

Thesis Oral

Grounded Knowledge Bases for Scientific Domains

Dana Movshovitz-Attias

August 26, 2015

Thesis Committee:

William Cohen, Chair

Tom Mitchell

Roni Rosenfeld

Alon Halevy, Google Research



Computer
Science
Department

 Who is Barack Obama's wife?

Who is Barack Obama's wife?

Michelle Obama (m. 1992)

Barack Obama, Spouse



Michelle LaVaughn Robinson Obama is an American lawyer and writer. She is married to the 44th and current President of the United States, Barack Obama, and is the first African-American First Lady of the United States. [Wikipedia](#)

More about Michelle Obama

Family of Barack Obama - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/Family_of_Barack_Obama - Wikipedia

Michelle Obama, née Robinson, the **wife** of **Barack Obama**, was born on January 17, 1964, in Chicago, Illinois. She is a lawyer and was a University of Chicago ...
[Sidwell Friends School](#) - [Marian Shields Robinson](#) - [Bo](#) - [Charles T. Payne](#)

Michelle Obama - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/Michelle_Obama - Wikipedia

Michelle LaVaughn Robinson **Obama** (born January 17, 1964) is an American lawyer and writer. She is the **wife** of the 44th and current **President** of the United ...
[Craig Robinson \(basketball\)](#) - [Hyde Park, Chicago](#) - [Sidley Austin](#) - [Valerie Jarrett](#)

Michelle Obama - Biography - U.S. First Lady, Lawyer ...

www.biography.com/people/michelle-obama-307592 - FYI

Explore the life of **Michelle Obama**, the 44th first lady and **wife** of President **Barack Obama**. Learn more at Biography.com.

First Lady Michelle Obama | whitehouse.gov

<https://www.whitehouse.gov/.../first-lady-michelle-obama> - White House

First Lady Michelle LaVaughn Robinson Obama is a lawyer, writer, and the **wife** of the 44th and current President, **Barack Obama**. She is the first ...

Barack Obama was asked about 'his first wife' by a woman ...

www.telegraph.co.uk/.../Barack_Obama - The Daily Telegraph

Jan 22, 2015 - **Barack Obama** was asked about his 'first **wife**' by a woman who took a ... when she gave Obama a gift of green lipstick for **Michelle Obama**, who ...

Michelle Obama - First Lady and wife of President Barack ...

www.telegraph.co.uk/News/World_News - The Daily Telegraph

Michelle Obama - Biography - U.S. First Lady, Lawyer ...



www.biography.com/people/michelle-obama-307592

Explore the life of Michelle Obama, the 44th first lady and **wife** of President **Barack Obama**. Learn more at ...

Michelle Obama - First Lady and wife of President Barack ...

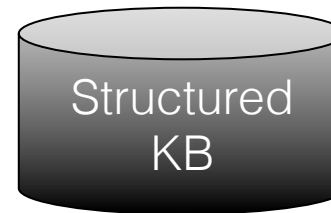
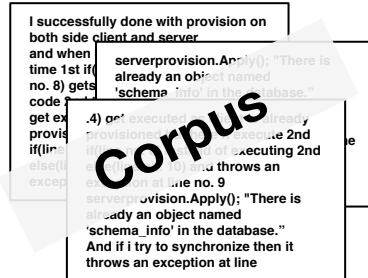
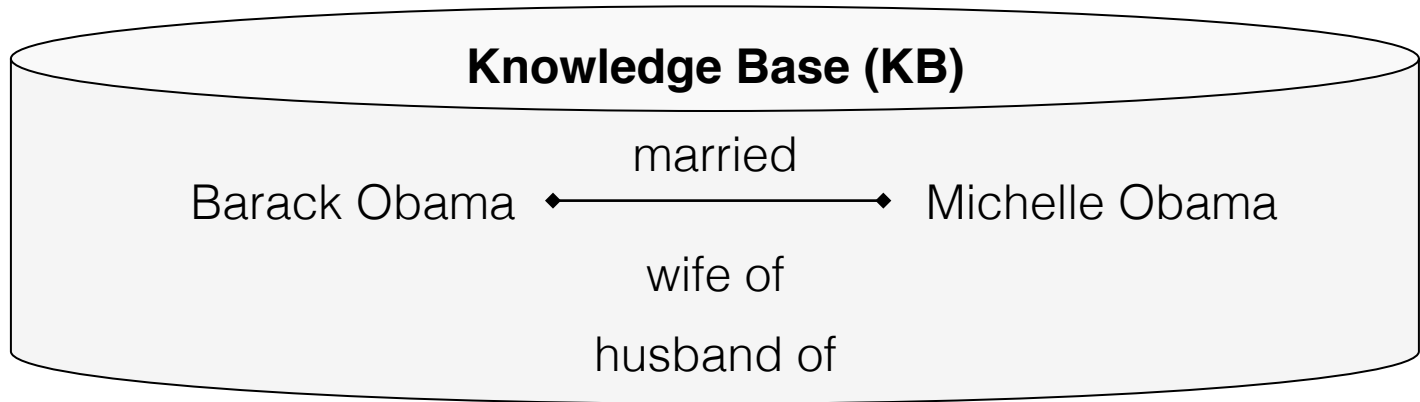


