure 3: DS3

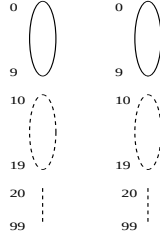


Figure 4: DS1:STIRR's O/P

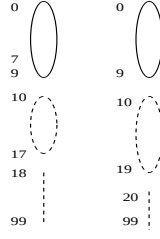


Figure 5: DS2:STIRR's O/P

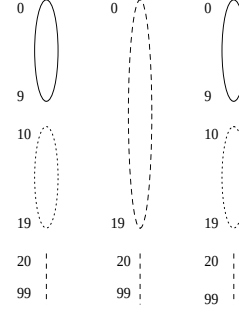


Figure 6: DS3:STIRR's O/P

We ran STIRR on the datasets shown in Figures 1, 2, and 3, and manually selected the basin that assigns positive and negative weights respectively to attribute values in different cluster-projections. To identify the cluster projections, we observed the weights allocated by STIRR and isolated two groups such that the weights in each group have large magnitude and are close to each other. The cluster-projections identified by STIRR are shown in Figures 4, 5, and 6.

STIRR recognized the cluster-projections for DS1 on the first non-principal basin (b_2) for every attribute (as shown in Figure 4). When run on the dataset DS2, the first non-principal basin (b_2) on A_1 identifies the two groups: $\{0, \dots, 9\}$ and $\{10, \dots, 17\}$ (as shown in Figure 5). The second non-principal basin (b_3) on A_1 identifies the following two groups: $\{0, \dots, 6\}$ and $\{7, \dots, 17\}$. Thus, no basin identifies the overlap between the cluster-projections. It may be possible to identify such overlaps through a non-trivial post processing step. However, it is not clear how many basins are required and how to recognize that cluster-projections overlap from the weights on attribute values. We believe that any such post-processing step itself will be similar to the CACTUS algorithm. The result of running STIRR on the dataset DS3 is shown in Figure 6. STIRR merged the two cluster-projections on the second attribute, possibly because one of the cluster-projections participates in more than one cluster.

From these experiments, we observe that STIRR fails to discover the following classes of clusters: (1) clusters consisting of overlapping cluster-projections on any attribute, (2) clusters where two or more clusters share the same cluster-projection. However, intuitively, these two classes of clusters

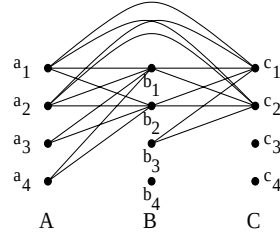


Figure 7: Σ_{IJ}

A w.r.t. B	B w.r.t. C	C w.r.t. B
$a_1, a_2:2$	$b_1, b_2:2$	$c_1, c_2:3$
$a_1, a_3:2$	$b_1, b_3:2$	$c_1, c_3:2$
$a_1, a_4:2$	$b_2, b_3:2$	
$a_2, a_3:2$		
$a_2, a_4:2$		
$a_3, a_4:2$		

Figure 8: Σ_{II}

should be valid classes of clusters, and our cluster definition includes these classes. CACTUS correctly discovers all the implanted clusters from the datasets DS1, DS2, and DS3. Thus, our definition of a cluster and hence CACTUS, which discovers all clusters allowed by our definition, seems to identify a broader class of clusters than that discovered by STIRR. Since it is not possible to characterize clusters discovered by STIRR, we could not construct any example datasets from which CACTUS does not retrieve the expected clusters and STIRR does. However, it is possible that such types of clusters exist.

4 CACTUS

In this section, we describe our three-phase clustering algorithm CACTUS. The central idea behind CACTUS is that a summary of the entire dataset is sufficient to compute a set

of “candidate” clusters which can then be validated to determine the actual set of clusters. CACTUS consists of three phases: *summarization*, *clustering*, and *validation*. In the summarization phase, we compute the summary information from the dataset. In the clustering phase, we use the summary information to discover a set of candidate clusters. In the validation phase, we determine the actual set of clusters from the set of candidate clusters. We introduce a hypothetical example which we use throughout the paper to illustrate the successive phases in the algorithm. Consider a dataset with three attributes A, B , and C with domains $\{a_1, a_2, a_3, a_4\}$, $\{b_1, b_2, b_3, b_4\}$, and $\{c_1, c_2, c_3, c_4\}$, respectively. Let the strongly connected attribute value pairs be as shown in Figures 7 and 8.

4.1 Summarization Phase

In this section, we describe the summarization phase of CACTUS. We show how to efficiently compute the inter-attribute and the intra-attribute summaries, and then describe the resource requirements for maintaining these summaries.

Categorical attributes usually have *small* domains. Typical categorical attribute domains considered for clustering consist of less than a hundred or, rarely, a thousand attribute values. An important implication of the compactness of categorical domains is that the inter-attribute summary Σ_{ij} for any pair of attributes A_i and A_j fits into main memory because the number of all possible attribute value pairs from A_i and A_j equals $|\mathcal{D}_i| \cdot |\mathcal{D}_j|$. For the rest of this section, we assume that the inter-attribute summary of any pair of attributes fits easily into main memory. (We will give an example later to support this assumption, and to show that typically inter-attribute summaries for many pairs of attributes together fit into main memory.) However, for the sake of completeness, we extend our techniques in Section 5 to handle cases where this trait is violated. The same argument holds for the intra-attribute summaries as well.

