Mining Approximate Acyclic Schemes from Relations

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ABSTRACT

Acyclic schemes have numerous applications in databases and in machine learning, such as improved design, more efficient storage, and increased performance for queries and machine learning algorithms. Multivalued dependencies (MVDs) are the building blocks of acyclic schemes. The discovery from data of both MVDs and acyclic schemes is more challenging than other forms of data dependencies, such as Functional Dependencies, because these dependencies do not hold on subsets of data, and because they are very sensitive to noise in the data; for example a single wrong or missing tuple may invalidate the schema. In this paper we present Maimon, a system for discovering approximate acyclic schemes and MVDs from data. We give a principled definition of approximation, by using notions from information theory, then describe the two components of Maimon: mining for approximate MVDs, then reconstructing acyclic schemes from approximate MVDs. We conduct an experimental evaluation of Maimon on 20 real-world datasets, and show that it can scale up to 1M rows, and up to 30 columns.

1 INTRODUCTION

Acyclic schemes have numerous applications in databases and in machine learning. Originally introduced by Beeri [5], they have lead to Yannakakis celebrated linear time query evaluation algorithms [42], and are used widely today in database design [13, 31], to speed up query evaluation with multiple aggregates [25], and to speed up machine learning applications such as ridge linear regression, classification trees, and regression trees [24, 39, 40]. When considering which types of schemes to fit the data, acyclic schemes are the natural choice due to their many desirable properties [6]. In this paper we study the following discovery problem: given a database consisting of a single relation, generate a set of acyclic schemes that fit the data to a large extent. For a simple illustration, consider the database shown on the left of Figure 1. It can be decomposed into an acyclic schema with four relations, shown on the right.

The building blocks of an acyclic schema are Multivalued Dependencies, MVDs. Every acyclic schema can be fully specified by the set of MVDs that it implies, which we call its *support*. Therefore, when mining acyclic schemes, the first

step is to mine the MVDs satisfied by the data. MVDs were first introduced by Fagin [13], which used them to introduce the 4th normal form, a generalization of the Boyce-Codd normal form (BCNF) [10]. They were studied extensively in the database literature [2, 4, 14, 28], have been proven to be equivalent to Saturated Conditional Independence in graphical models [17], and have recently been used as part of a data repairing solution to enforce fairness of ML systems [36, 37]. The methods used to synthesize an acyclic schema from a set of MVDs are well known [3, 7, 13, 32]. However, despite their importance, there is little research on the *discovery* of MVDs from data [1].

Work most closely related to the discovery of MVDs has been on discovering Functional Dependencies (FDs) and Unique Column Combinations (UCCs) [8, 21, 26, 27, 33, 35, 41]. These are special cases of MVDs, but MVDs are more general. Discovering all FDs and all UCCs is insufficient for discovering acyclic schemes. The only work that addressed the discovery problem for MVDs is by Savnik and Flach [38] and a master thesis by Draeger [12], and none of them address the more challenging task of discovering acyclic schemes.

There are two major challenges that make the discovery of MVDs and acyclic schemes, much harder than that of FDs and UCCs. First, they don't hold on subsets of the data. If a relation satisfies an FD, or a UCC, then every subset also satisfies the FD, or UCC, and this is exploited by many discovery algorithms, e.g FastFD [41] mines FDs in all subsets of size 2, while HyFD [35] mines FDs in a small subset extracted from the data. This property fails for MVDs, preventing us from considering subsets of the data. Second, MVDs and acyclic schemes are much more sensitive to data errors than FDs and UCCs. Even a single missing tuple may invalidate an MVD or schema. Real-world data often has important dependencies that do not hold exactly, but, if discovered, are very useful for a variety of applications. For that reason, in this paper we study the problem of discovering approximate MVDs and consequently, approximate acyclic schemes.

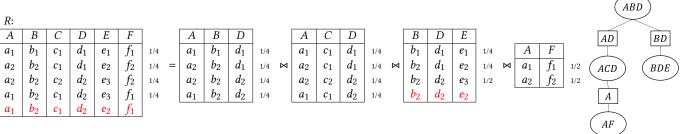


Fig. 1 A relation R and it's decomposition into an acylic schema

Fig. 2 Join Tree

We present Maimon¹, the first system for discovering approximate MVDs and acyclic schemes in the data. We introduce a principled notion of approximation, based on information theory, and develop the necessary theory for reasoning about approximate MVDs and schemes. We then describe algorithms for mining MVDs and schemes, and evaluate their scalability on real-world datasets of up to 1M rows, and 30 attributes. By allowing approximations, Maimon finds more interesting schemes without incurring too high a loss (i.e., spurious tuples). We make several contributions.

Our first contribution is to introduce a principled definition of approximation, and study its properties. Kivinen and Mannila [26] give three definitions of approximate functional dependencies, and Kruese and Naumann use one of them in their approximate FDs and UCCs discovery algorithm [27]. We propose an alternative metric of approximation, based on information theory. Each MVD or acyclic schema is associated with an information theoretic expression, and its value represents the degree of approximation. Our definition builds on early work by Lee [30].

Second, we propose novel algorithms for mining approximate MVDs and approximate acyclic schemes. For mining MVDs, our theoretical results prove that we do not need to discover *all* approximate MVDs, but only the so-called *full* MVDs with *minimal* separators. Our algorithm builds on previous results by Gunopulos et al. [20] for discovering the most *specific* sentences in the data that meet a certain criterion (e.g., maximal sets of items whose frequency in the data is above a given threshold). Following the discovery of the MVDs that hold in the data, we turn to the task of enumerating the acyclic schemes that can be synthesized from the set of discovered MVDs. Our algorithm is based on an approach for efficiently enumerating the maximal independent sets of a graph [11, 22], which has also been applied to the problem of enumerating tree decompositions [9].

Third, we evaluate Maimon on 20 real-world datasets that are part of the Metanome project that provides a repository of benchmarks for a variety of data profiling tasks that include the discovery of data dependencies. The datasets chosen for evaluation have been used in a large body of work on mining exact and approximate FDs [8, 12, 27, 33–35]. We show that Maimon scales up to 1M rows, and up to 30 columns. We empirically show that the loss entailed by the generated acyclic schemes (i.e., number of spurious tuples), monotonically depends on and the information theoretic measure of approximation we develop herein. We also show that a larger degree of approximation enables the discovery of schemes that exhibit a larger degree of decomposition, that leads to significant savings in storage. These schemes generally have more relations, and the *width* of the schema (i.e., relation with the largest number of attributes), is smaller.

The most expensive operation of Maimon is the computation of the entropy H(X) of a set of attributes X. Each such computation requires a full scan over the data, and this is prohibitively expensive due to the exponential number of subsets of attributes. We describe a novel, efficient approach to computing entropy, which reduces the problem to a set of main-memory SQL queries. Our method is inspired by the PLI cache (Position List Indices) data structure used for mining both exact and approximate FDs [21, 27].

To sum up, the contributions of this work are as follows:

- We define a principled notion of approximate data dependencies based on information theory, and study its properties; Sec. 4 and 5.
- (2) We describe a novel MVD enumeration algorithms and acylic schema enumeration algorithm; Sec. 6 and 7.
- (3) We conduct an extensive experimental evaluation on 20 real datasets; Sec. 8.

2 RUNNING EXAMPLE

We will use the following running example in this paper. Consider the relation R over the signature $\Omega = \{A, B, C, D, E, F\}$ in Figure 1. Ignore the probabilities, we will use them in Sec. 3. Also, ignore for now the last row (in red). The table with four rows can be decomposed into four tables, shown in the figure. More precisely, the following join dependency holds: $R = R[ABD] \bowtie R[ACD] \bowtie R[BDE] \bowtie R[AF]$. The schema of these four tables is acyclic, because it admits a join tree,

 $^{^1}$ Maimon stands for $\underline{M}ultivalued$ $\underline{A}pproximate$ Inference $\underline{M}ining$ and $\underline{NO}rmalization.$

Consider the 5'th row in R, shown in red. By adding it, we need to add a 4'th row to R[BDE], also shown in red. However, now the join dependency no longer holds exactly, because $R[ABD] \bowtie R[ACD] \bowtie R[BDE] \bowtie R[AF]$ contains a spurious tuple, namely $(a_2, b_2, c_2, d_2, e_2, f_2)$, which is not in R (it is not shown in the Figure); the first two MVDs no longer hold, only $A \rightarrow F|BCDE$ still holds, and the acyclic schema is no longer a correct decomposition of R. Yet the schema can still be useful for many applications, even it if leads to a spurious tuple. Insisting on exact acyclic schemas would severely restrict their applications, and also make them very brittle since the addition of one single tuple would invalidate the schema. In this paper we compute approximate acyclic schemas, and approximate MVDs. By allowing approximations, the schema shown in the figure is still considered valid for the data, despite the spurious tuple.

3 BACKGROUND

Table 1 summarizes the notations in this paper. We denote by $[n] = \{1, ..., n\}$. Let Ω be a set of variables, also called attributes. If $X, Y \subseteq \Omega$, then XY denotes $X \cup Y$.

3.1 Data Dependencies

Fix a relation instance R of size N = |R|, and schema Ω . For $Y \subseteq \Omega$ we let R[Y] denote the projection of R onto the attributes Y.

Let $X, Y, Z \subseteq \Omega$. A schema is a set $S = \{\Omega_1, \dots, \Omega_k\}$ such that $\bigcup_{i=1}^k \Omega_i = \Omega$ and $\Omega_i \nsubseteq \Omega_j$ for $i \neq j$. We say that the relation instance R satisfies the *join dependency* JD(S), and write $R \models \text{JD}(S)$, if $R = \bowtie_{i=1}^k R[\Omega_i]$. We say that R satisfies the multivalued dependency (MVD) $\phi = X \twoheadrightarrow Y_1 | Y_2 | \dots | Y_m$ where $m \geq 2$, the Y_i s are pairwise disjoint, and $XY_1 \cdots Y_m = \Omega$, if $R = R[XY_1] \bowtie \cdots \bowtie R[XY_m]$. We call X the key of the MVD and $\{Y_1, \dots, Y_m\}$ it's dependents, denoted key(ϕ) = X and dep(ϕ) = $\{Y_1, \dots, Y_m\}$. Most of the literature considers only MVDs with m = 2, which we call here standard MVDs.

Ω	set of variables (attributes)
$n = \Omega $	number of variables (attributes)
X, Y, A, B, \dots	sets of variables $\subseteq \Omega$
S	a schema = $\{\Omega_1, \ldots, \Omega_m\}$
$X \rightarrow Y Z$	a standard MVD
$X \rightarrow Y_1 Y_2 \cdots Y_m$	an MVD [4]
(\mathcal{T},χ)	a join tree
H(X)	entropy of a set of variables X
H(Y X), I(Y;Z X)	entropic measures
$\mathcal{J}(\mathcal{T},\chi)$	the entropic measure in Eq.(6)
$\mathcal{J}(S)$	${\cal J}$ of any join tree for S
$\mathcal{J}(X \twoheadrightarrow Y_1 \cdots Y_m)$	\mathcal{J} of the schema $\{XY_1,\ldots,XY_m\}$
$\mathcal{J}(X \twoheadrightarrow Y Z)$	=I(Y;Z X)
R	a relation
N = R	number of tuples
$R \models AJD(S)$	R satisfies an acyclic
	join dependency
$R \models_{\varepsilon} AJD(S)$	R ε-satisfies an acyclic
	join dependency

Table 1: Notations

Beeri et al. [4] noted that a generalized MVD can encode concisely multiple MVDs; for example X woheadrightarrow A|B|C holds iff X woheadrightarrow AB|C, X woheadrightarrow A|BC and X woheadrightarrow AC|B hold. We review a *join tree* from [6]:

Definition 3.1. A join tree is a pair (\mathcal{T}, χ) where \mathcal{T} is an undirected tree, and χ is a function that maps each $u \in \mathsf{nodes}(\mathcal{T})$ to a set of variables $\chi(u)$, called a *bag*, such that the following *running intersection* property holds: for every variable X, the set $\{u \in \mathsf{nodes}(\mathcal{T}) \mid X \in \chi(u)\}$ is a connected component of \mathcal{T} . We denote by $\chi(\mathcal{T}) \stackrel{\mathsf{def}}{=} \bigcup_u \chi(u)$, the set of variables of the join tree.