www.telegraph.co.uk/News/World_News

Jul 1, 2015

Michelle LaVaughn Obama, First Lady and **wife** of US President **Barack Obama**: All the latest news and ...

Who is **Barack Obama's wife**?



TextRunner

NELL

YAGO

Knowledge Vault



Software

“What is the **run time** of **quick sort**?”

Quicksort - Wikipedia, the free encyclopedia

<https://en.wikipedia.org/wiki/Quicksort> ▾ Wikipedia ▾

Animated visualization of the **quicksort** algorithm. The horizontal lines are pivot values.

Quicksort (sometimes called partition-exchange **sort**) is an efficient **sorting** algorithm, serving as a systematic method for placing the elements of an array in order.

Tony Hoare - Dutch national flag problem - Robert Sedgewick - Flashsort

Running Time of Quicksort - HackerRank

<https://www.hackerrank.com/challenges/quicksort4> ▾

Mar 4, 2013 - The **running time** of **Quicksort** will depend on how balanced the partitions are. If you are unlucky and select the greatest or the smallest element ...

Quicksort Running Time - Math StackExchange

math.stackexchange.com/.../quicksort-running-time ▾ Stack Exchange ▾

Feb 18, 2011 - ... the recurrence will be: The above recurrence has the solution (I will prove this later): Hence the **running time** of **QUICKSORT** in this case is ...

Quick Sort - Personal.kent.edu

www.personal.kent.edu/~rmuhamma/Algorithms/.../Sorting/quickSort.ht... ▾

The **running time** of **quick sort** depends on whether partition is balanced or unbalanced, which in turn depends on which elements of an array to be **sorted** are used for partitioning. A very good partition splits an array up into two equal sized arrays.

[PDF] Quick Sort

<https://www.cse.ust.hk...> ▾ Hong Kong University of Science and Technology ▾

P, followed by the results of **quicksort**(S. 2.)) ... void **quicksort**(int A[], int left, int right).

...the average case running time is $\theta(n \log n)$...

[PDF] Quicksort

www.bowdoin.edu/~ltoma/...quicksort/quicksort.pdf ▾ Bowdoin College ▾

Quicksort(A, q + 1, r). Fl. Sort using **Quicksort**(A, 1, n). If $q = n/2$ and we divide in $\Theta(n)$ time, we again get the recurrence $T(n) = 2T(n/2) + \Theta(n)$ for the **running time** ...

Biomedical

“What is the **molecular mass** of **BamA**?”

[PDF] Quiz 2 answers - with worked solutions - Bama.ua.edu

www.bama.ua.edu/.../quiz2_key_with_solutions.p... ▾ University of Alabama ▾

Quiz 2 answers - with worked solutions. 1. What is average mass, in grams, of one atoms of iron? use mol wt of iron (= **molar mass** = mass for one mol of Fe ...

[PPT] Polymers: Introduction - Bama.ua.edu

bama.ua.edu/~kshaughn/ch338/.../poly-lecture.ppt ▾ University of Alabama ▾

Monomer: Low **molecular weight** compound that can be connected together to give a poymer; Oligomer: Short polymer chain; Copolymer: polymer made up of 2 ...

[PDF] Hydrogen/Deuterium exchange mass spectrometry - Bam...

bama.ua.edu/.../Busenlehner_ABBreview_2005.p... ▾ University of Alabama ▾

by LS Busenlehner - 2005 - Cited by 143 - Related articles

Oct 5, 2004 - exchange mass spectrometry (H/D exchange MS) is emerging as an efficient ... proteins having **molecular masses** in excess of 50 kDa.

