

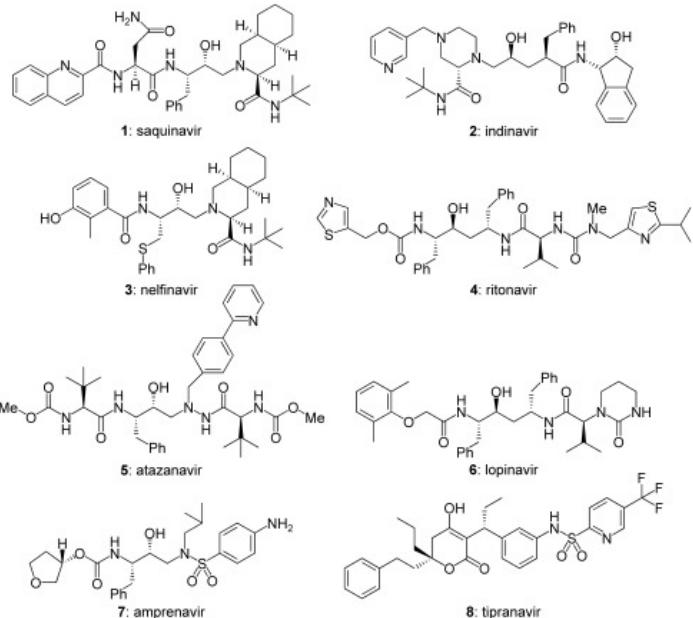
Schema Independent Relational Learning

Jose Picado, Arash Termehchy, Alan Fern, Parisa Ataei

Information and Data Management and Analytics (**IDEA**) Lab



Design a drug to treat HIV



What is the structure
of compounds that
have **anti-HIV** activity?

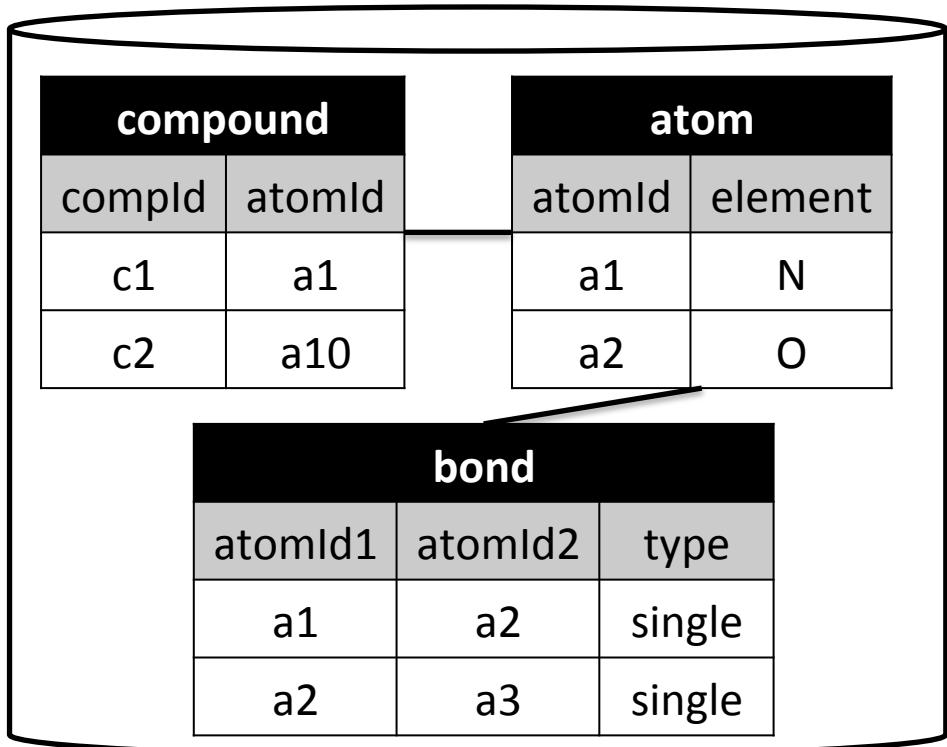


Oracle

A compound has **anti-HIV** activity if it has the
following substructure:



Relational learning



- Leverages the structure of the relational database
- Learns a Datalog definition

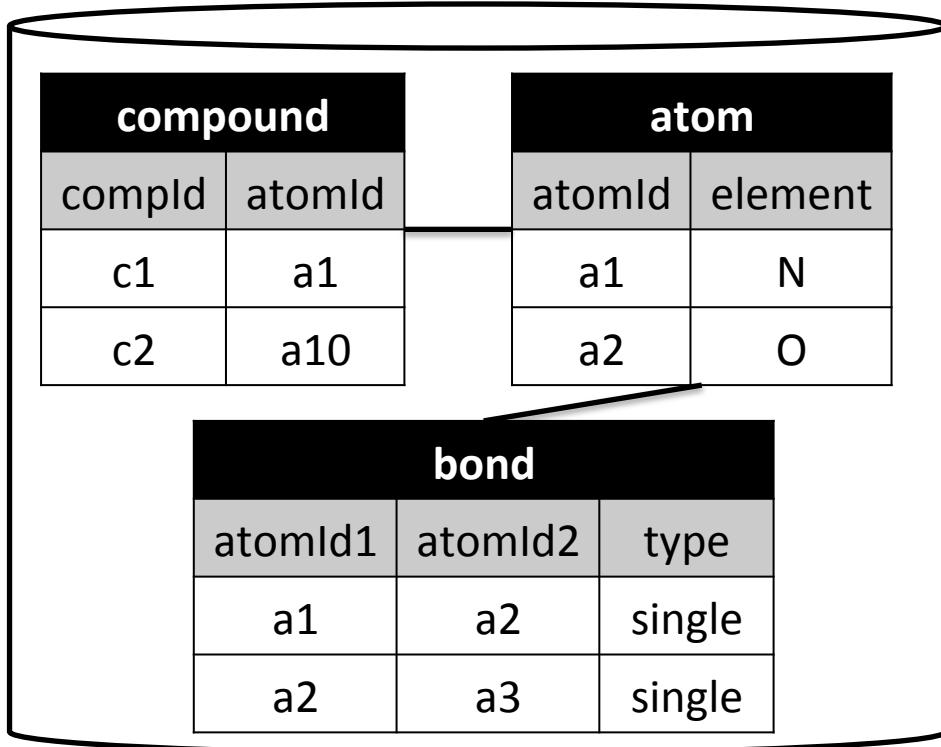
Training data:

anti-HIV	no-anti-HIV
compld	compld
c1	c2
c3	c4

Relational learning
algorithm

anti-HIV(x) :- compound(x,u), atom(u,N),
compound(x,v), atom(v,O),
compound(x,w), atom(w,N),
bond(u,v,single), bond(v,w,single).

Benefits of relational learning



✓ Leverage the structure of data and learn over complex schemas with multiple tables

✓ Automatic feature extraction and selection

✓ Results are interpretable (Datalog)

FOIL, Progol, ...
Castor (new algorithm)

anti-HIV(x) :- compound(x,u), atom(u,N),
compound(x,v), atom(v,O),
compound(x,w), atom(w,N),
bond(u,v,single), bond(v,w,single).

Existing algorithms

Schema 1

paperAuthor		author		authorAffiliation	
paperId	authorId	id	name	id	affiliation
p1	mad	mad	Madden	mad	MIT
p1	bai	sto	Stonebraker	sto	MIT
p2	soc	soc	Socher	soc	Stanford
p2	man	man	Manning	man	Stanford
p3	mad	bai	Bailis	bai	Stanford

paper		paperYear		paperConf	
id	title	id	year	id	conf
p1	MacroBase: Priori...	p1	2017	p1	SIGMOD
p2	GloVe: Global Vect...	p2	2014	p2	EMNLP

Which authors are
collaborators?

collaborators	
person1	person2
Madden	Bailis
Socher	Manning
Madden	Stonebraker

non-collaborators

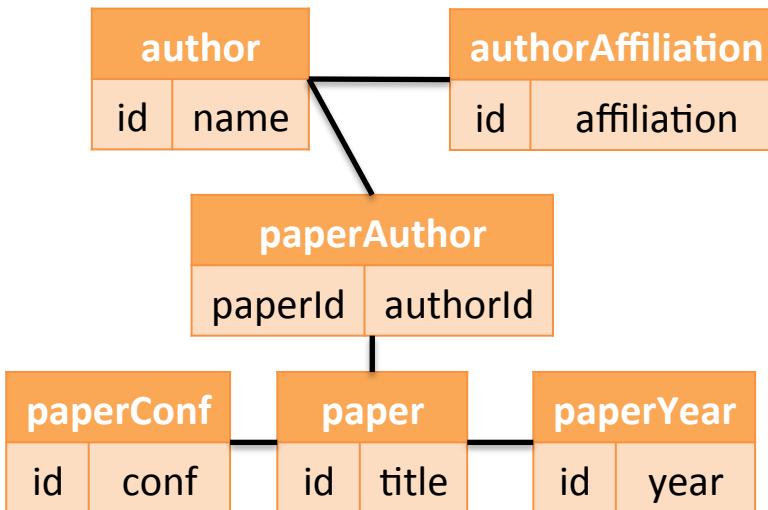
person1	person2
Madden	Socher
Manning	Bailis

FOIL learning
algorithm

?

FOIL: relational learning algorithm

Schema 1



collaborators(x,y) :-

Scoring function $f: P - N$

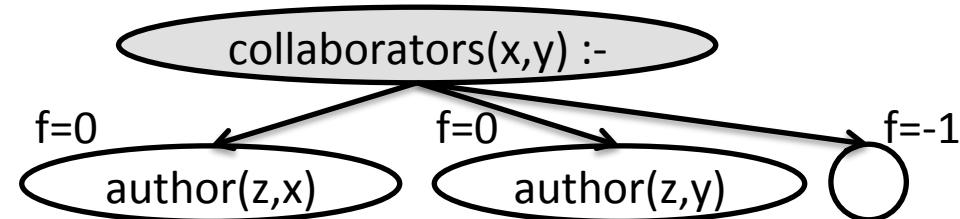
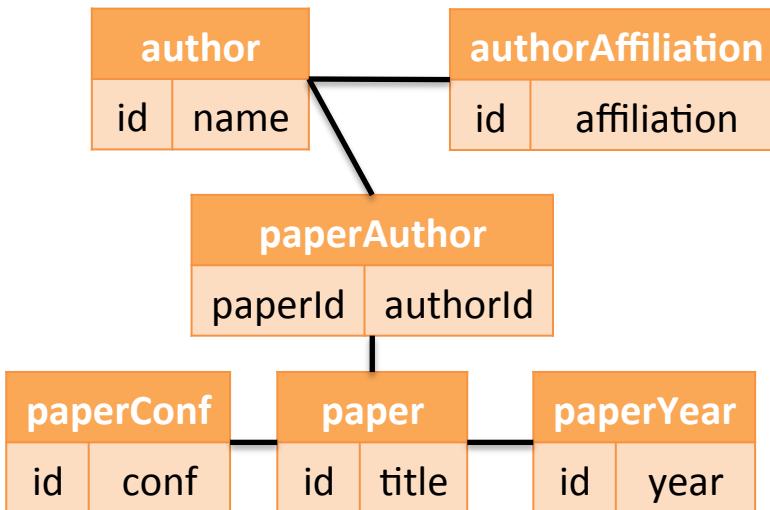
P: positive examples covered

N: negative examples covered

collaborators(x,y) :-
true.

FOIL: relational learning algorithm

Schema 1



Scoring function $f: P - N$

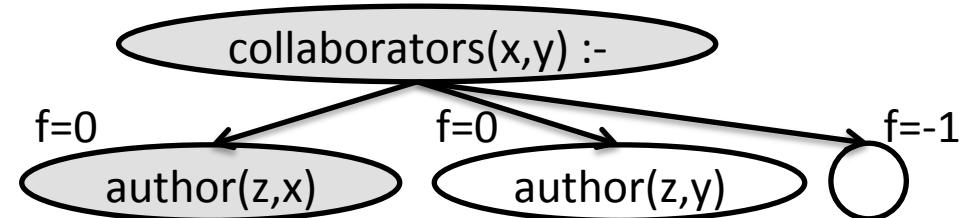
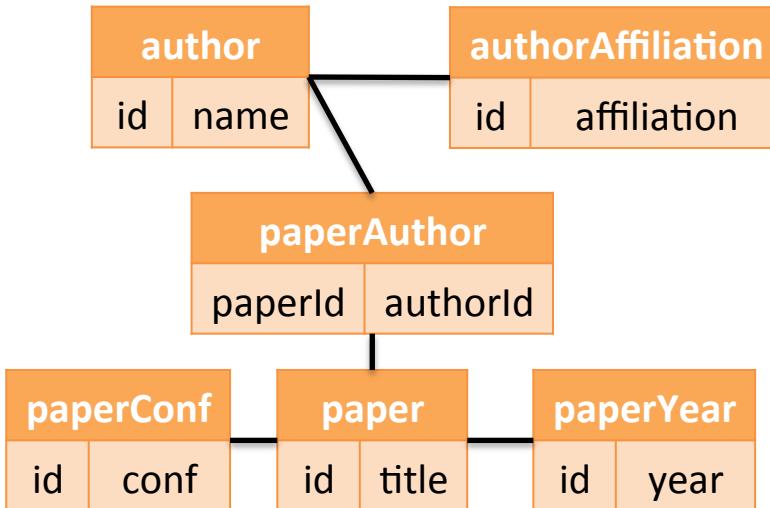
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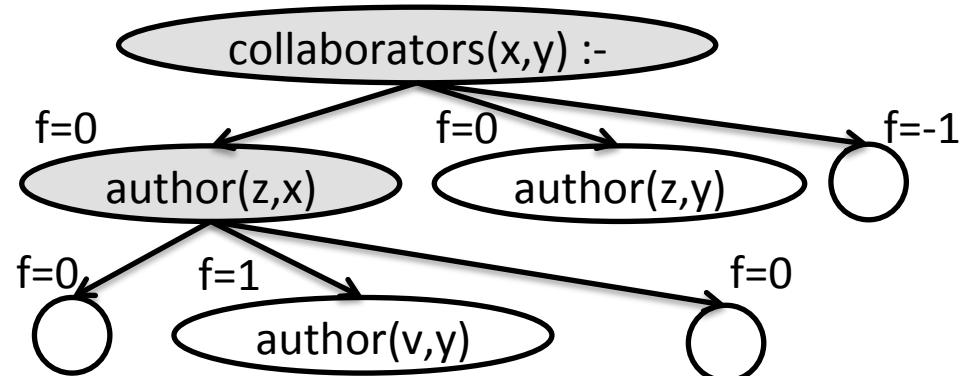
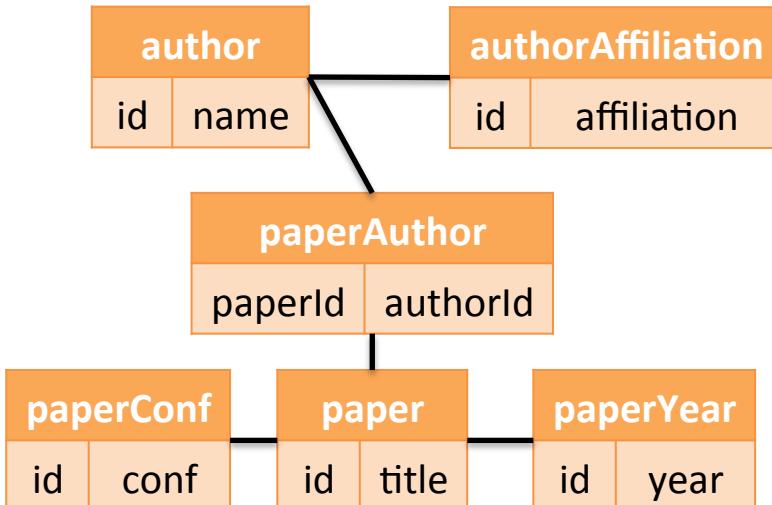
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N: negative examples covered

collaborators(x,y) :-
author(z,x).