4.1.1 Inter-attribute Summaries

We now discuss the computation of the inter-attribute summaries. Consider the computation of Σ_{ij} , $i \neq j$. We initialize a counter to zero for each pair of attribute values $(a_i, a_j) \in \mathcal{D}_i \times \mathcal{D}_j$, and start scanning the dataset D . For each tuple $t \in D$, we increment the counter for the pair $(t.A_i, t.A_j)$. After the scan of D is completed, we compute σ^* by setting to zero all counters whose value is less than the threshold $\kappa_{ij} = \alpha \cdot \frac{|\mathcal{D}|}{|\mathcal{D}_i| \times |\mathcal{D}_j|}$. Thus, counts of only the strongly connected pairs are retained. The number of strongly connected pairs is usually much smaller than $|\mathcal{D}_i| \cdot |\mathcal{D}_j|$. Therefore, the set of strongly connected pairs can be maintained in specialized data structures designed for sparse matrices [DER86].⁶

We now present a hypothetical example to illustrate the resource requirements of the simple strategy described above. Consider a dataset with 50 attributes each consisting of 100

attribute values. Suppose we have 100 MB of main memory (easily available on current desktop systems). Assuming that each counter requires 4 bytes we can maintain counters for 2500 ($= \frac{100 \times 10^6}{100 \times 100 \times 4}$) attribute pairs simultaneously. With 50 attributes, we have to evaluate 1225 attribute pairs. Therefore, we can compute all inter-attribute summaries together in just one scan of the dataset. The computational and space requirements here are similar to that of obtaining counts of pairs of items while computing frequent itemsets [AMS⁺96].

Quite often, a single scan is sufficient for computing Σ_{IJ} . In some cases, we may need to scan D multiple times—each scan computing Σ_{ij} for a different set of (i, j) pairs. The computation of the inter-attribute summaries is CPU-intensive, especially when the number of attributes n is high, because for each tuple in the dataset, we have to increment $\frac{n(n-1)}{2}$ counters. Even if we require multiple scans of the dataset, the I/O time for scanning the dataset goes up but the total CPU time—for incrementing the counters—remains the same. Since the CPU time dominates the overall summary-construction time, the relative increase due to multiple scans is not significant. For instance, consider a dataset of 1 million tuples defined on 50 attributes, each consisting of 100 attribute values. Experimentally, we found that the total time for computing the inter-attribute summaries of the dataset with 1 million tuples is 1040 seconds, whereas a scan of the dataset takes just 28 seconds. Suppose we partition all the 1225 pairs of attributes into three groups consisting of 408, 408, and 409 pairs respectively. The computation of the inter-attribute summaries of attribute pairs in each group requires a scan of the dataset. The total computation time will be around 1096 seconds, which is only slightly higher than computing the summary in one scan.

4.1.2 Intra-attribute Summaries

In this section, we describe the computation of the intra-attribute summaries. We again exploit the characteristic that categorical domains are very small and thus assume that the intra-attribute summary of any attribute A_i fits in main memory. Our procedure for computing Σ_{ii}^j reflects the evaluation of the following SQL query:

```

Select    T1.A, T2.A, count(*)
From       $\Sigma_{ij}$  as T1(A,B),  $\Sigma_{ij}$  as T2(A,B)
Where     T1.A  $\neq$  T2.A and T1.B = T2.B
Group by  T1.A, T2.A
Having    count > 0;

```

The above query joins Σ_{ij} with itself to compute the set of attribute value pairs of A_i strongly connected to each other with respect to A_j .⁷ Since Σ_{ij} fits in main memory the self-join and hence the computation of Σ_{ii}^j is very fast. We will observe in the next section that, at any stage of our algorithm, we only require Σ_{ii}^j for a particular pair of attributes A_i and

⁶In our current implementation, we maintain the counts of strongly connected pairs in an array and do not optimize for space.

⁷For an exposition of join processing, see any standard textbook on database systems, e.g., [Ram97].

A_j . Therefore, we compute Σ_{ii}^j , ($j \neq i$), for each (i, j) pair whenever it is required.

Consider the example shown in Figure 7. (We use the notation Σ_{XY} to denote the inter-attribute summary between attributes X and Y .) The inter-attribute summaries Σ_{AB} , Σ_{BC} , and Σ_{AC} correspond to the edges between attribute values in the figure. The intra-attribute summaries Σ_{AA}^B , Σ_{BB}^C , Σ_{CC}^A are shown in Figure 8.

4.2 Clustering Phase

In this section, we describe the two-step clustering phase of CACTUS that uses the attribute summaries to compute candidate clusters in the data. In the first step, we analyze each attribute to compute all cluster-projections on it. In the second step, we synthesize, in a level-wise manner, candidate clusters on sets of attributes from the cluster-projections on individual attributes. That is, we determine candidate clusters on a pair of attributes, then extend the pair to a set of three attributes, and so on. We now describe each step in detail.

4.2.1 Computing Cluster-Projections on Attributes

Let $A_1, \dots, A_n$ be the set of attributes and $\mathcal{D}_1, \dots, \mathcal{D}_n$ be their domains. The central idea for computing all cluster-projections on an attribute is that a cluster $\langle C_1, \dots, C_n \rangle$ over the set of attributes $\{A_1, \dots, A_n\}$ induces a sub-cluster over any attribute pair (A_i, A_j) , $i \neq j$. In addition, the cluster-projection C_i on A_i of the cluster C is the intersection of the cluster-projections on A_i of 2-clusters over attribute pairs (A_i, A_j) , $j \neq i$. For example, the cluster-projection $\{b_1, b_2\}$ on the attribute B in Figure 7 is the intersection of $\{b_1, b_2, b_3\}$ (the cluster-projection on B of the 2-cluster $\langle \{b_1, b_2, b_3\}, \{c_1, c_2\} \rangle$) and $\{b_1, b_2\}$ (the cluster-projection on B of the 2-cluster $\langle \{a_1, a_2, a_3, a_4\}, \{b_1, b_2\} \rangle$). We formalize the idea in the following lemma.

