

Computing Multi-Relational Sufficient Statistics for Large Databases

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ABSTRACT

Databases contain information about which relationships do and do not hold among entities. To make this information accessible for statistical analysis requires computing sufficient statistics that combine information from different database tables. Such statistics may involve any number of *positive and negative* relationships. With a naive enumeration approach, computing sufficient statistics for negative relationships is feasible only for small databases. We solve this problem with a new dynamic programming algorithm that performs a virtual join, where the requisite counts are computed without materializing join tables. Contingency table algebra is a new extension of relational algebra, that facilitates the efficient implementation of this Möbius virtual join operation. The Möbius Join scales to large datasets (over 1M tuples) with complex schemas. Empirical evaluation with seven benchmark datasets showed that information about the presence and absence of links can be exploited in feature selection, association rule mining, and Bayesian network learning.

Categories and Subject Descriptors

H.2.8 [Database Applications]: Data mining; H.2.4 [Systems]: Relational databases

Keywords

sufficient statistics; multi-relational databases; virtual join; relational algebra

1. INTRODUCTION

Relational databases contain information about attributes of entities, and which relationships do and do not hold among entities. To make this information accessible for knowledge discovery requires computing *sufficient statistics*. For discrete data, these sufficient statistics are instantiation counts for conjunctive queries. For relational statistical analysis to discover cross-table correlations, sufficient statistics must combine information from different database

tables. This paper describes a new dynamic programming algorithm for computing cross-table sufficient statistics that may contain any number of *positive and negative* relationships. Negative relationships concern the nonexistence of a relationship. Our algorithm makes the joint presence/absence of relationships available as features for the statistical analysis of databases. For instance, such statistics are important for learning correlations between different relationship types (e.g., if user u performs a web search for item i , is it likely that u watches a video about i ?).

Whereas sufficient statistics with positive relationships only can be efficiently computed by SQL joins of existing database tables, a table join approach is not feasible for negative relationships. This is because we would have to enumerate all tuples of entities that are *not* related (consider the number of user pairs who are *not* friends on Facebook). The cost of the enumeration approach is close to materializing the Cartesian cross product of entity sets, which grows exponentially with the number of entity sets involved. It may therefore seem that sufficient statistics with negative relationships can be computed only for small databases. We show that on the contrary, assuming that sufficient statistics with positive relationships are available, extending them to negative relationships can be achieved in a highly scalable manner, which does not depend on the size of the database.

Virtual Join Approach. Our approach to this problem introduces a new virtual join operation. A virtual join algorithm computes sufficient statistics *without* materializing a cross product [16]. Sufficient statistics can be represented in contingency tables [6]. Our virtual join operation is a dynamic programming algorithm that successively builds up a large contingency table from smaller ones, *without a need to access the original data tables*. We refer to it as the Möbius Join since it is based on the Möbius extension theorem [12].

We introduce algebraic operations on contingency tables that generalize standard relational algebra operators. We establish a contingency table algebraic identity that reduces the computation of sufficient statistics with $k + 1$ negative relationships to the computation of sufficient statistics with only k negative relationships. The Möbius Join applies the identity to construct contingency tables that involve $1, 2, \dots, \ell$ relationships (positive and negative), until we obtain a joint contingency table for all tables in the database. A theoretical upper bound for the number of contingency table operations required by the algorithm is $O(r \log r)$, where r

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CIKM'14, November 3–7, 2014, Shanghai, China.
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<http://dx.doi.org/10.1145/2661829.2662010>

is the number of sufficient statistics involving negative relationships. In other words, the number of table operations is nearly linear in the size of the required output.

Evaluation. We evaluate the Möbius Join algorithm by computing contingency tables for seven real-world databases. The observed computation times exhibit the near-linear growth predicted by our theoretical analysis. They range from two seconds on the simpler database schemas to just over two hours for the most complex schema with over 1 million tuples from the IMDB database.

Given that computing sufficient statistics for negative relationships is *feasible*, the remainder of our experiments evaluate their *usefulness*. These sufficient statistics allow statistical analysis to utilize the absence or presence of a relationship as a feature. Our benchmark datasets provide evidence that the positive and negative relationship features enhance different types of statistical analysis, as follows. (1) Feature selection: When provided with sufficient statistics for negative and positive relationships, a standard feature selection method selects relationship features for classification. (2) Association Rule Mining: A standard association rule learning method includes many association rules with relationship conditions in its top 20 list. (3) Bayesian network learning. A Bayesian network provides a graphical summary of the probabilistic dependencies among relationships and attributes in a database. On the two databases with the most complex schemas, enhanced sufficient statistics lead to a clearly superior model (better data fit with fewer parameters). This includes a database that is an order of magnitude larger than the databases for which graphical models have been learned previously [11].

Contributions. Our main contributions are as follows.

1. A dynamic program to compute a joint contingency table for sufficient statistics that combine several tables, and that may involve any number of *positive and negative* relationships.
2. An extension of relational algebra for contingency tables that supports the dynamic program conceptually and computationally.

We contribute open-source code that implements the Möbius Join. All code and datasets are available on-line[4]. Our implementation makes extensive use of RDBMS capabilities. Like the BayesStore system [15], our system treats statistical components as first-class citizens in the database. Contingency tables are stored as database tables in addition to the original data tables. We use SQL queries to construct initial contingency tables and to implement contingency table algebra operations.

Paper Organization. We review background for relational databases and statistical concepts. The main part of the paper describes the dynamic programming algorithm for computing a joint contingency table for all random variables. We define the contingency table algebra. A complexity analysis establishes feasible upper bounds on the number of contingency table operations required by the Möbius Join algorithm. We also investigate the scalability of the algorithm

empirically. The final set of experiments examines how the cached sufficient statistics support the analysis of cross-table dependencies for different learning and data mining tasks.

2. BACKGROUND AND NOTATION

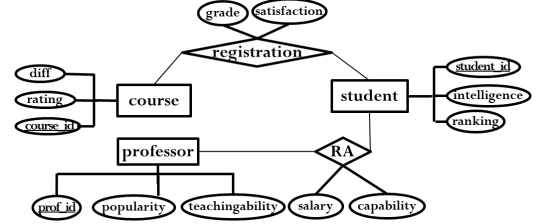


Figure 1: A relational ER Design. Registration and RA are many-to-many relationships.

We assume a standard **relational schema** containing a set of tables, each with key fields, descriptive attributes, and possibly foreign key pointers. A **database instance** specifies the tuples contained in the tables of a given database schema. We assume that tables in the relational schema can be divided into *entity tables* and *relationship tables*. This is the case whenever a relational schema is derived from an entity-relationship model (ER model) [14, Ch.2.2]. A **table join** of two or more tables contains the rows in the Cartesian products of the tables whose values match on common fields.

