

# Responsible Data Science

Association rule mining  
data profiling continued

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**Prof. Julia Stoyanovich**

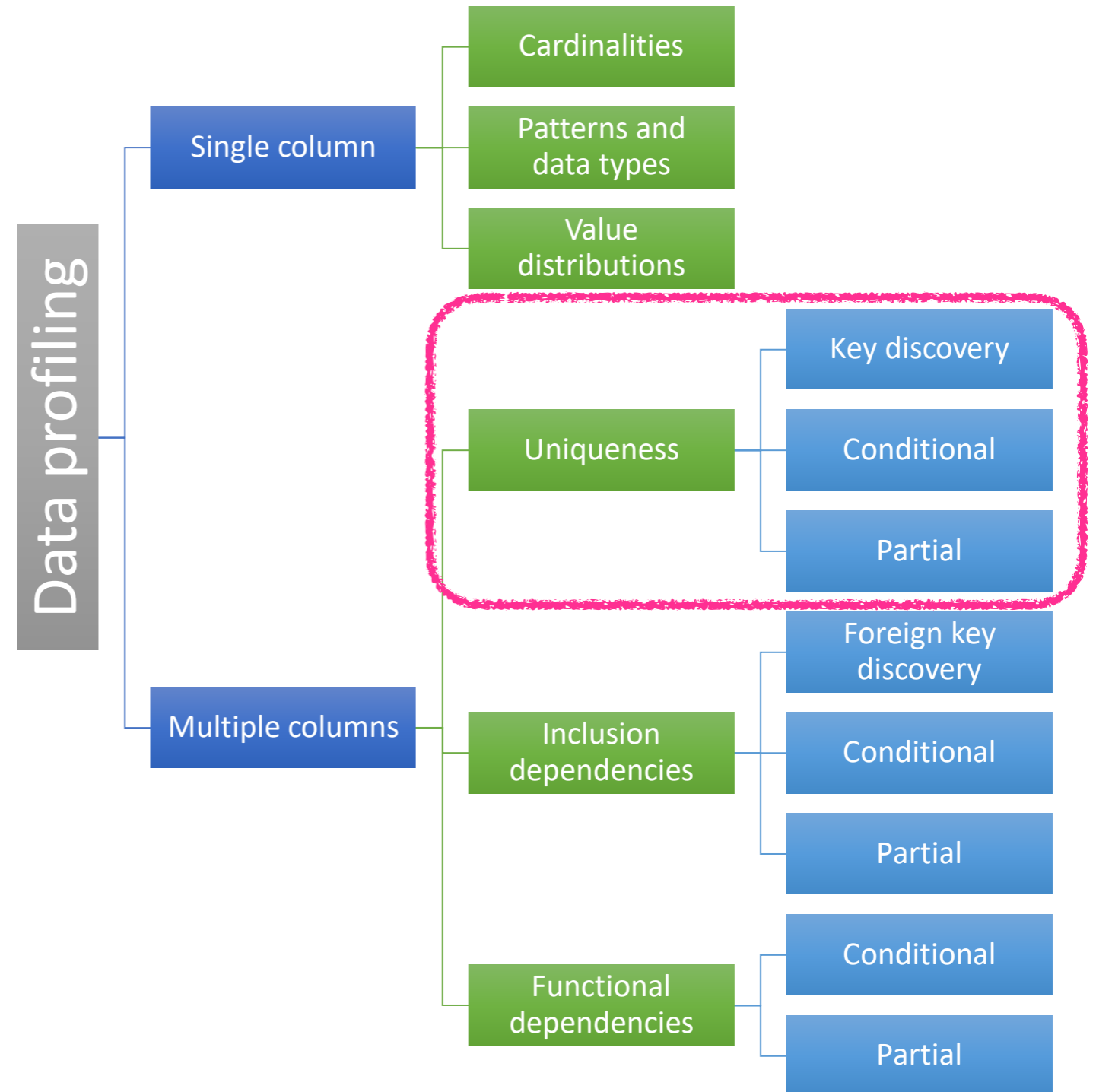
Center for Data Science &  
Computer Science and Engineering  
New York University

# Classification of data profiling tasks

[Abedjan, Golab, Naumann; *SIGMOD 2017*]

	A	B	C	D	E	F	G	H
1	UID	sex	race	MarriageSta	DateOfBirth	age	juv_fel_cour	decile_score
2	1	0	1	1	4/18/47	69	0	1
3	2	0	2	1	1/22/82	34	0	3
4	3	0	2	1	5/14/91	24	0	4
5	4	0	2	1	1/21/93	23	0	8
6	5	0	1	2	1/22/73	43	0	1
7	6	0	1	3	8/22/71	44	0	1
8	7	0	3	1	7/23/74	41	0	6
9	8	0	1	2	2/25/73	43	0	4
10	9	0	3	1	6/10/94	21	0	3
11	10	0	3	1	6/1/88	27	0	4
12	11	1	3	2	8/22/78	37	0	1
13	12	0	2	1	12/2/74	41	0	4
14	13	1	3	1	6/14/68	47	0	1
15	14	0	2	1	3/25/85	31	0	3
16	15	0	4	4	1/25/79	37	0	1
17	16	0	2	1	6/22/90	25	0	10
18	17	0	3	1	12/24/84	31	0	5
19	18	0	3	1	1/8/85	31	0	3
20	19	0	2	3	6/28/51	64	0	6
21	20	0	2	1	11/29/94	21	0	9
22	21	0	3	1	8/6/88	27	0	2
23	22	1	3	1	3/22/95	21	0	4
24	23	0	4	1	1/23/92	24	0	4
25	24	0	3	3	1/10/73	43	0	1
26	25	0	1	1	8/24/83	32	0	3
27	26	0	2	1	2/8/89	27	0	3
28	27	1	3	1	9/3/79	36	0	3
29	28	0	2	1	4/27/88	26	0	7

relational data (here: just one table)