TP0326, a Treponema pallidum β -Barrel Assembly ...

www.ncbi.nlm.nih.gov/... ▾ National Center for Biotechnology Information ▾

by DC Desrosiers - 2011 - Cited by 32 - Related articles

Apr 27, 2011 - In E. coli, **BamA** is the central component of a multi-protein complex consisting Native TP0326 forms part of a high **molecular mass** complex.

The crystal structure of BamB suggests interactions with ...

www.ncbi.nlm.nih.gov/... ▾ National Center for Biotechnology Information ▾

by N Noinaj - 2011 - Cited by 47 - Related articles

Jan 26, 2011 - It interacts with the periplasmic domain of **BamA**, an integral outer We determined the **molecular mass** of BamB in solution using size ...

...BamA at its expected molecular weight (~90 kDa)...

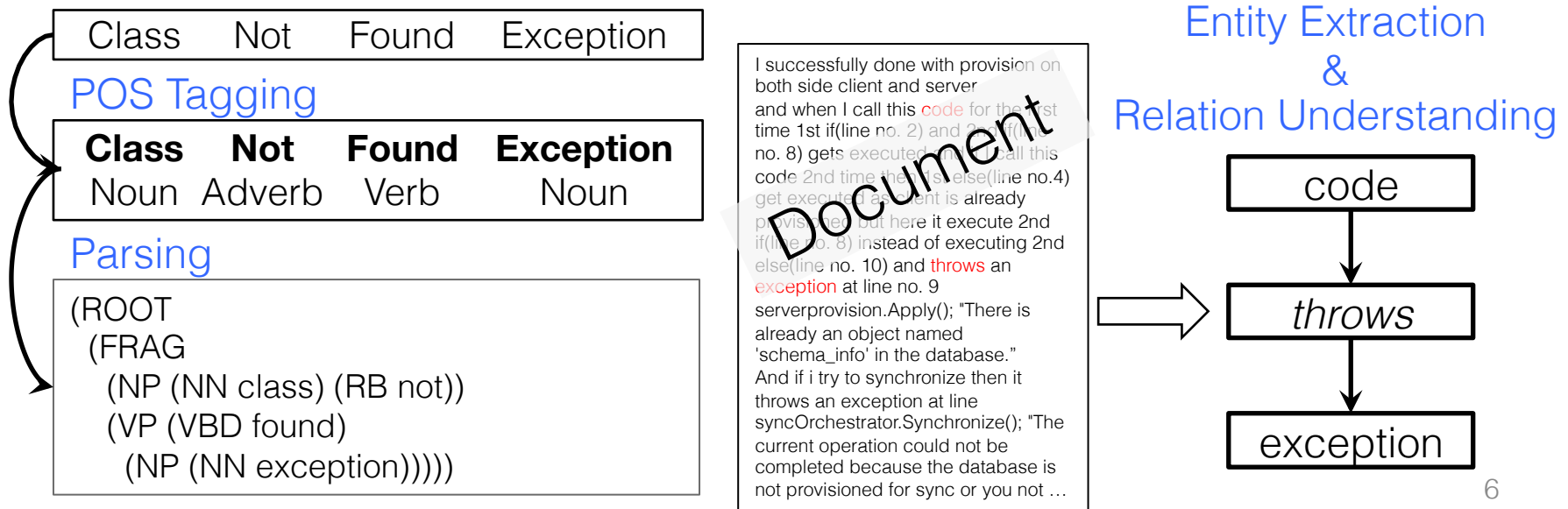
BAMA Course Survey: ... Use masses listed above to calculate the **molecular mass**. ...

This keeps the shape of the molecule "straight" or "linear" allowing these ...