FOIL: relational learning algorithm

Schema 1



Scoring function $f: P - N$

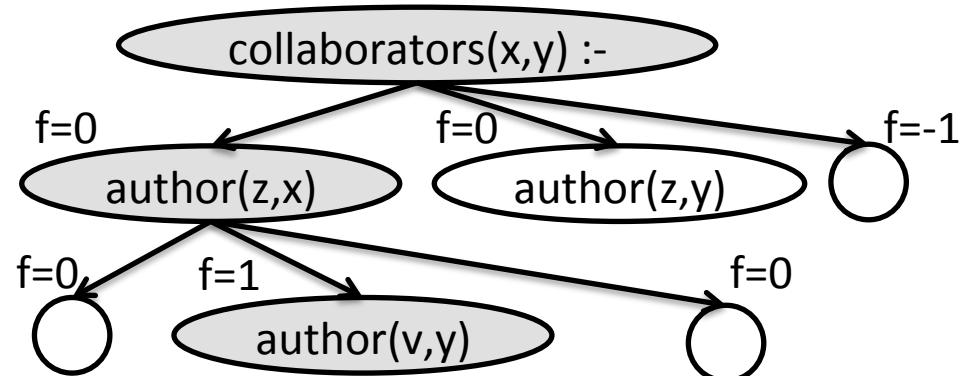
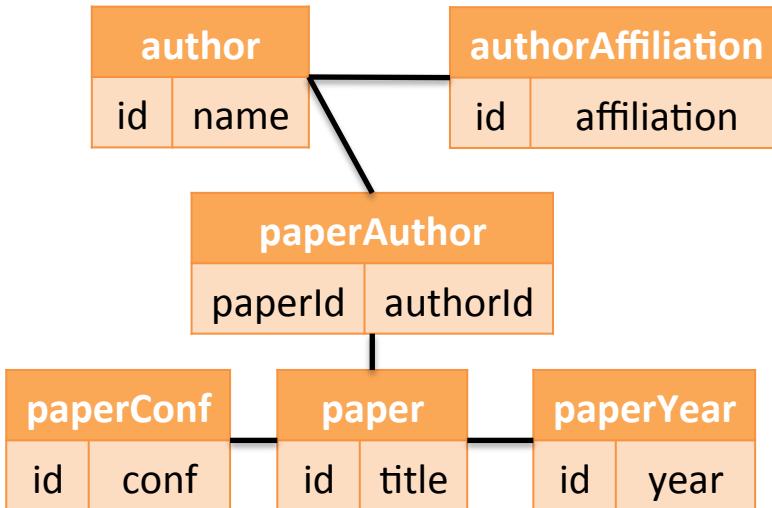
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Schema 1



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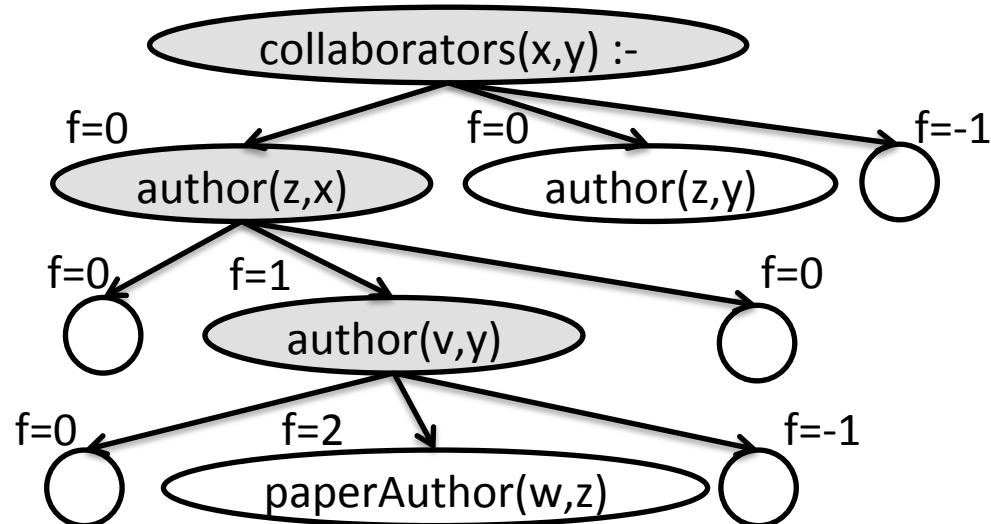
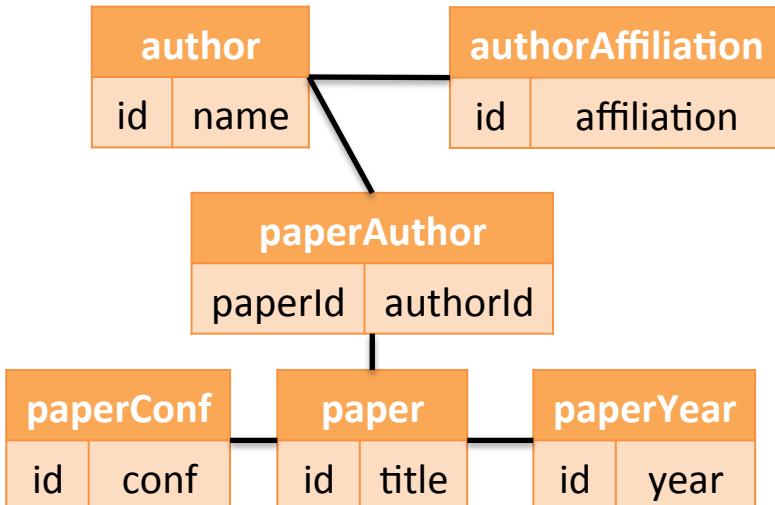
P: positive examples covered

N: negative examples covered

`collaborators(x,y) :-
author(z,x), author(v,y).`

FOIL: relational learning algorithm

Schema 1



Scoring function $f: P - N$

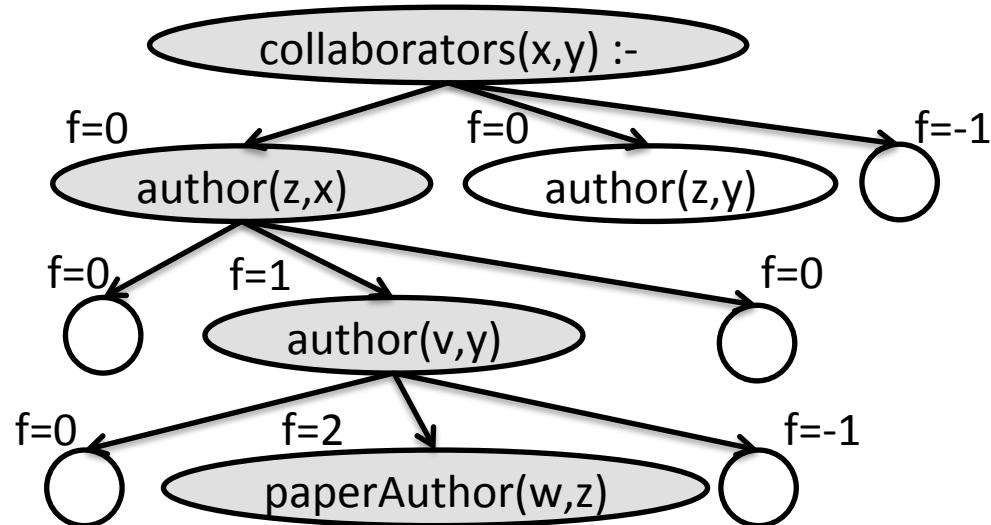
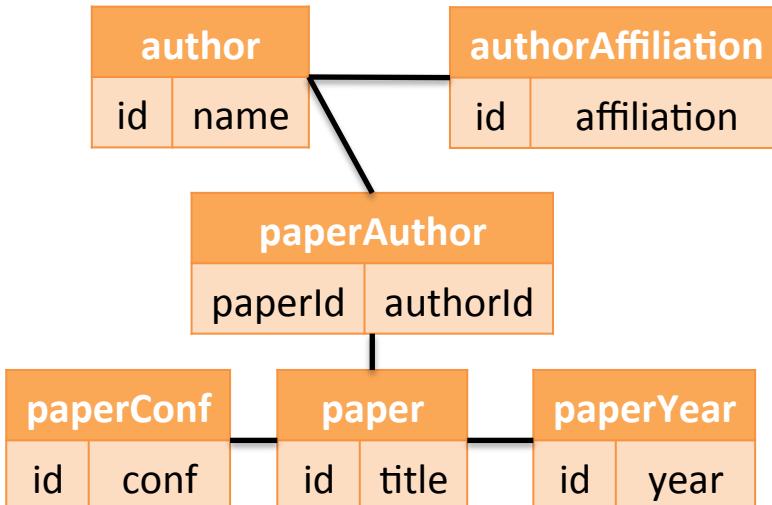
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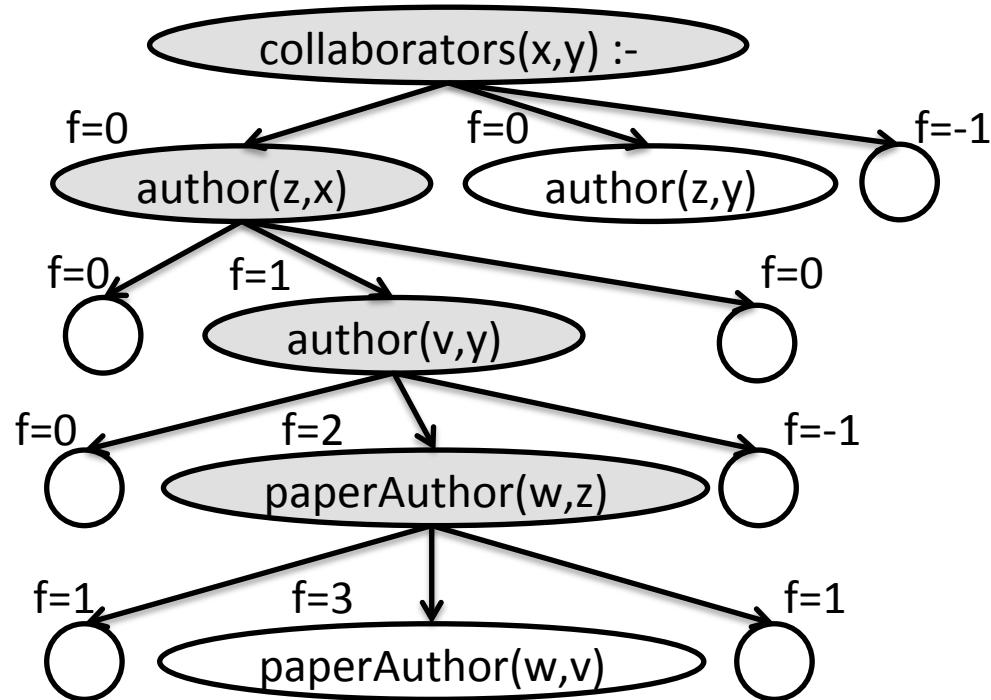
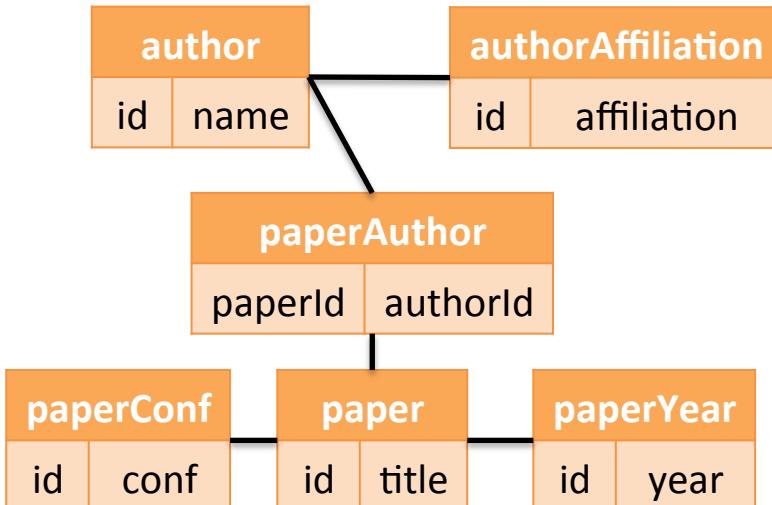
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`collaborators(x,y) :-
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FOIL: relational learning algorithm

