Hasso Plattner Institute
Information Systems Group

Data Profiling
–
Efficient Discovery of Dependencies

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Abstract

Data profiling is the computer science discipline of analyzing a given dataset for its metadata. The types of metadata range from basic statistics, such as tuple counts, column aggregations, and value distributions, to much more complex structures, in particular inclusion dependencies (INDs), unique column combinations (UCCs), and functional dependencies (FDs). If present, these statistics and structures serve to efficiently store, query, change, and understand the data. Most datasets, however, do not provide their metadata explicitly so that data scientists need to profile them.

While basic statistics are relatively easy to calculate, more complex structures present difficult, mostly NP-complete discovery tasks; even with good domain knowledge, it is hardly possible to detect them manually. Therefore, various profiling algorithms have been developed to automate the discovery. None of them, however, can process datasets of typical real-world size, because their resource consumptions and/or execution times exceed effective limits.

In this thesis, we propose novel profiling algorithms that automatically discover the three most popular types of complex metadata, namely INDs, UCCs, and FDs, which all describe different kinds of *key dependencies*. The task is to extract all valid occurrences from a given relational instance. The three algorithms build upon known techniques from related work and complement them with algorithmic paradigms, such as divide & conquer, hybrid search, progressivity, memory sensitivity, parallelization, and additional pruning to greatly improve upon current limitations. Our experiments show that the proposed algorithms are orders of magnitude faster than related work. They are, in particular, now able to process datasets of real-world, i.e., multiple gigabytes size with reasonable memory and time consumption.

Due to the importance of data profiling in practice, industry has built various profiling tools to support data scientists in their quest for metadata. These tools provide good support for basic statistics and they are also able to validate individual dependencies, but they lack real *discovery* features even though some fundamental discovery techniques are known for more than 15 years. To close this gap, we developed Metanome, an extensible profiling platform that incorporates not only our own algorithms but also many further algorithms from other researchers. With Metanome, we make our research accessible to all data scientists and IT-professionals that are tasked with data profiling. Besides the actual metadata discovery, the platform also offers support for the ranking and visualization of metadata result sets.

Being able to discover the entire set of syntactically valid metadata naturally introduces the subsequent task of extracting only the semantically meaningful parts. This is challenge, because the complete metadata results are surprisingly large (sometimes larger than the datasets itself) and judging their use case dependent semantic relevance is difficult. To show that the completeness of these metadata sets is extremely valuable for their usage, we finally exemplify the efficient processing and effective assessment of functional dependencies for the use case of schema normalization.

Zusammenfassung

Data Profiling ist eine Disziplin der Informatik, die sich mit der Analyse von Datensätzen auf deren Metadaten beschäftigt. Die verschiedenen Typen von Metadaten reichen von einfachen Statistiken wie Tupelzahlen, Spaltenaggregationen und Wertverteilungen bis hin zu weit komplexeren Strukturen, insbesondere Inklusionsabhängigkeiten (INDs), eindeutige Spaltenkombinationen (UCCs) und funktionale Abhängigkeiten (FDs). Diese Statistiken und Strukturen dienen, sofern vorhanden, dazu die Daten effizient zu speichern, zu lesen, zu ändern und zu verstehen. Die meisten Datensätze stellen ihre Metadaten aber nicht explizit zur Verfügung, so dass Informatiker sie mittels Data Profiling bestimmen müssen.

Während einfache Statistiken noch relativ schnell zu berechnen sind, stellen die komplexen Strukturen schwere, zumeist NP-vollständige Entdeckungsaufgaben dar. Es ist daher auch mit gutem Domänenwissen in der Regel nicht möglich sie manuell zu entdecken. Aus diesem Grund wurden verschiedenste Profiling Algorithmen entwickelt, die die Entdeckung automatisieren. Keiner dieser Algorithmen kann allerdings Datensätze von heutzutage typischer Größe verarbeiten, weil entweder der Ressourcenverbrauch oder die Rechenzeit effektive Grenzen überschreiten.

In dieser Arbeit stellen wir neuartige Profiling Algorithmen vor, die automatisch die drei populärsten Typen komplexer Metadaten entdecken können, nämlich INDs, UCCs, und FDs, die alle unterschiedliche Formen von Schlüssel-Abhängigkeiten beschreiben. Die Aufgabe dieser Algorithmen ist es alle gültigen Vorkommen der drei Metadaten-Typen aus einer gegebenen relationalen Instanz zu extrahieren. Sie nutzen dazu bekannte Entdeckungstechniken aus verwandten Arbeiten und ergänzen diese um algorithmische Paradigmen wie Teile-und-Herrsche, hybrides Suchen, Progressivität, Speichersensibilität, Parallelisierung und zusätzliche Streichungsregeln. Unsere Experimente zeigen, dass die vorgeschlagenen Algorithmen mit den neuen Techniken nicht nur um Größenordnungen schneller sind als alle verwandten Arbeiten, sie erweitern auch aktuelle Beschränkungen deutlich. Sie können insbesondere nun Datensätze realer Größe, d.h. mehrerer Gigabyte Größe mit vernünftigem Speicher- und Zeitverbrauch verarbeiten.

Aufgrund der praktischen Relevanz von Data Profiling hat die Industrie verschiedene Profiling Werkzeuge entwickelt, die Informatiker in ihrer Suche nach Metadaten unterstützen sollen. Diese Werkzeuge bieten eine gute Unterstützung für die Berechnung einfacher Statistiken. Sie sind auch in der

Lage einzelne Abhängigkeiten zu validieren, allerdings mangelt es ihnen an Funktionen zur echten *Entdeckung* von Metadaten, obwohl grundlegende Entdeckungstechniken schon mehr als 15 Jahre bekannt sind. Um diese Lücke zu schließen haben wir METANOME entwickelt, eine erweiterbare Profiling Plattform, die nicht nur unsere eigenen Algorithmen sondern auch viele weitere Algorithmen anderer Forscher integriert. Mit METANOME machen wir unsere Forschungsergebnisse für alle Informatiker und IT-Fachkräfte zugänglich, die ein modernes Data Profiling Werkzeug benötigen. Neben der tatsächlichen Metadaten-Entdeckung bietet die Plattform zusätzlich Unterstützung bei der Bewertung und Visualisierung gefundener Metadaten.

Alle syntaktisch korrekten Metadaten effizient finden zu können führt natürlicherweise zur Folgeaufgabe daraus nur die semantisch bedeutsamen Teile zu extrahieren. Das ist eine Herausforderung, weil zum einen die Mengen der gefundenen Metadaten überraschenderweise groß sind (manchmal größer als der untersuchte Datensatz selbst) und zum anderen die Entscheidung über die Anwendungsfall-spezifische semantische Relevanz einzelner Metadaten-Aussagen schwierig ist. Um zu zeigen, dass die Vollständigkeit der Metadaten sehr wertvoll für ihre Nutzung ist, veranschaulichen wir die effiziente Verarbeitung und effektive Bewertung von funktionalen Abhängigkeiten am Anwendungsfall Schema Normalisierung.

Acknowledgements

I want to dedicate the first lines to my advisor Felix Naumann, who owns my deepest appreciation and gratitude. As the epitome of a responsible and caring mentor, he supported me from the very beginning and taught me every detail of scientific working. We have spent countless hours discussing ideas, hitting walls, and then coming up with solutions. Not only did his knowledge provide me guidance throughout my journey, his support in difficult times always helped me to get back on track. For all that I am truly thankful.

My gratitude also goes to all my wonderful colleagues for their help and friendship. This PhD would not have been such a wonderful experience without all the people with whom I had the pleasure to work and consort with. Here, I want to express special thanks go to my close co-workers Sebastian Kruse, Hazar Harmouch, Anja Jentzsch, Tobias Bleifuß, and Maximilian Jenders with whom I could always share and discuss problems, ideas, and solutions. Also, many thanks to Jorgé-Arnulfo Quiané-Ruiz and Arvid Heise, who dragged me through my first publications with remarkable patience and became valuable co-advisors to me.

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Contents

1

Data Profiling

Whenever a data scientist receives a new dataset, she needs to inspect the dataset's format, its schema, and some example entries to determine what the dataset has to offer. Then, she probably measures the dataset's physical size, its length and width, followed by the density and distribution of values in certain attributes. In this way, the data scientist develops a basic understanding of the data that allows her to effectively store, query, and manipulate it. We call these and further actions that systematically extract knowledge about the structure of a dataset *data profiling* and the gained knowledge *metadata* [Naumann, 2013].

Of course, data profiling does not end with the inspection of value distributions. Many further profiling steps, such as data type inference and dependency discovery, are necessary to fully understand the data. The gathered metadata, then, enable the data scientist to not only use but also manage the data, which includes data cleaning, normalization, integration, and many further important maintenance tasks. Consequently, data profiling is – and ever was – an essential toolbox for data scientists.

A closer look into the profiling toolbox reveals that the state-of-the-art profiling techniques perform very well for most basic types of metadata, such as data types, value aggregations, and distribution statistics. According to Gardner [Judah et al., 2016], market leaders for commercial profiling solutions in this segment are Informatica, IBM, SAP, and SAS with their individual data analytic platforms. Research prototypes for the same purpose are, for instance, Bellman [Dasu et al., 2002], Profiler [Kandel et al., 2012], and MADLib [Hellerstein et al., 2012], but a data scientist can profile most basic metadata types likewise with a text editor, SQL or very simple programming. Profiling techniques for the discovery of more complex structures, such as functional dependencies or denial constraints, are, however, largely infeasible for most real-world datasets, because their discovery strategies do not scale well with the size of the data. For this reason, most profiling tools refrain from providing true *discovery* features; instead, they usually offer only checking methods for individual metadata candidates or try to approximate the metadata.

The trend of ever growing datasets fuels this problem: We produce, measure, record, and generate new data at an enormous rate and, thus, often lose control of what and how we store. In these cases, regaining the comprehension of the data is a downstream task for data profiling. Many discovery techniques are, however, hopelessly overloaded with such large datasets.

In this thesis, we focus on profiling techniques for the discovery of unique column combinations (UCCs), functional dependencies (FDs), and inclusion dependencies (INDs), which are the most important types of metadata in the group of currently overloaded discovery algorithms [Levene and Vincent, 1999; Toman and Weddell, 2008]. All three types of metadata describe different forms of key dependencies, i.e., keys *of* a table, *within* a table, and *between* tables. They form, inter alia, the basis for Wiederhold's and El-Masri's structural model of database systems [Wiederhold and El-Masri, 1979] and are essential for the interpretation of relational schemata as entity-relationship models [Chen, 1976]. In other words, UCCs, FDs, and INDs are essential to understand the semantics of a dataset.

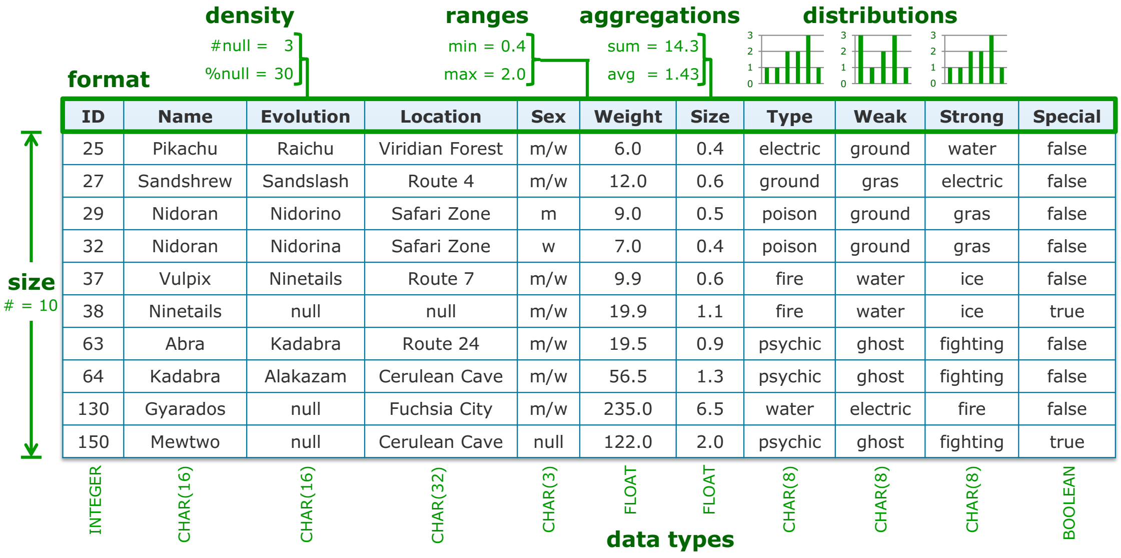
In this introductory chapter, we first give an overview on the different types of metadata. Afterwards, we set the focus on UCCs, FDs, and INDs and discuss their importance for a selection of popular data management use cases. We then introduce the research questions for this thesis, our concrete contributions, and the structure for the following chapters.

1.1 An overview of metadata

There are many ways to categorize the different types of metadata: One could, for instance, use their importance, their use cases, or their semantic properties. The most insightful categorization, however, is to group the metadata types by their relational scope, which is either *single-column* or *multi-column* as proposed in [Naumann, 2013]. Single-column metadata types provide structural information about individual columns, whereas multi-column metadata types make statements about groups of columns and their correlations.

To illustrate a few concrete metadata statements, we use a dataset from `bulbagarden.net` on Pokémon – small, fictional pocket monsters for children. The original *Pokemon* dataset contains more than 800 records. A sample of 10 records is depicted in Figures 1.1 and 1.2. The former figure annotates the sample with some single-column metadata and the latter with some multi-column metadata.

Figure 1.1 highlights the *format* of the dataset as one single-column metadata type. The format in this example is relational, but it could as well be, for instance, XML, RDF, or Json. The format basically indicates the representation of each attribute and, therefore, an attribute's schema, position, and, if present, heading. These information give us a basic understanding on how to read and parse the data. The *size*, then, refers to the number of records in the relation and the relations physical size, which both indicate storage requirements. The attributes' *data types* define how the individual values should be parsed and what value modifications are possible. Together, these three types of metadata are the minimum one reasonably needs to make use of a dataset. The remaining types of single-column metadata have more statistical nature: The *density*, for instance, describes the information content of an attribute, which is useful to judge its

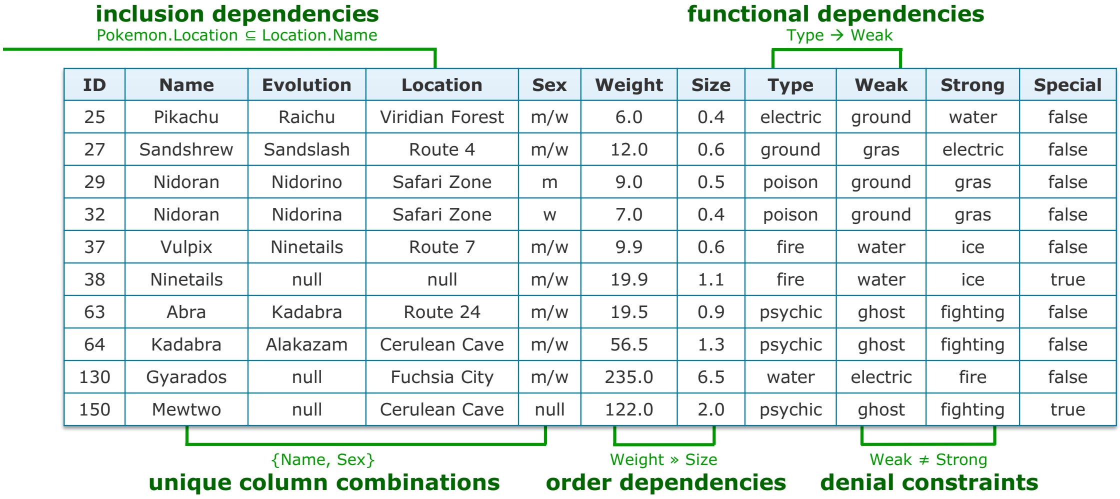


ID	Name	Evolution	Location	Sex	Weight	Size	Type	Weak	Strong	Special
25	Pikachu	Raichu	Viridian Forest	m/w	6.0	0.4	electric	ground	water	false
27	Sandshrew	Sandslash	Route 4	m/w	12.0	0.6	ground	gras	electric	false
29	Nidoran	Nidorino	Safari Zone	m	9.0	0.5	poison	ground	gras	false
32	Nidoran	Nidorina	Safari Zone	w	7.0	0.4	poison	ground	gras	false
37	Vulpix	Ninetails	Route 7	m/w	9.9	0.6	fire	water	ice	false
38	Ninetails	null	null	m/w	19.9	1.1	fire	water	ice	true
63	Abra	Kadabra	Route 24	m/w	19.5	0.9	psychic	ghost	fighting	false
64	Kadabra	Alakazam	Cerulean Cave	m/w	56.5	1.3	psychic	ghost	fighting	false
130	Gyarados	null	Fuchsia City	m/w	235.0	6.5	water	electric	fire	false
150	Mewtwo	null	Cerulean Cave	null	122.0	2.0	psychic	ghost	fighting	true

Figure 1.1: Example relation on Pokémon with *single-column* metadata.

relevance and the quality of the dataset; *range* information and *aggregations* help to query and analyse certain properties of the data; and detailed *distribution* statistics enable domain investigations and error detection. For example, distributions that follow certain laws, such as Zipf's law [Powers, 1998] or Benford's law [Berger and Hill, 2011] indicate specific domains and suspicious outliers. Overall, single-column metadata enable a basic understanding of their datasets; we can calculate them in linear or at least polynomial time. For further reading on single-column metadata, we refer to [Loshin, 2010].

Multi-column metadata, as shown in Figure 1.2, provide much deeper insights into implicit connections and relationships. *Implicit* means that these connections and relationships are (usually) no technical constraints – although declaring them as such often makes sense for technical reasons; they are, instead, determined by those real-world entities, facts, and processes that the data tries to describe. So we find, for instance, attributes or sets of attributes that naturally identify each entity in the relation. In our Pokémon example, it is a combination of name and sex that is unique for each pocket monster. Information like this are provided by *unique column combinations*. Furthermore, an *inclusion dependency* states that all values in one specific attribute(set) are also contained in some other attribute(set) so that we can connect, i.e., join these two sets. In our example, we find that all locations of our Pokémon also occur in a different table, which might offer additional information on these locations. Moreover, an *order dependency* shows that sorting the listed Pokémon by their weight also sorts them by their size, which is a useful information for query optimization and indexing. The *functional dependency* in our example expresses that the type of a Pokémon defines its weakness, which means that there are no two Pokémon with same type but different weakness. So if we know a Pokémon's type and the general type-weakness mapping, we can easily infer its weakness. The *denial constraint* in our example tells us that weaknesses are always different from strengths, a general insight that helps, for example, to understand the meaning of the attributes weak and strong.



inclusion dependencies
Pokemon.Location ⊆ Location.Name
functional dependencies
Type → Weak
{Name, Sex}
unique column combinations
Weight » Size
order dependencies
Weak ≠ Strong
denial constraints

ID	Name	Evolution	Location	Sex	Weight	Size	Type	Weak	Strong	Special
25	Pikachu	Raichu	Viridian Forest	m/w	6.0	0.4	electric	ground	water	false
27	Sandshrew	Sandslash	Route 4	m/w	12.0	0.6	ground	gras	electric	false
29	Nidoran	Nidorino	Safari Zone	m	9.0	0.5	poison	ground	gras	false
32	Nidoran	Nidorina	Safari Zone	w	7.0	0.4	poison	ground	gras	false
37	Vulpix	Ninetails	Route 7	m/w	9.9	0.6	fire	water	ice	false
38	Ninetails	null	null	m/w	19.9	1.1	fire	water	ice	true
63	Abra	Kadabra	Route 24	m/w	19.5	0.9	psychic	ghost	fighting	false
64	Kadabra	Alakazam	Cerulean Cave	m/w	56.5	1.3	psychic	ghost	fighting	false
130	Gyarados	null	Fuchsia City	m/w	235.0	6.5	water	electric	fire	false
150	Mewtwo	null	Cerulean Cave	null	122.0	2.0	psychic	ghost	fighting	true

Figure 1.2: Example relation on Pokémon with *multi-column* metadata.

Multi-column metadata types are much harder to discover than single-column metadata types, because they not only depend on the values in one but many columns and the combinations of these values: Both, the name and the sex attribute of a Pokémon, for instance, are not unique, but their combination is. Multi-column metadata discovery is generally an NP-complete problem that is infeasible to solve by hand. The first *automatic* approach to multi-column metadata discovery was published by Mannila in 1987 on functional dependency discovery and, since then, research contributed ever faster search techniques. A comprehensive survey on profiling techniques and data profiling in general is the work of Abedian et al. [Abedjan et al., 2015]. Another not so recent but more fundamental work on data profiling is Theodore Johnson's Chapter in the Encyclopedia of Database Systems [Johnson, 2009]

In Chapter 2, we define the three multi-column metadata types UCCs, FDs, and INDs as well as their properties and discovery problems in more depth. For more details on further multi-column metadata types, we recomment the survey [Caruccio et al., 2016] and the text book [Abiteboul et al., 1995]. We also refer to the following publications:

Order dependencies have first been published in [Ginsburg and Hull, 1983]. The work of [Szlichta et al., 2013] studies order dependencies in more depth and [Langer and Naumann, 2016] describes a discovery algorithm that was co-developed in the same research context as this thesis. The most efficient order dependency discovery algorithm at the time is, however, published in [Szlichta et al., 2017].

Multivalued dependencies have been defined by Fagin in [Fagin, 1977] for creating the fourth normal form (4NF) – a successor of the well-known Boyce-Codd normal form (BCNF). Multivalued dependencies and their use in schema normalization are also well described in database literature, such as [Ullman, 1990] and [Garcia-Molina et al., 2008]. The first discovery algorithm for multivalued dependency was published in [Flach and Savnik, 1999]. Our work on multivalued dependency discovery, however, improves significantly on this algorithm [Draeger, 2016].

Denial constraints are a universally quantified first order logic formalism, i.e., a rule language with certain predicates [Bertossi, 2011]. Denial constraints can express most other dependencies and are, therefore, particularly hard to fully discover. A first discovery algorithm has already been published in [Chu et al., 2013]; another, more efficient discovery algorithm that is based on the discovery techniques for functional dependencies introduced in this thesis can be found in [Bleifuß, 2016].

Matching dependencies are an extension of functional dependencies that incorporate a notion of value similarity, which is, certain values can be similar instead of strictly equal [Fan, 2008]. Due to the incorporated similarity, matching dependencies are especially valuable for data cleaning, but the similarity also makes them extremely hard to discover. A first discovery approach has been published in [Song and Chen, 2009]. Our approach to this discovery problem is slightly faster but also only scales to very small, i.e., kilobyte-sized datasets [Mascher, 2013].

1.2 Use cases in need for metadata

As we motivated earlier, every action that touches data requires some basic metadata, which makes metadata an asset for practically all data management tasks. In the following, however, we focus on the most traditional use cases for UCCs, FDs, and INDs. We provide intuitive explanations and references for further reading; detailed discussions are out of the scope of this thesis.

1.2.1 Data Exploration

Data exploration describes the process of improving the understanding of a dataset's semantic and structure. Because it is about increasing knowledge, data exploration always involves a human who usually runs the process interactively. In [Johnson, 2009], Johnson defines data profiling as follows: "Data profiling refers to the activity of creating small but informative summaries of a database". The purpose of metadata is, therefore, by definition to inform, create knowledge and offer special insights.

In this context, unique column combinations identify attributes with special meaning, as these attributes provide significant information for each entity in the data, e.g., with *Name* and *Sex* we can identify each Pokémon in our example dataset. Functional dependencies highlight structural laws and mark attributes with special relationships, such as *Type*, *Weak*, and *Strong* in our example that stand for elements and their interaction. Inclusion dependencies, finally, suggest relationships between different entities, e.g., all Pokémon of our example relation link to locations in another relation.

1.2.2 Schema Engineering

Schema engineering covers the *reverse engineering* of a schema from its data and the *redesign* of this schema. Both tasks require metadata: Schema reverse engineering uses, among other things, unique column combinations to rediscover the keys of the relational instance [Saiedian and Spencer, 1996] and inclusion dependencies to identify foreign-keys [Zhang et al., 2010]; schema redesign can, then, use the UCCs, FDs, and INDs to interpret the schema as an entity-relationship diagram [Andersson, 1994] – a representation of the data that is easier to understand and manipulate than bare schema definitions in, for example, DDL statements.

A further subtask of schema redesign is *schema normalization*. The goal of schema normalization is to remove redundancy in a relational instance by decomposing its relations into more compact relations. One popular normal form based on functional dependencies is the Boyce-Codd normal form (BCNF) [Codd, 1970]. In the normalization process, FDs represent the redundancy that is to be removed, whereas UCCs and INDs contribute new keys and foreign-keys [Zhang et al., 2010]. An extension of BCNF is the Inclusion Dependency normal form (IDNF), which additionally requires INDs to be noncircular and key-based [Levene and Vincent, 1999]. We deal with the normalization use case in much more detail in Chapter 7.

1.2.3 Data Cleaning

Data cleaning is the most popular use case for data profiling results, which is why most data profiling capabilities are actually offered in data cleaning tools, such as Bellman [Dasu et al., 2002], Profiler [Kandel et al., 2012], Potter's Wheel [Raman and Hellerstein, 2001], or Data Auditor [Golab et al., 2010], which all focus on data cleaning. The general idea for data cleaning with metadata is the same as for all rule based error detection systems: The metadata statements, which we can extract from the data, are rules and all records that contradict a rule are potential errors. To repair these errors, *equality-generating* dependencies, such as functional dependencies, enforce equal values in certain attributes if their records match in certain other attributes; *tuple-generating* dependencies, such as inclusion dependencies, on the other hand, enforce the existence of a new tuple if some other tuple was observed. So in general, equality-generating dependencies impose consistency and tuple-generating dependencies impose completeness of the data [Golab et al., 2011].

Of course, metadata discovered with an *exact* discovery algorithm, which all three algorithms proposed in this thesis are, will have no contradictions in the data. To allow the discovery of these contradictions, one could approximate the discovery process by, for instance, only discovering metadata on a (hopefully clean) sample of records [Diallo et al., 2012]. This is the preferred approach in related work, not only because it introduces contradictions, but also because current discovery algorithms do not scale up to larger datasets. With our new discovery algorithms, we instead propose to calculate the exact metadata and, then, generalize the discovered statements gradually: The UCC {*Name*, *Sex*}, for instance, would become {*Name*} and {*Sex*} – two UCCs that could be true but made invalid by errors. The former UCC {*Name*} has only one contradiction in our example Table 1.2, which is the value "Nidoran" occurring twice, but the latter has seven contradictions, which are all "m/w". We, therefore, conclude that "Nidoran" could be an error and {*Name*} a UCC, while {*Sex*} is most likely no UCC. This systematic approach does not assume a clean sample; it also approaches the true metadata more carefully, i.e., metadata calculated on a sample can be arbitrarily wrong.

Most state-of-the-art approaches for metadata-based data cleaning, such as [Bohannon et al., 2007], [Fan et al., 2008], and [Dallachiesa et al., 2013], build upon *conditional* metadata, i.e., metadata that counterbalance contradictions in the data with conditions (more on conditional metadata in Chapter 2). The discovery of such conditional statements is usually based on exact discovery algorithms, e.g. CTane is based on Tane [Fan et al., 2011] and CFun, CFD_Miner, and FastCFDs are based on Fun, FD_Mine, and FastFDs, respectively [Diallo et al., 2012]. For this reason, one could likewise use the algorithms proposed in this thesis for the same purpose. The cleaning procedure with conditional metadata is, then, the same as for exact metadata; the only difference is that conditional metadata captures inconsistencies better than their exact counterparts [Cong et al., 2007].

A subtask of data cleaning is *integrity checking*. Errors in this use case are not only wrong but also missing and out of place records. One example for an integrity rule are inclusion dependencies that assure referential integrity [Casanova et al., 1988]: If an IND is violated, the data contains a record referencing a non-existent record so that either the first record is out of place or the second is missing.

Due to the importance of data quality in practice, many further data cleaning and repairing methods with metadata exist. For a broader survey on such methods, we refer to the work of Fan [Fan, 2008].

1.2.4 Query Optimization

Query optimization with metadata aims to improve query loads by either optimizing query execution or rewriting queries. The former strategy, query execution optimization, is the more traditional approach that primarily uses query plan rewriting and indexing [Chaudhuri, 1998]; it is extensively used in all modern database management systems. The latter strategy, query rewriting, tries to reformulate parts of queries with semantically equivalent, more efficient query terms [Gryz, 1999]; if possible, it also removes parts of the queries that are obsolete. To achieve this, query rewriting requires more in-depth knowledge about the data and its metadata.

To illustrate the advantages of query rewriting, Figure 1.3 depicts the SQL query *"Find all Java-developer by name that work on the backend of our website and already received a paycheck."*.

```
SELECT DISTINCT employee.name
FROM employee, paycheck
WHERE employee.ID = paycheck.employee
AND employee.expertise = 'Java'
AND employee.workspace = '\product\backend';
```

Figure 1.3: Example SQL-query that can be optimized with metadata.

The query joins the `employee` table with the `paycheck` table to filter only those employees that received a paycheck. If we know that *all* employees did receive a paycheck, i.e., we know that the IND `employee.ID` $\subseteq$ `paycheck.employee` holds, then we find that the join is superfluous and can be removed from the query [Gryz, 1998].

Let us now assume that, for our particular dataset, {`employee.name`} is a UCC, i.e., there exist no two employees with same names. Then, the `DISTINCT` duplicate elimination is superfluous. And if, by chance, {`employee.expertise`} is another UCC, meaning that each employee has a unique expertise in the company, we can support the "Java"-expertise filter with an index on `employee.expertise` [Paulley and Larson, 1993].

We might, furthermore, find that the expertise of an employee defines her workspace. This would be reflected as an FD `employee.expertise` $\rightarrow$ `employee.workspace`. If the mapping "Java"-expertise to "backend"-workspace in the query is correct, then we can remove the obsolete "backend"-workspace filter [Paulley, 2000]. In case we do not use the FD for query rewriting, the query optimizer should definitely use this information to more accurately estimate the selectivity of the workspace filter whose selectivity is 1, i.e., no record is removed, because the expertise filter dominates the workspace filter.

```
SELECT employee.name
FROM employee
WHERE employee.expertise = 'Java';
```

Figure 1.4: Example SQL-query that was rewritten using metadata.

Figure 1.4 depicts the fully optimized query. Interestingly, it is irrelevant for this use case whether or not the used metadata statements have semantic meaning; it is only important that they are valid at the time the query is asked. All our profiling results are, for this reason, directly applicable to query optimization.

1.2.5 Data Integration

Data integration, also referred to as information integration or data fusion, is the activity of matching different schemata and transforming their data into a joined representation [Bellahsene et al., 2011]. The matching part usually leads to a new, integrated schema that subsumes the most important features of the given schemata [Rahm and Bernstein, 2001]; this schema can also be a view [Ullman, 1997]. The main challenge in this process is to find correspondences between the different individual schemata. These correspondences are difficult to find, because attribute labels usually differ and expert knowledge for the different schemata is scarce [Kang and Naughton, 2003]. However, certain schema elements exhibit very characteristic metadata signatures that can well be used to identify and match similar schema elements [Madhavan et al., 2001]. In fact, all sophisticated schema matching techniques, such as the Clio project [Miller et al., 2001], rely heavily on structural metadata, such as data types, statistics, and the various types of dependencies: The foreign-key graph of schema A, for instance, will probably match the foreign-key graph of schema B to some extend; a key of type integer with constant length 8 in schema A will probably correspond to a key of type integer with constant length 8 in schema B; and a group of functional dependent attributes in schema A will probably find its counterpart in schema B as well [Kang and Naughton, 2008].

A task related to data integration is *data linkage*. The goal of data linkage is not to merge but to connect schemata. This can be done by finding join paths and key-foreign relationships between the different schemata. Because inclusion dependencies are able to indicate such relationships, they are indispensable for this task [Zhang et al., 2010].

1.3 Research questions

The data profiling toolbox is basically as old as the relational data model itself. Still, research is continuously adding new tools and new issues open as others are solved. In this study, we pursue the following three research questions:

(1) How to efficiently discover all UCCs, FDs, and INDs in large datasets?
Despite their importance for many use cases, UCCs, FDs, and INDs are not known for most datasets. For this reason, data scientists need discovery algorithms that are able to find all occurrences of a certain type in a given relational dataset. This is a particularly difficult task, because all three discovery problems are NP-complete. Current state-of-the-art discovery algorithms do not present satisfactory solutions, because their resource consumptions and/or execution times on large datasets exceed effective limits.

(2) How to make discovery algorithms accessible?
Although many data profiling tools and tools with data profiling capabilities have been developed in the past, these tools are largely incapable of providing real *discovery* features to their users – instead they provide only *checking* features for individual metadata candidates. This is because current discovery algorithms are very sensitive to the data and not reliable enough to be put into a profiling product: The user must know the existing discovery algorithms, their strengths and weaknesses very well and apply the algorithms correctly, otherwise their executions will crash.

(3) How to serve concrete use cases with discovered metadata?
Most use cases for UCCs, FDs, and INDs assume that the metadata is given by a domain expert, which is why they assume that the amount of metadata is manageably small. This is a false assumption if the metadata was not hand-picked but automatically discovered: Discovered metadata result sets can be huge, even larger the data itself, and among the many syntactically correct results only a small subset is also semantically correct. Efficiently dealing with the entire result set and identifying the semantically correct subsets is, therefore, a new key challenge for many use cases in order to put discovered metadata into use.

1.4 Structure and contributions

This thesis focuses on the discovery, provision and utilization of unique column combinations (UCCs), functional dependencies (FDs), and inclusion dependencies (INDs). In particular, we make the following contributions:

(1) Three novel metadata discovery algorithms
We propose three novel metadata discovery algorithms: HyUCC for UCC discovery, HyFD for FD discovery, and Binder for IND discovery. The algorithms build upon known techniques from related work and complement them with algorithmic paradigms, such as additional pruning, divide-and-conquer, hybrid search, progressivity, memory sensitivity, and parallelization to greatly improve upon current limitations. Our experiments show that the proposed solutions are orders of magnitude faster than related work. They are, in particular, now able to process real-world datasets, i.e., multiple gigabytes size with reasonable memory and time consumption.

(2) A novel profiling platform
We present Metanome, a profiling platform for various metadata discovery algorithms. The platform supports researchers in the development of new profiling algorithms by providing a development framework and access to legacy algorithms for testing; it also supports data scientists and IT-professions in the application of these algorithms by easing the algorithm parametrization and providing features for result management. The idea of the Metanome framework is to treat profiling algorithms as external resources. In this way, it is very easy to extend Metanome with new profiling capabilities, which keeps the functionality up-to-date and supports collaborative research.

(3) Novel metadata processing techniques
We exemplify the efficient processing and effective assessment of functional dependencies for the use case of schema normalization with a novel algorithm called Normalize. This algorithm closes the gab between the discovered results and an actual use case: It shows how to efficiently calculate the closure of complete sets of FDs and how to effectively select semantically correct FDs as foreign-keys. Normalize, in general, shows that discovered metadata sets are not despite their size, but because of it extremely supportive for many use cases.

The remainder of this study is structured as follows: In Chapter 2, we discuss the theoretical foundations for key dependencies and their discovery. Then, we introduce our FD discovery algorithm HyFD in Chapter 3 [Papenbrock and Naumann, 2016], our UCC discovery algorithm HyUCC in Chapter 4 [Papenbrock and Naumann, 2017a], and our IND discovery algorithm Binder in Chapter 5 [Papenbrock et al., 2015d]. All three algorithms (and others) have been implemented for Metanome – a data profiling platform that we present in Chapter 6 [Papenbrock et al., 2015a]. In Chapter 7, we then propose the (semi-)automatic algorithm Normalize that demonstrates how discovered metadata, i.e., functional dependencies can be used to efficiently and effectively solve schema normalization tasks [Papenbrock and Naumann, 2017b]. We finally conclude this study in Chapter 8 by summing up our results and discussing open research questions for future work on data profiling.

2

Key Dependencies

This section discusses the theoretical foundations of functional dependencies, unique column combinations, and inclusion dependencies. We refer to these three types of metadata as *key dependencies*, because they propose attributes that serve as valid key or foreign-key constraints for certain other attributes. After reviewing the relational data model in Section 2.1, we carefully define the three key dependencies in Section 2.2 and survey their relaxations in Section 2.3. Section 2.4 then introduces the discovery problem and basic discovery techniques. We end in Section 2.5 with a discussion on `null` semantics.

2.1 The relational data model

A data model is a notation for describing data. It consists of three parts [Garcia-Molina et al., 2008]: The *structure* defines the physical and conceptual data layout; the *constraints* define inherent limitations and rules of the data; and the *operations* define possible methods to query and modify the data. In this thesis, we focus on the *relational data model* [Codd, 1970], which is not only the preferred model for the leading database management systems [Edjlali and Beyer, 2016] but also is today's most widely used model for data [DB-ENGINES, 2017]. The structure of the relational model consists of the two building blocks *schema* and *instance*:

Schema A *relational schema* R is a named, non-empty set of attributes. In theory, these attibutes have no order in the schema, but we usually assign an order for practical reasons, such as consistent presentation of a schema and its data. Each attribute $A \in R$ represents a property of the entities described by the schema. The possible values of an attribute A are drawn from its domain *dom(A)*. Because datasets usually consist of multiple schemata, we call the set of schemata a *database schema*. For illustration, the schema of our Pokémon dataset introduced in Section 1.1 is

$$\mathsf{Pokemon(ID, Name, Evolution, Location, Sex, Weight, Size, Type, Weak, Strong, Special)}$$

Instance The *relational instance*, or relation r for short, of a schema R is a set of records. A record t of a relational schema R is a function $t : R \rightarrow \bigcup_{A \in R} dom(A)$ that assigns to every attribute $A \in R$ a value $t[A] \in dom(A)$. Note that we use the notation $t[X]$ to denote the projection of record t to the values of $X \subseteq R$. Because we consider the attributes to be ordered, we often refer to records as tuples, which are ordered lists of $|R|$ values [Elmasri and Navathe, 2016]. So the first tuple in our Pokémon dataset is

(25, Pikachu, Raichu, Viridian Forest, m/w, 6.0, 0.4, electric, ground, water, false)

Operations permitted in the relational data model are those defined by relational algebra and relational calculus. The structured query language (SQL) is a practical implementation and extension of these [Abiteboul et al., 1995]; it is the defacto standard for all relational database systems [ISO/IEC 9075-1:2008]. In this thesis, however, we focus on the constraints part of the relational model, i.e., inherent rules and dependencies of relational datasets.

The most important constraint in the relational model is a *key* [Codd, 1970]. A key is a set of attributes $X \subseteq R$ that contains no entry more than once. So all values in X are *unique* and distinctively describe their records. A *primary key* is a key that was explicitly chosen as the main identifier for all records; while there can be arbitrary many keys, a schema defines only one primary key. A *foreign-key* is a set of attributes in one schema that uniquely identify records in *another* schema; a foreign-key can contain duplicate entries, i.e., it is not a key for its own schema, but it must reference a key in the other schema.

The enforcement of keys and constraints in general requires special structures, so called *integrity constraints* that prevent inconsistent states. Because such integrity constraints are expensive to maintain, most constraints are not explicitly stated. The records in a relational instance, however, naturally obey all their constraints, which means that every relational instance r implies its set of metadata Σ. We express this implication as $r \models \Sigma$ [Fagin and Vardi, 1984]. The observation that relational instances imply their metadata is crucial to justify data profiling, i.e., the discovery of metadata from relational instances.

Although we focus on profiling techniques for the relational data model in this thesis, other data models and their model-specific constraints are, of course, also subject to data profiling. Key dependencies, for instance, are also relevant in XML [Buneman et al., 2001] and RDF [Jentzsch et al., 2015] datasets. The most promising profiling tool for the discovery of metadata in RDF datasets is ProLOD++, which is a sister project of our Metanome tool [Abedjan et al., 2014a]. In general, however, research on profiling techniques for non-relational data is still scarce.

2.2 Types of key dependencies

Unique column combinations, functional dependencies, and inclusion dependencies describe keys *of* a table, *within* a table, and *between* tables, respectively [Toman and Weddell, 2008]. In this section, we formally define all three types of key dependencies in detail and state our notations. Note that we often write XY or X, Y to mean $X \cup Y$, i.e., the union of attributes or attribute sets X and Y.

2.2.1 Functional Dependencies

A *functional dependency* (FD) written as $X \to A$ expresses that all pairs of records with same values in attribute combination X must also have same values in attribute A [Codd, 1971]. The values in A *functionally depend* on the values in X. More formally, functional dependencies are defined as follows [Ullman, 1990]:

Definition 2.1 (Functional dependency)**.** Given a relational instance r for a schema R. The *functional dependency* $X \to A$ with $X \subseteq R$ and $A \in R$ is *valid* in r, iff $\forall t_i, t_j \in r : t_i[X] = t_j[X] \Rightarrow t_i[A] = t_j[A]$.

We call the determinant part X of an FD the *left-hand-side*, in short Lhs, and the dependent part A the *right hand side*, in short Rhs. Moreover, an FD $X \to A$ is a *generalization* of another FD $Y \to A$ if $X \subset Y$ and it is a *specialization* if $X \supset Y$. Functional dependencies with the same Lhs, such as $X \to A$ and $X \to B$ can be grouped so that we write $X \to A, B$ or $X \to Y$ for attributs A and B with $\{A, B\} = Y$. Using this notation, Armstrong formulated the following three axioms for functional dependencies on attribute sets X, Y, and Z [Armstrong, 1974; Beeri and Bernstein, 1979]:

1. *Reflexivity*: If $Y \subseteq X$, then $X \to Y$.
2. *Augmentation*: If $X \to Y$, then $X \cup Z \to Y \cup Z$.
3. *Transitivity*: If $X \to Y$ and $Y \to Z$, then $X \to Z$.

An FD $X \to Y$ is called *trivial* if $Y \subseteq X$, because all such FDs are valid according to Armstrong's reflexivity axiom; vice versa, the FD is *non-trivial* if $X \nsubseteq Y$ and *fully non-trivial* if $X \cap Y = \emptyset$. Furthermore, an FD is *minimal* if no B exists such that $X \backslash B \to A$ is a valid FD, i.e., if no valid generalization exists. To discover all FDs in a given relational instance r, it suffices to discover all minimal, non-trivial FDs, because all Lhs-subsets are non-dependencies and all Lhs-supersets are dependencies by logical inference following Armstrong's augmentation rule.

Because keys in relational datasets uniquely determine all other attributes, they are the most popular kinds of FDs, i.e., every key X is a functional dependeny $X \to R \setminus X$. Functional dependencies also arise naturally from real-world entities described in relational datasets. In our Pokémon dataset of Section 1.1, for instance, the elemental type of a pocket monster defines its weakness, i.e., *Type* $\to$ *Weak*.

2.2.2 Unique Column Combinations

A *unique column combination* (UCC) X is a set of attributes $X \subseteq R \backslash X$ whose projection contains no duplicate entry on a given relational instance r [Lucchesi and Osborn, 1978]. Unique column combinations or *uniques* for short are formally defined as follows [Heise et al., 2013]:

Definition 2.2 (Unique column combination)**.** Given a relational instance r for a schema R. The *unique column combination* X with $X \subseteq R$ is *valid* in r, iff $\forall t_i, t_j \in r, i \neq j : t_i[X] \neq t_j[X]$.

By this definition, every UCC X is also a valid FD, namely $X \rightarrow R \setminus X$. For this reason, UCCs and FDs share various properties: A UCC X is a *generalization* of another UCC Y if $X \subset Y$ and it is a *specialization* if $X \supset Y$. Furthermore, if X is a valid UCC, then any $X \cup Z$ with $Z \subseteq R$ is a valid UCC, because Armstrong's augmentation rule also applies to UCCs. According to this augmentation rule, a UCC is *minimal* if no B exists such that $X \backslash B$ is still a valid UCC, i.e., if no valid generalization exists. To discover all UCCs in a given relational instance r, it suffices to discover all minimal UCCs, because all subsets are non-unqiue and all supersets are unique by logical inference.

From the use case perspective, every unique column combination indicates a syntactically valid key. In our example dataset of Section 1.1, for instance, the column combinations $\{ID\}$, $\{Name, Sex\}$, and $\{Weight\}$ are unique and, hence, possible keys for pocket monsters. Although UCCs and keys are technically the same, we usually make the distinction that keys are UCCs with semantic meaning, i.e., they not only hold by chance in a relational instance but for a semantic reason in any instance of a given schema [Abedjan et al., 2015].

Because every valid UCC is also a valid FD, functional dependencies seem to subsume unique column combinations. However, considering the two types of key dependentencies separately makes sense for the following reasons:

1. *Non-trivial inference*: A minimal UCC is not necessarily a minimal FD, because UCCs are minimal w.r.t. R and FDs are minimal w.r.t. some $A \in R$. If, for instance, X is a minimal UCC, then $X \rightarrow R$ is a valid FD and no $Y \subset X$ exists such that $X \setminus Y \rightarrow R$ is still valid. However, $X \setminus Y \rightarrow A$ with $A \in R$ can still be a valid and minimal. For this reason, not all minimal UCCs can directly be inferred from the set of minimal FDs; to infer all minimal UCCs, one must systematically specialize the FDs, check if these specializations determine R entirely, and if they do, check whether they are minimal w.r.t. R.

2. *Duplicate row problem*: The FD $X \rightarrow R \setminus X$ does not necessarily define a UCC X if duplicate records are allowed in the relational instance r of R. A duplicate record invalidates all possible UCCs, because it puts a duplicate value in every attribute and attribute combination. A duplicate record, however, invalidates no FD, because only differing values on an FD's Rhs can invalidate it. As stated in Section 2.1, the relational model in fact forbids duplicate records and most relational database management systems also prevent duplicate records; still duplicate records occur in practice, because file formats such as CSV cannot ensure their absence.

3. *Discovery advantage*: UCC discovery can be done more efficient than FD discovery, because UCCs are easier to check and the search space is smaller. We show this in Section 2.4 and Chapter 4. So if a data scientist must only discover UCCs, making a detour over FDs in the discovery is generally a bad decision.