Challenges in Mining Scientific Text

- Specialized terminology
- Domain-specific language constructs

Affected NLP Techniques

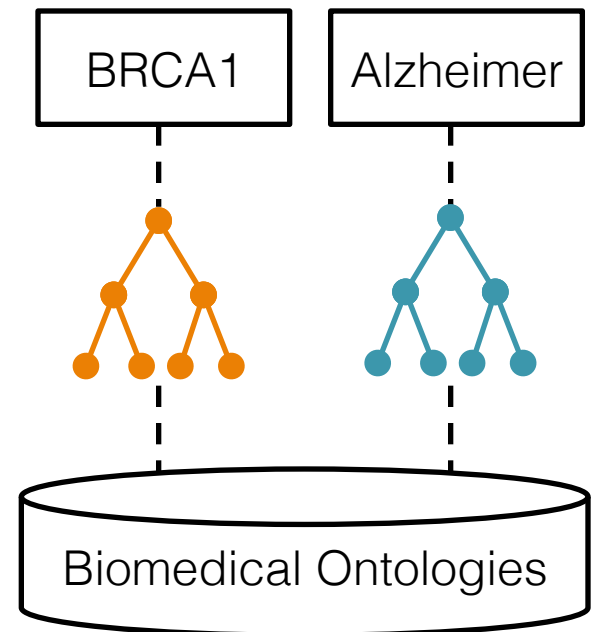
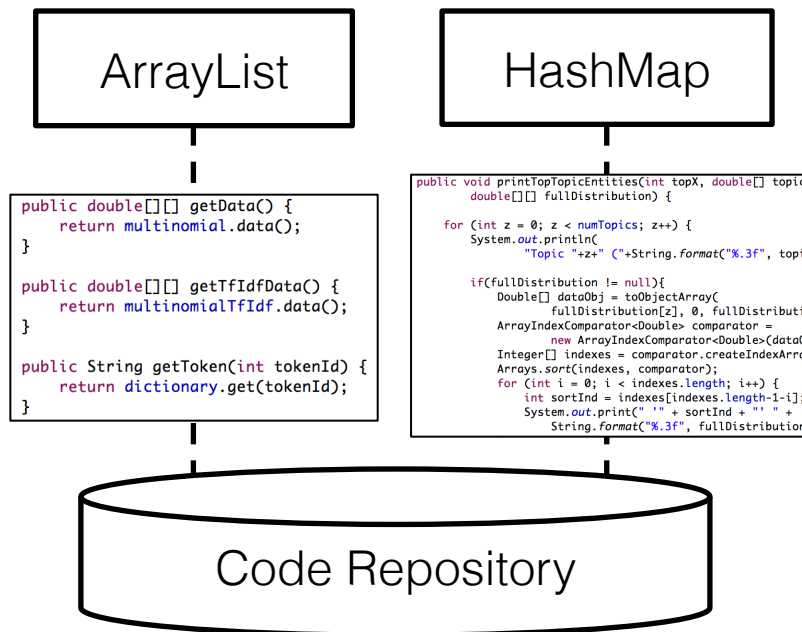