# Discovering uniques

Given a relation schema  $R(A, B, C, D)$  and a relation instance  $r$ , a **unique column combination** (or a “**unique**” for short) is a set of attributes  $X$  whose **projection** contains no duplicates in  $r$

*Episodes*(*season, num, title, viewers*)

season	num	title	viewers
1	1	Winter is Coming	2.2 M
1	2	The Kingsroad	2.2 M
2	1	The North Remembers	3.9 M

**Projection** is a relational algebra operation that takes as input relation  $R$  and returns a new relation  $R'$  with a subset of the columns of  $R$ .

$\pi_{season}(Episodes)$

season
1
1
2

non-unique

$\pi_{season,num}(Episodes)$

season	num
1	1
1	2
2	1

unique

$\pi_{title}(Episodes)$

title
Winter is Coming
The Kingsroad
The North Remembers

unique

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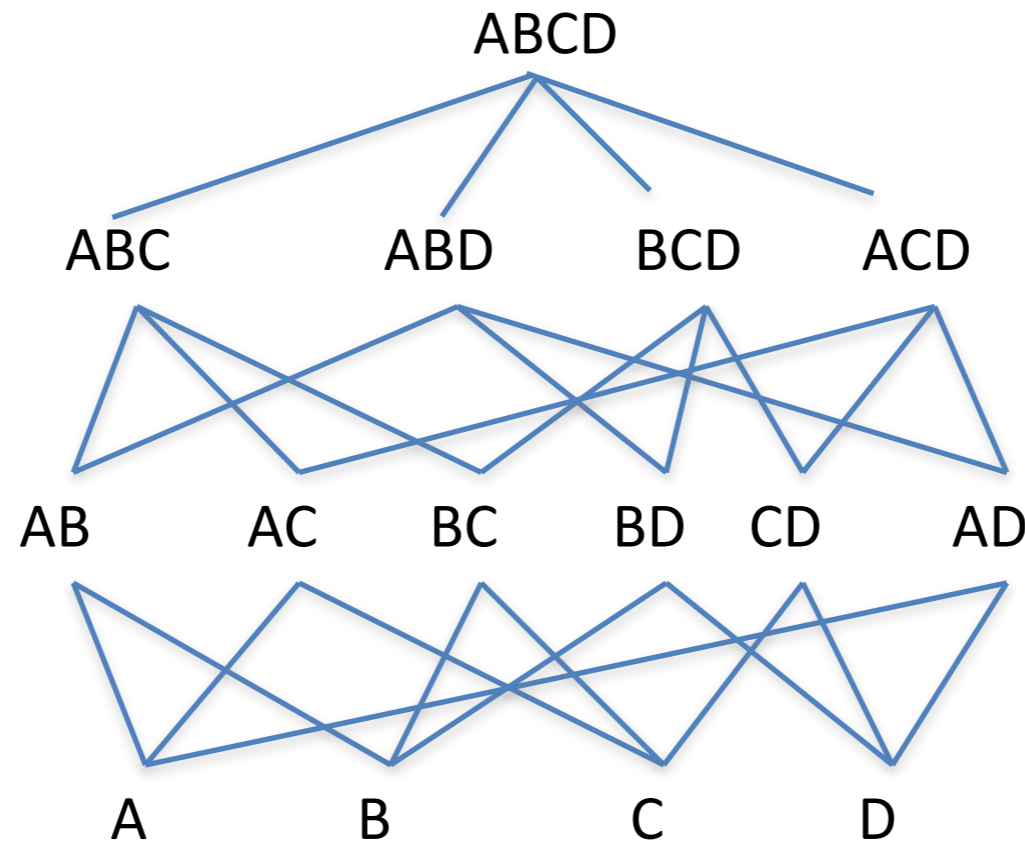
**Projection** is a relational algebra operation that takes as input relation  $R$  and returns a new relation  $R'$  with a subset of the columns of  $R$ .

- Recall that more than one set of attributes  $X$  may be unique
- It may be the case that  $X$  and  $Y$  are both unique, and that they are not disjoint. When is this interesting?