Lemma 4.1 Let $C = \langle C_1, \dots, C_n \rangle$ be a cluster on the set of attributes $\{A_1, \dots, A_n\}$. Then,

- (1) For all $i \neq j$, $i, j \in \{1, \dots, n\}$, $\langle C_i, C_j \rangle$ is a sub-cluster over the pair of attributes (A_i, A_j) .
- (2) There exists a set $\{C_i^j : j \neq i \text{ and } \langle C_i^j, C_j^i \rangle \text{ is a 2-cluster over } (A_i, A_j)\}$ such that $C_i = \bigcap_{j \neq i} C_i^j$.

Lemma 4.1 motivates the following two-step approach. In the first *pairwise cluster-projection* step, we cluster each attribute A_i with respect to every other attribute A_j , $j \neq i$ to find all cluster-projections on A_i of 2-clusters over (A_i, A_j) . In the second *intersection* step, we compute all the cluster-projections on A_i of clusters over $\{A_1, \dots, A_n\}$ by intersecting sets of cluster-projections from 2-clusters computed in the first step. However, the problem of computing cluster-projections of 2-clusters in the pairwise cluster-projection step is at least as hard as the NP-complete *clique* problem [GJ79].⁸

⁸A *clique* in $\mathcal{G}_i^j$ is a set of vertices that are connected to each other by edges with non-zero weights. Given a graph $\mathcal{G} = \langle V, \mathcal{E} \rangle$ and a constant J , the clique problem determines if $\mathcal{G}$ consists of a clique of size at least J .

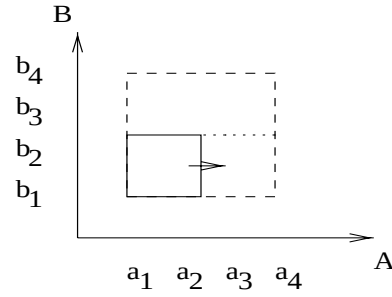


Figure 9: Extending $\{a_1, a_2\}$ w.r.t. B

The following lemma formalizes the computational complexity. The proof is given in the full paper [GGR99].

Lemma 4.2 Let A_i and A_j be two attributes. The problem of computing all cluster-projections on A_i of 2-clusters over (A_i, A_j) is NP-complete.

To reduce the computational complexity of the cluster-projection problem, we exploit the following property which, we believe, is usually exhibited by clusters in the categorical domain. If a cluster-projection C_i on A_i of one (or more) cluster(s) is larger than a fixed positive integer, called the *distinguishing number* (denoted κ), then it consists of a small identifying set—which we call the *distinguishing set*—of attribute values such that they will not *together* be contained in any other cluster-projection on A_i . Thus, the distinguishing set distinguishes C_i from other cluster-projections on A_i . Note that a proper subset of the distinguishing set may still belong to another cluster-projection, and that two distinct clusters may share an identical cluster-projection (as in Figure 1).

We believe that the distinguishing subset assumption holds in almost all cases. Even for the most restrictive version, which occurs when the distinguishing number is 1 and all cluster-projections of the set of clusters are distinct, the assumption only requires that each cluster consist of a set of attribute values—one on each attribute—that does not belong to any other cluster. For the example in Figure 7, the sets $\{a_1\}$ or $\{a_2\}$ identify the cluster-projection $\{a_1, a_2\}$ on the attribute A . We now formally state the assumption.

Distinguishing Subset Assumption: Let C_i and C'_i each of size greater than κ be two distinct cluster-projections on the attribute A_i . Then there exist two sets S_i and S'_i such that

$$|S_i| \leq \kappa, S_i \subset C_i, |S'_i| \leq \kappa, S'_i \subset C'_i, \text{ and } S_i \not\subset C'_i, S'_i \not\subset C_i$$

We call κ the *distinguishing number*.

Pairwise Cluster-Projections

We compute cluster-projections on A_i of 2-clusters over the attribute pair (A_i, A_j) in two steps. In the first step, we find all possible distinguishing sets (of size less than or equal to κ) on A_i . In the second step, we extend with respect to A_j some

of these distinguishing sets to compute cluster-projections on A_i . Henceforth, we write “cluster-projection on A_i ” instead of a “cluster-projection on A_i of a 2-cluster over (A_i, A_j) .”

Distinguishing Set Computation: In the first step, we rely on the following two properties to find all possible distinguishing sets on A_i . (1) All pairs of attribute values in a distinguishing set are strongly connected; that is the distinguishing set forms a *clique*. (2) Any subset of a distinguishing set is also a clique (*monotonicity property*). These two properties allow a level-wise clique generation similar to the candidate generation in apriori [AMS⁺96]. That is, we first compute all cliques of size 2, then use them to compute cliques of size 3, and so on until we compute all cliques of size less than or equal to κ .

Let C_k denote the set of all cliques of size equal to k . We give an inductive description of the procedure to generate the set C_k . The base case C_2 when $k = 2$ consists of all pairs of strongly connected attribute values in $\mathcal{D}_i$. These pairs can easily be found from Σ_{ii}^j . The set C_{k+1} is computed from the set C_k ($k \geq 2$) by “joining” C_k with itself. The join is the subset join—used in the candidate generation step of the frequent itemset computation in the apriori algorithm [AMS⁺96]. We also remove all the candidates in C_{k+1} that contain a proper k -subset not in C_k (a la subset pruning in apriori).