Grounding Scientific Entities

Scientific data is not
found only in text



Opportunity:
Domain-specific
resources

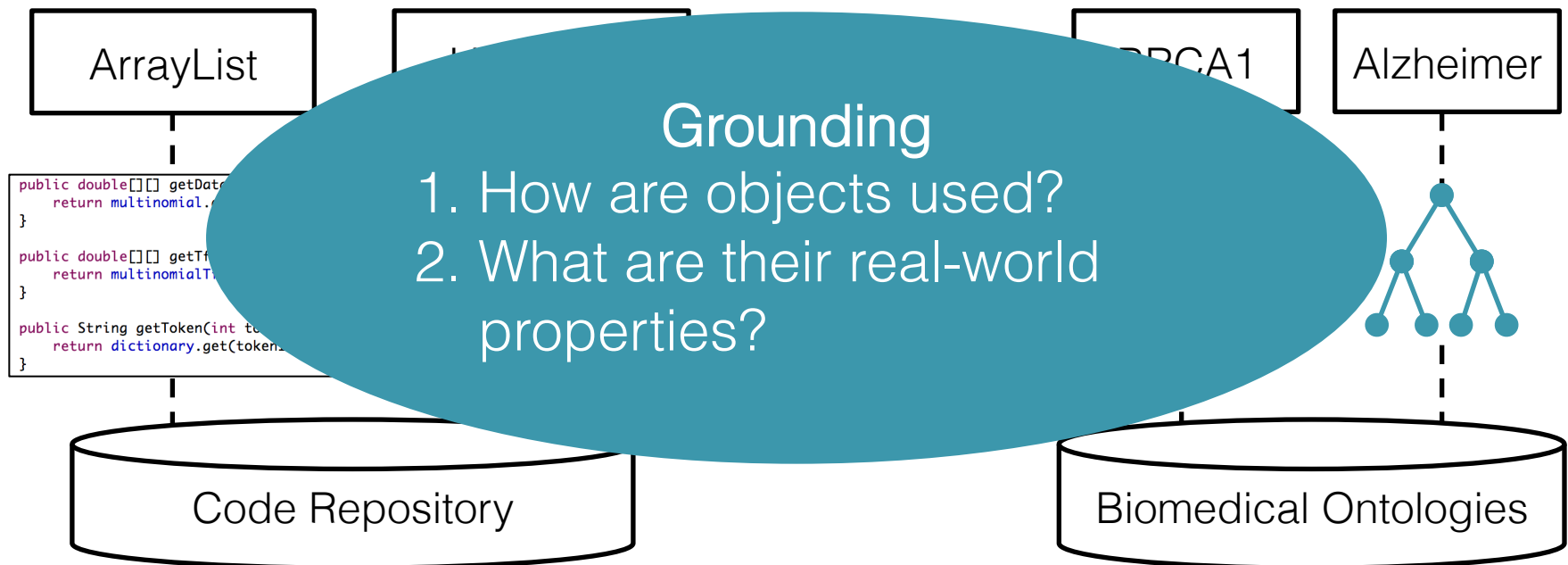


Grounding Scientific Entities

Scientific data is not
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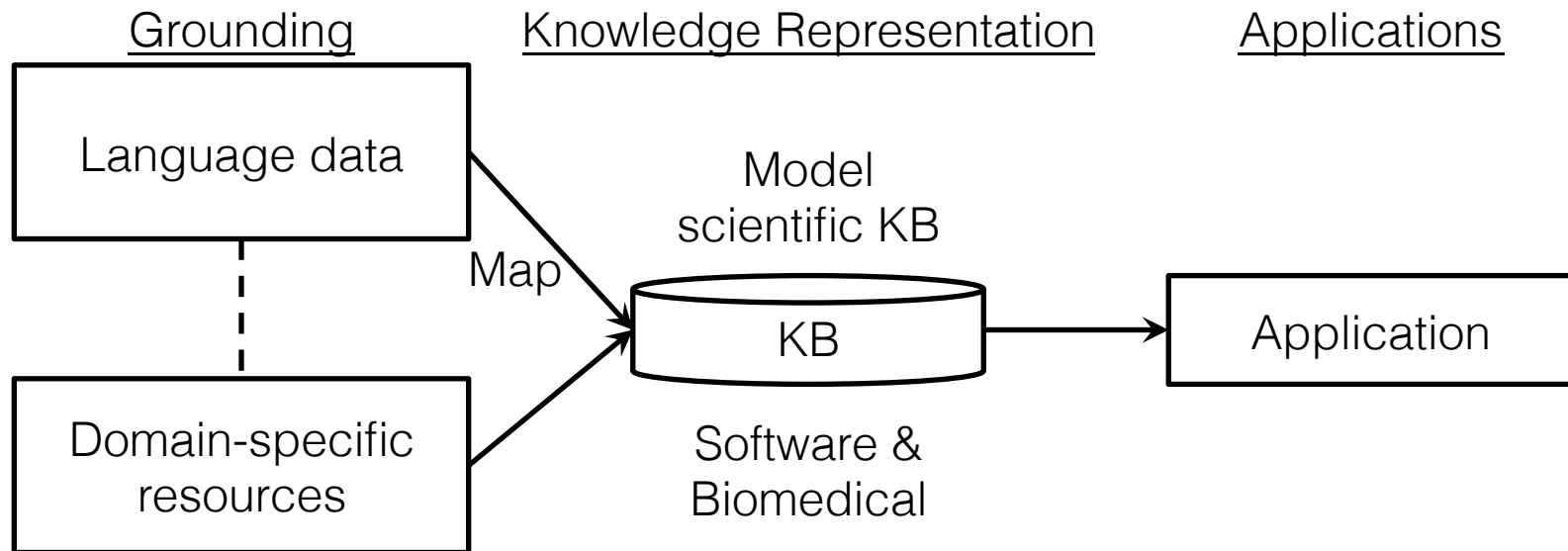


Opportunity:
Domain-specific
resources



Thesis Statement

“**Grounding entities** to specialized data from a scientific domain facilitates improved unsupervised and semi-supervised algorithms for **Knowledge Base construction** for that domain“