2.2.3 Inclusion Dependencies

An *inclusion dependency* (IND) $R_i[X] \subseteq R_j[Y]$ over the relational schemata R_i and R_j states that all entries in X are also contained in Y [Casanova et al., 1982]. We use the short notations $X \subseteq Y$ for INDs $R_i[X] \subseteq R_j[Y]$ if it is clear from the context that $X \subseteq Y$ denotes an IND (and not an inclusion of same attributes). Inclusion dependencies are formally defined as follows [Marchi et al., 2009]:

Definition 2.3 (Inclusion dependency)**.** Given two relational instances r_i and r_j for the schemata R_i, and R_j, respectively. The *inclusion dependency* $R_i[X] \subseteq R_j[Y]$ (short $X \subseteq Y$) with $X \subseteq R_i$, $Y \subseteq R_j$ and $|X| = |Y|$ is *valid*, iff $\forall t_i[X] \in r_i, \exists t_j[Y] \in r_j : t_i[X] = t_j[Y]$.

We call the dependent part X of an IND the *left-hand-side*, short Lhs, and the referenced part Y the *right hand side*, short Rhs. An IND $X \subseteq Y$ is a *generalization* of another IND $X' \to Y'$ if $X \subset X'$ and $Y \subset Y'$ and it is a *specialization* if $X \supset X'$ and $Y \supset Y'$. The *size* or *arity* n of an IND is defined by $n = |X| = |Y|$. We call INDs with $n = 1$ *unary* inclusion dependecies and INDs with $n > 1$ *n-ary* inclusion dependecies. A sound and complete axiomatization for INDs is given by the following three inference rules on schemata R_i, R_j, and R_k [Casanova et al., 1982]:

1. *Reflexivity*: If $i = j$ and $X = Y$, then $R_i[X] \subseteq R_j[Y]$.
2. *Permutation*: If $R_i[A_1, ..., A_n] \subseteq R_j[B_1, ..., B_n]$, then $R_i[A_{\sigma 1}, ..., A_{\sigma m}] \subseteq R_j[B_{\sigma 1}, ..., B_{\sigma m}]$ for each sequence $\sigma 1, ..., \sigma m$ of distinct integers from $\{1, ..., m\}$.
3. *Transitivity*: If $R_i[X] \subseteq R_j[Y]$ and $R_j[Y] \subseteq R_k[Z]$, then $R_i[X] \subseteq R_k[Z]$.

An IND $R_i[X] \subseteq R_i[X]$ for any i and X is said to be *trivial*, as it is always valid according to the reflexivity rule. For valid INDs, all generalizations are also valid INDs, i.e., if $R_i[X] \subseteq R_j[Y]$ is valid, then $R_i[X \setminus A_k] \subseteq R_j[Y \setminus B_k]$ with same attribute indices k is valid as well [Marchi et al., 2009]. Specializations of a valid IND can, however, be valid or invalid. An IND $R_i[X] \subseteq R_j[Y]$ is called *maximal*, iff $R_i[XA] \subseteq R_j[YB]$ is *invalid* for all attributes $A \in R_i$ and $B \in R_j$ whose unary inclusion $R_i[A] \subseteq R_j[B]$ is no generalization of $R_i[X] \subseteq R_j[Y]$. If $R_i[A] \subseteq R_j[B]$ is a generalization, then adding it to $R_i[X] \subseteq R_j[Y]$ always results in a valid IND, but the mapping of A to B would be *redundant* and, therefore, superfluous – the maximal IND would, in a sense, not be minimal. To discover all INDs of a given relational instance r, it therefore suffices to discover all maximal, non-trivial INDs.

Usually, data scientists are interested in inclusion dependencies between *different* relations R_i and R_j, such as *Pokemon*[*Location*] $\subseteq$ *Location*[*Name*] in our Pokémon dataset of Section 1.1, because these INDs indicate foreign-key relationships. Inclusion dependencies inside the same shema are, however, also interesting for query optimization, integrity checking, and data exploration. In our example, for instance, we also find the IND *Pokemon*[*Evolution*] $\subseteq$ *Pokemon*[*Name*], which tells us that every evolution of a pocket monster must be a pocket monster as well.

2.3 Relaxation of key dependencies

An *exact* dependency must be syntactically correct for the given relational instance. The correctness exactly follows the definition of the dependency and it does not allow contradictions, exceptions or special cases. When we talk about dependencies in this work, we always refer to exact dependencies. For many use cases, however, it is beneficial to relax the definition of a dependency. The three most popular types of relaxed dependencies are *approximate*, *partial*, and *conditional* dependencies [Abedjan et al., 2015]. These relaxations apply equally to all key dependencies – in fact, they also apply to most other dependencies, such as order, multivalued, and matching dependencies. For this reason, we use the notation $X \vdash Y$ to denote a generic type of dependency $\vdash$. In the following, we discuss the three relaxation types in more detail:

Approximate: An *approximate* or *soft* dependency relaxes the hard correctness constraint of an exact dependency [Ilyas et al., 2004]. Although an approximate dependency is supposed to be correct, its correctness is not guaranteed. This means that contradictions might exist in the relational instance, but their number and location is unknown. In some scenarios, however, it is possible to guess the confidence of an approximate dependency or to state a certain worst-case confidence [Kruse et al., 2017]. Because approximate dependencies must not assure their correctness, their discovery can be much more efficient than the discovery of exact dependencies [Kivinen and Mannila, 1995]. Common techniques for approximate dependency discovery are sampling [Brown and Hass, 2003; Ilyas et al., 2004] and summarization [Bleifuß et al., 2016; Cormode et al., 2012; Kruse et al., 2017; Zhang et al., 2010]. Note that a *set of dependencies* is called approximate if it relaxes completeness, correctness, and/or minimality of its elements [Bleifuß et al., 2016].

Partial: A *partial* dependency also relaxes the correctness constraint of an exact dependency, but in contrast to approximate dependencies the error is known and intended [Abedjan et al., 2015]. Partial dependencies do not approximate exact dependencies; instead, their validity is strictly defined given a certain error threshold: The dependency $X \vdash_{\Psi \leq \epsilon} Y$ is valid, iff the known error Ψ of $X \vdash Y$ is smaller or equal than the error threshold ϵ [Caruccio et al., 2016]. A partial dependency is minimal, iff all generalizations (or specializations for INDs) exceed the error threshold. Partial dependencies are useful if the given data is expected to contain errors, because such errors can, if not deliberately ignored, hide semantically meaningful dependencies. A popular error measure is *the minimum number of records that must be removed to make the partial dependency exact* [Huhtala et al., 1999], but other measures exist [Caruccio et al., 2016; Kivinen and Mannila, 1995]. Note that despite the fundamental difference between approximate and partial dependencies, many related works, such as [Huhtala et al., 1999] and [Marchi et al., 2009], do not explicitly distinguish partial and approximate.

Conditional: A *conditional* dependency, such as a conditional IND [Bravo et al., 2007] or a conditional FD [Fan et al., 2008], complements a partial dependency with conditions. These conditions restrict the scope of a partial dependency to only those records that exactly satisfy the dependency. The common way to formulate such conditions are sets of *pattern tuples* that mismatch all dependency contradicting tuples while at the same time match possibly many dependency satisfying tuples in the relational instance. The set of pattern tuples is called *pattern tableau* or simply *tableau* [Bohannon et al., 2007]. Formally, a conditional dependency is a pair $(X \vdash Y, T_p)$ of a dependency $X \vdash Y$ and a pattern tableau T_p. The pattern tableau T_p is a set of tuples $t \in T_p$ where each $t[A]$ with $A \in X \cup Y$ is either a constant or wildcard [Bravo et al., 2007]. With these pattern tableaux, conditional dependencies are not only able to circumvent errors in the data, they also provide additional semantics about the described dependencies, namely which parts of the data fulfill a certain criterion and which do not. The discovery of conditional dependencies is, however, much more difficult than the discovery of exact, approximate and partial dependencies [Diallo et al., 2012], because the generation of pattern tableaux is expensive: Finding one *optimal* tableau for one partial dependency is an NP-complete task, which was proven in [Golab et al., 2008].

For a much broader survey on relaxation properties, we refer to [Caruccio et al., 2016]. In this thesis, we propose three efficient algorithms for the discovery of *exact* dependencies. In [Kruse et al., 2017] and [Bleifuß et al., 2016], we show that their sister algorithms, i.e., algorithms that use similar ideas, can discover *approximate* dependencies even faster. We do not cover the discovery of *partial* and *conditional* dependencies in this work, because most discovery algorithms in these categories build upon exact discovery algorithms [Diallo et al., 2012; Fan et al., 2011] and, as motivated in Chapter 1, no current algorithm is able to efficiently discover exact dependencies in real-world sized datasets.

2.4 Discovery of key dependencies

The focus of this thesis is the descovery of *all minimal, non-trivial* unique column combinations, *all minimal, non-trivial* functional dependecies, and *all maximal, non-trivial* inclusion dependencies. The search space for all three discovery tasks can best be modeled as a graph coloring problem – in fact, we model the search spaces for most multi-column metadata in this way: The basis of this model is a *power set* of attribute combinations [Devlin, 1979]; every possible combination of attributes represents one set. Such a power set is a *partially ordered set*, because reflexivity, antisymmetry and transitivity hold between the attribute combinations [Deshpande, 1968]. Due to the partial order, every two elements have a unique supremum and a unique infimum. Hence, we can model the partially ordered set as a *lattice*, i.e., a graph of attribute combination nodes that connects each node $X \subseteq R$ to its direct subsets $X \setminus A$ and direct supersets $X \cup B$ (with $A \in X$, $B \in R$ and $B \notin X$). For more details on lattice theory, we refer to [Crawley and Dilworth, 1973]. A nice visualization of such lattices are Hasse diagrams, named after Helmut Hasse (1898–1979), who did not invent but made this type of diagram popular [Birkhoff, 1940]. Figure 2.1 I depicts an example lattice as Hasse diagram for an example relation $R(A, B, C, D)$. Note that we do not include $X = \emptyset$ as a node, because $\emptyset$ is neither a valid UCC candidate and nor is $\emptyset \subseteq Y$ a valid IND candidate for any $Y \subseteq R$. Any FD candidate $\emptyset \rightarrow Y$, however, is possible and valid, if the column Y is constant, i.e., it contains only one value.

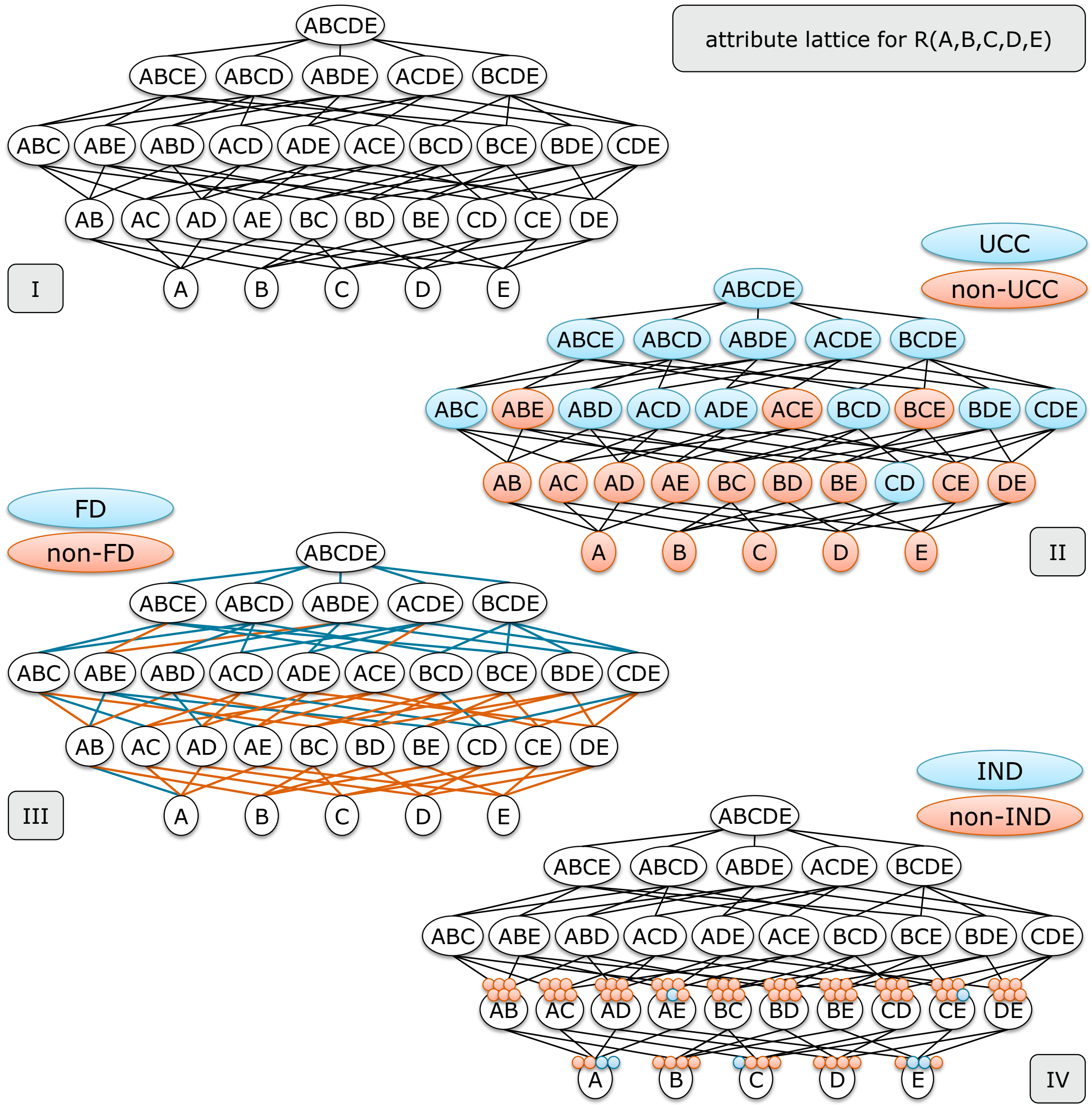
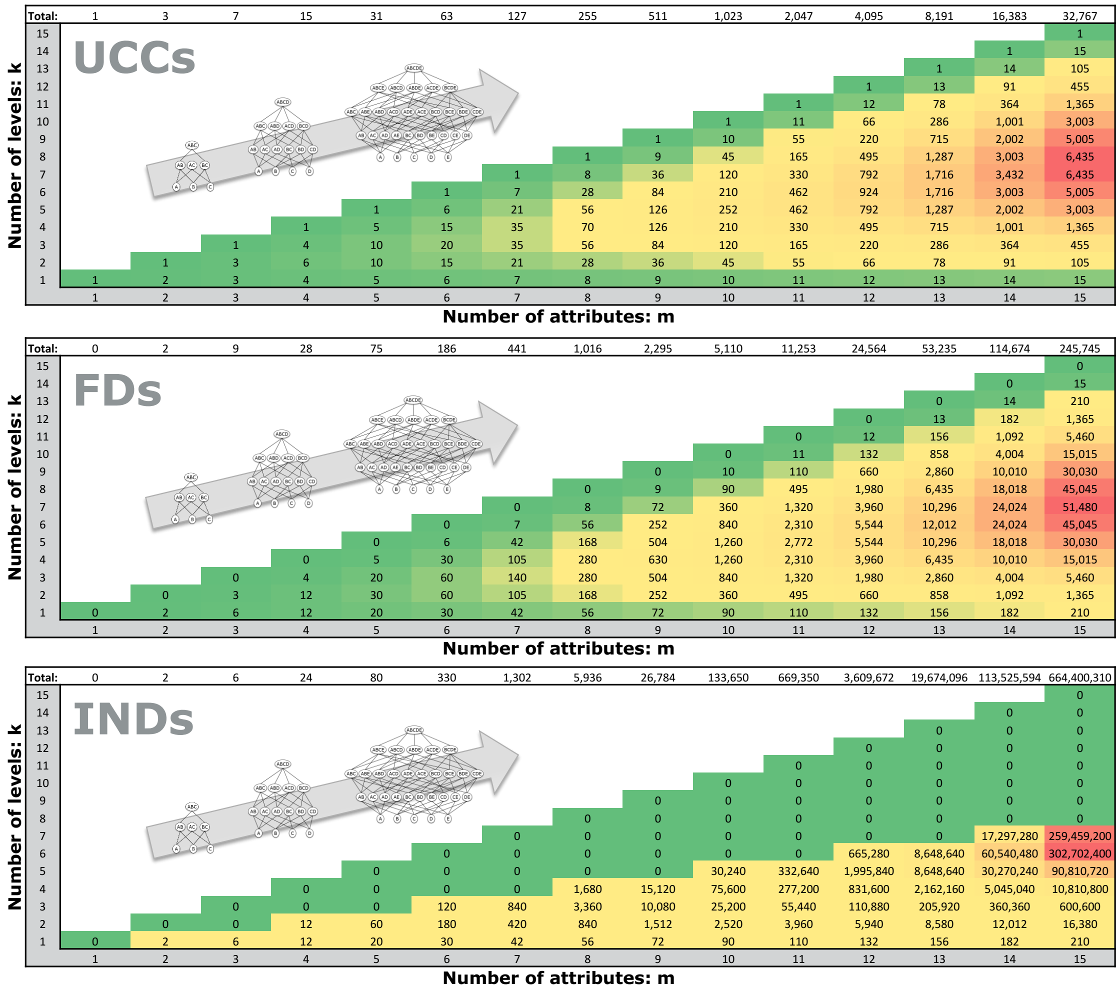

attribute lattice for R(A,B,C,D,E)
I
II
III
IV
UCC
non-UCC
FD
non-FD
IND
non-IND
ABCDE
ABCE ABCD ABDE ACDE BCDE
ABC ABE ABD ACD ADE ACE BCD BCE BDE CDE
AB AC AD AE BC BD BE CD CE DE
A B C D E

Figure 2.1: The search spaces of UCCs, FDs, and INDs visualized as lattices.

We now map the search spaces for UCCs, FDs, and INDs to the lattice of attribute combinations:

UCC discovery: For UCC discovery, each *node* X represents one UCC candidate, i.e., an attribute combination that is either unique or non-unique with respect to a given relational instance. To discover all UCCs, we need to classify all nodes in the graph and color them accordingly. Figure 2.1 II shows an examplary result of this process. In all such lattices, UCCs are located in the upper part of the lattice while non-UCCs are located at the bottom. The number of UCC candidates in level k for m attributes is $\binom{m}{k}$, which makes the total number of UCC candidates for m attributes $\sum_{k=1}^{m}\binom{m}{k} = 2^m - 1$. Figure 2.2 visualizes the growth of the UCC candidate search space with an increasing number of attributes. The depicted growth is exponential in the number of attributes.



UCCs

Total:	1	3	7	15	31	63	127	255	511	1,023	2,047	4,095	8,191	16,383	32,767
15															1
14														1	15
13													1	14	105
12												1	13	91	455
11											1	12	78	364	1,365
10										1	11	66	286	1,001	3,003
9									1	10	55	220	715	2,002	5,005
8								1	9	45	165	495	1,287	3,003	6,435
7							1	8	36	120	330	792	1,716	3,432	6,435
6						1	7	28	84	210	462	924	1,716	3,003	5,005
5					1	6	21	56	126	252	462	792	1,287	2,002	3,003
4				1	5	15	35	70	126	210	330	495	715	1,001	1,365
3			1	4	10	20	35	56	84	120	165	220	286	364	455
2		1	3	6	10	15	21	28	36	45	55	66	78	91	105
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15

FDs

Total:	0	2	9	28	75	186	441	1,016	2,295	5,110	11,253	24,564	53,235	114,674	245,745
15															0
14														0	15
13													0	14	210
12												0	13	182	1,365
11											0	12	156	1,092	5,460
10										0	11	132	858	4,004	15,015
9									0	10	110	660	2,860	10,010	30,030
8								0	9	90	495	1,980	6,435	18,018	45,045
7							0	8	72	360	1,320	3,960	10,296	24,024	51,480
6						0	7	56	252	840	2,310	5,544	12,012	24,024	45,045
5					0	6	42	168	504	1,260	2,772	5,544	10,296	18,018	30,030
4				0	5	30	105	280	630	1,260	2,310	3,960	6,435	10,010	15,015
3			0	4	20	60	140	280	504	840	1,320	1,980	2,860	4,004	5,460
2		0	3	12	30	60	105	168	252	360	495	660	858	1,092	1,365
1	0	2	6	12	20	30	42	56	72	90	110	132	156	182	210
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15

INDs

Total:	0	2	6	24	80	330	1,302	5,936	26,784	133,650	669,350	3,609,672	19,674,096	113,525,594	664,400,310
15															0
14														0	0
13													0	0	0
12												0	0	0	0
11											0	0	0	0	0
10										0	0	0	0	0	0
9									0	0	0	0	0	0	0
8								0	0	0	0	0	0	0	0
7							0	0	0	0	0	0	0	17,297,280	259,459,200
6						0	0	0	0	0	0	665,280	8,648,640	60,540,480	302,702,400
5					0	0	0	0	0	30,240	332,640	1,995,840	8,648,640	30,270,240	90,810,720
4				0	0	0	0	1,680	15,120	75,600	277,200	831,600	2,162,160	5,045,040	10,810,800
3			0	0	0	120	840	3,360	10,080	25,200	55,440	110,880	205,920	360,360	600,600
2		0	0	12	60	180	420	840	1,512	2,520	3,960	5,940	8,580	12,012	16,380
1	0	2	6	12	20	30	42	56	72	90	110	132	156	182	210
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15

Figure 2.2: Search space sizes for UCCs, FDs, and INDs.

FD discovery: For FD discovery, we map each *edge* between the nodes X and XA to an FD candidate $X \rightarrow A$. This mapping automatically ensures that only non-trivial candidates are represented in the model. In the discovery process, we now classify all edges in the graph as either valid or invalid FDs in a given relational instance. In Figure 2.1 III, we depict an example for an FD labelled lattice. Like UCCs, valid FDs are located in the upper part of the lattice and non-FDs in the lower part. The number of FD candidates in level k for m attributes is $\binom{m}{k} \cdot (m-k)$ where $m-k$ is the number upper edges of a node in the lattice; the total number of FD candidates is accordingly $\sum_{k=1}^{m} \binom{m}{k} \cdot (m-k)$. Note that the sum starts with $k=0$, if we consider $\emptyset$ as a node; then, the number of FD candidates is $\sum_{k=0}^{m} \binom{m}{k} \cdot (m-k) \leq \frac{m}{2} \cdot 2^m$. The growth of the FD candidate space with respect to the number of attributes is visualized in Figure 2.2. It is also exponential and even stronger than the growth of the UCC candidate space.

IND discovery: For IND discovery, we would need to annotate each node X in the lattice with all permutation of attribute sets Y of same size, i.e., all permutations of $Y \subset R$ with $|Y| = |X|$. Each such *annotation* then represents an IND candidate $X \subseteq Y$

and can be classified as either valid or invalid with respect to a given relational instance. By the definition of an IND, these annotations also include trivial combinations, such as $A \subseteq A$ and $X \subseteq X$, and combinations with duplicate attributes, such as $AA \subseteq BC$ and $ABC \subseteq BCB$. Most IND discovery algorithms, however, ignore trivial combinations and combinations with duplicates, because these INDs have hardly practical relevance. The number of candidates is even without these kinds of INDs still so high that we restrict our visualization of the search space even further – note that this is necessary only for the exploration of the search space in this chapter and that our discovery algorithm can overrule this last restriction: We consider only those INDs $X \subseteq Y$ where $Y \cap X = \emptyset$, which was also done in [Liu et al., 2012]. The example in Figure 2.1 IV then shows that due to $Y \cap X = \emptyset$ the annotations only exist up to level $\lfloor \frac{m}{2} \rfloor$. It also shows that, other than UCCs and FDs, valid INDs are located at the *bottom* and the invalid INDs at the top of the lattice – as stated in Section 2.2.3, INDs might become invalid when adding attributes while UCCs and FDs remain (or become) valid. The number of IND candidates in level k for m attributes is with the $Y \cap X = \emptyset$ restriction still $\binom{m}{k} \cdot \binom{m-k}{k} \cdot k!$ where $\binom{m-k}{k}$ are all non-overlapping attribute sets of a lattice node and $k!$ all permutations of such a non-overlapping attribute set. With that, we can quantify the total number of IND candidates as $\sum_{k=1}^{m} \binom{m}{k} \cdot \binom{m-k}{k} \cdot k!$. Figure 2.2 shows that this number of candidates is much larger than the number of UCC or FD candidates on same size schemata although IND candidates only reach to half the lattice height.

The discovery of UCCs, FDs, and INDs is a process that, in one form or another, involves data preparation, search space traversal, candidate generation, and candidate checking. The candidate checks are the most expensive action in the discovery processes. For this reason, most algorithms utilize the inference rules discussed in Section 2.2 as pruning rules to quickly infer the (in-)validity of larger sub-graphs. For instance, if X was identified as a UCC, all X' with $X' \supset X$ must also be valid UCCs. In this way, the algorithms avoid checking each and every candidate. To maximize the pruning effect, various checking strategies have been proposed based on the lattice search space model, most importantly *breadth-first bottom-up* [Huhtala et al., 1999], *breadth-first top-down* [Marchi and Petit, 2003], and *depth-first random walk* [Heise et al., 2013].

To improve the efficiency of the UCC and FD candidate checks, many discovery algorithms rely on an index structure called *position list index* (Pli), which are also known as *stripped partitions* [Cosmadakis et al., 1986]. A Pli, denoted by π_X, groups tuples into equivalence classes by their values of attribute set X. Thereby, two tuples t_1 and t_2 of an attribute set X belong to the same equivalence class if $\forall A \in X : t_1[A] = t_2[A]$. These equivalence classes are also called *clusters*, because they cluster records by same values. For compression, a Pli does not store clusters with only a single entry, because tuples that do not occur in any cluster of π_X can be inferred to be unique in X. Consider, for example, the relation Class(Teacher, Subject) and its example instance in Table 2.1. The Plis $\pi_{\{Teacher\}}$ and $\pi_{\{Subject\}}$, which are also depicted in Table 2.1, represent the partitions of the two individual columns; the Pli $\pi_{\{Teacher,Subject\}} = \pi_{\{Teacher\}} \cap \pi_{\{Subject\}}$ describes their intersection, which is the Pli of the column combination $\{$*Teacher, Subject*$\}$.

A unique column combination X is valid, iff the π_X contains no cluster. In this case, all clusters in π_X have size 1 and no value combination in X occurs more than once. To

Table 2.1: An example instance for the schema Class(Teacher, Subject) and its PLIs.

	Teacher	**Subject**
t_1	Brown	Math
t_2	Walker	Math
t_3	Brown	English
t_4	Miller	English
t_5	Brown	Math

$$\pi_{\{Teacher\}} = \{\{1,3,5\}\}$$
$$\pi_{\{Subject\}} = \{\{1,2,5\},\{3,4\}\}$$
$$\pi_{\{Teacher,Subject\}} = \{\{1,5\}\}$$

check a functional dependency $X \to A$, we test if every cluster in π_X is a subset of some cluster of π_A. If this holds true, then all tuples with same values in X have also same values in A, which is the definition of an FD. This check is called *refinement* and was first introduced in [Huhtala et al., 1999].

Despite their practical importance, the pruning rules and position list indixes do not change the complexity of the discovery tasks. Beeri et al. have shown that the following problem is NP-complete [Beeri et al., 1984]: Given a relation scheme and an integer $i > 1$, decide whether there exists a key of cardinality less than i. So finding *one* key, which is, one unique column combination is already an NP-complete problem. The same also holds for functional dependencies [Davies and Russell., 1994] and inclusion dependencies [Kantola et al., 1992]. The discovery of *all minimal* UCCs, FDs, and INDs are, therefore, by nature NP-complete tasks; they require exponential time in the number attributes m and, if nested loop joins are used for candidate validation, quadratic time in the number of records n. More specifically, UCC discovery is in $\mathcal{O}(n^2 \cdot 2^m)$, FD discovery is in $\mathcal{O}(n^2 \cdot 2^m \cdot (\frac{m}{2})^2)$, and IND discovery is in $\mathcal{O}(n^2 \cdot 2^m \cdot m!)$ (note that $m!$ is a simplification and n^2 is a worst case consideration that can be improved using, for instance, sorting- or hashing-based candidate validation techniques) [Liu et al., 2012]. This makes UCC discovery the easiest of the three tasks and IND discovery the most difficult one.

Within the class of NP-complete problems, some problems are still easier to solve than others, as we often find parameters k that determine the exponential complexity while the rest of the algorithm is polynomial in the size of the input n. More formally, we find an algorithm that runs in $\mathcal{O}(f(k) \cdot p(n))$ with exponential function f and polynomial function p [Downey and Fellows, 1999]. If such an algorithm exists for an NP-complete problem, the problem is called *fixed-parameter tractable* (FPT). An FPT solution to an NP-complete problem is efficient, if the parameter k is small (or even fixed) due to some practical assumption. For our key dependencies, k could, for instance, be the maximum size of a dependency – a parameter that we can easily enforce. However, Bläsius et al. have shown that the three problems do *not* admit FPT algorithms [Bläsius et al., 2017]: Regarding the W-hierarchy, which is a classification of computational complexities, UCC discovery and FD discovery are $W[2]$-complete and IND discovery is $W[3]$-complete. This makes IND discovery one of the hardest natural problems known today; the only other known $W[t]$-complete natural problem with $t > 2$ is related to supply chain management [Chen and Zhang, 2006].

2.5 Null semantics for key dependencies

Data is often incomplete, which means that we either do not know the value of a certain attribute or that the attribute does not apply to all entities in the relation. In such cases, `null` values $\perp$ are used to signal *no value* [Garcia-Molina et al., 2008]. For the discovery of dependencies, `null` values are an issue, because the validity of a dependency relies on the existence of values that either support or contradict it.

The standard solution for `null` values in data profiling is to define a semantics for `null` comparisons: Expressions of the form `null` $= x$ with some value x always evaluate to `false`, because one `null` value is usually compared to many different x values and the assumption that the same `null` value is simultaneously equal to all these x values leads to inconsistent conclusions. The expression `null` = `null`, however, consistently evaluates to `true` or `false` – either we consider all `null` values to represent the same value or different values.

The decision for either the `null` = `null` or the `null` $\neq$ `null` semantic has a direct influence on the key dependencies. Consider, for example, the schema $R(A, B)$ with two tuples $t_1 = (\perp, 1)$ and $t_2 = (\perp, 2)$. Depending on whether we choose `null` = `null` or `null` $\neq$ `null`, the UCC $\{A\}$ and the FD $A \rightarrow B$ are both either `false` or `true`. When switching the semantics from `null` $\neq$ `null` to `null` = `null`, the minimal UCCs of a dataset tend to become larger on average, because more attributes are needed to make attribute combinations with `null` values unique. The minimal FDs, however, can become both smaller and larger, i.e., `null` values in Lhs attributes introduce violations that demand for additional Lhs attributes and `null` values in Rhs attributes resolve violations that must no longer be counterbalanced with certain Lhs attributes. In general, `null` = `null` is the *pessimistic* perspective and `null` $\neq$ `null` the *optimistic* perspective for key dependencies.

To choose between the two `null` semantics, one obvious idea is to consult the handling of `null` values in SQL. In SQL, `null` = `null` evaluates to `unknown`, which is neither `true` nor `false` [Garcia-Molina et al., 2008]. In some cases, `unknown` is effectively treated as `false`, e.g., `null` values do not match in join statements. In other cases, however, `unknown` is treated as `true`, e.g., in group-by statements. For this reason, SQL does not help to decide for one of the two semantics.

The algorithms proposed in this work support both `null` semantics. In our experiments, we use the pessimistic `null` = `null` semantics for the following three reasons: First, we believe it to be more intuitive, because a completely empty column, for instance, should not functionally determine all other columns; second, it is the more challenging semantics, because many dependencies are located on higher lattice levels; third, the `null` = `null` semantics was chosen in all related works so that we use the same semantics for a comparable evaluation [Papenbrock et al., 2015b].

Note that the agreement on a `null` semantics is in fact a simplification of the `null` problem. A precise interpretation of a `null` value is *no information* [Zaniolo, 1984], which was first introduced for functional dependencies and constraints in [Atzeni and Morfuni, 1986]. Köhler and Link derived two validity models for this `null` interpretation, namely the *possible world* model and the *certain world* model: A dependency is valid in the possible world model, iff at least *one* replacement of all `null` values exists that satisfies the dependency; the dependency is valid in the certain world model, iff *every* replacement of the `null` values satisfies the dependency [Köhler and Link, 2016; Köhler et al., 2015]. To ensure possible and certain world validity, the discovery algorithms require some additional reasoning on `null` replacements. Because `null` reasoning is not the focus of this work, we use the traditional `null` semantics. For more details on possible and certain world key dependencies, we refer to [Le, 2014].

3

Functional Dependency Discovery

The *discovery of functional dependencies* aims to automatically detect *all* functional dependencies that hold in a given relational instance. As discussed in Section 2.2, it suffices to find all *minimal*, *non-trivial* FDs, because the remaining FDs can be efficiently inferred using Armstrong axioms. Due to the importance of functional dependencies for various use cases, many discovery algorithms have already been proposed. None of them is, however, able to process datasets of real-world size, i.e., datasets with more than 50 columns and a million rows, as we could show in [Papenbrock et al., 2015b]. Because the need for functional dependency discovery usually increases with growing dataset sizes, larger datasets are those for which FDs are most urgently needed. The reason why current algorithms fail on larger datasets is that they optimize for either many records *or* many attributes. This is a problem, because the discovery of functional dependencies is, as discussed in Section 2.4, by nature exponential in the number attributes and, for naïve approaches, quadratic in the number of records. Therefore, any truly scalable algorithm must be able to cope with both large schemata *and* many rows.

In this chapter, we present a hybrid discovery algorithm called HyFD, which is also described in [Papenbrock and Naumann, 2016]. HyFD dynamically switches its discovery method depending on which method currently performs best: The first discovery method carefully extracts a small subset of records from the input data and calculates only the FDs of this non-random sample. Due to this use of a non-random subset of records, this method performs particularly column-efficiently. The result is a set of FDs that are either valid or almost valid with respect to the complete dataset. The second discovery method of HyFD validates the discovered FDs on the entire dataset and refines such FDs that do not yet hold. This method is row-efficient, because it uses the previously discovered FDs to effectively prune the search space. If the validations become inefficient, HyFD is able to switch back to the first method and continue there with all results discovered so far. This alternating, two-phased discovery strategy experimentally outperforms all existing algorithms in terms of runtime and scalability, while still discovering *all minimal FDs*. In detail, our contributions are the following:

(1) *FD discovery.* We introduce HyFD, a hybrid FD discovery algorithm that is faster and able to handle much larger datasets than state-of-the-art algorithms.

(2) *Focused sampling.* We present sampling techniques that leverage the advantages of dependency induction algorithms while, at the same time, requiring far fewer comparisons.

(3) *Direct validation.* We contribute an efficient validation technique that leverages the advantages of lattice traversal algorithms with minimal memory consumption.

(4) *Robust scaling.* We propose a best-effort strategy that dynamically limits the size of resulting FDs if these would otherwise exhaust the available memory capacities.

(5) *Comprehensive evaluation.* We evaluate our algorithm on more than 20 real-world datasets and compare it to seven state-of-the-art FD discovery algorithms.

In the following, Section 3.1 discusses related work. Then, Section 3.2 provides the theoretical foundations for our hybrid discovery strategy and Section 3.3 an overview on our algorithm HyFD. Sections 3.4, 3.5, 3.6, and 3.7 describe the different components of HyFD in more detail. Section 3.9 evaluates our algorithm and compares it against seven algorithms from related work. We then conclude in Section 3.10 and discuss other algorithms that HyFD has inspired.

3.1 Related Work

In [Papenbrock et al., 2015b], we compared seven popular algorithms for functional dependency discovery and demonstrated their individual strengths and weaknesses. Some effort has also been spent on the discovery of *approximate* [Huhtala et al., 1999] and *conditional* [Bohannon et al., 2007; Cormode et al., 2009] functional dependencies, but those approaches are orthogonal to our research: We aim to discover *all minimal* functional dependencies without any restrictions or relaxations. Parallel and distributed dependency discovery systems, such as [Garnaud et al., 2014] and [Li et al., 2015], form another orthogonal branch of research. They rely on massive parallelization rather than efficient pruning to cope with the discovery problem. We focus on more sophisticated search techniques and show that these can still be parallelized accordingly. In the following, we briefly summarize current state-of-the-art in non-distributed FD discovery.

Lattice traversal algorithms: The algorithms Tane [Huhtala et al., 1999], Fun [Novelli and Cicchetti, 2001], FD_Mine [Yao et al., 2002], and Dfd [Abedjan et al., 2014c] conceptually arrange all possible FD candidates in a powerset lattice of attribute combinations and then traverse this lattice. The first three algorithms search through the candidate lattice level-wise bottom-up using the *apriori-gen* candidate generation [Agrawal and Srikant, 1994], whereas Dfd applies a depth-first random walk. Lattice traversal algorithms in general make intensive use of pruning rules and their candidate validation is based on position list indixes (see Section 2.4). They have been shown to perform well on long datasets, i.e., datasets with many records, but due to their candidate-driven search strategy, they scale poorly with the number of columns in the input dataset. In this chapter, we adopt the pruning rules and the position list index data structure from these algorithms for the validation of functional dependencies.

Difference- and agree-set algorithms: The algorithms Dep-Miner [Lopes et al., 2000] and FastFDs [Wyss et al., 2001] analyze a dataset for sets of attributes that agree on the values in certain tuple pairs. These so-called agree-sets are transformed into difference-sets from which all valid FDs can be derived. This discovery strategy scales better with the number of attributes than lattice traversal strategies, because FD candidates are generated only from concrete observations rather than being generated systematically. The required maximization of agree-sets or minimization of difference-sets respectively, however, reduces this advantage significantly. Furthermore, Dep-Miner and FastFDs scale much worse than the previous algorithms with the number of records, because they need to compare all pairs of records. Our algorithm HyFD also compares records pair-wise, but we carefully *choose* these comparisons.

Dependency induction algorithms: The Fdep [Flach and Savnik, 1999] algorithm also compares all records pair-wise to find all *invalid* functional dependencies. This set is called *negative cover* and is stored in a prefix tree. In contrast to Dep-Miner and FastFDs, Fdep translates this negative cover into the set of valid functional dependencies, i.e., the *positive cover*, not by forming complements but by successive specialization: The positive cover initially assumes that each attribute functionally determines all other attributes; these functional dependencies are then refined with every single non-FD in the negative cover. Apart from the fact that the pair-wise comparisons do not scale with the number of records in the input dataset, this discovery strategy has proven to scale well with the number of attributes. For this reason, we follow a similar approach during the induction of functional dependency candidates. However, we compress records before their comparison, store the negative cover in a more efficient data structure, and optimize the specialization process.

Parallel algorithms: Parallelization is besides a clever discovery strategy and effective pruning rules a third technique to improve the efficiency of the FD discovery. PaRaDe [Garnaud et al., 2014] is currently the only known FD discovery algorithm that implements parallelization techniques for compute-intensive subtasks. Similarly, we can use parallelization in HyFD for such subtasks that are independent from one another, i.e., record comparisons and FD validations.

The evaluation section of this chapter provides a comparison of our algorithm HyFD with *all* mentioned related work algorithms.

3.2 Hybrid FD discovery

Before we dive into the technical details of our algorithm, this section explains the intuition of our hybrid FD discovery. To aid the understanding, we first revisit the search space lattice of Section 2.4. Figure 3.1 depicts an example lattice with its FDs and non-FDs. In all such lattices, FDs are located in the upper part of the lattice; non-FDs are located at the bottom. In this lattice, we also explicitly distinguish between minimal and non-minimal FDs, because a discovery algorithm only searches for the minimal FDs. Now note that a virtual border separates the FDs and non-FDs. All minimal FDs, which we aim to discover, reside on this virtual border line. Our hybrid discovery approach

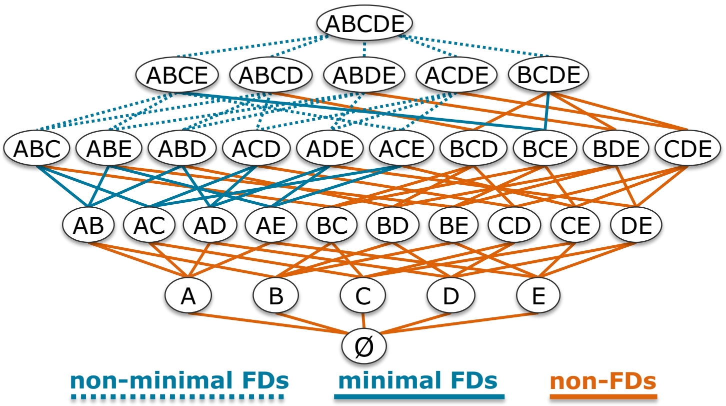


Figure 3.1: FD discovery in a power set lattice.

uses this observation: We use sampling techniques to approximate the minimal FDs from below and pruning rules to discard non-minimal FDs in the upper part of the lattice.

Sampling-based FD discovery. For a relational instance r, a sample r' of r contains only a subset of records $r' \subset r$. Because r' is (much) smaller than r, discovering all minimal FDs on r' is expected to be cheaper than discovering all minimal FDs on r (with any FD discovery algorithm). The resulting r'-FDs can, then, be valid or invalid in r, but they exhibit three properties that are important for our hybrid algorithm:

(1) *Completeness:* The set of r'-FDs implies the set of r-FDs, i.e., we find an $X' \rightarrow A$ in r' for each valid $X \rightarrow A$ in r with $X' \subseteq X$. Hence, all $X \rightarrow A$ are also valid in r' and the sampling result is complete. To prove this, assume $X \rightarrow A$ is valid in r but invalid in r'. Then r' must invalidate $X \rightarrow A$ with two records that do not exist in r. So it is $r' \not\subset r$, which contradicts $r' \subset r$.

(2) *Minimality:* If a minimal r'-FD is *valid* on the entire instance r, then the FD must also be minimal in r. This means that the sampling cannot produce non-minimal or incomplete results. In other words, a functional dependency cannot be valid in r but invalid in r'. This property is easily proven: If $X \rightarrow A$ is invalid in r', then r' contains two records with same X values but different A values. Because $r' \subset r$, the same records must also exist in r. Therefore, $X \rightarrow A$ must be invalid in r as well.

(3) *Proximity:* If a minimal r'-FD is *invalid* on the entire instance r, then the r'-FD is still expected to be *close* to specializations that are valid in r. In other words, r'-FDs are always located closer to the virtual border, which holds the true r-FDs, than the FDs at the bottom of the lattice, which are the FDs that are traditionally checked first. Therefore, any sampling-based FD discovery algorithm approximates the real FDs. The distance between r'-FDs and r-FDs still depends on the sampling algorithm and the entire data.

In summary, a sampling-based FD discovery algorithm calculates a set of r'-FDs that are either r-FDs or possibly close generalizations of r-FDs. In terms of Figure 3.1, the result of the sampling is a subset of solid lines.

The hybrid approach. In [Papenbrock et al., 2015b], we made the observation that current FD discovery algorithms either scale well with the number of records (e.g., DFD) or they scale well with the number of attributes (e.g., FDEP). None of the algorithms, however, addresses both dimensions equally well. Therefore, we propose a hybrid algorithm that combines column-efficient FD induction techniques with row-efficient FD search techniques in two alternating phases.

In Phase 1, the algorithm uses column-efficient FD induction techniques. Because these are sensitive to the number of rows, we process only a small sample of the input. The idea is to produce with low effort a set of FD candidates that are according to property (3) *proximity* close to the real FDs. To achieve this, we propose focused sampling techniques that let the algorithm select samples with a possibly large impact on the result's precision. Due to sampling properties (1) *completeness* and (2) *minimality*, these techniques cannot produce non-minimal or incomplete results.

In Phase 2, the algorithm uses row-efficient FD search techniques to validate the FD candidates given by Phase 1. Because the FD candidates and their specializations represent only a small subset of the search space, the number of columns in the input dataset has a much smaller impact on the row-efficient FD search techniques. Furthermore, the FD candidates should be valid FDs or close to valid specializations due to sampling property (3) *proximity.* The task of the second phase is, hence, to check all FD candidates and to find valid specializations if a candidate is invalid.

Although the two phases match perfectly, finding an appropriate, dataset-independent criterion for when to switch from Phase 1 into Phase 2 and back is difficult. If we switch too early into Phase 2, the FD candidates approximate the real FDs only poorly and the search space remains large; if we remain too long in Phase 1, we might end up analyzing the entire dataset with only column-efficient FD induction techniques, which is very expensive on many rows. For this reason, we propose to switch between the two phases back and forth whenever the currently running strategy becomes inefficient.

For Phase 1, we track the *sampling efficiency*, which is defined as the number of new observations per comparison. If this efficiency falls below an optimistic threshold, the algorithm switches into Phase 2. In Phase 2, we then track the *validation efficiency*, which is the number of discovered valid FDs per validation. Again, if this efficiency drops below a given threshold, the validation process can be considered inefficient and we switch back into Phase 1. In this case, the previous sampling threshold was too optimistic, so the algorithm dynamically increases it.

When switching back and forth between the two phases, the algorithm can share insights between the different strategies: The validation phase obviously profits from the FD candidates produced by the sampling phase; the sampling phase, in turn, profits from the validation phase, because the validation hints on interesting tuples that already invalidated some FD candidates. The hybrid FD discovery terminates when Phase 2 finally validated all FD candidates. We typically observe three to eight switches from Phase 2 back into Phase 1 until the algorithm finds the complete set of minimal functional dependencies. This result is correct, complete, and minimal, because Phase 1 is complete and minimal, as we have shown, and Phase 2 finally releases a correct, complete, and minimal result as shown by [Huhtala et al., 1999].

3.3 The HyFD algorithm

We implemented the hybrid FD discovery idea as the HyFD algorithm. Figure 3.2 gives an overview of HyFD showing its components and the control flow between them. In the following, we briefly introduce each component and their tasks in the FD discovery process. Each component is later explained in detail in their respective sections. Note that the `Sampler` and the `Inductor` component together implement Phase 1 and the `Validator` component implements Phase 2.