Extension Operation: In the second step, we “extend” some of the candidate distinguishing sets computed in the first step to compute cluster-projections on A_i of 2-clusters on (A_i, A_j) . The intuition behind the extension operation is illustrated in Figure 9. Suppose we want to extend $\{a_1, a_2\}$ on A with respect to B . We compute the set $\{b_1, b_2\}$ of attribute values on B strongly connected with $\{a_1, a_2\}$. We then extend $\{a_1, a_2\}$ with the set of all other values $\{a_3, a_4\}$ on A that is strongly connected with $\{b_1, b_2\}$.

Informally, the extension of a distinguishing set $S \subset \mathcal{D}_i$ adds to S all attribute values in $\mathcal{D}_i$ that are strongly connected with the set of all attribute values in $\mathcal{D}_j$ that S is strongly connected with. We now introduce the concepts of *sibling set*, *subset flag*, and the *participation count* to formally describe the extension operation.

Definition 4.1 Let A_i and A_j be two attributes with domains $\mathcal{D}_i$ and $\mathcal{D}_j$. Let $\mathcal{CS}_i^j$ be the set of cluster-projections on A_i of 2-clusters over (A_i, A_j) . Let $\mathcal{DS}_i^j$ be a set of candidate distinguishing sets, with respect to A_j , on attribute A_i . The *sibling set* S_i^j of $S_i \in \mathcal{DS}_i^j$ with respect to the attribute A_j is defined as follows:

$$S_i^j = \{a_j \in \mathcal{D}_j : \text{for all } a_i \in S_i, \sigma^*(a_i, a_j) > 0\}$$

$|S_i^j|$ is called the *sibling strength* of S_i with respect to A_j .

The *subset flag* of $S_i \in \mathcal{DS}_i^j$ with respect to a collection of sets $\mathcal{C}_s$ is said to be *set* (to 1) if there exists a set $S \in \mathcal{C}_s$ such that $S_i \subseteq S$. Otherwise, the subset flag of S_i is not set.

The *participation count* of $S_i \in \mathcal{DS}_i^j$ with respect to $\mathcal{C}_s$ is the sum of the sibling strengths with respect to A_j of all supersets of S_i in $\mathcal{C}_s$.

Informally, the subset flag and the participation count serve the following two purposes. First, a cluster-projection may consist of more than one distinguishing set in $\mathcal{DS}_i^j$. Therefore, if we extend each set in $\mathcal{DS}_i^j$ a particular cluster-projection may be generated several times, once for each distinguishing set it contains. To avoid the repeated generation of the same cluster-projection, we associate with each distinguishing set a subset flag. The subset flag indicates whether the distinguishing set is a subset of an existing cluster-projection in $\mathcal{CS}_i^j$. Therefore, if the subset flag is set then the distinguishing set need not be extended. For the example shown in Figure 7, the distinguishing sets $\{a_1\}$ and $\{a_2\}$ on A can both be extended to the cluster-projection $\{a_1, a_2\}$. Second, the distinguishing subset assumption applies only to cluster-projections of size greater than κ . Therefore, a clique of size less than or equal to κ may be a cluster-projection on its own even though it may be a subset of some other cluster-projection. To recognize such small cluster-projections, we associate a participation count with each distinguishing set. If the participation count of a distinguishing set with respect to $\mathcal{CS}_i^j$ is less than its sibling strength then it may be a small cluster-projection.

Algorithm 4.1 $\text{Extend}(\mathcal{DS}_i^j, \Sigma_{ij})$

/* Output: $\mathcal{CS}_i^j$ */

/* Initialization */

$\mathcal{CS}_i^j = \phi$

Reset the subset flags and the participation counts of all distinguishing sets in $\mathcal{DS}_i^j$ to zero

foreach $S_i \in \mathcal{DS}_i^j$

 if the subset flag of S_i is not set then

 Extend S_i to C_i^S

 Set the subset flags and increment by the sibling strength of S_i the participation counts of all subsets of C_i^S in $\mathcal{DS}_i^j$.

 end /*if*/

end /*for*/

Identify and add small cluster-projections (of size $\leq \kappa$) to $\mathcal{CS}_i^j$

The pseudocode for the computation of $\mathcal{CS}_i^j$ is shown in Algorithm 4.1. Below, we describe each step in detail.

Initialization: The first two steps initialize the procedure: we set $\mathcal{CS}_i^j = \phi$, and the subset flags and their participation counts of all distinguishing sets in $\mathcal{DS}_i^j$ to zero.

Extending S_i : Let S_i^j be the sibling set of S_i with respect to A_j . Let C_i^S be the sibling set of S_i^j with respect to A_i . Then, we extend S_i to the cluster-projection C_i^S . Add C_i^S to $\mathcal{CS}_i^j$.

Prune subsets of C_i^S : Suppose C_i^S was extended from S_i . Then, by definition, subsets of C_i^S cannot be the distinguishing sets of other cluster projections on A_i . Therefore, we set (to 1) all subset flags of subsets of C_i^S (including S_i) in $\mathcal{DS}_i^j$. The participation count of each of these subsets is also increased by $|S_i^j|$ —the sibling strength of S_i .

Identifying small cluster-projections: While extending distinguishing sets, we only choose sets whose subset flags are not set. We check if each unextended distinguishing set S_i whose subset flag is set can be a small (of size less than κ) cluster-projection. If the participation count of S_i equals its sibling strength, then S_i cannot be a cluster-projection on its own. Otherwise, S_i may be a cluster-projection. Therefore, we add S_i to $\mathcal{CS}_i^j$.