# Discovering uniques

R (A, B, C, D)

attribute lattice of **R**



$$\binom{4}{4} = 1$$
$$\binom{4}{3} = 4$$
$$\binom{4}{2} = 6$$
$$\binom{4}{1} = 4$$

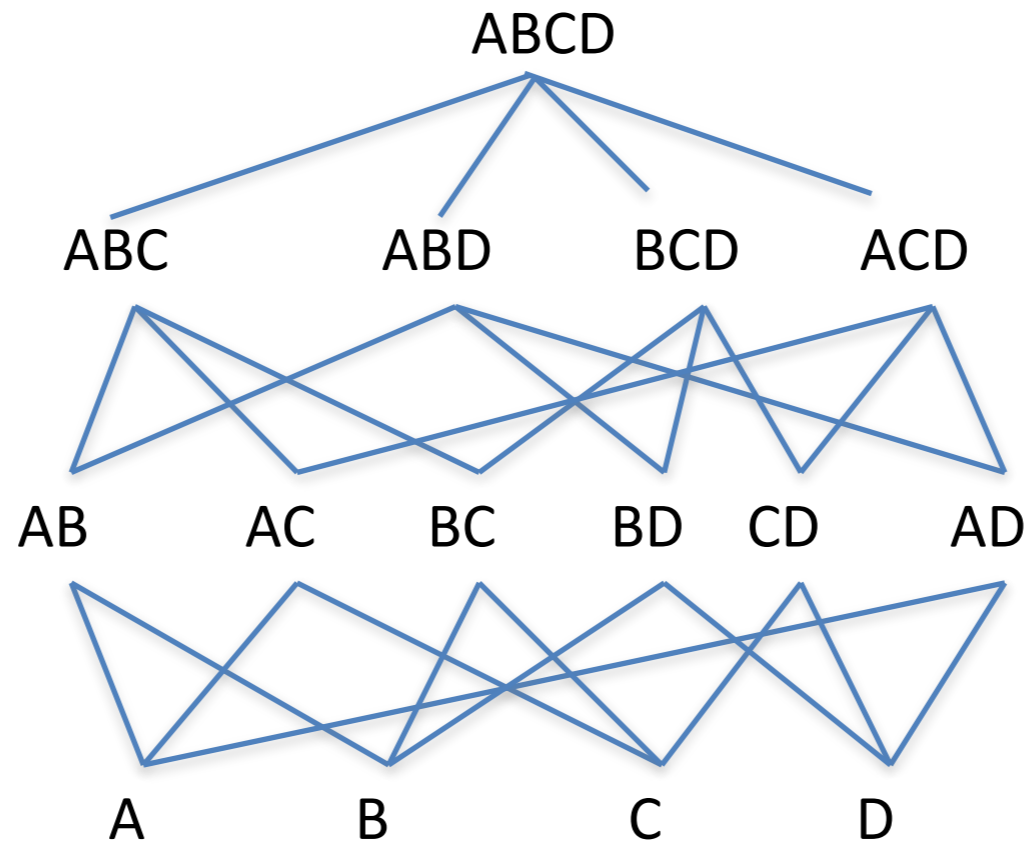
What's the size of the attribute lattice of **R**?

**Look at all attribute combinations?**

# Discovering uniques

R (A, B, C, D)

attribute lattice of R



- If **X** is unique, then what can we say about its **superset Y**?
- If **X** is non-unique, then what can we say about its **subset Z**?