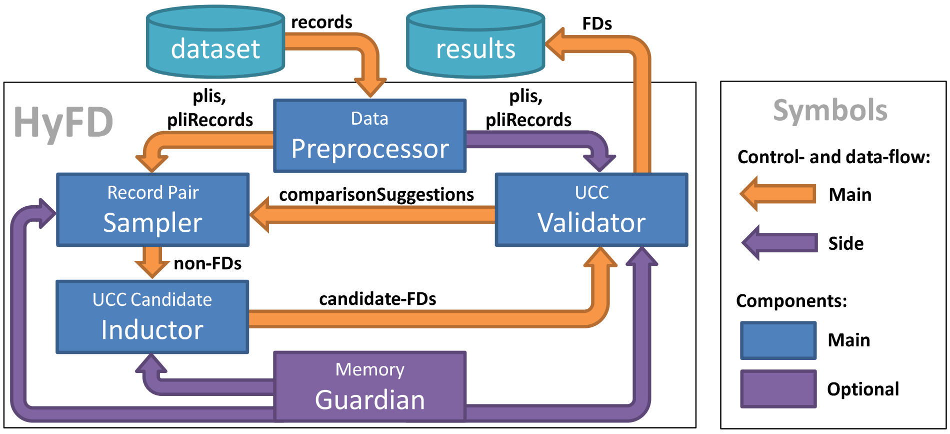


Figure 3.2: Overview of HyFD and its components.

(1) `Preprocessor`. To discover functional dependencies, we must know the positions of same values for each attribute, because same values in an FD's LHS can make it invalid if the according RHS values differ. The values itself, however, must not be known. Therefore, HyFD's `Preprocessor` component first transforms the records of a given dataset into compact *position list indexes* (PLIs). For performance reasons, the component also pre-calculates the inverse of this index, which is later used in the validation step. Because HyFD uses sampling to combine row- with column-efficient discovery techniques, it still needs to access the input dataset's records. For this purpose, the `Preprocessor` compresses the records via dictionary compression using the PLIs.

(2) `Sampler`. The `Sampler` component implements the first part of a column-efficient FD induction technique: It starts the FD discovery by checking the compressed records for FD-violations. An FD-violation is a pair of two records that match in one or more attribute values. From such record pairs, the algorithm infers that the matching attributes, i.e., the *agree sets* cannot functionally determine any of the non-matching attributes. Hence, they indicate non-valid FDs or short *non-FDs*. The schema $R(A, B, C)$, for instance, could hold the two records $r_1(1, 2, 3)$ and $r_2(1, 4, 5)$. Because the A-values match and the B- and C-values differ, $A \not\rightarrow B$ and $A \not\rightarrow C$ are two non-FDs in R. Finding all such non-FDs requires to systematically match all records pair-wise, which has quadratic complexity. To reduce these costs, the `Sampler` carefully selects only a subset of record pairs, namely those that indicate possibly many FD-violations. For the selection of record pairs, the component uses a deterministic, focused sampling technique that we call *cluster windowing*.

(3) `Inductor`. The `Inductor` component implements the second part of the column-efficient FD induction technique: From the `Sampler`, it receives a rich set of non-FDs that must be converted into *FD-candidates*. An FD-candidate is an FD that is minimal and valid with respect to the chosen sample – whether this candidate is actually valid on the entire dataset is determined in Phase 2. The conversion technique is similar to the conversion technique in the FDEP algorithm [Flach and Savnik, 1999]: We first assume that the empty set functionally determines all attributes; then, we successively specialize this assumption with every known non-FD. Recall the example schema $R(A, B, C)$ and its known non-FD $A \not\rightarrow B$. Initially, we define our result to be $\emptyset \rightarrow ABC$, which is a short notation for the FDs $\emptyset \rightarrow A$, $\emptyset \rightarrow B$, and $\emptyset \rightarrow C$. Because $A \not\rightarrow B$, the FD $\emptyset \rightarrow B$, which is a generalization of our known non-FD, must be invalid as well. Therefore, we remove it and add all valid, minimal, non-trivial specializations. Because this is only $C \rightarrow B$, our new result set is $\emptyset \rightarrow AC$ and $C \rightarrow B$. To execute the specialization process efficiently, the `Inductor` component maintains the valid FDs in a prefix tree that allows for fast generalization look-ups. If the `Inductor` is called again, it can continue specializing the FDs that it already knows, so it does not start with an empty prefix tree.

(4) `Validator`. The `Validator` component implements a row-efficient FD search technique: It takes the candidate-FDs from the `Inductor` and validates them against the entire dataset, which is given as a set of PLIs from the `Preprocessor`. When modeling the FD search space as a powerset lattice, the given candidate-FDs approximate the final FDs from below, i.e., a candidate-FD is either a valid FD or a generalization of a valid FD. Therefore, the `Validator` checks the candidate-FDs level-wise bottom-up: Whenever the algorithm finds an invalid FD, it removed this FD from the candidate space; from the removed FD, it then generates all minimal, non-trivial specializations and adds those specializations back to the candidate space that may still be valid and minimal using common pruning rules for lattice traversal algorithms [Huhtala et al., 1999]. If the previous calculations of Phase 1 yielded a good approximation of the valid FDs, only few FD candidates need to be specialized; otherwise, the number of invalid FDs increases rapidly from level to level and the `Validator` switches back to `Sampler`. The FD validations themselves build upon direct refinement checks and avoid the costly hierarchical PLI intersections that are typical in all current lattice traversal algorithms. In the end, the `Validator` outputs all minimal, non-trivial FDs for the given input dataset.

(5) `Guardian`. FD result sets can grow exponentially with the number of attributes in the input relation. For this reason, discovering complete result sets can sooner or later exhaust any memory-limit, regardless of how compact intermediate data structures, such as PLIs or results, are stored. Therefore, a robust algorithm must prune the results in some reasonable way, if memory threatens to be exhausted. This is the task of HYFD's `Guardian` component: Whenever the prefix tree, which contains the valid FDs, grows, the `Guardian` checks the current memory consumption and prunes the FD tree, if necessary. The idea is to give up FDs with largest left-hand-sides, because these FDs mostly hold accidentally in a given instance but not semantically in the according schema. Overall, however, the `Guardian` is an optional component in the HYFD algorithm and does not contribute in the discovery process itself. Our overarching goal remains to find the *complete* set of minimal FDs.

3.4 Preprocessing

The `Preprocessor` is responsible for transforming the input data into two compact data structures: *plis* and *pliRecords*. The first data structure *plis* is an array of *position list indexes* (Pli), which we already introduced in Section 2.4. A Pli π_X groups tuples into equivalence classes by their values of attribute set X. Such Plis can efficiently be implemented as sets of record ID sets, which we wrap in Pli objects. A functional dependency $X \rightarrow A$ is then checked by testing if every cluster in π_X is a subset of some cluster of π_A, which is true iff the FD is valid. This check is called *refinement* (see Section 3.7) and was first introduced in [Huhtala et al., 1999].

Algorithm 1 shows the `Preprocessor` component and the two data structures it produces: The already discussed *plis* and a Pli-compressed representation of all records, which we call *pliRecords*. For their creation, the algorithm first determines the number of input records *numRecs* and the number of attributes *numAttrs* (Lines 1 and 2). Then, it builds the *plis* array – one π for each attribute. This is done by hashing each value to a list of record IDs and then simply collecting these lists in a Pli object (Line 4). We call the lists of record IDs *cluster*, because they cluster records with a same value in the respective attribute. When created, the `Preprocessor` sorts the array of Plis in descending order by the number of clusters (including clusters of size one, whose number is implicitly known). This sorting improves the focussed sampling of non-FDs in the `Sampler` component (see Section 3.5), because it groups *effective* attributes, i.e., attributes that contain violations to potentially many FD candidates at the beginning of the list and non-effective attributes at the end; the sorting also improves the FD-candidate validations in the `Validator` component (see Section 3.7), because the attributes at the beginning of the sorted list then constitute the most efficient pivot elements.

Algorithm 1: Data Preprocessing

```
   Data: records
   Result: plis, invertedPlis, pliRecords
1  numRecs ← |records|;
2  numAttrs ← |records[0]|;
3  array plis size numAttrs as Pli;
4  plis ← buildPlis(records);
5  plis ← sort(plis, DESCENDING);
6  array invertedPlis size numAttrs × numRecs as Integer;
7  invertedPlis ← invert(plis);
8  array pliRecords size numRecs × numAttrs as Integer;
9  pliRecords ← createRecords(invertedPlis);
10 return plis, invertedPlis, pliRecords;
```

The clusters in each Pli object are stored in an arbitrary but fixed order so that we can enumerate the clusters. This allows the `Preprocessor` to calculate the inverse of each Pli, i.e., an array that maps each record ID to its corresponding cluster ID (Lines 6 and 7). If no cluster exists for a particular record, its value must be unique in this attribute and we store -1 as a special ID for unique values. With the *invertedPlis*, the

`Preprocessor` finally creates dictionary compressed representations of all records, the *pliRecords* (Lines 8 and 9). A compressed record is an array of cluster IDs where each field denotes the record's cluster in attribute $A \in [0, numAttrs[$. We extract these representations from the *plis* that already map cluster IDs to record IDs for each attribute. The PLI-compressed records are needed in the sampling phase to find FD-violations and in the validation phase to find LHS- and RHS-cluster IDs for certain records.

3.5 Sampling

The idea of the `Sampler` component is to analyze a dataset, which is represented by the *pliRecords*, for FD-violations, i.e., non-FDs that can later be converted into FDs. To derive FD-violations, the component compares records pair-wise. These pair-wise record comparisons are robust against the number of columns, but comparing all pairs of records scales quadratically with their number. Therefore, the `Sampler` uses only a subset, i.e., a sample of record pairs for the non-FD calculations. The record pairs in this subset should be chosen carefully, because some pairs are more likely to reveal FD-violations than others. In the following, we first discuss how non-FDs are identified; then, we present a deterministic focused sampling technique, which extracts a non-random subset of promising record pairs for the non-FD discovery; lastly, we propose an implementation of our sampling technique.

Retrieving non-FDs. A functional dependency $X \rightarrow A$ can be invalidated with two records that have matching X and differing A values. Therefore, the non-FD search is based on pair-wise record comparisons: If two records match in their values for attribute set Y and differ in their values for attribute set Z, then they invalidate all $X \rightarrow A$ with $X \subseteq Y$ and $A \in Z$. The corresponding FD-violation $Y \not\rightarrow Z$ can be efficiently stored in bitsets that hold a 1 for each matching attribute of Y and a 0 for each differing attribute Z. To calculate these bitsets, we use the ***match***()-function, which compares two PLI-compressed records element-wise. Because the records are given as Integer arrays (and not as, for instance, String arrays), this function is cheap in contrast to the validation and specialization functions used by other components of HYFD.

Sometimes, the sampling discovers the same FD-violations with different record pairs. For this reason, the bitsets are stored in a set called *nonFds*, which automatically eliminates duplicate observations. For the same task, related algorithms, such as FDEP [Flach and Savnik, 1999], proposed prefix-trees, but our evaluation in Section 3.9 and in particular the experiments in Section 3.9.5 show that these data structures consume much more memory and do not yield a better performance. Reconsidering Figure 3.1, we can easily see that the number of non-FDs is much larger than the number of minimal FDs, so storing the non-FDs in a memory-efficient data structure is crucial.

Focused sampling. FD-violations are retrieved from record pairs, and while certain record pairs indicate important FD-violations, the same two records may not offer any new insights when compared with other records. So an important aspect of focused sampling is that we sample *record pairs* and not *records*. Thereby, only record pairs that match in at least one attribute can reveal FD-violations; comparing records with no overlap should be avoided. A focused sampling algorithm can easily assure this by comparing only those records that co-occur in at least one Pli-cluster. But due to columns that contain only few distinct values, most record pairs co-occur in some cluster. Therefore, more sophisticated pair selection techniques are needed.

The problem of finding promising comparison candidates is a well known problem in duplicate detection research. A popular solution for this problem is the *sorted neighborhood* pair selection algorithm [Hernández and Stolfo, 1998]. The idea is to first sort the data by some domain-dependent key that sorts similar records close to one another; then, the algorithm compares all records to their w closest neighbors, where w is a *windowing*. Because our problem of finding violating record pairs is similar to finding matching record pairs, we use the same idea for our focused sampling algorithm.

At first, we sort similar records, i.e., records that co-occur in certain Pli-clusters, close to one-another. We do this for all clusters in all Plis with different sorting keys each (we discuss possible sorting keys soon). Then, we slide a window of size $w = 2$ over the clusters of each Pli and compare all record pairs within this window, which are all direct neighbors. Because some Plis produce better sortations than others in the sense that they reveal more FD-violations than others, the algorithm shall automatically prefer more efficient sortations over less efficient ones. This can be done with a progressive selection technique, which is also known from duplicate detection [Papenbrock et al., 2015c]: The algorithm first compares all records to their direct neighbors and counts the results; afterwards, the result counts are ranked and the sortation with the most results is chosen to run a slightly larger window $(w + 1)$. The algorithm stops continuing best sortations, when all sortations have become inefficient. In this way, the algorithm automatically chooses most profitable comparisons. When adapting the same strategy for our FD-violation search, we can save many comparisons: Because efficient sortations anticipate most informative comparisons, less efficient sortations become quickly inefficient.

Finally, the focused sampling must decide on when the comparisons of records in a certain sortation, i.e., for a certain Pli, become inefficient. We propose to start with a rather strict definition of efficiency, because HyFD returns into the sampling phase anyway, if the number of identified FD-violations was too low. So an efficiency threshold could be 0.01, which is one new FD-violation within 100 comparisons – in fact, Section 3.9 shows that this threshold performs well on *all* tested dataset sizes. To relax this threshold in subsequent iterations, we double the number of comparisons whenever the algorithm returns to the sampling phase.

The sampling algorithm. Algorithm 2 implements the focused sampling strategy introduced above. It requires the *plis* and *pliRecords* from the `Preprocessor` and the *comparisonSuggestions* from the `Validator`. Figure 3.3 illustrates the algorithm with an example.

The priority queue *efficiencyQueue* is a local data structure that ranks the Plis by their sampling efficiency. If the *efficiencyQueue* is empty (Line 1), this is the first time the `Sampler` is called. In this case, we need to sort the records in all clusters by some Pli-dependent sorting key (Lines 2 to 4). As shown in Figure 3.3.1, we sort the records in each cluster of attribute A_i's Pli by their cluster number in attribute A_{i-1}; if numbers are equal or unknown, the sorting uses the cluster number in A_{i+1} as a tiebreaker. The

Algorithm 2: Record Pair Sampling

```
Data: plis, pliRecords, comparisonSuggestions
Result: nonFds
if efficiencyQueue = ∅ then
    for pli ∈ plis do
        for cluster ∈ pli do
            cluster ← sort(cluster, ATTR_LEFT_RIGHT);
    nonFds ← ∅;
    efficiencyThreshold ← 0.01;
    efficiencyQueue ← new PriorityQueue;
    for attr ∈ [0, numAttributes[ do
        efficiency ← new Efficiency;
        efficiency.attribute ← attr;
        efficiency.window ← 2;
        efficiency.comps ← 0;
        efficiency.results ← 0;
        runWindow(efficiency, plis[attr], nonFds);
        efficiencyQueue.append(efficiency);
else
    efficiencyThreshold ← efficiencyThreshold / 2;
    for sug ∈ comparisonSuggestions do
        nonFds ← nonFds ∪ match(sug[0], sug[1]);
while true do
    bestEff ← efficiencyQueue.peek();
    if bestEff.eval() < efficiencyThreshold then
        break;
    bestEff.window ← bestEff.window + 1;
    runWindow(bestEff, plis[bestEff.attribute], nonFds);
return newFDsIn(nonFds);
function runWindow(efficiency, pli, nonFds)
prevNumNonFds ← |nonFds|;
for cluster ∈ pli do
    for i ∈ [0, |cluster| − efficiency.window [ do
        pivot ← pliRecords[cluster[i]];
        partner ← pliRecords[cluster[i + window − 1]];
        nonFds ← nonFds ∪ match(pivot, partner);
        efficiency.comps ← efficiency.comps + 1;
newResults ← |nonFds| − prevNumNonFds;
efficiency.results ← efficiency.results + newResults;
```

intuition here is that attribute A_{i-1} has more clusters than A_i, due to the sorting of *plis* in the `Preprocessor`, which makes it a promising key; some unique values in A_{i-1}, on the other hand, do not have a cluster number, so the sorting also checks the Pli of attribute A_{i+1} that has larger clusters than A_i. However, the important point in choosing sorting

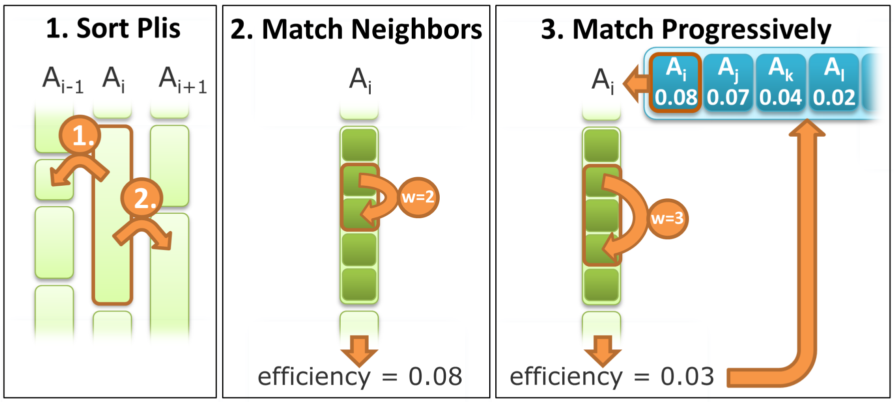


Figure 3.3: Focused sampling: Sorting of Pli clusters (1); record matching to direct neighbors (2); progressive record matching (3).

keys is not which $A_{i+/-x}$ to take but to take different sorting keys for each Pli. In this way, the neighborhood of one record differs in each of its Pli clusters.

When the sorting is done, the algorithm initializes the *efficiencyQueue* with first *efficiency* measurements. The efficiency of an attribute's Pli is an object that stores the Pli's sampling performance: It holds the attribute identifier, the last window size, the number of comparisons within this window, and the number of results, i.e., FD-violations that were first revealed with these comparisons. An efficiency object can calculate its efficiency by dividing the number of results by the number of comparisons. For instance, 8 new FD-violations in 100 comparisons yield an efficiency of 0.08. To initialize the efficiency object of each attribute, the `Sampler` runs a window of size 2 over the attribute's Pli clusters (Line 14) using the *runWindow*()-function shown in Lines 27 to 35. Figure 3.3 (2) illustrates how this function compares all direct neighbors in the clusters with window size 2.

If the `Sampler` is not called for the first time, the Pli clusters are already sorted and the last efficiency measurements are also present. We must, however, relax the efficiency threshold (Line 17) and execute the suggested comparisons (Lines 18 and 19). The suggested comparisons are record pairs that violated at least one FD candidate in Phase 2 of the HyFD algorithm; hence, it is probable that they also violate some more FDs. With the suggested comparisons, Phase 1 incorporates knowledge from Phase 2 to focus the sampling.

No matter whether this is the first or a subsequent call of the `Sampler`, the algorithm finally starts a progressive search for more FD-violations (Lines 20 to 25): It selects the efficiency object *bestEff* with the highest efficiency in the *efficiencyQueue* (Line 21) and executes the next window size on its Pli (Line 25). This updates the efficiency of *bestEff* so that it might get re-ranked in the priority queue. Figure 3.3 (3) illustrates one such progressive selection step for a best attribute A_i with efficiency 0.08 and next window size three: After matching all records within this window, the efficiency drops to 0.03, which makes A_j the new best attribute.

The `Sampler` algorithm continues running ever larger windows over the PLIs until all efficiencies have fallen below the current *efficiencyThreshold* (Line 22). At this point, the row-efficient discovery technique has apparently become inefficient and the algorithm decides to proceed with a column-efficient discovery technique.

3.6 Induction

The `Inductor` component concludes the column-efficient discovery phase and leads over into the row-efficient discovery phase. Its task is to convert the *nonFds* given by the `Sampler` component into corresponding minimal FD-candidates *fds* – a process that is known as *cover inversion* as it translates the negative cover, which are all non-FDs, into the positive cover, which are all FDs. While the non-FDs are given as a set of bitsets, the FD-candidates will be stored in a data structure called *FDTree*, which is a prefix-tree optimized for functional dependencies. Figure 3.4 shows three such FDTrees with example FDs. First introduced in [Flach and Savnik, 1999], an FDTree maps the LHS of FDs to nodes in the tree and the RHS of these FDs to bitsets, which are attached to the nodes. A RHS attribute in the bitsets is marked if it is at the end of an FD's LHS path, i.e., if the current path of nodes describes the entire LHS to which the RHS belongs.

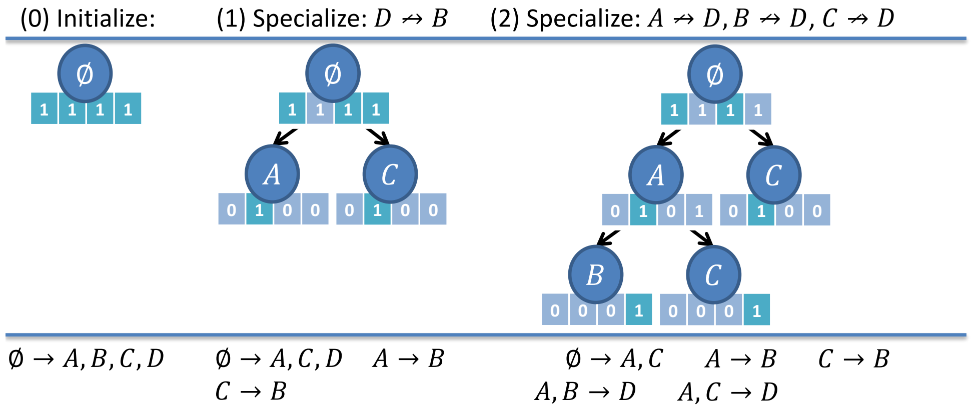

(0) Initialize:
(1) Specialize: $D \nrightarrow B$
(2) Specialize: $A \nrightarrow D, B \nrightarrow D, C \nrightarrow D$
∅
1 1 1 1
∅
1 1 1 1
A
0 1 0 0
C
0 1 0 0
∅
1 1 1 1
A
0 1 0 1
C
0 1 0 0
B
0 0 0 1
C
0 0 0 1
$\emptyset \rightarrow A, B, C, D$
$\emptyset \rightarrow A, C, D$ $A \rightarrow B$
$C \rightarrow B$
$\emptyset \rightarrow A, C$ $A \rightarrow B$ $C \rightarrow B$
$A, B \rightarrow D$ $A, C \rightarrow D$

Figure 3.4: Specializing the FDTree with non-FDs.

Algorithm 3 shows the conversion process in detail. The `Inductor` first sorts the *nonFds* in descending order by their cardinality, i.e., the number of set bits (Line 1). The sorting of FD-violations is important, because it lets HYFD convert non-FDs with long LHSs into FD-candidates first and non-FDs with ever shorter LHSs gradually later. In this way, the number of changes made to the FDTree is minimized, because many large FD-violations cover smaller FD-violations and their impact on the FD-candidates. The FD-violations $\{A, B\}$ and $\{A, C\}$, for example, together cover all non-FDs that also the FD-violation $\{A\}$ implies, namely $A \nrightarrow R$. For this reason, $\{A\}$ causes no changes to the FDTree, if the `Inductor` handles the larger supersets $\{A, B\}$ and $\{A, C\}$ first.

When the `Inductor` is called for the first time, the FDTree *fds* has not been created yet and is initialized with a schema R's most general FDs $\emptyset \rightarrow R$, where the attributes in R are represented as integers (Line 4); otherwise, the algorithm continues with the

Algorithm 3: Functional Dependency Induction

```
   Data: nonFds
   Result: fds
 1 nonFds ← sort(nonFds, CARDINALITY_DESCENDING);
 2 if fds = null then
 3     fds ← new FDTree;
 4     fds.add(∅ → {0, 1, ..., numAttributes});
 5 for lhs ∈ nonFds do
 6     rhss ← lhs.clone().flip();
 7     for rhs ∈ rhss do
 8         specialize(fds, lhs, rhs);
 9 return fds;
   function specialize(fds, lhs, rhs)
10 invalidLhss ← fds.getFdAndGenerals(lhs, rhs);
11 for invalidLhs ∈ invalidLhss do
12     fds.remove(invalidLhs, rhs);
13     for attr ∈ [0, numAttributes[ do
14         if invalidLhs.get(attr) ∨
15           rhs = attr then
16             continue;
17         newLhs ← invalidLhs ∪ attr;
18         if fds.findFdOrGeneral(newLhs, rhs) then
19             continue;
20         fds.add(newLhs, rhs);
```

previously calculated *fds*. The task is to specialize the *fds* with every bitset in *nonFds*: Each bitset describes the LHS of several non-FDs (Line 5) and each zero-bit in these bitsets describes a RHS of a non-FD (Lines 6 and 7). Once retrieved from the bitsets, each non-FD is used to specialize the FDTree *fds* (Line 8).

Figure 3.4 exemplarily shows the specialization of the initial FDTree for the non-FD $D \not\rightarrow B$ in (1): First, the *specialize*-function recursively collects the invalid FD and all its generalizations from the *fds* (Line 10), because these must be invalid as well. In our example, the only invalid FD in the tree is $\emptyset \rightarrow B$. HYFD then successively removes these non-FDs from the FDTree *fds* (Line 12). Once removed, the non-FDs are specialized, which means that the algorithm *extends* the LHS of each non-FD to generate still valid specializations (Line 17). In our example, these are $A \rightarrow B$ and $C \rightarrow B$. Before adding these specializations, the `Inductor` assures that the new candidate-FDs are minimal by searching for generalizations in the known *fds* (Line 18). Figure 3.4 also shows the result when inducing three more non-FDs into the FDTree. After specializing the *fds* with all *nonFds*, the prefix-tree holds the entire set of valid, minimal FDs with respect to these given non-FDs [Flach and Savnik, 1999].

3.7 Validation

The `Validator` component takes the previously calculated FDTree *fds* and validates the contained FD-candidates against the entire input dataset, which is represented by the *plis* and the *invertedPlis*. For this validation process, the component uses a row-efficient lattice traversal strategy. We first discuss the lattice traversal; then, we introduce our direct candidate validation technique; and finally, we present the specialization method of invalid FD-candidates. The `Validator` component is shown in detail in Algorithm 4.

Traversal. Usually, lattice traversal algorithms need to traverse a huge candidate lattice, because FDs can be everywhere (see Figure 3.1 in Section 3.2). Due to the previous, sampling-based discovery, HyFD already starts the lattice traversal with a set of promising FD-candidates *fds* that are organized in an FDTree. Because this FDTree maps directly to the FD search space, i.e., the candidate lattice, HyFD can use it to systematically check all necessary FD candidates: Beginning from the root of the tree, the `Validator` component traverses the candidate set breadh-first level by level.

When the `Validator` component is called for the first time (Line 1), it initializes the *currentLevelNumber* to zero (Line 2); otherwise, it continues the traversal from where it stopped before. During the traversal, the set *currentLevel* holds all FDTree nodes of the current level. Before entering the level-wise traversal in Line 5, the `Validator` initializes the *currentLevel* using the ***getLevel***()-function (Line 3). This function recursively collects all nodes with depth *currentLevelNumber* from the prefix-tree *fds*.

On each level (Line 5), the algorithm first validates all FD-candidates removing those from the FDTree that are invalid (Lines 6 to 16); then, the algorithm collects all child-nodes of the current level to form the next level (Lines 17 to 20); finally, it specializes the invalid FDs of the current level which generates new, minimal FD-candidates for the next level (Lines 21 to 33). The level-wise traversal stops when the validation process becomes inefficient (Lines 36 and 37). Here, this means that more than 1% of the FD-candidates of the current level were invalid and the search space started growing rapidly. HyFD then returns into the sampling phase. We use 1% as a static threshold for efficiency in this phase, but our experiments in Section 3.9.5 show that any small percentage performs well here, because the number of invalid FD-candidates grows exponentially fast if many candidates are invalid. The validation terminates when the next level is empty (Line 5) and all FDs in the FDTree *fds* are valid. This also ends the entire HyFD algorithm.

Validation. Each node in an FDTree can harbor multiple FDs with the same Lhs and different Rhss (see Figure 3.4 in Section 3.6): The Lhs attributes are described by a node's path in the tree and the Rhs attributes that form FDs with the current Lhs are marked. The `Validator` component validates all FD-candidates of a node simultaneously using the ***refines***()-function (Line 11). This function checks which Rhs attributes are *refined* by the current Lhs using the *plis* and *pliRecords*. The refined Rhs attributes indicate valid FDs, while all other Rhs attributes indicate invalid FDs.

Figure 3.5 illustrates how the ***refines***()-function works: Let $X \to Y$ be the set of FD-candidates that is to be validated. At first, the function selects the *pli* of the first Lhs attribute X_0. Due to the sorting of *plis* in the `Preprocessor` component, this is the Pli

Algorithm 4: Functional Dependency Validation

```
Data: $fds$, $plis$, $pliRecords$
Result: $fds$, $comparisonSuggestions$
if $currentLevel$ = null then
    $currentLevelNumber \leftarrow 0$;
$currentLevel \leftarrow fds.$getLevel$(currentLevelNumber)$;
$comparisonSuggestions \leftarrow \emptyset$;
while $currentLevel \neq \emptyset$ do
    /* Validate all FDs on the current level                         */
    $invalidFds \leftarrow \emptyset$;
    $numValidFds \leftarrow 0$;
    for $node \in currentLevel$ do
        $lhs \leftarrow node.$getLhs$()$;
        $rhss \leftarrow node.$getRhss$()$;
        $validRhss \leftarrow$ refines$(lhs, rhss, plis, pliRecords, comparisonSuggestions)$;
        $numValidFds \leftarrow numValidFds + |validRhss|$;
        $invalidRhss \leftarrow rhss.$andNot$(validRhss)$;
        $node.$setFds$(validRhss)$;
        for $invalidRhs \in invalidRhss$ do
            $invalidFds \leftarrow invalidFds \cup (lhs, invalidRhs)$;
    /* Add all children to the next level                            */
    $nextLevel \leftarrow \emptyset$;
    for $node \in currentLevel$ do
        for $child \in node.$getChildren$()$ do
            $nextLevel \leftarrow nextLevel \cup child$;
    /* Specialize all invalid FDs                                    */
    for $invalidFd \in invalidFds$ do
        $lhs, rhs \leftarrow invalidFd$;
        for $attr \in [0, numAttributes[$ do
            if $lhs.$get$(attr) \lor rhs = attr \lor$
              $fds.$findFdOrGeneral$(lhs, attr) \lor$
              $fds.$findFd$(attr, rhs)$ then
                continue;
            $newLhs \leftarrow lhs \cup attr$;
            if $fds.$findFdOrGeneral$(newLhs, rhs)$ then
                continue;
            $child \leftarrow fds.$addAndGetIfNew$(newLhs, rhs)$;
            if $child \neq$ null then
                $nextLevel \leftarrow nextLevel \cup child$;
    $currentLevel \leftarrow nextLevel$;
    $currentLevelNumber \leftarrow currentLevelNumber + 1$;
    /* Judge efficiency of validation process                        */
    if $|invalidFds| > 0.01 * numValidFds$ then
        return $fds$, $comparisonSuggestions$;
return $fds$, $\emptyset$;
```

with the most and, hence, the smallest clusters of all Lhs attributes. For each cluster in X_0's Pli, the algorithm iterates all record IDs r_i in this cluster and retrieves the according compressed records from the *pliRecords*. A compressed record contains all cluster IDs in which a record is contained. Hence, the algorithm can create one array containing the Lhs cluster IDs of X and one array containing the Rhs cluster IDs of Y. The Lhs array, then, describes the cluster of r_i regarding attribute combination X. To check which Rhs Pli these Lhs clusters refine, we map the Lhs clusters to the corresponding array of Rhs clusters. We fill this map while iterating the record IDs of a cluster. If an array of Lhs clusters already exists in this map, the array of Rhs clusters must match the existing one. All non-matching Rhs clusters indicate refinement-violations and, hence, invalid Rhs attributes. The algorithm immediately stops checking such Rhs attributes so that only valid Rhs attributes survive until the end.

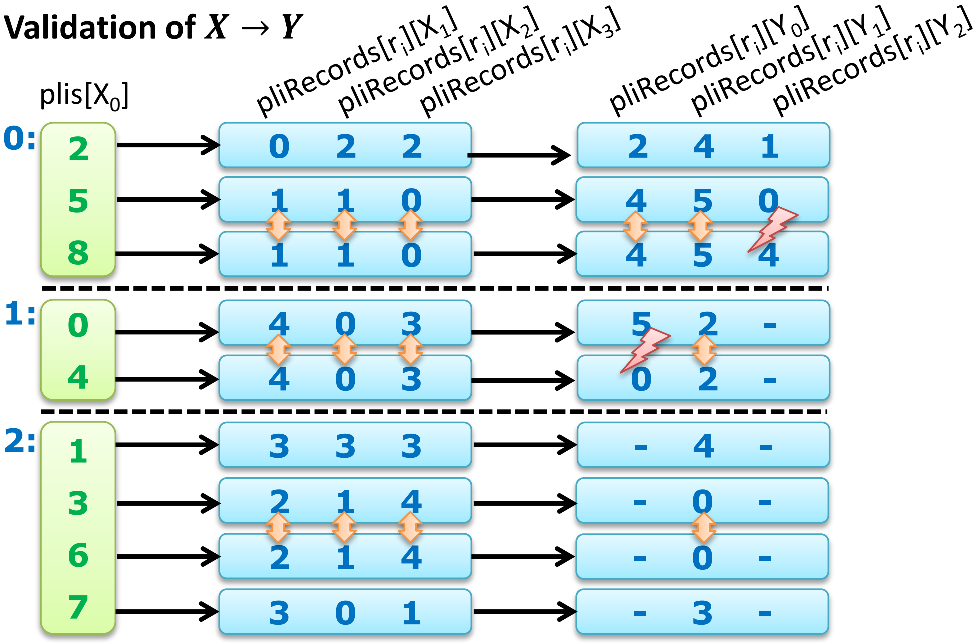


Figure 3.5: Directly validating FD-candidates $X \rightarrow Y$.

In comparison to other Pli-based algorithms, such as Tane, HyFD's validation technique avoids the costly hierarchical Pli intersections. By mapping the Lhs clusters to Rhs clusters, the checks are independent of other checks and do not require intermediate Plis. The direct validation is important, because the `Validator`'s starting FD candidates are – due to the sampling-based induction part – on much higher lattice levels and successively intersecting lower level Plis would undo this advantage. Furthermore, HyFD can terminate refinement checks very early if all Rhs attributes are invalid, because the results of the intersections, i.e., the intersected Plis are not needed for later intersections. Not storing intermediate Plis also has the advantage of demanding much less memory – most Pli-based algorithms fail at processing larger datasets, for exactly this reason [Papenbrock et al., 2015b].

Specialization. The validation of FD candidates identifies all invalid FDs and collects them in the set *invalidFds*. The specialization part of Algorithm 4, then, extends these invalid FDs in order to generate new FD candidates for the next higher level: For each invalid FD represented by *lhs* and *rhs* (Line 21), the algorithm checks for all attributes *attr* (Line 23) if they specialize the invalid FD into a new minimal, non-trivial FD candidate *lhs* ∪ *attr* → *rhs*. To assure minimality and non-triviality of the new candidate, the algorithm assures the following:

(1) *Non-triviality*: $attr \notin lhs$ and $attr \neq rhs$ (Line 24)

(2) *Minimality 1*: $lhs \not\to attr$ (Line 25)

(3) *Minimality 2*: $lhs \cup attr \not\to rhs$ (Lines 26 and 29)

For the minimality checks, `Validator` recursively searches for generalizations in the FDTree *fds*. This is possible, because all generalizations in the FDTree have already been validated and must, therefore, be correct. The generalization look-ups also include the new FD candidate itself, because if this is already present in the tree, it does not need to be added again. The minimality checks logically correspond to candidate pruning rules, as used by lattice traversal algorithms, such as Tane, Fun, and Dfd.

If a minimal, non-trivial specialization has been found, the algorithm adds it to the FDTree *fds* (Line 31). The adding of a new FD into the FDTree might create a new node in the graph. To handle these new nodes on the next level, the algorithm must also add them to *nextLevel*. When the specialization has finished with all invalid FDs, the `Validator` moves to the next level. If the next level is empty, all FD-candidates have been validated and *fds* contains all minimal, non-trivial FDs of the input dataset.

3.8 Memory Guardian

The memory `Guardian` is an optional component in HyFD and enables a best-effort strategy for FD discovery for very large inputs. Its task is to observe the memory consumption and to free resources if HyFD is about to reach the memory limit. Observing memory consumption is a standard task in any programming language. So the question is, what resources the `Guardian` can free if the memory is exhausted.

The Pli data structures grow linearly with the input dataset's size and are relatively small. The number of FD-violations found in the sampling step grows exponentially with the number of attributes, but it takes quite some attributes to exhaust the memory with these compact bitsets. The data structure that grows by far the fastest is the FDTree *fds*, which is constantly specialized by the `Inductor` and `Validator` components. Hence, this is the data structure the `Guardian` must prune.

Obviously, shrinking the *fds* is only possible by giving up some results, i.e., giving up completeness of the algorithm. In our implementation of the `Guardian`, we decided to successively reduce the maximum Lhs size of our results; we provide three reasons: First, FDs with a long Lhs usually occur accidentally, meaning that they hold for a particular instance but not for the relation in general. Second, FDs with long Lhss are less useful in most use cases, e.g., they become worse key/foreign-key candidates when used for normalization and they are less likely to match a query when used for query optimization. Third, FDs with long LHSs consume more memory, because they are physically larger, and preferentially removing them retains more FDs in total.

To restrict the maximum size of the FDs' LHSs, we need to add some additional logic into the FDTree: It must hold the maximum LHS size as a variable, which the `Guardian` component can control; whenever this variable is decremented, the FDTree recursively removes all FDs with larger LHSs and sets their memory resources free. The FDTree also refuses to add any new FD with a larger LHS. In this way, the result pruning works without changing any of the other four components. However, note that the `Guardian` component prunes only such results whose size would otherwise exceed the memory capacity, which means that the component in general does not take action.

3.9 Evaluation

FD discovery has shown to be exponential in the number of attributes m, simply because the results can become exponentially large (see Section 2.4). For this reason, HYFD's runtime is in $\mathcal{O}(m^2 \cdot 2^m)$ as well: In Phase 1, the comparison costs for record pairs are linear in m, but the induction of the positive cover is in $\mathcal{O}(m^2 \cdot 2^m)$, because in the worst case 2^{m-1} LHS attribute combinations must be refined on average $\frac{m-1}{2}$ times in the negative cover for each of the m possible RHS attributes – HYFD prevents the worst case by sorting the non-FDs descendingly in the negative cover before inducing the positive cover. Phase 2 is in $\mathcal{O}(m^2 \cdot 2^m)$, because this represents the worst case number of FD candidates that need to be tested – HYFD reduces this number via minimality pruning and the use of Phase 1's results. Due to the threshold-bounded windowing in Phase 1 and the PLI-based validations in Phase 2, HYFD's runtime is (like other runtimes of lattice-based FD algorithms) about linear in the number of records n.

Note that each phase can (potentially) discover all minimal FDs without the other. The following experiments, however, show that HYFD is able to process significantly larger datasets than state-of-the-art FD discovery algorithms in less runtime. At first, we introduce our experimental setup. Then, we evaluate the scalability of HYFD with both a dataset's number of rows and columns. Afterwards, we show that HYFD performs well on different datasets. In all these experiments, we compare HYFD to seven state-of-the-art FD discovery algorithms. We, finally, analyze some characteristics of HYFD in more detail and discuss the results of the discovery process.

3.9.1 Experimental setup

Metanome. HYFD and all algorithms from related work have been implemented for the *Metanome* data profiling framework (`www.metanome.de`), which defines standard interfaces for different kinds of profiling algorithms. Metanome also provided the various implementations of the state of the art. Common tasks, such as input parsing, result formatting, and performance measurement are standardized by the framework and decoupled from the algorithms. We cover more details on METANOME in Chapter 6.

Hardware. We run all our experiments on a Dell PowerEdge R620 with two Intel Xeon E5-2650 2.00 GHz CPUs and 128 GB RAM. The server runs on CentOS 6.4 and uses OpenJDK 64-Bit Server VM 1.7.0_25 as Java environment.

Null Semantics. As discussed in Section 2.5, real-world data often contains `null` values and depending on which semantics we choose for `null` comparisons, some functional dependency are either `true` or `false`. So because the `null` semantics changes the results of the FD discovery, HyFD supports both settings, which means that the semantics can be switched in the `Preprocessor` (Pli-construction) and in the `Sampler` (*match*()-function) with a parameter. For our experiments, however, we use `null` = `null`, because this is how related work treats `null` values [Papenbrock et al., 2015b].

Datasets. We evaluate HyFD on various synthetic and real-world datasets. Table 3.1 in Section 3.9.4 and Table 3.2 in Section 3.9.5 give an overview of these datasets. The data shown in Table 3.1 includes the *plista* dataset on web log data [Kille et al., 2013a], the *uniprot*[1] dataset on protein sequences, and the *ncvoter*[2] dataset on public voter statistics; the remaining datasets originate from the UCI machine learning repository[3]. The datasets listed in Table 3.2 are the *CD* dataset on CD-product data, the synthetic *TPC-H* dataset on business data, the *PDB* dataset on protein sequence data, and the *SAP_R3* dataset, which contains data of a real SAP R3 ERP system. These datasets have never been analyzed for FDs before, because they are much larger than the datasets of Table 3.1 and most of them cannot be processed with any of the related seven FD discovery algorithms within reasonable time (<1 month) and memory (<100 GB).

3.9.2 Varying the number of rows

Our first experiment measures the runtime of HyFD on different row numbers. The experiment uses the *ncvoter* dataset with 19 columns and the *uniprot* dataset with 30 columns. The results, which also include the runtimes of the other seven FD discovery algorithms, are shown in Figure 3.6. A series of measurements stops if either the memory consumption exceeded 128 GB or the runtime exceeded 10,000 seconds. The dotted line shows the number of FDs in the input using the second y-axis: This number first increases, because more tuples invalidate more FDs so that more larger FDs arise; then it decreases, because even the larger FDs get invalidated and no further minimal specializations exist.

With our HyFD algorithm, we could process the 19 column version of the *ncvoter* dataset in 97 seconds and the 30 column version of the *uniprot* dataset in 89 seconds for the largest row size. This makes HyFD more than 20 times faster on *ncvoter* and more than 416 times faster on *uniprot* than the best state-of-the-art algorithm respectively. The reason why HyFD performs so much better than current lattice traversal algorithms is that the number of FD-candidates that need to be validated against the many rows is greatly reduced by the `Sampler` component.

[1] `http://uniprot.org` *(Accessed: 2017-04-12)*

[2] `http://ncsbe.gov/ncsbe/data-statistics` *(Accessed: 2017-04-12)*

[3] `http://archive.ics.uci.edu/ml` *(Accessed: 2017-04-12)*

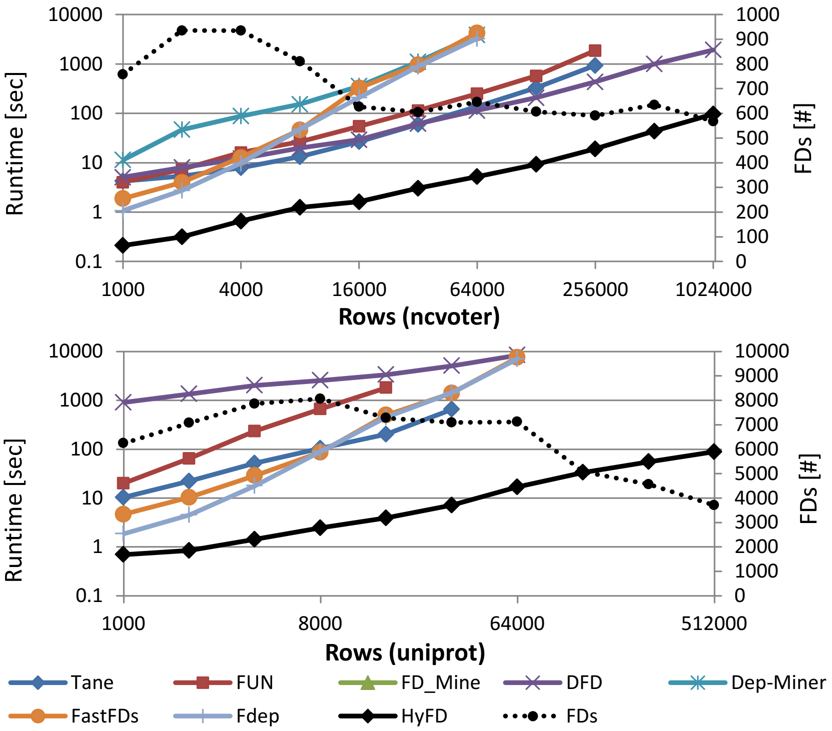


Figure 3.6: Row scalability on *ncvoter* and *uniprot*.

3.9.3 Varying the number of columns

In our second experiment, we measure HyFD's runtime on different column numbers using the *uniprot* dataset and the *plista* dataset with 1,000 records each. Again, we plot the measurements of HyFD with the measurements of the other FD discovery algorithms and cut the runtimes at 10,000 seconds. Figure 3.7 shows the result of this experiment.

We first notice that HyFD's runtime rather scales with the number of FDs, i.e., with the result size than with the number of columns. This is a desirable behavior, because the increasing effort is compensated by an also increasing gain. We further see that HyFD again outperforms all existing algorithms. The improvement factor is, however, smaller in this experiment, because the two datasets are with 1,000 rows so small that comparing all pairs of records, as Fdep does, is feasible and probably the best way to proceed. HyFD is still slightly faster than Fdep, because it does not compare all record pairs; the overhead of creating Plis is compensated by then being able to compare Pli compressed records rather than String-represented records.