2.1 Relational Random Variables

We adopt function-based notation from logic for combining statistical and relational concepts [9]. A domain or **population** is a set of individuals. Individuals are denoted by lower case expressions (e.g., *bob*). A **functor** represents a mapping $f : \mathcal{P}_1, \dots, \mathcal{P}_a \rightarrow V_f$ where f is the name of the functor, each \mathcal{P}_i is a population, and V_f is the output type or **range** of the functor. In this paper we consider only functors with a finite range, disjoint from all populations. If $V_f = \{T, F\}$, the functor f is a (Boolean) **predicate**. A predicate with more than one argument is called a **relationship**; other functors are called **attributes**. We use uppercase for predicates and lowercase for other functors. Throughout this paper we assume that all relationships are binary, though this is not essential for our algorithm.

A (**Parametrized**) **random variable** (PRV) is of the form $f(\mathbb{X}_1, \dots, \mathbb{X}_a)$, where each \mathbb{X}_i is a first-order variable [8]. Each first-order variable is associated with a population/type.

Student			Course			Professor		
s_id	intelligence	ranking	c_id	rating	difficulty	p_id	popularity	teachingability
jack	3	1	101	3	2	jim	2	1
kim	2	1	102	2	1	oliver	3	1
paul	1	2	103	2	1	david	2	2

(a)

RA			
s_id	p_id	salary	capability
jack	oliver	High	3
kim	oliver	Low	1
paul	jim	Med	2
kim	david	High	2

(d)

Registration			
s_id	c_id	grade	satisfaction
jack	101	1	1
jack	102	2	2
kim	102	3	1
paul	101	2	1

(e)

Figure 2: Database Instance based on Figure 1.

ER Diagram	Type	Functor	Random Variable
Relation Tables	RVars	RA	$RA(\mathbb{P}, \mathbb{S})$
Entity Attributes	$1Atts$	intelligence, ranking	$\{intelligence(\mathbb{S}), ranking(\mathbb{S})\} = 1Atts(\mathbb{S})$
Relationship Attributes	$2Atts$	capability, salary	$\{capability(\mathbb{P}, \mathbb{S}), salary(\mathbb{P}, \mathbb{S})\} = 2Atts(RA(\mathbb{P}, \mathbb{S}))$

Table 1: Translation from ER Diagram to Random Variables.

The functor formalism is rich enough to represent the constraints of an entity-relationship schema via the following translation: Entity sets correspond to populations, descriptive attributes to functions, relationship tables to relationships, and foreign key constraints to type constraints on the arguments of relationship predicates. Table 1 illustrates this translation, distinguishing attributes of entities ($1Atts$) and attributes of relationships ($2Atts$).

2.2 Contingency Tables

Sufficient statistics can be represented in *contingency tables* as follows [6].

Consider a fixed list of random variables. A **query** is a set of (*variable* = *value*) pairs where each value is of a valid type for the random variable. The **result set** of a query in a database \mathcal{D} is the set of instantiations of the first-order variables such that the query evaluates as true in \mathcal{D} . For example, in the database of Figure 2 the result set for the query ($intelligence(\mathbb{S}) = 2$, $rank(\mathbb{S}) = 1$, $popularity(\mathbb{P}) = 3$, $teachingability(\mathbb{P}) = 1$, $RA(\mathbb{P}, \mathbb{S}) = T$) is the singleton $\{(kim, oliver)\}$. The **count** of a query is the cardinality of its result set.

For every set of variables $\mathbf{V} = \{V_1, \dots, V_n\}$ there is a **contingency table** $ct(\mathbf{V})$. This is a table with a row for each of the possible assignments of values to the variables in \mathbf{V} , and a special integer column called *count*. The value of the *count* column in a row corresponding to $V_1 = v_1, \dots, V_n = v_n$ records the count of the corresponding query. Figure 3 shows the contingency table for the university database. The value of a relationship attribute is undefined for entities that are not related. Following [9], we indicate this by writing $capability(\mathbb{P}, \mathbb{S}) = n/a$ for a reserved constant n/a . The assertion $capability(\mathbb{P}, \mathbb{S}) = n/a$ is therefore equivalent to the assertion that $RA(\mathbb{P}, \mathbb{S}) = F$. A **conditional contingency**

Count	Diff.	Rat.	Pop.	Teach.	Intel.	Rank.	Cap.	Sal.	Grade	Sat.	RA	Reg.
1	1	1	1	2	3	1	3	High	1	1	T	T
1	1	2	1	2	2	2	n/a	n/a	2	2	F	T
3	1	2	1	2	2	2	1	Med	n/a	n/a	T	F
24	2	1	1	2	1	5	n/a	n/a	n/a	n/a	F	F
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1	2	1	2	2	1	4	n/a	n/a	3	2	F	T

Figure 3: Excerpt from the joint contingency table for the university database of Figure 2.

table, written

$$ct(V_1, \dots, V_k | V_{k+1} = v_{k+1}, \dots, V_{k+m} = v_{k+m})$$

is the contingency table whose column headers are V_1, \dots, V_k and whose rows comprise the subset that match the conditions to the right of the $|$ symbol. We assume that contingency tables omit rows with count 0.

3. RELATIONAL CONTINGENCY TABLES

Many relational learning algorithms take an iterative deepening approach: explore correlations along a single relationship, then along relationship chains of length 2, 3, etc. Chains of relationships form a natural lattice structure, where iterative deepening corresponds to moving from the bottom to the top. The Möbius Join algorithm computes contingency tables by reusing the results for smaller relationships for larger relationship chains.

A relationship variable set is a **chain** if it can be ordered as a list $[R_1(\tau_1), \dots, R_k(\tau_k)]$ such that each relationship variable $R_{i+1}(\tau_{i+1})$ shares at least one first-order variable with the preceding terms $R_1(\tau_1), \dots, R_i(\tau_i)$. All sets in the lattice are constrained to form a chain. For instance, in the University schema of Figure 1, a chain is formed by the two relationship variables

$$Registration(\mathbb{S}, \mathbb{C}), RA(\mathbb{P}, \mathbb{S}).$$

If relationship variable $Teaches(\mathbb{P}, \mathbb{C})$ is added, we may have a three-element chain

$$Registration(\mathbb{S}, \mathbb{C}), RA(\mathbb{P}, \mathbb{S}), Teaches(\mathbb{P}, \mathbb{C}).$$

The subset ordering defines a lattice on relationship sets/chains. Figure 4 illustrates the lattice for the relationship variables in the university schema. For reasons that we explain below, entity tables are also included in the lattice and linked to relationships that involve the entity in question. With