We often denote the join tree as \mathcal{T} , dropping χ when it is clear from the context. The *schema* defined by \mathcal{T} is $S = \{\Omega_1, \ldots, \Omega_m\}$, where $\Omega_1, \ldots, \Omega_m$ are the bags of \mathcal{T} . We call a schema S *acyclic* if there exists a join tree whose schema is S. Since we required $\Omega_i \nsubseteq \Omega_j$ for $i \neq j$, one can prove that any acyclic schema with n attributes and m relations satisfies $m \leq n$. We say that a relation R satisfies the *acyclic join dependency* S, and denote $R \models AJD(S)$, if S is acyclic and $R \models JD(S)$. An MVD $X \twoheadrightarrow Y_1 | \cdots | Y_m$ represents a simple acyclic schema, namely $S = \{XY_1, XY_2, \ldots, XY_m\}$.

Let $S = \{\Omega_1, \ldots, \Omega_m\}$ be an acyclic schema with join tree (\mathcal{T}, χ) . We associate to every $(u, v) \in \text{edges}(\mathcal{T})$ an MVD $\phi_{u,v}$ as follows. Let \mathcal{T}_u and \mathcal{T}_v be the two subtrees obtained by removing the edge (u, v). Then, we denote by $\phi_{u,v} \stackrel{\text{def}}{=} \chi(u) \cap \chi(v) \twoheadrightarrow \chi(\mathcal{T}_u) | \chi(\mathcal{T}_v)$. We call the *support of* \mathcal{T} the set of m-1 MVDs associated to its edges, in notation MVD(\mathcal{T}) = $\{\phi_{u,v} \mid (u,v) \in \text{edges}(\mathcal{T})\}$. If \mathcal{T} defines the acyclic schema

S, then it satisfies $R \models AJD(S)$ iff it satisfies all MVDs in its support: $R \models \phi_{u,v}$ for all $\phi_{u,v} \in MVD(\mathcal{T})$ [6, Thm. 8.8].

Example 3.2. We will illustrate with the running example from Sec. 2. The tree in Fig. 2 is a join tree. Its bags are the ovals labeled AF, ACD, ABD, and BDE, and it is custom to show the intersection of two bags on the connecting edge. $MVD(\mathcal{T}) = \{BD \twoheadrightarrow E|ACF, AD \twoheadrightarrow CF|BE, A \twoheadrightarrow F|BCDE\}.$

3.2 Information Theory

Lee [29, 30] gave an equivalent formulation of data dependencies in terms of information measures; we review this briefly here, after a short background on information theory.

Let *X* be a random variable with a finite domain \mathcal{D} and probability mass p (thus, $\sum_{x \in \mathcal{D}} p(x) = 1$). Its entropy is:

$$H(X) \stackrel{\text{def}}{=} \sum_{x \in \mathcal{D}} p(x) \log \frac{1}{p(x)} \tag{1}$$

If $N = |\mathcal{D}|$ then $H(X) \leq \log N$, and equality holds iff p is uniform. For a set of jointly distributed random variables $\Omega = \{X_1, \dots, X_n\}$ we define the function $H : 2^{\Omega} \to \mathbb{R}$ as the entropy of the joint random variables in the For example, $H(X_1X_2) = \sum_{x_1 \in \mathcal{D}_1, x_2 \in \mathcal{D}_2} p(x_1, x_2) \log \frac{1}{p(x_1, x_2)}$. Let $A, B, C \subseteq \Omega$. The mutual information I(B; C|A) is defined as:

$$I(B;C|A) \stackrel{\text{def}}{=} H(AB) + H(AC) - H(ABC) - H(A)$$
 (2)

It is known that the conditional independence $p \models B \perp C \mid A$ (i.e., B is independent of C given A) holds iff $I(B; C \mid A) = 0$.

In this paper we use only the following two properties of the mutual information:

$$I(B;C|A) \ge 0 \tag{3}$$

$$I(B;CD|A) = I(B;C|A) + I(B;D|AC)$$
(4)

The first inequality follows from monotonicity and submodularity (it is in fact equivalent to them); the second equality is called the *chain rule*. All consequences of these two (in)equalities are called *Shannon inequalities*; for example, monotonicity $H(AB) \ge H(A)$ is a Shannon inequality because it follows from (3) by setting B = C.

Let R be relation with attributes $\Omega = \{X_1, \ldots, X_n\}$ and N tuples. The *empirical distribution* is the uniform distribution over its tuples: $\forall t \in R, p(t) = 1/N$. It's entropy satisfies $H(\Omega) = \log N$. For $\alpha \subseteq [n]$, we denote by X_α the set of variables X_i , $i \in \alpha$, and denote by $R(X_\alpha = x_\alpha)$ the subset of tuples $t \in R$ where $t[X_\alpha] = x_\alpha$, for fixed values x_α . By uniformity, the marginal probability is $p(X_\alpha = x_\alpha) = \frac{|R(X_\alpha = x_\alpha)|}{N}$, and therefore:

$$H(X_{\alpha}) \stackrel{\text{def}}{=} \log N - \frac{1}{N} \sum_{x_{\alpha} \in \mathcal{D}_{\alpha}} |R(X_{\alpha} = x_{\alpha})| \log |R(X_{\alpha} = x_{\alpha})|$$
 (5)

The sum above can be computed using a simple SQL query: Select X_{α} , count(*)×log(count(*)) From R Group By X_{α} .

Lee [29, 30] formalized the following connection between database constraints, and entropic measures. Let (\mathcal{T}, χ) be a join tree. We define the following expression:

$$\mathcal{J}(\mathcal{T},\chi) \stackrel{\text{def}}{=} \sum_{\substack{v \in \\ \mathsf{nodes}(\mathcal{T})}} H(\chi(v)) - \sum_{\substack{(v_1,v_2) \in \\ \mathsf{edges}(\mathcal{T})}} H(\chi(v_1) \cap \chi(v_2)) - H(\chi(\mathcal{T}))$$

We abbreviate it with $\mathcal{J}(\mathcal{T})$, or \mathcal{J} , when \mathcal{T} , χ are clear from the context; we will prove later (Th. 5.1) that $\mathcal{J} \geq 0$ is a Shannon inequality. Lee proved that \mathcal{J} depends only on the schema S defined by the join tree, and not on the tree itself. To see this on a simple example, consider the MVD $X \rightarrow$ U|V|W and its associated acyclic schema $\{XU, XV, XW\}$. If we consider the join tree XU - XV - XW, then $\mathcal{J} =$ H(XU) + H(XV) + H(XW) - 2H(X) - H(XUVW). Another join tree is XU - XW - XV, and \mathcal{J} is the same. Therefore, if S is acyclic, then we write $\mathcal{J}(S)$ to denote $\mathcal{J}(\mathcal{T})$ for any join tree of S. We denote by $\mathcal{J}(X \to Y_1 | \cdots | Y_m) \stackrel{\text{def}}{=}$ $H(XY_1) + \cdots + H(XY_m) - (m-1)H(X) - H(XY_1 \cdots Y_m)$ for any sets of variables X, Y_1, \ldots, Y_m where Y_1, \ldots, Y_m are pairwise disjoint, even when $XY_1 \cdots Y_m$ is not necessarily Ω . When m = 2, then $J(X \rightarrow Y|Z) = I(Y;Z|X)$. Lee proved the following:

Theorem 3.3. ([30]) Let H be the entropy of the empirical distribution on R, and let S be any acyclic schema. Then $R \models A \mathcal{J}D(S)$ iff $\mathcal{J}(S) = 0$.

In the particular case of a standard MVD, Lee's result implies that $R \models X \twoheadrightarrow Y | Z$ if and only if I(Y; Z | X) = 0.

Example 3.4. Continuing Example 3.2, the empirical distribution of the relation R in Fig 1 (without the red tuple) assigns probability 1/4 to each tuple. Thus, $H(ABCDEF) = \log 4 = 2$. The marginal probabilities need not be uniform, e.g. the marginals for BDE are 1/4, 1/4, 1/2, and thus $H(BDE) = 1/4 \log 4 + 1/4 \log 4 + 1/2 \log 2 = 3/2$. The value of $\mathcal J$ is: $\mathcal J(\mathcal T) = H(AF) + H(ACD) + H(ABD) + H(BDE) - H(A) - H(AD) - H(BD) - H(ABCDEF)$. For the empirical distribution in the figure, this quantity is 0.

4 PROBLEM STATEMENT

Our main goal is to discover an acyclic schema for a given relation instance *R*. Since exact schemas are very sensitive to data errors, Maimon discovers approximate schemas.

Definition 4.1 (Approximate Acyclic Schema). Fix a relation instance R, and $\varepsilon \ge 0$. We say that an acyclic schema S is an ε -schema for R, or simply approximate schema, if $\mathcal{J}(S) \le \varepsilon$. In notation, $R \models_{\varepsilon} AJD(S)$.

Maimon takes as input $\varepsilon \ge 0$ and discovers approximate acyclic schemas for R. By Lee's theorem, if we set $\varepsilon = 0$, then Maimon returns exact schemas. In practice, a relation

R may not have any exact schemas, or may have very limited schemas; by allowing $\varepsilon \ge 0$ we may find approximate schemas that are quite useful for many applications.

Problem 4.1 (Schema Enumeration Problem). Given a relational instance R, enumerate the approximate acyclic schemas of R.

In practice, we are not interested in enumerating *all* approximate acyclic schemas of R. This would take a prohibitively long time, and some acyclic schemas are superior to others. For example, consider a relation over four attributes that satisfies the acyclic join dependency $S = \{XA, XB, XC\}$. The following acyclic join dependencies also hold in $R: \{XAB, XC\}$, $\{XAC, XB\}$, and $\{XA, XBC\}$. The latter schemas are less useful than $S = \{XA, XB, XC\}$ that leads to a larger degree of decomposition. Therefore, in this paper we address the problem of enumerating acyclic schemas that cannot be extended (i.e., with additional relational instances) while continuing to satisfy the accuracy threshold.

We derive the approximate schemas from the MVDs in their support. Since an MVD is, in particular, an acyclic schema, Def. 4.1 applies to them as well: a ε -MVD is one for which $\mathcal{J}(X \twoheadrightarrow Y_1 | \cdots | Y_m) \leq \varepsilon$. Our second problem is:

Problem 4.2 (MVD Enumeration Problem). Given a relational instance R, enumerate the approximate MVDs of R.

Maimon works as follows. The user provides a parameter $\varepsilon \geq 0$. In the first phase, Maimon enumerates ε -MVDs, using the algorithm in Sec. 6. When it finishes, or after a timeout, it starts the second phase, where it enumerates approximate schemas with support from the set returned by the first phase, using the algorithm in Sec. 7. Since the support of a schema consists of m-1 MVDs, the algorithm reports schemas with $\mathcal{J}(S) \leq (m-1)\varepsilon$, where m is the number of relations in S but, since the enumeration algorithm is exhaustive, all schemas with $\mathcal{J} \leq \varepsilon$ are reported eventually.

5 THREE MAIN TECHNIQUES

We describe here three main techniques that allow us to design efficient schema- and MVD-discovery algorithms. The first reduces the approximate schema discovery to approximate MVD discovery, the next two reduce the number of MVD's that need to be discovered.