3.9.4 Varying the datasets

To show that HyFD is not sensitive to any dataset peculiarity, the next experiment evaluates the algorithm on many different datasets. For this experiment, we set a time limit (TL) of 4 hours and a memory limit (ML) of 100 GB. Table 3.1 summarizes the runtimes of the different algorithms.

Dataset	Cols [#]	Rows [#]	Size [KB]	FDs [#]	Tane	Fun	FD_Mine	Dfd	Dep-Miner	FastFDs	Fdep	HyFD
iris	5	150	5	4	1.1	**0.1**	0.2	0.2	0.2	0.2	**0.1**	**0.1**
balance-scale	5	625	7	1	1.2	**0.1**	0.2	0.3	0.3	0.3	0.2	**0.1**
chess	7	28,056	519	1	2.9	1.1	3.8	1.0	174.6	164.2	125.5	**0.2**
abalone	9	4,177	187	137	2.1	0.6	1.8	1.1	3.0	2.9	3.8	**0.2**
nursery	9	12,960	1,024	1	4.1	1.8	7.1	0.9	121.2	118.9	46.8	**0.5**
breast-cancer	11	699	20	46	2.3	0.6	2.2	0.8	1.1	1.1	0.5	**0.2**
bridges	13	108	6	142	2.2	0.6	4.2	0.9	0.5	0.6	0.2	**0.1**
echocardiogram	13	132	6	527	1.6	0.4	69.9	1.2	0.5	0.5	0.2	**0.1**
adult	14	48,842	3,528	78	67.4	111.6	531.5	5.9	6039.2	6033.8	860.2	**1.1**
letter	17	20,000	695	61	260.0	529.0	7204.8	6.0	1090.0	1015.5	291.3	**3.4**
ncvoter	19	1,000	151	758	4.3	4.0	ML	5.1	11.4	1.9	1.1	**0.4**
hepatitis	20	155	8	8,250	12.2	175.9	ML	326.7	5576.5	9.5	0.8	**0.6**
horse	27	368	25	128,727	457.0	TL	ML	TL	TL	385.8	7.2	**7.1**
fd-reduced-30	30	250,000	69,581	89,571	**41.1**	77.7	ML	TL	377.2	382.4	TL	513.0
plista	63	1,000	568	178,152	ML	ML	ML	TL	TL	TL	26.9	**21.8**
flight	109	1,000	575	982,631	ML	ML	ML	TL	TL	TL	216.5	**53.4**
uniprot	223	1,000	2,439	>2,437,556	ML	ML	ML	TL	TL	TL	ML	>**5254.7**

Results larger than 1,000 FDs are only counted **TL**: time limit of 4 hours exceeded **ML**: memory limit of 100 GB exceeded

Table 3.1: Runtimes in seconds for several real-world datasets.

Tane [Huhtala et al., 1999] Fun [Novelli and Cicchetti, 2001] FD_Mine [Yao et al., 2002] Dfd [Abedjan et al., 2014c]
Dep-Miner [Lopes et al., 2000] FastFDs [Wyss et al., 2001] Fdep [Flach and Savnik, 1999] HyFD [Papenbrock and Naumann, 2016]

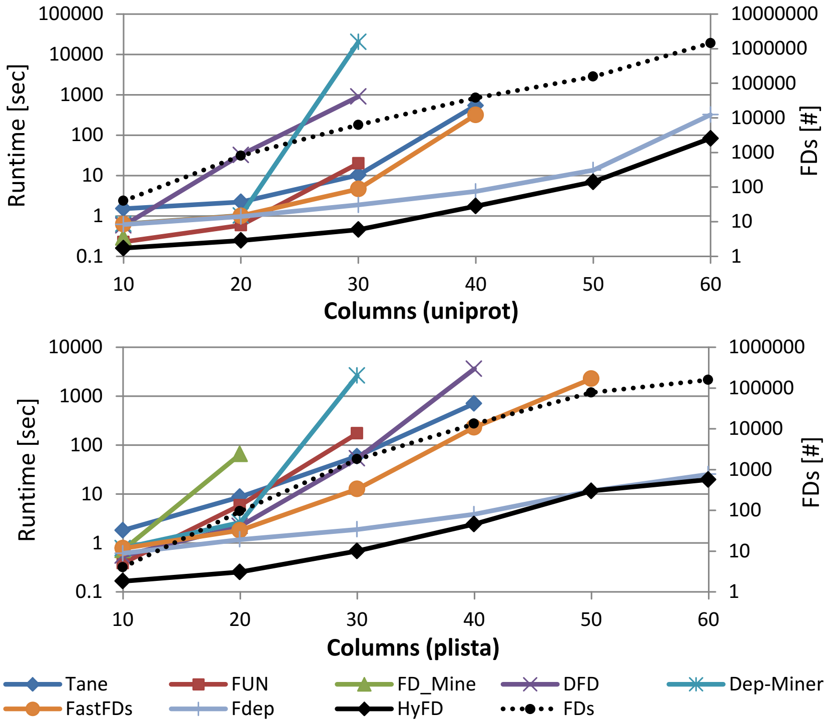


Figure 3.7: Column scalability on *uniprot* and *plista*.

The measurements show that HyFD was able to process all datasets and that it usually performed best. There are only two runtimes, namely those for the *fd-reduced-30* and for the *uniprot* dataset, that are in need of explanation: First, the *fd-reduced-30* dataset is a generated dataset that exclusively contains random values. Due to these random values, all FDs are accidental and do not have any semantic meaning. Also, all FDs are of same size, i.e., 99% of the 89,571 minimal FDs reside on lattice level three and none of them above this level. Thus, bottom-up lattice traversal algorithms, such as Tane and Fun, and algorithms that have bottom-up characteristics, such as Dep-Miner and FastFDs, perform very well on such an unusual dataset. The runtime of HyFD, which is about 9 minutes, is an adequate runtime for any dataset with 30 columns and 250,000 rows.

The *uniprot* dataset is another extreme, but real-world dataset: Because it comprises 223 columns, the total number of minimal FDs in this dataset is much larger than 100 million. This is, as Figure 3.7 shows, due to the fact that the number of FDs in this dataset grows exponentially with the number of columns. For this reason, we limited HyFD's result size to 4 GB and let the algorithm's `Guardian` component assure that the result does not become larger. In this way, HyFD discovered all minimal FDs with a Lhs of up to four attributes; all FDs on lattice level five and above have been successively pruned, because they would exceed the 4 GB memory limit. So HyFD discovered the first 2.5 million FDs in about 1.5 hours. One can compute more FDs on *uniprot* with HyFD using more memory, but the entire result set is – at the time – infeasible to store.

The datasets in Table 3.1 brought all state-of-the-art algorithms to their limits, but they are still quite small in comparison to most real-world datasets. Therefore, we also evaluated HyFD on much larger datasets. In this experiment, we report only HyFD's runtimes, because no other algorithm can process the datasets within reasonable time and memory limits. Table 3.2 lists the results for the single-threaded implementation of HyFD (left column) that we also used in the previous experiments and a multi-threaded implementation (right column), which we explain below.

Dataset	Cols	Rows	Size	FDs	HyFD	
	[#]	[#]	[MB]	[#]	[s/m/h/d]	
TPC-H.lineitem	16	6 m	1,051	4 k	**39 m**	4 m
PDB.POLY_SEQ	13	17 m	1,256	68	**4 m**	3 m
PDB.ATOM_SITE	31	27 m	5,042	10 k	**12 h**	64 m
SAP_R3.ZBC00DT	35	3 m	783	211	**4 m**	2 m
SAP_R3.ILOA	48	45 m	8,731	16 k	**35 h**	8 h
SAP_R3.CE4HI01	65	2 m	649	2 k	**17 m**	10 m
NCVoter.statewide	71	1 m	561	5 m	**10 d**	31 h
CD.cd	107	10 k	5	36 k	**5 s**	3 s

Table 3.2: Single- and multi-threaded runtimes on larger real-world datasets.

The measurements show that HyFD's runtime depends on the number of FDs, which is fine, because the increased effort pays off in more results. Intuitively, the more FDs are to be validated, the longer the discovery takes. But the *CD* dataset shows that the runtime also depends on the number of rows, i.e., the FD-candidate validations are much less expensive if only a few values need to be checked. If both the number of rows and columns becomes large, which is when they exceed 50 columns and 10 million rows, HyFD might run multiple days. This is due to the exponential complexity of the FD-discovery problem. However, HyFD was able to process all such datasets and because no other algorithm is able to achieve this, obtaining a complete result within some days is the first actual solution to the problem.

Multiple threads. We introduced and tested a single-threaded implementation of HyFD to compare its runtime with the single-threaded state-of-the-art algorithms. HyFD can, however, easily be parallelized: All comparisons in the `Sampler` component and all validations in the `Validator` component are independent of one another and can, therefore, be executed in parallel. We implemented these simple parallelizations and the runtimes reduced to the measurements shown in the right column of Table 3.2 using 32 parallel threads. Compared to the parallel FD discovery algorithm ParaDe [Garnaud et al., 2014], HyFD is 8x (*POLY_SEQ*), 38x (*lineitem*), 89x (*CE4HI01*), and 1178x (*cd*) faster due to its novel, hybrid search strategy – for the other datasets, we stopped ParaDe after two weeks each.

3.9.5 In-depth experiments

Memory consumption. Many FD discovery algorithms demand a lot of main memory to store intermediate data structures. The following experiment contrasts the memory consumption of HyFD with its three most efficient competitors Tane, Dfd, and Fdep on different datasets (the memory consumption of Fun and FD_Mine is worse than Tane's; Dep-Miner and FastFDs are similar to Fdep [Papenbrock et al., 2015b]). To measure the memory consumption, we limited the available memory successively to 1 MB, 2 MB, ..., 10 MB, 15 MB, ..., 100 MB, 110 MB, ..., 300 MB, 350 MB, ..., 1 GB, 2 GB, ..., 10 GB, 15 GB, ..., 100 GB and stopped increasing the memory when an algorithm finished without memory issues. Table 3.3 lists the results. Note that the memory consumption is given for complete results and HyFD can produce smaller results on less memory using the Guardian component. Because Dfd takes more than 4 hours, which is our time limit, to process *horse*, *plista*, and *flight*, we could not measure the algorithm's memory consumption on these datasets.

Dataset	Tane	Dfd	Fdep	HyFD
hepatitis	400 MB	300 MB	9 MB	**5 MB**
adult	5 GB	300 MB	100 MB	**10 MB**
letter	30 GB	400 MB	90 MB	**25 MB**
horse	25 GB	TL	100 MB	**65 MB**
plista	ML	TL	800 MB	**110 MB**
flight	ML	TL	900 MB	**200 MB**

ML: memory limit of 100 GB exceeded **TL**: time limit of 4 hours exceeded

Table 3.3: Memory consumption

Due to the excessive construction of Plis, Tane of course consumes the most memory. Dfd manages the Plis in a Pli-store using a least-recently-used strategy to discard Plis when memory is exhausted, but the minimum number of required Plis is still very large. Also, Dfd becomes very slow on low memory. Fdep has a relatively small memory footprint, because it does not use Plis at all. HyFD uses the same data structures as Tane and Fdep and some additional data structures, such as the comparison suggestions, but it still has the overall smallest memory consumption: In contrast to Tane, HyFD generates much fewer candidates and requires only the single-column Plis for its direct validation technique; in contrast to Fdep, it stores the non-FDs in bitsets rather than index lists and uses the Plis instead of the original data for the record comparisons.

Efficiency threshold. HyFD requires a parameter that determines when Phase 1 or Phase 2 become inefficient: It stops the record matching in the Sampler component if less than x percent matches delivered new FD-violations and it stops the FD-candidate validations in the Validator component if more than x percent candidates have shown to be invalid. In the explanation of the algorithm and in all previous experiments, we set this parameter to 1% regardless of the datasets being analyzed. The following experiment evaluates different parameter settings on the *ncvoter_statewide* dataset with ten thousand records. Note that this experiment produced similar results on different datasets, which is why we only show the results for one dataset here.

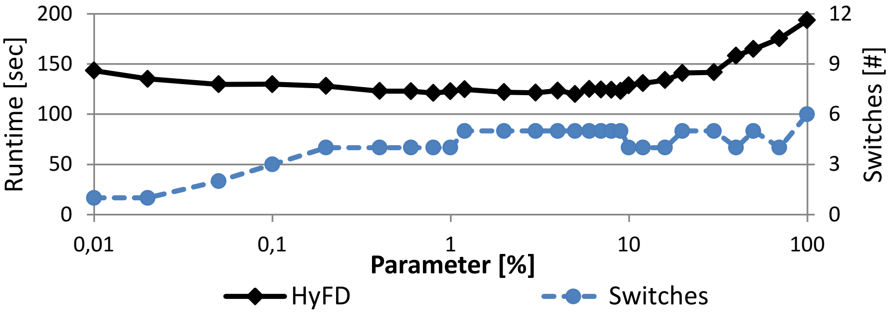


Figure 3.8: Effect of HyFD's only parameter on 10 thousand records of the *ncvoter_statewide* dataset.

The first line in Figure 3.8 plots HyFD's runtime for parameter values between 0.01% and 100%. It shows that HyFD's performance is not very sensitive to the efficiency threshold parameter. In fact, the performance is almost the same for any value between 0.1% and 10%. This is because the efficiency of either phase falls suddenly and fast so that all low efficiency values are met quickly: The progressive sampling identifies most matches very early and the validation generates many new, largely also invalid FD-candidates for every candidate tested as invalid.

However, if we set the parameter higher than 10%, then HyFD starts validating some lattice levels with too many invalid FD-candidates, which affects the performance negatively; if we, on the other hand, set the value lower than 0.1%, HyFD invests too much time on sampling than actually needed, which means that it keeps matching records although all results have already been found. Because the efficiency threshold has also shown a stable performance between 0.1% and 10% for other datasets, we propose 1% as a default value for HyFD.

The second line in Table 3.8 depicts the number of switches from Phase 2 back into Phase 1 that HyFD made with the different parameter settings. We observe that four to five phase-switches are necessary on *ncvoter_statewide* and doing fewer or more switches is disadvantageous for the performance. Note that HyFD did these switches on different lattice-levels depending on the parameter setting, i.e., with low thresholds it switches earlier; with high thresholds later.

Comparison suggestions. The strongest and most obvious advantage of HyFD over related work is that the sampling in Phase 1 effectively prunes many FD-candidates with low effort, which significantly reduces the number of validations in Phase 2. In turn, Phase 2 reports comparison suggestions to Phase 1 as hints for missing FD-violations. To investigate the effect of these comparison suggestions, we also measured the runtime of HyFD with and without comparison suggestions. Note that we do not use parallelization in this experiment. The results are shown in Table 3.4.

In the comparison suggestion experiment, we measured three variables: The *performance* impact of the comparison suggestions, which is the runtime difference of using and not using comparison suggestions; the sum of all *window* runs over all attributes; and the number of *switches* from Phase 2 back into Phase 1. The results in Table 3.4 show

Dataset	Performance	Windows	Switches
bridges	0.00%	90 ↘ 90	0 ↘ 0
plista	9.09%	2263 ↘ 1725	3 ↘ 1
TPC-H.lineitem	10.06%	89 ↘ 52	7 ↘ 6
PDB.POLY_SEQ	24.52%	33 ↘ 21	6 ↘ 3
SAP_R3.ZBC00DT	38.11%	111 ↘ 50	7 ↘ 4
NCVoter.statewide (100k rows)	80.89%	15120 ↘ 13025	20 ↘ 9

Table 3.4: Performance gains of the comparison suggestions.

that the comparison suggestions effectively improve the focus of the comparisons, which reduces the runtime of HyFD by up to 80% (in this experiment). This performance gain has two causes: First, the decrease in window runs tells us that with the comparison suggestions fewer tuple comparisons are necessary in Phase 1. Second, the decrease in phase switches shows that, due to the comparison suggestions, many more false candidates, which otherwise cause these phase switches, can be pruned and, therefore, fewer validations are needed in Phase 2. The results on the *bridges* dataset also show that the comparison suggestions only then have a performance impact if at least one switch from Phase 2 back into Phase 1 occurs. Very short datasets with less than a few hundred rows often cause no back-switches, because the number of row pairs is so small that the initial window runs already cover most of the comparisons; hence, they already produce very good approximations of the real FDs. For datasets larger than few hundred rows, we can, however, expect performance improvements of 9% and more, which is shown by the *plista* dataset. So the comparison suggestions are an important factor in HyFD's performance especially on longer datasets.

3.9.6 Result analysis

The number of FDs that HyFD can discover is very large. In fact, the size of the discovered metadata can easily exceed the size of the original dataset (see the *uniprot* dataset in Section 3.9.4). A reasonable question is, hence, whether complete results, i.e., *all* minimal FDs, are actually needed. Schema normalization, for instance, requires only a small subset of FDs to transform a current schema into a new schema with smaller memory footprint. Data integration also requires only a subset of all FDs, namely those that overlap with a second schema. In short, most use-cases for FDs indeed require only a subset of all results.

However, one must inspect all functional dependencies to identify these subsets: Schema normalization, for instance, is based on closure calculation and data integration is based on dependency mapping, both requiring complete FD result sets to find the optimal solutions. Furthermore, in query optimization, a subset of FDs that optimizes a given query workload by 10% is very good at first sight, but if a different subset of FDs could have saved 20% of the query load, one would have missed optimization potential. For these reasons and because we cannot know which other use cases HyFD will have to serve, we discover all functional dependencies – or at least as many as possible.

3.10 Conclusion & Future Work

In this chapter, we proposed HyFD, a hybrid FD discovery algorithm that discovers all minimal, non-trivial functional dependencies in relational datasets. Because HyFD combines row- and column-efficient discovery techniques, it is able to process datasets that are both long and wide. This makes HyFD the first algorithm that can process datasets of relevant real-world size, i.e., datasets with more than 50 attributes and a million records. On smaller datasets, which some other FD discovery algorithms can already process, HyFD offers the smallest memory footprints and the fastest runtimes; in many cases, our algorithm is orders of magnitude faster than the best state-of-the-art algorithm. Because the number of FDs can grow exponentially with the number of attributes, we also proposed a component that dynamically prunes the result set, if the available memory is exhausted.

The two-phased search technique of HyFD has also inspired the development of other algorithms in the area of dependency discovery. Our algorithm Aid-FD [Bleifuß et al., 2016], for example, uses the same combination of sampling and validation phases to discover *approximate FDs*, i.e., we sacrifice the guarantee for a correct result in return for further performance improvements. Other sister algorithms of HyFD are MvdDetector [Draeger, 2016], an algorithm for the discovery of *multivalued dependencies*, and Hydra [Bleifuß, 2016], an algorithm for the discovery of *denial constraints*. In the next chapter, we also present HyUCC, a sister algorithm of HyFD that discovers all unique column combinations in relational datasets.

A task for future work in FD discovery is the development of use-case-specific algorithms that leverage FD result sets for query optimization, data integration, data cleansing, and many other tasks. In addition, knowledge of the use-case might help develop specific semantic pruning rules to further speed-up detection. The only general semantic pruning we found was removing FDs with largest left-hand-sides, because these are most prone to being accidental, and we only apply it when absolutely necessary.

4

Unique Column Combination Discovery

Given a relational datasets, the *discovery of unique column combinations* is a task that aims to automatically detect *all* unique column combinations, i.e., attribute sets whose projection has no duplicate entries. To achieve this, it suffices to find all *minimal* UCCs, because we can infer all other UCCs with Armstrong's augmentation rule (see Section 2.2.2). Furthermore, most use cases, such as database key discovery [Mancas, 2016], are interested in only the minimal UCCs. The need for unique column combinations in many applications has led to the development of various discovery algorithms, such as GORDIAN [Sismanis et al., 2006], HCA [Abedjan and Naumann, 2011], and DUCC [Heise et al., 2013]. All these approaches experience serious difficulties when datasets of typical real-world size, i.e., datasets with more than 50 attributes and a million records, need to be processed. Similar to the task of FD discovery, this is because most of these algorithms focus on only one discovery strategy that either performs well for many columns or many rows in a dataset.

In this chapter, we present the hybrid discovery algorithm HYUCC that automatically detects *all minimal unique column combinations* in relational datasets. This algorithm and most parts of this chapter have been published in [Papenbrock and Naumann, 2017a]. HYUCC uses the same combination of row- and column-efficient techniques as its sister algorithm HYFD, which we introduced in Chapter 3: The interplay of fast candidate approximation and efficient candidate validation allows HYUCC to process datasets that are both wide and long. The hybrid search not only outperforms all existing approaches, it also scales to much larger datasets. In fact, with HYUCC the discovery time becomes less of an issue than the ability of the executing machine to cope with the size of the UCC result set, which can grow exponentially large. The main contributions of HYUCC can thus be summarized as follows:

The two algorithms HYFD and HYUCC are, in fact, very similar, which means that only few changes are necessary to let HYUCC discover UCCs instead of FDs. These changes are, in a nutshell: the use of a prefix tree for UCCs, a cover inversion algorithm for UCCs, a candidate validation function for UCCs, and pruning rules for UCCs. As these changes are relatively straightforward, the main contribution of HYUCC and its evaluation is a proof of concept that the hybrid discovery strategies, which we originally developed for FD discovery, work as well for other discovery problems in data profiling.

The remainder of chapter is structured as follows: Section 4.1first discusses related work. Then, we introduce the intuition of our hybrid approach for UCCs in Section 4.2. Section 4.3 shows how these ideas can be algorithmically implemented and emphasizes the differences between HyUCC and HyFD. In Section 4.4, we evaluate our algorithm and conclude in Section 4.5.

4.1 Related Work

There are basically two classes of UCC discovery algorithms: row-based discovery algorithms, such as Gordian [Sismanis et al., 2006], and column-based algorithms, such as Hca [Abedjan and Naumann, 2011]. Row-based algorithms compare pairs of records in the dataset, derive so-called agree or disagree sets, and finally derive the UCCs from these sets. This discovery strategy performs well with increasing numbers of attributes, but falls short when the number of rows is high. Column-based algorithms model the search space as a powerset lattice and then traverse this lattice to identify the UCCs. The traversal strategies usually differ, but all algorithms of this kind make extensive use of pruning rules, i.e., they remove subsets of falsified candidates from the search space (these must be false as well) and supersets of validated candidates (which must be valid and not minimal). The column-based family of discovery algorithms scales well with larger numbers of records, but large numbers of attributes render them infeasible. Because both row- and column-efficient algorithms have their strengths, we combine these two search strategies in our HyUCC algorithm.

A previous, efficient UCC discovery algorithm, which also belongs to the column-based algorithm family, is Ducc [Heise et al., 2013]. The algorithm pursues a random walk approach in the search space lattice to maximize the effect of the known superset- und subset-pruning rules. Because this algorithm was shown to be faster than both Gordian and Hca, it serves as a baseline for our evaluation.

4.2 Hybrid UCC discovery

The core idea of hybrid UCC discovery is to combine techniques from column-based and row-based discovery algorithms into one algorithm that automatically switches back and forth between these techniques, depending on which technique currently performs better. The challenge for these switches is to decide when to switch and to convert the intermediate results from one model into the other, which is necessary to let the strategies support each other. In the following, we first describe the two discovery strategies for UCCs; then, we discuss when and how intermediate results can be synchronized.

Row-efficient strategy. Column-based UCC discovery algorithms, which are the family of algorithms that perform well on many rows, model the search space as a powerset lattice of attribute combinations where each node represents a UCC candidate. The

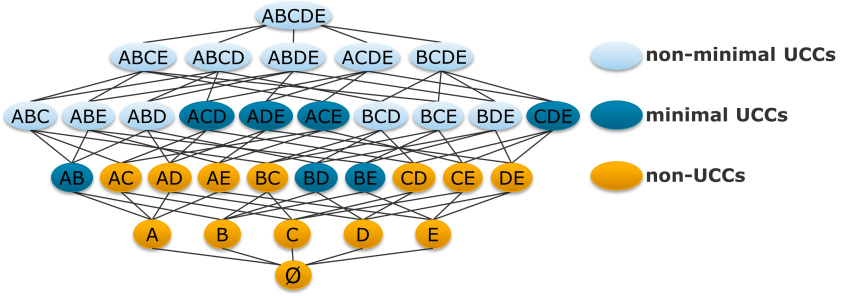


Figure 4.1: UCC discovery in a powerset lattice.

search strategy is then a classification problem of labelling each node as non-UCC, minimal UCC, or non-minimal UCC. Figure 4.1 depicts an example lattice for five attributes A, B, C, D, and E with labeled nodes.

For our hybrid algorithm, we propose a simple bottom-up traversal strategy: First, we test all candidates of size one, then of size two and so on. The lattice is generated level-wise using the *apriori-gen* algorithm [Agrawal and Srikant, 1994]. Minimality pruning assures that no implicitly valid UCCs, i.e., non-minimal UCCs are ever generated [Heise et al., 2013]. All discovered minimal UCCs must be stored as the algorithm's result.

An important characteristic of this discovery strategy is that, during the discovery, all intermediate results are correct but the set of results is still incomplete, that is, each discovered UCCs must be valid but not all UCCs have been discovered. Because correctness is guaranteed, we will always end the hybrid algorithm in a phase with this discovery strategy. Another characteristic of the bottom-up lattice traversal is that it might have to wade through many non-UCCs until it reaches the true UCCs, because these are all placed along the virtual border between non-UCCs (below in the lattice) and true UCCs (above in the lattice). The fact that the number of these non-UCCs increases exponentially with the number of columns hinders algorithms of this family to scale well with increasing numbers of attributes – the lattice becomes extremely "wide". Hence, we need to utilize an alternative discovery strategy that skips most of the non-UCC nodes to reach the true UCCs faster.

Column-efficient strategy. Row-based / column-efficient UCC discovery strategies compare all records pair-wise and derive so-called agree sets from these comparisons. An agree set is a negative observation, i.e., a set of attributes that have same values in the two compared records and can, therefore, not be a UCC; so agree sets directly correspond to non-UCCs in the attribute lattice. When all (or some) agree sets have been collected, we can use the techniques proposed in [Flach and Savnik, 1999] with small changes to turn them into true UCCs.

A major weakness of this discovery strategy is that comparing all records pair-wise is usually infeasible. So we propose to stop the comparison of records at some time during the discovery; we basically compare only a sample r' of all r record pairs. When turning whatever agree sets we found so far into UCCs, these UCCs are most likely not all correct, because the sampling might have missed some important agree sets. However, the intermediate result has three important properties (see Chapter 3 for proofs):

1. *Completeness:* Because all supersets of UCCs in the result are also assumed to be correct UCCs, the set of r'-UCCs is complete: It implies the entire set of r-UCCs, i.e., we find at least one X' in the r'-UCCs for each valid X in r-UCCs with $X' \subseteq X$.

2. *Minimality:* If a minimal r'-UCC is truly valid, then the UCC must also be minimal with respect to the real result. For this reason, the early stopping cannot lead to non-minimal or incomplete results.

3. *Proximity:* If a minimal r'-UCC is in fact invalid for the entire r, then the r'-UCC is still expected to be *close* to one or more specializations that are valid. In other words, most r'-UCCs need fewer specializations to reach the true r-UCCs on the virtual border than the unary UCCs at the bottom of the lattice so that the early stopping approximates the real UCCs.

Hybrid strategy. Although the row- and column-efficient search strategies for UCCs differ slightly from their FD counterparts, the hybrid combination of these strategies is exactly the same: We again refer to the column-efficient search as the *sampling phase*, because it inspects carefully chosen subsets of record pairs for agree sets, and to the row-efficient search as the *validation phase*, because it directly validates individual UCC candidates. Intuitively, the hybrid discovery uses the sampling phase to jump over possibly many non-UCCs and the validation phase to produce a valid result. We start with the sampling phase, then switch back and forth between phases, and finally end with the validation phase. The questions that remain are *when* and *how* to switch between the phases.

The best moment to leave the sampling phase is when most of the non-UCCs have been identified and finding more non-UCCs becomes more expensive than simply directly checking their candidates. Of course, this moment is known neither a-priori nor during the process, because one would need to already know the result to calculate the moment. For this reason, we switch optimistically back and forth whenever a phase becomes *inefficient*: The sampling becomes inefficient, when the number of newly discovered agree sets per comparison falls below a certain threshold; the validation becomes inefficient, when the number of valid UCCs per non-UCC falls below a certain threshold. With every switch, we relax this threshold a bit, so that the phases are considered efficient again. In this way, the hybrid discovery always progressively pursues the currently most efficient strategy.

To exchange intermediate results between phases, the hybrid algorithm must maintain all currently valid UCCs in a central data structure (we later propose a prefix-tree). When switching from sampling to validation, all agree sets must be applied to this central data structure, refining all UCCs in it for which a negative observation, i.e., an agree set exists. The validation phase, then, directly operates on this data structure so that many non-UCCs are already excluded from the validation procedure. When switching from the validation to the sampling, the algorithm must not explicitly update the central data structure, because the validation already performs all changes directly to it. However, the validation automatically identifies record pairs that violated certain UCC candidates, and these record pairs should be suggested to the sampling phase for full comparisons as it is very likely that they indicate larger agree sets. In this way, both phases can benefit from one another, as we already showed for FDs in Section 3.9.5.

4.3 The HyUCC algorithm

We now describe our implementation of the hybrid UCC discovery strategy HyUCC. Because this algorithm is largely equal to the FD discovery algorithm HyFD, we omit various details that can be found in Chapter 3. The differences that make HyUCC discover unique column combinations instead of functional dependencies are in particular a prefix tree (trie) to store the UCCs, a cover inversion algorithm for UCCs, a UCC-specific validation, and UCC-specific pruning rules.

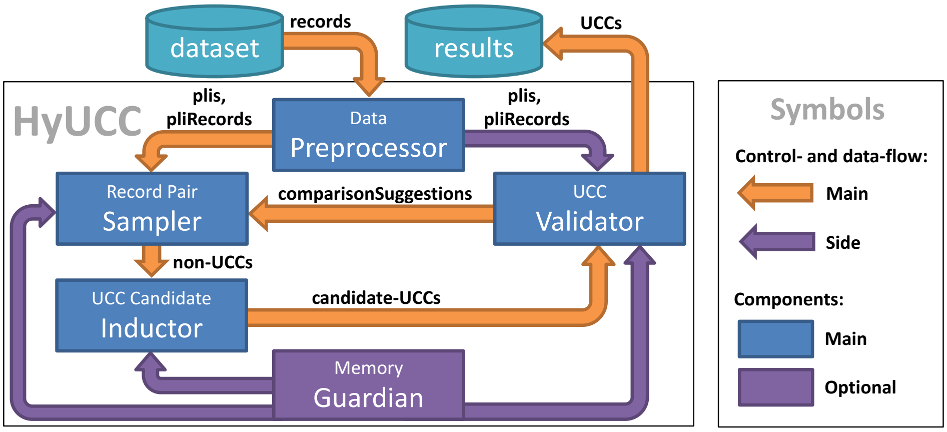


Figure 4.2: Overview of HyUCC and its components.

Figure 4.2 gives an overview of HyUCC and its components. Given a relational dataset as a collection of records, the algorithm first runs them through a `Preprocessor` component that transforms the records into the two smaller index structures Plis and PliRecords. Then, HyUCC starts the sampling phase in the `Sampler` component. When the sampling has become inefficient, the algorithm passes the discovered agree sets, i.e., the non-UCCs, to the `Inductor` component, which turns them into candidate-UCCs: UCCs that hold true on the sample of record pairs that was seen so far. Afterwards, the algorithm switches to the validation phase in the `Validator` component. This component systematically (level-wise, bottom-up) checks and creates candidate-UCCs. If the checking becomes inefficient, HyUCC switches back into the sampling phase handing over a set of comparison suggestions; otherwise, the validation continues until all candidates have been checked and all true UCCs can be returned. We now discuss the components of HyUCC in more detail.

Data Preprocessor. The `Preprocessor` in HyUCC is the same as the `Preprocessor` HyFD: It transforms all records into compact *position list indexes* (Plis) and dictionary compressed PliRecords. These two data structures are needed for the record comparisons in the `Sampler` component and the UCC candidate validations in the `Validator` component.

Record Pair Sampler. The `Sampler` component compares the PliRecords to derive agree sets, i.e., non-UCCs. As stated earlier, a non-UCC is simply a set of attributes that have same values in at least two records. Because the sampling phase should be maximally efficient, the `Sampler` chooses the record pairs for the comparisons deliberately: Record pairs that are more likely to reveal non-UCCs are progressively chosen earlier in the process and less promising record pairs later. Intuitively, the more values two records share, the higher their probability of delivering a new non-UCC is. Vice versa, records that do not share any values cannot deliver any non-UCC and should not be compared at all.

To focus the comparisons on those record pairs that share possibly many values, we use these same progressive strategy as in the HyFD algorithm: Because the Plis group records with at least one identical value, HyUCC compares only records within same Pli clusters. For all records within same Pli clusters, we must define a possibly effective comparison order. For this purpose, we again first sort all clusters in all Plis with a different sorting key (see Section 3.5). This produces different neighborhoods for each record in each of the record's clusters, even if the record co-occurs with same other records in its clusters. After sorting, the `Sampler` iterates all Plis and compares each record to its direct neighbor. In this step, the algorithm also calculates the *number of discovered non-UCCs per comparison* for each Pli. This number indicates the sampling efficiency achieved with this particular Pli. In a third step, the `Sampler` can then rank the different Plis by their efficiency, pick the most efficient Pli, and use it to compare each record to its second neighbor. This comparison run updates the efficiency of the used Pli, so that it is re-ranked with the other. The `Sampler` then again picks the most efficient Pli for the next round of comparisons. This process of comparing records to their $n+1$ next neighbors progressively chooses most promising comparisons; it continues until the top ranked Pli is not efficient any more, which is the condition to switch to the validation phase.

UCC Candidate Inductor. The `Inductor` component updates the intermediate result of UCCs with the non-UCCs from the `Sampler` component. We store these UCCs in a prefix tree, i.e., a trie, where each node represents exactly one attribute and each path a UCC. Such a *UCC tree* allows for fast subset-lookups, which is the most frequent operation on the intermediate results of UCCs. The UCC tree in HyUCC is much leaner than the FD tree used in HyFD, because no additional right-hand-sides must be stored in the nodes; the paths alone suffice to identify the UCCs.

Initially, the UCC tree contains all individual attributes, assuming that each of them is unique. The `Inductor` then refines this initial UCC tree with every non-UCC that it receives from the `Sampler`: For every non-UCC, remove the UCC and all of its subsets from the UCC tree, because these must all be non-unique. Then, create all possible specializations of each removed non-UCC by adding one additional attribute; these could still be true UCCs. For each specialization, check the UCC tree for existing subsets (generalizations) or supersets (specialization). If a generalization exists, the created UCC is not minimal; if a specialization exists, it is invalid. In both cases, we ignore the generated UCC; otherwise, we add it to the UCC tree as a new candidate.

UCC Validator. The `Validator` component traverses the UCC tree level-wise from bottom to top. This traversal is implemented as a simple breadth-first search. Each leaf-node represents a UCC candidate X that the algorithm validates. If the validation returns a positive result, the `Validator` keeps the UCC in the lattice; otherwise, it removes the non-UCC X and adds all XA to the tree with $A \notin X$ and XA is both minimal (XA has no specialization in the UCC tree) and valid (XA has no generalization in the UCC tree). After validating an entire level of UCC candidates, the `Validator` calculates the number of valid UCCs per validation. If this efficiency value does not meet a current threshold, HyUCC switches back into the sampling phase; the `Validator`, then, continues with the next level when it gets the control flow back.

To validate a column combination X, the `Validator` intersects the PLIs of all columns in X. Intersecting a PLI with one or more other PLIs means to intersect all the record clusters that they contain. The result is again a PLI. If this PLI contains no clusters of size greater than one, its column combination X is unique; otherwise, X is non-unique and the records in the clusters greater than one violate it. The algorithm suggests these records to the `Sampler` as interesting comparison candidates, because they have not yet been compared and may reveal additional non-UCCs of greater size.

For the validation of a UCC candidate via PLI intersection, it suffices to find one cluster of size greater than one; if no such cluster exists, the candidate is valid. An efficient way to find this cluster is a validation algorithm that works similar to the validation algorithm of FDs introduced in Section 3.7: The input is a UCC candidate X, the PLIs *plis* and the PLI compressed records *pliRecords* – the latter two structures are given by the `Preprocessor`. The task, which we visualized in Figure 4.3, is to intersect all PLIs of attributes $X_i \in X$ until the first cluster reaches size two. We start the intersection by selecting the PLI with the fewest records as the *pivot* PLI (recall that PLIs do not contain clusters of size one so that the numbers of records in the PLIs usually

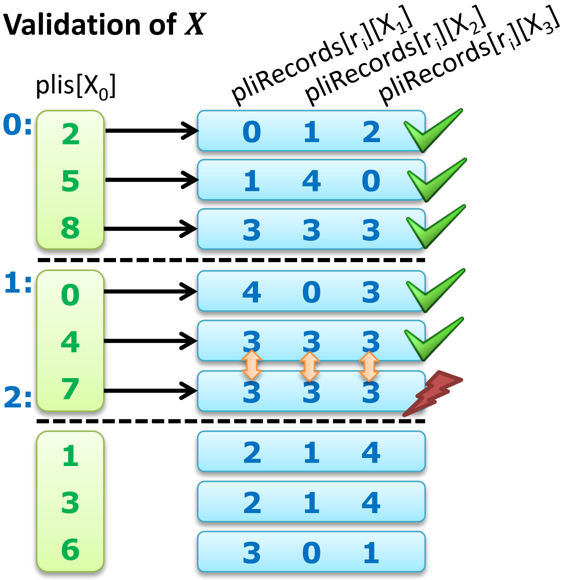


Figure 4.3: Directly validating a UCC candidate X.

differ). This pivot PLI requires the least number of intersection look-ups with the other PLIS to become unique. For each cluster in the pivot PLI, the validation algorithm now does the following: It iterates all record IDs and, for each record ID, looks-up the cluster numbers of all other attributes of X in the *pliRecords*; then, it stores each retrieved list of cluster numbers in a set – each element represents a cluster of the intersection result and contains, if the candidate is a unique, only one record. If this set already contains a cluster number sequence equal to the sequence the `Validator` wants to insert, then the algorithm found a violation and can stop the validation process for this candidate. In Figure 4.3, this happens in the second cluster. The current record and the record referring to the cluster number sequence in the set are, in the end, sent to the `Sampler` as a new comparison suggestion.

Memory Guardian. The `Guardian` is an optional component that monitors the memory consumption of HYUCC. If at any point the memory threatens to become exhausted, this component gradually reduces the maximum size of UCCs in the result until sufficient memory becomes available. Of course, the result is then not complete any more, but correctness and minimality of all reported UCCs is still guaranteed. Also, the result limitation only happens if the *result* becomes so large that the executing machine cannot store it any more; other algorithms would break in such cases. To reduce the size, the `Guardian` deletes all agree sets and UCC candidates that exceed a certain maximum size. It then forbids further insertions of any new elements of this or greater size.

4.4 Evaluation

We evaluate HYUCC and compare it to its sister algorithm HYFD [Papenbrock and Naumann, 2016] and to the state-of-the-art UCC discovery algorithm DUCC [Heise et al., 2013]. All three algorithms have been implemented for our METANOME data profiling framework (`www.metanome.de`) in order to use the framework's standard functionality for data I/O and result management. Our experiments use a Dell PowerEdge R620 with two Intel Xeon E5-2650 2.00 GHz CPUs and 128 GB RAM. The server runs on CentOS 6.4 and uses OpenJDK 64-Bit Server VM 1.7.0_25 as Java environment. Details about our experimental datasets can be found in Section 3.9 and on our repeatability website[1]. Note that the experiments use the `null` = `null` semantics, because this was also used in related work; HYUCC can compute UCCs with `null` ≠ `null` as well, which makes the search faster, because columns with `null` values become unique more quickly.

4.4.1 Varying the datasets

In this first experiment, we measure the discovery times for the three algorithms on eight real-world datasets. The datasets, their characteristics, and the runtimes are listed in Table 4.1. The results show that HYUCC clearly outperforms the current state-of-the-art algorithm DUCC: On most datasets, HYUCC is about 4 times faster than DUCC; on the *flight* dataset, it is even more than 1,000 times faster. Only on *zbc00dt* DUCC

[1] `www.hpi.de/naumann/projects/repeatability.html`

Dataset	Cols [#]	Rows [#]	Size [MB]	FDs [#]	UCCs [#]	DUCC	HyFD	HyUCC	HyFD parallel	HyUCC parallel
ncvoter	19	8 m	1,263.5	822	96	706.1	1,009.6	220.1	239.8	157.9
hepatitis	20	155	0.1	8,250	348	0.6	0.4	0.1	0.4	0.1
horse	27	368	0.1	128,727	253	0.8	5.8	0.2	3.7	0.2
zbc00dt	35	3 m	783.0	211	1	57.7	191.1	58.2	69.4	58.2
ncvoter_c	71	100 k	55.7	208,470	1,980	170.3	2,561.6	51.3	533.4	14.9
ncvoter_s	71	7 m	4,167.6	>5 m	32,385	>8 h	>8 h	>8 h	>8 h	1.6 h
flight	109	1 k	0.6	982,631	26,652	4,212.5	54.1	3.7	19.5	1.5
uniprot	120	1 k	2.1	>10 m	1,973,734	>8 h	>1 h	92.5	>1 h	76.7
isolet	200	6 k	12.9	244 m	1,241,149	>8 h	1,653.7	410.9	482.3	45.1

Table 4.1: Runtimes in seconds for several real-world datasets

is slightly faster, because only one UCC was to be discovered and Ducc does not precompute PliRecords or inverted Plis as HyUCC does. Furthermore, the runtimes of HyFD show that UCC discovery is considerably faster than FD discovery. This is due to the smaller result sets, because HyFD and HyUCC use similar discovery techniques.

Because we can easily parallelize the validations in HyUCC and HyFD, the experiment also lists the runtimes for their parallel versions. Because our evaluation server has 32 cores, the parallel algorithms use the same number of threads. On the given datasets, HyUCC could in this way achieve 1.2 (*uniprot*) to more than 9 (*isolet*) times faster runtimes than its single-threaded version (less than 32, because only the validations run in parallel); on *ncvoter_s*, the parallel version of HyUCC was the only algorithm that was able to produce a result within 8 hours.

4.4.2 Varying columns and rows

We now evaluate the scalability of HyUCC with the input dataset's number of rows and columns. The row-scalability is evaluated on the *ncvoter_s* dataset with 71 columns and the column-scalability on the *isolet* dataset with 6238 rows. Figure 4.4 shows the results of these experiments for Ducc and HyUCC. The results also include the runtimes for the parallel version of HyUCC; the dotted line indicates the number of UCCs for each measurement point.

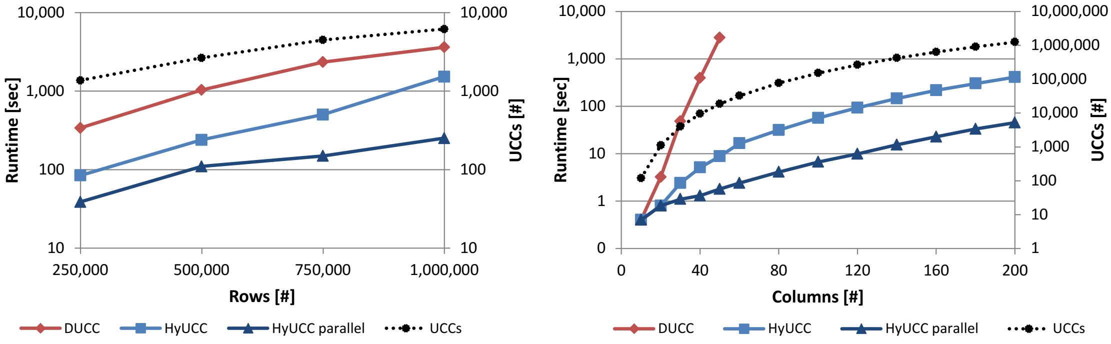


Figure 4.4: Row scalability on *ncvoter_s* (71 columns) and column scalability on *isolet* (6238 rows).

The graphs show that the runtimes of both algorithms scale with the number of UCCs in the result, which is a desirable discovery behavior. However, HyUCC still outperforms Ducc in both dimensions – even in the row-dimension that Ducc is optimized for: It is about 4 times faster in the row-scalability experiment and 4 to more than 310 times faster in the column-scalability experiment (because Ducc exceeded our time limit of eight hours in the latter experiment, we cannot report the improvements after 50 attributes). HyUCC's advantage in the column-dimension is clearly the fact that the non-UCCs derived from the sampling phase allow the algorithm to skip most of the lower-level UCC candidates (and the number of these candidates increases exponentially with the number of columns); the advantage in the row-dimension is also this sampling phase of HyUCC, allowing it to skip many candidates and, because the number of UCCs also increases when increasing the number of rows, this gives HyUCC a significant advantage.

4.5 Conclusion & Future Work

In this chapter, we proposed HyUCC, a hybrid UCC discovery algorithm that combines row- and column-efficient techniques to process relational datasets with both many records and many attributes. On most real-world datasets, HyUCC outperforms all existing UCC discovery algorithms by orders of magnitude.

HyUCC and its sister algorithms HyFD [Papenbrock and Naumann, 2016] for FDs, MvdDetector [Draeger, 2016] for MvDs, and Hydra [Bleifuß, 2016] for DCs show that the hybrid search strategy serves the discovery of different types of metadata. We also investigated the changes necessary to discover order dependencies (ODs) using the hybrid search strategy and are confident that an actual implementation would work, too. The strength of the hybrid search is to quickly narrow the search space – a particular advantage for dependencies that tend to occur on higher lattice levels. Some dependencies, such as inclusion dependencies, that largely occur on the lowest lattice levels cannot benefit from this strength much. For this reason, we propose different search and evaluation strategies for IND discovery in Chapter 5.

For future work, we suggest to find novel techniques to deal with the often huge amount of results. Currently, HyUCC limits its results if these exceed main memory capacity, but one might consider using disk or flash memory in addition for these cases.