Note that the computation of cluster-projections on A_i requires only the inter-attribute summary Σ_{ij} and the intra-attribute summary Σ_{ii}^j . Since Σ_{ij} and Σ_{ii}^j fit into main memory, the computation is very fast.

Intersection of Cluster-projections

Informally, the intersection step computes the set of cluster-projections on A_i of clusters over $\{A_1, \dots, A_n\}$ by successively joining sets of cluster-projections on A_i of 2-clusters over attribute pairs (A_i, A_j) , $j \neq i$. For describing the procedure, we require the following definition.

Definition 4.2 Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be two collections of sets of attribute values on A_i . We define the *intersection join* $\mathcal{S}_1 \sqcap \mathcal{S}_2$ between $\mathcal{S}_1$ and $\mathcal{S}_2$ as follows: $\mathcal{S}_1 \sqcap \mathcal{S}_2 \stackrel{\text{def}}{=} \{s : \exists s_1 \in \mathcal{S}_1 \text{ and } s_2 \in \mathcal{S}_2 \text{ such that } s = s_1 \cap s_2 \text{ and } |s| > 1\}$

Let $\mathcal{CS}_i^j$ be the set of cluster-projections on A_i with respect to A_j , $j \neq i$. Let $j_1 = 1$ if $i > 1$, else $j_1 = 2$. Starting with $S = \mathcal{CS}_i^{j_1}$, the intersection step executes the following operation for all $k \neq i$.

$$S = S \sqcap \mathcal{CS}_i^k, \text{ if } k \neq i$$

The resulting set S is the set of cluster-projections on A_i of clusters over $\{A_1, \dots, A_n\}$. Besides being a main-memory operation, the number of cluster-projections on A_i with respect to any other attribute A_j is usually small; therefore, the intersection step is quite fast.

Further optimizations are possible over the basic strategy described above for computing cluster projections. For instance, we can combine the computation of $\mathcal{CS}_i^j$ and that of $\mathcal{CS}_j^i$ because, for each cluster-projection in $\mathcal{CS}_i^j$, we compute its sibling set which is a cluster-projection in $\mathcal{CS}_j^i$. However, we do not consider such optimizations because the clustering phase takes a small fraction (less than 10%) of the time taken by the summarization phase. (Our experiments in Section 6 confirm this observation.)

4.2.2 Level-wise Synthesis of Clusters

In this section, we describe the synthesis of candidate clusters from the cluster-projections on individual attributes (computed as described in Section 4.2). The central idea is that a

cluster on a set of attributes induces a sub-cluster on any subset of the attributes (*monotonicity property*). The monotonicity property follows directly from the definition of a cluster. We also exploit the fact that we want to compute clusters over the set of all attributes $\{A_1, \dots, A_n\}$. Informally, we start with cluster-projections on A_1 and then extend them to clusters over (A_1, A_2) , then to clusters over (A_1, A_2, A_3) , and so on.

Let $\mathcal{C}_i$ be the set of cluster-projections on the attribute A_i , $i = 1, \dots, n$. Let $\mathcal{C}^k$ denote the set of candidate clusters defined over the set of attributes $A_1, \dots, A_k$. Therefore, $\mathcal{C}^1 = \mathcal{C}_1$. We successively generate $\mathcal{C}^{k+1}$ from $\mathcal{C}^k$ until $\mathcal{C}^n$ is generated or $\mathcal{C}^{k+1}$ is empty for some $k + 1 < n$. The generation of $\mathcal{C}^{k+1}$ from $\mathcal{C}^k$ proceeds as follows. Set $\mathcal{C}^{k+1} = \phi$. For each element $c^k = \langle c_1, \dots, c_k \rangle \in \mathcal{C}^k$, we attempt to augment c^k with a cluster projection c_{k+1} on the attribute A_{k+1} . If for all $i \in \{1, \dots, k\}$, $\langle c_i, c_{k+1} \rangle$ is a sub-cluster on (A_i, A_{k+1}) —which can be checked by looking up $\Sigma_{i(k+1)}$ —we augment c^k to $c^{k+1} = \langle c_1, \dots, c_{k+1} \rangle$ and add c^{k+1} to $\mathcal{C}^{k+1}$.

For the example in Figure 7, the computation of the set of candidate clusters proceeds as follows. We start with the set $\{a_1, a_2\}$ on A . We then find the candidate 2-cluster $\{\langle \{a_1, a_2\}, \{b_1, b_2\} \rangle\}$ over the attribute pair (A, B) , and then the candidate 3-cluster $\{\langle \{a_1, a_2\}, \{b_1, b_2\}, \{c_1, c_2\} \rangle\}$ over $\{A, B, C\}$.

4.3 Validation

We now describe a procedure to compute the set of actual clusters from the set of candidate clusters. Some of the candidate clusters may not have enough support because some of the 2-clusters that combine to form a candidate cluster may be due to different sets of tuples. To recognize such false candidates, we check if the support of each candidate cluster is greater than the required threshold. Only clusters whose support on D passes the threshold requirement are retained.

After setting the supports of all candidate clusters to zero, we start scanning the dataset D . For each tuple $t \in D$, we increment the support of the candidate cluster to which t belongs. (Because the set of clusters correspond to disjoint interval regions, t can belong to at most one cluster.) At the end of the scan, we delete all candidate clusters whose support in the dataset D is less than the required threshold: α times the expected support of the cluster under the attribute-independence assumption.