Schema 1



Scoring function $f: P - N$

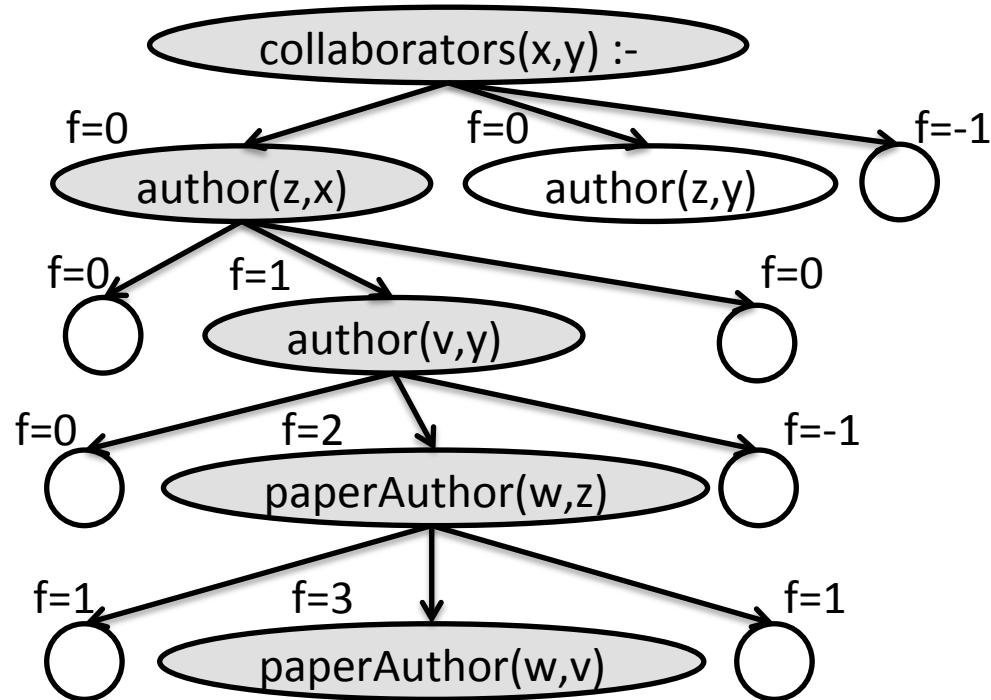
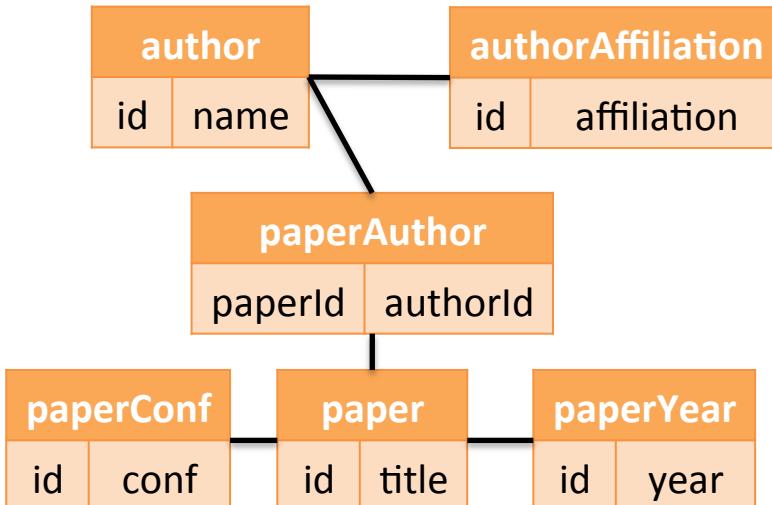
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Schema 1



Scoring function $f: P - N$

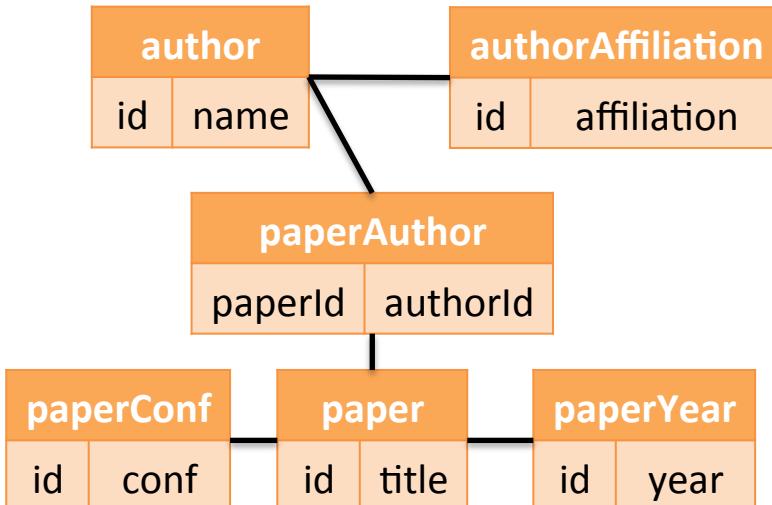
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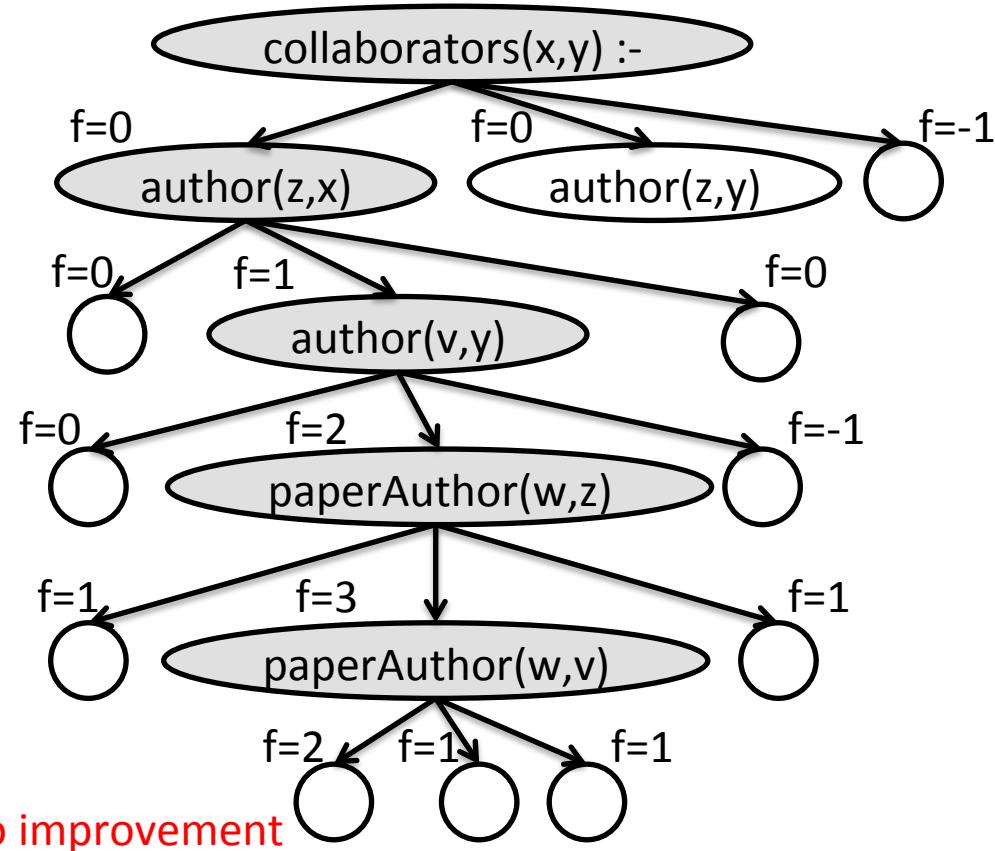
Schema 1



Scoring function $f: P - N$

P: positive examples covered

N: negative examples covered



```

collaborators(x,y) :-
    author(z,x), author(v,y),
    paperAuthor(w,z), paperAuthor(w,v).
  
```

Schema 1

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paperId	authorId	id	name	id	affiliation
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id	title	id	year	id	conf
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Which authors are **collaborators**?

collaborators	
person1	person2
Madden	Bailis
Socher	Manning
Madden	Stonebraker

non-collaborators	
person1	person2
Madden	Socher
Manning	Bailis

f=3

FOIL learning algorithm

collaborators(x,y) :-
 author(z,x), author(v,y),
 paperAuthor(w,z), paperAuthor(w,v).

Two people are collaborators if they are co-authors.

People represent the same data using different schemas

author	
id	name
mad	Madden
sto	Stonebraker
soc	Socher
man	Manning
bai	Bailis

authorAffiliation	
id	affiliation
mad	MIT
sto	MIT
soc	Stanford
man	Stanford
bai	Stanford

author		
id	name	affiliation
mad	Madden	MIT
sto	Stonebraker	MIT
soc	Socher	Stanford
man	Manning	Stanford
bai	Bailis	Stanford

paper	
id	title
p1	MacroBase: Priori...
p2	GloVe: Global Vect...

paperYear	
id	year
p1	2017
p2	2014

paperConf	
id	conf
p1	SIGMOD
p2	EMNLP

Composition
Denormalization
better performance



Schema 2

paperAuthor		author		
paperId	authorId	id	name	affiliation
p1	mad	mad	Madden	MIT
p1	bai	sto	Stonebraker	MIT
p2	soc	soc	Socher	Stanford
p2	man	man	Manning	Stanford
p3	mad	bai	Bailis	Stanford

paper			
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Which authors are
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collaborators	
person1	person2
Madden	Bailis
Socher	Manning
Madden	Stonebraker

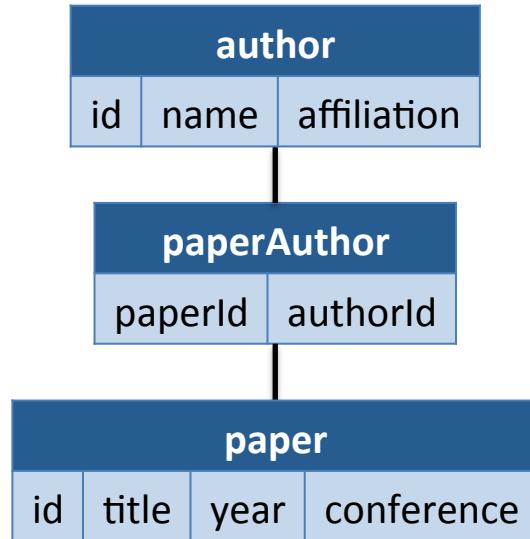
non-collaborators	
person1	person2
Madden	Socher
Manning	Bailis

FOIL learning
algorithm

?

FOIL: relational learning algorithm

Schema 2



collaborators(x,y) :-

Scoring function $f: P - N$

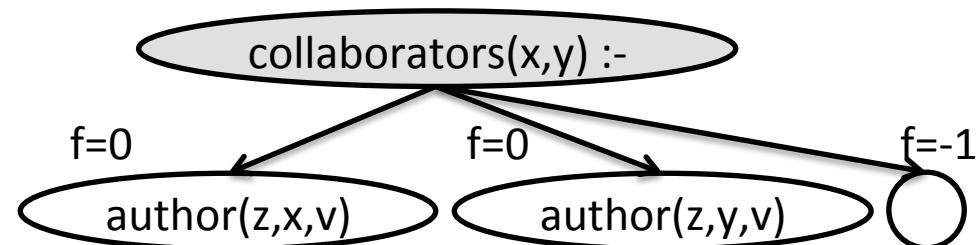
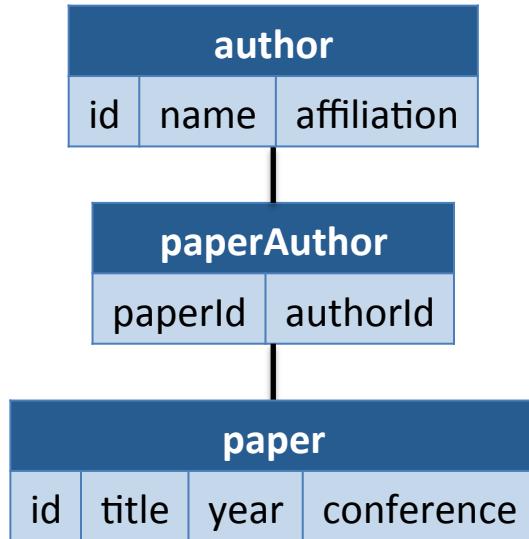
P: positive examples covered

N: negative examples covered

collaborators(x,y) :-
true.

FOIL: relational learning algorithm

Schema 2



Scoring function $f: P - N$

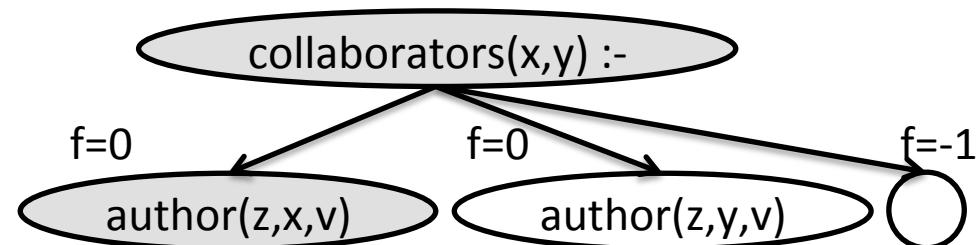
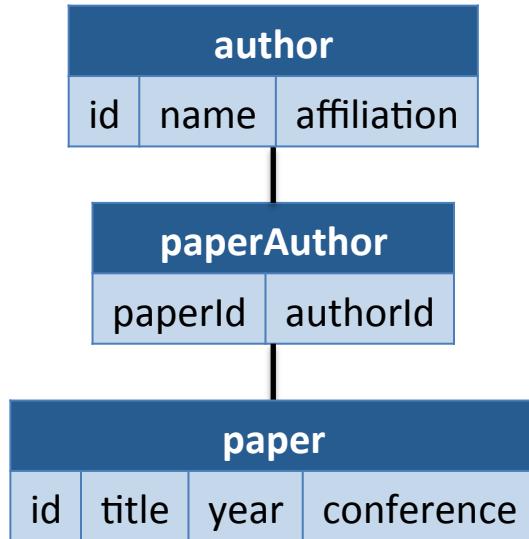
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collaborateurs(x,y) :-
true.