5

Inclusion Dependency Discovery

The *discovery of all inclusion dependencies* in a relational dataset is an important part of any data profiling effort. Apart from the detection of foreign key relationships, INDs support data integration, query optimization, integrity checking, schema (re-)design, and many further use cases. We have shown in Section 2.4 that the discovery of inclusion dependencies is one of the hardest tasks in data profiling: Appart from the complexity of the search problem, aggravating circumstances are the relatively high costs for candidate checks, which require the actual values and not only positions of same values, and the limited effect of candidate pruning, i.e., subset-pruning, because most INDs reside on the lowest lattice levels. Current state-of-the-art IND discovery algorithms propose several, quite efficient discovery techniques based on inverted indexes or specialized sort-merge joins to cope with these issues. Still, each of these algorithms has certain shortcomings when the dataset volumes increase and most them solve the IND discovery problem only for either unary or higher level n-ary INDs.

To this end, this chapter presents Binder, an IND detection algorithm that is capable of detecting both unary and n-ary INDs. The algorithm and most parts of this chapter were published in [Papenbrock et al., 2015d]. Binder utilizes divide & conquer techniques to split the data and with it the overall discovery problem into smaller chunks allowing it to scale with the size of the input data. In contrast to most related works, Binder does not rely on existing database functionality nor does it assume that inspected datasets fit into main memory. With its own method for candidate validation, Binder outperforms related algorithms in both unary (Spider [Bauckmann et al., 2006]) and n-ary (Mind [Marchi et al., 2009]) IND discovery contributing the following:

(1) *Divide & conquer-based IND discovery.* We propose an approach to efficiently divide datasets into smaller partitions that fit in main memory, lazily refining too large partitions. This lazy refinement strategy piggybacks on the actual IND validation process, saving many expensive I/O operations.

(2) *Dual-index-based validation.* We propose a fast IND validation strategy that is based on two different indexes ("inverted" and "dense") instead of on a single index or on sorting. Additionally, our IND validation strategy applies two new non-statistics-based pruning techniques to speed up the process.

(3) *Systematic candidate generation.* We present a robust IND candidate generation technique that allows BINDER to apply the same strategy to discover both all unary and all higher level n-ary INDs, i.e., with n > 1. This makes BINDER easy to maintain.

(4) *Comprehensive evaluation.* We present an exhaustive validation of BINDER on many real-world datasets as well as on two synthetic datasets. We experimentally compare it with two other state-of-the-art approaches: SPIDER [Bauckmann et al., 2006] and MIND [Marchi et al., 2009]. The results show the high superiority of BINDER. It is up to more than one order of magnitude (26 times) faster than SPIDER and up to more than three orders of magnitude (more than 2500 times) faster than MIND.

The rest of this chapter is structures as follows: We first introduce related work in Section 5.1. We give an overview of BINDER in Section 5.2 and then present the three major components of BINDER in detail: the `Bucketizer` (Section 5.3), the `Validator` (Section 5.4), and the `CandidateGenerator` (Section 5.5). We discuss our experimental results in Section 5.6 and finally conclude with Section 5.7.

5.1 Related Work

The discovery of inclusion dependencies is a task that has been shown to be not only NP-complete but also PSPACE-complete [Casanova et al., 1988]. The algorithms that aim to solve this task can be grouped into three classes: Unary IND discovery algorithms, which discover only unary INDs; n-ary IND discovery algorithms, which also solve the discovery task for INDs of size greater than one; and foreign key discovery algorithms, which discover INDs only between relations and often apply additional pruning for non-foreign-key-like INDs. Our algorithm BINDER solves the discovery task for unary and n-ary INDs; it can also easily be restricted to discover only inter-relation INDs. Note that our related work focuses on exact discovery algorithms, because any approximation significantly simplifies the problem and most use cases for INDs require exact results.

Unary IND discovery. Bell and Brockhausen introduced an algorithm [Bell and Brockhausen, 1995] that first derives all unary IND *candidates* from previously collected data statistics, such as data types and min-max values. It then validates these IND candidates using SQL `join`-statements. Once validated, IND candidates can be used to prune yet untested candidates. The SQL-based validations require the data to be stored in a database and each candidate validation must access the data on disk, which is very costly. For this reason, efficient discovery algorithms could adapt the statistics-based candidate generation, but the validation technique is infeasible for larger candidate sets.

De Marchi et al. proposed an algorithm [Marchi et al., 2009] that transforms the data into an inverted index pointing each value to the set of all attributes containing the value. One can then retrieve valid INDs from the attribute sets by intersecting them. Despite this efficient technique, the algorithm yields poor performance, because it applies the attribute set intersections for all values, without being able to discard attributes that have already been removed from all their IND candidates. Furthermore, building such an inverted index for large datasets that do not fit in main memory is very costly, because it involves many I/O operations. BINDER solves both of these issues.

Bauckmann et al. proposed Spider [Bauckmann et al., 2006], which is an adapted sort-merge-join approach. First, it individually sorts the values of each attribute, removes duplicate values, and writes these sorted lists to disk. Then it applies an adapted (for early termination) sort-merge join approach to validate IND candidates. Spider also prunes those attributes from the validation process that have been removed from all their IND candidates. This technique makes Spider the most efficient algorithm for unary IND detection in related work. However, Spider still comes with a large sorting overhead that cannot be reduced by its attribute pruning. And if a column does not fit into main memory, external sorting is required. Furthermore, Spider's scalability in the number of attributes is technically limited by most operating systems, because they limit the number of simultaneously open file handles and Spider requires one per attribute.

Another algorithm for unary IND discovery is S-IndD [Shaabani and Meinel, 2015], which was developed at the same time as our algorithm Binder. The authors of the algorithm claim that S-IndD is a special case of Spider and the similarity is, in fact, so clear that we cannot reproduce the experiments that show S-IndD being superior to Spider: Both algorithms use, inter alia, sorting to build their intermediate data structures, early termination for the IND candidate validations, and value files on disk. No explanation is given for the performance improvement. However, S-IndD circumvents Spider's file-handle-issue by merging the value lists in multiple phases.

N-ary IND discovery. De Marchi et al. introduced the bottom-up level-wise algorithm Mind [Marchi et al., 2009] to detect n-ary INDs with n > 1. Mind first utilizes the algorithm of [Marchi et al., 2009] to detect unary INDs; then, it applies an apriori-gen-based approach [Agrawal and Srikant, 1994] for n-ary IND candidate generation and validates these candides using SQL-join-statements. Because Mind validates all candidates individually and using costly SQL-statements, Binder outperforms this algorithm in n-ary IND detection with a more efficient validation strategy based on data partitioning.

With Find2 [Koeller and Rundensteiner, 2002], Koeller and Rundensteiner proposed an efficient algorithm for the discovery of high-dimensional n-ary INDs. The algorithm models known INDs as hypergraphs, finds hypercliques in these hypergraphs and forms IND candidates from the discovered hypercliques. In this way, Find2 effectively generates candidates of high arity. The ZigZag algorithm [Marchi and Petit, 2003] by De Marchi and Petit also proposes a technique to identify large n-ary INDs: It combines a pessimistic bottom-up with an optimistic depth-first search. Both of these approaches, Find2 and ZigZag, again, test the IND candidates using costly SQL-statements, which does not scale well with the number of INDs. The Clim approach [Marchi, 2011] discusses an idea to avoid these single SQL checks by applying closed item set mining techniques on a new kind of index structure. The feasibility of such an algorithm has, however, not been shown. Another algorithm for the discovery of high-dimensional n-ary INDs is Mind2 [Shaabani and Meinel, 2016] by Shaabani and Meinel: First, Mind2 uses the S-IndD [Shaabani and Meinel, 2015] algorithm to detect all unary INDs; then, the algorithm calculates so called *IND coordinates* for the unary INDs, from which it can directly infer all maximal n-ary INDs – a technique that has shown to outperform the Find2 algorithm. The basic assumption of all these algorithms, i.e., Find2, ZigZag, Clim, and Mind2 is that most n-ary INDs are very large and, hence, occur on high lattice levels. If this is true for a particular dataset, their sophisticated, more complex search strategies are justified. In practice, however, we observe that most INDs in real-world datasets are in fact small making apriori-gen-based candidate generation the optimal search strategy.

In contrast to all state-of-the-art IND discovery algorithms, Binder is the only system that utilizes the same techniques for both unary and n-ary IND discovery: The data partitioning techniques ensure that the algorithm can handle increasing input sizes and the candidate validation methods ensure that the algorithm processes all candidates efficiently. In particular, using the same techniques for the entire discovery process makes Binder easier to implement and maintain than other approaches.

Foreign Key Discovery. The primary use case for INDs is the discovery of foreign keys. In general, this is an orthogonal task that uses IND discovery as a preprocessing step. For instance, Rostin et al. proposed rule-based discovery techniques based on machine learning to derive foreign keys from INDs [Rostin et al., 2009]. Zhang et al., in contrast, integrated the IND detection in the foreign key discovery by using approximation techniques [Zhang et al., 2010]. Their specialization on foreign key discovery makes their approach less useful to other IND use cases, such as query optimization [Gryz, 1998], integrity checking [Casanova et al., 1988], or schema matching [Levene and Vincent, 1999], which prefer complete and/or non-approximate results.

5.2 BINDER Overview

Binder, which is short for ***B**ucketing **IN**clusion **D**ependency **E**xtracto**R***, is an algorithm for the efficient discovery of *all exact* n-ary INDs in relational datasets. The algorithm uses the divide & conquer paradigm to discover INDs even in very large datasets. The main idea is to partition the input into smaller buckets that can be better mapped into main memory and, then, check these buckets successively for INDs. Intuitively, Binder implements an adapted distinct hash-join to test for INDs, whereas its main competitor, i.e., Spider implements an adapted sort-merge-join.

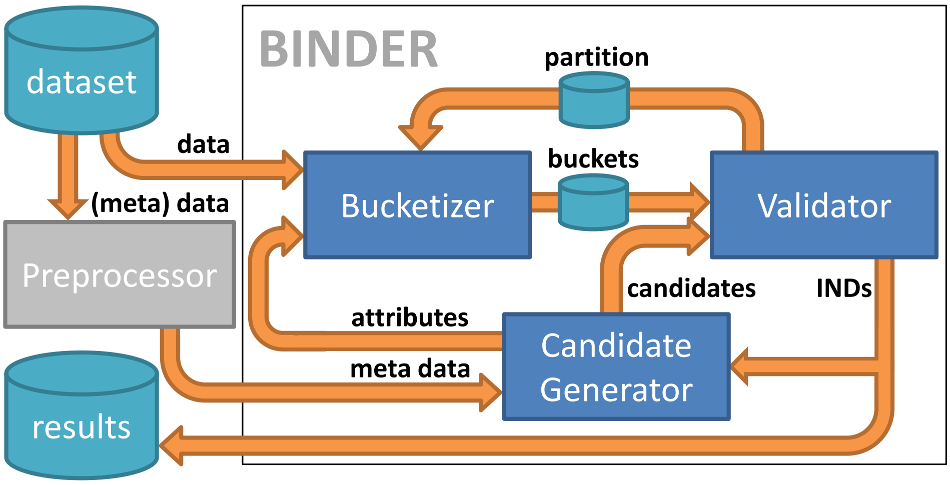
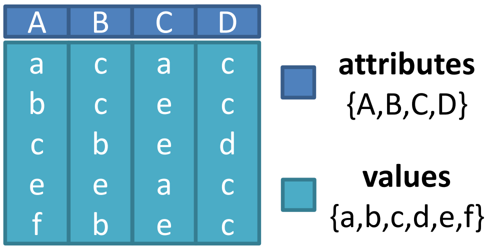


Figure 5.1: Overview of Binder and its components.

Figure 5.1 depicts the architecture of BINDER, which consists of three major components: `Bucketizer`, `Validator`, and `CandidateGenerator`. The additional `Preprocessor` is required by BINDER to find some structural properties needed for the IND discovery, such as table identifiers, attribute identifiers, and attribute types. Note that every IND detection system requires such a preprocessing phase for unknown datasets [Bauckmann et al., 2006; Bell and Brockhausen, 1995; Marchi et al., 2009]. Like all these works, BINDER uses standard techniques for the extraction of structural properties, i.e., the algorithm parses the properties from the headline of a CSV-file (file sources) or it reads the properties from metadata tables (database sources). It is also worth noting that, in terms of performance, the preprocessing step is negligible. Therefore, we do not consider it as a major component of BINDER. Below, we briefly discuss each of BINDER's three major components. For clarity, we use the dataset in Figure 5.2, which is an instance of a relational table with four attributes and a universe of six String values.

(1) `Bucketizer`. Given an input dataset, BINDER starts by splitting the datasets into several smaller parts (*buckets*) that allow for efficient IND discovery. A bucket is a (potentially deduplicated) subset of values from a certain single attribute. The `Bucketizer` splits a dataset using hash-partitioning on the attributes values. More precisely, it sequentially reads an input dataset and places each value into a specific bucket according to a given hash-function. The `Bucketizer` uses hash-partitioning instead of a range- or list-partitioning, because hash-partitioning satisfies two important criteria: It puts equal values into same buckets and, with a good hash-function, it distributes the values evenly across all buckets. At the end of this process, the partitioning writes the generated buckets to disk.



A	B	C	D
a	c	a	c
b	c	e	c
c	b	e	d
e	e	a	c
f	b	e	c

🟦 **attributes** {A,B,C,D}

🟦 **values** {a,b,c,d,e,f}

Figure 5.2: A relational table with example data.

Let us illustrate this process with our example dataset from Figure 5.2. Figure 5.3 shows an output produced by the `Bucketizer` for this dataset. Each box of attribute values represents one bucket. We denote a bucket using the tuple (a, n), where a is the attribute of the bucket and n is the bucket's hash-number. For instance, the bucket $(A, 2)$ is the second bucket of attribute A. Then, a *partition* is the collection of all buckets with the same hash-number, $p_i = \{(a, n) \mid n = i\}$. Each row in Figure 5.3 represents a different partition. Note that for the following validation process, an entire partition needs to fit in main memory. If this is not the case, BINDER re-calls the `Bucketizer` to dynamically refine a partition into smaller sub-partitions that each fit in main memory. Section 5.3 explains the `Bucketizer` in more detail.

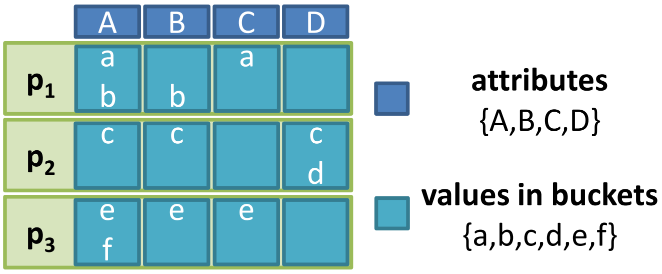


Figure 5.3: The example dataset bucketized into 12 buckets.

(2) `Validator`. Having divided the input dataset into a set of buckets, Binder starts to successively validate all possible unary IND candidates against this set. The `Validator` component, which is illustrated in Figure 5.4, is in charge of this validation process and proceeds partition-wise: First, it loads the current partition, i.e., all buckets with the same hash-number into main memory. If too few (and thus large) partitions have been created, so that a partition does not fit into main memory entirely, the `Validator` instructs the `Bucketizer` to refine that partition; then, the `Validator` continues with the sub-partitions.

Once a partition or sub-partition has been loaded, the `Validator` creates two indexes per partition: an inverted index and a dense index. The inverted index allows the efficient checking of candidates, whereas the dense index is used to prune irrelevant candidate checks for a current partition. When moving to the next partition, the `Validator` also prunes entire attributes as *inactive* if all their IND candidates have been falsified (gray buckets in Figure 5.4). In this way, subsequent partitions become smaller during the validation process, which can reduce the number of lazily executed partition refinements. The `Validator` returns all valid INDs, which are the candidates that "survived" all checks. In Figure 5.4, this is the IND $F \subseteq A$. We further discuss the `Validator` in Section 5.4.

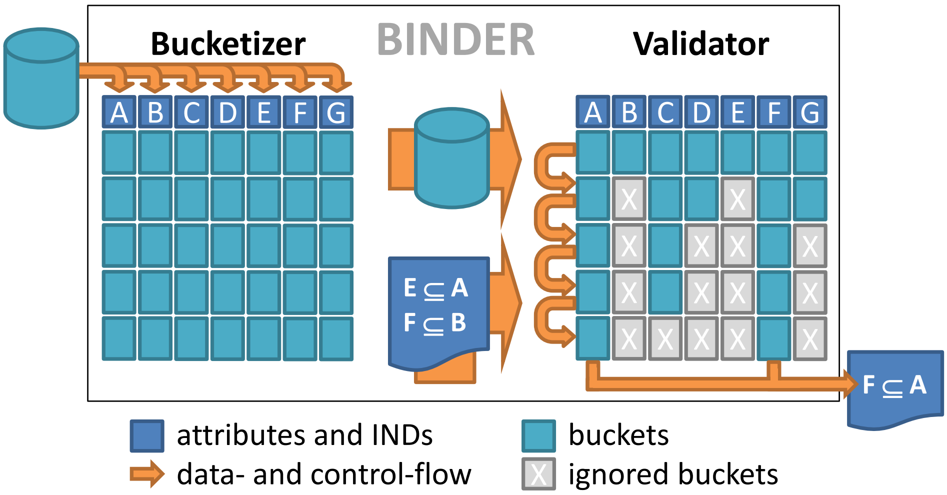


Figure 5.4: Illustration of the bucketing and validation processes.

(3) `CandidateGenerator`**.** This is the driver component that defines the set of IND candidates and calls the `Bucketizer` and `Validator` components. Initially, it generates all unary IND candidates from the dataset's metadata and sends them into the IND discovery process. If only unary INDs shall be detected, the component stops the detection process when it retrieves the valid unary INDs; otherwise, it uses them to generate and process all binary IND candidates, then ternary IND candidates, etc. The `CandidateGenerator` keeps generating and processing (n+1)-ary IND candidates from discovered n-ary INDs until no more candidates can be generated. We present the `CandidateGenerator` component in detail in Section 5.5.

5.3 Efficiently Dividing Datasets

As discussed in the previous section, Binder first uses the `Bucketizer` component to split the input dataset into a fixed number of partitions, which are ideally of equal size. Each partition contains one bucket per attribute. A bucket is an unordered collection of attribute values whose hashes lie within the same range.

Algorithm 5 shows the bucketing process in detail. The `Bucketizer` takes three input parameters: the *attributes* that should be bucketized, the *tables* that point to the actual data, and the *number of partitions* into which the dataset should be split. We show in Section 5.6.5 that Binder's performance is not sensitive to the parameter *nPartitions*, so we set it to 10 by default. We call the partitions *seed partitions*, because Binder might lazily refine them into smaller sub-partitions later on, in case they become too large to fit in main memory.

Overall, the bucketing process consists of three parts: (i) *value partitioning* (ll. 1-14), which reads the data and splits it into buckets, (ii) *dynamic memory handling* (ll. 15-21), which spills buckets to disk if main memory is exhausted, and (iii) *bucket management* (ll. 22-30), which writes the buckets to disk while piggybacking some additional statistics. We describe each of these parts in the following three subsections. In the fourth, we discuss the *lazy partition refinement* algorithm.

5.3.1 Value partitioning

The `Bucketizer` starts the partitioning by iterating the input dataset table-wise in order to keep possibly all buckets for one table in main memory at a time (l. 3). For each table, the `Bucketizer` reads the values in a tuple-wise manner (l. 6). It then fetches all those values from each tuple that belong to the attributes that it has to bucketize (ll. 7 & 8). For each non-`null` value, it calculates the partition number, *partitionNr*, via hash-partitioning (l. 11): The partition number for the current value is its hash-code modulo the number of partitions. Thus, same attribute values are placed into the same partitions, which preserves valid INDs across different partitions. By using a good, data-type specific hash function, the values are distributed evenly on the partitions. Then, if the current value is new, i.e., it does not yet exist in its bucket, the `Bucketizer` simply stores it (ll. 12 & 13). At the same time, the algorithm piggybacks a value counter for

Algorithm 5: Bucketing

```
   Data: attributes, tables, nPartitions
   Result: attrSizes, checkOrder
1  array attrSizes size | attributes | as Long;
2  array emptyBuckets size nPartitions as Integer;
3  foreach table $\in$ tables do
4      array buckets size | table.attr | $\times$ nPartitions as Bucket;
5      array nValsPerAttr size | table.attr | as Integer;
6      foreach tuple $\in$ read(table) do
7          foreach attr $\in$ table.attr do
8              if attr $\notin$ attributes then continue;
9              value $\leftarrow$ line[attr];
10             if value = null then continue;
11             partitionNr $\leftarrow$ hashCode(value) % nPartitions;
12             if value $\notin$ buckets[attr][partitionNr] then
13                 buckets[attr][partitionNr] $\leftarrow$ buckets[attr][partitionNr] $\cup$ value;
14                 nValsPerAttr[attr] $\leftarrow$ nValsPerAttr[attr] + 1;
15         if memoryExhausted() then
16             lAttr $\leftarrow$ max(nValsPerAttr);
17             foreach bucket $\in$ buckets[lAttr] do
18                 attrSizes[lAttr] $\leftarrow$ attrSizes[lAttr] + sizeOf(bucket);
19                 writeToDisk(bucket);
20                 bucket $\leftarrow \emptyset$;
21             nValsPerAttr[lAttr] $\leftarrow$ 0;
22     foreach attr $\in$ table.attr do
23         foreach bucket $\in$ buckets[attr] do
24             if bucket = $\emptyset$ then
25                 emptyBuckets[attr] $\leftarrow$ emptyBuckets[attr] + 1;
26             else
27                 attrSizes[attr] $\leftarrow$ attrSizes[attr] + sizeOf(bucket);
28                 writeToDisk(bucket);
29 checkOrder $\leftarrow$ orderBy(emptyBuckets);
30 return checkOrder, attrSizes;
```

each attribute, *nValsPerAttr*, that it increases with every new value (l. 14). *nValsPerAttr* is an array that Binder uses later, to decide which buckets should be spilled to disk if main memory is exhausted.

5.3.2 Dynamic memory handling

Every time the `Bucketizer` partitions a tuple, it checks the overall memory consumption. If the main memory is exhausted (e.g., if less than 10% of the memory is free), it spills the buckets with the largest number of attribute values, *nValsPerAttr*, to disk (ll. 15 & 21). Spilling only the largest buckets has two major benefits: First, spilling small buckets introduces the same file handling overhead as for large buckets, but the gain in terms of freed memory is smaller. Second, spilling to disk might cause duplicate values within a bucket, because the values on disk cannot be checked again in the remainder of the bucketing process for efficiency reasons; large buckets contain many different values anyway and are, hence, less likely to receive same values over and over again, which causes them to generate fewer duplicate values when being spilled to disk. The buckets of a table's primary key attribute, for instance, contain no duplicates. To find the largest attribute *lAttr* (and hence the largest buckets), the max() function queries an index that keeps track of the maximum value in the *nValsPerAttr* array (l. 16). Then, the `Bucketizer` iterates the largest buckets and writes them to disk (ll. 17-19). Afterwards, it clears the spilled buckets to free main memory and resets the spilled attribute in the *nValsPerAttr*-field (ll. 20 & 21).

5.3.3 Bucket management

Once the `Bucketizer` has partitioned a table, it writes all current buckets to disk from where the `Validator` can read them later on (ll. 22-28). In this way, it can reuse the entire main memory for bucketing the next table. While writing buckets to disk, the component also piggybacks the collection of two statistics: *attrSizes* and *emptyBuckets* (ll. 25 & 27). We describe each of these below:

(1) The attribute sizes array, *attrSizes*, stores the in-memory size of each bucketized attribute. It is later used to identify partitions that do not fit in main memory in the validation process. The `Bucketizer` computes the byte-size of a bucket as follows:

$$sizeOf(bucket) = \sum_{string \in bucket} 8 + 8 \cdot \left\lceil \frac{64 + 2 \cdot |string|}{8} \right\rceil$$

This calculation assumes an implementation in Java and a 64 bit system, on which strings need 64 byte for pointers, headers, and length and 2 bytes for each character. After normalizing to a multiple of 8 byte, which is the smallest addressable unit, we add another 8 byte for index-structures needed in the validation phase. For instance, the size of bucket (A,1) in our running example (see Figure 5.3) is 160 byte, because it contains two values of length one.

(2) The empty buckets array, *emptyBuckets*, counts the number of empty buckets in each partition to later determine the most promising checking order, *checkOrder*, for the `Validator`. The intuition is to prioritize the partitions with the smallest number of empty buckets, because the `Validator` cannot use empty buckets to invalidate IND candidates. So, the `Validator` aims at identifying and discarding inactive attributes early on by checking those attributes with the lowest number of empty buckets first. For instance, the *emptyBuckets* array for our example in Figure 5.3 is [1,1,1], because each partition contains one empty bucket. If all buckets contain the same number of empty buckets – like in this example – the *emptyBuckets* array does not indicate an optimal checking order and the partitions' initial order is used. Note that empty buckets mainly arise from attributes containing only a few distinct values, such as *gender*-attributes, which typically contain only two unique values.

5.3.4 Lazy partition refinement

Once the `Bucketizer` has finished splitting an input dataset into buckets, the `Validator` successively uploads seed partitions into main memory to validate IND candidates. Sometimes, however, seed partitions are larger than the main memory capacity. Thus, the `Bucketizer` needs to refine such seed partitions, which means that it splits a partition into smaller sub-partitions that fit into main memory. Refining a seed partition is, however, a costly operation as one has to read and write most values again. We could, indeed, collect some statistics about the input data, such as its size or length, to estimate the right number of seed partitions and avoid refining them. Unfortunately, collecting such statistics would introduce a significant overhead to the preprocessing step; the perfectly partitioned initial bucketing could also become very fine-grained for large datasets, i.e., it would cause the creation of numerous superfluous bucket-files on disk that lead to many file operations (create, open, and close) and, hence, could dominate the execution time of the bucketing process and with it the execution time of the entire IND discovery. For this reason, BINDER does not try to estimate the perfect bucketing a priori.

Instead, the `Bucketizer` *lazily* refines the partitions whenever necessary. The main idea is to split large seed partitions into smaller sub-partitions while validating INDs. Assume, for instance, that BINDER needs to check p_1 of Figure 5.3 and that only two values fit into main memory; BINDER then lazily refines p_1 into [{a},{ },{a},{ }] and [{b},{b},{ },{ }]. This lazy refinement also allows BINDER to dynamically reduce the number of sub-partitions when the number of active attributes decreases from one seed partition to the next one. For instance, if all IND candidates of an attribute are invalidated in some partition, BINDER does not need to refine the attribute's buckets in all subsequent partitions, saving much I/O. In contrast to estimating the number of seed partitions, lazy refinement creates much fewer files and, therefore, much less overhead for three reasons: (i) the number of required sub-partitions can be determined more precisely in the validation process, (ii) the number of files decreases with every invalidated attribute, and (iii) some small attributes can even stay in memory after refinement.

Algorithm 6 details the lazy refinement process. To refine a partition, the `Bucketizer` requires three inputs: *attrSizes* (size of the attributes' buckets in byte), *partitionNr* (identifier of the partition to be refined), and *activeAttr* (attributes to consider for refinement). Overall, the refinement process consists of two parts: (i) the *sub-partition number calculation* (ll. 1-5), which calculates the number of sub-partitions in which a seed partition has to be split, and (ii) the *value re-bucketing* (ll. 6-11), which splits a large partition into smaller sub-partitions. We explain these two parts below.

Algorithm 6: Lazy Refinement

```
    Data: $activeAttr$, $attrSizes$, $partitionNr$
    Result: $attrSizes$, $checkOrder$
 1  $availMem \leftarrow$ getAvailableMemory();
 2  $partSize \leftarrow 0$;
 3  foreach $attr \in activeAttr$ do
 4      $partSize \leftarrow partSize + attrSizes[attr]/nPartitions$;
 5  $nSubPartitions \leftarrow \lceil partSize/availMem \rceil$;
 6  $tables \leftarrow$ getTablesFromFiles($activeAttr$, $partitionNr$);
 7  if $nPartitions > 1$ then
 8      $checkOrder$, $attrSizes \leftarrow$ bucketize($activeAttr$, $tables$, $nSubPartitions$);
 9      return $checkOrder$;
10  else
11      return $\{partitionNr\}$;
```

(1) *Sub-partition number calculation.* To decide if a split is necessary, the `Bucketizer` needs to know the in-memory size of each attribute in a partition. The component can get this information from the *attrSizes* array, which it collected during the bucketing process (see Section 5.3.3). Let *availMem* be the available main memory and *attr* one attribute. As the hash function created seed partitions of equal size, the `Bucketizer` can now calculate the size of an attributes's bucket independently of the actual bucket number as:

$$size(attr) = attrSizes[attr]/nPartitions$$

The `Bucketizer` then calculates the size of a partition *partitionNr* as the sum of the sizes of all its active attributes:

$$partSize = \sum_{attr \in activeAttr} size(attr)$$

Thus, given a seed partition, the `Bucketizer` simply returns the seed partition number without refinement if $availMem > partSize$. Otherwise, it needs to split the seed partition into *nPartitions* sub-partitions as follows:

$$nSubPartitions = \lceil partSize/availMem \rceil$$

(2) *Value re-bucketing.* If refinement is needed, Binder re-applies the bucketing process depicted in Algorithm 5 on the bucket files. To this end, the `Bucketizer` first calls the function `getTablesFromFiles()`, which interprets each bucket as a table containing only one attribute (l. 6). Then, it successively reads the buckets of the current partition, re-hashes their values, and writes the new buckets back to disk (l. 8).

It is worth noting that distributing values from a bucket into different sub-partitions in an efficient manner is challenging for two reasons: *(i)* the values in each bucket are already similar with respect to their hash-values and thus redistributing them becomes harder, and *(ii)* refining seed partitions requires two additional I/O operations (for reading from and writing back to disk) for each value of an active attribute in a seed partition. BINDER addresses these two aspects as follows:

(i) To redistribute the values in a bucket, the `Bucketizer` re-partitions the values into *nSubPartitions* as follows:

$$x = \frac{\mathit{hash}(\mathit{value}) \ \% \ (\mathit{nPartitions} \cdot \mathit{nSubPartitions}) - \mathit{partitionNr}}{\mathit{nPartitions}}$$

Here, x is the sub-bucket number with $x \in [0, \mathit{nSubPartitions}{-}1]$ denoting the sub-bucket for the given *value*. Taking the hashes of the values modulo the number of seed partitions *nPartitions* multiplied by the number of required sub-partitions *nSubPartitions* leaves us with *nSubPartitions* different numbers. For instance, if $\mathit{nPartitions} = 10$, $\mathit{partitionNr} = 8$, and $\mathit{nSubPartitions} = 2$, we obtain numbers in $\{8, 18\}$, because the hash-values modulo *nPartitions* always give us the same number, which is *partitionNr*. By subtracting the current partition number *partitionNr* from the modulo and, then, dividing by *nPartitions*, we get an integer x in $[0, \mathit{nSubPartitions}{-}1]$ assigning the current value to its sub-bucket.

(ii) Concerning the additional I/O operations, we consider that each attribute can allocate at most $m = \mathit{availMem}/\,|\mathit{activeAttr}|$ memory for each of its buckets. However, in practice, most buckets are much smaller than m. Thus, our `Bucketizer` saves many I/O operations by not writing and reading again the sub-buckets of such small buckets, i.e., whenever $m < \mathit{size}_{\mathit{attr}}$.

5.4 Fast IND Discovery

Given a set of IND candidates, the `Validator` component successively checks them against the bucketized dataset. Algorithm 7 shows the validation process in detail. While the `Validator` reads the bucketized dataset directly from disk, it requires three additional inputs: the IND *candidates* that should be checked, the *checkOrder* defining the checking order of the partitions, and the *attrSizes* indicating the in-memory size of each bucket. See Section 5.3.3 for details about the *checkOrder* and *attrSizes* structures. The *candidates* input is a map that points each possible dependent attribute (i.e., included attribute) to all those attributes that it might reference (i.e., that it might be included in).

During the validation process, the `Validator` removes all invalid INDs from the *candidates* map so that only the valid INDs survive until the end of the process. Overall, the validation process consists of two parts: (i) the *partition traversal* (ll. 1-6), which iterates the partitions and maintains the attributes, and (ii) the *candidate validation* (ll. 7-22), which checks the candidates against a current partition. We explain both parts in the following two sections. Afterwards, we take a closer look at the candidate pruning capabilities of BINDER and discuss our design decisions.

Algorithm 7: Validation

```
   Data: candidates, checkOrder, attrSizes
   Result: candidates
 1 activeAttr ← getKeysAndValues(candidates);
 2 foreach partitionNr ∈ checkOrder do
 3     subPrtNrs ← refine(activeAttr, attrSizes, partitionNr);
 4     foreach subPartitionNr ∈ subPrtNrs do
 5         activeAttr ← getKeysAndValues(candidates);
 6         if activeAttr = ∅ then break all;
 7         map attr2value as Integer to {};
 8         map value2attr as String to {};
 9         foreach attr ∈ activeAttr do
10             bucket ← readFromDisk(attr, subPartitionNr);
11             attr2value.get(attr) ← bucket;
12             foreach value ∈ bucket do
13                 value2attr.get(value) ← value2attr.get(value) ∪ attr;
14         foreach attr ∈ activeAttr do
15             foreach value ∈ attr2value.get(attr) do
16                 if candidates.get(attr) = ∅ then break;
17                 if value ∉ value2attr.keys then continue;
18                 attrGrp ← value2attr.get(value);
19                 foreach dep ∈ attrGrp do
20                     candidates.get(dep) ← candidates.get(dep) \ attrGrp;
21                 value2attr.remove(value);
22 return candidates;
```

5.4.1 Partition traversal

As its first step, the `Validator` collects all active attributes *activeAttr*, which are all attributes that participate in at least one IND candidate (l. 1). The `Validator` uses *activeAttr* to prune inactive attributes during the validation (l. 6): If an attribute is removed from all IND candidates, it is also removed from this set and ignored for the rest of the validation process. The `Validator` checks the IND candidates against the bucketized dataset in the checking order, *checkOrder*, previously defined by the `Bucketizer` (l. 2). Before validation, the `Validator` calls the `Bucketizer` to refine the current seed partition into smaller sub-partitions if necessary (l. 3), which is, if the partition does not fit in main memory (see Section 5.3.4). Notice that the current seed partition is the only sub-partition if no refinement was needed.

After the refinement process, the `Validator` iterates the sub-partitions to check the candidates against them (l. 4). As the `Validator` might invalidate candidates on the current sub-partition in each iteration, it first updates the *activeAttr* set before starting the validation of the current iteration (l. 5). If no active attributes are left, which means that all IND candidates became invalid, the `Validator` stops the partition traversal (l. 6); otherwise, it proceeds with the IND candidate validations.

5.4.2 Candidate validation

The `Validator` first loads the current sub-partition into main memory and then checks the IND candidates on this sub-partition. To support fast checking, the `Validator` now builds two indexes upon the partition's values: the dense index *attr2values* and the inverted index *values2attr*. For the following illustration, assume that our running example dataset shown in Figure 5.2 has been bucketized into only one partition. Figure 5.5 then shows the two index structures that the `Validator` would create for this single partition.

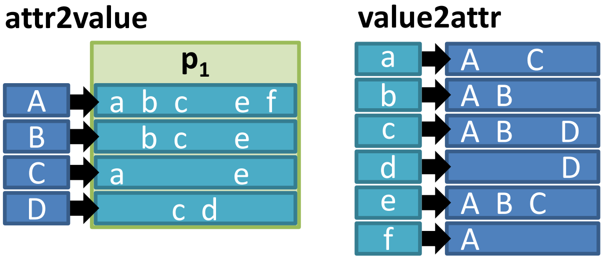


Figure 5.5: Dense index *attr2value* and inverted index *value2attr* for our example attributes {A,B,C,D} and values {a,b,c,d,e,f}.

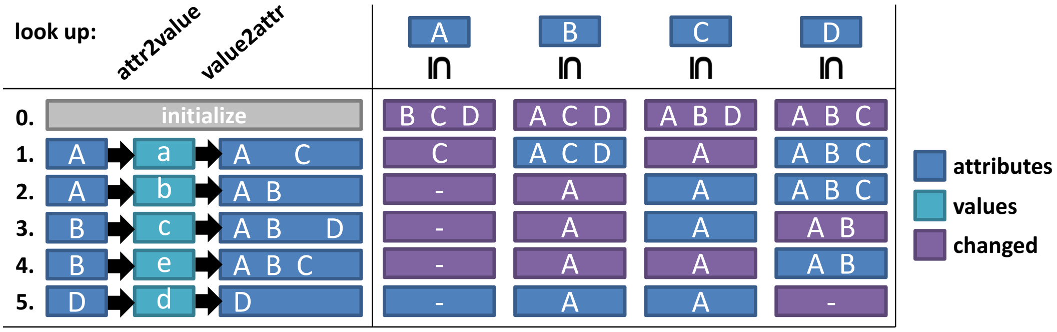
(1) *Dense Index.* The index *attr2values* maps each attribute to the set of values contained in this attribute. The `Validator` constructs the index when loading a partition into main memory in a bucket-wise manner. As each bucket represents the values of one attribute, the `Validator` can easily build this index with a negligible overhead. When validating a current partition, the `Validator` uses *attr2values* to discard attributes that become independent of all other attributes, which means that they are not included in any other attribute.

(2) *Inverted Index.* The inverted index *values2attr* maps each value to all those attributes that contain this value. Similar to DeMarchi's algorithm [Marchi et al., 2009] and Bauckmann's Spider algorithm [Bauckmann et al., 2006], the `Validator` uses the sets of attributes containing a common value to efficiently validate IND candidates via set intersection.

Index initialization. The `Validator` initializes the two indexes attribute-wise (ll. 9-13): For each active attribute, it reads the corresponding bucket from disk. Then, it points the active attribute to the read values in the *attr2values* index (left side of Figure 5.5). To initialize the *values2attr* index, the `Validator` inverts the key-value pairs and points each value to all those attributes where it occurs in (right side of Figure 5.5).

IND validation. Having initialized the two indexes with the current sub-partition, the `Validator` then uses them to efficiently remove non-inclusions from the set of IND *candidates*: Tt again iterates all active attributes and, for each active attribute, all the attribute's values (ll. 14 & 15). If the current attribute does not depend on any other attribute anymore, i.e., its *candidate* entry is empty, the `Validator` does not check any other values of this attribute and it can proceed with the next active attribute (l. 16).

Sometimes, the current value has already been handled with a different attribute and the inverted index does not contain the value anymore. Then, the `Validator` proceeds with the next value of the same attribute (l. 17); otherwise, it retrieves the group of attributes *attrGrp* containing the current value and intersects the set of referenced attributes of each of the group's members with this group (ll. 18-20). The intuition behind this intersection is that none of the *attrGrp* attributes can be included in an attribute that is not part of this group, because it would not contain the value of this particular attribute group. When the intersections are done, the `Validator` removes the current value from the inverted index *values2attr* to avoid checking the same attribute group again for different members of the group (l. 21).



look up:	attr2value	value2attr		A ⊆	B ⊆	C ⊆	D ⊆
0.	initialize			B C D	A C D	A B D	A B C
1.	A	a	A C	C	A C D	A	A B C
2.	A	b	A B	-	A	A	A B C
3.	B	c	A B D	-	A	A	A B
4.	B	e	A B C	-	A	A	A B
5.	D	d	D	-	A	A	-

Figure 5.6: Checking process over the example indexes of Figure 5.5

Example. Let us walk through the validation process once again with the example indexes shown in Figure 5.5. We use Figure 5.6 to list the intermediate results of the validation process. Each column in the table represents a dependent attribute and the cells list the attributes that are referenced by the respective dependent attribute. When reading the table from top to bottom, the initial IND candidates assume that each attribute is included in all three other attributes. Then, the `Validator` starts to check these candidates by looking up attribute A in the *attr2values* index and its first value a in the *values2attr* index. There, the `Validator` finds the attribute group $\{A, C\}$. Then, it intersects the referenced attribute sets of A and C, which are all the attributes of the previously retrieved attribute group $\{A, C\}$, with the set $\{A, C\}$. Thereby, we retrieve $\{C\}$ for attribute A and $\{A\}$ for attribute C. Since, we now handled the index entry of a in *values2attr*, we can remove it from the index.

Next, the `Validator` continues with the second value of attribute A, which is b, and finds the attribute group $\{A, B\}$. After intersecting attribute A's and attribute B's sets of referenced attributes with this attribute group, attribute A's set is empty. Thus, the `Validator` stops the checking of attribute A entirely after deleting the b-entry from the inverted index. We now continue with attribute B in the *attr2values* index. For attribute B, the `Validator` cannot find its first value b in the inverted *values2attr* index anymore, because it has already been handled. Therefore, it continues with value c and handles the corresponding attribute group $\{A, B, D\}$. The same follows for e. Because the `Validator` has checked all values of B now, it moves to attribute C. As all of attribute C's values have also been handled, it directly continues checking attribute D. Here, it finds the value d unchecked, which disassociates attribute D from A and B. Finally, the `Validator` terminates yielding the two inclusion dependencies $B \subseteq A$ and $C \subseteq A$.

5.4.3 Candidate pruning

A common practice to prune IND candidates is to collect some statistics about the buckets, such as min and max values, with which the algorithm can prune some attributes before even reading their first buckets. However, in early evaluations, we found that collecting such statistics is often more expensive than their actual pruning effect: We observed that the bucketing process dominates the entire IND discovery process by taking up 95% of the execution time; hence, additional costs for statistics collection in this step dominate any possible pruning-gain. Therefore, the `Validator` relies on two non-statistics-based pruning techniques to significantly speed up the validation process: *intra-partition* and *inter-partition* pruning.

Intra-partition pruning. During the validation of a partition, some attributes become independent of all other attributes, such as attribute A in our example. This means that they no longer appear as a dependent attribute in any IND candidate. In these cases, the `Validator` directly prunes the rest of the attribute's values from the validation process by skipping to the next active attribute in the *attr2values* index. The value f in our example, for instance, is never checked. In real-world datasets, many of such values exist, because attributes containing a large number of different values have an especially high chance of not being included in any other attribute.

Inter-partition pruning. After validating a partition, attributes become inactive if they neither depend on other attributes nor get referenced. Thus, by frequently updating the *activeAttr* set, the `Validator` can prune entire attributes from further validation processes. In consequence, the partitions become smaller and smaller, which continuously reduces the time needed for partition refinement, bucket loading, and index creation. Fewer attributes also reduce the average size of attribute groups in the *values2attr* index, which in turn makes the intersections faster.

In summary, the `Validator` does not need to read and check all attributes entirely due to the two indexes and its lazy bucketing and refinement techniques (if not all attributes participate in any inclusion dependency). All candidates that "survive" the validation on all partitions are valid inclusion dependencies.

5.5 IND Candidate Generation

The `CandidateGenerator` is the driver component of the entire IND discovery process. It first generates the IND candidates, then it instructs the `Bucketizer` to partition the data accordingly, thereafter it calls the `Validator` to check the candidates on the bucketized dataset and finally the component restarts the process for the next larger IND candidates. This iterative process allows Binder to use the same efficient components, i.e., bucketing, validation, and candidate generation to discover both unary and n-ary INDs. Using the same algorithm for all sizes of INDs also improves the maintainability of Binder.

With Algorithm 8, we show the candidate generation process in detail. It takes four parameters: the three arrays *attributes*, *tables*, and *dataTypes*, which store metadata about the dataset, and the *nPartitions* variable, which defines the number of seed partitions. At first, the `CandidateGenerator` generates all unary IND candidates and runs them through the bucketing and validation processes (ll. 1-12). If n-ary INDs should be detected as well, the `CandidateGenerator` then starts a level-wise generation and validation process for n-ary IND candidates (ll. 13-21). Each level represents the INDs of size i. The iterative process uses the already discovered INDs of size i to generate IND candidates of size $i + 1$. While this traversal strategy is already known from previous works [Agrawal and Srikant, 1994; Marchi et al., 2009], our candidate validation techniques contribute a significant improvement and simplification to the checking of n-ary IND candidates.

5.5.1 Unary IND detection

The `CandidateGenerator` starts by defining the *dep2refs* map, in which we store all valid INDs, and the *candidates* map, in which we store the IND candidates that still need to be checked (ll. 1 & 2). Both data structures map dependent attributes to lists of referenced attributes. The algorithm then calls the `Bucketizer` to partition the dataset for the unary IND detection (l. 3). The `Bucketizer` splits all *attributes* of all *tables* into *nPartitions* buckets as explained in Section 5.3. Next, the `CandidateGenerator` collects all empty attributes in the *emptyAttr* set using the previously measured attribute sizes (l. 4). An empty attribute is an attribute that contains no values. Using the attributes, their data types, and the set of empty attributes, the `CandidateGenerator` iterates the set of all possible unary IND candidates, which is the cross product of all attributes (l. 5). Each candidate *cand* is a pair of one dependent attribute *cand*[0] and one referenced attribute *cand*[1]. If both are the same, the IND is trivial and is discarded (l. 6).

Like most state-of-the-art IND discovery algorithms, such as [Marchi et al., 2009] and [Bauckmann et al., 2006], the `CandidateGenerator` also discards candidates containing differently typed attributes (l. 7). However, if INDs between differently typed attributes are of interest, e.g., if numeric columns can be included in string columns, this type-filter can be omitted. Furthermore, the `CandidateGenerator` excludes empty attributes, which are contained in all other attributes by definition, from the validation process and adds their INDs directly to the output (ll. 8-10). After discarding some first candidates, the remaining candidates are either valid per definition, which is when their dependent attribute is empty (l. 9), or they need to be checked against the data (l. 11). For the latter, the `CandidateGenerator` calls the `Validator` to check the IND candidates (see Secion 5.4) and places the valid INDs into the *dep2refs* map (l. 12). If only unary INDs are required, the algorithm stops here; otherwise, it continues with the discovery of n-ary INDs.