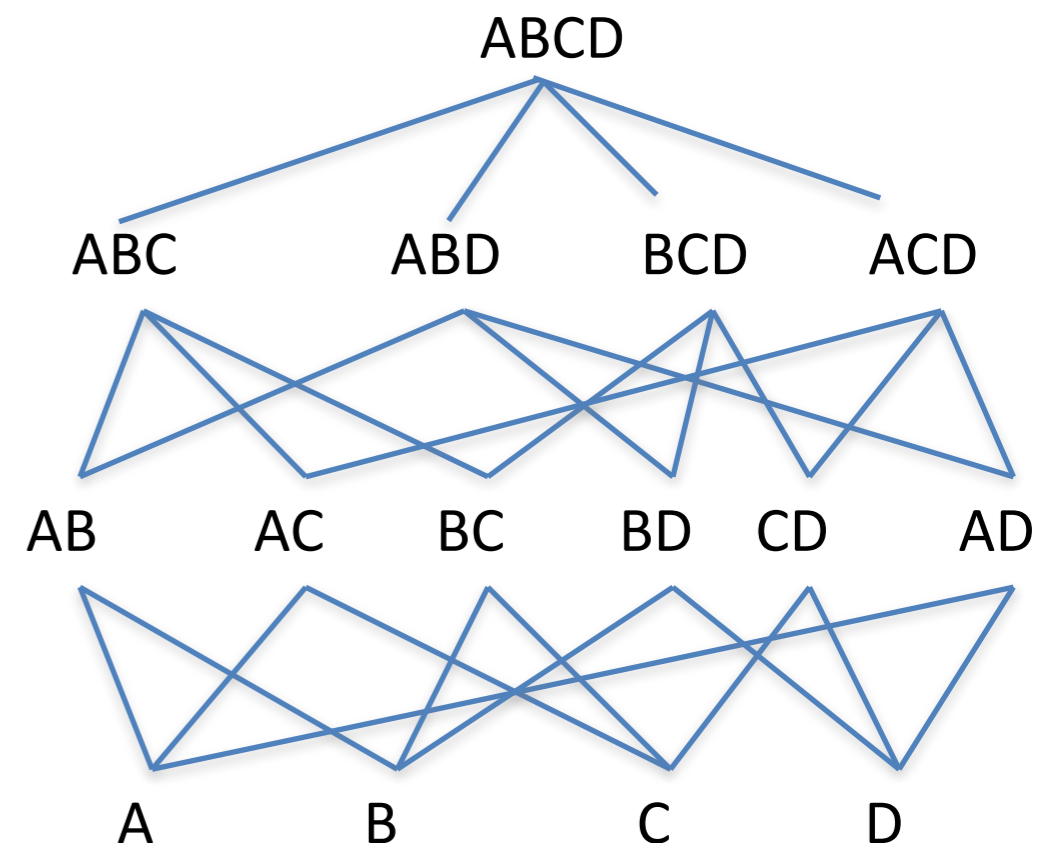
# Discovering uniques

Given a relation schema  $R (A, B, C, D)$  and a relation instance  $r$ , a **unique column combination** (or a “**unique**” for short) is a set of attributes  $X$  whose **projection** contains no duplicates in  $r$

Given a relation schema  $R (A, B, C, D)$  and a relation instance  $r$ , a set of attributes  $Y$  is **non-unique** if its projection contains duplicates in  $r$

$X$  is **minimal unique** if every subset  $Y$  of  $X$  is non-unique

$Y$  is maximal non-unique if every superset  $X$  of  $Y$  is unique



# From uniques to candidate keys

Given a relation schema  $R(A, B, C, D)$  and a relation instance  $r$ , a **unique column combination** is a set of attributes  $X$  whose **projection** contains no duplicates in  $r$

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A set of attributes is a **candidate key** for a relation if:

- (1) no two distinct tuples can have the same values for all key attributes (candidate key **uniquely identifies** a tuple), *and*
- (2) this is not true for any subset of the key attributes (candidate key **is minimal**)

**A minimal unique of a relation instance is a (possible) candidate key of the relation schema.** To find all possible candidate keys, find all minimal uniques in a relation instance.





**association rule  
mining**

# The early days of data mining

- Problem formulation due to Agrawal, Imielinski, Swami, SIGMOD 1993
- Solution: the **Apriori** algorithm by Agrawal & Srikant, VLDB 1994
- Initially for **market-basket data** analysis, has many other applications, we'll see one today
- We wish to answer two related questions:
  - **Frequent itemsets:** Which items are often purchased together, e.g., milk and cookies are often bought together
  - **Association rules:** Which items will likely be purchased, based on other purchased items, e.g., if diapers are bought in a transaction, beer is also likely bought in the same transaction

# Market-basket data

- $I = \{i_1, i_2, \dots, i_m\}$  is the set of available items, e.g., a product catalog of a store
- $X \subseteq I$  is an **itemset**, e.g., {milk, bread, cereal}
- **Transaction**  $t$  is a set of items purchased together,  $t \subseteq I$ , has a transaction id (TID)
  - $t_1$ : {bread, cheese, milk}
  - $t_2$ : {apple, eggs, salt, yogurt}
  - $t_3$ : {biscuit, cheese, eggs, milk}
- Database  $T$  is a set of transactions  $\{t_1, t_2, \dots, t_n\}$
- A transaction  $t$  **supports** an itemset  $X$  if  $X \subseteq t$
- Itemsets supported by at least **minSupp** transactions are called **frequent itemsets**

**minSupp, which can be a number or a percentage, is specified by the user**

# Itemsets

TID	Items
1	A
2	A C
3	A B D
4	A C
5	A B C
6	A B C

**minSupp** = 2 transactions

How many possible itemsets are there (excluding the empty itemset)?

$$2^4 - 1 = 15$$

	itemset	support
★	A	6
★	B	3
★	C	4
	D	1
★	A B	3
★	A C	4
	A D	1
★	B C	2
	B D	1
	C D	0
★	A B C	2
	A B D	1
	B C D	0
	A C D	0
	A B C D	0

# Association rules

An **association rule** is an implication  $X \rightarrow Y$ , where  $X, Y \subset I$ , and  $X \cap Y = \emptyset$

example:  $\{\text{milk, bread}\} \rightarrow \{\text{cereal}\}$

“A customer who purchased  $X$  is also likely to have purchased  $Y$  in the same transaction”

we are interested in rules with a **single item** in  $Y$

can we represent  $\{\text{milk, bread}\} \rightarrow \{\text{cereal, cheese}\}$ ?