FOIL: relational learning algorithm

Schema 2



Scoring function $f: P - N$

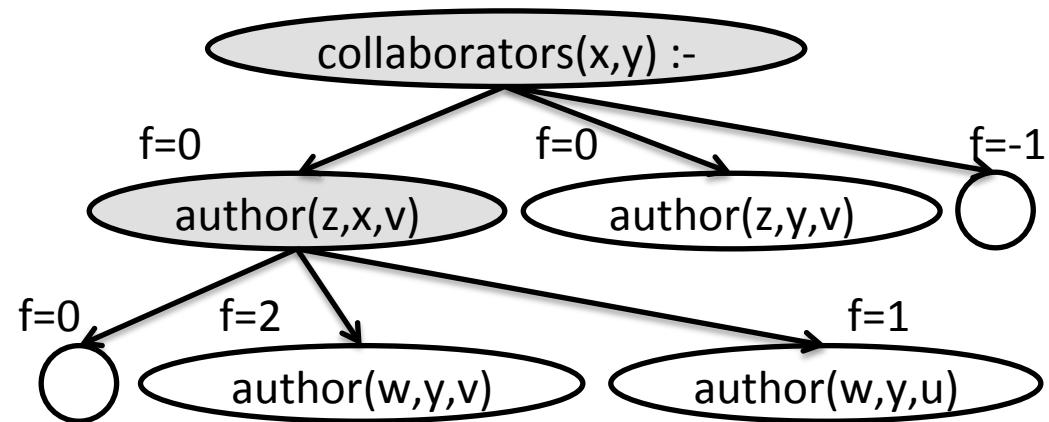
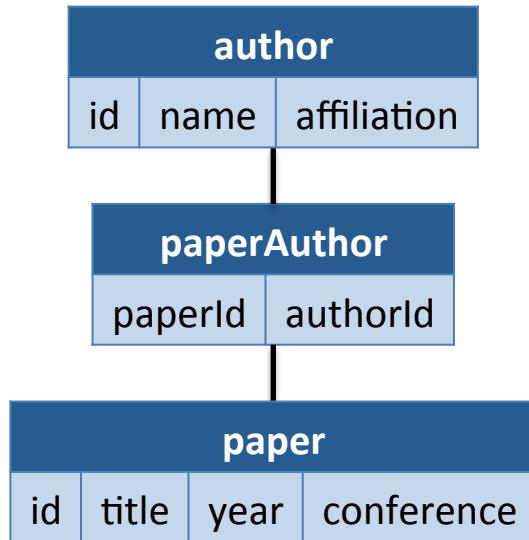
P: positive examples covered

N: negative examples covered

```
collaborators(x,y) :-  
    author(z,x,v).  
    author(z,y,v).
```

FOIL: relational learning algorithm

Schema 2



Scoring function $f: P - N$

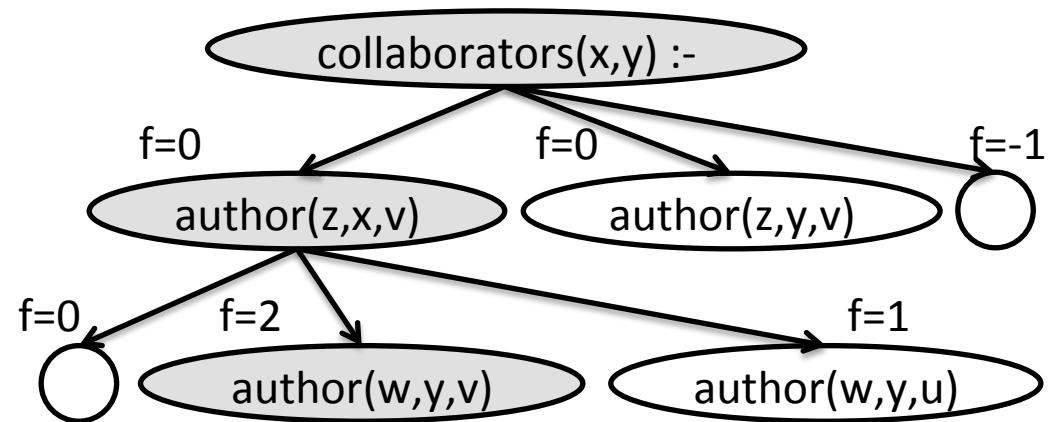
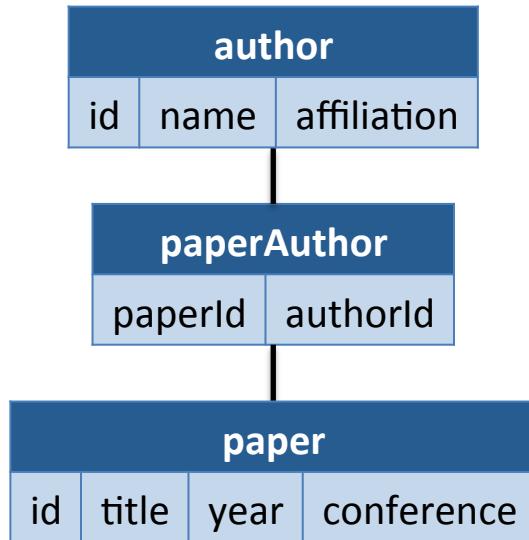
P: positive examples covered

N: negative examples covered

collaborators(x,y) :-
author(z,x,v).

FOIL: relational learning algorithm

Schema 2



Scoring function $f: P - N$

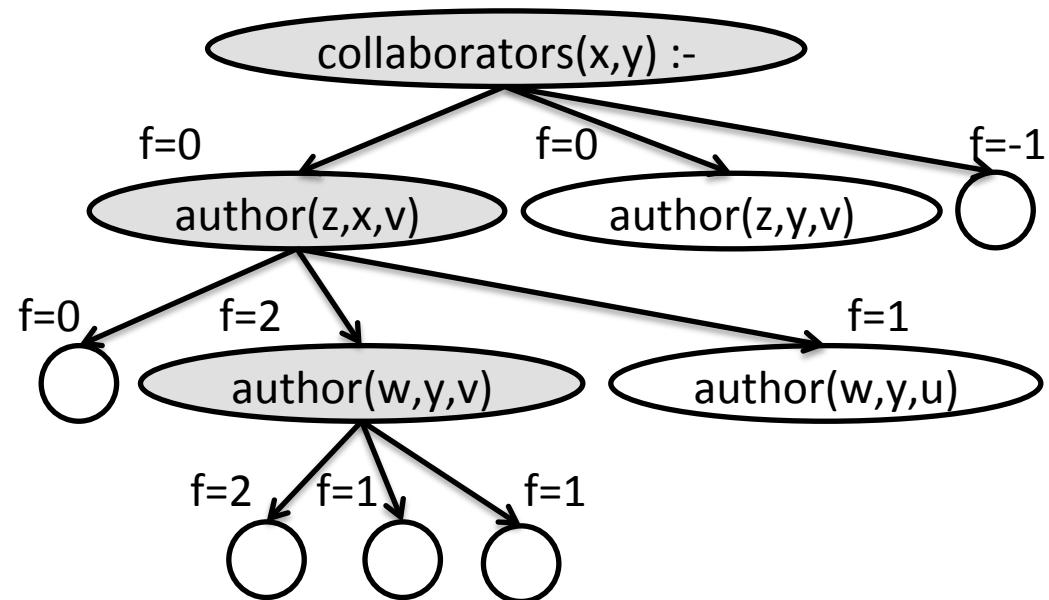
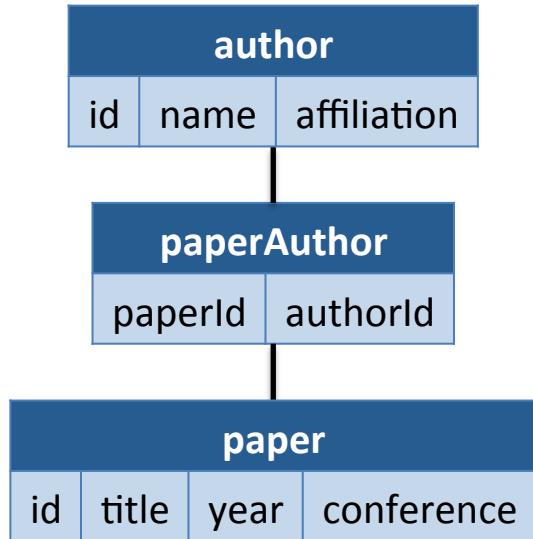
P: positive examples covered

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collaborators(x,y) :-
author(z,x,v), author(w,y,v).

FOIL: relational learning algorithm

Schema 2



No improvement

Scoring function $f: P - N$

P: positive examples covered

N: negative examples covered

collaborators(x,y) :-
author(z,x,v), author(w,y,v).

Schema 2

paperAuthor		author		
paperId	authorId	id	name	affiliation
p1	mad	mad	Madden	MIT
p1	bai	sto	Stonebraker	MIT
p2	soc	soc	Socher	Stanford
p2	man	man	Manning	Stanford
p3	mad	bai	Bailis	Stanford

paper			
id	title	year	conference
p1	MacroBase: Priori...	2017	SIGMOD
p2	GloVe: Global Vect...	2014	EMNLP

Which authors are
collaborators?

collaborators	
person1	person2
Madden	Bailis
Socher	Manning
Madden	Stonebraker

non-collaborators	
person1	person2
Madden	Socher
Manning	Bailis

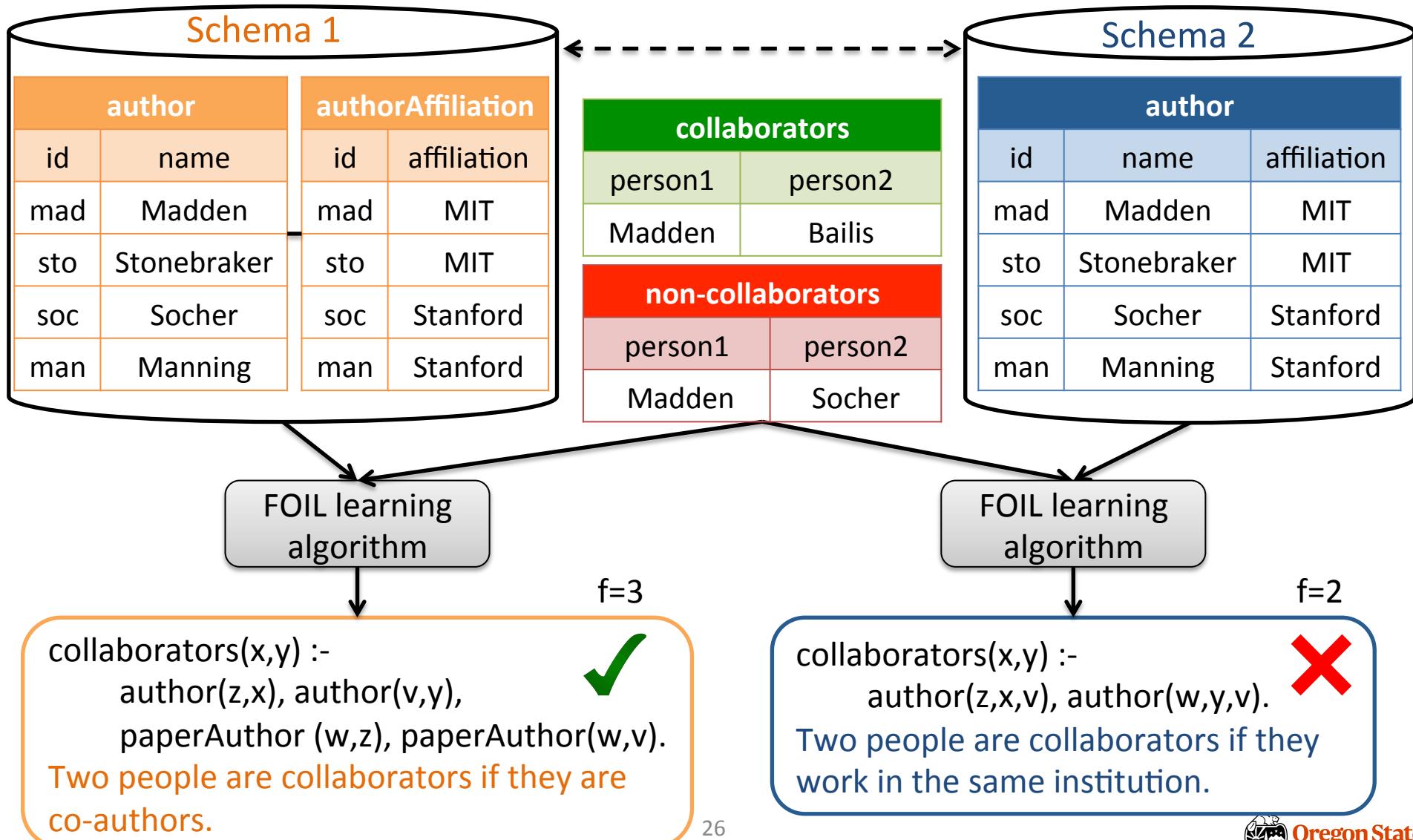
f=2

FOIL learning
algorithm

collaborators(x,y) :-
author(z,x,v), author(w,y,v).

Two people are collaborators if they work in the same institution.