5.1 From MVDs to Acyclic Schemas

Beeri at al. [6] showed that, for exact constraints, an acyclic schema over m relations is equivalent to the set of m-1 MVDs in its support. We give here a non-trivial generalization to approximate schemas and MVDs. We start with two simple inequalities which we need throughout the paper:

PROPOSITION 5.1. Let $Y_1, Z_1, ..., Y_m, Z_m$ be pairwise disjoint sets of variables, and let X be any set of variables. Then the following are Shannon inequalities:

$$\mathcal{J}(X \to Y_1 | \cdots | Y_m) \le \mathcal{J}(X \to Y_1 Z_1 | \cdots | Y_m Z_m) \tag{7}$$

$$\mathcal{J}(XZ_1\cdots Z_m \twoheadrightarrow Y_1|\cdots|Y_m) \leq \mathcal{J}(X \twoheadrightarrow Y_1Z_1|\cdots|Y_mZ_m) \quad (8)$$

PROOF. The first inequality follows from this chain of inequalities: $\mathcal{J}(X \twoheadrightarrow Y_1|\cdots|Y_m) \leq \mathcal{J}(X \twoheadrightarrow Y_1Z_1|Y_2|\cdots|Y_m) \leq \mathcal{J}(X \twoheadrightarrow Y_1Z_1|Y_2Z_2|\cdots|Y_m) \leq \cdots$; to prove it, we show only the first step (the others are similar), which follows by observing $\mathcal{J}(X \twoheadrightarrow Y_1|\cdots|Y_m) + I(Z_1;Y_2\cdots Y_m|XY_1) = \mathcal{J}(X \twoheadrightarrow Y_1Z_1|\cdots|Y_m)$ then using inequality (3). The second inequality follows from a similar chain, where the first step follows from $\mathcal{J}(XZ_1 \twoheadrightarrow Y_1|\cdots|Y_m) + \sum_{i=2}^m I(Y_i;Z_1|X) = \mathcal{J}(X \twoheadrightarrow Y_1Z_1|Y_2|\cdots|Y_m)$ and the inequality follows from (3).

Let (\mathcal{T}, χ) be a join tree, defining an acyclic schema S over the variables $\chi(\mathcal{T}) = \Omega$. Choose an arbitrary root, orient the tree accordingly, and let u_1, \ldots, u_m be a depth-first enumeration of $\operatorname{nodes}(\mathcal{T})$. Thus, u_1 is the root, and for every i > 1, $\operatorname{parent}(u_i)$ is some node u_j with j < i. For every i, we define $\Omega_i \stackrel{\operatorname{def}}{=} \chi(u_i)$, $\Omega_{i:j} \stackrel{\operatorname{def}}{=} \bigcup_{\ell=i,j} \Omega_\ell$, and $\Delta_i \stackrel{\operatorname{def}}{=} \chi(\operatorname{parent}(u_i)) \cap \chi(u_i)$ (by the running intersection property this is equal to $\Omega_{1:(i-1)} \cap \Omega_i$). We prove:

Theorem 5.1. The following hold:

$$\mathcal{J}(\mathcal{T}) = \sum_{i=2}^{m} I(\Omega_{1:(i-1)}; \Omega_i | \Delta_i)$$
 (9)

$$\max_{i=2,m} I(\Omega_{1:(i-1)}; \Omega_{i:m} | \Delta_i) \le \mathcal{J}(\mathcal{T}) \le \sum_{i=2}^m I(\Omega_{1:(i-1)}; \Omega_{i:m} | \Delta_i)$$
(10)

The first is an identity, and the second is a Shannon inequality.

The identity (9) captures precisely the intuition that the information measure associated with a join tree $\mathcal T$ is equivalent to m-1 mutual information. This identity implies that $\mathcal J(\mathcal T)\geq 0$, because $I(\cdots)\geq 0$. But the expressions $I(\cdots)$ in (9) do not correspond to MVDs, because they do not include all variables Ω . The Shannon inequality (10) rectifies this, by showing that $\mathcal J(\mathcal T)$ lies between the max and the sum of m-1 MVDs. Notice that the MVDs $\Delta_i \twoheadrightarrow \Omega_{1:(i-1)}|\Omega_{i:m},$ i=2,m are precisely the support, MVD($\mathcal T$), thus (10) generalizes Beeri's observation to approximate schemas. An immediate consequence of (10) is the following relationship between an acyclic schema S and its support.

COROLLARY 5.2. Let S be an acyclic schema with join tree (\mathcal{T}, χ) . Then: (1) if $R \models_{\varepsilon} A\mathcal{J}D(S)$ then $R \models_{\varepsilon} MVD(\mathcal{T})$. (2) If $R \models_{\varepsilon} MVD(\mathcal{T})$ then $R \models_{(m-1)\varepsilon} A\mathcal{J}D(S)$. In particular, (1) and (2) are equivalent if $\varepsilon = 0$. Here $R \models_{\varepsilon} MVD(\mathcal{T})$ means $R \models_{\varepsilon} \phi$, forall $\phi \in MVD(\mathcal{T})$.

PROOF. (of Theorem 5.1) Let \mathcal{T}_i denote the subtree consisting of the nodes u_1, \ldots, u_i . We prove (9) by induction

on m. Assume the identity holds for m-1. Compared to \mathcal{T}_{m-1} , the tree \mathcal{T}_m has one extra node u_m and one extra edge (parent(u_m), u_m), hence by the definition of \mathcal{J} in (6):

$$\begin{split} \mathcal{J}(\mathcal{T}_m) = & \mathcal{J}(\mathcal{T}_{m-1}) + H(\chi(u_m)) - H(\chi(u_m)) \cap \chi(\mathsf{parent}(u_m)) \\ & + H(\chi(\mathcal{T}_{m-1})) - H(\chi(\mathcal{T}_m)) \\ = & \mathcal{J}(\mathcal{T}_{m-1}) + H(\Omega_m) - H(\Delta_m) + H(\Omega_{1:(m-1)}) - H(\Omega_{1:m}) \\ = & \mathcal{J}(\mathcal{T}_{m-1}) + I(\Omega_{1:(m-1)}; \Omega_m | \Delta_m) \end{split}$$

The claim follows from the induction hypothesis on $\mathcal{J}(\mathcal{T}_{m-1})$. We prove (10). The right inequality follows from the fact that $I(\Omega_{1:(i-1)};\Omega_i|\Delta_i)\leq I(\Omega_{1:(i-1)};\Omega_{i:m}|\Delta_i)$ (which holds by Eq. (8)). For the left inequality, we make the following observation. If \mathcal{T} is any join tree and \mathcal{T}' is obtained by mergining two adjacent nodes $(u,v)\in \operatorname{edges}(\mathcal{T})$, then $\mathcal{J}(\mathcal{T})\geq \mathcal{J}(\mathcal{T}')$. This is because $\mathcal{J}(\mathcal{T})=\mathcal{J}(\mathcal{T}')+H(\chi(u))+H(\chi(v))-H(\chi(u)\cap\chi(v))-H(\chi(u)\cup\chi(v))=\mathcal{J}(\mathcal{T}')+I(\chi(u);\chi(v)|\chi(u)\cap\chi(v))$. To prove (10), we fix one edge (parent(u_i), u_i) and repeatedly merge all other edges, until we end with a tree \mathcal{T}' with two bags, $\Omega_{1:(i-1)}$ and $\Omega_{i:m}$ respectively. Then $\mathcal{J}(\mathcal{T})\geq \mathcal{J}(\mathcal{T}')=I(\Omega_{1:(i-1)};\Omega_{i:m}|\Delta_i)$. The claim follows from the fact that this holds for any i=2,m.

Example 5.3. We illustrate the first part of the theorem on the running example in Fig. 2 and Example 3.4. Enumerating the nodes depth-first (*ABD*, *ACD*, *AF*, *BDE*), Eq. (9) and (10) become:

$$\mathcal{J}(\mathcal{T}) = I(C; B|AD) + I(F; BCD|A) + I(ACF; E|BD)$$

$$\max(\cdots) \le \mathcal{J}(\mathcal{T}) \le I(CF; BE|AD) + I(F; BCDE|A) + I(ACF; E|BD)$$

5.2 Full MVDs

The number of candidate MVD's is very large: there are $(3^n + 1)/2 - 2^n = O(3^n)$ standard MVD's X woheadrightarrow Y|Z, which is too large to consider for practical datasets. Here, and in the next section, we describe two techniques that allow us to restrict the search space. Consider a fixed key X. Beeri at al. [4] noted that, in the exact case, if any MVD X woheadrightarrow ... holds on the data, then there exists a "best" one. For example if both X woheadrightarrow AB|C and X woheadrightarrow A|BC hold exactly, then so does X woheadrightarrow A|B|C, and it suffices to discover only the latter. Unfortunately, this fails for approximate MVDs, as we explain here.

We say that $\phi = X \twoheadrightarrow A_1 | \dots | A_m$ refines $\psi = X \twoheadrightarrow B_1 | \dots | B_k$, denoted by $\phi \ge \psi$ if they both have the same key (i.e., $\ker(\phi) = \ker(\psi) = X$) and for every $A_i \in \operatorname{dep}(\phi)$ there exists $B_j \in \operatorname{dep}(\psi)$ such that $A_i \subseteq B_j$. For example, $X \twoheadrightarrow A|B|C$ refines $X \twoheadrightarrow AB|C$.

Proposition 5.2. If $\phi \geq \psi$ then $\mathcal{J}(\phi) \geq \mathcal{J}(\psi)$.

Proof. It suffices to consider the case when two dependents in ϕ are replaced by their union in ψ , e.g. $\phi = X \rightarrow A|B|\cdots$ and $\psi = X \rightarrow AB|\cdots$, since any refinement is a sequence of such steps. In that case, by inspecting Eq.(6) we observe $\mathcal{J}(\phi) = \mathcal{J}(\psi) + H(XA) + H(XB) - H(XAB) - H(X) = \mathcal{J}(\psi) + I(A;B|X) \geq \mathcal{J}(\psi)$ proving the claim.

We say that an MVD ψ is ε -full, or simply full, if $R \models_{\varepsilon} \psi$ and, for all strict refinements $\phi > \psi$, $R \not\models_{\varepsilon} \phi$. We denote by FullMVD $_{\varepsilon}(R,X)$ the set of all full ε -MVDs with key X. Thus, we only need to discover the sets FullMVD $_{\varepsilon}(R,X)$, for all $X \subseteq \Omega$, because all other MVDs can be derived using Shannon inequalities.

Beeri proved that, in the exact case, FullMVD₀(R,X) has at most one element. We next present Lemma 5.4 that shows what happens in the approximate case, and allows us to derive Beeri's result as a special case. Given two MVDs $\phi = X \twoheadrightarrow A_1 | \dots | A_m$ and $\psi = X \twoheadrightarrow B_1 | \dots | B_k$, define their join as $\phi \lor \psi = X \twoheadrightarrow C_{11} | C_{12} | \dots | C_{mk}$, where $C_{ij} = A_i \cap B_j$. Clearly, $\phi \lor \psi$ refines both ϕ and ψ , i.e. $\mathcal{J}(\phi \lor \psi) \ge \max(\mathcal{J}(\phi), \mathcal{J}(\psi))$. We prove a weak form of converse:

LEMMA 5.4. The following are Shannon inequalities: $\mathcal{J}(\phi \lor \psi) \leq \mathcal{J}(\phi) + m\mathcal{J}(\psi)$ and $\mathcal{J}(\phi \lor \psi) \leq k\mathcal{J}(\phi) + \mathcal{J}(\psi)$.

By this result, $\mathcal{J}(\phi) = \mathcal{J}(\psi) = 0$ implies $\mathcal{J}(\phi \vee \psi) = 0$, which proves Beeri's theorem that $\text{FULLMVD}_{\varepsilon}(R, X)$ has at most one element, because if ϕ_1, ϕ_2, \cdots are all MVD's with key X that hold exactly on R, then $\phi_1 \vee \phi_2 \vee \cdots$ refines all of them and holds too. This property was also used by Draeger [12] in his MVD discovery algorithm. When $\varepsilon > 0$ however, then this fails. For a very simple example, consider

a relation with two tuples, $\begin{bmatrix} A & A & B & C \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \end{bmatrix}$ and fix $\varepsilon = 1$. Then $R \models_{\varepsilon} X \twoheadrightarrow AB \mid C, X \twoheadrightarrow AC \mid B, X \twoheadrightarrow BC \mid A$, but $\not\models_{\varepsilon} X \twoheadrightarrow A \mid B \mid C$; indeed, $H(\emptyset) = H(X) = 0$ and H(W) = 1 for all other sets W, and the reader can check $\mathcal{J}(X \twoheadrightarrow AB \mid C) = \mathcal{J}(X \twoheadrightarrow AC \mid B) = \mathcal{J}(X \twoheadrightarrow BC \mid A) = 1$ but $\mathcal{J}(X \twoheadrightarrow AB \mid C) = 2$.