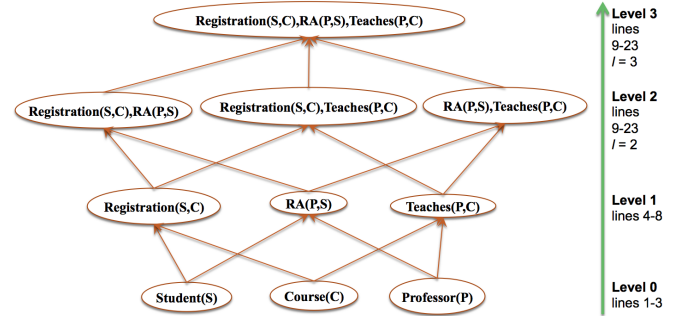


Figure 4: A lattice of relationship sets for the university schema of Figure 1. The Möbius Join constructs contingency table tables for each relationship chain for each level ℓ of the lattice. We reference the lines of the pseudo-code in Algorithm 2.

each relationship chain \mathbf{R} (Rchain for short) is associated a *ct*-table $ct_{\mathbf{R}}$. The variables in the *ct*-table $ct_{\mathbf{R}}$ comprise the relationship variables in \mathbf{R} , and the unary/binary descriptive attributes associated with each of the relationships. To define these, we introduce the following notation (cf. Table 1).

- $1Atts(\mathbb{A})$ denotes the attribute variables of a first-order variable \mathbb{A} collectively (1 for unary).

- $1Atts(\mathbf{R})$ denotes the set of entity attribute variables for the first-order variables that are involved in the relationships in \mathbf{R} .
- $2Atts(\mathbf{R})$ denotes the set of relationship attribute variables for the relationships in \mathbf{R} (2 for binary).
- $Atts(\mathbf{R}) \equiv 1Atts(\mathbf{R}) \cup 2Atts(\mathbf{R})$ is the set of all attribute variables in the relationship chain \mathbf{R} .

In this notation, the variables in the ct -table $ct_{\mathbf{R}}$ are denoted as $\mathbf{R} \cup Atts(\mathbf{R})$. The goal of the Möbius Join algorithm is to compute a contingency table for each chain \mathbf{R} . In the example of Figure 4, the algorithm computes 10 contingency tables. The ct -table for the top element of the lattice is the **joint ct -table** for the entire database.

If a conjunctive query involves only positive relationships, then it can be computed using SQL's count aggregate function applied to a table join. To illustrate, we show the SQL for computing the positive relationship part of the ct -table for the $RA(\mathbb{P}, \mathbb{S})$ chain.

```
CREATE TABLE  $ct_T$  AS
SELECT Count(*) as count, student.ranking,
student.intelligence, professor.popularity,
professor.teachingability, RA.capability, RA.salary
FROM professor, student, RA
WHERE
RA.p_id = professor.p_id and RA.s_id = student.s_id
GROUP BY student.ranking, student.intelligence,
professor.popularity, professor.teachingability, RA.capability,
RA.salary
```

Even more efficient than SQL count queries is the Tuple ID propagation method, a Möbius Join method for computing query counts with positive relationships only [16]. In the next section we assume that contingency tables for positive relationships only have been computed already, and consider how such tables can be extended to full contingency tables with both positive and negative relationships.

4. COMPUTING CONTINGENCY TABLES FOR NEGATIVE RELATIONSHIPS

We describe a Virtual Join algorithm that computes the required sufficient statistics without materializing a cross product of entity sets. First, we introduce an extension of relational algebra that we term **contingency table algebra**. The purpose of this extension is to show that query counts using $k + 1$ negative relationships can be computed from two query counts that each involve at most k relationships. Second, a dynamic programming algorithm applies the algebraic identify repeatedly to build up a complete contingency table from partial tables.

4.1 Contingency Table Algebra

We introduce relational algebra style operations defined on contingency tables.

4.1.1 Unary Operators

Selection $\sigma_{\phi} ct$ selects a subset of the rows in the ct -table that satisfy condition ϕ . This is the standard relational algebra operation except that the selection condition ϕ may not involve the *count* column.

Projection $\pi_{V_1, \dots, V_k} ct$ selects a subset of the columns in the ct -table, excluding the count column. The counts in the projected subtable are the sum of counts of rows that satisfy the query in the subtable. The ct -table projection $\pi_{V_1, \dots, V_k} ct$ can be defined by the following SQL code template:

```
SELECT SUM(count) AS count,  $V_1, \dots, V_k$ 
FROM  $ct$ 
GROUP BY  $V_1, \dots, V_k$ 
```

Conditioning $\chi_{\phi} ct$ returns a conditional contingency table. Ordering the columns as $(V_1, \dots, V_k, \dots, V_{k+j})$, suppose that the selection condition is a conjunction of values of the form

$$\phi = (V_{k+1} = v_{k+1}, \dots, V_{k+j} = v_{k+j}).$$

Conditioning can be defined in terms of selection and projection by the equation:

$$\chi_{\phi} ct = \pi_{V_1, \dots, V_k} (\sigma_{\phi} ct)$$

4.1.2 Binary Operators

We use \mathbf{V} , \mathbf{U} in SQL templates to denote a list of column names in arbitrary order. The notation $ct_1.\mathbf{V} = ct_2.\mathbf{V}$ indicates an equijoin condition: the contingency tables ct_1 and ct_2 have the same column set \mathbf{V} and matching columns from the different tables have the same values.

Cross Product The **cross-product** of $ct_1(\mathbf{U})$, $ct_2(\mathbf{V})$ is the Cartesian product of the rows, where the product counts are the products of count. The cross-product can be defined by the following SQL template:

```
SELECT
( $ct_1.count * ct_2.count$ ) AS count,  $\mathbf{U}, \mathbf{V}$ 
FROM  $ct_1, ct_2$ 
```

Addition The **count addition** $ct_1(\mathbf{V}) + ct_2(\mathbf{V})$ adds the counts of matching rows, as in the following SQL template.

```
SELECT  $ct_1.count + ct_2.count$  AS count,  $\mathbf{V}$ 
FROM  $ct_1, ct_2$ 
WHERE  $ct_1.\mathbf{V} = ct_2.\mathbf{V}$ 
```

If a row appears in one ct -table but not the other, we include the row with the count of the table that contains the row.

Subtraction The **count difference** $ct_1(\mathbf{V}) - ct_2(\mathbf{V})$ equals $ct_1(\mathbf{V}) + (-ct_2(\mathbf{V}))$ where $-ct_2(\mathbf{V})$ is the same as $ct_2(\mathbf{V})$ but with negative counts. Table subtraction is defined only if (i) without the *count* column, the rows in ct_1 are a superset of those in ct_2 , and (ii) for each row that appears in both tables, the count in ct_1 is at least as great as the count in ct_2 .