Rule  $X \rightarrow Y$  holds with **support**  $supp$  in  $T$  if  $supp$  of transactions contain  $X \cup Y$

Rule  $X \rightarrow Y$  holds with **confidence**  $conf$  in  $T$  if  $conf$  % of transactions that contain  $X$  also contain  $Y$

$$conf \approx \Pr(Y | X)$$

$$conf(X \rightarrow Y) = \frac{supp(X \cup Y)}{supp(X)}$$

# Association rules

**minSupp** = 2 transactions  
**minConf** = 0.75

supp = 3	
$A \rightarrow B$	conf = $3 / 6 = 0.5$
$B \rightarrow A$	conf = $3 / 3 = 1.0$ ★
<hr/>	
supp = 2	
$B \rightarrow C$	conf = $2 / 3 = 0.67$
$C \rightarrow B$	conf = $2 / 4 = 0.5$
<hr/>	
supp = 4	
$A \rightarrow C$	conf = $4 / 6 = 0.67$
$C \rightarrow A$	conf = $4 / 4 = 1.0$ ★
<hr/>	
supp = 2	
$AB \rightarrow C$	conf = $2 / 3 = 0.67$
$AC \rightarrow B$	conf = $2 / 4 = 0.5$
$BC \rightarrow A$	conf = $2 / 2 = 1.0$ ★

itemset	support
★ A	6
★ B	3
★ C	4
D	1
<hr/>	
★ A B	3
★ A C	4
A D	1
★ B C	2
B D	1
C D	0
<hr/>	
★ A B C	2
A B D	1
B C D	0
A C D	0
<hr/>	
A B C D	0

$$conf(X \rightarrow Y) = \frac{supp(X \cup Y)}{supp(X)}$$

# Association rule mining

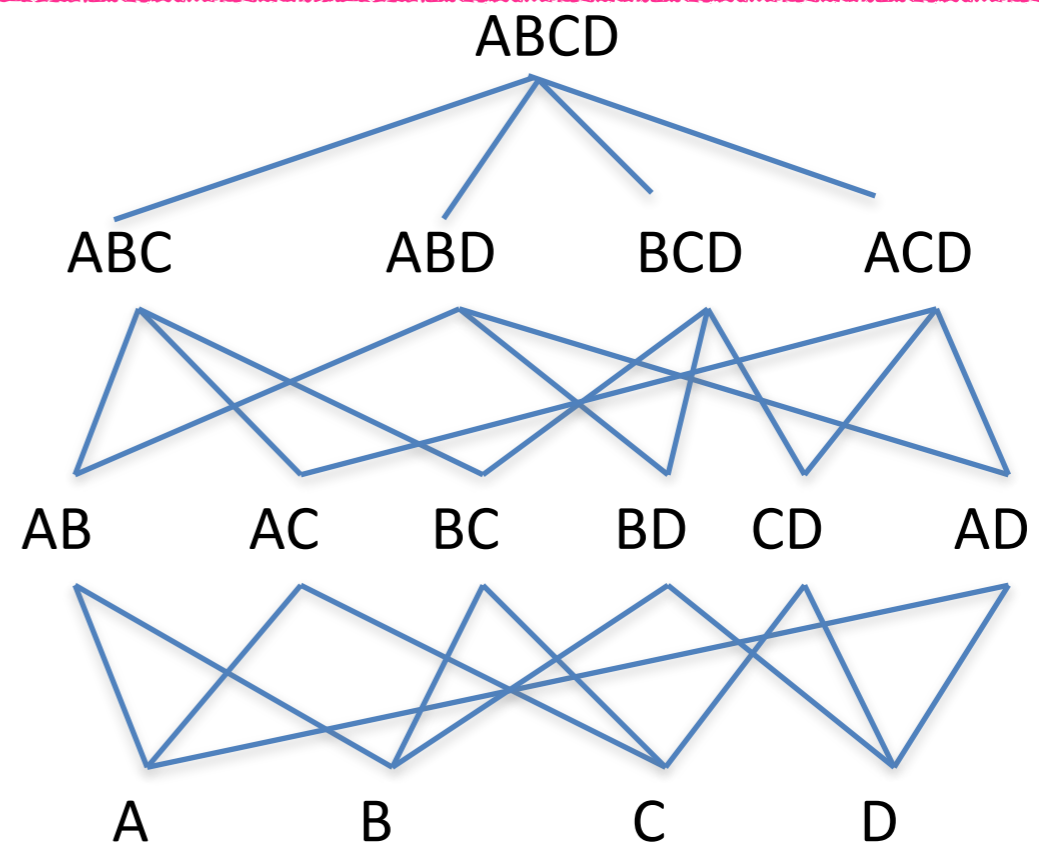
- Goal: find all association rules that satisfy the user-specified minimum support and minimum confidence
- Algorithm outline
  - Step 1: find all frequent itemsets
  - Step 2: find association rules
- Take 1: naïve algorithm for frequent itemset mining
  - Enumerate all subsets of  $I$ , check their support in  $T$
  - **What is the complexity?**

# Key idea: downward closure

itemset	support
★ A	6
★ B	3
★ C	4
D	1
<hr/>	
★ A B	3
★ A C	4
A D	1
★ B C	2
B D	1
C D	0
<hr/>	
★ A B C	2
A B D	1
B C D	0
A C D	0
<hr/>	
A B C D	0

All subsets of a frequent itemset **X** are themselves frequent

So, if some subset of  $X$  is infrequent, then  $X$  cannot be frequent, we know this **apriori**



The converse is not true! If all subsets of **X** are frequent, **X** is not guaranteed to be frequent