By construction, CACTUS discovers all clusters that satisfy our cluster definition, and hence the following theorem holds.

Theorem 4.1 Given that the distinguishing subset assumption holds, CACTUS finds all and only those clusters that satisfy Definition 3.3.

5 Extensions

In this section, we extend CACTUS to handle unusually large attribute value domains as well as to identify clusters in subspaces.

5.1 Large Attribute Value Domains

Until now, we assumed that the domains of categorical attributes are such that the inter-attribute summary of any pair of attributes and the intra-attribute summary of any attribute fits in main memory. For the sake of completeness, we modify the summarization phase of CACTUS to handle arbitrarily large domain sizes.

Recall that the summary information only consists of strongly connected pairs of attribute values. For large domain sizes, the number of strongly connected attribute value pairs (either from the same or from different attributes) relative to the number of all possible attribute value pairs is very small. We exploit this observation to collapse sets of attribute values on each attribute into a single attribute value thus creating a new domain of smaller size. The intuition is that if a pair of attribute values in the original domain are strongly connected, then the corresponding pair of transformed attribute values are also strongly connected, provided the threshold for strong connectivity between attribute values in the transformed domain is the same as that for the original domain.

Let A_i be an attribute with an unusually large domain $\mathcal{D}_i$. Without loss of generality, let $\mathcal{D}_i$ be the set $\{1, \dots, |\mathcal{D}_i|\}$. Let $M < |\mathcal{D}_i|$ be the maximum number of attribute values per attribute so that the inter-attribute summaries and the intra-attribute summaries fit into main memory. Let $c = \lceil \frac{|\mathcal{D}_i|}{M} \rceil$. We construct $\mathcal{D}'_i$ of size M from $\mathcal{D}_i$ by mapping for a given $x \in \{0, \dots, M-1\}$, the set of attribute values $\{x \cdot c + 1, \dots, x \cdot c + c\}$ to the value $x + 1$. Formally,

$$\mathcal{D}'_i = \{f(1), \dots, f(|\mathcal{D}_i|)\}, \text{ where } f(i) = \lfloor \frac{i}{c} \rfloor + 1$$

We set the threshold for the strong connectivity involving attribute values in $\mathcal{D}'_i$ as if $\mathcal{D}_i$ was being used. We then compute the inter-attribute summaries involving A_i using the transformed domain $\mathcal{D}'_i$. For each attribute value $a'_i \in \mathcal{D}'_i$ that participates in a strongly connected pair (a'_i, a_j) ($a_j \in \mathcal{D}_j$, $j \neq i$), we expand a'_i to the set of all attribute values $\{a'_i \cdot c + 1, \dots, a'_i \cdot c + c\} \subset \mathcal{D}_i$ that map into a'_i and form the pairs $(a'_i \cdot c + 1, a_j), \dots, (a'_i \cdot c + c, a_j)$. We then scan the dataset D to count the supports of all these pairs, and select the strongly connected pairs among them; they constitute the inter-attribute summary Σ_{ij} .

The number of new pairs whose supports are to be counted is less than or equal to $c \cdot |\Sigma_{ij}|$ where $|\Sigma_{ij}|$ represents the number of strongly connected pairs in $\mathcal{D}_i \times \mathcal{D}_j$. If this set of pairs is still larger than main memory, we can repeat the above transformation trick. However, we believe that such repeated application will be rare.

5.2 Clusters in Subspaces

CACTUS does not discover clusters in subspaces for the following reason. The order $A_1, \dots, A_n$ in which cluster-projections on individual attributes are combined may not be the right order to find a subspace cluster C . For instance, if C spans the subspace defined by a set of attributes $\{A_2, A_3, A_4\}$

(when $n \geq 4$) then the level-wise synthesis described in Section 4.2.2 will not find C .

The extension to find subspace clusters exploits the monotonicity property of subspace clusters. That is, a cluster in a subspace S induces a subcluster on any subset of S . The monotonicity property again motivates the apriori-style level-wise synthesis of candidate clusters from the cluster-projections on individual attributes. The algorithm differs in two ways from the algorithm to find clusters over all attributes. The first difference is that we do not restrict that a cluster-projection on an attribute should participate in 2-cluster with every other attribute. The second difference is in the procedure for generating the set of candidate clusters. We now discuss both differences.

We skip the intersection of cluster-projections on each attribute A_i with respect to every other attribute A_j ($j \neq i$) for the following two reasons. First, a cluster in subspace S may not induce a 2-cluster on a pair of attributes not in S , and hence the intersection of cluster-projections on an attribute in S with respect to every other attribute may return an empty set. Second, the intersection may cause the loss of maximality (condition (2) in Definition 3.3) of a subspace cluster. For instance, a cluster-projection on A_i with respect to A_j corresponds to a 2-cluster over (A_i, A_j) which, by definition, is a subspace cluster; truncating such a cluster-projection in the intersection step will no longer yield a maximal cluster on (A_i, A_j) .

In the candidate generation algorithm, we let $\mathcal{C}^k$ denote the set of candidate clusters defined on any set of k -attributes (not necessarily $\{A_1, \dots, A_k\}$). Otherwise, the candidate generation proceeds exactly as in Section 4.2.2. The reason is that a subspace cluster on k attributes may not always be in the first k attributes.