4.1.3 Implementation

The selection operator can be implemented using SQL as with standard relational algebra. Projection with *ct*-tables requires use of the GROUP BY construct as shown in Section 4.1.1.

For addition/subtraction, assuming that a sort-merge join is used [14], a standard analysis shows that the cost of a sort-merge join is $size(table1) + size(table2) +$ the cost of sorting both tables.

The cross product is easily implemented in SQL as shown in Section 4.1.2. The cross product size is quadratic in the size of the input tables.

4.2 Lattice Computation of Contingency Tables

This section describes a method for computing the contingency tables level-wise in the relationship chain lattice. We start with a contingency table algebra equivalence that allows us to compute counts for rows with negative relationships from rows with positive relations. Following [6], we use a “don’t care” value $*$ to indicate that a query does not specify the value of a node. For instance, the query $R_1 = T, R_2 = *$ is equivalent to the query $R_1 = T$.

Algorithm 1: The Pivot function returns a conditional contingency table for a set of attribute variables and all possible values of the relationship R_{pivot} , including $R_{pivot} = F$. The set of conditional relationships $\mathbf{R} = (R_{pivot}, \dots, R_\ell)$ may be empty in which case the Pivot computes an unconditional *ct*-table.

Input: Two conditional contingency tables

$ct_T := ct(Vars, 2Atts(R_{pivot}) | R_{pivot} = T, \mathbf{R} = T)$
and $ct_* := ct(Vars | R_{pivot} = *, \mathbf{R} = T)$.

Precondition: The set *Vars* does not contain the relationship variable R_{pivot} nor any of its descriptive attributes $2Atts(R_{pivot})$.

Output: The conditional contingency table

$ct(Vars, 2Atts(R_{pivot}), R_{pivot} | \mathbf{R} = T)$.

- 1: $ct_F := ct_* - \pi_{Vars} ct_T$.
 {Implements the algebra Equation 1 in proposition 1.}
 - 2: $ct_F^+ := \text{extend } ct_F \text{ with columns } R_{pivot} \text{ everywhere false and } 2Atts(R_{pivot}) \text{ everywhere } n/a$.
 - 3: $ct_T^+ := \text{extend } ct_T \text{ with columns } R_{pivot} \text{ everywhere true}$.
 - 4: **return** $ct_F^+ \cup ct_T^+$
-

PROPOSITION 1. *Let R be a relationship variable and let \mathbf{R} be a set of relationship variables. Let *Vars* be a set of variables that does not contain R nor any of the $2Atts$ of R . Let $\mathbb{X}_1, \dots, \mathbb{X}_l$ be the first-order variables that appear in R but not in *Vars*, where l is possibly zero. Then we have*

$$\begin{aligned} ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = F) = \\ ct(Vars | \mathbf{R} = T, R = *) \times ct(\mathbb{X}_1) \times \dots \times ct(\mathbb{X}_l) \\ - ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = T). \end{aligned} \quad (1)$$

If $l = 0$, the equation holds without the cross-product term.

PROOF. The equation

$$\begin{aligned} ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = *) = \\ ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = T) + \\ ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = F) \end{aligned} \quad (2)$$

holds because the set $Vars \cup 1Atts(R)$ contains all first-order variables in R .¹ Equation (2) implies

$$\begin{aligned} ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = F) = \\ ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = *) - \\ ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = T). \end{aligned} \quad (3)$$

To compute the *ct*-table conditional on the relationship R being unspecified, we use the equation

$$\begin{aligned} ct(Vars \cup 1Atts(R) | \mathbf{R} = T, R = *) = \\ ct(Vars | \mathbf{R} = T, R = *) \times ct(\mathbb{X}_1) \times \dots \times ct(\mathbb{X}_l) \end{aligned} \quad (4)$$

which holds because if the set *Vars* does not contain a first-order variable of R , then the counts of the associated $1Atts(R)$ are independent of the counts for *Vars*. If $l = 0$, there is no new first-order variable, and Equation (4) holds without the cross-product term. Together Equations (3) and (4) establish the proposition. \square

Figure 5 illustrates Equation (1). The construction of the ct_F table in Algorithm 1 provides pseudo-code for applying Equation (1) to compute a complete *ct*-table, given a partial table where a specified relationship variable R is true, and another partial table that does not contain the relationship variable. We refer to R as the **pivot** variable. For extra generality, Algorithm 1 applies Equation (1) with a condition that lists a set of relationship variables fixed to be true. Figure 5 illustrates the Pivot computation for the case of only one relationship. Algorithm 2 shows how the Pivot operation can be applied repeatedly to find all contingency tables in the relationship lattice.

Initialization. Compute *ct*-tables for entity tables. Compute *ct*-tables for each single relationship variable R , conditional on $R = T$. If $R = *$, then no link is specified between the first-order variables involved in the relation R . Therefore the individual counts for each first-order variable are independent of each other and the joint counts can be obtained by the cross product operation. Apply the Pivot function to construct the complete *ct*-table for relationship variable R .

Lattice Computation. The goal is to compute *ct*-tables for all relationship chains of length > 1 . For each relationship chain, order the relationship variables in the chain arbitrarily. Make each relationship variable in order the Pivot variable R_i . For the current Pivot variable R_i , find the conditional *ct*-table where R_i is unspecified, and the subsequent relations R_j with $j > i$ are true. This *ct*-table can be computed from a *ct*-table for a shorter chain that has been constructed already. The conditional *ct*-table has been constructed already, where R_i is true, and the subsequent relations are true (see loop invariant). Apply the Pivot function to construct the complete *ct*-table, for any Pivot vari-

¹We assume here that for each first-order variable, there is at least one *1Att*, i.e., descriptive attribute.