Schema dependence: schema affects the learning outcomes



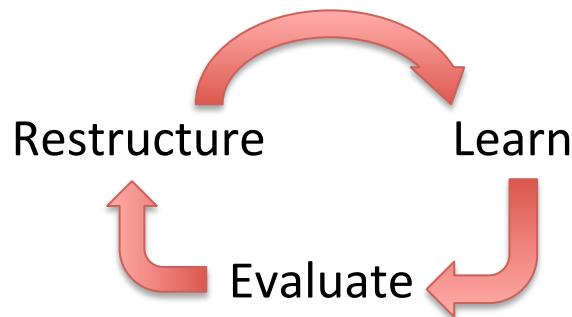
Current solutions

author		
id	name	affiliation
mad	Madden	MIT

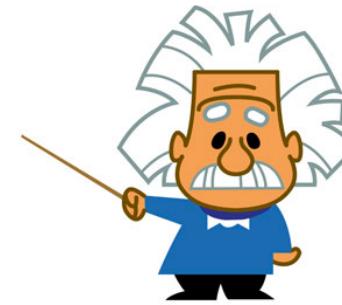
→

author		authorAffiliation	
id	name	id	affiliation
mad	Madden	mad	MIT

Users must restructure databases

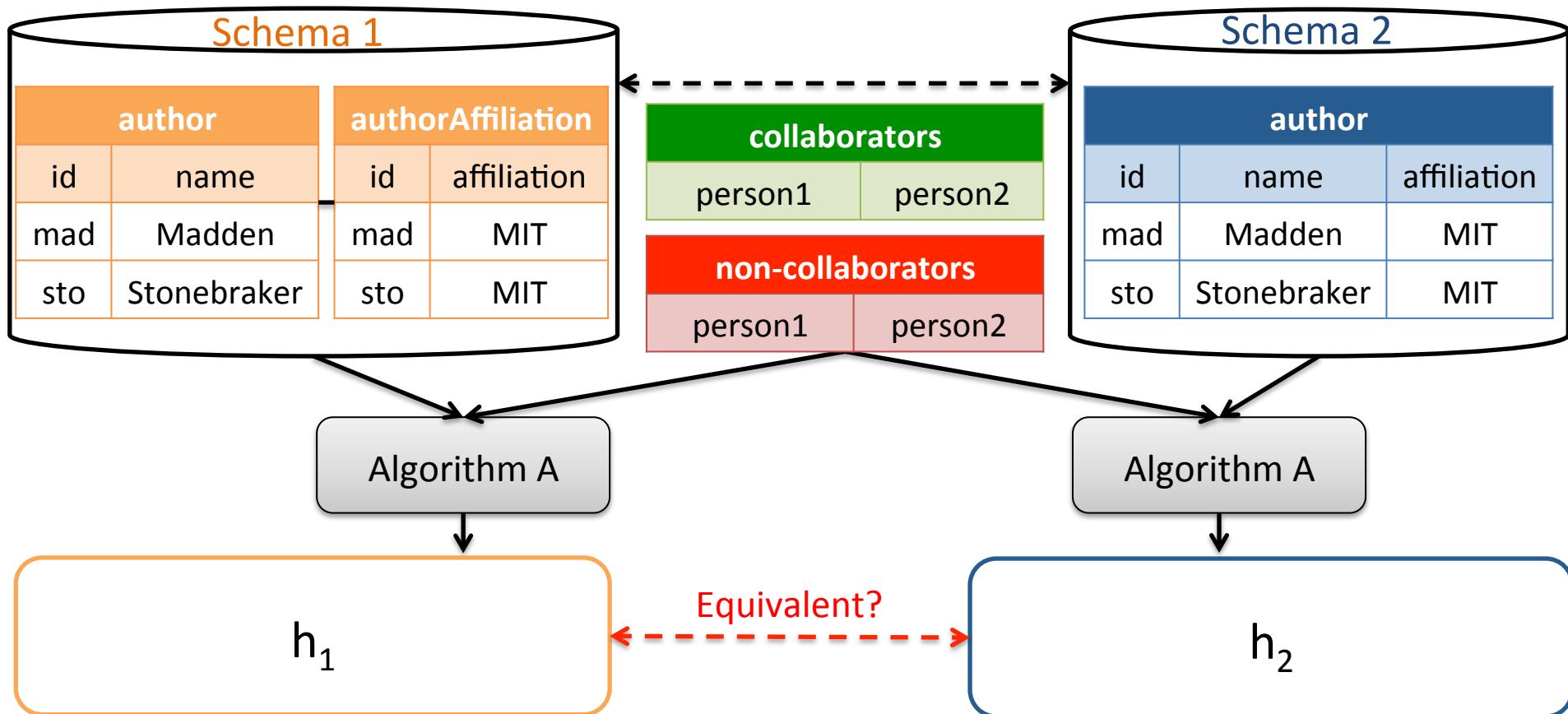


Which is the best schema?

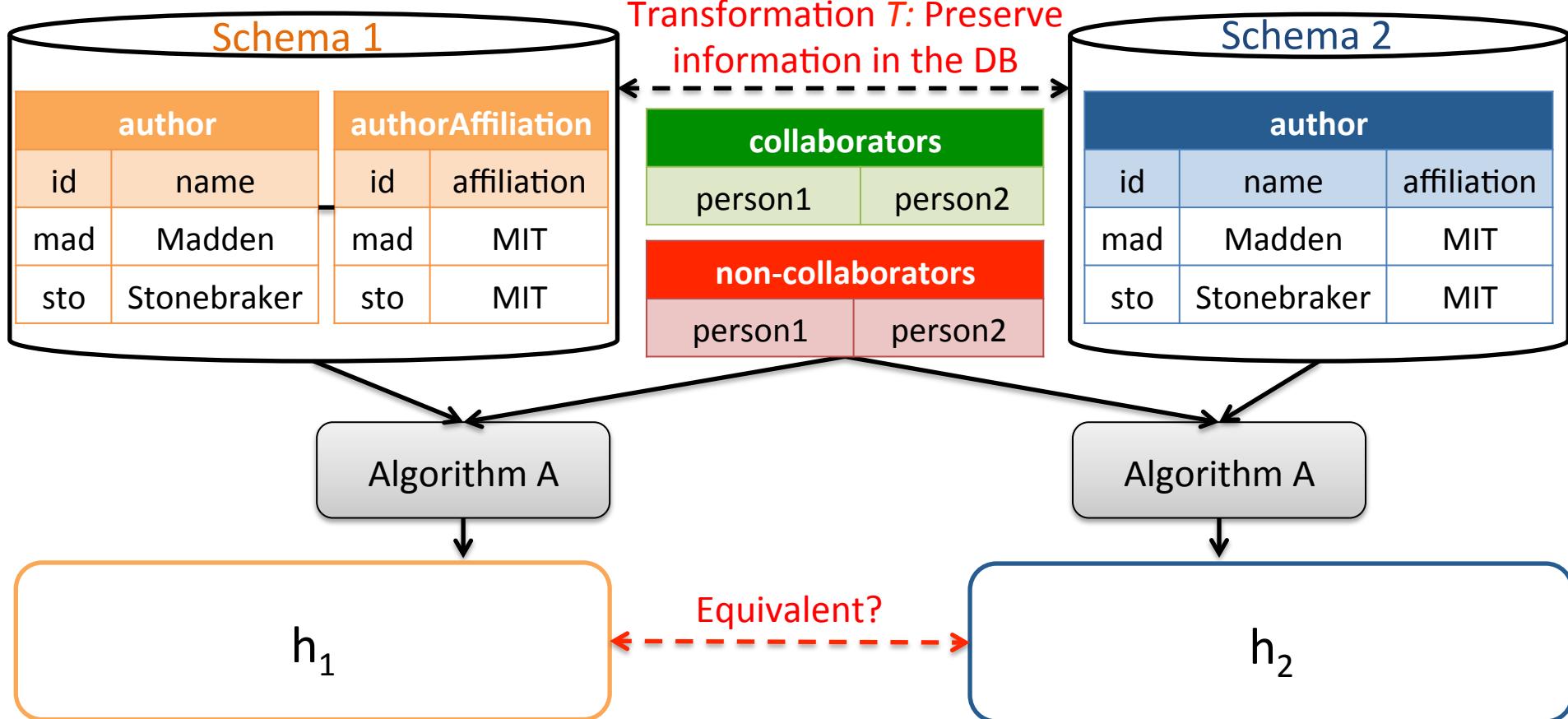


Expert attention

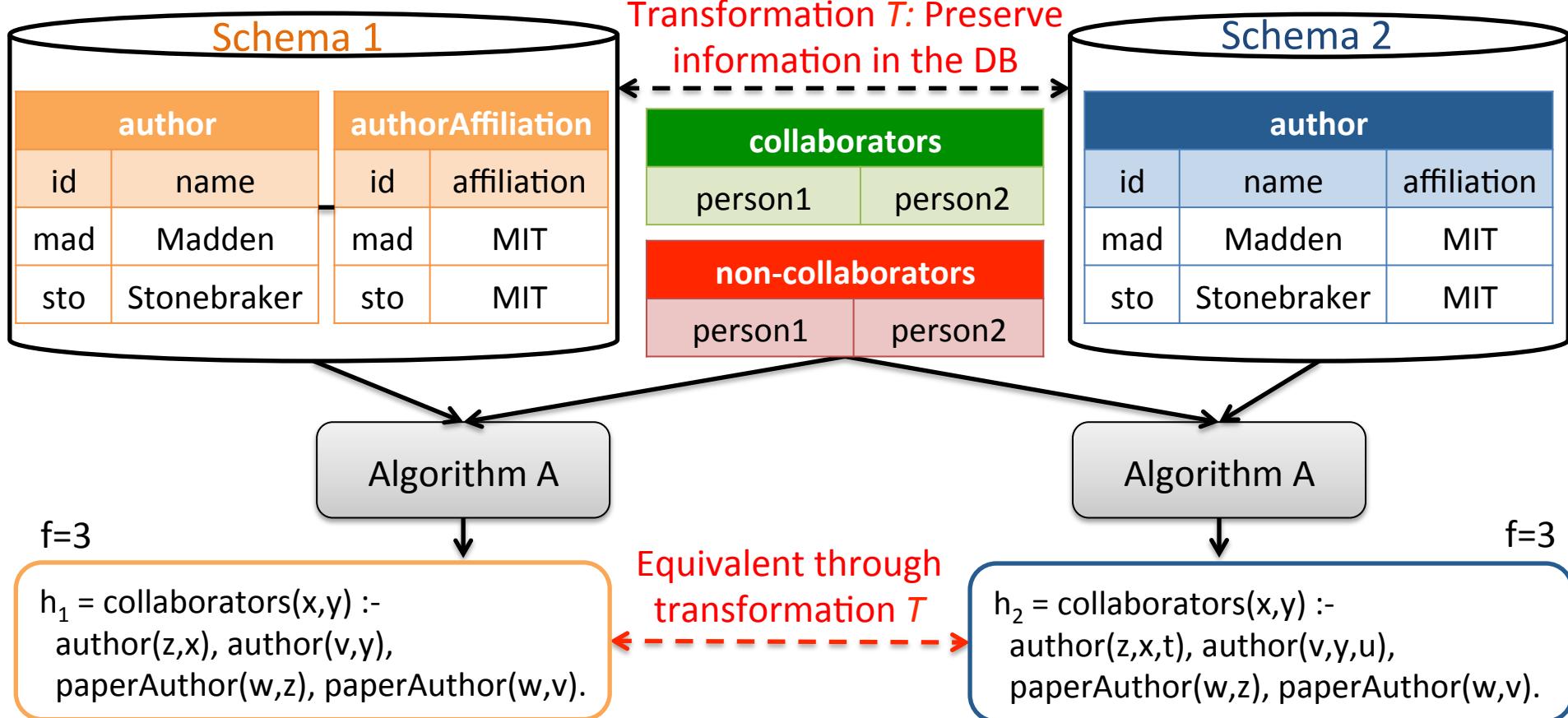
Definition of schema independence



Definition of schema independence

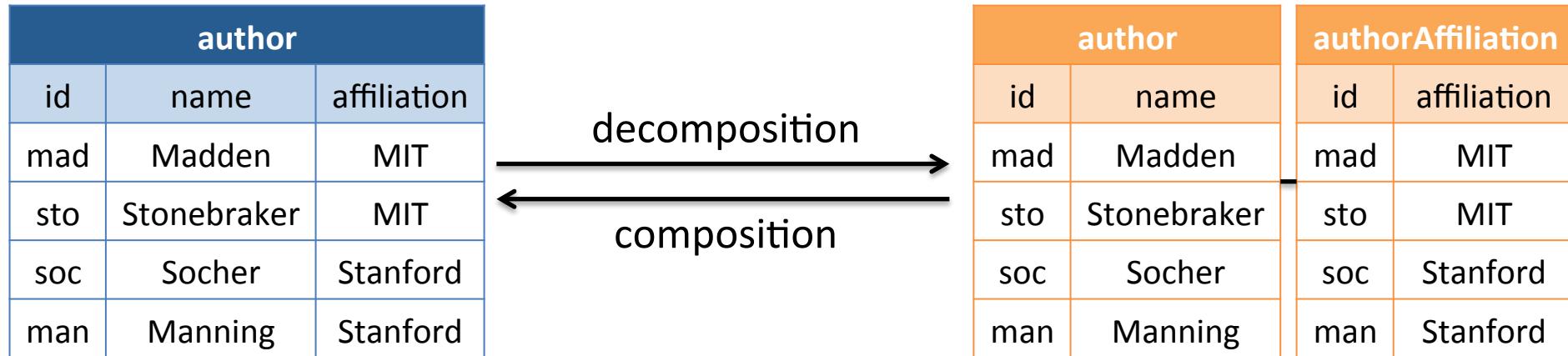


Definition of schema independence



Algorithm A is **schema independent** under T iff
for all pairs of databases (I, J) and training examples E ,
 h_1 and h_2 are equivalent

We focus on schema independence under composition/decomposition



Inclusion dependencies
(referential integrity constraints):
 $\text{author}[\text{id}] \subseteq \text{authorAffiliation}[\text{id}]$

- Most common schema transformations
- Used in normalization and denormalization
- We support combinations of compositions and decompositions