In summary, our algorithm discovers $\text{FullMVD}_{\varepsilon}(R, X)$, for every X. Unlike the exact case, $\text{FullMVD}_{\varepsilon}(R, X)$ may contain more than one element.

5.3 Minimal Separators

We now show that it is not necessary to discover the sets $\text{FullMVD}_{\varepsilon}(R, X)$ for all subset of attributes $X \subset \Omega$, but only those where X is a *minimal separator*.

Definition 5.5. Fix a relation R and $\varepsilon \geq 0$. We say that a set X separates two variables $A, B \notin X$ if there exists an ε -MVD $X \to Y_1 | \cdots | Y_m$ that separates A, B, i.e. A, B occur in different sets Y_i, Y_j . We say X is a minimal A, B-separator if there is no $X_0 \subsetneq X$ that separates A, B.

 $^{^2}$ There are 3^n ways to partition Ω into three sets $X,\,Y,\,Z.$ We rule out the 2^n partitions that have $Y=\emptyset$ and the 2^n partitions that have $Z=\emptyset,$ and add back the 1 partition that has $Y=Z=\emptyset,$ for a total of $3^n-2^{n+1}+1.$ Finally, we divide by 2 since $X \twoheadrightarrow Y|Z$ and $X \twoheadrightarrow Z|Y$ are the same MVD.

For a pair $A, B \in \Omega$, we denote by MINSEP_{ε}(R, A, B) the set of minimal A, B separators in R, and for a minimal AB separator X we denote by FullMVD_{ε}(R, X, A, B) the set of full MVDs that separate A, B. Notice that:

$$\mathrm{FullMVD}_{\varepsilon}(R,X) = \bigcup_{A,B \in \Omega \backslash X} \mathrm{FullMVD}_{\varepsilon}(R,X,A,B).$$

Example 5.6. Let R be a relation over $\Omega = \{A, \ldots, E\}$. Suppose $R \models_{\varepsilon} CD \twoheadrightarrow A | BE$. By (8) we also have $R \models_{\varepsilon} CDE \twoheadrightarrow A | B$, which means that CDE cannot be a minimal separator for A, B. To check that CD is a minimal A, B-separator, we need to check that neither C nor D separates A, B

The main result in this section is that we only need to compute the full MVDs with minimal separators, denoted as:

$$\mathcal{M}_{\varepsilon} \stackrel{\text{def}}{=} \bigcup_{\substack{X \in \\ \text{MINSEP.}(R, A, B)}} \bigvee_{X \in \\ \text{MINSEP.}(R, A, B)} \text{FULLMVD}_{\varepsilon}(R, X, A, B) \tag{11}$$

because, as we show, every ε -MVD can be derived from the set $\mathcal{M}_{\varepsilon}$ by a Shannon inequality.

THEOREM 5.7. Let X woheadrightarrow Y|Z be an ε -MVD for R. Then there exist $\phi_1, \ldots, \phi_m \in \mathcal{M}_{\varepsilon}$, where $m = |Y| \cdot |Z|$, such that the following is a Shannon inequality: $I(Y; Z|X) \leq \sum_i \mathcal{J}(\phi_i)$.

In summary, our algorithm will iterate over pairs of attributes A, B, will compute $MinSep_{\varepsilon}(R, A, B)$, then, for each X in this set will compute $FullMVD_{\varepsilon}(R, X, A, B)$, and return their union, $\mathcal{M}_{\varepsilon}$; we describe it in the next section. We end this section with the proof of Theorem 5.7.

PROOF. Let $Y = A_1 ... A_m$, and $Z = B_1 ... B_k$. By the chain rule (4) it holds that:

$$I(Y;Z|X) = \sum_{i=1}^{m} \sum_{j=1}^{k} I(A_i; B_j | XA_1 \dots A_{i-1}B_1 \dots B_{j-1})$$

It suffices to prove that, for each i, j, there exists an MVD $\phi \in \mathcal{M}_{\varepsilon}$ such that the following is a Shannon inequality:

$$I(A_i; B_i | XA_1 \cdots A_{i-1}B_1 \cdots B_{i-1}) \leq \mathcal{J}(\phi)$$

Since X woheadrightarrow Y|Z is a ε -MVD for the relation R, then X is an A_i, B_j separator. Let $S \subseteq X$ be any minimal A_i, B_j separator, thus $S \in \text{MINSEP}_{\varepsilon}(R, A_i, B_j)$, and let $\phi = S woheadrightarrow U_1|\cdots|U_p$ be a full MVD in FullMVD $_{\varepsilon}(R, S, A_i, B_j) \subseteq \mathcal{M}_{\varepsilon}$ that separates A_i, B_j . Assume w.l.o.g. $A_i \in U_1, B_j \in U_2$, and let $\psi \stackrel{\text{def}}{=} S woheadrightarrow W|V$, where $W = U_1, V = U_2U_3\cdots U_p$. Thus, $\phi \succeq \psi$, and therefore by Prop. 5.2 the following Shannon inequality holds: $\mathcal{J}(\phi) \geq \mathcal{J}(\psi)$. Write ψ as $\psi = S woheadrightarrow W_0 | V \cap (XA_1 \cdots A_iB_1 \cdots B_j), W_1 = W - W_0$, and similarly $V_0 = V \cap (XA_1 \cdots A_iB_1 \cdots B_j), V_1 = V - V_0$. By Prop. 5.1 (7) we have the following Shannon inequality $\mathcal{J}(\psi) = \mathcal{J}(S woheadrightarrow W_0 | V_0 V_1) \geq \mathcal{J}(S woheadrightarrow W_0 | V_0)$. Finally, we notice that the

Algorithm MVDMiner(R, Ω , ε)

```
1: \mathcal{M}_{\varepsilon} \leftarrow \emptyset

2: for all pairs A, B \in \Omega do

3: MINSEP_{\varepsilon}(R, A, B) \leftarrow \text{MineMinSeps}(R, \Omega, \varepsilon, (A, B))

4: for all X \in \text{MINSEP}_{\varepsilon}(R, A, B) do

5: \mathcal{M}_{\varepsilon} \leftarrow \mathcal{M}_{\varepsilon} \cup \text{getFullMVDs}(X, \varepsilon, (A, B), \infty)

6: return \mathcal{M}_{\varepsilon}
```

Fig. 3 Discover the set $\mathcal{M}_{\varepsilon} = \bigcup_{S \in MINSEPR} FULLMVD_{\varepsilon}(S)$.

set SW_0V_0 is the same as $XA_1 \cdots A_iB_1 \cdots B_j$ and that $A_i \in W_0$, $B_j \in V_0$, therefore by Prop. 5.1, (8), $\mathcal{J}(S \to W_0|V_0) \geq \mathcal{J}(XA_1 \cdots A_{i-1}B_1 \cdots B_{j-1} \to A_i|B_j)$, proving the claim. \square

6 DISCOVERING ε -MVDS

In this section we present the first phase of Maimon: the algorithm for the discovery of ε -MVDs in a relation R, called MVDMiner, and shown in Figure 3. As explained, the algorithm returns the set $\mathcal{M}_{\varepsilon}$, defined in Eq.(11); this set is used in the second phase of Maimon to compute ε -schemes.

MVDMiner iterates over all pairs of attributes $A, B \in \Omega$. It first computes the set $\operatorname{MinSep}_{\mathcal{E}}(R,A,B)$ of minimal A,B-separators (line 3): we describe this step in Sec. 6.1. Then, for each $X \in \operatorname{MinSep}_{\mathcal{E}}(R,A,B)$, it computes $\operatorname{FullMVD}_{\mathcal{E}}(R,X,A,B)$ (line 5): we describe this step in Sec. 6.2. Finally, the algorithm returns their union, $\mathcal{M}_{\mathcal{E}}$. Both steps require access to an oracle getEntropy_R(X) for computing the entropy H(X), according to Eq. (5), where H is the entropy associated with the empirical distribution over R. We describe the implementation and optimization of getEntropy_R(X) in Section 6.3.

6.1 Discovering the Minimal Separators

We describe here how we compute all minimal A, B-separators, $MINSep_{\varepsilon}(R,A,B)$ (line 3 of MVDMiner). One possible way to do this could be to iterate over sets X top down, because it enables pruning: if X is not an A, B-separator, then neither is any subset of X, by (8) in Prop. 5.1. This suggests a top-down algorithm, which starts from the largest set $X = \Omega \setminus \{A, B\}$, and checks if it is an A, B-separator. If not, then none exists. Otherwise it exhaustively searches over subsets of X, from largest to smallest, returning the minimal (with regard to inclusion) sets that separate A, B. Such an exhaustive search will explore all separators, while we only want to find the minimal ones. Our approach takes advantage of the fact that we need to find only the minimal separators, and builds on a result by Gunopulos et al. [20].

Let $\mathbf{C} = \{C_1, \dots, C_m\}$ be a set of distinct subsets of Ω . A set $D \subset \Omega$ is a *transversal* of \mathbf{C} if $D \cap C_i \neq \emptyset$ for every $C_i \in \mathbf{C}$. For a set $D \subseteq \Omega$, we denote by \overline{D} the complement set $\Omega \setminus D$.

THEOREM 6.1. Let $C = \{C_1, \ldots, C_n\}$ denote a set of minimal A, B separators in R. Then there exists a minimal A, B-separator $X \notin C$ iff there exists a minimal transversal D of C such that \overline{D} is an A, B-separator.

PROOF. **only if.** Since *D* is a transversal of **C** then:

$$\bigwedge_{i=1}^{n} (C_i \cap D \neq \emptyset) \iff \bigwedge_{i=1}^{n} (\overline{D} \not\supseteq C_i)$$
 (12)

Since \overline{D} is an A, B separator, there exists some minimal separator $X \subseteq \overline{D}$. Assume, by contradiction, that $X \supseteq C_i$ for some $C_i \in \mathbb{C}$. Then $\overline{D} \supseteq X \supseteq C_i$, contradicting (12).

if. Since X is a minimal A, B separator that is not in \mathbb{C} , then $\bigwedge_{i=1}^{n} (X \not\supseteq C_i)$, meaning that \overline{X} is a transveral of \mathbb{C} . Then any minimal transversal $D \subseteq \overline{X}$ satisfies the claim. \square

Algorithm MineMinSeps (Fig. 5) for discovering all minimal A, B separators, MinSep $_{\varepsilon}(R, A, B)$ is based on Theorem 6.1, and proceeds as follows:

- (1) Initialize **C** with a single minimal *A*, *B*-separator (Line 3-5).
- (2) Iterate over all minimal transversals D of \mathbb{C} (Line 8):
- (3) If \overline{D} separates A, B (Line 11), then:
 - (a) Find any minimal A, B separator $X \subseteq \overline{D}$ (Line 12).
 - (b) $\mathbf{C} \leftarrow \mathbf{C} \cup \{X\}$.

The function ReduceMinSep called in lines 4 and 12 takes a separator ($\Omega\setminus\{A,B\}$ or \overline{D} respectively) and finds any subset that is a minimal separator; this is done greedily in ReduceMinSep (Fig. 4). The function getFullMVDs called in line 10 of MineMinSeps, and in line 4 of ReduceMinSep, takes as input an attribute set X, a pair of attributes A, B, and a threshold ε , and computes full ε -MVDs with key X that separate A, B; a parameter K>0 is used to limit the number of full MVDs returned, and here we set K=1 because we only check if one exists; in line 5 of the main algorithm (Fig. 3) we set $K=\infty$.