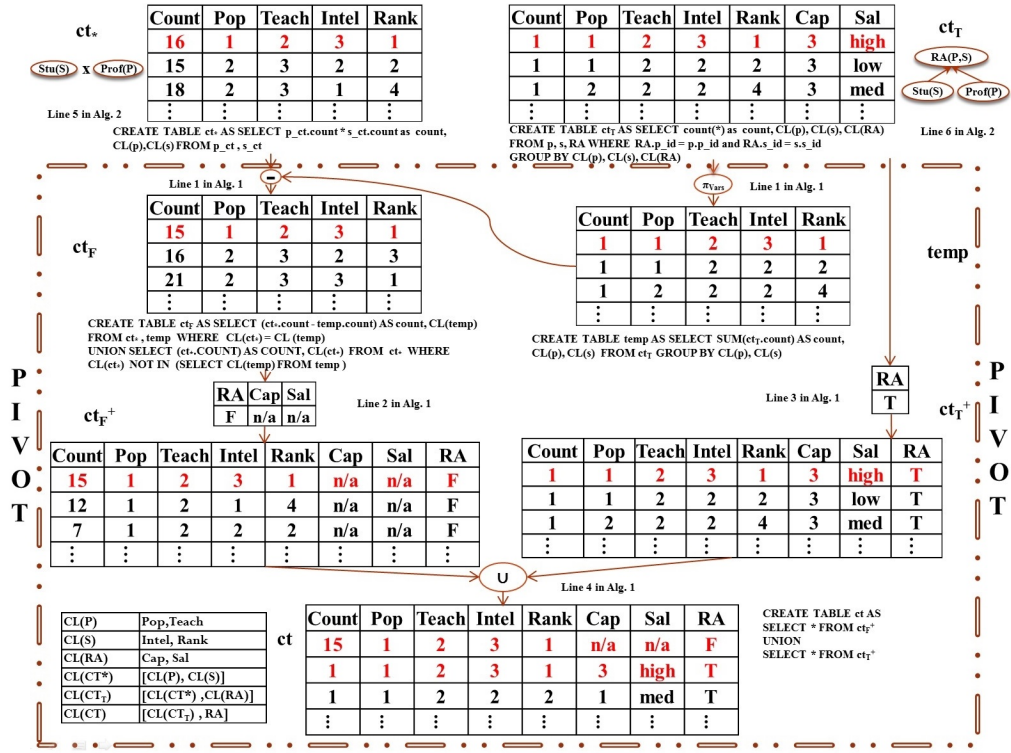


Figure 5: Top: Equation (1) is used to compute the conditional contingency table $ct_F = ct(1Atts(R)|R = F)$. (Set $Vars = \emptyset$, $R = RA(P, S)$, $R = \emptyset$). **Bottom:** The Pivot operation computes the contingency table $ct_{RA(P, S)}$ for the relationship $RA(P, S) := R_{pivot}$. The ct -table operations are implemented using dynamic SQL queries as shown. Lists of column names are abbreviated as shown and also as follows. $CL(ct_*) = CL(temp) = CL(ct_F)$, $CL(ct) = CL(ct_F^+) = CL(ct_T^+)$. We reference the corresponding lines of Algorithms 1 and 2.

able R_i , conditional on the subsequent relations being true.

lines	Operation	Resulting ct-table
11	$Reg(S, C) = T, RA(P, S) = T$	Current_ct
13-14	$i = 1, Reg(S, C) = *, RA(P, S) = T$	ct_*
20	PIVOT	Current_ct
16-18	$i = 2, RA(P, S) = *$	ct_*
20	PIVOT	Final ct-table for $Reg(S, C), RA(P, S)$

Figure 6: Illustrates the relationship chain loop of Algorithm 2 (lines 11-21) for the chain $R = Reg(S, C), RA(P, S)$. This loop is executed for each relationship chain at each level.

4.3 Complexity Analysis

The key point about the Möbius Join (MJ) algorithm is that it avoids materializing the cross product of entity tuples. The algorithm accesses only *existing* tuples, never constructs nonexisting tuples. The number of ct -table operation is therefore independent of the number of data records in the original database. We bound the total number of ct -

algebra operations performed by the Möbius Join algorithm in terms of the size of its output: the number of sufficient statistics that involve negative relationships.

PROPOSITION 2. The number of ct -table operations performed by the Möbius Join algorithm is bounded as

$$\#ct_ops = O(r \cdot \log_2 r)$$

where r is the number of sufficient statistics that involve negative relationships.

To analyze the computational cost, we examine the total number of ct -algebra operations performed by the Möbius Join algorithm. We provide upper bounds in terms of two parameters: the number of relationship nodes m , and the number of rows r in the ct -table that involve negative relationships. For these parameters we establish that

$$\#ct_ops = O(r \cdot \log_2 r) = O(m \cdot 2^m).$$

This shows the efficiency of our algorithm for the following reasons. (i) Since the time cost of any algorithm must be at least as great as the time for writing the output, which is at least as great as r , the Möbius Join algorithm adds at most a logarithmic factor to this lower bound. (ii) The second upper bound means that the number of ct -algebra

Algorithm 2: Möbius Join algorithm for Computing the Contingency Table for Input Database

Input: A relational database \mathcal{D} ; a set of variables

Output: A contingency table that lists the count in the database D for each possible assignment of values to each variable.

```
1: for all first-order variables  $\mathbb{X}$  do
2:   compute  $ct(1Atts(\mathbb{X}))$  using SQL queries.
3: end for
4: for all relationship variable  $R$  do
5:    $ct_* := ct(\mathbb{X}) \times ct(\mathbb{Y})$  where  $\mathbb{X}, \mathbb{Y}$  are the first-order variables in  $R$ .
6:    $ct_T := ct(1Atts(R)|R = T)$  using SQL joins.
7:   Call  $Pivot(ct_T, ct_*)$  to compute  $ct(1Atts(R), 2Atts(R), R)$ .
8: end for
9: for Rchain length  $\ell = 2$  to  $m$  do
10:  for all Rchains  $\mathbf{R} = R_1, \dots, R_\ell$  do
11:     $Current\_ct := ct(1Atts(R_1, \dots, R_\ell), 2Atts(R_1, \dots, R_\ell)|R_1 = T, \dots, R_\ell = T)$  using SQL joins.
12:    for  $i = 1$  to  $\ell$  do
13:      if  $i$  equals 1 then
14:         $ct_* := ct(1Atts(R_2, \dots, R_\ell), 2Atts(R_2, \dots, R_\ell)|R_1 = *, R_2 = T, \dots, R_\ell = T) \times ct(\mathbb{X})$  where  $\mathbb{X}$  is the first-order variable in  $R_1$ , if any, that does not appear in  $R_2, \dots, R_\ell$  { $ct_*$  can be computed from a  $ct$ -table for a Rchain of length  $\ell - 1$ .}
15:      else
16:         $1Atts_i := 1Atts(R_1, \dots, R_{i-1}, R_{i+1}, \dots, R_\ell)$ .
17:         $2Atts_i := 2Atts(R_1, \dots, R_{i-1}, R_{i+1}, \dots, R_\ell)$ .
18:         $ct_* := ct(1Atts_i, 2Atts_i, R_1, \dots, R_{i-1})|R_i = *, R_{i+1} = T, \dots, R_\ell = T) \times ct(\mathbb{Y})$  where  $\mathbb{Y}$  is the first-order variable in  $R_i$ , if any, that does not appear in  $\mathbf{R}$ .
19:      end if
20:       $Current\_ct := Pivot(Current\_ct, ct_*)$ .
21:    end for {Loop Invariant: After iteration  $i$ , the table  $Current\_ct$  equals  $ct(1Atts(R_1, \dots, R_\ell), 2Atts(R_1, \dots, R_\ell), R_1, \dots, R_i|R_{i+1} = T, \dots, R_\ell = T)$ }
22:  end for {Loop Invariant: The  $ct$ -tables for all Rchains of length  $\ell$  have been computed.}
23: end for
24: return the  $ct$ -table for the Rchain involves all the relationship variables.
```

operations is fixed-parameter tractable with respect to m .² In practice the number m is on the order of the number of tables in the database, which is very small compared to the number of tuples in the tables.