# The *Apriori* algorithm

```
Algorithm Apriori( $T, minSupp$ )
   $F_1 = \{\text{frequent 1-itemsets}\};$ 
  for ( $k = 2; F_{k-1} \neq \emptyset; k++$ ) do
     $C_k \leftarrow \text{candidate-gen}(F_{k-1});$ 
    for each transaction  $t \in T$  do
      for each candidate  $c \in C_k$  do
        if  $c$  is contained in  $t$  then
           $c.count++;$ 
        end
      end
    end
     $F_k \leftarrow \{c \in C_k \mid c.count \geq minSupp\}$ 
  end
  return  $F \leftarrow \bigcup_k F_k;$ 
```

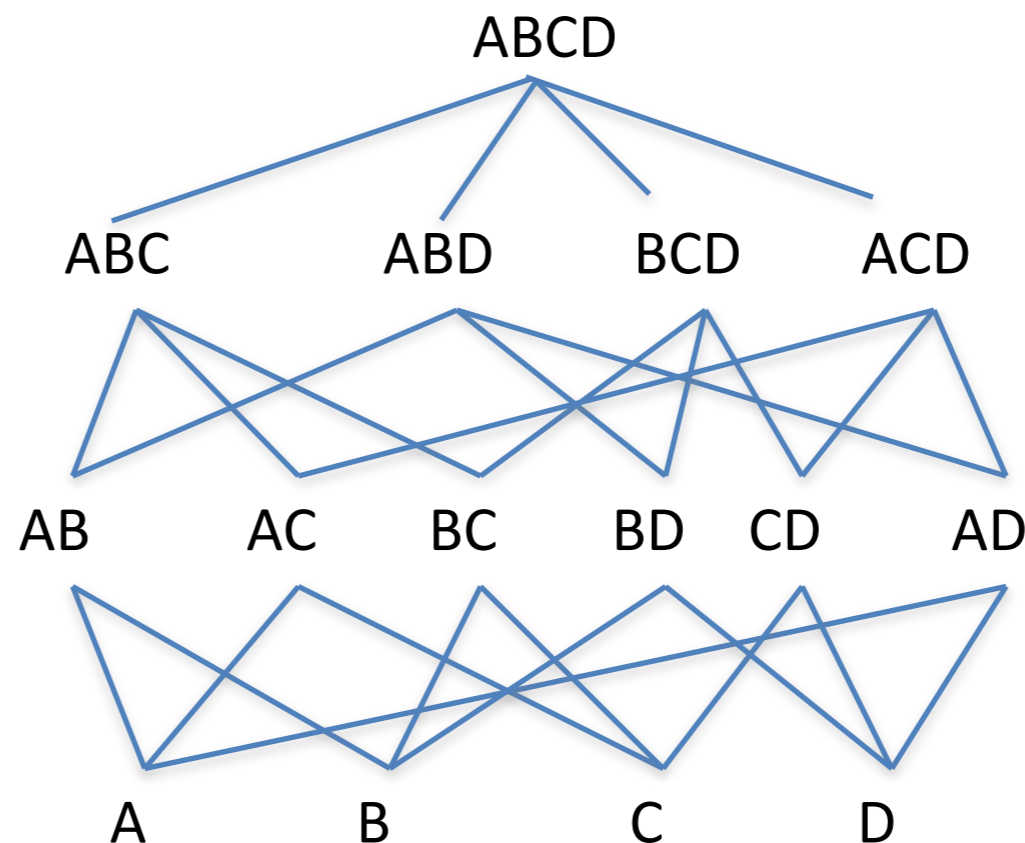
	itemset	support
★	A	6
★	B	3
★	C	4
	D	1
<hr/>		
★	A B	3
★	A C	4
	A D	1
★	B C	2
	B D	1
	C D	0
<hr/>		
★	A B C	2
	A B D	1
	B C D	0
	A C D	0
<hr/>		
	A B C D	0

# Candidate generation

The **candidate-gen** function takes  $F_{k-1}$  and returns a superset (called the candidates) of the set of all frequent  $k$ -itemsets. It has two steps:

**Join:** generate all possible candidate itemsets  $C_k$  of length  $k$

**Prune:** optionally remove those candidates in  $C_k$  that have infrequent subsets



# Candidate generation: join

```

Insert into  $C_k$  (
select  p.item1, p.item2, ..., p.itemk-1, q.itemk-1
from     $F_{k-1}$  p,  $F_{k-1}$  q
where   p.item1 = q.item1
        and      p.item2 = q.item2
        and      ...
        and      p.itemk-1 < q.itemk-1)
    
```

$F_1$  as p

A
B
C

$F_1$  as q

A
B
C

$C_2$

A	B
A	C
B	C

	itemset	support
★	A	6
★	B	3
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★	A B	3
★	A C	4
	A D	1
★	B C	2
	B D	1
	C D	0
★	A B C	2
	A B D	1
	B C D	0
	A C D	0
	A B C D	0

# Candidate generation: join

Insert into  $C_k$  (  
 select  $p.item_1, p.item_2, \dots, p.item_{k-1}, q.item_{k-1}$   
 from  $F_{k-1} p, F_{k-1} q$   
 where  $p.item_1 = q.item_1$   
 and  $p.item_2 = q.item_2$   
 and ...  
 and  $p.item_{k-1} < q.item_{k-1}$ )