Current relational learning algorithms are NOT schema independent

Theorems:

- FOIL
- Progol
- ProGolem



are **NOT** schema independent
under composition/decomposition

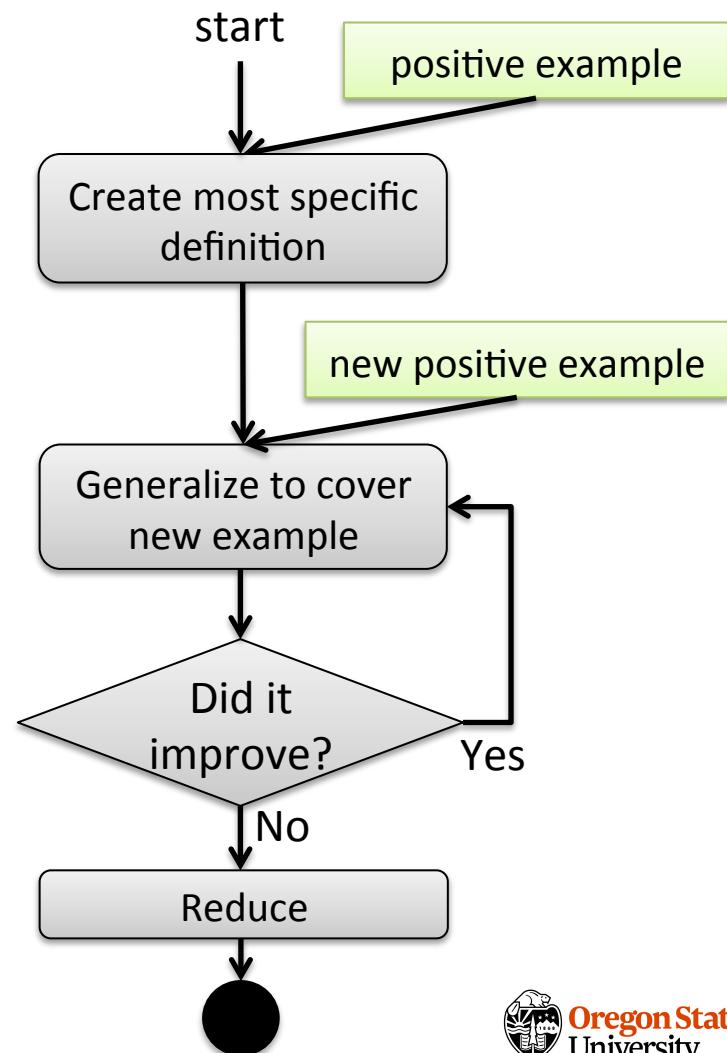


Reasons for schema dependence:

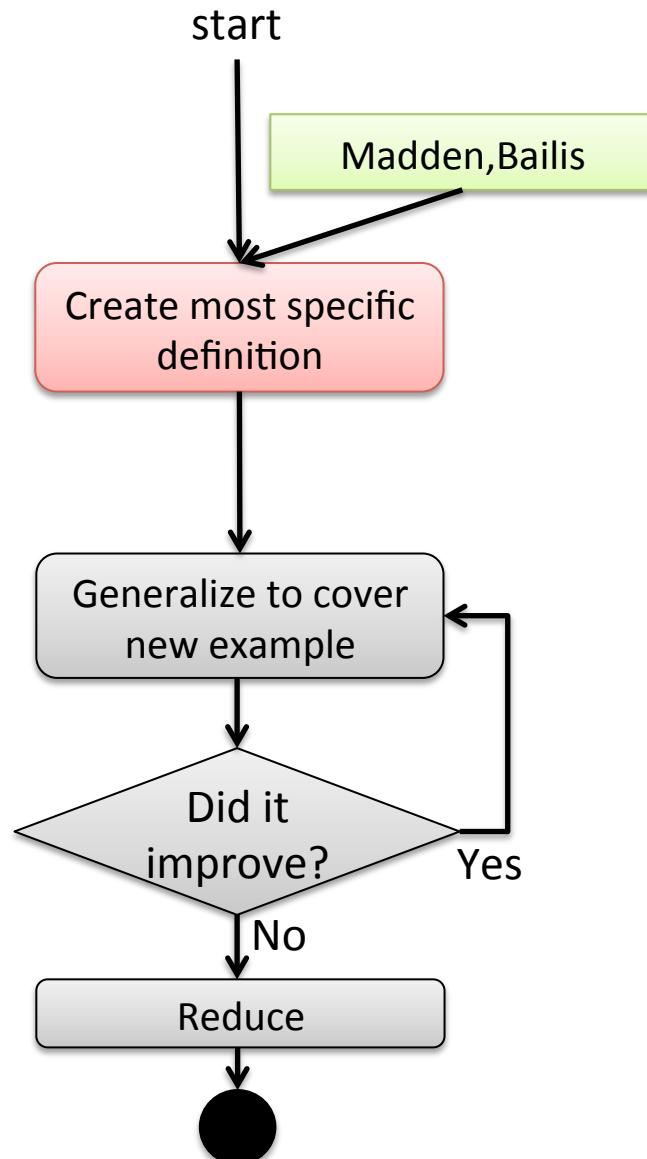
- Search process affected by schema
- Greedy search strategies

Our algorithm: Castor schema independent algorithm

- Specific to general definitions
- Uses database constraints to achieve schema independence



Step 1: Create most specific definition

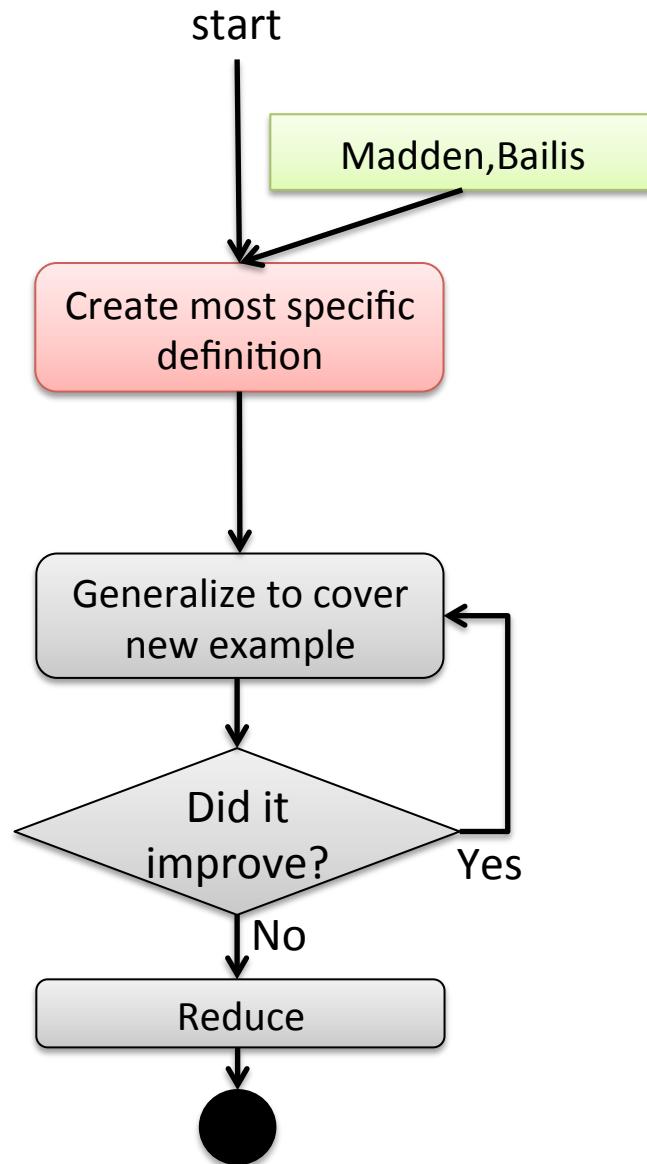


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p1	mad	mad	Madden	mad	MIT
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p1	MacroBase: Priori...	p1	2017	p1	SIGMOD
p2	GloVe: Global Vect...	p2	2014	p2	EMNLP

collaborators(v_1, v_2) :-

Step 1: Create most specific definition

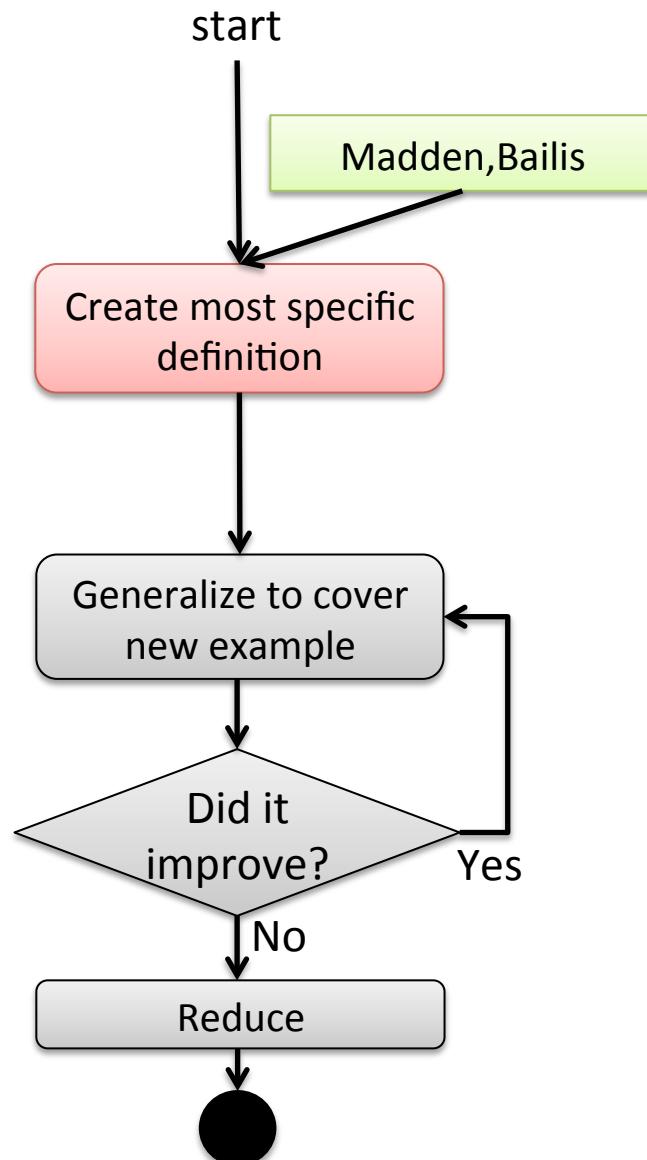


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p1	MacroBase: Priori...	p1	2017	p1	SIGMOD
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collaborators(v_1, v_2) :-
author(v_3, v_1), author(v_4, v_2).

Step 1: Create most specific definition

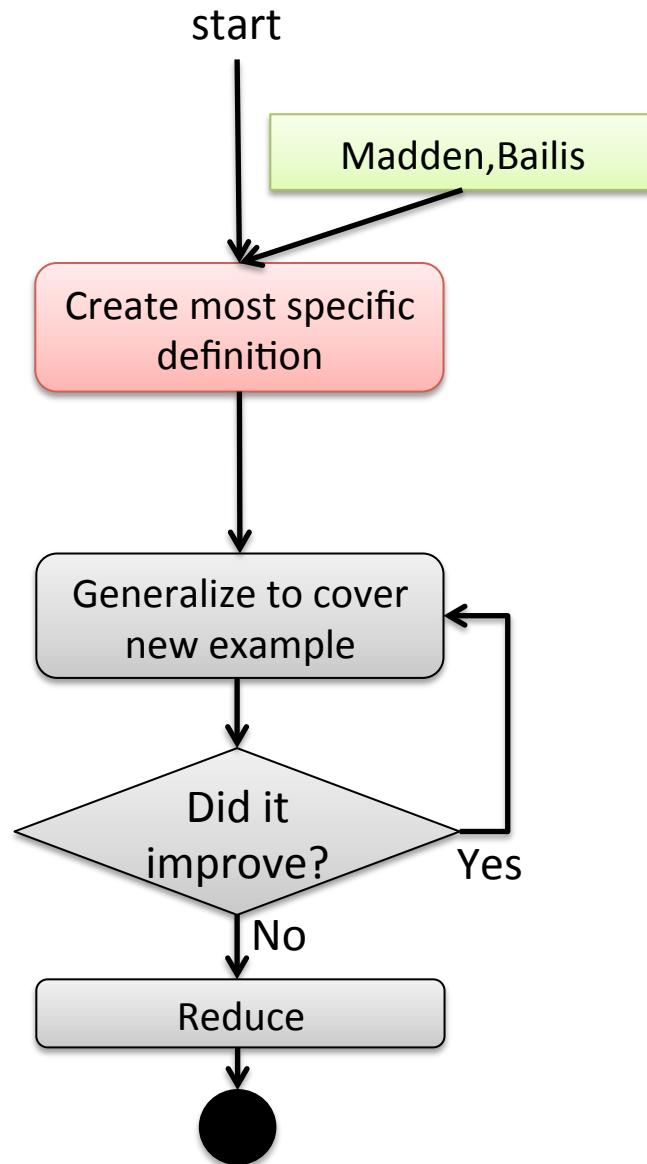


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collaborators(v_1, v_2) :-
author(v_3, v_1), author(v_4, v_2),
authorAffiliation(v_3 , MIT), authorAffiliation(v_3, v_5),
authorAffiliation(v_4 , Stanford), authorAffiliation(v_4, v_6).

Step 1: Create most specific definition



A diagram showing a relational database schema with four tables: paperAuthor, author, authorAffiliation, and paper. The paperAuthor table links paperId (p1) to authorId (mad, bai). The author table links authorId (mad, bai) to name (Madden, Bailis). The authorAffiliation table links authorId (mad, bai) to affiliation (MIT, Stanford). The paper table links id (p1, p2) to title (MacroBase: Priori..., GloVe: Global Vect...).