Derivation of Upper Bounds. For a given relationship chain of length ℓ , the Möbius Join algorithm goes through the chain linearly (Algorithm 2 inner for loop line 12). At each iteration, it computes a ct_* table with a single cross product, then performs a single Pivot operation. Each Pivot operation requires three ct -algebra operations. Thus overall, the number of ct -algebra operations for a relationship chain of length ℓ is $6 \cdot \ell = O(\ell)$. For a fixed length ℓ , there are at most $\binom{m}{\ell}$ relationship chains. Using the known identity³

$$\sum_{\ell=1}^m \binom{m}{\ell} \cdot \ell = m \cdot 2^{m-1} \quad (5)$$

we obtain the $O(m \cdot 2^{m-1}) = O(m \cdot 2^m)$ upper bound.

For the upper bound in terms of ct -table rows r , we note that the output ct -table can be decomposed into 2^m subtables, one for each assignment of values to the m relationship nodes. Each of these subtables contains the same number of rows d , one for each possible assignment of values to the attribute nodes. Thus the total number of rows is given by

²For arbitrary m , the problem of computing a ct table in a relational structure is #P-complete [1, Prop.12.4].

³math.wikia.com/wiki/Binomial_coefficient, Equation 6a

$r = d \cdot 2^m$. Therefore we have $m \cdot 2^m = \log_2(r/d) \cdot r/d \leq \log_2(r) \cdot r$. Thus the total number of ct -algebra operations is $O(r \cdot \log_2(r))$.

From this analysis we see that both upper bounds are over-estimates. (1) Because relationship chains must be linked by foreign key constraints, the number of valid relationship chains of length ℓ is usually much smaller than the number of all possible subsets $\binom{m}{\ell}$. (2) The constant factor d grows exponentially with the number of attribute nodes, so $\log_2(r) \cdot r$ is a loose upper bound on $\log_2(r/d) \cdot r/d$. We conclude that the number of ct -algebra operations is not the critical factor for scalability, but rather the cost of carrying out a single ct -algebra operation.

This means that if the number r of sufficient statistics is a feasible bound on computational time and space, then computing the sufficient statistics is feasible. In our benchmark datasets, the number of sufficient statistics was feasible, as we report below. In Section 8 below we discuss options in case the number of sufficient statistics grows too large.

5. EVALUATION OF CONTINGENCY TABLE COMPUTATION

We describe the system and the datasets we used. Code was written in Java, JRE 1.7.0. and executed with 8GB of RAM and a single Intel Core 2 QUAD Processor Q6700 with a clock speed of 2.66GHz (no hyper-threading). The operating system was Linux Centos 2.6.32. The MySQL Server version

5.5.34 was run with 8GB of RAM and a single core processor of 2.2GHz. All code and datasets are available on-line [4].

Dataset	#Relationship Tables/ Total	#Self Relationships	#Tuples	#Attributes
MovieLens	1 / 3	0	1,010,051	7
Mutagenesis	2 / 4	0	14,540	11
Financial	3 / 7	0	225,932	15
Hepatitis	3 / 7	0	12,927	19
IMDB	3 / 7	0	1,354,134	17
Mondial	2 / 4	1	870	18
UW-CSE	2 / 4	2	712	14

Table 2: Datasets characteristics. #Tuples = total number of tuples over all tables in the dataset.

5.1 Datasets

We used seven benchmark real-world databases. For detailed descriptions and the sources of the databases, please see reference [11]. Table 2 summarizes basic information about the benchmark datasets. A self-relationship relates two entities of the same type (e.g. *Borders* relates two countries in Mondial). Random variables for each database were defined as described in Section 2.1 (see also [11]). IMDB is the largest dataset in terms of number of total tuples (more than 1.3M tuples) and schema complexity. It combines the MovieLens database⁴ with data from the Internet Movie Database (IMDB)⁵ following [7].

5.2 Contingency Tables With Negative Relationships: Cross Product vs. Möbius Join

In this subsection we compare two different approaches for constructing the joint contingency tables for all variables together, for each database: Our Möbius Join algorithm (MJ) vs. materializing the cross product (CP) of the entity tables for each first-order variable (primary keys). Cross-checking the MJ contingency tables with the cross-product contingency tables confirmed the correctness of our implementation. Table 3 compares the time and space costs of the MJ vs. the CP approach. The cross product was materialized using an SQL query. The ratio of the cross product size to the number of statistics in the *ct*-table measures how much compression the *ct*-table provides compared to enumerating the cross product. It shows that cross product materialization requires an infeasible amount of space resources. The *ct*-table provides a substantial compression of the statistical information in the database, by a factor of over 4,500 for the largest database IMDB.

Dataset	MJ-time(s)	CP-time(s)	CP-#tuples	#Statistics	Compress Ratio
MovieLens	2.70	703.99	23M	252	93,053.32
Mutagenesis	1.67	1096.00	1M	1,631	555.00
Financial	1421.87	N.T.	149,046,585M	3,013,011	49,467,653.90
Hepatitis	3536.76	N.T.	17,846M	12,374,892	1,442.19
IMDB	7467.85	N.T.	5,030,412,758M	15,538,430	323,740,092.05
Mondial	1112.84	132.13	5M	1,746,870	2.67
UW-CSE	3.84	350.30	10M	2,828	3,607.32

Table 3: Constructing the contingency table for each dataset. M = million. N.T. = non-termination. Compress Ratio = CP-#tuples/#Statistics.

Computation Time. The numbers shown are the complete computation time for all statistics. For faster processing,

⁴www.grouplens.org, 1M version

⁵www.imdb.com, July 2013

both methods used a B+tree index built on each column in the original dataset. The MJ method also utilized B+ indexes on the *ct*-tables. We include the cost of building these indexes in the reported time. The Möbius Join algorithm returned a contingency table with negative relationships in feasible time. On the biggest dataset IMDB with 1.3 million tuples, it took just over 2 hours.

The cross product construction did not always terminate, crashing after around 4, 5, and 10 hours on Financial, IMDB and Hepatitis respectively. When it did terminate, it took orders of magnitude longer than the MJ method except for the Mondial dataset. Generally the higher the compression ratio, the higher the time savings. On Mondial the compression ratio is unusually low, so materializing the cross-product was faster.