For a cluster $c \in \mathcal{C}^k$ in a subspace consisting of k attributes, the above candidate generation procedure examines $2^k - (k + 1)$ candidates. Depending on the value of k (say, larger than 15), the number of candidate clusters can be prohibitively high. The problem of examining a large number of candidate clusters has been addressed by Agrawal et al. [AGGR98]. They use the *minimum description length* principle to prune the number of candidate clusters. Their techniques apply directly in our scenario as well. Therefore, we do not address this problem; instead, we refer the reader to the original paper [AGGR98].

6 Performance Evaluation

In this section, we show the results of a detailed evaluation of the speed and scalability of CACTUS on synthetic and real datasets. We also compared the performance of CACTUS with the performance of STIRR.⁹ Our results show that CACTUS is very fast and scalable; it outperforms STIRR by a factor between 3 and 10.

⁹We intend to compare CACTUS and ROCK after our ongoing implementation of ROCK is complete.

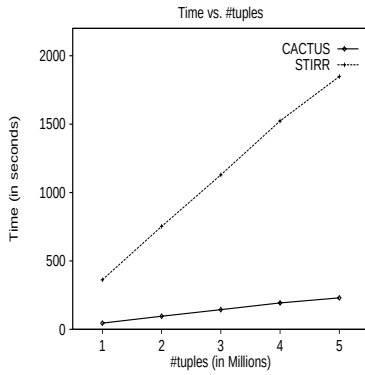


Figure 10: Time vs. #Tuples

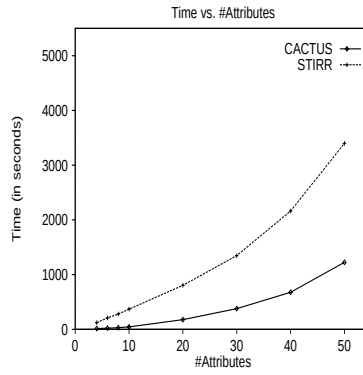


Figure 11: Time vs. #Attributes

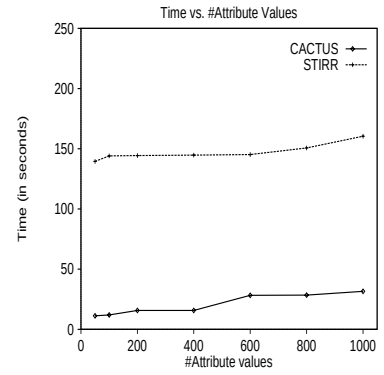


Figure 12: Time vs. #Attr-values

First Author	First Author (contd.)	Second Author	Second Author (contd.)
Katz, Stonebraker, Wong	Ceri, Navathe	Katz, Wong	Ceri, Navathe
DeWitt, Hsiao	Abiteboul, Grumbach	DeWitt, David	Vianu, Grumbach
DeWitt, Ghandeharizadeh	Korth, Levy	DeWitt, Ghandeharizadeh	Silberschatz, Levy
Kanellakis, Beer, Vardi	Agrawal, Gehani	Abiteboul, Beer	Jagadish, Gehani
Ramakrishnan, Beer	Chen, Hua, Su	Beer, Srivastava	Su, Chen, Chu
Bancilhon, Kifer	Chen, Hua, Lam	Ramakrishnan, Kim	Su, Lee
Afrati, Cosmadakis	Collmeyer, King, Shemer	Papadimitriou, Cosmadakis	Collmeyer, Shemer
Alonso, Barbara, GarciaMolina	Copeland, Lipovski, Su	GarciaMolina, Barbara	Su, Lipovski, Copeland
Devor, Elmasri	Cornell, Dan, Iyer, Yu	Devor, ElMasri, Weeldreyer	Yu, Dias
Barsolou, Keller, Wiederhold	Chang, Gupta	Keller, Wiederhold	Lee, Cheng
Barsalou, Keller, Shalom	Fischer, Griffeth, Lynch	Keller, Wiederhold	Griffeth, Fischer

Table 1: 2-clusters on the pair of first author and second author attributes

6.1 Synthetic Datasets

We first present our experiments on synthetic datasets. The test datasets were generated using the data generator developed by Gibson et al. [GKR98] to evaluate STIRR. (See Section 3.2 for a description of the data generator.) We set the number of tuples to 1 million, the number of attributes to 10 and the number of attribute values for each attribute to 100. In all datasets, the cluster-projections on each attribute were $[0, 9]$ and $[10, 19]$ (as shown in Figure 1). We fix the value of α at 3, and the value of the distinguishing number κ at 2. For STIRR, we fixed the number of iterations to be 10—as suggested by Gibson et al. [GKR98].

CACTUS discovered the clusters in the input datasets shown in Figures 1, 2, and 3.

Figure 10 plots the running time while increasing the number of tuples from 1 to 5 million. Figure 11 plots the running time while increasing the number of attributes from 4 to 50. Figure 12 plots the running time while increasing the number of attribute values from 50 to 1000 while fixing the number of attributes at 4. While varying the number of attribute values, we assumed that until 500 attribute values, the inter-attribute summaries would fit into main memory; for a larger number of attribute values we took the multi-layered approach described in Section 5. In all cases, CACTUS is 3 to 10 times faster than STIRR.

6.2 Real Datasets

In this section, we discuss an application of CACTUS to a combination of two sets of bibliographic entries. The results from the application show that CACTUS finds intuitively meaningful clusters from the dataset thus supporting our definition of a cluster.