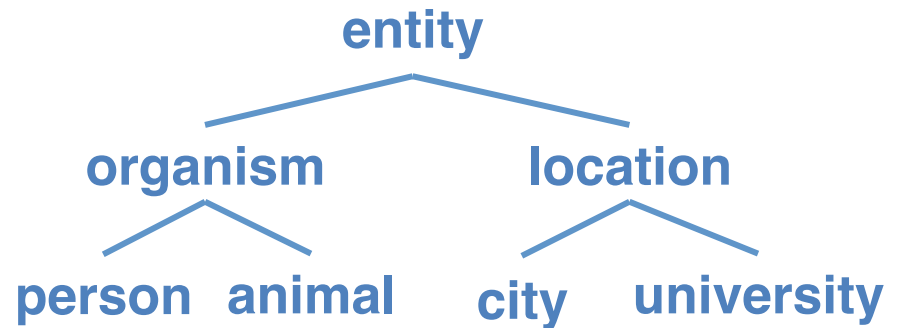
Knowledge Base Construction

Open IE

(**Beijing**, *is the capital of*, **China**)
(**Penticton**, *has very*, **warm summers**)
(**Goods**, *can be defined in*, **a variety of ways**)

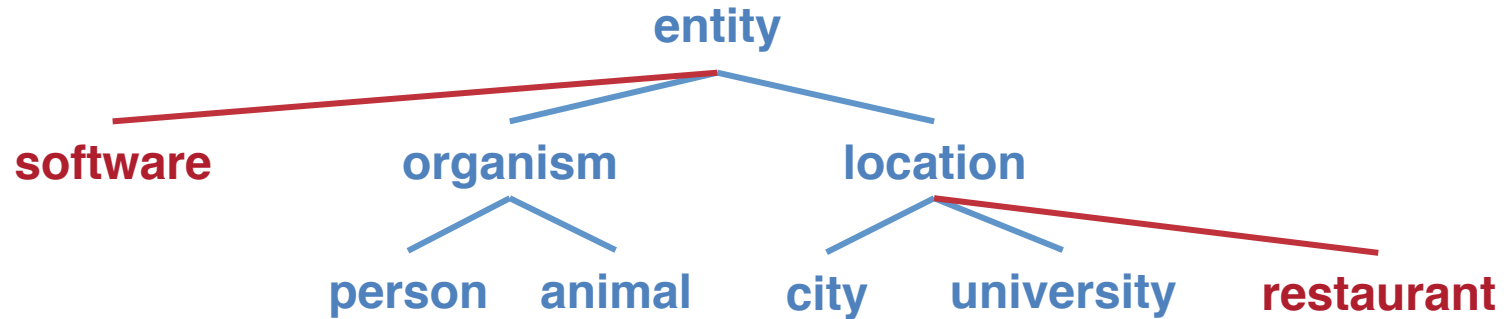
- ReVerb [Fader et al., 2011]
- TextRunner [Yates et al., 2007]

Ontology-Guided Construction



- NELL [Carlson et al., 2010]
- FreeBase [Google, 2011]
- Yago [Suchanek et al., 2007, 2008]
- Knowledge Vault [Dong et al., 2014]

Reasoning with Ontologies



- ✓ Ontologies give information context
- ✓ Easy to extract domain-specific information
- ✗ Ontologies are
 - expensive
 - require prior knowledge
- ✗ Manual ontology does not reflect language statistics

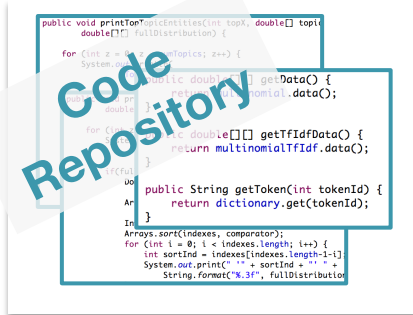
Roadmap

Statistical Language Model for
Software Domain Application

```
/* comment prediction */
```