Dataset	Link On	Link Off	#extra statistics	extra time (s)
MovieLens	252	210	42	0.27
Mutagenesis	1,631	565	1,066	0.99
Financial	3,013,011	8,733	3,004,278	1416.21
Hepatitis	12,374,892	2,487	12,372,405	3535.51
IMDB	15,538,430	1,098,132	14,440,298	4538.62
Mondial	1,746,870	0	1,746,870	1112.31
UW-CSE	2,828	2	2,826	3.41

Table 4: Number of Sufficient Statistics for Link Analysis On and Off. Extra Time refers to the total MJ time (Table 3 Col.2) minus the time for computing the positive statistics only.

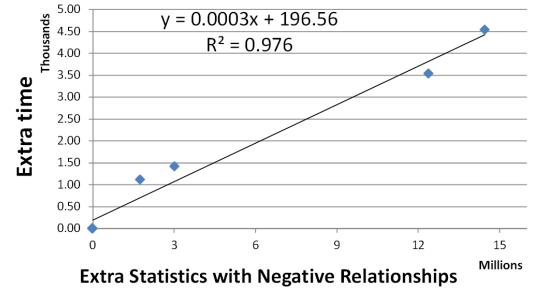


Figure 7: Möbius Join Extra Time (s)

5.3 Contingency Tables with Negative Relationships vs. Positive Relationships Only

In this section we compare the time and space costs of computing both positive and negative relationships, vs. positive relationships only. We use the following terminology. **Link Analysis On** refers to using a contingency table with sufficient statistics for both positive and negative relationships. An example is table *ct* in Figure 5. **Link Analysis Off** refers to using a contingency table with sufficient statistics for positive relationships only. An example is table *ct*_T in Figure 5. Table 4 shows the number of sufficient statistics required for link analysis on vs. off. The difference between the link analysis on statistics and the link analysis off statistics is the number of Extra Statistics. The Extra Time column shows how much time the MJ algorithm requires to compute the Extra Statistics *after* the contingency tables for positive relationships are constructed using SQL joins.

As Figure 7 illustrates, the Extra Time stands in a nearly linear relationship to the number of Extra Statistics, which confirms the analysis of Section 4.3. Figure 8 shows that most of the MJ run time is spent on the Pivot component (Algorithm 1) rather than the main loop (Algorithm 2). In terms of *ct*-table operations, most time is spent on subtraction/union rather than cross product.

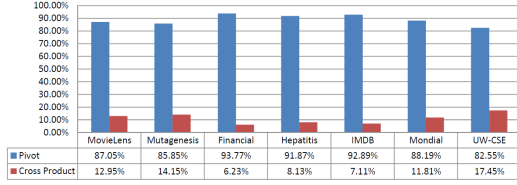


Figure 8: Breakdown of MJ Total Running Time

6. STATISTICAL APPLICATIONS

We evaluate using link analysis on three different types of cross-table statistical analysis: feature selection, association rule mining, and learning a Bayesian network.

6.1 Feature Selection

For each database, we selected a target for classification, then used Weka’s CFS feature subset selection method (Version 3.6.7) to select features for classification [3], given a contingency table. The idea is that if the existence of relationships is relevant to classification, then there should be a difference between the set selected with link analysis on and that selected with link analysis off. We measure how different two feature sets are by 1-Jaccard’s coefficient:

$$Distinctness(A, B) = 1 - \frac{A \cap B}{A \cup B}.$$

Dataset	Target variable	# Selected Attributes		Distinctness
		Link Analysis Off	Link Analysis On / Rvars	
MovieLens	Horror(M)	2	2 / 0	0.0
Mutagenesis	inda(M)	3	3 / 0	0.0
Financial	balance(T)	3	2 / 1	1.0
Hepatitis	sex(D)	1	2 / 1	0.5
IMDB	avg_revenue(D)	5	2 / 1	1.0
Mondial	percentage(C)	Empty CT	4 / 0	1.0
UW-CSE	courseLevel(C)	1	4 / 2	1.0

Table 5: Selected Features for Target variables for Link Analysis Off vs. Link Analysis On. Rvars denotes the number of relationship features selected.

Distinctness measures how different the selected feature subset is with link analysis on and off, on a scale from 0 to 1. Here 1 = maximum dissimilarity. Table 5 compares the feature sets selected. In almost all datasets, sufficient statistics about negative relationships generate new relevant features for classification. In 4/7 datasets, the feature sets are disjoint (coefficient = 1). For the Mutagenesis and MovieLens data sets, no new features are selected.

While Table 5 provides evidence that relationship features are relevant to the class label, it is not straightforward to

evaluate their usefulness by adding them to a relational classifier. The reason for this is that relational classification requires some kind of mechanism for aggregating/combining information from a target entity’s relational neighborhood. There is no standard method for performing this aggregation [2], so one needs to study the interaction of the aggregation mechanism with relationship features. We leave for future work experiments that utilize relationship features in combination with different relational classifiers.

6.2 Association Rules

A widely studied task is finding interesting association rules in a database. We considered association rules of the form *body* \rightarrow *head*, where *body* and *head* are conjunctive queries. An example of a cross-table association rule for Financial is

$$statement_freq.(Acc) = monthly \rightarrow HasLoan(Acc, Loan) = T.$$

We searched for interesting rules using both the link analysis off and the link analysis on contingency tables for each database. The idea is that if a relationship variable is relevant for other features, it should appear in an association rule. With link analysis off, all relationship variables always have the value T, so they do not appear in any association rule. We used Weka’s Apriori implementation to search for association rules in both modes. The interestingness metric was Lift. Parameters were set to their default values. Table 6 shows the number of rules that utilize relationship variables with link analysis on, out of the top 20 rules. In all cases, a majority of rules utilize relationship variables, in Mutagenesis and IMDB all of them do.

Dataset	MovieLens	Mutagenesis	Financial	Hepatitis	IMDB	Mondial	UW-CSE
# rules	14/20	20/20	12/20	15/20	20/20	16/20	12/20

Table 6: Number of top 20 Association Rules that utilize relationship variables.

6.3 Learning Bayesian Networks

Our most challenging application is constructing a Bayesian network (BN) for a relational database. For single-table data, Bayesian network learning has been considered as a benchmark application for precomputing sufficient statistics [6, 5]. A Bayesian network structure is a directly acyclic graph whose nodes are random variables. Given an assignment of values to its parameters, a Bayesian network represents a joint distribution over both attributes and relationships in a relational database. Several researchers have noted the usefulness of constructing a graphical statistical model for a relational database [13, 15]. For data exploration, a Bayes net model provides a succinct graphical representation of complex statistical-relational correlations. The model also supports probabilistic reasoning for answering “what-if” queries about the probabilities of uncertain outcomes.