The only sets of attributes returned in MineMinSeps are minimal *AB*-separators returned by ReduceMinSep in lines 4 and 12. The proof of completeness (i.e., the algorithm returns all minimal *AB*-separators) follows techniques similar to those by Gunopulos et al. [20], and is given in the full version of the paper:

THEOREM 6.2. Algorithm MineMinSeps in Figure 5 enumerates all minimal A, B-separators in R.

We now analyze the runtime between consecutive discoveries of minimal A, B-separators in MineMinSeps. We let Ω be a finite set of cardinality n, and let $\mathbf{C} \subseteq 2^{\Omega}$ be a

Algorithm ReduceMinSep(ε , X, (A,B))

```
    Let p = X<sub>1</sub>,..., X<sub>m</sub> be a predefined ordering of X.
    S ← X
    for all i = 1 to m do
    M<sub>i</sub> ← getFullMVDs(S\{X<sub>i</sub>}, ε, (A, B), 1)
    if M<sub>i</sub> ≠ ∅ then
    S ← S\{X<sub>i</sub>}
    return S
```

Fig. 4 Given a set $X \subset \Omega$, and a pair $(A, B) \in \Omega \backslash X$, find a subset $S \subseteq X$ s.t. S is a minimal A, B-separator in R.

Algorithm MineMinSeps(R, Ω , ε , (A, B))

```
1: C ← Ø
 2: X \leftarrow nil
 3: if I(A; B|\Omega \setminus \{A, B\}) \le \varepsilon {by getEntropy<sub>R</sub>} then
          X \leftarrow \mathsf{ReduceMinSep}(\varepsilon, \Omega \setminus \{A, B\}, (A, B))
           \mathbf{C} \leftarrow \mathbf{C} \cup \{X\}
 6: else
           Return Ø
      while (D \leftarrow nextMinTransversal(C)) \neq nil do
          \overline{D} \leftarrow \Omega \backslash D
           \phi \leftarrow \text{getFullMVDs}(\overline{D}, \varepsilon, (A, B), 1)
          if \phi \neq \emptyset then
11:
               X \leftarrow \mathsf{ReduceMinSep}(\varepsilon, \overline{D}, (A, B))
12:
13:
               \mathbf{C} \leftarrow \mathbf{C} \cup \{X\}
14: return C
```

Fig. 5 Given a relation R with schema Ω , two attributes $A, B \in \Omega$, and a threshold ε enumerate all minimal A, B-separators in R.

finite set of sets. The problem of discovering all minimal transversals of ${\bf C}$ is called the *hypergraph transversal problem* [23]. The theoretically best known algorithm for solving the hypergraph transversal problem is due to Fredman and Khachiyan [16] and has a quasi incremental-polynomial delay of $poly(n) + m^{O(\log^2 m)}$ where $m = |{\bf C}| + n$. Note the dependence on the size of the discovered minimal separators $|{\bf C}|$. We denote by $T_{minTrans}(n,{\bf C})$ the delay of the minimal transversal algorithm. However, not every minimal transversal D leads to the discovery of a minimal separator if \overline{D} does not separate A and B (i.e., $\phi = \emptyset$ in line 11 of MineMinSeps).

In the full version of this paper we show that the number of minimal transversals processed in lines 9-13 before a new minimal separator is discovered (e.g., in line 12), or before the loop exists, is bounded by $n \cdot |\mathbf{C}|$. This allows us to formalize the delay between the discovery of minimal A, B-separators. We denote by T(getFullMVDs) the runtime of getFullMVDs, which we analyze in the next section.

COROLLARY 6.3. Algorithm MineAllMinseps enumerates the minimal A, B-separators in R with a delay of $O(n \cdot |C| \cdot T_{minTrans}(n, C) \cdot T(\text{getFullMVDs}))$, where $n = |\Omega|$.

6.2 Discovering the Full MVDs

Returning to our main algorithm, MVDMiner, we have shown how to compute $\text{MinSep}_{\mathcal{E}}(R,A,B)$, the set of minimal A,B separators in R. Next, for each minimal A,B separator $X \in \text{MinSep}_{\mathcal{E}}(R,A,B)$, we compute all full MVDs with key X that separate A and B, i.e. the set $\text{FullMVD}_{\mathcal{E}}(R,X,A,B)$; this is line 5 of MVDMiner. Recall that full means that the MVD cannot be further refined.

The algorithm getFullMVDs starts by checking the most refined MVD with key X, namely $\varphi = X \twoheadrightarrow Y_1|\dots|Y_n$ where Y_1,\dots,Y_n are all attributes not in X (including A,B). If $\mathcal{J}(\varphi) \leq \varepsilon$ then we are done. Otherwise, the algorithm considers all possible ways to *merge* two dependents, while keeping A and B in different dependents; i.e. it tries $X \twoheadrightarrow Y_1Y_2|\dots|Y_n,X \twoheadrightarrow Y_1Y_3|Y_2|\dots|Y_n$, etc. We denote the MVD that results from merging dependents Y_i and Y_j in $\operatorname{dep}(\varphi)$ by $\operatorname{merge}_{ij}(\varphi)$. Since φ refines $\operatorname{merge}_{ij}(\varphi)$ then, by Proposition 5.2, it holds that $\mathcal{J}(\operatorname{merge}_{ij}(\varphi)) \leq \mathcal{J}(\varphi)$. This procedure for searching for a full ε -MVD can be viewed as a graph traversal algorithm where every node φ is an ε -MVD candidate with key X, dependents Z_1,\dots,Z_k , and its neighbors $\operatorname{Nbr}(\varphi)$ are the ε -MVD candidates:

$$Nbr(\phi) \stackrel{\text{def}}{=} \{merge_{ij}(\phi) : Z_i, Z_j \in dep(\phi), A, B \notin Z_i Z_j \}$$
 (13)

Clearly, if A, B were separated in ϕ , then they remain separated in every MVD in Nbr(ϕ). We present the algorithm as a depth-first traversal, which is how we implemented it. The pseudocode is presented in Figure 6.

6.2.1 An Optimization to getFullMVDs. In the worst case, Algorithm getFullMVDs will traverse the search space of possible ways to partition n attributes into $k \in \{2, ..., n-1\}$ sets, and there can be $O(\frac{k^n}{k!})$ such such partitions 3 . While, in general, this is unavoidable, we implemented an optimization, described in the complete version of this paper, that leads to a significant reduction in the search space.

Algorithm getFullMVDs(S, ε , (A, B), K)

```
1: \mathcal{P} \leftarrow \emptyset {Output set}
 2: Q \leftarrow \emptyset \{Q \text{ is a stack}\}
 3: \phi_0 = S \rightarrow X_1 | \dots | X_n where X_i are singletons.
 4: Q.push(\phi_0)
 5: while Q \neq \emptyset
                                 |\mathcal{P}| < K  do
          \varphi \leftarrow Q.pop()
 6:
          Compute \mathcal{J}(\varphi) {using getEntropy<sub>R</sub>}
 7:
 8:
          if \mathcal{J}(\varphi) \leq \varepsilon then
              \mathcal{P} \leftarrow \mathcal{P} \cup \{\varphi\}
 9:
10:
          else
              for all \phi \in Nbr(\phi) do
11:
                  Q.push(\phi) {See (13)}
12:
13: return \mathcal{P}
```

Fig. 6 Returns a set of at most K full MVDs with key S that approximately hold in R (w.r.t ε) in which A and B are in distinct components.

6.3 Computing Entropies Efficiently

We describe the procedure getEntropy_R for calculating the joint entropy of a set of attributes. The efficiency of this procedure is crucial to the performance of MVDMiner, which needs to repeatedly compute mutual information values I(Y; Z|X), and each such computation requires four entropic values H(XY), H(XZ), H(XYZ), and H(X). Repeatedly computing values of the form $H(X_{\alpha})$, for $\alpha \subseteq [n]$ requires multiple scans over the data that resides in external memory.

We build on ideas introduced in the PLI cache data structure [21, 27], and reduce the problem of computing $H(X_{\alpha})$ to a main memory join-group-by query. To describe the algorithm, we repeat here the entropy formula (5) for convenience:

$$H(X_{\alpha}) \stackrel{\text{def}}{=} \log N - \frac{1}{N} \sum_{X_{\alpha} \in \mathcal{D}_{\alpha}} |R(X_{\alpha} = x_{\alpha}) \log |R(X_{\alpha} = x_{\alpha})| \quad (14)$$

The algorithm uses two ideas: (1) if x_{α} is a singleton (i.,e., its frequency $|R(X_{\alpha}=x_{\alpha})|=1$) then it can be ignored because its contribution to the total entropy in (14) is 0 (due to the logarithm), and (2) given two relations mapping the distinct values of attribute sets X_{α} , and X_{β} , respectively, to the tuple ids in the relation R that contain them, then we can derive this mapping for $X_{\alpha} \cup X_{\beta}$ by simply joining the two mappings on the tuple IDs. Ignoring singleton valuations makes these mappings highly compressed, enabling us to store them in main memory and perform the join using a main memory database system. We used the in-memory database H2 [44]. We describe the details next. We let Hash denote a hash function. In our implementation we use the hash function provided by the database system.

³These are *Stirling numbers of the second kind:* https://en.wikipedia.org/wiki/Stirling_numbers_of_the_second_kind

Alg. getEntropy_R maintains two sets of relations indexed by $\alpha \subseteq [n]$: CNT $_{\alpha}$ (val, cnt) and TID $_{\alpha}$ (val, tid) defined as:

```
\begin{split} & \text{CNT}_{\alpha} \!=\! \{(Hash(x_{\alpha}), \text{cnt}) \mid \text{cnt} = |R(X_{\alpha} = x_{\alpha})|, \text{cnt} > 1\} \\ & \text{TID}_{\alpha} \!=\! \{(Hash(x_{\alpha}), t[\text{tid}]) \mid t \!\in\! R, t[X_{\alpha}] \!=\! x_{\alpha}, Hash(x_{\alpha}) \!\in\! \Pi_{\text{val}}(\text{CNT}_{\alpha})\} \end{split}
```

We compute $H(X_{\alpha})$ by scanning table CNT_{α} . The algorithm starts by computing two sets of relations: (1) $\{\mathrm{CNT}_{\{i\}}\}$ and (2) $\{\mathrm{TID}_{\{i\}}\}$ for every $i \in [n]$. Assume that we have computed the relations CNT_{α} , CNT_{β} and TID_{α} , TID_{β} for some subsets $\alpha, \beta \subset [n]$ such that $\alpha \cap \beta = \emptyset$. We first compute $\mathrm{CNT}_{\alpha \cup \beta}$ as:

```
Select Hash(A.val, B.val) as val, count(*) as cnt From TID_{\alpha} A, TID_{\beta} B Where A.tid = B.tid Group By Hash(A.val, B.val) Having count(*) > 1
```

Next, we compute $TID_{\alpha \cup \beta}$ as:

```
Select Hash(A.val, B.val) as val, A.tid as tid From TID_{\alpha} A, TID_{\beta} B, CNT_{\alpha \cup \beta} Z Where A.tid = B.tid and Hash(A.val, B.val) = Z.val
```

Pruning the singleton values makes this technique very effective, because as we move up the lattice from smaller α 's to larger α 's, many more tuples x_{α} are unique in the data, and the tables CNT_{α} and TID_{α} become smaller.

Example 6.4. For a simple illustration, Fig. 7 shows the tables generated for a 3-attribute relation *R*. Both types of relations only contain values corresponding to non-singleton valuations in *R*.

However, even with our compression, generating and storing all 2^n-1 tables CNT_α , and TID_α is intractable. Instead, we perform the following optimization. Fix a parameter L (in our implementation we chose L=10), and partition the set Ω into $\left\lceil \frac{n}{L} \right\rceil$ disjoint subsets $\Omega_1, \Omega_2, \ldots$ each of size at most L. For each i, compute the tables TID_α and CNT_α for all subsets $\alpha \subseteq \Omega_i$; thus the total number of tables precomputed is $2 \left\lceil \frac{n}{L} \right\rceil \cdot 2^L$. In order to compute $H(X_\alpha)$, we express $\alpha = (\alpha \cap \Omega_1) \cup (\alpha \cap \Omega_2) \cup \ldots$, where each union is treated as explained above for $\alpha \cup \beta$.