Algorithm 8: Candidate Generation

```
   Data: $attributes$, $tables$, $dataTypes$, $nPartitions$
   Result: $dep2refs$
 1 map $dep2refs$ as Integer to {};
 2 map $candidates$ as Integer to {};
   // Unary IND detection
 3 $checkOrder$, $attrSizes \leftarrow$ bucketize($attributes$, $tables$, $nPartitions$);
 4 $emptyAttr \leftarrow \{a \in attributes \mid attrSizes[a] = 0\}$;
 5 foreach $cand \in attributes \times attributes$ do
 6     if $cand[0] = cand[1]$ then continue;
 7     if $dataTypes[cand[0]] \neq dataTypes[cand[1]]$ then continue;
 8     if $cand[0] \in emptyAttr$ then
 9         $dep2refs.get(cand[0]) \leftarrow dep2refs.get(cand[0]) \cup cand[1]$;
10         continue;
11     $candidates.get(cand[0]) \leftarrow candidates.get(cand[0]) \cup cand[1]$;
12 $dep2refs \leftarrow dep2refs \cup$ validate($candidates$, $checkOrder$, $attrSizes$);
   // N-ary IND detection
13 $lastDep2ref \leftarrow dep2refs$;
14 while $lastDep2ref \neq \emptyset$ do
15     $candidates \leftarrow$ generateNext($lastDep2ref$);
16     if $candidates = \emptyset$ then break;
17     $attrCombinations \leftarrow$ getKeysAndValues($candidates$);
18     $checkOrder$, $attrSizes \leftarrow$ bucketize($attrCombinations$, $tables$, $nPartitions$);
19     $lastDep2ref \leftarrow$ validate($candidates$, $checkOrder$, $attrSizes$);
20     $dep2refs \leftarrow dep2refs \cup lastDep2ref$
21 return $dep2refs$;
```

5.5.2 N-ary IND detection

For the discovery of n-ary INDs, the `CandidateGenerator` incrementally generates and checks ever larger candidates. The generation is based on the apriori-gen algorithm, which traverses the lattice of attribute combinations level-wise [Agrawal and Srikant, 1994]. In detail, the `CandidateGenerator` first copies the already discovered unary INDs into the *lastDep2ref* map (l. 13), which stores all discovered INDs of the lastly finished lattice level, i.e., the last validation iteration. While the *lastDep2ref* map is not empty, i.e., the last validation iteration found at least one new inclusion dependency, the `CandidateGenerator` keeps generating and checking ever larger INDs (ll. 14-20).

Candidate generation. To generate the n-ary IND candidates *nAryCandidates* of size $n+1$ from the valid INDs *lastDep2ref* of size n, the `CandidateGenerator` uses the generateNext() function (l. 15). Given that X and Y are attribute sets, A, B, C, and D are single attributes, and $R_j[XA] \subseteq R_k[YC]$ and $R_j[XB] \subseteq R_k[YD]$ are known INDs of size $n = |XA|$, then this function forms the IND candidate $R_j[XAB] \subseteq R_k[YCD]$ of size $n+1$, iff $A < C$ and $B \neq D$. Note that we consider the attributes to be ordered so that X and Y respectively are same prefixes for the single attributes in the INDs of size n. The matching prefixes together with $A < C$ assure that the algorithm creates no candidate twice; otherwise, $R_j[XAB] \subseteq R_k[YCD]$ and $R_j[BAX] \subseteq R_k[DCY]$ would represent the same IND due to the permutation property of INDs. Because the number of $R_j[XAB] \subseteq R_k[YCD]$ candidates is huge and most use cases require only those INDs for which the dependent and referenced attributes are disjoint, Binder and related algorithms also use $XAB \cap YCD = \emptyset$ as a rule to reduce the number of candidates.

Re-bucketing. Having generated the next *nAryCandidates*, the `CandidateGenerator` needs to bucketize again the dataset according to these new candidates. It cannot reuse the bucketized dataset from the previous run, because the information about co-occurring values of different attributes gets lost when the values are bucketized. For instance, if the `CandidateGenerator` has to check the candidate $R_j[AB] \subseteq R_k[CD]$, then it checks if $\forall r \in R_j[AB] : r \in R_k[CD]$. As record r cannot be reconstructed from previous bucketings, the `CandidateGenerator` has to re-execute the bucketing algorithm with one small difference: Instead of single attribute values, Algorithm 5 bucketizes records from attribute combinations *attrCombinations* that either occur as a dependent or referenced attribute combination in any IND candidate. Technically, the `Bucketizer` can simply combine the values of such records with a *dedicated* separator character to then bucketize the combined values. For instance, consider that we need to check the IND candidate $R_j[AB] \subseteq R_k[CD]$. Now, assume that the `Bucketizer` reads the record (f, b, e, c) from our example schema $R_1[A, B, C, D]$. Then, it partitions the value $'f\#b'$ for $R_1[AB]$ and $'e\#c'$ for $R_1[CD]$.

It is worth emphasizing that the resulting buckets can become much larger than the buckets created for the unary IND checking: First, the combined values for n-ary IND candidates of size i are i-times larger on average than the single values, without counting the separator character. Second, the number of non-duplicate values increases exponentially with the size of the IND candidates so that more values are to be stored. Binder can still handle this space complexity through its dynamic memory handling (Section 5.3.2) and the lazy partition refinement (Section 5.3.4) techniques.

Validation. After the bucketing, the `CandidateGenerator` calls the `Validator` with the current set of n-ary IND candidates. Here, the validation of n-ary candidates is the same as the validation of unary candidates. The `Validator` has just to consider that the buckets refer to attribute combinations, e.g., to $R[AB]$. After validating the n-ary IND candidates of size $n+1$, the `CandidateGenerator` supplements the final result *dep2ref* with the set of newly discovered INDs. In case that no new INDs are found, the `CandidateGenerator` stops the level-wise search, because all unary and n-ary INDs have already been discovered. As a result, Binder reports the *dep2ref* map that now contains all valid INDs.

5.6 Evaluation

We evaluate and compare the performance of BINDER with two state-of-the-art systems for IND discovery. In particular, we carried out this evaluation with five questions in mind: How good does BINDER perform when (i) *varying the number of rows* (Section 5.6.2) and (ii) *varying the number of columns* (Section 5.6.3)? How well does BINDER behave when processing (iii) *different datasets* (Section 5.6.4)? What is the performance impact regarding the (iv) *internal techniques* of BINDER (Section 5.6.5) and how does BINDER perform for (v) *discovering n-ary INDs with* $n > 1$ (Section 5.6.6)?

5.6.1 Experimental setup

Our experiments compare BINDER against two other algorithms from related work, namely SPIDER [Bauckmann et al., 2006], which to date is the fastest algorithm for unary IND discovery, and MIND [Marchi et al., 2009], which is the most cited algorithm for n-ary IND discovery with n > 1. We implemented all three algorithms within our METANOME data profiling tool (`www.metanome.de`) using Java 7. BINDER and the other algorithms' binaries are publicly available[1]. For all experiments, we set BINDER's input parameter *nPartitions* to 10 and show in Section 5.6.5 why this is a good default value.

Hardware. All experiments were run on a Dell PowerEdge R620 with two Intel Xeon E5-2650 2.00 GHz CPUs and 128 GB DDR3 RAM. The server runs CentOS 6.4 as operating system. For some experiments, we reduce the server's memory to 8 GB in order to evaluate the algorithm's performance on limited memory resources.

Data storage. Our experiments consider both a database and raw files as data storage, because this choice influences the system's runtimes. SPIDER, for instance, uses SQL order-by statements on database inputs for its sorting phase and external memory sorting on files. MIND uses SQL for all inclusion checks and, hence, only runs on databases. BINDER reads an input dataset only once and then maintains the data itself, which is why the algorithm executes equally on both storage types. In our experiments, we use CSV-formatted files and the IBM DB2 9.7 database in its default setup. For database inputs, no indexes other than the relations' primary key indexes are given.

Datasets. Our experiments build upon both synthetic and real-world datasets. The real-world datasets we use are: COMA, WIKIPEDIA, and WIKIRANK, which are small datasets containing image descriptions, page statistics, and link information, respectively, that we crawled from the Wikipedia knowledge base; SCOP, BIOSQL, ENSEMBLE, CATH, and PDB, which are all excerpts from biological databases on proteins, dna, and genomes; CENSUS, which contains data about peoples' life circumstances, education, and income; LOD, which is an excerpt of linked open data on famous persons and stores many RDF-triples in relational format; and PLISTA [Kille et al., 2013b], which contains anonymized web-log data provided by the advertisement company Plista. The last two datasets TESMA and TPC-H are synthetic datasets, which we generated with the dbtesma tool for person data and the dbgen tool for business data, respectively. Table 5.1

[1] http://hpi.de/en/naumann/projects/repeatability/data-profiling/ind

Table 5.1: Datasets and their characteristics

Name	File Size	Attributes	Unary INDs	N-ary INDs	$\mathbf{n_{max}}$
COMA	20 KB	4	0	0	1
SCOP	16 MB	22	43	40	4
CENSUS	112 MB	48	73	147	6
WIKIPEDIA	540 MB	14	2	0	1
BIOSQL	560 MB	148	12463	22	2
WIKIRANK	697 MB	35	321	339	7
LOD	830 MB	41	298	1361005	8
ENSEMBL	836 MB	448	142510	100	4
CATH	908 MB	115	62	81	3
TESMA	1,1 GB	128	1780	0	1
PDB	44 GB	2790	800651	unknown	
PLISTA	61 GB	140	4877	unknown	
TPC-H	100 GB	61	90	6	2

lists these datasets with their *file size* on disk, number of *attributes*, number of all *unary* INDs, number of all *n-ary* INDs with $n > 1$, and the INDs' maximum arity n_{max}. Usually, most n-ary INDs are of size $n = 2$, but in the LOD dataset most n-ary INDs are of size $n = 4$. A link collection to these datasets and the data generation tools is available online[1].

5.6.2 Varying the number of rows

We start evaluating BINDER with regard to the length of the dataset, i.e., the number of rows. For this experiment we generated five TPC-H datasets with different scale factors from 1 to 70. The two left-side charts in Figure 5.7 show the result of the experiment for 128 GB (top) and 8 GB (bottom) of main memory.

We observe that with 128 GB of main memory, BINDER is up to 6.2 times faster on file inputs and up to 1.6 times faster on a database than SPIDER. BINDER outperforms SPIDER for three main reasons: First, building indexes for the IND validation is faster than SPIDER's sorting. Second, the indexes are not constructed for all attribute values, because some inactive attributes can be discarded early on. Third, BINDER reads the data once, whereas SPIDER queries the data multiple times in order to sort the different attributes. The results also show that BINDER performs worse on database inputs than on file inputs although the algorithm is exactly the same. In fact, its execution time almost doubles. The reason is the database overhead of query parsing, record formatting, and, in particular, inter-process data transfer. SPIDER, on the other hand, profits from a database: It uses the databases' built-in sorting algorithms, which are highly optimized for data that lives inside the database. Additionally, by directly eliminating duplicate values, the database also reduces the amount of data that it sends to the validation process. Despite these advantages, BINDER still clearly outperforms SPIDER even on database inputs.

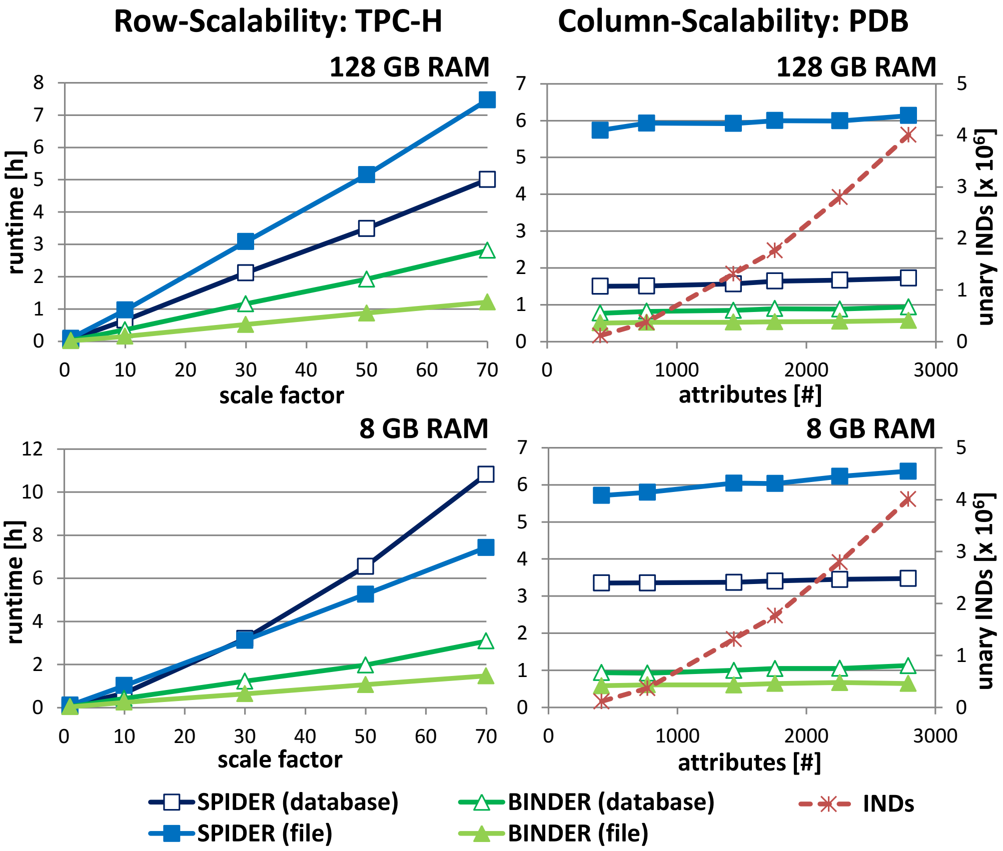


Figure 5.7: Runtimes measured scaling rows or columns

We also observe that with 8 GB of main memory, both algorithms become slower, as expected. The runtimes of BINDER increased by 8-9% and the runtimes of SPIDER by 10%. This is because both need their external memory techniques, which is spilling and refinement in BINDER and external memory sorting in SPIDER. However, we observe that the runtime of SPIDER on the database significantly increased, because the database sorting algorithm is apparently less performant on insufficient main memory. As a result, BINDER is now up to 3.5 times faster than SPIDER. When using raw files as input, BINDER is up to 5.1 times faster than SPIDER. This is a bit less than when having 128 GB of RAM, because the refinement strategy of BINDER requires slightly more spills to disk.

In summary, BINDER significantly outperforms SPIDER on both database and file inputs. It scales linearly with an increasing number of rows, because the bucketing process scales linearly and dominates the overall runtime of BINDER with 92-95%; in fact, the scalability is slightly super-linear, because the relative runtime costs for the validation process decreased with the length of the data from 8 to 5% due to our pruning techniques.

5.6.3 Varying the number of columns

We now evaluate Binder with regard to the width of the dataset, i.e., the number of attributes. In these experiments we used the PDB dataset, which comprises 2,790 attributes in total. We start with a subset of 411 attributes and continuously add tables from the PDB dataset to its subset. Note that we had to increase the open files limit in the operating system from 1,024 to 4,096 for Spider, to avoid the "Too many open files" exception.

The two right-side charts in Figure 5.7 show the result of the experiment for 128 GB (top) and 8 GB (bottom). We additionally plot the number of discovered INDs (red line in the charts) in these charts as they increase with the number of attributes. Similar to the row scalability experiment, Binder significantly outperforms Spider: (i) it is up to 1.8 times faster on a database and up to 10.7 times faster on raw files with 128 GB of main memory; and (ii) it is up to 3.1 times faster on a database and up to 9.9 times faster on raw files with 8 GB of main memory. We see that these improvement factors stay constant when adding more attributes, because the two IND validation strategies have the same complexity with respect to the number of attributes. However, it is worth noting that although the number of INDs increases rapidly, the runtimes of both algorithms only increase slightly. This is because the bucketing (for Binder) and sorting (for Spider) processes dominate the runtimes with 95% and 99% respectively.

5.6.4 Varying the datasets

The previous sections have shown that Binder's performance does not depend on the number of rows or columns in the dataset. As the following experiments on several real-world and two synthetic datasets will show, it instead depends on four other characteristics of the input datasets: (i) the *dataset size*, (ii) the *number of duplicate values per attribute*, (iii) the *average number of attributes per table*, and (iv) the *number of prunable attributes*, i.e., attributes not being part of any IND. Thus, to better evaluate Binder under the influence of these characteristics, we evaluated it on different datasets and compare its performance to that of Spider.

Figure 5.8 shows the results of these experiments. We again executed all experiments with 128 GB (top) and 8 GB (bottom) main memory. Notice that only the runtimes for the large datasets differ across the two memory settings. Overall, we observe that Binder outperforms Spider on all datasets, except the very small COMA and SCOP datasets. We now examine these results with respect to the four characteristics mentioned above:

(1) Dataset size. As we observed in the scalability experiments in Sections 5.6.2 and 5.6.3, the improvement of Binder over Spider does not depend on the number of rows or columns if the datasets are sufficiently large. The current results, however, show that Binder is slower than Spider if the datasets are very small, such as the COMA dataset with only 20 KB. This is because the file creation costs on disk dominate the runtimes of Binder: The algorithm creates ten files per attribute[2] whereas Spider

[2] In contrast to Spider, Binder only opens one of these files at a time.

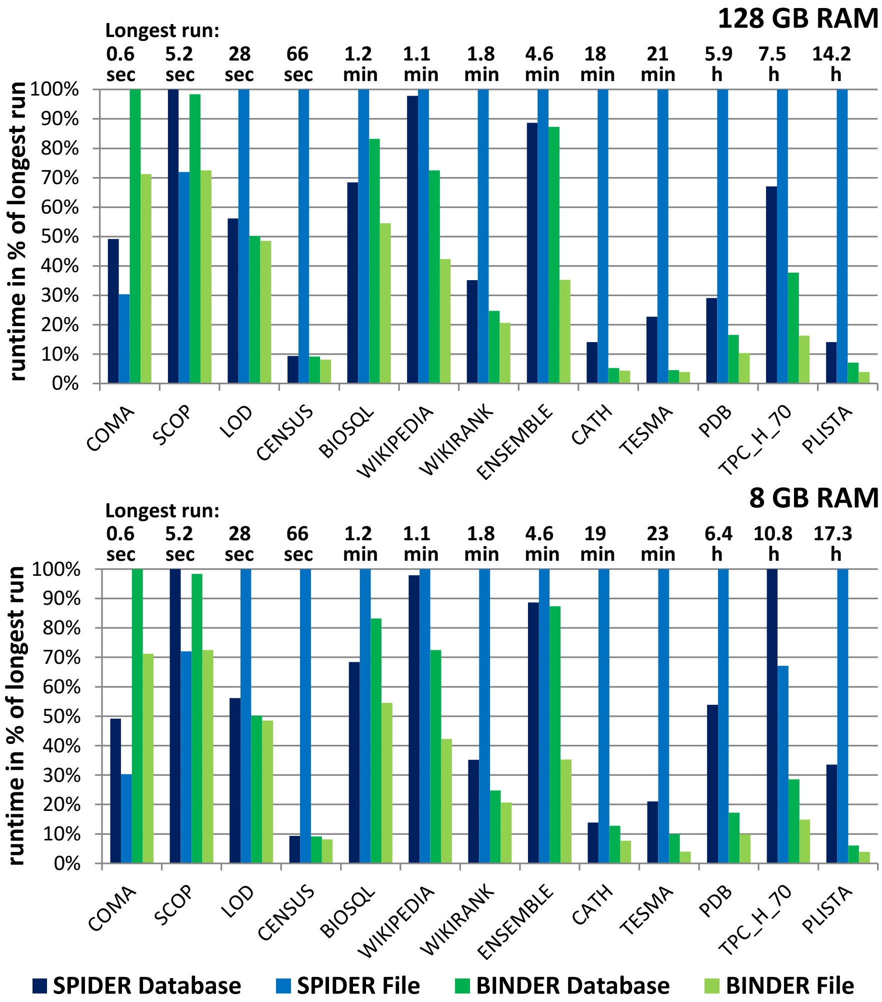


Figure 5.8: Runtime comparison on different datasets

only creates one file per attribute. For large datasets, however, the file creation costs are negligible in Binder. Therefore, Binder could for small datasets simply keep its buckets in main memory to further improve its performance.

(2) Number of duplicate values per attribute. Spider has an advantage over Binder if the input dataset contains many duplicate values and the IND detection is executed on a database. This is because Spider uses database functionality to remove such duplicates. The results for the CENSUS, BIOSSQL, and ENSEMBL datasets, which contain many duplicate values, show that Spider on a database can compete against Binder on a database. This also shows the efficiency of Binder to eliminate duplicate values in the bucketing process. In contrast to these results, when running on top of raw datasets, Binder again significantly outperforms Spider. We also observe that Binder is much better than Spider for the generated TESMA dataset, which contains only few duplicate values.

(3) Average number of attributes per table. The experiments in Section 5.6.3 have shown that the overall number of attributes does not influence the performance difference between Binder and Spider. However, we particularly observed that if the average number of attributes per table is high, Binder's performance is not affected as much as the performance of Spider: Spider needs to access a large table once for reading each of its attributes, which introduces a large overhead especially if the dataset needs to be read from files. Binder, on the other hand, needs to spill buckets more often to disk, but this introduces only a small overhead as the buckets are written to disk anyway. The results for the TESMA and PLISTA dataset show this aspect best: Having 32 and 35 attributes per table on average, respectively, Binder significantly outperforms Spider.

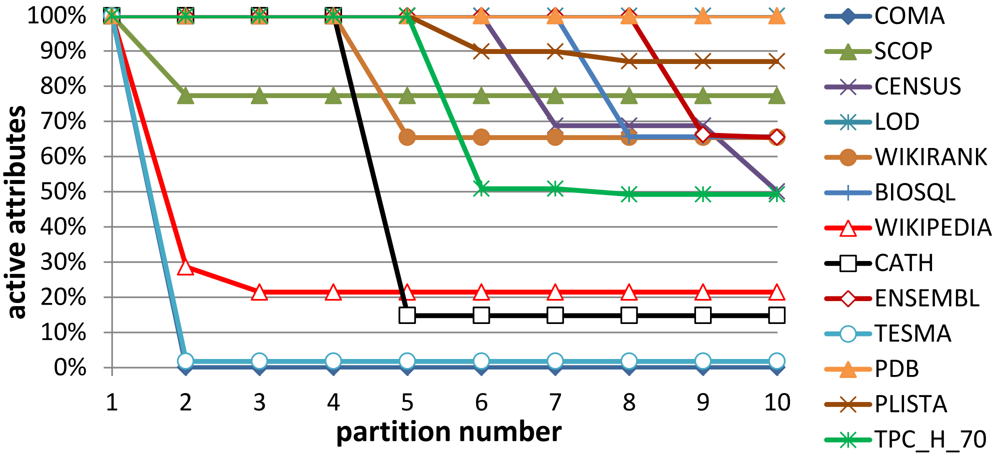


Figure 5.9: Active attributes per partition for the different datasets

(4) Number of prunable attributes. In contrast to Spider, which cannot prune inactive attributes before or during sorting values, Binder fully profits from attributes that are not part of any IND thanks to the inter-partition pruning (Section 5.4.3). For the SCOP dataset, for instance, Binder performs as good as Spider even if this dataset is still very small (16 MB). This is because Binder already prunes all attributes that are not part of any IND while processing the first partition. In this way, Binder saves significant indexing time whereas Spider cannot save sorting time for prunable attributes. Figure 5.9 shows the pruning effect in more detail: It lists the percentage of active attributes for the different partitions showing how many attributes Binder pruned in the different partitions. Notice that all attributes that survive as active attributes until Partition 10 are part of at least one valid IND. For instance, 50% of the attributes finally appear in at least one IND for the TPC-H dataset. The experiment shows that Binder achieved the highest pruning effect on the COMA, TESMA, WIKIPEDIA, and SCOP datasets: It pruned almost all unimportant attributes within the first partitions. This means that the values of these attributes are not read, indexed, or compared in the following partitions. Nonetheless, we see that the pruning capabilities of Binder have no effect for the LOD and PDB datasets, because all of their attributes either depend on another attribute or reference another attribute.

5.6.5 BINDER in-depth

So far, we have shown BINDER's advantage over SPIDER for unary IND discovery. We now evaluate BINDER to study the impact of: (i) the *nPartitions* parameter; (ii) the data structures used in the validation process; and (iii) the index-based candidate checking.

(1) Number of seed buckets. Recall that the *nPartitions* parameter specifies the number of seed buckets that BINDER initially creates. Although one could use any value for this parameter – thanks to the lazy refinement used in the validations –, the number of seed buckets influences the performance of BINDER as shown in Figure 5.10. It shows both the runtime of BINDER for different *nPartitions* values and the percentage of refined partitions for each number of seed buckets on the TPC-H 70 dataset. Note that we observed identical results for the PLISTA and PDB datasets and very similar results for the other datasets. As expected, on the one hand, we observe that taking a small number of seed partitions (two to three) decreases the performance of BINDER, because the algorithm needs more costly bucket refinements. On the other hand, we observe that choosing a large number of seed partitions, e.g., 50, also reduces the performance of BINDER, because more initial partitions increase the file overhead: BINDER creates more files than it actually needs. In between very small and very large values, we see that BINDER is not sensitive but robust to the *nPartitions* parameter. It is worth noting that SPIDER takes 7.4 hours to compute the same dataset, which is still more than 4 times slower than the worst choice of *nPartitions* in BINDER.

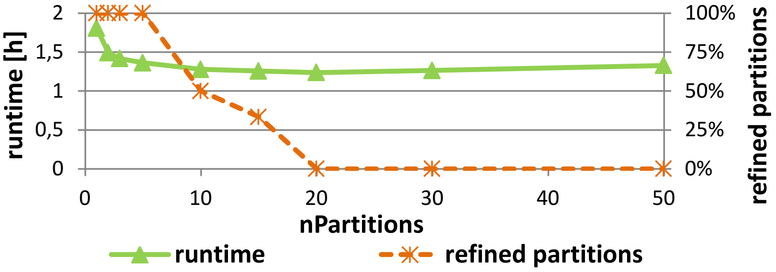


Figure 5.10: The nPartitions parameter on TPC-H 70 using 8 GB RAM

(2) Lists vs. BitSets. In the validation process, BINDER checks the generated IND candidates against the bucketized dataset by intersecting the candidates referenced attribute sets with those sets of attributes that all contain a same value. Technically, we can maintain the attribute sets as Lists or BitSets. BitSets have two advantages over Lists if most bits are set: They offer a smaller memory footprint and their intersection is faster. Thus, we implemented and tested both data structures. In our experiments, we did not observe a clear performance difference between the two data structures. This is because the attribute sets are typically very small and the intersection costs become almost constant [Marchi et al., 2009]. However, we observed a higher memory consumption for BitSets on datasets with many attributes, e.g., 41% higher on the PDB dataset, because they are very sparsely populated. Furthermore, the number of candidates increases quadratically with the number of attributes but while the candidate number shrinks over time using Lists, they stay large using BitSets. For these reasons, BINDER uses Lists.

(3) Indexing vs. sorting. Recall that the `Validator` component checks the IND candidates using two indexes, but it could also use Spider's sort-merge join approach instead. One can imagine that the sort-based approach might be faster than using indexes, because it does not need an external memory sorting algorithm due to Binder's bucketing phase. Thus, this approach would be clearly faster than the original Spider algorithm. However, we observed in our experiments that this sort-based approach is still 2.6 times slower than the indexing approach on average.

5.6.6 N-ary IND discovery

We now evaluate the performance of Binder when discovering all n-ary INDs of a dataset. Due to Binder's dynamic memory management and lazy partition refinement techniques, it can find n-ary INDs using the same, efficient discovery methods as for unary INDs. As related work algorithms use different approaches for unary and n-ary IND discovery (with n > 1), we compare Binder's runtime to the runtime of Mind– an algorithm specifically designed for n-ary IND discovery. Notice that we had to conduct these experiments on database inputs only, because Mind uses SQL queries for candidate evaluations.

Our first experiment measures Binder's and Mind's runtime while scaling the number of attributes on the PDB dataset. We report the results in the left chart of Figure 5.11. We also show in the right chart of Figure 5.11 the increase of n-ary candidates and n-ary INDs in this experiment. We observe that Mind is very sensitive to the number of IND candidates and becomes inapplicable (runtime longer than two days) already when the number of candidate checks is in the order of hundreds. Binder, however, scales well with the number of candidates and in particular with the number of discovered INDs, because it efficiently reuses bucketized attributes for multiple validations. We observe that while MIND runs in 2.4 days for 150 attributes, Binder runs under 20 minutes for up to 350 attributes and under 30 minutes for 600 attributes. In contrast to Mind, we also observe that Binder is not considerably influenced by the IND's arity (max level line in the right chart of Figure 5.11), because it reuses data buckets whenever possible while Mind combines data values again with every SQL validation.

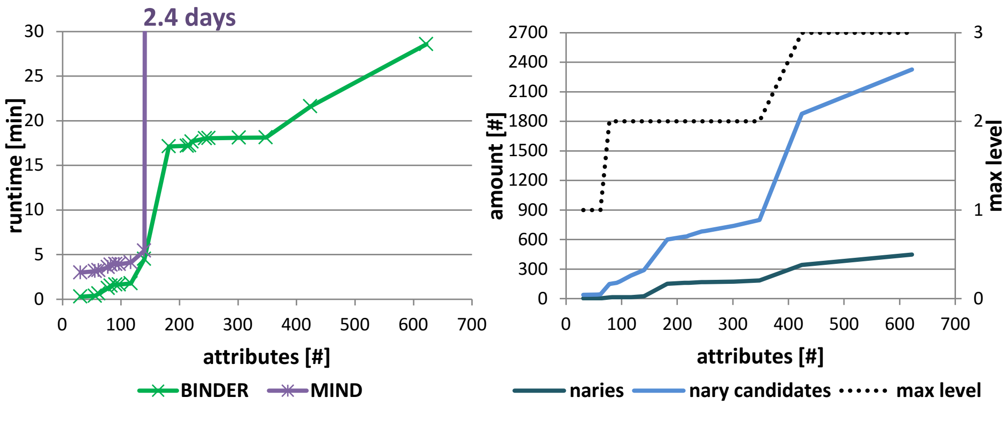


Figure 5.11: Runtimes of Binder and Mind scaling columns for PDB

To see how BINDER's discovery techniques perform in general, we evaluated the two algorithms on different datasets. Figure 5.12 depicts the measured runtimes. The experimental results together with the information on the datasets given in Table 5.1 show that, overall, the runtimes of BINDER and MIND correlate with the size of the dataset *and* the number of n-ary INDs, i.e., both input size and output size strongly influence the algorithms' runtimes. In detail, we observe that if no (or only few) INDs are to be discovered, as in the COMA, WIKIPEDIA, and TESMA datasets, BINDER's bucketing process does not pay off and single SQL queries may perform better. However, if a dataset contains n-ary INDs, which is the default in practice, BINDER is orders of magnitude faster than MIND. We measured improvements by up to more than three orders of magnitude in comparison to MIND (e.g., for CENSUS). This is because MIND, on the one hand, checks each IND candidate separately, which makes it access attributes and values multiple times; BINDER, on the other hand, re-uses the powerful unary candidate validation for the n-ary candidates, which lets it validate many candidates simultaneously. Considering that data access is the most expensive operation, BINDER's complexity in terms of I/O is in $O(n)$ whereas MIND complexity is in $O(2^n)$, where n is the number of attributes. Thus, even though MIND also uses pruning techniques for the IND checks, i.e., it stops matching the values of two attributes if one value is already missing, the single checks are already much too costly.

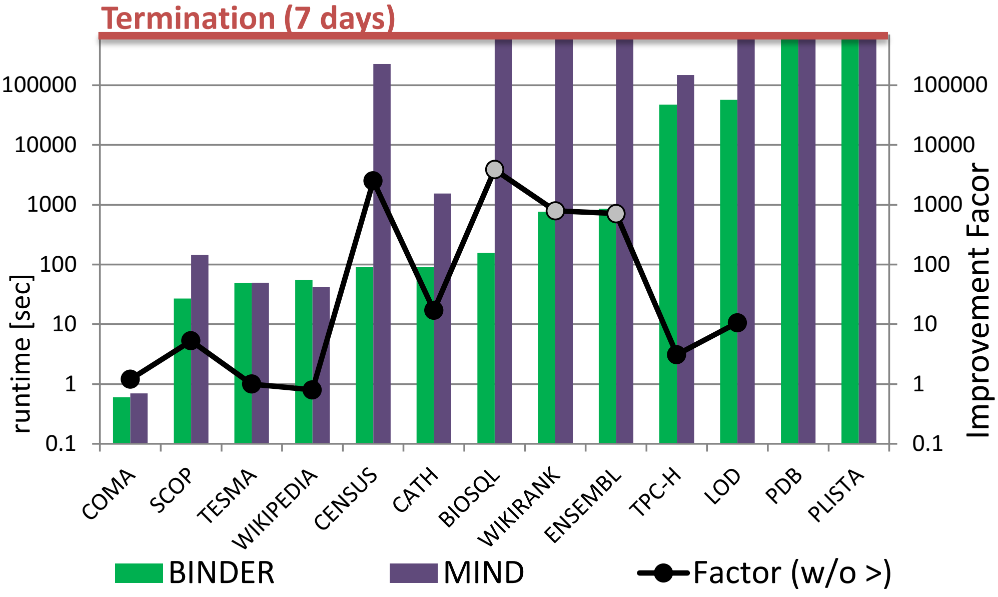


Figure 5.12: Comparing BINDER and MIND in n-ary IND detection

As Figure 5.12 shows, we had to terminate MIND after seven days for six datasets. BINDER could process four of these datasets in less than a day, but also exceeds seven days for PDB and PLISTA. This is because both datasets contain an extremely high number of n-ary INDs. In PDB, we found a set of almost duplicate tables and PLISTA contains two tables, `statistics` and `requests`, with same schema. At some point, this causes the generation of an exponential number of IND candidates. As BINDER scales with the size of the result, its execution time also increases exponentially.

With the TPC-H dataset, the experiment proves that even though the number of INDs (and IND candidates) is low, Binder can still outperform Mind. This is because the SQL checks become unproportionally expensive on high numbers of attribute values. Note that we tried different validation queries based on `LEFT OUTER JOIN`, `NOT IN`, and `EXCEPT` statements (limited on the first not joinable tuple) for Mind all showing the same limitation. Especially when the tables or the IND candidates' left and right hand sides become larger, the SQL-queries become clearly slower.

In summary, our experiments showed that only if tables are small and their number of n-ary IND candidates is low, Mind can compete with Binder. But as most real world datasets are large and contain many n-ary INDs, Binder is by far the most efficient algorithm for exact and complete n-ary IND discovery.

5.7 Conclusion & Future Work

We presented Binder, the currently most effective algorithm for exact and complete unary and n-ary IND discovery. The use of the divide & conquer principle allows it to efficiently handle very large datasets. Due to the partitioning, the algorithm can apply known pruning techniques and a novel IND-checking strategy at partition-level. In contrast to most related work, Binder does not rely on existing database functionality nor does it assume that the dataset fits into main memory. Our experimental results show that Binder is more than one order of magnitude (26 times) faster than Spider and up to more than three orders of magnitude (more than 2500 times) faster than Mind. The experimental results also show that Binder scales to much larger datasets than the state-of-the-art.

Because Binder's performance is I/O bound, we also developed a distributed IND discovery algorithm called Sindy [Kruse et al., 2015]. The distribution in Sindy comes at the cost of a less effective candidate pruning, but the gains in parallel I/O can compensate this disadvantage at some point. Another sister algorithm of Binder is Faida [Kruse et al., 2017]. In Faida, we relax the *correctness* constraint of the result to improve the discovery performance even further. Relaxing correctness means that the result set of discovered INDs is still complete, but false positives might occur – in fact, however, Faida's result sets were 100% correct on all tested datasets. In another line of research, we studied IND discovery on short tables, because Binder's divide & conquer strategy is an optimization only for long datasets with many thousand records and more. Some datasets, such as web table data or sample data, however, consist of rather short tables that only have 10 or less records per table on average. To efficiently process datasets of such unusual shortness, we developed Many [Tschirschnitz et al., 2017], an algorithm that, first, heavily prunes the search space using Bloomfilters and, then, validates the remaining candidates in memory. Within the same project scope of Binder, we also developed the RDFind algorithm [Kruse et al., 2016a]. This algorithm was designed to discover conditional INDs in RDF datasets, i.e., INDs that hold for certain subsets of RDF triples. Hence, RDFind is orthogonal research to Binder, as we left the relational world and found an alternative definition for INDs in the RDF format.

IND discovery is the most difficult task known in data profiling. Binder is currently the most efficient, exact solution for this problem, but its memory consumption on disk can still be an issue for n-ary IND discovery: The number of candidates can grow exponentially and with it the algorithm's memory consumption. In future work, we aim to solve this problem with additional, use case specific pruning rules that a priori reduce the number of attributes and, hence, buckets on disk. To find foreign keys, one could, for instance, drop all attributes with boolean or floating point values, because these are inappropriate data types for key constraints.

6

Metanome

Data profiling is an important preparation step for many practical use cases. For this reason, data scientists and IT professionals are frequently confronted with this special task. Only very few of these people have a technical unterstanding of data profiling and know how profiling algorithms work – they are usually experts for their use case but not necessarily in dependency discovery. So their success in data profiling relies mostly on available tool support for this task. As we already discussed in Chapter 1, current profiling tools, indeed, offer comprehensive functionality for basic types of metadata, which are easy to compute, but they usually lack automatic and efficient discovery functionality for complex metadata types; in particular, tool support for those metadata types that involve multiple columns, such as functional dependencies, unique column combinations, and inclusion dependencies, is sparse.

In this chapter, we propose METANOME[1], an extensible and open profiling platform that incorporates many state-of-the-art profiling algorithms for relational data. The first fully functional version of METANOME was presented as a demonstration in [Papenbrock et al., 2015a]. The profiling platform is able to calculate simple profiling statistics, but its main focus lies on the automatic *discovery* of *complex* metadata, i.e., those tasks that related profiling tools have difficulties with. For this purpose, METANOME's goal is to make novel profiling algorithms from research accessible to all experts tasked with data profiling: It guides the configuration and execution of metadata discovery algorithms and offers ranking and visualization features for the discovered metadata result sets. Through its modular and extensible architecture, METANOME also supports developers in building, testing, and evaluating new algorithms: The framework itself handles common functionality for data access and result management and defines standard interfaces for fair algorithm benchmarking. Note that all algorithms of this thesis, which are HYFD, HYUCC, BINDER, and their sister algorithms, have been implemented in this framework. In summary, the contributions of METANOME are the following:

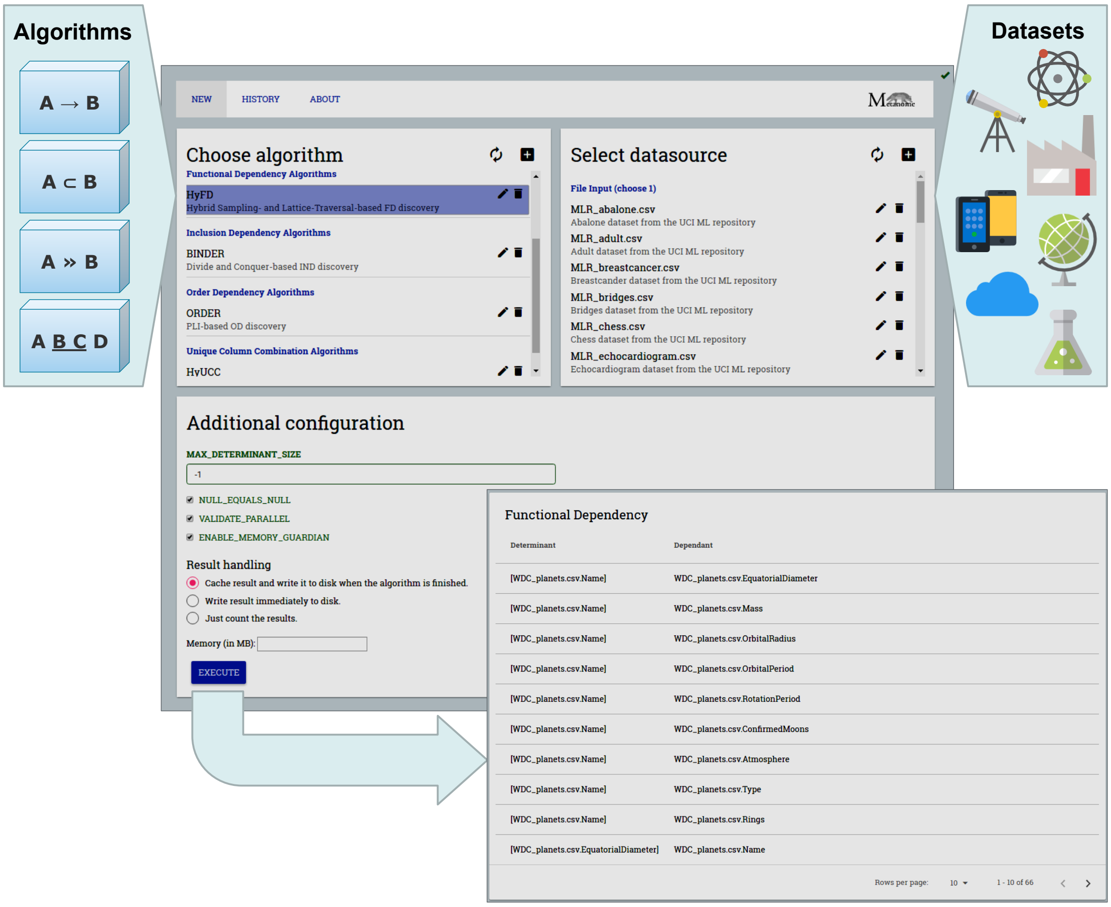
(1) *Data profiling support.* METANOME assists database administrators and IT professionals with state-of-the-art discovery algorithms in their effort to analyze relational datasets for metadata.

[1] www.metanome.de

(2) *Algorithm development support.* METANOME provides a framework to developers and researchers for building, testing, and maintaining new metadata discovery algorithms.

(3) *Metadata management support.* METANOME helps data scientists to interpret profiling results with the aid of ranking and visualization techniques.

Figure 6.1 shows a visualization of METANOME including two screenshots of its user interface: One screenshot shows the execution planning view, in which the user chooses the algorithm and dataset(s) for the next profiling job; the second screenshot shows the rankable result listing for a result set of INDs. Both algorithms and datasets are external resources for METANOME. We discuss the details of this architecture, i.e., the modularization of algorithms, the user interaction, and the result handling more accurately in the following Section 6.1. Section 6.2 then shows how data profiling with METANOME works from the user perspective and describes how METANOME supports the development of new algorithms. Afterwards, Section 6.3 discusses first practical uses of METANOME in research and industry.



Choose algorithm

Functional Dependency Algorithms

HyFD
Hybrid Sampling- and Lattice-Traversal-based FD discovery

Inclusion Dependency Algorithms

BINDER
Divide and Conquer-based IND discovery

Order Dependency Algorithms

ORDER
PLI-based OD discovery

Unique Column Combination Algorithms

HyUCC

Select datasource

File Input (choose 1)

MLR_abalone.csv
Abalone dataset from the UCI ML repository

MLR_adult.csv
Adult dataset from the UCI ML repository

MLR_breastcancer.csv
Breastcander dataset from the UCI ML repository

MLR_bridges.csv
Bridges dataset from the UCI ML repository

MLR_chess.csv
Chess dataset from the UCI ML repository

MLR_echocardiogram.csv
Echocardiogram dataset from the UCI ML repository

Additional configuration

MAX_DETERMINANT_SIZE: -1

☑ NULL_EQUALS_NULL
☑ VALIDATE_PARALLEL
☑ ENABLE_MEMORY_GUARDIAN

Result handling

● Cache result and write it to disk when the algorithm is finished.
○ Write result immediately to disk.
○ Just count the results.

Memory (in MB):

Functional Dependency

Determinant	Dependant
[WDC_planets.csv.Name]	WDC_planets.csv.EquatorialDiameter
[WDC_planets.csv.Name]	WDC_planets.csv.Mass
[WDC_planets.csv.Name]	WDC_planets.csv.OrbitalRadius
[WDC_planets.csv.Name]	WDC_planets.csv.OrbitalPeriod
[WDC_planets.csv.Name]	WDC_planets.csv.RotationPeriod
[WDC_planets.csv.Name]	WDC_planets.csv.ConfirmedMoons
[WDC_planets.csv.Name]	WDC_planets.csv.Atmosphere
[WDC_planets.csv.Name]	WDC_planets.csv.Type
[WDC_planets.csv.Name]	WDC_planets.csv.Rings
[WDC_planets.csv.EquatorialDiameter]	WDC_planets.csv.Name

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Figure 6.1: A visualization of the METANOME profiling platform with a screenshot of the execution planning view (center) and a screenshot of the result view for INDs (front).

6.1 The Data Profiling Platform

In this section, we discuss the architecture of METANOME. The METANOME project is an open source project available on GitHub[2]. Links to the most recent builds and to more detailed documentation for both users and developers can be found on the same page. The overall development of METANOME goes by the following three design goals:

1. *Simplicity:* METANOME should be easy to setup and use, i.e., a user should be able to simply download and start the tool, add data, and begin to profile it.
2. *Extensibility:* New algorithms and datasets should be easily connectable to the system without needing to change the system itself.
3. *Standardization:* All common tasks, such as tooling, input parsing, and result handling, should be integrated into the METANOME framework allowing the algorithms to focus on their specific solution strategies and allowing competitive evaluations to fairly compare algorithms by their performance.
4. *Flexibility:* METANOME should make as few restrictions to the algorithms as possible in order to enable possibly many algorithmic ideas.

In the following, we describe how these goals influenced METANOME's architecture, the framework's tasks, and the modularization of profiling algorithms.

6.1.1 Architecture

METANOME is a web-application that builds upon a classical three-tier architecture. Figure 6.2 illustrates this architecture: The data tier comprises the *Metanome store*, the *input sources*, and the *profiling algorithms*; the logic tier appears as *backend* component; and the presentation tier is represented by the *frontend* component. The division into a server (data and logic tier) and a client (presentation tier) component is an important design decision, because data profiling is usually conducted from an IT professional's workstation (client) on a remote machine (server) that holds the data and the necessary compute resources. Hence, the client can steer the profiling and analysis processes while the server performs the expensive profiling. For small profiling tasks, however, METANOME can also run as a desktop application. We now discuss the three tiers in more detail:

Data tier. The *Metanome store* is a light-weight HSQLDB database that stores operational metadata for the tool, such as configuration parameters, links to external resources, and statistics about previous profiling runs. The database is shipped with the METANOME tool and does not need to be installed separately. The data tier further comprises the *input sources*, which can be files or databases, and the *profiling algorithms*, which are precompiled jar-files. Both sources and algorithms are managed dynamically, meaning that they can be added or removed at runtime.