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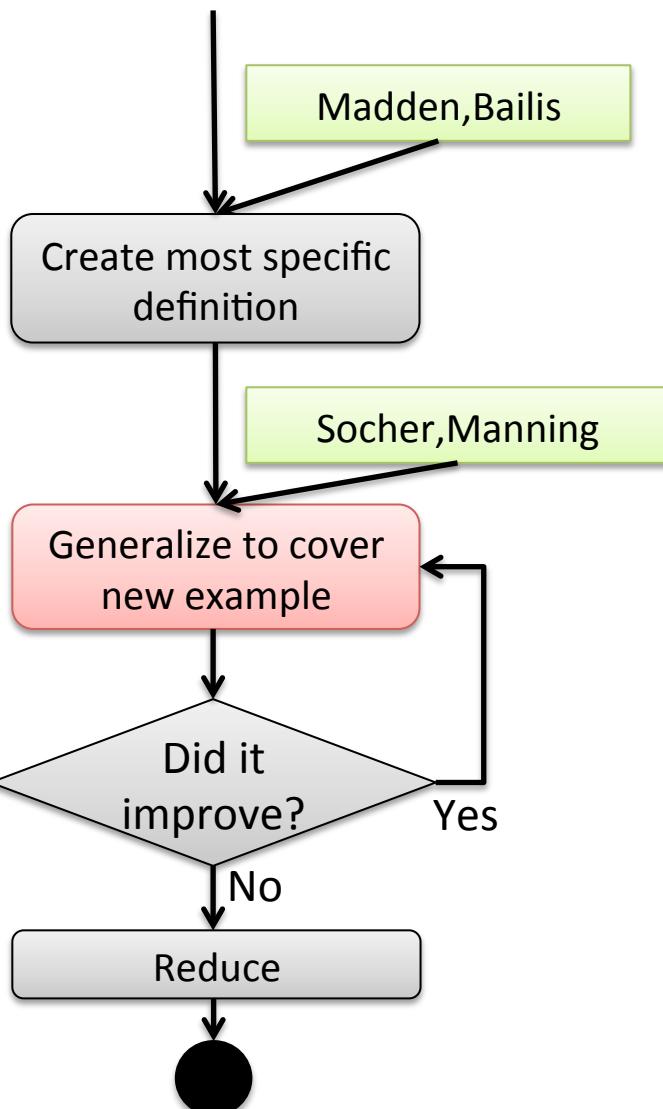
paper		paperYear		paperConf	
id	title	id	year	id	conf
p1	MacroBase: Priori...	p1	2017	p1	SIGMOD
p2	GloVe: Global Vect...	p2	2014	p2	EMNLP

$$f = P - N = 1$$

collaborators(v_1, v_2) :-
 author(v_3, v_1), author(v_4, v_2),
 authorAffiliation(v_3 , MIT), authorAffiliation(v_3, v_5),
 authorAffiliation(v_4 , Stanford), authorAffiliation(v_4, v_6),
 paperAuthor(v_7, v_3), paperAuthor(v_7, v_4).

Step 2: Generalize definition

start



paperAuthor		author		authorAffiliation	
paperId	authorId	id	name	id	affiliation
p2	soc	soc	Socher	soc	Stanford
p2	man		Manning		Stanford

paper		paperYear		paperConf	
id	title	id	year	id	conf
p2	GloVe: Global Vect...	p2	2014	p2	EMNLP

$v_1 \rightarrow$ Socher

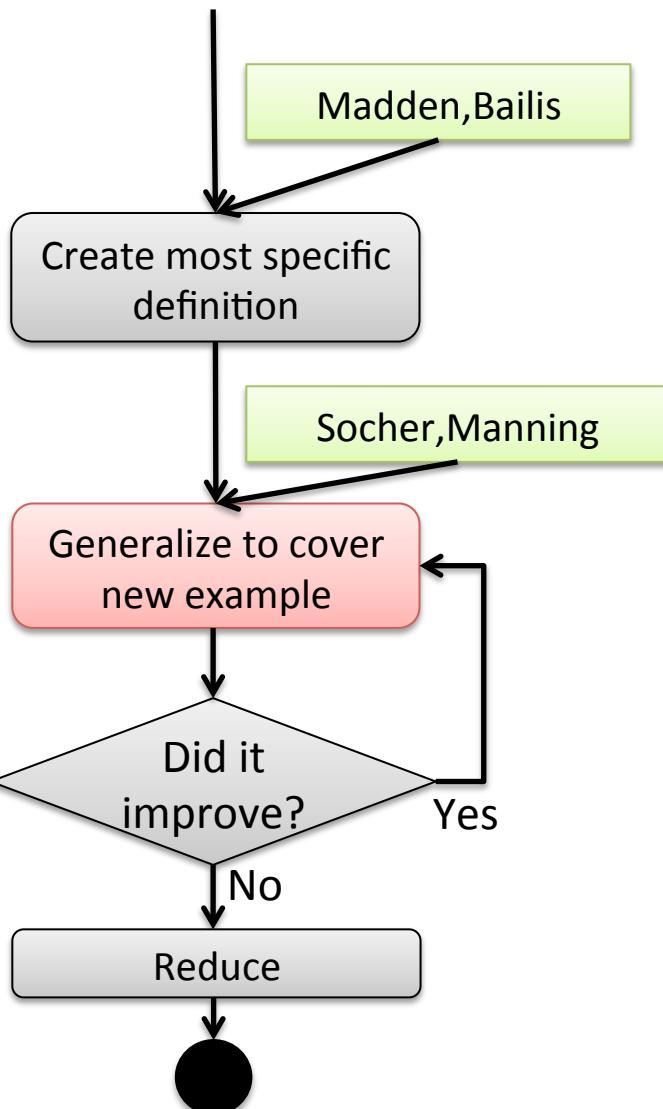
$v_2 \rightarrow$ Manning

$$f = P - N = 1$$

collaborators(v_1, v_2) :-
 author(v_3, v_1), author(v_4, v_2),
~~authorAffiliation(v_3, MIT)~~, authorAffiliation(v_3, v_5),
 authorAffiliation($v_4, Stanford$), authorAffiliation(v_4, v_6),
 paperAuthor(v_7, v_3), paperAuthor(v_7, v_4).

Step 2: Generalize definition

start



paperAuthor		author		authorAffiliation	
paperId	authorId	id	name	id	affiliation
p2	soc	soc	Socher	soc	Stanford
p2	man		Manning		Stanford

paper		paperYear		paperConf	
id	title	id	year	id	conf
p2	GloVe: Global Vect...	p2	2014	p2	EMNLP

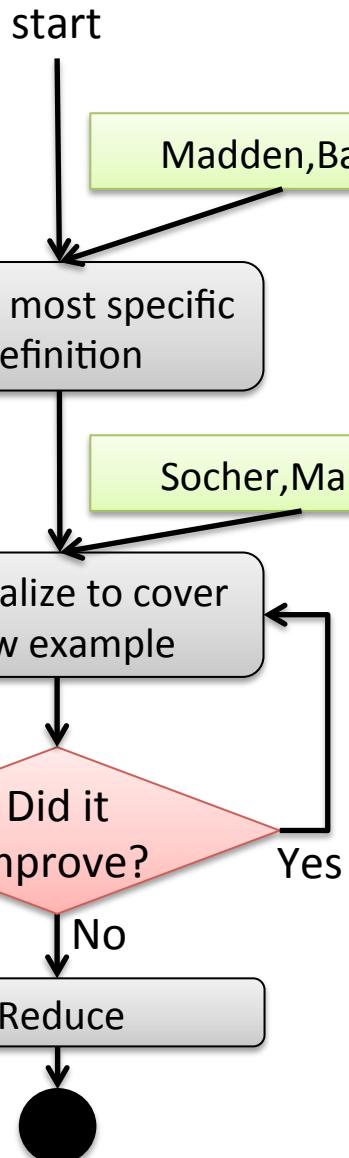
$v_1 \rightarrow$ Socher

$v_2 \rightarrow$ Manning

$$f = P - N = 2$$

collaborators(v_1, v_2) :-
 author(v_3, v_1), author(v_4, v_2),
 authorAffiliation(v_3, v_5),
 authorAffiliation($v_4, \text{Stanford}$), authorAffiliation(v_4, v_6),
 paperAuthor(v_7, v_3), paperAuthor(v_7, v_4).

Step 2: Generalize definition



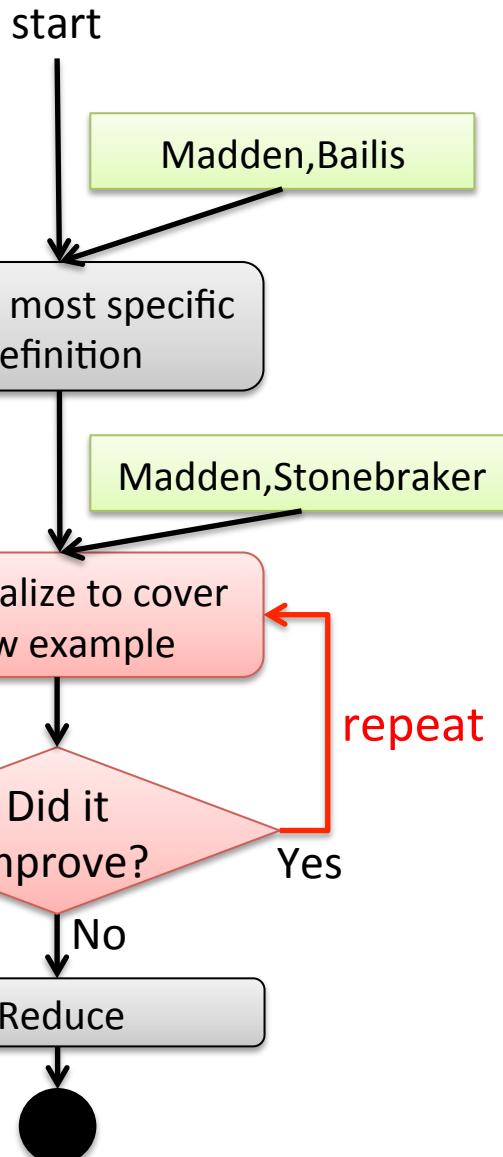
paperAuthor		author		authorAffiliation	
paperId	authorId	id	name	id	affiliation
p2	soc	soc	Socher	soc	Stanford
p2	man	man	Manning	man	Stanford

paper		paperYear		paperConf	
id	title	id	year	id	conf
p2	GloVe: Global Vect...	p2	2014	p2	EMNLP

$$f = P - N = 2$$

collaborators(v_1, v_2) :-
 author(v_3, v_1), author(v_4, v_2),
 authorAffiliation(v_3, v_5),
 authorAffiliation($v_4, \text{Stanford}$), authorAffiliation(v_4, v_6),
 paperAuthor(v_7, v_3), paperAuthor(v_7, v_4).

Step 2: Generalize definition



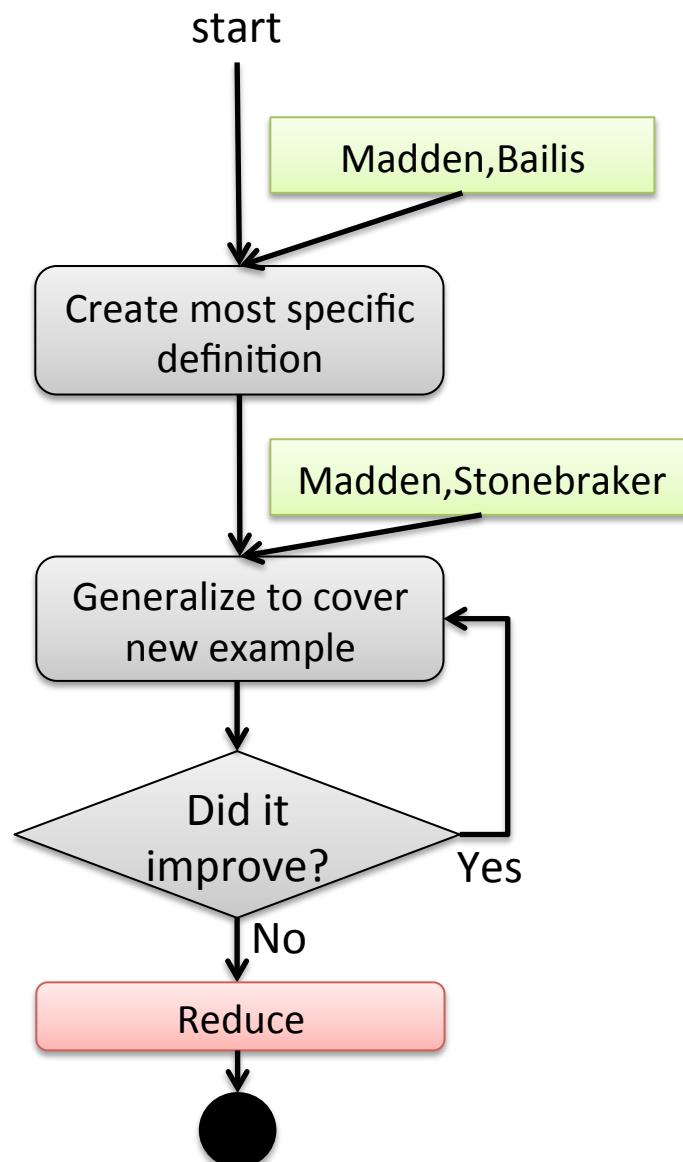
paperAuthor		author		authorAffiliation	
paperId	authorId	id	name	id	affiliation
p3	mad	mad	Madden	mad	MIT
p3	sto	mad	Stonebraker	sto	MIT

paper		paperYear		paperConf	
id	title	id	year	id	conf
p3	The Data Civilizer...	p3	2017	p3	CIDR