7 ENUMERATING ACYCLIC SCHEMAS

In this section we present the second phase of Maimon: given the set $\mathcal{M}_{\varepsilon}$ of full ε -MVDs (Eq. (11)), generate acyclic ε -schemes. The algorithm ASMiner is shown in Fig. 8. It searches for subsets of MVDs $Q \subseteq \mathcal{M}_{\varepsilon}$, and reconstructs a schema from that set. The key to the algorithm's efficiency is our new definition of compatibility:

R										
tid	Α	В	С							
t_1	a_1	b_2	<i>c</i> ₃	CNT	CNT_A		CNT_B		CNT_C	
t_2	a_2	b_1	c_1	val	CNT	val	CNT	val	CNT	
t_3	a_2	b_2	c_2	a_2	2	b_2	2	<i>c</i> ₃	2	
t_4	a_3	b_3	c_3	a_3	2	b_3	2			
t_5	a_3	b_3	c_4	TID_A	TID_A		TID_B		TID_C	
CNT	AB			val	tid	val	tid	val	tid	
	/al		CNT	a_2	t_2	b_2	t_1	c_3	t_4	
Hash	$a(a_3, b)$	$b_3)$	2	a_2	t_3	b_2	t_3	c_3	t_4	
TID_A	AB			a_3	t_4	b_3	t_4			
	/al		tid	a_3	t_5	b_3	t_5			
Hash	$a(a_3, b)$	(b_3)	t_4							
Hash	$a(a_3, b)$	$b_3)$	t_5							

Fig. 7 getEntropy_R *example*.

Algorithm ASMiner($\mathcal{M}_{\varepsilon}$)

- 1: $schemes = \emptyset$
- 2: Construct the graph $G = \{(\phi, \psi) \mid \phi, \psi \in \mathcal{M}_{\varepsilon}, \phi \sharp \psi\}$
- 3: for all $Q \in MaxIndependentSet(G)$ do
- 4: schemes ← schemes \cup {BuildAcyclicSchema(Q)}
- 5: return schemas

Fig. 8 Generate Acyclic Schemas from $\mathcal{M}_{\varepsilon}$.

Algorithm BuildAcyclicSchema(*Q*)

- 1: $S \leftarrow \{\Omega\}$
- 2: Sort Q by ascending order of key cardinality {e.g., X woheadrightarrow A|B before XY woheadrightarrow C|D}
- 3: for all $\phi \in Q$ do
- 4: Let $\phi = X \rightarrow C_1 | \dots | C_m$
- 5: Let $\Omega_i \in S$ s.t. $X \subseteq \Omega_i$
- 6: $\mathbf{D}_{\phi} \leftarrow \{C_i X \cap \Omega_i \mid j \in [i, m]\} \setminus \{X\}$
- 7: **if** $|\mathbf{D}_{\phi}| \geq 2$ **then**
- 8: Replace $\Omega_i \in S$ with $\mathbf{D}_{\phi} \{ \phi \text{ is non-redundant} \}$
- 9: return S

Fig. 9 Gets a set Q of pairwise compatible MVDs, and returns an acyclic schema.

Definition 7.1. Let $\phi_1 = X \twoheadrightarrow A_1 | \dots | A_m$ and $\phi_2 = Y \twoheadrightarrow B_1 | \dots | B_k$ be two ε -MVDs. We say that ϕ_1 and ϕ_2 are *compatible* if there exist an $i \in \{1, \dots, m\}$, and $j \in \{1, \dots, k\}$ such that:

- (1) $Y \subseteq XA_i$, and $X \subseteq YB_j$. In this case we say that the two MVDs are *split-free* [6, 15, 19, 28].
- (2) There exist two distinct indexes $j_1, j_2 \in \{1, ..., k\}$ such that $XA_i \cap B_{j_1} \neq \emptyset$, and $XA_i \cap B_{j_2} \neq \emptyset$. Likewise, there exist two distinct indexes $i_1, i_2 \in \{1, ..., m\}$ such that $YB_j \cap A_{i_1} \neq \emptyset$, and $YB_j \cap A_{i_2} \neq \emptyset$.

We write $\phi_1 \sharp \phi_2$ to denote the fact that ϕ_1, ϕ_2 are *in*compatible.

We say that a set Q of ε -MVDs is *pairwise compatible* if every pair of ε -MVDs in Q is compatible. Recall that every join tree \mathcal{T} with m nodes defines a set of m-1 MVDs called its *support* and denoted by MVD(\mathcal{T}).

THEOREM 7.2. Let S be an acyclic schema with join tree (\mathcal{T}, χ) . Then the set $MVD(\mathcal{T})$ is pairwise compatible.

Thus, it suffices to iterate over sets of pairwise compatible ε -MVDs. Specifically, our algorithm enumerates the *maximal* sets of pairwise compatible ε -MVDs, and for this task we use a graph algorithm from the literature. Define the graph $G(\mathcal{M}_{\varepsilon}, E)$ as follows:

$$E = \{ (\phi_1, \phi_2) : \phi_1, \phi_2 \in \mathcal{M}_{\varepsilon} \text{ and } \phi_1 \sharp \phi_2 \}$$
 (15)

By this definition every maximal independent set in G corresponds to a maximal set of pairwise compatible ε -MVDs. We apply the following result.

Theorem 7.3. ([11, 22]) Let G(V, E) be a graph. The maximal independent sets of G can be enumerated such that the delay between consecutive outputs is in $O(|V|^3)$.

In summary, algorithm ASMiner in Fig. 8 enumerates all maximal independent sets Q, then for each of them constructs one acyclic schema S, by calling BuildAcyclicSchema shown in Fig. 9, and described next.

Algorithm BuildAcyclicSchema starts with a schema that contains a single relation with all attributes (i.e., $S = \{\Omega\}$). It then builds the acyclic schema for R by repeatedly using an ε -MVD from Q to decompose one of the relations in S. The MVDs are processed in ascending order of the cardinality of their keys. Therefore, when an MVD $S \rightarrow C_1 | \ldots | C_m$ is processed, then we know that S is contained in exactly one of the relations in S (e.g., otherwise, S must be contained in a key of a previously processed ε -MVD). The algorithm then applies this ε -MVD to the single relation that contains it, and continues until all ε -MVDs in Q have been processed. An MVD is said to be *redundant* [18] if it does not split the single relation that contains it (i.e., condition of line 7 does not hold). Redundant MVDs are simply ignored in BuildAcyclicSchema.

THEOREM 7.4. Algorithm BuildAcyclicSchema generates an acyclic schema S with join tree (\mathcal{T}, χ) such that $MVD(\mathcal{T}) \subseteq Q$. If Q is a non-redundant set of ε -MVDs then $MVD(\mathcal{T}) = Q$. The algorithm runs in time $O(n^3)$.

 $\begin{array}{c} \text{Dataset} & \text{Full MVDs} \\ & \text{threshold=0.0} \end{array}$

Dataset	Cols.	Rows	Runtime [sec]	Full MVDs
Ditag Feature	13	3960124	TL	NA
Four Square (Spots)	15	973516	17017	105
Image	12	777676	3747	151
FD_Reduced_30	30	250000	8024	21
FD_Reduced_15	15	250000	1006	21
Census	42	199524	TL	NA
SG_Bioentry	7	184292	101	3
Atom Sites	26	160000	TL	242
Classification	12	70859	1327	27
Adult	15	32561	1083	58
Entity Source	33	26139	14155	153
Reflns	27	24769	TL	543
Letter	17	20000	605	44
School Results	27	14384	7202	2394
Voter State	45	10000	TL	262
Abalone	9	4177	602	36
Breast-Cancer	11	699	5	30
Hepatitis	20	155	479	2953
Echocardiogram	13	132	6	104
Bridges	13	108	3.8	60

Table 2: Datasets used in the experiments. We show the runtimes (in seconds) for mining full MVDs with threshold 0.0, with a time limit (TL) of 5 hours.

The novel insight of our algorithm is the characterization of (in)compatibility in Definition 7.1, which depends only on the pairwise relationship between the MVDs, and therefore enables the reduction to enumerating maximal independent sets in graphs. Previous characterizations [6, 15, 19, 28] are for entire sets of MVDs, and are not pairwise (more precisely, they have a different second condition called intersection which relies on the existence of a third MVD in the set). Goodman and Tay [18] present an algorithm for synthesizing an acyclic schema from a set Q of MVDs that satisfy the subset property. As in Theorem 7.4, they show that if the set Q is non-redundant then the synthesized acyclic schema has a join tree whose support is precisely the set Q. However, we are not aware of any characterization of non-redundant MVDs. While the subset property is pairwise, it is applicable only to binary MVDs, while our MVDs may have any number of dependents. Algorithms for constructing a (single) acyclic schema from data dependencies have been previously developed by Bernstein [7] where the input is a set of functional dependencies, and by Beeri et al. and Lien whose algorithms work by combining conflict-free MVDs [6, 32].

EVALUATION

In this section we conduct an experimental evaluation of Maimon. We start with an end-to-end evaluation of its usefulness in Section 8.1, then evaluate the accuracy of the approximate schemas in terms of the relationship between the *J*-measure and number of spurious tuples in Section 8.2. Next, we evaluate the efficiency and scalability of Maimon, measuring the time to find the minimal separators in Section 8.3. Finally, we report the rate of enumeration, and some quality metrics of the generated acyclic schemes in Section 8.4.

We used 20 real-world datsets [43] that are part of the Metanome data profiling project [34], shown in Table 2 (we discuss the runtimes in Sec. 8.3). Maimon was implemented in Java 1.8 and all experiments are conducted on a 64bit Linux machine with 120 CPUs and 1 TB of memory, running Ubuntu 5.4.0; our algorithm is single-threaded and runs on a single core.

8.1 A Use Case: Nursery

To evaluate the usefulness of Maimon we applied it to the Nursery dataset⁴, a training data for classifying and ranking applications for nursery schools. The dataset contains eight attributes describing occupational, financial, social and health conditions of the family, and a classification attribute that indicates the priority of the application; we renamed the attributes $A \dots I$ for brevity. The data has 12960 tuples and a total of 12960 * 9 = 116640 cells. By increasing the threshold J from 0 to 0.5, we found 415 acyclic schemes (Fig 11), and show ten of them in detail in Fig. 10. As one can see in Fig. 10(a), when J = 0, no exact decomposition is possible; a traditional (exact) decomposition of this data is not possible. As we increase J, however, we find better and better schemas in Fig. 10 (b)-(j), in the sense that it decomposes into more relations, each with fewer attributes. For example, the schema in (h) (J = 0.277) has 4 relations, BEGI, ABDEHI, CDE, DEF. For each scheme we report the percentage cell savings, S, and the percentage of spurious tuples, E. There is a good tradeoff between space savings and error rate: several schemes have under 10% spurious tuples yet achieve over 80% space saving. The space savings are very high (e.g. over 90%), because the Nursery data is dense: the attribute domains have sizes 3, 5, 4, 4, 3, 2, 3, 3, 5. For example, the extreme schema where each attribute is a separate relation (not shown in the Figure) has 3+5+4+4+3+2+3+3+5 = 32 cells and a savings of (116640 - 32)/116640 i.e. S = 99.9725%; however, its fraction of spurious tuples is (3*5*4*4*3*2*3*3*5-12960)/12960 = 4, i.e. E = 400%. Fig. 11 shows the values S, E for all 415 schemes. Users are likely to select the pareto optimal schemes, i.e. whose *S*, *E* values are not dominated by any other schemes: the ten pareto optimal schemes in this graph are connected

by a line, and are precisely those we have selected to show in detail in Fig. 10. In addition to savings S and spurious tuples E, applications are likely to define their own domain specific quality measure and choose the optimal schema for that application.