[2] `https://github.com/HPI-Information-Systems/Metanome`

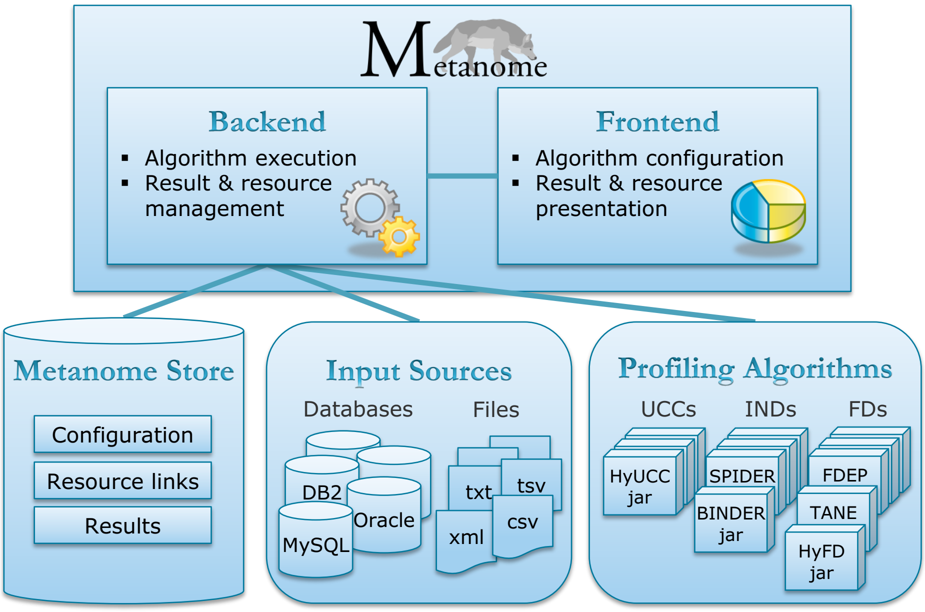

Figure 6.2: Architecture of the METANOME profiling platform.

Logic tier. The *backend* executes the algorithms and manages the results. Through a well-defined interface, the backend provides the algorithms with several standard functions for common tasks: Input parsing, output processing, and algorithm parametrization are, in this way, standardized. This makes the profiling algorithms easier to develop, evaluate, and compare.

Presentation tier. The *frontend* provides a graphical web-interface to the user. This interface allows the user to add/remove input sources and profiling algorithms, configure and start profiling processes, and list and visualize profiling results. It also provides access to previous profiling runs and their results so that a user can review all metadata grouped by their dataset. The frontend is developed in AngularJS and communicates over a RESTful API with the backend component.

METANOME is shipped with its own Tomcat web-server so that it runs out of the box, requiring only a JRE 1.7 or higher to be installed. No further software is required by METANOME itself, but the tool can read data from an existing database or run algorithms that utilize external frameworks, such as SPARK or MATLAB.

6.1.2 Profiling Framework

METANOME acts as a framework for different kinds of profiling algorithms. Because most of the algorithms perform the same common tasks, METANOME provides standardized functionality for them. In the following, we discuss the four most important tasks and the provided functionality:

Input Parsing. The first task of the METANOME framework is to build an abstraction around input sources, because specific data formats, such as separator characters in CSV-files, are irrelevant for the profiling algorithms. Hence, algorithms can choose between four standardized types of inputs:

1. *Relational:* The algorithm accepts any kind of relational input. The input source can be a file or a table in a database. The input is read sequentially while Metanome performs the parsing of records depending on the actual source.
2. *File:* The algorithm accepts raw files as input. It can, then, decide to either read and parse the content itself or, if the content is relational, to use Metanome functionality for the parsing. In this way, a Metanome algorithm can read non-relational formats, such as JSON, RDF, or XML if it handles the parsing itself.
3. *Table:* The algorithm accepts database tables as input. The advantage of only accepting database tables is that the algorithm is able to use database functionality when reading the tables. For instance, the tables can be read sorted or filtered by some criterion.
4. *Database:* The algorithm accepts an entire database as input. It must, then, select the tables itself, but it is also able to access metadata tables containing schema and data type information that can be used in the profiling process. To do so, Metanome also provides the type of database, e.g., DB2, MySQL, or Oracle, to the algorithm, because the name and location of metadata tables is vendor-specific.

Output Processing. Metanome's second task is to standardize the output formats depending on the type of metadata that the algorithm discovers. This is important, because Metanome can process and automatically analyze the results if it knows their type. To build a graphical visualization of an inclusion dependency graph, for instance, Metanome must know that the output contains inclusion dependencies and it must distinguish their dependent and referenced attributes. The most important, currently supported types of metadata are *unique column combinations* (UCCs), *inclusion dependencies* (INDs), *functional dependencies* (FDs), *order dependencies* (ODs), *multivalued dependencies* (MvDs), and *basic statistics*. The metadata type "basic statistics" is designed for simple types of metadata, such as minimum, maximum, average, or median that do not require individual output formats; it also captures those types of metadata that have no dedicated implementation in Metanome, yet, such as *denial constraints* (DCs), *matching dependencies* (MDs), and several *conditional* dependencies.

Parametrization Handling. Besides input and output standardization, Metanome also handles the parametrization of its algorithms. For this purpose, the profiling algorithms need to expose their configuration variables and preferably default values. The variables can then be set by the user. In this way, an algorithm can, for example, ask for a maximum number of results or a search strategy option.

Temporary Data Management. Sometimes, algorithms must write intermediate results or operational data to disk, for instance, if memory capacity is low. For these cases, Metanome provides dedicated temp-files. An algorithm can store its temporary data in such files, while Metanome places them on disk and cleans them when the algorithm has finished.

6.1.3 Profiling Algorithms

To run within METANOME, a profiling algorithm needs to implement a set of light-weight interfaces: The first interface defines the algorithm's output type and the second interface its input type as described in Section 6.1.2. Choosing one output and one input type is mandatory. A holistic profiling algorithm, i.e., an algorithm that discovers multiple types of metadata, might choose more than one output type. Further interfaces can optionally be added to request certain types of parameters or temp files. For instance, an algorithm could request a regular expression for input filtering using the String-parameter interface. The algorithm can also define the number of required parameter values. An IND discovery algorithm, for instance, would require multiple relations to discover foreign key candidates between them.

Apart from the interface, the profiling algorithms work fully autonomously, i.e., they are treated as foreign code modules that manage themselves, providing maximum flexibility for their design. So an algorithm is able to, for instance, use distributed systems like MAPREDUCE, machine learning frameworks like WEKA, or subroutines in other programming languages like C without needing to change the METANOME framework. This freedom is also a risk for METANOME, because foreign code can produce memory leaks if it crashes or is terminated. Therefore, algorithms are executed in separate processes with their own address spaces. Apart from memory protection, this also allows METANOME to limit the memory consumption of profiling runs. Of course, METANOME cannot protect itself against intentionally harmful algorithms; the profiling platform is rather designed for a trusted research community. The following algorithms are already contained in METANOME *and* publicly available[3]:

- **UCCs:** DUCC [Heise et al., 2013], HYUCC [Papenbrock and Naumann, 2017a]
- **INDs:** SPIDER [Bauckmann et al., 2006], BINDER [Papenbrock et al., 2015d], FAIDA [Kruse et al., 2017], MANY [Tschirschnitz et al., 2017]
- **FDs:** TANE [Huhtala et al., 1999], FUN [Novelli and Cicchetti, 2001], FD_MINE [Yao et al., 2002], DFD [Abedjan et al., 2014c], DEP-MINER [Lopes et al., 2000], FAST-FDS [Wyss et al., 2001], FDEP [Flach and Savnik, 1999], HYFD [Papenbrock and Naumann, 2016], AID-FD [Bleifuß et al., 2016]
- **ODs:** ORDER [Langer and Naumann, 2016]
- **MvDs:** MVDDETECTOR [Draeger, 2016]
- **Statistics:** SCDP

6.2 Profiling with Metanome

In this section, we examine METANOME from two user perspectives: an IT professional, who uses METANOME as a profiling tool on his data, and a scientist, who develops a new profiling algorithm using METANOME as a framework.

[3] https://hpi.de/naumann/projects/data-profiling-and-analytics/metanome-data-profiling/algorithms.html

6.2.1 Metadata Discovery

Given a single dependency candidate, it is easy to *validate* it on some dataset. The challenge in data profiling is to *discover* all dependencies, i.e., to answer requests such as *"Show me all dependencies of type X that hold in a given dataset"*. Metanome is designed for exactly such requests. To start a profiling run, an IT professional needs to specify at least a dataset and the type of dependency that should be discovered.

The need for data profiling usually arises when IT professionals already possess the data or have access to it. This data can be in file or database format. To profile the data, a user must register the dataset with its format definition, e.g., the separator, quote, and escape characters for file sources or the URL, username, and password for database sources. After registration, the new dataset appears in Metanome's list of profilable datasets (see Figure 6.1 center screenshot right list).

To add a new profiling algorithm, the user simply copies the algorithm's jar-file into Metanome's algorithm folder and, then, selects it in the frontend. This will make the algorithm appear in the list of profiling algorithms. Each algorithm defines the type(s) of metadata that can be discovered (see Figure 6.1 center screenshot left list).

Starting a profiling run is easy: Select an algorithm, choose a data source and, if needed, set some algorithm-specific parameters; pressing the *execute* button, then, starts the profiling task (see Figure 6.1 center screenshot bottom panel). Metanome executes the profiling tasks in seperate processes to control their resources and protect the application's own memory; it also starts the profiling tasks asynchronously, which allows the user to run multiple tasks in parallel.

During execution, Metanome measures the algorithm's runtime and reports on its progress if the algorithm's implementation supports progress measurement. In case an execution lasts too long, users can safely cancel it, which will shoutdown the respective process. On regular termination, the results are listed in the frontend (see Figure 6.1 front screenshot). As profiling results can be numerous, Metanome uses pagination and loads only a subset of any large result set into the frontend. The list of results can then be browsed, ranked, and visualized to find interesting dependencies.

Because already small datasets can harbor large amounts of metadata, Metanome introduces various result management techniques for metadata management: When a profiling run has finished, the user is first provided with a list of profiling results. This list can be scrolled, filtered, and sorted by different criteria, such as lexicographical order, length, or coverage. For some types of metadata, such as INDs, FDs, and UCCs, Metanome then proposes different visualizations. These higher level abstractions provide an overview on the data and indicate certain patterns.

For the visualization of functional dependencies, for instance, Metanome uses collapsible prefix-trees (see Figure 6.3) and zoom-able sunburst diagrams (see Figure 6.4). These visualizations, which were developed in [Neubert et al., 2014], let the user explore the results incrementally. The sunburst diagram, in particular, also indicates if one attribute is determined by particularly many other attributes or if its relatively independent, which is an indicator for redundance in this attribute.

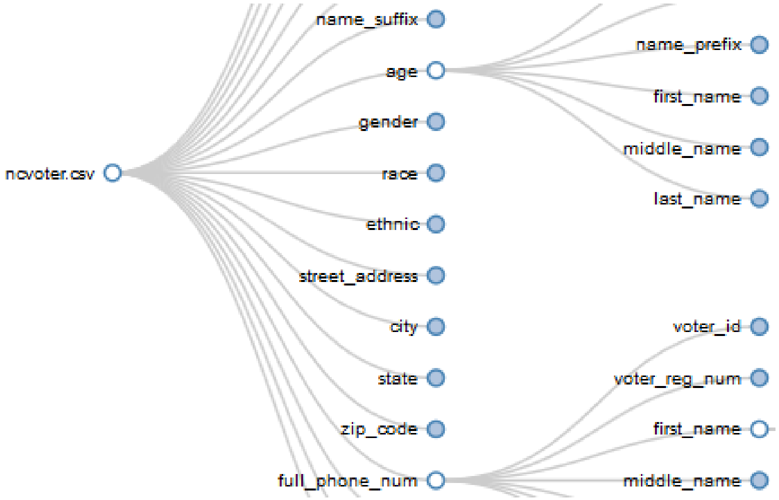

Figure 6.3: *Prefix-tree* visualization of functional dependencies [Neubert et al., 2014].

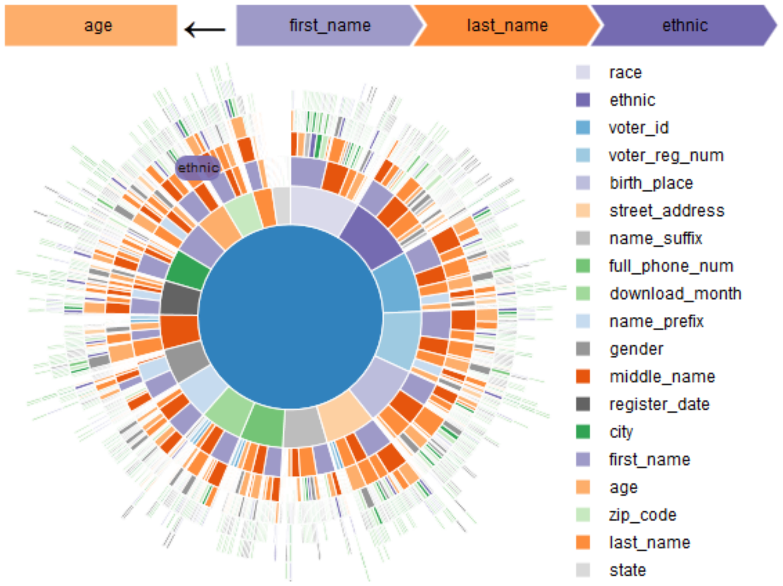

Figure 6.4: *Sunburst* visualization of functional dependencies [Neubert et al., 2014].

Figure 6.5, shows an exemplary visualization of inclusion dependencies: The bubble chart on the left indicates inclusion dependency clusters, i.e., sets of tables that are connected via INDs. These connections indicate possible foreign-key relationships and, hence, possible join paths. Clicking one cluster in the left chart opens its graph representation on the right side. Each node represents a table, and each edge one (or more) inclusion dependencies. This visualization not only allows the user to find topic-wise related tables but also shows how to link their information. We recently published the IND visualization in [Tschirschnitz et al., 2017] and its integration into the METANOME platform is currently work in progress.

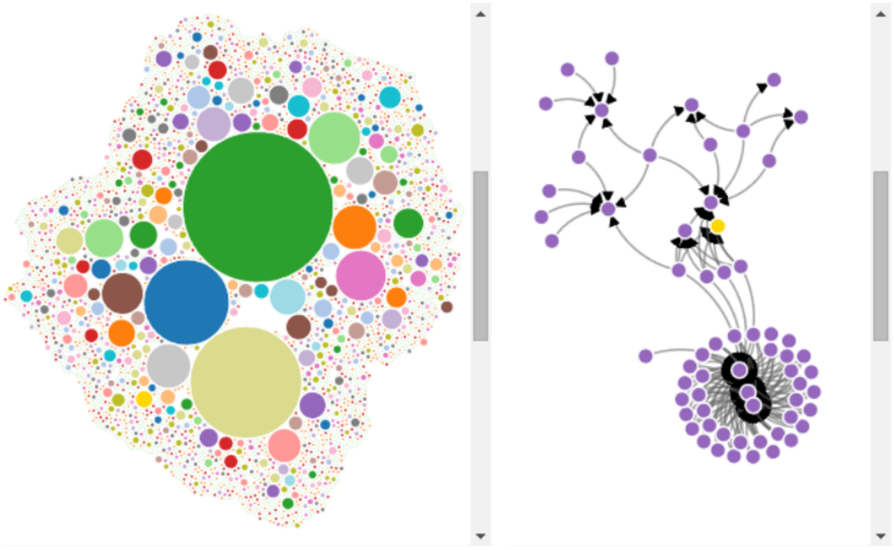

Figure 6.5: Visualization of inclusion dependency clusters (left) and the table join graph of one cluster (right) [Tschirschnitz et al., 2017].

6.2.2 Algorithm Development

To offer state-of-the-art profiling algorithms in Metanome, it must be easy for developers to integrate their work. As discussed in Section 6.1.3, an algorithm must specify its input type, the type of metadata that it calculates, and the parameter it needs via interfaces. The easiest way to develop a new algorithm is to use the template algorithm provided on Metanome's homepage and extend it. In order to obtain the Metanome interfaces that connect the algorithm with the frameworks standardized I/O, UI, and runtime features, we recommend using Apache Maven; all Metanome components are available as Maven dependencies.

During development, Metanome supports developers by providing standard components for common tasks. But Metanome also supports the testing and evaluation of new algorithms, because a developer can easily compare the results and runtimes of her solution to previous algorithms by using the same execution environment.

6.3 System Successes

Since Metanome's inception, the platform was used by various stakeholders in several projects. In this section, we give an overview of Metanome's successful employments:

Research. As a research prototype, Metanome supported the creation of various research papers. Meanwhile, more than 20 papers have been published in the context of the Metanome data profiling project. Most of these papers propose novel discovery algorithms for different types of metadata. The collection of papers also includes a demo paper on Metanome itself [Papenbrock et al., 2015a], an experimental evaluation paper for the different FD discovery algorithms [Papenbrock et al., 2015b], and a paper on an holistic discovery algorithm that jointly discovers INDs, UCCs, and FDs [Ehrlich et al., 2016]. Metanome also enabled a scientific case study on data anamnesis using the MusicBrainz dataset [Kruse et al., 2016b]. We furthermore know that Metanome and/or Metanome algorithms are used by research groups in France, Italy, USA, Canada, New Zealand, India, and China, because researchers from these countries contacted us via email; we hope that further, anonymous users of Metanome exist.

Industry. We used the Metanome platform not only in research but also in two industry projects: With FlixBus, a European logistics company, we successfully used Metanome to analyze travel data for business objects, patterns, and optimization potential; with idealo, a German online price comparison service, we deployed Metanome for data exploration and data preparation. Besides these industry projects, we also cooperated with data profiling teams of IBM and SAP: IBM re-implemented most core ideas of Metanome, such as external algorithm management and I/O standardization, for their own Open Discovery Framework (ODF) and we currently collaborate to make Metanome algorithms also executable within ODF; SAP also successfully took over some ideas from Metanome and its algorithms into their data profiling tool suite and we are now extending our collaboration with a long-term project on utilizing data profiling results in concrete use cases.

Teaching. Metanome served as a teaching vehicle in various lectures, seminars, and student projects: On the one hand, the platform and its algorithms were used to explain the different, existing profiling algorithms; on the other hand, meanwhile more than 200 studends used Metanome for the development of own profiling algorithms as part of their course-work, through master's theses, and as homework assignments. Only the best algorithms are included in the distribution of Metanome.

Competition. Most recently, the Metanome project won the business idea competition of the German *10. Nationalen IT-Gipfel*, which not only shows the need for modern profiling solutions in industry and academia but also Metanome's potential for sparking a spin-off company.

7

Data-driven Schema Normalization

Our experiments with Metanome have shown that discovered metadata result sets can be huge, i.e., millions of dependencies and more. For most use cases, only a small subset of these dependencies is actually relevant and processing the entire result set with use case specific standard solutions is infeasible. Hence, dependency discovery research created a paradigm shift from hard-to-understand datasets to hard-to-understand metadata sets.

The new challenge for data profiling is now to find metadata management techniques that are able to whittle discovered metadata sets down to such subsets that are actually relevant. Unfortunately, this task has no universal solution, because the *relevance* of a discovered dependency depends on the use case: For data exploration, relevant dependencies are those that express insightful rules; for schema normalization, we require dependencies that yield reliable foreign-key constraints; for query optimization, the dependencies must match the SQL expressions in some query load; and for data cleaning, useful dependencies are those that indicate data errors – to mention just a few examples for use case specific demands. We call a use case *data-driven* if it uses metadata that was obtained from the data via profiling; thus, use cases that use expert-defined, i.e., manually obtained metadata are non-data-driven.

One relevance criterion that appears in multiple use cases is *sematic correctness*, i.e., the question if a dependency is only incidentally true on a given instance or if it expresses a real-world rule that makes it logically true on all instances of a given schema. In fact, the majority of discovered dependencies are incidental and only few dependencies are semantically meaningful. This is because the candidate space for dependencies is, as shown in Section 2.4, exponentially large although only a few of these candidates have a semantic meaning; and only a limited number of the meaningless candidates finds an invalidation in their relational instances.

In this chapter, we exemplify efficient and effective metadata management for the concrete use case of schema normalization. The aim of schema normalization is to change the schema of a relational instance in a way that reduces redundancy in the data without reducing the schema's capacity. Like many other use cases that are based on discovered metadata, schema normalization introduces two challenges: On the computational level, we need an efficient algorithmic solution to cope with the size of discovered metadata sets in reasonable time and resource consumption; on the interpretation level, we must correctly assess the relevance of the dependencies and choose those that serve our use case appropriately. For the latter challenge, we also propose an approach to evaluate the semantic correctness of the dependencies.

We begin this chapter, which is based on [Papenbrock and Naumann, 2017b], with a motivation for the Boyce-Codd Normal Form (BCNF) and data-driven normalization in Section 7.1. Then, we discuss related work in Section 7.2 and introduce our schema normalization algorithm Normalize in Section 7.3. The following sections go into more detail, explaining efficient techniques for closure calculation (Section 7.4), key derivation (Section 7.5), and violation detection (Section 7.6). Section 7.7, then, introduces assessment techniques for key and foreign-key candidates. Finally, we evaluate Normalize in Section 7.8 and conclude in Section 7.9.

7.1 The Boyce-Codd Normal Form

Ensuring Boyce-Codd Normal Form (BCNF) [Codd, 1971] is a popular way to remove redundancy and anomalies from datasets. Normalization to BCNF forces functional dependencies (FDs) into keys and foreign keys, which eliminates redundant values and makes data constraints explicit. In this section, we first explain the BCNF normalization with an example; then, we discuss our normalization objective and the research challenges for data-driven schema normalization; finally, we list the contributions of this chapter.

7.1.1 Normalization example

Consider, as an example, the address dataset in Table 7.1. The two functional dependencies Postcode→City and Postcode→Mayor hold true in this dataset. Because both FDs have the same Lhs, we aggregate them to Postcode→City,Mayor. The presence of this FD introduces anomalies in the dataset, because the values Potsdam, Frankfurt, Jakobs, and Feldmann are stored redundantly and updating these values might cause inconsistencies. So if, for instance, some Mr. Schmidt was elected as the new mayor of Potsdam, we must correctly change all three occurrences of Jakobs to Schmidt.

Table 7.1: Example address dataset

First	Last	Postcode	City	Mayor
Thomas	Miller	14482	Potsdam	Jakobs
Sarah	Miller	14482	Potsdam	Jakobs
Peter	Smith	60329	Frankfurt	Feldmann
Jasmine	Cone	01069	Dresden	Orosz
Mike	Cone	14482	Potsdam	Jakobs
Thomas	Moore	60329	Frankfurt	Feldmann

Such anomalies can be avoided by normalizing relations into the Boyce-Codd Normal Form (BCNF). A relational schema R is in BCNF, iff for all FDs $X \to A$ in R the Lhs X is either a key or superkey [Codd, 1971]. Because Postcode is neither a key nor a superkey in the example dataset, this relation does not meet the BCNF condition. To bring all relations of a schema into BCNF, one has to perform six steps, which are explained in more detail later: (1) discover all FDs, (2) extend the FDs, (3) derive all keys from the extended FDs, (4) identify the BCNF-violating FDs, (5) select a violating FD for decomposition (6) split the relation according to the chosen violating FD. The steps (3) to (5) repeat until step (4) finds no more violating FDs and the resulting schema is BCNF-conform. Several FD discovery algorithms, such as Tane [Huhtala et al., 1999] and HyFD [Papenbrock and Naumann, 2016], exist to automatically solve step (1), but there are, thus far, no algorithms available to efficiently and automatically solve the steps (2) to (6).

For the example dataset, an FD discovery algorithm would find twelve valid FDs in step (1). These FDs must be aggregated and transitively extended in step (2) so that we find, inter alia, First,Last→Postcode,City,Mayor and Postcode→City,Mayor. In step (3), the former FD lets us derive the key $\{\textsf{First}, \textsf{Last}\}$, because these two attributes functionally determine all other attributes of the relation. Step (4), then, determines that the second FD violates the BCNF condition, because its Lhs Postcode is neither a key nor superkey. If we assume that step (5) is able to automatically select the second FD for decomposition, step (6) decomposes the example relation into $R_1(\underline{\textsf{First}}, \underline{\textsf{Last}}, \textsf{Postcode})$ and $R_2(\underline{\textsf{Postcode}}, \textsf{City}, \textsf{Mayor})$ with $\{\textsf{First}, \textsf{Last}\}$ and $\{\textsf{Postcode}\}$ being primary keys and $R_1.\textsf{Postcode} \to R_2.\textsf{Postcode}$ a foreign key constraint. Table 7.2 shows this result. When again checking for violating FDs, we do not find any and stop the normalization process with a BCNF-conform result. Note that the redundancy in City and Mayor has been removed and the total size of the dataset was reduced from 36 to 27 values.

Table 7.2: Normalized example address dataset

First	**Last**	**Postcode**
Thomas	Miller	14482
Sarah	Miller	14482
Peter	Smith	60329
Jasmine	Cone	01069
Mike	Cone	14482
Thomas	Moore	60329

Postcode	**City**	**Mayor**
14482	Potsdam	Jakobs
60329	Frankfurt	Feldmann
01069	Dresden	Orosz

Despite being well researched in theory, converting the schema of an existing dataset into BCNF is still a complex, manual task, especially because the number of discoverable functional dependencies is huge and deriving keys and foreign keys is NP-hard. Our solution for the BCNF schema normalization task is a data-driven normalization algorithm called Normalize. Data-driven schema normalization means that redundancy is removed only where it can actually be observed in a given relational instance. With Normalize, we propose a (semi-)automatic algorithm so that a user may or may not interfere with the normalization process. The algorithm introduces an efficient method for calculating the closure over sets of functional dependencies and novel features for choosing appropriate constraints. Our evaluation shows that Normalize can process millions of FDs within a few minutes and that the constraint selection techniques support the construction of meaningful relations during normalization.

7.1.2 Normalization objective

Because memory became a lot cheeper in the last years, there is a trend of not normalizing datasets for performance reasons. Normalization is, for this reason, today often claimed to be obsolete. This claim is false and ignoring normalization is dangerous for the following reasons [Date, 2012]:

1. Normalization removes redundancy and, in this way, decreases error susceptibility and memory consumption. While memory might be relatively cheep, data errors can have serious and expensive consequences and should be avoided at all costs.

2. Normalization does not necessarily decrease query performance; in fact, it can even increase the performance. Some queries might need some additional joins after normalization, but others can read the smaller relations much faster. Also, more focused locks can be set, increasing parallel access to the data, if the data has to be changed. So the performance impact of normalization is not determined by the normalized dataset but by the application that uses it.

3. Normalization increases the understanding of the schema and of queries against this schema: Relations become smaller and closer to the entities they describe; their complexity decreases making them easier to maintain and extend. Furthermore, queries become easier to formulate and many mistakes are easier to avoid. Aggregations over columns with redundant values, for instance, are hard to formulate correctly.

In summary, normalization should be the default and denormalization a conscious decision, i.e., “we should denormalize only at a last resort [and] back off from a fully normalized design only if all other strategies for improving performance have failed, somehow, to meet requiremnts”, C. J. Date, p. 88 [Date, 2012].

Our objective is to normalize a given relational instance into Boyce-Codd Normal Form. Note that we do not aim to recover a certain schema nor do we aim to design a new schema using business logic. To solve the normalization task, we propose a data-driven, (semi-)automatic normalization algorithm that removes all FD-related redundancy while still providing full information recoverability. Again, data-driven schema normalization means that all FDs used in the normalization process are extracted directly from the data so that all decomposition proposals are based solely on data-characteristics.

The advantage of a data-driven normalization approach over state-of-the-art schema-driven approaches is that it can use the data to expose all syntactically valid normalization options, i.e., functional dependencies with evidence in the data, so that the algorithm (or the user) must only *decide* for a normalization path and not *find* one. The number of FDs can, indeed, become large, but we show that an algorithm can effectively propose the semantically most appropriate options. Furthermore, knowing all FDs allows for a more efficient normalization algorithm as opposed to having only a subset of FDs.

7.1.3 Research challenges

In contrast to the vast amount of research on normalization in the past decades, we do not assume that the FDs are given, because this is almost never the case in practice. We also do not assume that a human data expert is able to manually identify them, because the search is difficult by nature and the actual FDs are often not obvious. The FD Postcode→City from our example, for instance, is commonly believed to be true although it is usually violated by exceptions where two cities share the same postcode; the FD Atmosphere→Rings, on the other hand, is difficult to discover for a human but in fact holds on various datasets about planets. For this reason, we automatically discover all (minimal) FDs. This introduces a new challenge, because we now deal with much larger, often spurious, but complete sets of FDs.

Using all FDs of a particular relational instance in the normalization process further introduces the challenge of selecting appropriate keys and foreign keys from the FDs (see Step (5)), because most of the FDs are coincidental, i.e., they are syntactically true but semantically false. This means that when the data changes these semantically invalid FDs could be violated and, hence, no longer work as a constraint. So we introduce features to automatically identify (and choose) reliable constraints from the set of FDs, which is usually too large for a human to manually examine.

Even if all FDs are semantically correct, selecting appropriate keys and foreign keys is still difficult. The decisions made here define which decompositions are executed, because decomposition options are often mutually exclusive: If, for instance, two violating FDs overlap, one split can make the other split infeasible. This happens, because BCNF normalization is not dependency preserving [Garcia-Molina et al., 2008]. In all these constellations, however, some violating FDs are semantically better choices than others, which is why violating FDs must not only be filtered but also ranked by such quality features. Based on these rankings, we propose a greedy selection approach, which always picks the in the current state most suitable FD for the next split.

Another challenge, besides guiding the normalization process in the right direction, is the computational complexity of the normalization. Beeri and Bernstein have proven that the question "Given a set of FDs and a relational schema that embodies it, does the schema violate BCNF?" is NP-complete in the number of attributes [Beeri and Bernstein, 1979]. To test this, we need to check that the Lhs of each of these FDs is a key or a super key, i.e., if each Lhs determines all other attributes. This is trivial if all FDs are transitively fully extended, i.e., they are transitively closed. For this reason, the complexity lies in calculating these closures (see Step (2)). Because no current algorithm is able to solve the closure calculation efficiently, we propose novel techniques for this sub-task of schema normalization.

7.1.4 Contributions

We propose a novel, instance-based schema normalization algorithm called Normalize that can perform the normalization of a relational dataset automatically or supervised by an expert. Allowing a human in the loop enables the algorithm to combine its analytical strengths with the domain knowledge of an expert. Normalize makes the following contributions:

(1) *Schema normalization.* We show how the entire schema normalization process can be implemented as one algorithm, which no previous work has done before. We discuss each component of this algorithm in detail. The main contribution of our (semi-)automatic approach is to incrementally weed out semantically false FDs by focusing on those FDs that are most likely true.

(2) *Closure calculation.* We present two efficient closure algorithms, one for general FD result sets and one for complete result sets. Their core innovations include a more focused extension procedure, the use of efficient index-structures, and parallelization. These algorithms are not only useful in the normalization context, but also for many other FD-related tasks, such as query optimization, data cleansing, or schema reverse-engineering.

(3) *Violation detection.* We propose a compact data structure, i.e., a prefix tree, to efficiently detect FDs that violate BCNF. This is the first approach to algorithmically improve this step. We also discuss how this step can be changed to discover violating FDs for normal forms other than BCNF.

(4) *Constraint selection.* We contribute several features to rate the probability of key and foreign key candidates for actually being constraints. With the results, the candidates can be ranked, filtered, and selected as constraints during the normalization process. The selection can be done by either an expert or by the algorithm itself. Because all previous works on schema normalization assumed all input FDs to be correct, this is the first solution for a problem that has been ignored until now.

(5) *Evaluation.* We evaluate our algorithms on several datasets demonstrating the efficiency of the closure calculation on complete, real-world FD result sets and the feasibility of (semi-)automatic schema normalization.

7.2 Related Work

Normal forms for relational data have been extensively studied since the proposal of the relational data model itself [Codd, 1969]. For this reason, many normal forms have been proposed. Instead of giving a survey on normal forms here, we refer the interested reader to [Fagin, 1979]. The Boyce-Codd Normal Form (BCNF) [Codd, 1971] is a popular normal form that removes most kinds of redundancy from relational schemata. This is why we focus on this particular normal form in this chapter. Most of the proposed techniques can, however, likewise be used to create other normal forms. The idea for our normalization algorithm follows the BCNF decomposition algorithm proposed in [Garcia-Molina et al., 2008] and many other text books on database systems. The algorithm eliminates all anomalies related to functional dependencies while still guaranteeing full information recoverability via natural joins.

Schema normalization and especially the normalization into BCNF are well studied problems [Beeri and Bernstein, 1979; Ceri and Gottlob, 1986; Mannila and Räihä, 1987]. Bernstein presents a complete procedure for performing schema synthesis based on functional dependencies [Bernstein, 1976]. In particular, he shows that calculating the closure over a set of FDs is a crucial step in the normalization process. He also lays the theoretical foundation for this chapter. But like most other works on schema normalization, Bernstein takes the functional dependencies and their semantic validity as a given – an assumption that hardly applies, because FDs are usually hidden in the data and must be discovered. For this reason, existing works on schema normalization greatly underestimate the number of valid FDs in non-normalized datasets and they also ignore the task of filtering the syntactically correct FDs for semantically meaningful ones. These reasons make those normalization approaches inapplicable in practice. In this chapter, we propose a normalization system that covers the entire process from FD discovery over constraint selection up to the final relation decomposition. We show the feasibility of this approach in practical experiments.

There are other works on schema normalization, such as the work of Diederich and Milton [Diederich and Milton, 1988], who understood that calculating the transitive closure over the FDs is a computationally complex task that becomes infeasible facing real-world FD sets. As a solution, they propose to remove so called *extraneous* attributes from the FDs before calculating the closure, which reduces the calculation costs significantly. However, if all FDs are minimal, which is the case in our normalization process, then no *extraneous* attributes exist, and the proposed pruning strategy is futile.

A major difference between traditional normalization approaches and our algorithm is that we retrieve *all minimal FDs* from a given relational instance to exploit them for closure calculation (syntactic step) and constraint selection (semantic step). The latter has received little attention in previous research. In [Andritsos et al., 2004], the authors proposed to rank the FDs used for normalization by the entropy of their attribute sets: The more duplication an FD removes, the better it is. The problem with this approach is that it weights the FDs only for effectiveness and not for semantic relevance. Entropy is also expensive to calculate, which is why we use different features. In fact, we use techniques inspired by [Rostin et al., 2009], who extracted foreign keys from INDs.

Schema normalization is a sub-task in schema design and evolution. There are numerous database administration tools, such as Navicat[1], Toad[2], and MySQL Workbench[3], that support these overall tasks. Most of them transform a given schema into an ER-diagram that a user can manipulate. All manipulations are then translated back to the schema and its data. Such tools are partly able to support normalization processes, but none of them can automatically propose normalizations with discovered FDs.

[1] `https://www.navicat.com/` *(Accessed: 2017-04-12)*

[2] `http://www.toadworld.com/` *(Accessed: 2017-04-12)*

[3] `http://www.mysql.com/products/workbench/` *(Accessed: 2017-04-12)*

In [Beeri and Bernstein, 1979], the authors propose an efficient algorithm for the membership problem, i.e., the problem of testing whether one given FD is in the cover or not. This algorithm does not solve the closure calculation problem, but the authors propose some improvements in that algorithm that our improved closure algorithm uses as well, e.g., testing only for missing attributes on the RHS. They also propose derivation trees as a model for FD derivations, i.e., deriving further FDs from a set of known FDs using Armstrong's inference rules. Because no algorithm is given for their model, we cannot compare our solution against it.

As stated above, the discovery of functional dependencies from relational data is a prerequisite for schema normalization. Fortunately, FD discovery is a well researched problem and we find various algorithms to solve it. For this work, we utilize our HyFD algorithm that we introduced in Chapter 3. HyFD discovers – like almost all FD discovery algorithms – the complete set of all minimal, syntactically valid FDs in a given relational dataset. We exploit these properties, i.e., minimality and completeness in our closure algorithm.

7.3 Schema Normalization

To normalize a schema into Boyce-Codd Normal Form (BCNF), we implement the straightforward BCNF decomposition algorithm shown in most textbooks on database systems, such as [Garcia-Molina et al., 2008]. The BCNF-conform schema produced by this algorithm is always a tree-shaped *snowflake schema*, i.e., the foreign key structure is hierarchical and cycle-free. Our normalization algorithm is, for this reason, not designed to (re-)construct arbitrary non-snowflake schemata. It, however, removes all FD related redundancy from the relations. If other schema design decisions that lead to alternative schema topologies are necessary, the user must (and can!) interactively choose different decompositions other than the ones our algorithm can propose.

In the following, we propose a normalization process that takes an arbitrary relational instance as input and returns a BCNF-conform schema for it. The input dataset can contain one or more relations, and no other metadata than the dataset's schema is required. This schema, which is incrementally changed during the normalization process, is globally known to all algorithmic components. We refer to a dataset's *schema* as its set of relations, specifying attributes, tables, and key/foreign key constraints. For instance, the schema of our example dataset in Table 7.2 is $\{R_1(\underline{\mathsf{First}}, \underline{\mathsf{Last}}, \mathsf{Postcode}), R_2(\underline{\mathsf{Postcode}}, \mathsf{City}, \mathsf{Mayor})\}$, where underlined attributes represent keys and same attribute names represent foreign keys.

Figure 7.1 gives an overview of the normalization algorithm NORMALIZE. In contrast to other normalization algorithms, such as those proposed in [Bernstein, 1976] or [Diederich and Milton, 1988], NORMALIZE does not have any components responsible for minimizing FDs or removing extraneous FDs. This is because the set of FDs on which we operate, is not arbitrary; it contains only minimal and, hence, no extraneous FDs due to the FD discovery step. We now introduce the components step by step and discuss the entire normalization process.

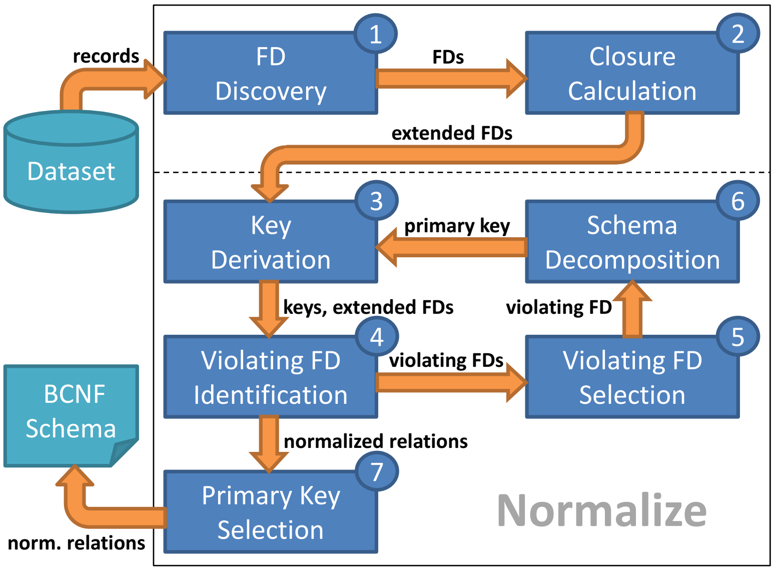

Figure 7.1: The algorithm NORMALIZE and its components.

(1) FD Discovery. Given a relational dataset, the first component is responsible for discovering all minimal functional dependencies. Any known FD discovery algorithm, such as TANE [Huhtala et al., 1999] or DFD [Abedjan et al., 2014c], can be used, because all these algorithms are able to discover the complete set of minimal FDs in relational datasets. We make use of our HYFD algorithm here (see Chapter 3), because it is the most efficient algorithm for this task and it offers special pruning capabilities that we can exploit later in the normalization process. In summary, the first component reads the data, discovers all FDs, and sends them to the second component.

(2) Closure Calculation. The second component calculates the closure over the given FDs. The closure is needed by subsequent components to infer keys and normal form violations. Formally, the *closure* X_F^+ *over a set of attributes* X given the FDs F is defined as the set of attributes X plus all additional attributes Y that we can add to X using F and Armstrong's axioms [Diederich and Milton, 1988]. If, for example, $X = \{A, B\}$ and $F = \{A \rightarrow C, C \rightarrow D\}$, then $X_F^+ = \{A, B, C, D\}$. We define the *closure* F^+ *over a set of FDs* F as a set of extended FDs: The RHS Y of each FD $X \rightarrow Y \in F$ is extended such that $X \cup Y = X_F^+$. In other words, each FD in F is maximized using Armstrong's transitivity axiom. As Beeri et al. have shown [Beeri and Bernstein, 1979], this is an NP-hard task with respect to the number of attributes in the input relation. Therefore, we propose an efficient FD extension algorithm that finds transitive dependencies via prefix tree lookups. This algorithm iterates the set of FDs only once and is able to parallelize its work. It exploits the fact that the given FDs are minimal and complete (Section 7.4).

(3) Key Derivation. The key derivation component collects those keys from the extended FDs that the algorithm requires for the normalization. Such a key X is a set of attributes for which $X \rightarrow Y \in F^+$ and $X \cup Y = R_i$ with R_i being *all* attributes of relation i. In other words, if X determines all other attributes, it is a key for its relation. Once discovered, these keys are passed to the next component. Our method of deriving keys from the extended FDs does not reveal all existing keys in the schema, but we prove in Section 7.5 that only the derived keys are needed for BCNF normalization.

(4) Violating FD Identification. Given the extended FDs and the set of keys, the violation detection component checks all relations for being BCNF-conform. Recall that a relation R is BCNF-conform, iff for all FDs $X \rightarrow A$ in that relation the LHS X is either a key or superkey. So NORMALIZE checks the LHS of each FD for having a (sub)set in the set of keys; if no such (sub)set can be found, the FD is reported as a BCNF violation. Note that one could setup other normalization criteria in this component to accomplish 3NF or other normal forms. If FD violations are identified, these are reported to the next component; otherwise, the schema is BCNF-conform and can be sent to the primary key selection. We propose an efficient technique to find all violating FDs in Section 7.6.

(5) Violating FD Selection. As long as some relations are not yet in BCNF, the violating FD selection component is called with a set of violating FDs. In this case, the component scores all violating FDs for being good foreign key constraints. With these scores, the algorithm creates a ranking of violating FDs for each non-BCNF relation. From each ranking, a user picks the most suitable violating FD for normalization; if no user is present, the algorithm automatically picks the top ranked FD. Note that the user, if present, can also decide to pick none of the FDs, which ends the normalization process for the current relation. This is reasonable if all presented FDs are obviously semantically incorrect, i.e., the FDs hold on the given data accidentally but have no real meaning. Such FDs are presented with a relatively low score at the end of the ranking. Eventually, the iterative process automatically weeds out most of the semantically incorrect FDs by selecting only semantically reliable FDs in each step. We discuss the violating FD selection together with the key selection in Section 7.7.

(6) Schema Decomposition. Knowing the violating FDs, the actual schema decomposition is a straight-forward task: A relation R, for which a violating FD $X \rightarrow Y$ is given, is split into two parts – one part without the redundant attributes $R_1 = R \backslash Y$ and one part with the FD's attributes $R_2 = X \cup Y$. Now X automatically becomes the new primary key in R_2 and a foreign key in R_1. With these new relations, the algorithm goes back into step (3), the key selection, because new keys might have appeared in R_2, namely those keys Z for which $Z \rightarrow X$ holds. Because the decomposition itself is straightforward, we do not go into more detail for this component.

(7) Primary Key Selection. The primary key selection is the last component in the normalization process. It makes sure that every BCNF-conform relation has a primary key constraint. Because the decomposition component already assigns keys and foreign keys when splitting relations, most relations already have a primary key. Only those relations that had no primary key at the beginning of the normalization process are processed by this component. For them, the algorithm (semi-)automatically assigns a primary key: All keys of the respective relation are scored for being a good primary key; then, the keys are ranked by their score and either a human picks a primary key from this ranking, or the algorithm automatically picks the highest ranked key as the relation's primary key. Section 7.7 describes the scoring and selection of keys in detail.

Once the closure of all FDs is calculated, the components (3) to (6) form a loop: This loop drives the normalization process until component (4) finds the schema to be in BCNF. Overall, the proposed components can be grouped into two classes: The first class includes the components (1), (2), (3), (4), and (6) and operates on a syntactic level;

the results in this class are well defined and the focus is set on performance optimization. The second class includes the components (5) and (7) and operates on a semantic level; the computations here are easy to execute but the choices are difficult and determine the quality of the result, which is why a user can influence decisions made in (5) and (7).

7.4 Closure Calculation

As already stated in Section 2.2.1, Armstrong formulated the following three axioms for functional dependencies on attribute sets X, Y, and Z:

1. *Reflexivity*: If $Y \subseteq X$, then $X \to Y$.
2. *Augmentation*: If $X \to Y$, then $X \cup Z \to Y \cup Z$.
3. *Transitivity*: If $X \to Y$ and $Y \to Z$, then $X \to Z$.

For schema normalization, we are given a set of FDs F and need to find a cover F^+ that maximizes the right hand side of each FD in F. The maximization of FDs is important to identify keys and to decompose relations correctly. In our running example, for instance, we might be given Postcode→City and City→Mayor. A correct decomposition with foreign key Postcode requires Postcode→City,Mayor; otherwise we would lose City→Mayor, because the attributes City and Mayor would end up in different relations. Therefore, we apply Armstrong's transitivity and reflexivity axioms on F to calculate its cover F^+. This means that each FD in F is maximized using these two axioms.