$$f = P - N = 3$$

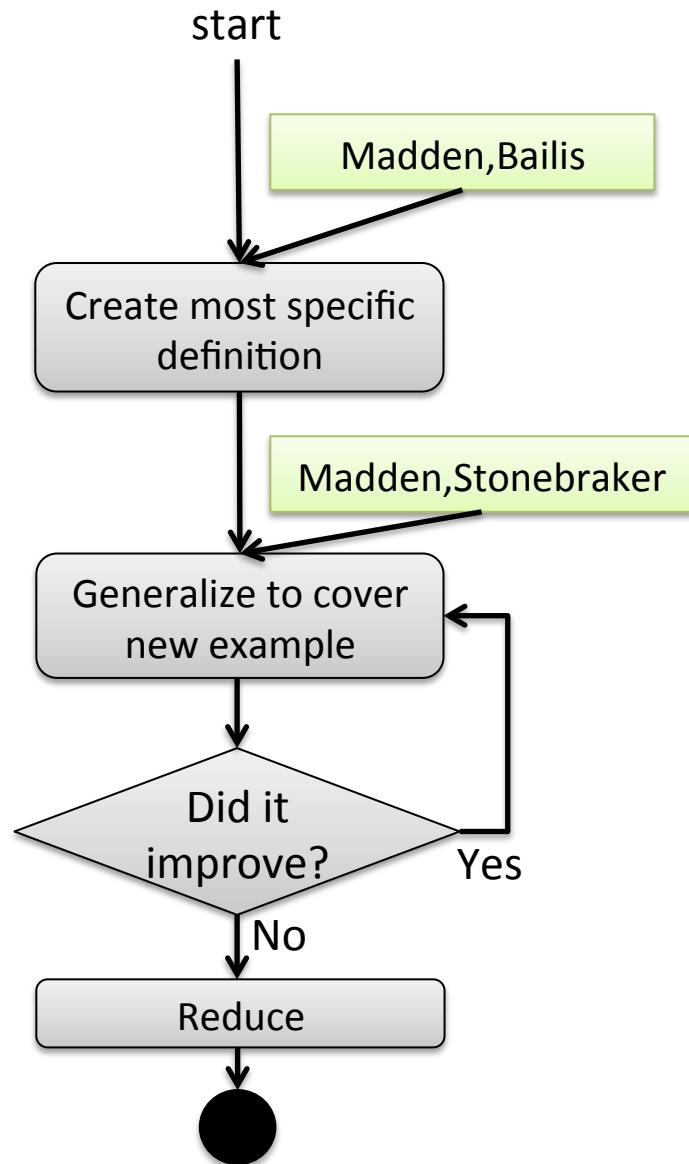
collaborators(v_1, v_2) :-
 author(v_3, v_1), author(v_4, v_2),
 authorAffiliation(v_3, v_5), authorAffiliation(v_4, v_6),
 paperAuthor(v_7, v_3), paperAuthor(v_7, v_4).

Step 3: Reduce definition



- Generalize even more to avoid overfitting
- Reduce definition using negative examples

Learned definition



$$f = P - N = 3$$

collaborators(v_1, v_2) :-
author(v_3, v_1), author(v_4, v_2),
paperAuthor(v_7, v_3), paperAuthor(v_7, v_4).

Two people are collaborators if they are co-authors.

Castor achieves schema independence by using database constraints

author	
id	name
mad	Madden
bai	Bailis

authorAffiliation	
id	affiliation
mad	MIT
bai	Stanford

paperAuthor	
paperId	authId
p3	mad
p3	sto

$\text{author[id]} \subseteq \text{authorAffiliation[id]}$
 $\text{author[id]} \subseteq \text{paperAuthor[authId]}$

author		
id	name	affiliation
mad	Madden	MIT
bai	Bailis	Stanford

paperAuthor	
paperId	authId
p3	mad
p3	sto

$\text{author[id]} \subseteq \text{paperAuthor[authId]}$

Step 1: Create most specific definition using database constraints

author	
id	name
mad	Madden
bai	Bailis

authorAffiliation	
id	affiliation
mad	MIT
bai	Stanford

Madden,Bailis

Create most specific definition

author		
id	name	affiliation
mad	Madden	MIT
bai	Bailis	Stanford

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ authorAffiliation[id]
author[id] ⊆ paperAuthor[authId]

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ paperAuthor[authId]

collaborators(v_1, v_2) :-

collaborators(v_1, v_2) :-

Step 1: Create most specific definition using database constraints

author	
id	name
mad	Madden
bai	Bailis

authorAffiliation	
id	affiliation
mad	MIT
bai	Stanford

Madden,Bailis

Create most specific definition

author		
id	name	affiliation
mad	Madden	MIT
bai	Bailis	Stanford

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ authorAffiliation[id]
 author[id] ⊆ paperAuthor[authId]

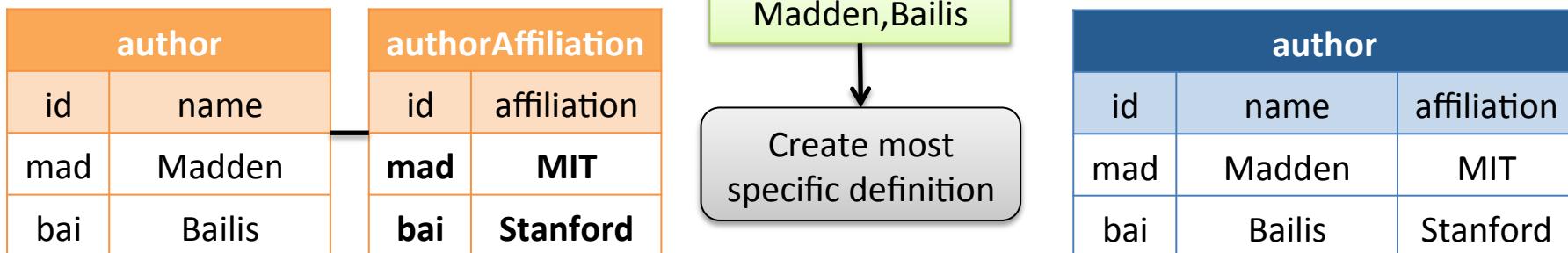
paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ paperAuthor[authId]

collaborators(v_1, v_2) :-
 author(v_3, v_1), author(v_4, v_2).

collaborators(v_1, v_2) :-
 author(v_3, v_1 , MIT), author(v_4, v_2 , Stanford).

Step 1: Create most specific definition using database constraints



$\text{author}[\text{id}] \subseteq \text{authorAffiliation}[\text{id}]$
 $\text{author}[\text{id}] \subseteq \text{paperAuthor}[\text{authId}]$

$\text{author}[\text{id}] \subseteq \text{paperAuthor}[\text{authId}]$

collaborators(v_1, v_2) :-
author(v_3, v_1), author(v_4, v_2),
authorAffiliation(v_3, MIT), paperAuthor(v_3, v_5),
authorAffiliation($v_4, \text{Stanford}$), paperAuthor(v_4, v_6).

collaborators(v_1, v_2) :-
author(v_3, v_1, MIT), author($v_4, v_2, \text{Stanford}$),
paperAuthor(v_3, v_5), paperAuthor(v_4, v_6).

Ensures that the algorithm accesses the same information over all schemas

Step 2 and 3: Generalization and reduction using database constraints

author	
id	name
mad	Madden
sto	Stonebraker

authorAffiliation	
id	affiliation
mad	MIT
sto	MIT

Madden,Stonebraker

Generalize to cover
new example

author		
id	name	affiliation
mad	Madden	MIT
sto	Stonebraker	MIT

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ authorAffiliation[id]
author[id] ⊆ paperAuthor[authId]

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ paperAuthor[authId]

collaborators(v_1, v_2) :-
author(v_3, v_1), authorAffiliation(v_3 , MIT),
author(v_4, v_2), ~~authorAffiliation(v_4 , Stanford)~~.

collaborators(v_1, v_2) :-
author(v_3, v_1 , MIT), ~~author(v_4, v_2 , Stanford)~~.

Step 2 and 3: Generalization and reduction using database constraints

author	
id	name
mad	Madden
sto	Stonebraker

authorAffiliation	
id	affiliation
mad	MIT
sto	MIT

Madden,Stonebraker

Generalize to cover
new example

author		
id	name	affiliation
mad	Madden	MIT
sto	Stonebraker	MIT

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ authorAffiliation[id]
author[id] ⊆ paperAuthor[authId]

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ paperAuthor[authId]

collaborators(v_1, v_2) :-
author(v_3, v_1), authorAffiliation(v_3 , MIT),
~~author(v_4, v_2), authorAffiliation(v_4 , Stanford)~~.

collaborators(v_1, v_2) :-
author(v_3, v_1 , MIT), ~~author(v_4, v_2 , Stanford)~~.

Step 2 and 3: Generalization and reduction using database constraints

author	
id	name
mad	Madden
sto	Stonebraker

authorAffiliation	
id	affiliation
mad	MIT
sto	MIT

Madden,Stonebraker

Generalize to cover
new example

author		
id	name	affiliation
mad	Madden	MIT
sto	Stonebraker	MIT

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ authorAffiliation[id]
author[id] ⊆ paperAuthor[authId]

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ paperAuthor[authId]

collaborators(v_1, v_2) :-
author(v_3, v_1), authorAffiliation(v_3, MIT).

collaborators(v_1, v_2) :-
author(v_3, v_1), MIT).

Step 2 and 3: Generalization and reduction using database constraints

author	
id	name
mad	Madden
sto	Stonebraker

authorAffiliation	
id	affiliation
mad	MIT
sto	MIT

Madden,Stonebraker

Generalize to cover
new example

author		
id	name	affiliation
mad	Madden	MIT
sto	Stonebraker	MIT

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ authorAffiliation[id]
author[id] ⊆ paperAuthor[authId]

paperAuthor	
paperId	authId
p3	mad
p3	sto

author[id] ⊆ paperAuthor[authId]

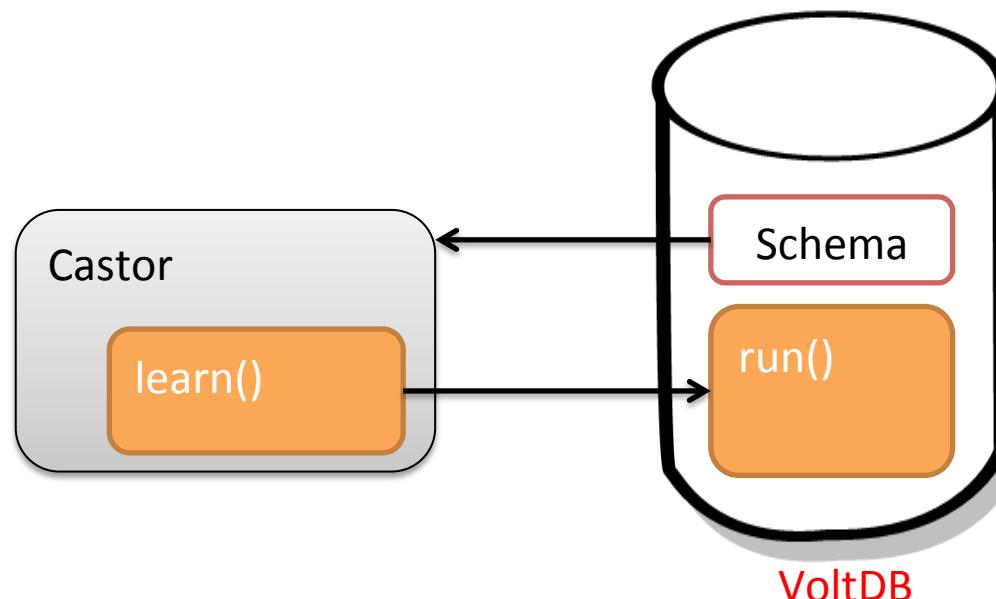
collaborators(v_1, v_2) :-
author(v_3, v_1), authorAffiliation(v_3, MIT).

collaborators(v_1, v_2) :-
author(v_3, v_1), MIT).

Theorem: Castor is schema independent under composition / decomposition.

Techniques to achieve efficiency

1. Castor is implemented on top of the in-memory RDBMS VoltDB
 - Exploit RDBMS mechanisms
 - Part of the algorithm implemented in a stored procedure
2. Approximate and efficient definition minimization



Techniques to achieve efficiency

3. Castor efficiently checks whether a definition covers an example

Alternative approach:

Datalog:

```
collaborators(x,y) :-  
    author(z,x), author(v,y), paperAuthor(w,z), paperAuthor(w,v).
```

SQL:

```
SELECT c.person1, c.person2  
FROM collaborators c, author a1, author s2, paperAuthor pa1, paperAuthor pa2  
WHERE  c.person1 = a1.name AND c.person2 = a2.name AND a1.id = pa1.authorId  
       AND a2.id = pa2.authorId AND pa1.id = pa2.id;
```

Castor's approach:

1. Compute most specific definition h_e for example e .
2. Definition h covers example e iff there is a substitution θ such that $h\theta \subseteq h_e$ (homomorphism).

✓ More efficient

Experimental results

- Database: UW-CSE – academic department
 - 9 relations, 2K tuples
 - 102 positive examples, 204 negative examples
- Target relation: advisedBy(student, professor)

Algorithm	Metric	Schema 1	Schema 2	Schema 3	Schema 4
FOIL	F1-score	0.49	0.49	0.54	0.61
	Time (s)	18.7	20.8	30.7	30.6
Progol	F1-score	0.68	0.61	0.53	0.38
	Time(s)	9.7	13.2	27.9	334.8
ProGolem	F1-score	0.68	0.68	0.60	0.61
	Time (s)	24.4	28.8	26.7	54.1
Castor	F1-score	0.68	0.68	0.68	0.68
	Time (s)	7.2	7.4	7.9	12.4

Experimental results

- Database: HIV – structure of chemical compounds
 - 80 relations, 14M tuples
 - 5K positive examples, 36K negative examples
- Target relation: anti-HIV(compound)

Algorithm	Metric	Schema 1	Schema 2
FOIL	F1-score	0.49	0.80
	Time (h)	3	0.9
Castor	F1-score	0.83	0.83
	Time(h)	3.5	1.9

Progol and ProGolem do not terminate after 5 days

Conclusions and future work

- Relational learning algorithms leverage the structure of data to learn Datalog definitions
- Schema independence is a desired property
- Current algorithms are not schema independent
- Castor is schema independent, accurate and efficient
- Future work:
 - Achieve schema independence over other transformations
 - Learn over different data sources

Thank you