8.2 Accuracy

Next, we analyzed the relationship between the *J*-measure of the acyclic schemes, and the percentage of spurious tuples. There is no tight theoretical connection between these two measures, except that J=0 iff there are no spurious tuples, hence the need for an empirical evaluation. The results are presented in Figure 12. We generated all acyclic schemes with a threshold $\varepsilon \in [0, 0.5]$, partitioned the schemes into buckets according to their *J*-measure, and report the quantiles of the number of spurious tuples in each bucket. The experiments confirm a consistent relationship between the *J*-measure and the percentage of spurious tuples. Assuming we want to have no more than 20% spurious tuples, then we can increase J up to 0.1-0.3, depending on the dataset. The width of the boxes represent the number of acyclic schemes in that bucket. In general, as J increases, the number of acyclic schemes will eventually decrease: this is particularly visible in Fig. 12 (d). The explanation lies in the fact that larger *J*'s reduce the size (and, hence, the number) of minimum separators. If we allowed I to increase further, eventually we find a single schema, where each attribute is a separate relation, and where the sole minimal separator is the empty set.

8.3 Scalability

Next, we evaluated the scalability of Maimon. We started by computing all exact MVDs ($\varepsilon = 0$) on all 20 datasets and report the runtimes in Table 2. On five of the datasets, our system timed out after 5h: for Atom Sites, REFLNS, and Voter State, it did report a large number of full MVDs, while for DITAG Feature and Census it did not find any within this limit, but it terminated on subsets, as we report below.

The discovery of acyclic schemes has three parts: computing all minimal separators (Sec. 6.1), discovering all full MVDs (Sec. 6.2), and enumerating the acyclic schemes (Sec. 7). We found that the first step by far dominates the total runtime, and we report it here; we report the other two runtimes in the technical report. We report here the time to compute all minimal separators as a function of #rows, and of #columns.

8.3.1 Row Scalability. We evaluated the algorithm over three large datsets: Image, foursquare, and Ditag Feature. We included all columns, and a subset of 10% to 100% of the tuples. The results are in Figure 13. In general, we found that the runtime increases mostly linearly with the size of the data even when the number of minimal separators is mostly constant, e.g. for Image and Ditag Feature.

⁴https://archive.ics.uci.edu/ml/datasets/nursery

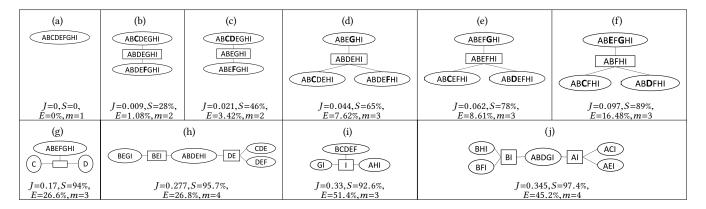


Fig. 10 The Nursery use case, showing the 10 pareto optimal schemes (out of 415). We encode the 9 attributes as A, B, \dots, I (top). The data does not admit a exact decomposition (a), but we obtain increasingly better schemes (b)-(j) as we increase the J-measure, with increased space savings S, at the cost of increased rate of spurious tuples E; for example, for J = 0.277 the data decomposes into 4 relations, S = 95.7% (see text for the explanation of why it is so high) and E = 26.8%.

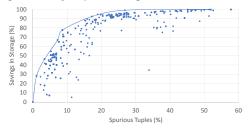


Fig. 11 All 415 schemes discovered for **Nursøry**. The plot shows the savings S v.s. the spurious tuples E. The line connects the ten pareto-optimal schemes further detailed in Fig. 10.

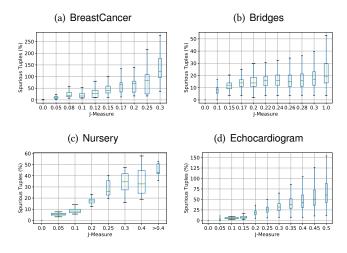


Fig. 12 Spurious Tuples (%) vs. J-measure (see Sec. 8.2).

8.3.2 Column Scalability. Next, we varied the number of columns. Here we kept all rows of the datasets, and included between 10% to 100% of the columns. The results are presented in Figure 14. We let the algorithm run for 5 hours

and measured the resulting number of minimal separators. For example, in the Voter State dataset with 32 columns Maimon discovered 682, 306 and 242 minimal separators for thresholds 0,0.01, and 0.1 respectively, within the 5h time limit. We found that the runtime is affected both by the number of attributes, and, quite significantly, by the number of minimal separators. This is explained by considering Corollary 6.3 that analyzes the delay between the output of minimal separators. First, we note that the delay depends exponentially on the number of attributes (via getFullMVDs, see Sec. 6.2.1) which explains why the delay significantly increases with the number of attributes, leading to an overall reduction in the number of minimal separators returned. Second, the delay also depends on the number of minimal separators generated up to that point, which explains the high runtime in cases where the data contains a large number of minimal separators.

8.4 Quality

We conducted an empirical evaluation of the quality of the schemes generated by Maimon, and report the results in Figure 15. Per threshold, we ran the enumeration algorithm for half an hour and measured the number of schemes generated (i.e., #schemes), and the following quality measures, for which we report on their aggregate values.

- (1) The number of relations in any scheme S generated, denoted #relations(S).
- (2) The *width* attained by any generated scheme, where width refers to the largest number of attributes in any relation of S. Formally⁵, width(S) $\stackrel{\text{def}}{=} \max_{i \in [1, m]} |\Omega_i|$.
- (3) The *intersection width* attained by any scheme generated, where intersection width refers to the the largest

⁵width(S) is precisely the treewidth plus one.

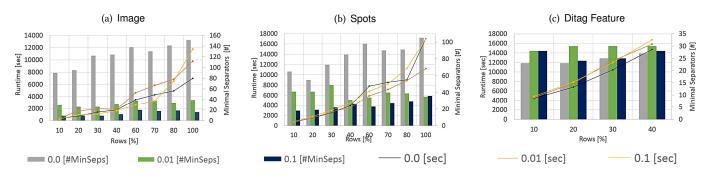


Fig. 13 Row scalability experiments, for $\varepsilon \in \{0., 0.01, 0.1\}$ (Sec 8.3.1).

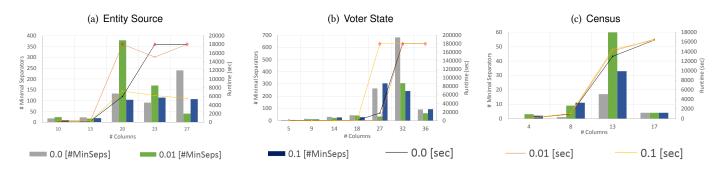


Fig. 14 Column scalability experiments for $\varepsilon \in \{0, 0.01, 0.1\}$ (Sec 8.3.1). We timed out at five hours (red clock).

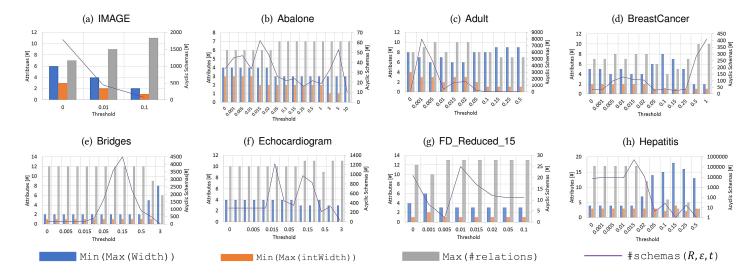


Fig. 15 Quality of approximate schemas (Sec. 8.4)

size of any separator of S. Formally, intWidth(S) $\stackrel{\text{def}}{=}$ $\max_{i,j\in[1,m]} |\Omega_i \cap \Omega_j|$.

In Figure 15 we increased the threshold ε , and report for each threshold the maximum #relations(S), and the minimum width(S), intWidth(S) for all schemas at that threshold. In general, we observed that, as we increase the threshold, the system can find more interesting schemes. For example,

for Image and Abalone, width (blue bar) decreases, which means that the number of attributes in the widest relation decreases. For Adult and BreastCancer the number of relations (#relations – gray bar) increases, another indicator of the quality of the schema.

9 CONCLUSIONS

We present Maimon, the first system for the discovery of approximate acyclic schemes and approximate MVDs from data. To define "approximate", we used concepts from information theory, where each MVD or acyclic schema is defined by an expression over entropic terms; when the expression is 0, then the MVD or acyclic schema holds exactly. We then presented the two main algorithms in Maimon, mining all full ε -MVDs with minimal separators, and discovering acyclic schemes from a set of ε -MVDs. Both algorithms improve over prior work in the literature. We conducted an experimental evaluation of Maimon on over 20 real-world data sets.

Our approach of using information theory to define approximate data dependencies differs from the previous definitions that rely mostly on counting the number of offending tuples. On one hand, our definitions provide us with more powerful mathematical tools, on the other hand the connection to the actual data quality is less intuitive. We leave it up to future work to explore the connection between information theory and data quality.

Depending on the dataset, Maimon generates hundreds and even thousands of acyclic ε -schemas in as little as 30 minutes. As part of future work we intend to investigate acyclic schema generation in *ranked order*. The categories to rank on may be the extent of decomposition (e.g., width of the schema), or other measures indicative of how well the schema meets the requirements of the application.

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10 APPENDIX

11 PROOFS FROM SECTION 5

Given two MVDs $\phi = S \twoheadrightarrow X_1 | \dots | X_m$ and $\psi = S \twoheadrightarrow Y_1 | \dots | Y_k$, define their *join* as $\phi \lor \psi = S \twoheadrightarrow Z_{11} | Z_{12} | \dots | Z_{mk}$, where $Z_{ij} = X_i \cap Y_j$. Clearly, $\phi \lor \psi$ refines both ϕ and ψ , i.e. $\mathcal{J}(\phi \lor \psi) \ge \max(\mathcal{J}(\phi), \mathcal{J}(\psi))$. We prove a weak form of converse:

LEMMA 5.4. The following are Shannon inequalities: $\mathcal{J}(\phi \lor \psi) \le \mathcal{J}(\phi) + m\mathcal{J}(\psi)$ and $\mathcal{J}(\phi \lor \psi) \le k\mathcal{J}(\phi) + \mathcal{J}(\psi)$.

PROOF. We prove the first inequality (the second is similar), and for that we need to show: $\left(\sum_{i=1}^{m} H(SX_i) - (m-1)H(S) - H(\Omega)\right) + m\left(\sum_{j=1}^{k} H(SY_j) - (k-1)H(S) - H(\Omega)\right) \ge \sum_{i,j} H(SZ_{i,j}) - (mk-1)H(S) - H(\Omega)$, or, equivalently:

$$\sum_{i=1}^{m} H(SX_i) + m \sum_{j=1}^{k} H(SY_j) \ge \sum_{ij} H(SZ_{ij}) + mH(\Omega)$$
(16)

For that we prove by induction on ℓ :

$$H(SX_i) + \sum_{j=1}^{\ell} H(SY_j) \ge \sum_{j=1}^{\ell} H(SZ_{ij}) + H(SX_iY_1 \dots Y_{\ell})$$
 (17)

Indeed, assuming the statement for $\ell-1$ holds, then the statement for ℓ follows from:

$$H(SY_{\ell}) + H(SX_iY_1 \dots Y_{\ell-1}) \ge H(SZ_{i\ell}) + H(SX_iY_1 \dots Y_{\ell})$$

which is the submodularity inequality, since $SY_{\ell} \cap (SX_iY_1 \dots Y_{\ell-1}) = SY_{\ell} \cap SX_i = SZ_{i\ell}$. Setting $\ell = k$ in (17) and summing over i = 1, m we obtain $\sum_{i=1}^m H(SX_i) + m \sum_{j=1}^k H(SY_j) \ge \sum_{ij} H(SZ_{ij}) + \sum_{i=1}^m H(SX_iY_1 \dots Y_k) = \sum_{ij} H(SZ_{ij}) + mH(\Omega)$, proving (16).