$F_2$  as  $p$

A	B
A	C
B	C

$F_2$  as  $q$

A	B
A	C
B	C

$C_3$

A	B	C
---	---	---

itemset	support
★ A	6
★ B	3
★ C	4
D	1
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A D	1
★ B C	2
B D	1
C D	0
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A B D	1
B C D	0
A C D	0
A B C D	0

# Candidate generation

Assume a lexicographic ordering of the items

## Join

```
Insert into  $C_k$  (  
  select   $p.item_1, p.item_2, \dots, p.item_{k-1}, q.item_{k-1}$   
  from     $F_{k-1} p, F_{k-1} q$   
  where    $p.item_1 = q.item_1$   
  and      $p.item_2 = q.item_2$   
  and     ...  
  and      $p.item_{k-1} < q.item_{k-1}$  ) why not  $p.item_{k-1} \neq q.item_{k-1}$ ?
```

## Prune

```
for each  $c$  in  $C_k$  do  
  for each  $(k-1)$  subset  $s$  of  $c$  do  
    if ( $s$  not in  $F_{k-1}$ ) then  
      delete  $c$  from  $C_k$ 
```

# Generating association rules

Rules =  $\emptyset$

**for** each frequent *k-itemset*  $X$  **do**

**for** each 1-itemset  $A \subset X$  **do**

        compute  $\text{conf}(X / A \rightarrow A) = \text{supp}(X) / \text{sup}(X / A)$

**if**  $\text{conf}(X / A \rightarrow A) \geq \text{minConf}$  **then**

            Rules  $\leftarrow$  " $X / A \rightarrow A$ "

**end**

**end**

**end**

**return** Rules

# Performance of *Apriori*

- The possible number of frequent itemsets is exponential,  $O(2^m)$ , where  $m$  is the number of items
- Apriori exploits sparseness and locality of data
  - Still, it may produce a large number of rules: thousands, tens of thousands, ....
  - So, thresholds should be set carefully. **What are some good heuristics?**

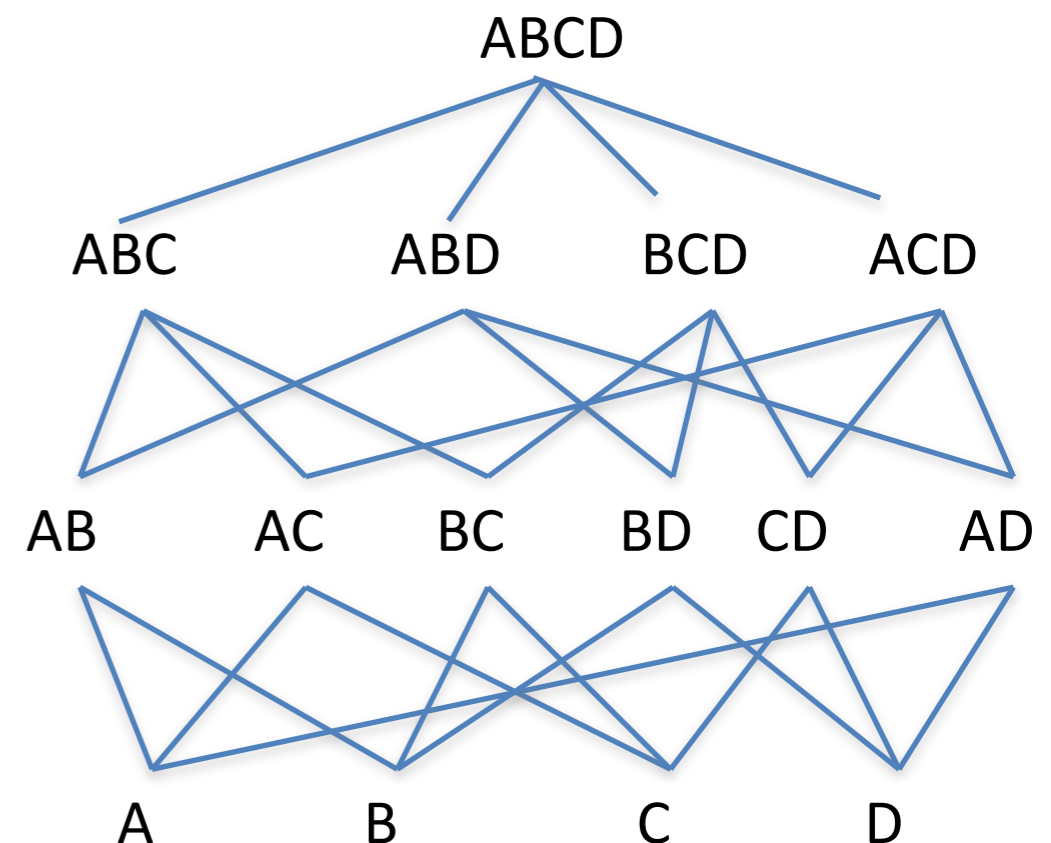
# Back to data profiling: Discovering uniques

Given a relation schema  $R (A, B, C, D)$  and a relation instance  $r$ , a **unique column combination** (or a “**unique**” for short) is a set of attributes  $X$  whose **projection** contains no duplicates in  $r$