We used the previously existing learn-and-join method (LAJ), which is the state of the art for Bayes net learning in relational databases [11]. The LAJ method takes as input a contingency table for the entire database, so we can apply it with both link analysis on and link analysis off to obtain two different BN structures for each database. Our experiment is the first evaluation of the LAJ method with link

Dataset	Link Analysis On	Link Analysis Off
MovieLens	1.53	1.44
Mutagenesis	1.78	1.96
Financial	96.31	3.19
Hepatitis	416.70	3.49
IMDB	551.64	26.16
Mondial	190.16	N/A
UW-CSE	2.89	2.47

Table 7: Model Structure Learning Time in seconds.

analysis on. We used the LAJ implementation provided by its creators. We score all learned graph structures using the same full contingency table with link analysis on, so that the scores are comparable. The idea is that turning link analysis on should lead to a different structure that represents correlations, involving relationship variables, that exist in the data.

6.3.1 Structure Learning Times

Table 7 provides the model search time for structure learning with link analysis on and off. Structure learning is fast, even for the largest contingency table IMDB (less than 10 minutes run-time). With link analysis on, structure learning takes more time as it processes more information. In both modes, the run-time for building the contingency tables (Table 3) dominates the structure learning cost. For the Mondial database, there is no case where all relationship variables are simultaneously true, so with link analysis off the contingency table is empty.

6.3.2 Statistical Scores.

We report two model metrics, the log-likelihood score, and the model complexity as measured by the number of parameters. The **log-likelihood** is denoted as $L(\hat{G}, \mathbf{d})$, where \hat{G} is the BN G with its parameters instantiated to be the maximum likelihood estimates given the dataset \mathbf{d} , and the quantity $L(\hat{G}, \mathbf{d})$ is the log-likelihood of \hat{G} on \mathbf{d} . We use the relational log-likelihood score defined in [10], which differs from the standard single-table Bayes net likelihood only by replacing counts by frequencies so that scores are comparable across different nodes and databases. To provide information about the qualitative graph structure learned, we report edges learned that point to a relationship variable as a child. Such edges can be learned only with link analysis on. We distinguish edges that link relationship variables—R2R—and that link attribute variables to relationships—A2R.

Structure learning can use the new type of dependencies to find a better, or at least different, trade-off between model complexity and model fit. On two datasets (IMDB and Financial), link analysis leads to a superior model that achieves better data fit with fewer parameters. These are also the datasets with the most complex relational schemas (see Table 2). On IMDB in particular, considering only positive links leads to a very poor structure with a huge number of parameters. On four datasets, extra sufficient statistics lead to different trade-offs: On MovieLens and Mutagenesis, link analysis leads to better data fit but higher model complexity, and the reverse for Hepatitis and UW-CSE.

7. RELATED WORK

MovieLens	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	-4.68	164	0	0
Link Analysis On	-3.44	292	0	3

Mutagenesis	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	-6.18	499	0	0
Link Analysis On	-5.96	721	1	5

Financial	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	-10.96	11,572	0	0
Link Analysis On	-10.74	2433	2	9

Hepatitis	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	-15.61	962	0	0
Link Analysis On	-16.58	569	3	6

IMDB	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	-13.63	181,896	0	0
Link Analysis On	-11.39	60,059	0	11

Mondial	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	N/A	N/A	N/A	N/A
Link Analysis On	-18.2	339	0	4

UW-CSE	log-likelihood	#Parameter	R2R	A2R
Link Analysis Off	-6.68	305	0	0
Link Analysis On	-8.13	241	0	2

Table 8: Comparison of Statistical Performance of Bayesian Network Learning.

Sufficient Statistics for Single Data Tables. Several data structures have been proposed for storing sufficient statistics defined on a *single* data table. One of the best-known are ADtrees [6]. An ADtree provides a memory-efficient data structure for *storing* and retrieving sufficient statistics once they have been computed. In this paper, we focus on the problem of *computing* the sufficient statistics, especially for the case where the relevant rows have not been materialized. Thus ADtrees and contingency tables are complementary representations for different purposes: contingency tables support a computationally efficient block access to sufficient statistics, whereas ADtrees provide a memory efficient compression of the sufficient statistics. An interesting direction for future work is to build an ADtree for the contingency table once it has been computed.

Relational Sufficient Statistics. Schulte *et al.* review previous methods for computing statistics with negative relationships [12]. They show that the fast Möbius transform can be used in the case of multiple negative relationships. Their evaluation considered only Bayes net parameter learning with only one relationship. We examined computing joint sufficient statistics over the entire database. Other novel aspects are the *ct*-table operations and using the relationship chain lattice to facilitate dynamic programming.

8. CONCLUSION

Utilizing the information in a relational database for statistical modelling and pattern mining requires fast access to multi-relational sufficient statistics, that combine information across database tables. We presented an efficient dynamic program that computes sufficient statistics for any

combination of positive *and* negative relationships, starting with a set of statistics for positive relationships only. Our dynamic program performs a virtual join operation, that counts the number of statistics in a table join without actually constructing the join. We showed that the run time of the algorithm is $O(r \log r)$, where r is the number of sufficient statistics to be computed. The computed statistics are stored in contingency tables. We introduced contingency table algebra, an extension of relational algebra, to elegantly describe and efficiently implement the dynamic program. Empirical evaluation on seven benchmark databases demonstrated the scalability of our algorithm; we compute sufficient statistics with positive and negative relationships in databases with over 1 million data records. Our experiments illustrated how access to sufficient statistics for both positive and negative relationships enhances feature selection, rule mining, and Bayesian network learning.

Limitations and Future Work. Our dynamic program scales well with the number of rows, but not with the number of columns and relationships in the database. This limitation stems from the fact that the contingency table size grows exponentially with the number of random variables in the table. In this paper, we applied the algorithm to construct a large table for *all* variables in the database. We emphasize that this is only one way to apply the algorithm. The Möbius Join algorithm efficiently finds cross-table statistics for any set of variables, not only for the complete set of all variables in the database. An alternative is to apply the virtual join only up to a prespecified relatively small relationship chain length. Another possibility is to use postcounting [5]: Rather than precompute a large contingency table prior to learning, compute many small contingency tables for small subsets of variables on demand during learning.

In sum, our Möbius Virtual Join algorithm efficiently computes query counts which may involve any number of *positive and negative* relationships. These sufficient statistics support a scalable statistical analysis of associations among both relationships and attributes in a relational database.

Acknowledgments

This research was supported by a Discovery grant to Oliver Schulte by the Natural Sciences and Engineering Research Council of Canada. Zhensong Qian was supported by a grant from the China Scholarship Council.

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