12 PROOFS AND DETAILS FROM SECTION 6

12.1 Correctness of Algorithm MineAllMinSeps

THEOREM 3.3. Algorithm MineMinSeps in Figure 5 enumerates all minimal A, B-separators in R.

PROOF. We first note that every set of attributes *S* that is added to *S* in lines 5 and 13 is a minimal *AB* separator. Therefore, we proceed by showing that *all* minimal *AB* separators are mined by MVDMiner.

Let $\Omega = X_1 \dots X_n$, and let $p = X_1, \dots, X_n$ be some predefined order over the attributes that is used in algorithm ReduceMinSep (Figure 4). We view every minimal AB-separator as a subsequence of p, whose letters (i.e., attributes) are ordered according to p. That is, the permutation p induces a lexicographic ordering over the subsets of Ω . For example, $X_3X_4X_9X_{15} > X_3X_4X_7X_{100}$. We prove the claim by backwards induction on the lexicographic ordering of the subsets of Ω . That is, for every subsequence p_S of p, over attributes S, we show that if S is a minimal AB separator, then S is discovered by the algorithm. The induction follows reverse lexicographic order of the sequences (e.g., $X_3X_4X_9X_{15}$ before $X_3X_4X_7X_{100}$).

Base case. : p_S is the lexicographically largest subsequence: $p_S = X_n$, or $S = X_n$. By Theorem 6.1, if S is a minimal AB separator that is not in S, then there exists a minimal transversal D of S such that $S \subseteq \overline{D}$. By Proposition 5.1 if X_n separates A and B, then so does each one of its supersets. Therefore, algorithm ReduceMinSep (Figure 4) that uses the attribute sequence p, will return the minimal AB separator $S = X_n$ when provided with input $\overline{D} \supseteq \{X_n\} = S$.

Step. : Let p_S denote the subsequence corresponding to the set $S \subset \Omega$. By the induction hypothesis, we assume that all minimal AB separators that are lexicographically larger than S have been mined and are in S. By Theorem 6.1, there exists a minimal transversal D of S such that $S \subseteq \overline{D}$. Now, let $p_S = X_{i_1}, \ldots, X_{i_m}$ denote the subsequence associated with S (i.e., $S = \{X_{i_1}, \ldots, X_{i_m}\}$). Now, consider how algorithm ReduceMinSep handles the input \overline{D} (line 12). Clearly, it will remove all attributes $X_j \in \overline{D}$ such that $X_{i_1} > X_j$ because the resulting set contains the minimal separator S (line 6 in ReduceMinSep). Now, suppose, by contradiction, that $X_{i_k} \in S$ is removed in line 6 of ReduceMinSep. This means that \overline{D} contains a minimal AB separator C that is lexicographically larger than S. But by the induction hypothesis, such a minimal separator C is already in S. Since $C \subseteq \overline{D}$, it means that $C \cap D = \emptyset$, contradicting the fact that D is a minimal transversal of S.

12.2 Runtime Analysis of MineAllMinSeps

Definition 12.1. Let S be a (not necessarily complete) set of minimal AB separators. We define the negative border of S to be:

$$BD^{-}(S) = \{ U \subset \Omega | U \notin S, \text{ there exists a } X_i \in \Omega \text{ s.t. } U \cup \{X_i\} \in S \}$$
 (18)

Since every minimal separator in S contains at most *n* attributes then $|BD^{-}(S)| \leq |S| \cdot n$.

THEOREM 12.2. The number of minimal transversals processed in lines 9-13 of algorithm MineAllMinseps is at most |BD⁻(S)|.

PROOF. Let D be a minimal transversal of S processed by in lines 9-13. It cannot be the case that $\overline{D} \supseteq C$ for any $C \in S$, and in particular $\overline{D} \notin S$. Since D is a minimal transversal, then for every attribute $Y \in D$ it holds that $D \setminus \{Y\}$ is no longer a transversal for S. That is, there is an AB minimal separator $C \in S$ such that $C \cap (D \setminus \{Y\}) = \emptyset$, or that $C \subseteq \overline{D} \setminus \{Y\}$. Noting that $\overline{D} \setminus \{Y\} = \overline{D} \cup \{Y\}$, we get that $C \subseteq \overline{D} \cup \{Y\}$, or that $C \setminus \{Y\} \subseteq \overline{D}$. So we get that $C \setminus \{Y\} \subseteq \overline{D}$, and that $C \not\subseteq \overline{D}$. In other words, every minimal transversal D processed corresponds to a set in $BD^-(S)$.

12.3 An Optimization to getFullMVDs

In the worst case, if *S* is *not* an *AB* separator then Algorithm getFullMVDs will traverse the complete search space of size $O(2^n)$. While, in general, this is unavoidable, we implemented an optimization, described in the complete version of this paper, that leads to a significant reduction in the search space.

By (7) in Proposition 5.1 it holds that if $I(A; B|S) > \varepsilon$ for a pair of attributes $A, B \in \Omega$, then for any MVD $\phi = S \twoheadrightarrow C_1 | \dots | C_m$ in which A and B are in distinct components it holds that $\mathcal{J}_H(\phi) > \varepsilon$.

We say that an MVD $\phi = S \twoheadrightarrow C_1 | \dots | C_m$ is *pairwise consistent* if $I(C_i; C_j | S) \le \varepsilon$ for every pair of distinct components $C_i, C_j \in \text{dep}(\phi)$. Since $I(C_i; C_j | S) \le \mathcal{F}(S \twoheadrightarrow C_1 | \dots | C_m)$, then we can prune an MVD $S \twoheadrightarrow C_1 | \dots | C_m$ if it is not pairwise consistent, and avoid traversing its neighbors and descendants. In Figure 16 we present the algorithm getPairwiseConsistentMVD that receives an MVD $\phi = S \twoheadrightarrow C_1 | \dots | C_m$ where A and B are in distinct components, and returns a *pairwise consistent* MVD where A and B are in distinct components, if one exists. In Figure 17 we present the optimized getFullMVDs that prunes MVDs that cannot lead (via merges to components) to an MVD in which A and B are in distinct components.

Algorithm getPairwiseConsistentMVD(ε , ϕ , (A, B))

- 1: **while** A and B are in distinct components of ϕ AND ϕ is not pairwise consistent ${\bf do}$
- 2: Let $C_i, C_i \in \text{dep}(\phi)$ s.t. $I(C_i; C_i|S) > \varepsilon$
- 3: $\phi \leftarrow \mathsf{merge}_{ii}(\phi)$
- 4: **if** A and B are in distinct components of ϕ **then**
- 5: return ϕ
- 6: return nil

Fig. 16 Return an MVD $S woheadrightarrow C_1 | \dots | C_m \text{ s.t. } I(C_i; C_j | S) \le \varepsilon \text{ for every pair } C_i, C_j, \text{ and } A \text{ and } B \text{ are in distinct components or nil if no such MVD exists.}$

Algorithm getFullMVDsOpt(S, ε , (A, B), K)

```
1: \mathcal{P} \leftarrow \emptyset {Output set}
 2: Q \leftarrow \emptyset \{Q \text{ is a stack}\}
     \phi_0 = S \rightarrow X_1 | \dots | X_n where X_i are singletons.
          \leftarrow getPairwiseConsistentMVD(\varepsilon, \phi, (A, B))
 5: if \phi'_0 = nil then
         return Ø
 7: Q.push(\phi'_0)
     while Q \neq \emptyset and |\mathcal{P}| < K do
         \varphi \leftarrow Q.pop()
         Computed \mathcal{J}_H(\varphi) {using getEntropy<sub>R</sub>}
10:
         if \mathcal{J}_H(\varphi) \leq \varepsilon then
11:
             \mathcal{P} \leftarrow \mathcal{P} \cup \{\varphi\}
12:
         else
13:
             for all \phi \in Nbr(\phi) do
14:
                 \phi' \leftarrow \text{getPairwiseConsistentMVD}(\varepsilon, \phi, (A, B))
15:
                 if \phi' \neq nil then
16:
                      Q.push(\phi') {See (13)}
17:
18: return \mathcal{P}
```

Fig. 17 Returns a set of at most K full MVDs with key S that approximately hold in R in which A and B are in distinct components.

13 PROOFS FROM SECTION 7

Theorem 7.2. Let S be an acyclic schema with join tree (\mathcal{T}, χ) . Then the set $MVD(\mathcal{T})$ is pairwise compatible.

PROOF. Every key of MVD(\mathcal{T}) is the label on an edge of \mathcal{T} , and thus contained in a bag of \mathcal{T} . Hence, the set MVD(\mathcal{T}) is split-free and satisfies the first condition of definition 7.1.

Let $\phi_1, \phi_2 \in \text{MVD}(\mathcal{T})$ corresponding to edges $e_1, e_2 \in \text{edges}(\mathcal{T})$. Let $\mathcal{T}_1, \mathcal{T}_2$, and \mathcal{T}_3 be the three connected subtrees resulting from removing e_1, e_2 from \mathcal{T} . W.l.o.g, any path from a node in nodes(\mathcal{T}_1) to a node in nodes(\mathcal{T}_3) must pass through a node in nodes(\mathcal{T}_2). Therefore, dep(ϕ_1) = { $\chi(\mathcal{T}_1)\setminus \text{key}(\phi_1)$, $\chi(\mathcal{T}_2)\cup \chi(\mathcal{T}_3)\setminus \text{key}(\phi_1)$ }, and dep(ϕ_2) = { $\chi(\mathcal{T}_3)\setminus \text{key}(\phi_2)$, $\chi(\mathcal{T}_1)\cup \chi(\mathcal{T}_2)\setminus \text{key}(\phi_2)$ }. In particular, ϕ_2 splits the set $\chi(\mathcal{T}_2)\cup \chi(\mathcal{T}_3)$, and ϕ_1 splits the set $\chi(\mathcal{T}_2)\cup \chi(\mathcal{T}_1)$. Hence, MVD(\mathcal{T}) satisfies the second condition of definition 7.1.

14 FURTHER EXPERIMENTS

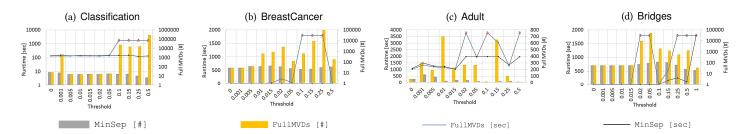


Fig. 18 Full MVDs Experiments. Red stopwatch indicates that the algorithm stopped after 30 minutes.

14.1 From minimal separators to full MVDs

We now experiment with the transition from minimal separators to full MVDs. We recall that an MVD ϕ is full with regard to ε if $R \models_{\varepsilon} \phi$ and for all MVDs $\psi > \phi$ that strictly refine ϕ then $R \not\models_{\varepsilon} \psi$.

In this set of experiments we have, for every pair of attributes $A, B \in \Omega$, the set MINSEP $_{\varepsilon,A,B}(R)$ of minimal AB-separators that hold in R w.r.t. ε , and we apply the algorithm for generating the set FULLMVD $_{\varepsilon,A,B}$ by calling getFullMVDs (Fig. 6) with the pair (A, B), and an unlimited number of MVDs to return (i.e., $K = \infty$). 6 In particular, the runtimes presented here do not include the time taken to mine the minimal separators. The performance of this phase is analyzed in Section 8.3 and Table 2.

We conduct the experiment as follows. For every dataset we vary the threshold in the range [0, 0.5], and for every threshold execute the procedure getFullMVDsOpt for a total of 30 minutes. The results are presented in Figure 18. When the threshold is $\varepsilon = 0$ then the number of full MVDs is identical to the number of minimal separators as expected by Lemma 5.4. In practice, when the threshold is 0, our algorithm for mining all minimal separators also discovers all full MVDs. As the threshold increases so does the difference between the number of minimal separators and the number of full MVDs. Overall, Algorithm getFullMVDsOpt for generating full MVDs is capable of reaching a rate of about 55 full MVDs per second for thresholds larger than 0.1 (see Figures 18(a), 18(b), and 18(d)).

 $^{^6}$ We actually call the optimized version of this algorithm, getFullMVDsOpt described in the full version of this paper.