The first set consists of 7766 bibliographic entries for articles related to database research [Wie] and the second set consists of 30919 bibliographic entries for articles related to Theoretical Computer Science and related areas [Sei]. For each article, we use the following four attributes: the first author, the second author, the conference or the journal of publication, and the year. If an article is singly-authored then the author’s name is repeated in the second author attribute as well. The sizes of the first author, the second author, the conference, and the year attribute domains for the database-related, the theory-related, and the combined sets are $\{3418, 3529, 1631, 44\}$, $\{8043, 8190, 690, 42\}$, and $\{10212, 10527, 2315, 52\}$ respectively. We combined the two sets together to check if CACTUS is able to identify the differences and the overlap between the two communities. Note that for these domains, some of the inter-attribute summaries and the intra-attribute summaries—especially those involving the first author and the second author dimensions—do not fit in main memory. However, we choose this particular dataset because it is easier to verify the validity of the resulting clusters (than for some other

Table 2: Cluster-projections on Conference w.r.t. the First Author

publicly available datasets, e.g., the MUSHROOM dataset from the UCI Machine Learning repository).

Table 5.1 shows some of the 2-clusters on the first author and the second author attribute pair. We only present the database-related cluster-projections to illustrate that CACTUS identifies the differences between the two communities. We verified the validity of each cluster-projection by querying on the *Database Systems and Logic Programming* bibliography at the web site maintained by Michael Ley [Ley]. Similar cluster-projections identifying groups of theory-related researchers as well as groups that contribute to both fields also exist. Due to space constraints, we show some cluster-projections corresponding to the latter two types in the full paper [GGR99].

Table 2 shows some of the cluster-projections on the conference attribute computed with respect to the first author attribute. The first row consists exclusively of a group of database-related conferences, the second consists exclusively of theory-related conferences, and the third a mixture of both reflecting a considerable overlap between the two communities.

7 Conclusions and Future Work

In this paper, we formalized the definition of a cluster when the data consists of categorical attributes, and then introduced a fast summarization-based algorithm CACTUS for discovering such clusters in categorical data. We then evaluated our algorithm against both synthetic and real datasets.

In future, we intend to extend CACTUS in the following three directions. First, we intend to relax the cluster definition by allowing sets of attribute values on each attribute which are “almost” strongly connected to each other. Second, motivated by the observation that inter-attribute summaries can be incrementally maintained under addition and deletion of tuples, we intend to derive an incremental clustering algorithm from CACTUS. Third, we intend to “rank” the clusters based on a measure of interestingness, say, some function of the support of a cluster.

Acknowledgements: We thank Prabhakar Raghavan for sending us the bibliographic data.

References

- [AGGR98] Rakesh Agrawal, Johannes Gehrke, Dimitrios Gunopulos, and Prabhakar Raghavan. Automatic subspace clustering of high dimensional data for data mining. In *Proceedings of the ACM SIGMOD Conference on Management of Data*, 1998.
- [AMS⁺96] Rakesh Agrawal, Heikki Mannila, Ramakrishnan Srikant, Hannu Toivonen, and A. Inkeri Verkamo. Fast Discovery of Association Rules. In Usama M. Fayyad, Gregory Piatetsky-Shapiro, Padhraic Smyth, and Ramasamy Uthurusamy, editors, *Advances in Knowledge Discovery and Data Mining*, chapter 12, pages 307–328. AAAI/MIT Press, 1996.
- [BD76] Peter J. Bickel and Kjell A. Doksum. *Mathematical Statistics: Basic Ideas and Selected Topics*. Prentice Hall, 1976.
- [CBM98] E. Keogh C. Blake and C.J. Merz. UCI repository of machine learning databases, 1998.
- [Cou95] Transaction Processing Performance Council, May 1995. <http://www.tpc.org>.
- [CS96] P. Cheeseman and J. Stutz. Bayesian classification (autoclass): Theory and results. In U. Fayyad, G. Piatetsky-Shapiro, P. Smyth, and R. Uthurusamy, editors, *Advances in Knowledge Discovery and Data Mining*, pages 153–180. MIT Press, 1996.
- [DER86] I.S. Duff, A.M. Erisman, and J.K. Reid. *Direct Methods for Sparse Matrices*. Oxford University Press, 1986.
- [DLR77] A.P. Dempster, N.M. Laird, and D.B. Rubin. Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal Statistical Society*, 1977.
- [GGR99] Venkatesh Ganti, Johannes Gehrke, and Raghu Ramakrishnan. Cactus-clustering categorical data using summaries. <http://www.cs.wisc.edu/~vganti/demon/cactus-full.ps>, March 1999.
- [GJ79] M. R. Garey and D. S. Johnson. Computers and intractability — A guide to the theory of NP-completeness. *Freeman; Bell Lab, Murray Hill NJ*, 1979.
- [GKR98] David Gibson, Jon Kleinberg, and Prabhakar Raghavan. Clustering categorical data: An approach based on dynamical systems. In *Proceedings of the 24th International Conference on Very Large Databases*, pages 311–323, New York City, New York, August 24-27 1998.
- [GRS99] Sudipto Guha, Rajeev Rastogi, and Kyuseok Shim. Rock: A robust clustering algorithm for categorical attributes. In *Proceedings of the IEEE International Conference on Data Engineering*, Sydney, March 1999.
- [Ley] Michael Ley. Computer science bibliography. <http://www.informatik.uni-trier.de/~ley/db/index.html>.
- [Ram97] Raghu Ramakrishnan. *Database Management Systems*. McGraw Hill, 1997.
- [Sei] J. Seiferas. Bibliography on theory of computer science. <http://iinwww.ira.uka.de/bibliography/Theory/Seiferas>.
- [Wie] G. Wiederhold. Bibliography on database systems. <http://iinwww.ira.uka.de/bibliography/Database/Wiederhold>.