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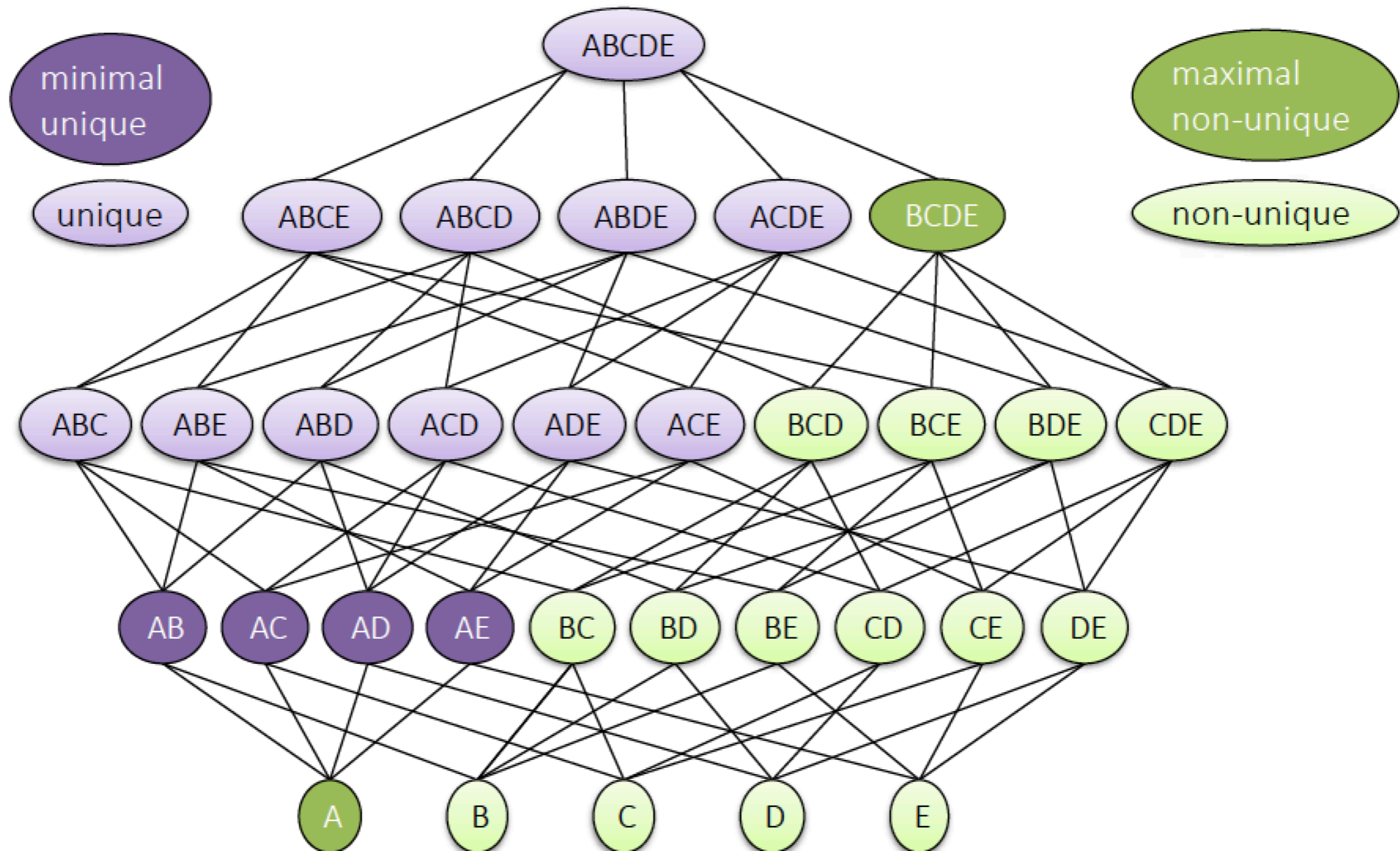
$X$  is **minimal unique** if every subset  $Y$  of  $X$  is non-unique

$Y$  is maximal non-unique if every superset  $X$  of  $Y$  is unique





# Output



Data Profiling | SIGMOD 2017 | Chicago

# From uniques to candidate keys

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- (2) this is not true for any subset of the key attributes (candidate key **is minimal**)

**A minimal unique of a relation instance is a (possible) candidate key of the relation schema.** To find such possible candidate keys, find all minimal uniques in a given relation instance.

# Apriori-style uniques discovery

[Abedjan, Golab, Naumann; *SIGMOD 2017*]

**A minimal unique** of a relation instance is a **(possible) candidate key** of the relation schema.

**Algorithm Uniques // sketch, similar to HCA**

$U_1 = \{1\text{-uniques}\}$      $N_1 = \{1\text{-non-uniques}\}$

**for** ( $k = 2; N_{k-1} \neq \emptyset; k++$ ) **do**

$C_k \leftarrow$  **candidate-gen**( $N_{k-1}$ )

$U_k \leftarrow$  **prune-then-check** ( $C_k$ )

        // prune candidates with unique sub-sets, and with **value distributions that cannot be unique**

        // check each candidate in pruned set for uniqueness

$N_k \leftarrow C_k \setminus U_k$

**end**

return  $U \leftarrow \bigcup_k U_k$ ;

**breadth-first bottom-up strategy for attribute lattice traversal**