Armstrong's augmentation rule does not need be used, because this rule generates new, non-minimal FDs instead of extending existing ones and the decomposition steps of the normalization process require the FDs to be minimal, because their left-hand-sides should become *minimal* keys after the decompositions.

The reflexivity axiom adds all Lhs attributes to an FD's Rhs. To reduce memory consumption, we make this extension only implicit: We assume that Lhs attributes always also belong to an FD's Rhs without explicitly storing them on that side. For this reason, we apply the transitivity axiom for attribute sets W, X, Y, and Z as follows: If $W \to X$, $Y \to Z$, and $Y \subseteq W \cup X$, then $W \to Z$. So if, for instance, the FD First,Last→Mayor is given, we can extend the FD First,Postcode→Last with the Rhs attribute Mayor, because {First, Last} $\subseteq$ {First, Postcode} $\cup$ {Last}.

In the following, we discuss three algorithms for calculating F^+ from F: A naive algorithm, an improved algorithm for arbitrary sets of FDs, and an optimized algorithm for complete sets of minimal FDs. While the second algorithm might be useful for closure calculation in other contexts, such as query optimization or data cleansing, we recommend the third algorithm for our normalization system. All three algorithms store F, which is transformed into F^+, in the variable *fds*. We evaluate the performance of these algorithms later in Section 7.8.2.

7.4.1 Naive closure algorithm

The naive closure algorithm, which was already introduced as such in [Diederich and Milton, 1988], is given as Algorithm 9. For each FD in *fds* (Line 3), the algorithm iterates all other FDs (Line 4) and tests whether these extend the current FD (Line 5). If an extension is possible, the current FD is updated (Line 6). These updates might enable further updates for already tested FDs. For this reason, the naive algorithm iterates the FDs until an entire pass has not added any further extensions (Line 7).

Algorithm 9: Naive Closure Calculation

```
   Data: $fds$
   Result: $fds$
1  while $somethingChanged$ do
2      $somethingChanged \leftarrow$ false;
3      foreach $fd \in fds$ do
4          foreach $otherFd \in fds$ do
5              if $otherFd.lhs \subseteq fd.lhs \cup fd.rhs$ then
6                  $fd.rhs \leftarrow fd.rhs \cup otherFd.rhs$;
7                  $somethingChanged \leftarrow$ true;
8  return $fds$;
```

7.4.2 Improved closure algorithm

There are several ways to improve the naive closure algorithm, some of which have already been proposed in similar form in [Diederich and Milton, 1988] and [Beeri and Bernstein, 1979]. In this section, we present an improved closure algorithm that solves the following three issues: First, the algorithm should not check all other FDs when extending one specific FD, but only those that can possibly link to a missing Rhs attribute. Second, when looking for a missing Rhs attribute, the algorithm should not check all other FDs that can provide it, but only those that have a subset-relation with the current FD, i.e., those that are relevant for extensions. Third, the change-loop should not iterate the entire FD set, because some FDs must be extended more often than others so that many extension tests are executed superfluously.

Algorithm 10 shows our improved version. First, we remove the nested loop over all other FDs and replace it with index lookups. The index structure we propose is a set of prefix-trees, aka. tries. Each trie stores all FD Lhss that have the same, trie-specific Rhs attribute. Having an index for each Rhs attribute allows the algorithm to check only those other FDs that can deliver a link to a Rhs attribute that a current FD is actually missing (Line 8).

The *lhsTries* are constructed before the algorithm starts extending the given FDs (Lines 1 to 4). Each index-lookup must then not iterate all FDs referencing the missing Rhs attribute; it instead performs a subset search in the according prefix tree, because the algorithm is specifically looking for an FD whose Lhs is contained in the current FD's Rhs attributes (Line 9). The subset search is much more effective than iterating all possible extension candidates and has already been proposed for FD generalization lookups in [Flach and Savnik, 1999].

Algorithm 10: Improved Closure Calculation

```
   Data: $fds$
   Result: $fds$
1  array $lhsTries$ size $|$ $schema.attributes$ $|$ as Trie;
2  foreach $fd \in fds$ do
3      foreach $rhsAttr \in fd.rhs$ do
4          $lhsTries[rhsAttr]$.insert($fd.lhs$);
5  foreach $fd \in fds$ do
6      while $somethingChanged$ do
7          $somethingChanged \leftarrow$ false;
8          foreach $attr \notin fd.rhs \cup fd.lhs$ do
9              if $fd.lhs \cup fd.rhs \supseteq lhsTries[attr]$ then
10                 $fd.rhs \leftarrow fd.rhs \cup attr$;
11                 $somethingChanged \leftarrow$ true;
12 return $fds$;
```

As the third optimization, we propose to move the change-loop inside the FD-loop (Line 6). Now, a single FD that requires many transitive extensions in subsequent iterations does not trigger the same number of iterations over all FDs, which mostly are already fully extended.

7.4.3 Optimized closure algorithm

Algorithm 10 works well for arbitrary sets of FDs, but we can further optimize the algorithm with the assumption that these sets contain *all minimal FDs*. Algorithm 11 shows this more efficient version for complete sets of minimal FDs.

Like Algorithm 10, the optimized closure algorithm also uses the Lhs tries for efficient FD extensions, but it does not require a change-loop so that it iterates the missing Rhs attributes of an FD only once. The algorithm also checks only the Lhs attributes of an FD for subsets and not all attributes of a current FD (Line 7). These two optimizations are possible, because the set of FDs is complete and minimal so that we always find a subset-FD for any valid extension attribute. The following lemma states this formally:

Lemma 7.1. *Let F be a complete set of minimal FDs. If $X \rightarrow A$ with $A \notin Y$ is valid and $X \rightarrow Y \in F$, then there must exist an $X' \subset X$ so that $X' \rightarrow A \in F$.*

Proof. Let F be a complete set of minimal FDs. If $X \rightarrow A$ with $A \notin Y$ is valid and $X \rightarrow A \notin F$, then $X \rightarrow A$ is not minimal and a minimal FD $X' \rightarrow A$ with $X' \subset X$ must exist. If $X' \rightarrow A \notin F$, then F is not a complete set of minimal FDs, which contradicts the premise that F is complete. □

Algorithm 11: Optimized Closure Calculation

```
   Data: $fds$
   Result: $fds$
1  array $lhsTries$ size | $schema.attributes$ | as Trie;
2  foreach $fd \in fds$ do
3      foreach $rhsAttr \in fd.rhs$ do
4          $lhsTries[rhsAttr]$.insert ($fd.lhs$);
5  foreach $fd \in fds$ do
6      foreach $attr \notin fd.rhs \cup fd.lhs$ do
7          if $fd.lhs \supseteq lhsTries[attr]$ then
8              $fd.rhs \leftarrow fd.rhs \cup attr$;
9  return $fds$;
```

The fact that all minimal FDs are required for Algorithm 11 to work correctly has the disadvantage that complete sets of FDs are usually much larger than sets of FDs that have already been reduced to meaningful FDs. Reducing a set of FDs to meaningful ones is, on the contrary, a difficult and use-case specific task that becomes more accurate if the FDs' closure is known. For this reason, we perform the closure calculation before the FD selection and accept the increased processing time and memory consumption.

In fact, the increased processing time is hardly an issue, because the performance gain of Algorithm 11 over Algorithm 10 on same sized inputs is so significant that larger sets of FDs can still easily be processed. We show this in Section 7.8. The increased memory consumption, on the other hand, becomes a problem if the complete set of minimal FDs is too large to be held in memory or maybe even too large to be held on disk. We then need to prune FDs. But which FDs can be pruned so that Algorithm 11 still computes a correct closure on the remainder? To fully extend an FD $X \rightarrow Y$, the algorithm requires all subset-FDs $X' \rightarrow Z$ with $X' \subset X$ to be available. So if we prune all superset-FDs with larger Lhs than $|X|$, the calculated closure for $X \rightarrow Y$ and all its subset-FDs $X' \rightarrow Z$ would still be correct. In general, we can define a maximum Lhs size and prune all FDs with a larger Lhs size while still being able to compute the complete and correct closure for the remaining FDs with Algorithm 11. This pruning fits our normalization use-case well, because FDs with shorter Lhs are semantically better candidates for key and foreign key constraints as we argue in Section 7.7. Normalize achieves the maximum Lhs size pruning for free, because it is already implemented in the HyFD algorithm that we proposed using for the FD discovery.

All three closure algorithms can easily be parallelized by splitting the FD-loops (Lines 3, 2, and 5 respectively) to different worker threads. This is possible, because each worker changes only its own FD and changes made to other FDs can, but do not have to be seen by this worker.

Considering the complexity of the three algorithms with respect to the number of input FDs, the naive algorithm is in $\mathcal{O}(|fds|^3)$, the improved in $\mathcal{O}(|fds|^2)$, and the optimized in $\mathcal{O}(|fds|)$. But because the number of FDs potentially increases exponentially with the number of attributes, all three algorithms are NP-complete in the number of attributes. We compare the algorithms experimentally in Section 7.8.

7.5 Key Derivation

Keys are important in normalization processes, because they do not contain any redundancy due to their uniqueness. So they do not cause anomalies in the data. Keys basically indicate normalized schema elements that do not need to be decomposed, i.e., decomposing them would not remove any redundancy in the given relational instance. In this section, we first discuss how keys can be derived from extended FDs. Then, we prove that the set of derived keys is sufficient for BCNF schema normalization.

Deriving keys from extended FDs. By definition, a key is any attribute or attribute combination whose values uniquely determine all other records [Codd, 1969]. In other words, the attributes of a key X functionally determine all other attributes Y of a relation R. So given the extended FDs, the keys can easily be found by checking each FD $X \rightarrow Y$ for $X \cup Y = R$.

The set of keys that we can directly derive from the extended FDs does, however, not necessarily contain *all* minimal keys of a given relation. Consider here, for instance, the relations $\mathsf{Professor}(\underline{\mathsf{name}}, \mathsf{department}, \mathsf{salary})$, $\mathsf{Teaches}(\underline{\mathsf{name}}, \underline{\mathsf{label}})$, and $\mathsf{Class}(\underline{\mathsf{label}}, \mathsf{room}, \mathsf{date})$ with Teaches being a join table for the n:m-relationship between Professor and Class. When we *denormalize* this schema by calculating $R = \mathsf{Professor} \bowtie \mathsf{Teaches} \bowtie \mathsf{Class}$, we get $R(\underline{\mathsf{name}}, \underline{\mathsf{label}}, \mathsf{department}, \mathsf{salary}, \mathsf{room}, \mathsf{date})$ with primary key $\{\mathsf{name}, \mathsf{label}\}$. This key *cannot* directly be derived from the minimal FDs, because $\mathsf{name,label}{\rightarrow}A$ is not a minimal FD for any $A \in R_i$; the two minimal FDs are $\mathsf{name}{\rightarrow}\mathsf{department,salary}$ and $\mathsf{label}{\rightarrow}\mathsf{room,date}$.

Skipping missing keys. The discovery of missing keys is an expensive task, especially when we consider the number of FDs that can be huge for non-normalized datasets. The BCNF-normalization, however, requires only those keys that we can directly derive from the extended FDs. We can basically ignore the missing keys, because the algorithm checks normal form violations only with keys that are *subsets* of an FD's Lhs (see Section 7.6) and all such keys can directly be derived. The following lemma states this more formally:

Lemma 7.2. *If X' is a key and $X \rightarrow Y \in F^+$ is an FD with $X' \subseteq X$, then X' can directly be derived from F^+.*

Proof. Let X' be a key of relation R and let $X \rightarrow Y \in F^+$ be an FD with $X' \subseteq X$. To directly derive the key X' from F^+, we must prove the existence of an FD $X' \rightarrow Z \in F^+$ with $Z = R \setminus X'$:
X must be a minimal Lhs in some FD $X \rightarrow Y'$ with $Y' \subseteq Y$, because $X \rightarrow Y \in F^+$ and F is the set of all minimal FDs. Now consider the precondition $X' \subseteq X$: If $X' \subset X$, then $X \rightarrow Y \notin F^+$, because X is a key and, hence, it determines any attribute A that X could contain more than X'. Therefore, $X = X'$ must be true. At this point, we have that $X \rightarrow Y' \in F^+$ and $X = X'$. So $X' \rightarrow Y' \in F^+$ must be true as well, which also shows that $Y' = Y = Z$, because X' is a key. □

The key derivation component in Normalize in fact discovers only those keys that are relevant for the normalization process by checking $X \cup Y = R$ for each FD $X \rightarrow Y$. The primary key selection component in the end of the normalization process must, however, discover all keys for those relations that did not receive a primary key from any previous decomposition operation. For this task, we use our HyUCC algorithm (see Chapter 4), which is specialized in unique column combination discovery, i.e., key candidate discovery. The key discovery is an NP complete problem, but because the normalized relations are much smaller than the non-normalized starting relations, it is a fast operation at this stage of the algorithm.

7.6 Violation Detection

Given the extended *fds* and the *keys*, detecting BCNF violations is straightforward: Each FD whose Lhs is neither a key nor a super-key must be classified as a violation. Algorithm 12 shows an efficient implementation of this check again using a prefix tree for subset searches.

Algorithm 12: Violation Detection

```
   Data: $fds$, $keys$
   Result: $violatingFds$
1  $keyTrie \leftarrow$ new Trie;
2  foreach $key \in keys$ do
3      $keyTrie$.insert($key$);
4  $violatingFds \leftarrow \emptyset$;
5  foreach $fd \in fds$ do
6      if $\perp \in$ valuesOf($fd.lhs$) then
7          continue;
8      if $fd.lhs \supseteq keyTrie$ then
9          continue;
10     if $currentSchema.primaryKey \neq$ null then
11         $fd.rhs \leftarrow fd.rhs - currentSchema.primaryKey$;
12     if $\exists\ fk \in currentSchema.foreignKeys$:
13         $(fk \cap fd.rhs \neq \emptyset) \wedge (fk \not\subseteq fd.lhs \cup fd.rhs)$ then
14         continue;
15     $violatingFds \leftarrow violatingFds \cup fd$;
16 return $violatingFds$;
```

At first, the violation detection algorithm inserts all given keys into a trie (Lines 1 to 3). Then, it iterates the *fds* and, for each FD, it checks if the values of the FD's Lhs contain a `null` value $\perp$. Such FDs do not need to be considered for decompositions, because the Lhs becomes a primary key constraint in the new, split off relation and SQL prohibits `null` values in key constraints. Note that there is, as discussed in Section 2.5, work on *possible/certain key constraints* that permit ⊥ values in keys [Köhler et al., 2015], but we continue with the standard for now. If the Lhs contains no `null` values, the algorithm queries the *keyTrie* for subsets of the FD's Lhs (Line 8). If a subset is found, the FD does not violate BCNF and we continue with the next FD; otherwise, the FD violates BCNF.

To preserve existing constraints, we remove all primary key attributes from a violating FD's Rhs, if a primary key is present (Line 11). Not removing the primary key attributes from the FD's Rhs could cause the decomposition step to break the primary key apart. Some key attributes would then be moved into another relation breaking the primary key constraint and possible foreign key constraints referencing this primary key. Because the current schema might also contain foreign key constraints, we test if the violating FD preserves all such constraints when used for decomposition: Each foreign key *fk* must stay intact in either of the two new relations or otherwise we do not use the violating FD for normalization (Line 13). The algorithm finally adds each constraint preserving violating FD to the *violatingFds* result set (Line 15). In Section 7.7 we propose a method to select one of them for decomposition.

When a violating FD $X \to Y$ is used to decompose a relation R, we obtain two new relations, which are $R_1(R \backslash Y \cup X)$ and $R_2(X \cup Y)$. Due to this split of attributes, not all previous FDs hold in R_1 and R_2. It is obvious that the FDs in R_1 are exactly those FDs $V \to W$ for which $V \cup W \subseteq R_1$ and $V \to W' \in F^+$ with $W \subseteq W'$, because the records for $V \to W$ are still the same in R_1; R_1 just lost some attributes that are irrelevant for all $V \to W$. The same observation holds for R_2 although the number of records has been reduced:

Lemma 7.3. *The relation $R_2(X \cup Y)$ produced by a decomposition on FD $X \to Y$ retains exactly all FDs $V \to W$, for which $V \cup W \subseteq R_2$ and $V \to W$ is valid in R.*

Proof. We need to show that (1) any $V \to W$ of R is still valid in R_2 and (2) no valid $V \to W$ of R_2 can be invalid in R:
(1) Any valid $V \to W$ of R is still valid in R_2: Assume that $V \to W$ is valid in R but invalid in R_2. Then R_2 must contain at least two records violating $V \to W$. Because the decomposition only *removes* records in $V \cup W$ and $V \cup W \subseteq R_2 \subseteq R$, these violating records must also exist in R. But such records cannot exist in R, because $V \to W$ is valid in R; hence, the FD must also be valid in R_2.
(2) No valid $V \to W$ of R_2 can be invalid in R: Assume $V \to W$ is valid in R_2 but invalid in R. Then R must contain at least two records violating $V \to W$. Because these two records are not completely equal in their $V \cup W$ values and $V \cup W \subseteq R_2$, the decomposition does not remove them and they also exist in R_2. So $V \to W$ must also be invalid in R_2. Therefore, there can be no FD valid in R_2 but invalid in R. □

Assume that, instead of BCNF, we would aim to assure 3NF, which is slightly less strict than BCNF: In contrast to BCNF, 3NF does not remove all FD-related redundancy, but it is dependency preserving. Consequently, no decomposition may split an FD other than the violating FD [Bernstein, 1976]. To calculate 3NF instead of BCNF, we could additionally remove all those groups of violating FDs from the result of Algorithm 12 that are mutually exclusive, i.e., any FD that would split the Lhs of some other FD. To calculate stricter normal forms than BCNF, we would need to have detected other kinds of dependencies. For example, constructing 4NF requires all multi-valued dependencies (MVDs) and, hence, an algorithm that discovers MVDs. The normalization algorithm, then, would work in the same manner.

7.7 Constraint Selection

During schema normalization, we need to define key and foreign key constraints. Syntactically, all keys are equally correct and all violating FDs form correct foreign keys, but semantically the choice of primary keys and violating FDs makes a difference. Judging the relevance of keys and FDs from a semantic point of view is a difficult task for an algorithm – and in many cases for humans as well – but in the following, we define some quality features that serve to automatically score keys and FDs for being "good" constraints, i.e., constraints that are not only valid on the given instance but are true for its schema.

The two selection components of Normalize, i.e., *primary key selection* and *violating FD selection* use the quality features to score the key and foreign-key candidates, respectively. Then, they sort the candidates by their score. The most reasonable candidates are presented at the top of the list and likely accidental candidates appear at the end. By default, Normalize uses the top-ranked candidate and proceeds; if a user is involved, she can choose the constraint or stop the process. The candidate list can, of course, become too large for a full manual inspection, but (1) the user always needs to pick only one element, i.e., she does not need to classify all elements in the list as either true or false, (2) the candidate list becomes shorter in every step of the algorithm as many options are implicitly weeded out, and (3) the problem of finding a split candidate in a ranked enumeration of options is easier than finding a split without any ordering, as it would be the case without our method.

7.7.1 Primary key selection

If a relation has no given primary key, we must assign one from the relation's set of keys. To find the semantically best key, Normalize scores all keys X using these features:

(1) Length score: $\frac{1}{|X|}$

Semantically correct keys are usually shorter than random keys (in their number of attributes $|X|$), because schema designers tend to use short keys: Short keys can more efficiently be indexed and they are easier to understand.

(2) Value score: $\frac{1}{max(1,|max(X)|-7)}$

The values in primary keys are typically short, because they serve to identify records and usually do not contain much business logic. Most relational database management systems (RDBMS) also restrict the maximum length of values in primary key attributes, because primary keys are indexed by default and indices with too long values are more difficult to manage. So we downgrade keys with values longer than 8 characters using the function *max(X)* that returns the longest value in attribute (combination) X; for multiple attributes, *max(X)* concatenates their values.

(3) Position score: $\frac{1}{2}(\frac{1}{|left(X)|+1} + \frac{1}{|between(X)|+1})$
When considering the order of attributes in their relations, key attributes are typically located further at the beginning and without non-key attributes between them. This is intuitive, because humans tend to place keys first and logically coherent attributes together. The position score exploits this by assigning decreasing score values to keys depending on the number of non-key attributes left *left(X)* and between *between(X)* key attributes X.

The formulas we propose for the ranking reflect only our intuition. The list of features is most likely also not complete, but the proposed features produce good results for key scoring in our experiments. For the final *key score*, we simply calculate the mean of the individual scores. In this way, the perfect key in our ranking has one attribute, a maximum value length of 8 characters and position one in the relation, which produces a key score of 1; less perfect keys have lower scores.

After scoring, Normalize ranks the keys by their score and lets the user choose a primary key amongst the top ranked keys; if no user interaction is desired (or possible), the algorithm automatically selects the top-ranked key.

7.7.2 Violating FD selection

During normalization, we need to select some violating FDs for the schema decompositions given the keys of the schema. Because the selected FDs become foreign key constraints after the decompositions, the violating FD selection problem is similar to the foreign key selection problem [Rostin et al., 2009], which scores inclusion dependencies (INDs) for being good foreign keys. The viewpoints are, however, different: Selecting foreign keys from INDs aims to identify semantically correct links between existing tables; selecting foreign keys from FDs, on the other hand, is about forming redundancy-free tables with appropriate keys.

Recall that selecting semantically correct violating FDs is crucial, because some decompositions are mutually exclusive. If possible, a user should also discard violating FDs that hold only accidentally in the given relational instance. Otherwise, Normalize might drive the normalization a bit too far by splitting attribute sets – in particular sparsely populated attributes – into separate relations. In the following, we discuss our features for scoring violating FDs $X \rightarrow Y$ as "good" foreign key constraints:

(1) Length score: $\frac{1}{2}(\frac{1}{|X|} + \frac{|Y|}{|R|-2})$
Because the Lhs X of a violating FD becomes a primary key for the Lhs attributes after decomposition, it should be short in length. The Rhs Y, on the contrary, should be long so that we create large new relations: Large right-hand sides not only raise the confidence of the FD to be semantically correct, they also make the decomposition more effective. Because the Rhs can be at most $|R| - 2$ attributes long in relation R (one

attribute must be X and one must not depend on X so that X is not a key in R), we weight the RHS's length by this factor.

(2) Value score: $\frac{1}{max(1,|max(X)|-7)}$
The value score for a violating FD is the same as the value score for a primary key X, because X becomes a primary key after decomposition.

(3) Position score: $\frac{1}{2}(\frac{1}{|between(X)|+1} + \frac{1}{|between(Y)|+1})$
The attributes of a semantically correct FD are most likely placed close to one another due to their common context. We expect this to hold for both the FD's LHS and RHS. The space between LHS and RHS attributes, however, is only a very weak indicator, and we ignore it. For this reason, we weight the violating FD anti-proportionally to the number of attributes *between* LHS attributes and *between* RHS attributes.

(4) Duplication score: $\frac{1}{2}(2 - \frac{|uniques(X)|}{|values(X)|} - \frac{|uniques(Y)|}{|values(Y)|})$
A violating FD is well suited for normalization if both LHS X and RHS Y contain possibly many duplicate values and, hence, much redundancy. The decomposition can, then, remove many of these redundant values. As for most scoring features, a high duplication score in the LHS values reduces the probability that the FD holds by coincidence, because only duplicate values in an FD's LHS can invalidate the FD and having many duplicate values in LHS X without any violation is a good indicator for its semantic correctness. For scoring, we estimate the number of unique values in X and Y with $|uniques()|$; because exactly calculating this number is computationally expensive, we create a Bloom-filter for each attribute and use their false positive probabilities to efficiently estimate the number of unique values.

We calculate the final *violating FD score* as the mean of the individual scores. In this way, the most promising violating FD is one that has a single LHS attribute determining almost the entire relation with short and few distinct values. Like for the key scoring, the proposed features reflect our intuitions and observations; they might not be optimal or complete, but they produce reasonable results for a difficult selection problem: In our experiments the top-ranked violating FDs usually indicate the semantically best decomposition points.

After choosing a violating FD for becoming a foreign key constraint, we could in principle decide to remove individual attributes from the FD's RHS. One reason might be that these attributes also appear in another FD's RHS and can be used in a subsequent decomposition. So when a user guides the normalization process, we present all RHS attributes that are also contained in other violating FDs. He/she can then decide to remove such attributes. If no user is present, nothing is removed.

7.8 Evaluation

In this section, we evaluate the efficiency and effectiveness of our normalization algorithm NORMALIZE. At first, we introduce our experimental setup. Then, we evaluate the performance of NORMALIZE and, in particular, its closure calculation component. In the end, we assess the quality of the normalization output.

7.8.1 Experimental setup

Hardware. We ran all our experiments on a Dell PowerEdge R620 with two Intel Xeon E5-2650 2.00 GHz CPUs and 128 GB DDR3 RAM. The server runs on CentOS 6.7 and uses OpenJDK 64-Bit 1.8.0_71 as Java environment.

Datasets. We primarily use the synthetic *TPC-H*[4] dataset (scale factor one), which models generic business data, and the *MusicBrainz*[5] dataset, which is a user-maintained encyclopedia on music and artists. To evaluate the effectiveness of NORMALIZE, we denormalized the two datasets by joining all their relations into a single, universal relation. In this way, we can compare the normalization result to the original datasets. For MusicBrainz, we had to restrict this join to eleven selected core tables, because the number of tables in this dataset is huge. We also limited the number of records for the denormalized MusicBrainz dataset, because the associative tables produce an enormous amount of records when used for complete joins. For the efficiency evaluation, we use four additional datasets, namely Horse, Plista, Amalgam1, and Flight. We provide these datasets and more detailed descriptions on our web-page[6]. In our evaluation, each dataset consists of one relation with the characteristics shown in Table 7.3; the input of NORMALIZE can, in general, consist of multiple relations.

Table 7.3: A summary of the datasets we used for our evaluations

Name	Size	Attributes	Records	FDs	FD-Keys
Horse	25.5 kB	27	368	128,727	40
Plista	588.8 kB	63	1000	178,152	1
Amalgam1	61.6 kB	87	50	450,020	2,737
Flight	582.2 kB	109	1000	982,631	25,260
MusicBrainz	1.2 GB	106	1,000,000	12,358,548	0
TPC-H	6.7 GB	52	6,001,215	13,262,106	347,805

7.8.2 Efficiency analysis

Table 7.3 lists six datasets with different properties. The amount of minimal functional dependencies in these datasets is between 128 thousand and 13 million, and thus too great to manually select meaningful ones. The column *FD-Keys* counts all those keys that we can directly derive from the FDs. Their number does not depend on the number of FDs but on the structure of the data: Amalgam1 and TPC-H have a snow-flake schema while, for instance, MusicBrainz has a more complex link structure in its schema.

We executed NORMALIZE on each of these datasets and measured the execution time for the components (1) FD Discovery, (2) Closure Calculation, (3) Key Derivation, and (4) Violating FD Identification. The results are shown in Table 7.4. The first two components, i.e., FD discovery and closure calculation are parallelized so that they fully

[4] `http://tpc.org/tpch`

[5] `https://musicbrainz.org`

[6] `https://hpi.de/naumann/projects/repeatability`

Table 7.4: The processing times of NORMALIZE's components on different datasets

Name	**FD Disc.**	**Closure$_{impr}$**	**Closure$_{opt}$**	**Key Der.**	**Viol. Iden.**
Horse	4,157 ms	1,765 ms	486 ms	40 ms	246 ms
Plista	9,847 ms	6,652 ms	857 ms	49 ms	55 ms
Amalgam1	3,462 ms	745 ms	333 ms	7 ms	25 ms
Flight	20,921 ms	132,085 ms	1,662 ms	77 ms	93 ms
MusicBrainz	2,132 min	215.5 min	1.4 min	331 ms	26 ms
TPC-H	3,651 min	3.8 min	0.5 min	163 ms	4093 ms

use all 32 cores of our evaluation machine. Despite the parallelization, the necessary discovery of the complete set of FDs still requires 36 and 61 hours on the two larger datasets, respectively.

First of all, we notice that the key derivation and violating FD identification steps are much faster than the FD discovery and closure calculation steps; they usually finish in less than a second. This is important, because the two components are executed multiple times in the normalization process and a user might be in the loop interacting with the system at the same time. In Table 7.4, we show only the execution times for the first call of these components; subsequent calls can be handled even faster, because their input sizes shrink continuously. The time needed to determine the violating FDs depends primarily on the number of FD-keys, because the search for LHS generalizations in the trie of keys is the most expensive operation. This explains the long execution time of 4 seconds for the TPC-H dataset.

For the closure calculation, Table 7.4 shows the execution times of the improved (*impr*) and optimized (*opt*) algorithm. The naive algorithm already took 13 seconds for the Amalgam1 dataset (compared to less than 1 s for both *impr* and *opt*), 23 minutes for Horse (<2 s and <1 s for *impr* and *opt*, respectively), and 41 minutes for Plista (<7 s and <1 s). These runtimes are so much worse than the improved and optimized algorithm versions that we stopped testing it. The optimized closure algorithm, then, outperforms the improved version by factors of 2 (Amalgam1) to 159 (MusicBrainz), because it can exploit the completeness of the given FD set. The more extensions of right-hand sides the algorithm must perform, the higher this advantage becomes. The average RHS size for Amalgam1 FDs, for instance, increases from 32 to 56, whereas the average RHS size for MusicBrainz FDs increases from 3 to 40. For TPC-H, the average RHS size increases from 10 to 23. The runtimes of the optimized closure calculation are, overall, acceptable when compared to the FD discovery time. Therefore, it is not necessary to filter FDs prior to the closure calculation.

Because closure calculation is not only important for normalization but for many other use cases as well, Figure 7.2 analyses the scalability of this step in more detail. The graphs show the execution times of the improved and the optimized algorithm for an increasing number of input FDs. The experiment takes these input FDs randomly from the 12 million MusicBrainz FDs; the number of attributes is kept constant to 106. We again omit the naive algorithm, because it is orders of magnitude slower than both other approaches.

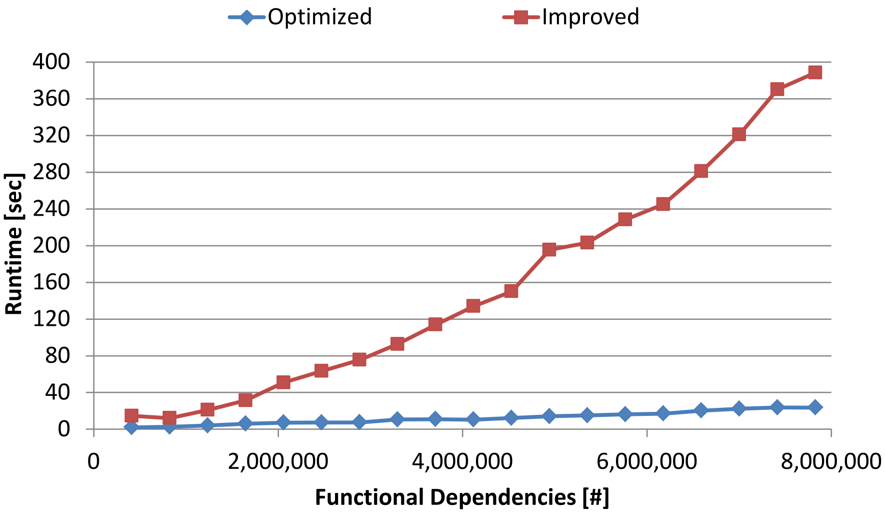

Figure 7.2: Scaling the number of input FDs for closure calculation.

Both runtimes in Figure 7.2 appear to scale almost linearly with the number of FDs, because the extension costs for each single FD are low due to the efficient index lookups. Nevertheless, the index lookups become more expensive with an increasing number of FDs in the indexes (and they would also become more numerous, if we would increase the number of attributes as well). Because the improved algorithm performs the index lookups more often than the optimized version (i.e. changed loop) and with larger search keys (i.e. Lhs and Rhs), the optimized version is faster and scales better with the number of FDs: It is from 4 to 16 times faster in this experiment.

7.8.3 Normalization quality

For a fair effectiveness analysis, we perform the normalization automatically, i.e., without human interaction. Under human supervision, better (but possibly also worse) schemata than presented below can be produced. For the following experiments, we focus on TPC-H and MusicBrainz, because we denormalized these datasets before so that we can use their original schemata as gold standards for their normalization results.

Figure 7.3 shows the BCNF normalized TPC-H dataset. The color coding indicates the original relations of the different attributes. We first notice that Normalize almost perfectly restored the original TPC-H schema: We can identify all original relations in the normalized result. The automatically selected constraints, i.e., keys and foreign keys are all correct w.r.t. the original schema, which is possible because the original schema was snow-flake shaped. Note that the normalization does not automatically produce meaningful table names for the new relations and we labeled the reconstruced relations with their previous names; finding good names for *new* relations is still an open research topic.

Nevertheless, we also observe two interesting flaws in the automatically normalized schema: First, Normalize decomposed the LINEITEM relation a bit too far; syntactically, the result is correct and perfectly BCNF-conform, but semantically, the splits with

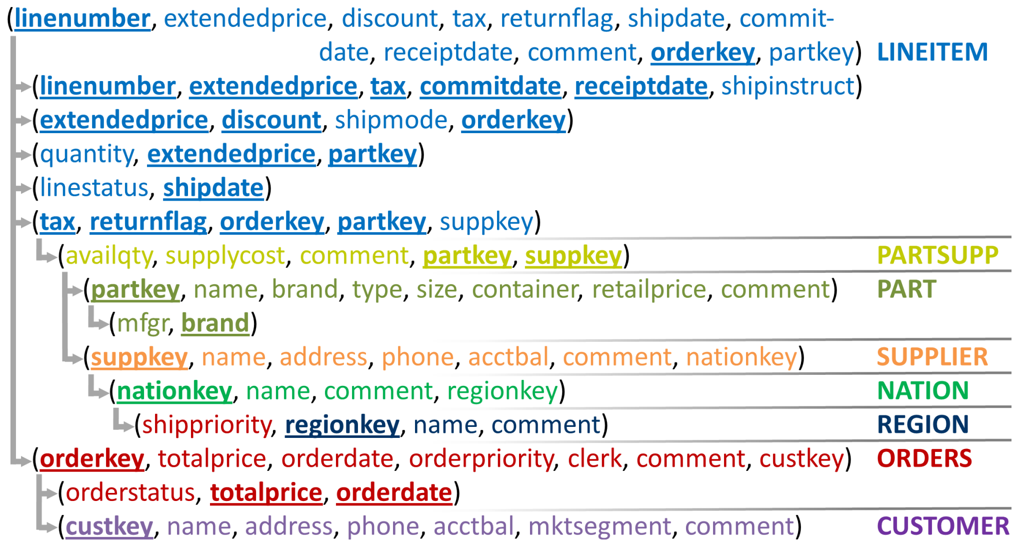
(linenumber, extendedprice, discount, tax, returnflag, shipdate, commitdate, receiptdate, comment, orderkey, partkey) LINEITEM
(linenumber, extendedprice, tax, commitdate, receiptdate, shipinstruct)
(extendedprice, discount, shipmode, orderkey)
(quantity, extendedprice, partkey)
(linestatus, shipdate)
(tax, returnflag, orderkey, partkey, suppkey)
(availqty, supplycost, comment, partkey, suppkey) PARTSUPP
(partkey, name, brand, type, size, container, retailprice, comment) PART
(mfgr, brand)
(suppkey, name, address, phone, acctbal, comment, nationkey) SUPPLIER
(nationkey, name, comment, regionkey) NATION
(shippriority, regionkey, name, comment) REGION
(orderkey, totalprice, orderdate, orderpriority, clerk, comment, custkey) ORDERS
(orderstatus, totalprice, orderdate)
(custkey, name, address, phone, acctbal, mktsegment, comment) CUSTOMER

Figure 7.3: Relations after normalizing TPC-H.

only one dependent and more than three foreign key attributes are not reasonable. Second, the attribute shippriority originally belongs to the ORDERS relation but was placed into the REGION relation. This is syntactically a good decision, because the region also determines the shipping priority in the given data and putting the attribute into this relation removes more redundant values than putting it into the ORDERS relation.

Figure 7.4 shows the BCNF-normalized MusicBrainz dataset. Although MusicBrainz has originally no snow-flake schema, Normalize was still able to reconstruct almost all original relations. Only ARTIST_CREDIT_NAME was not reconstructed and its attributes now lie in the semantically related ARTIST relation. Because MusicBrainz is originally not snow-flake shaped, the normalization produced a new top-level relation that represents all many-to-many relationships between artists, places, release labels, and tracks. This top-level relation can be likened to a fact table.

Most mistakes are made for the ARTIST_CREDIT relation, which was the first proposed split. This split took away some attributes from other relations, because these attributes do not contain many values and assigning them to the ARTIST_CREDIT relation makes syntactically sense. A human expert, if involved, would have likely avoided that, because Normalize does report to the user that these attributes are also dependent on other violating FDs Lhs attributes. Overall, however, the normalization result is quite satisfactory, keeping in mind that no human was involved in creating it.

We also tested Normalize on various other datasets with similar findings: If datasets have been de-normalized before, we can find the original tables in the proposed schema; if sparsely populated columns exist, these are often moved into smaller relations; and if no human is in the loop, some decompositions become detailed. All results were BCNF-conform and semantically understandable.

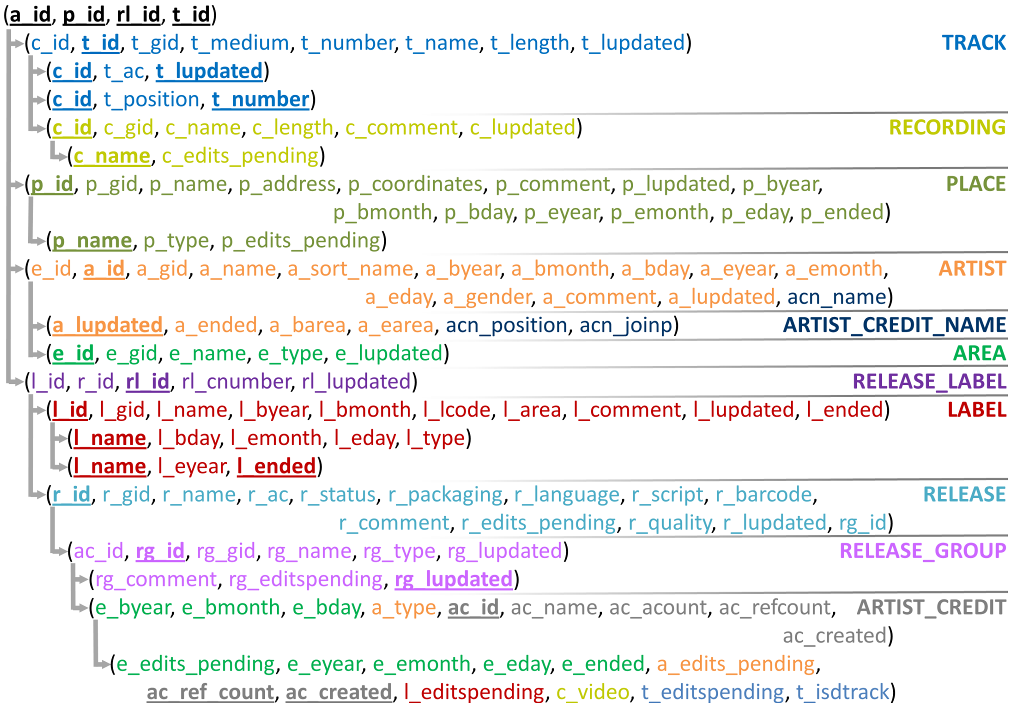
(a_id, p_id, rl_id, t_id)
(c_id, t_id, t_gid, t_medium, t_number, t_name, t_length, t_lupdated)
TRACK
(c_id, t_ac, t_lupdated)
(c_id, t_position, t_number)
(c_id, c_gid, c_name, c_length, c_comment, c_lupdated)
RECORDING
(c_name, c_edits_pending)
(p_id, p_gid, p_name, p_address, p_coordinates, p_comment, p_lupdated, p_byear, p_bmonth, p_bday, p_eyear, p_emonth, p_eday, p_ended)
PLACE
(p_name, p_type, p_edits_pending)
(e_id, a_id, a_gid, a_name, a_sort_name, a_byear, a_bmonth, a_bday, a_eyear, a_emonth, a_eday, a_gender, a_comment, a_lupdated, acn_name)
ARTIST
(a_lupdated, a_ended, a_barea, a_earea, acn_position, acn_joinp)
ARTIST_CREDIT_NAME
(e_id, e_gid, e_name, e_type, e_lupdated)
AREA
(l_id, r_id, rl_id, rl_cnumber, rl_lupdated)
RELEASE_LABEL
(l_id, l_gid, l_name, l_byear, l_bmonth, l_lcode, l_area, l_comment, l_lupdated, l_ended)
LABEL
(l_name, l_bday, l_emonth, l_eday, l_type)
(l_name, l_eyear, l_ended)
(r_id, r_gid, r_name, r_ac, r_status, r_packaging, r_language, r_script, r_barcode, r_comment, r_edits_pending, r_quality, r_lupdated, rg_id)
RELEASE
(ac_id, rg_id, rg_gid, rg_name, rg_type, rg_lupdated)
RELEASE_GROUP
(rg_comment, rg_editspending, rg_lupdated)
(e_byear, e_bmonth, e_bday, a_type, ac_id, ac_name, ac_acount, ac_refcount, ac_created)
ARTIST_CREDIT
(e_edits_pending, e_eyear, e_emonth, e_eday, e_ended, a_edits_pending, ac_ref_count, ac_created, l_editspending, c_video, t_editspending, t_isdtrack)

Figure 7.4: Relations after normalizing MusicBrainz.

7.9 Conclusion & Future Work

We proposed Normalize, an instance-driven, (semi-) automatic algorithm for schema normalization. The algorithm has shown that functional dependency profiling results of any size can efficiently be used for the specific task of schema normalization. We also presented techniques for guiding the BCNF decomposition algorithm in order to produce semantically good normalization results that also conform to changes of the data.

Our implementation is publicly available at `http://hpi.de/naumann/projects/repeatability`. It is currently console-based, offering only basic user interaction. Future work shall concentrate on emphasizing the user-in-the-loop, for instance, by employing graphical previews of normalized relations and their connections. We also suggest research on other features for the key and foreign key selection that may yield even better results. Another open research question is how normalization processes should handle dynamic data and errors in the data.

8

Conclusion and Future Work

In this thesis, we introduced the three novel profiling algorithms HyFD, HyUCC, and Binder for the discovery of the three most popular types of complex metadata: FDs, UCCs, and INDs. With the use of algorithmic paradigms, such as divide-and-conquer, hybrid search, progressivity, memory sensitivity, parallelization, and additional pruning, our algorithms greatly improve upon the performance of related discovery algorithms; in particular, they are now able to process datasets of real-world, i.e., multiple gigabytes size. The algorithms also sparked the development of various further profiling algorithms that discover other types of metadata with the same algorithmic techniques.

We also developed Metanome, a prototype for a next generation profiling platform. Metanome was built to make state-of-the-art profiling techniques available to data scientists and IT-professionals. Its core features are the flexible integration of profiling algorithms, the standardization of the profiling process, and first metadata management features. The prototype already influenced the development of commercial profiling products at SAP and IBM.

Being able to discover large amounds of metadata introduced a new challenge to data profiling, namely the utilization of these results for actual use cases. With Normalize, we showed how these large metadata sets can be used to efficiently and effectively transform a schema into BCNF: The algorithm proposes a data-driven, (semi-)automatic normalization process that iteratively selects semantically most suitable dependencies. Other use cases might require alternative solutions, but Normalize exemplified that complete, discovered metadata sets can improve the way these use cases are solved.

During my PhD-study, I also co-developed several profiling algorithms that I could not discuss in this thesis due to its limited scope. These algorithms include MDMinder [Mascher, 2013], Sindy [Kruse et al., 2015], Aid-FD [Bleifuß et al., 2016], MvdDetector [Draeger, 2016], RDFind [Kruse et al., 2016a], Muds [Ehrlich et al., 2016], Faida [Kruse et al., 2017], and Many [Tschirschnitz et al., 2017].

Although we could already improve several aspects of data profiling within the Metanome project, several profiling tasks are still insufficiently solved and, therefore, demand for future work:

Partial and conditional dependencies In this work, we focussed on the *exact* discovery of dependencies. The next step is to extend the discovery algorithms for partial and conditional versions of these dependencies. To achive this, the algorithms require a notion of error tolerance and the ability to counterbalance these errors with conditions. As discussed in Section 1.2.3, related work has already shown how such extensions could be build.

Distributed data profiling The use of parallelization has clearly improved the runtime of HyFD and HyUCC. We did not use parallelization in Binder, because Binder is mostly I/O bound, i.e., reading and writing bucket files. Distributing these and other profiling algorithms could, therefore, have further beneficial effects on their performances, because it allows to not only parellelize processing efforts but also I/O operations. The challenge in developing distribution profiling algorithms is to efficiently communicate necessary pruning decisions between the different computing nodes. For IND discovery, our Sindy algorithm [Kruse et al., 2015], which is not contained in this thesis, has shown that distribution does pay off at a certain degree of parallelization.

Data-driven use cases Data profiling algorithms are now able to discover the metadata of real-world sized datasets and these metadata results are surprisingly large – larger, in particular, than most state-of-the-art solutions for use cases of metadata expect. A task for future work is, therefore, to develop new solutions that are able to utilize these large metadata sets. With Normalize, we already exemplified the deployment of discovered functional dependencies for the use case of schema normalization. Other use cases that still require data-driven solutions are, for instance, data exploration, query optimization, schema matching, and data cleaning.

Incremental data profiling Most datasets are non-static, i.e., they are subject to change. Changes, which are inserts, updates, and deletes, also change the datasets' metadata making it necessary to frequently re-profile the data. Because exhaustive data profiling processes are expensive, incremental profiling methods are needed to maintain the metadata under the event of data changes. The works of [Wang et al., 2003] and [Abedjan et al., 2014b] are first approaches to this research area.

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Selbstständigkeitserklärung

Ich erkläre hiermit, dass ich die vorliegende Doktorarbeit mit dem Thema:

Data Profiling – Efficient Discovery of Dependencies

selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe.

Potsdam, den 29. Juni 2017