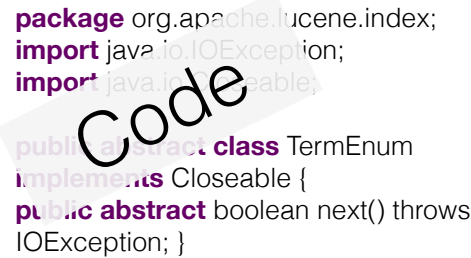
Predicting Code Comments

Model code with statistical language models



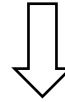
```
public void printTopicsEntities(int topic, double[] topics,
double[] fullDistribution) {
    for (int z = 0; z < topics.length; z++) {
        System.out.print("Topic: ");
        public double[] getData() {
            return multinomialTFidf.data();
        }
        for (int i = 0; i < fullDistribution.length; i++) {
            double[] data = getTFidfData();
            return multinomialTFidf.data();
        }
    }
    public String getToken(int tokenId) {
        return dictionary.getTokenId();
    }
}
Arrays.sort(indexes, comparator);
for (int i = 0; i < indexes.length; i++) {
    int sortInd = indexes[i].length - 1;
    System.out.print(" " + sortInd + " " +
        String.format("%.3f", fullDistribution
```

Predict class comment



```
package org.apache.lucene.index;
import java.io.IOException;
import java.io.Closeable;

public abstract class TermEnum
implements Closeable {
    public abstract boolean next() throws
    IOException;
}
```



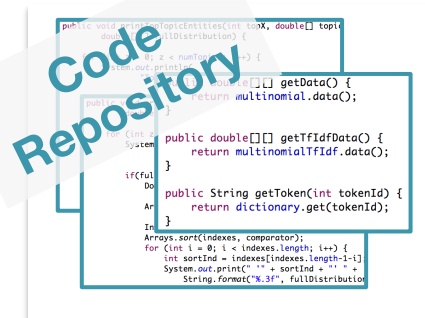
```
Abstract class for enumerating terms.
<p>Term enumeration always
ordered by Term.compareTo(). Each
term in
the enumeration is greater than all
that precede it.
```

Evaluate how much typing can we save?

Up to 47% !

Train a named-entity extractor

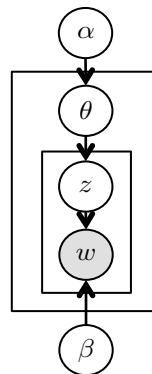
Code Modeling



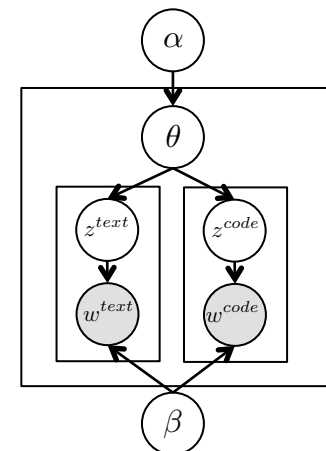
Language and domain understanding

1. Shallow statistical model
N-gram

2. BOW topic model
LDA



3. Basic domain encoding
(code vs. text entities)
Link-LDA

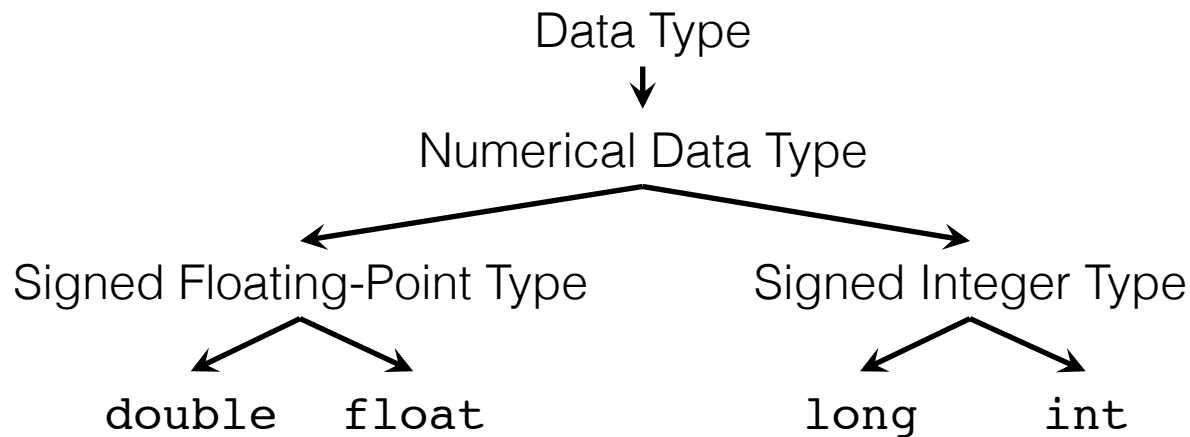


Predicting Code Comments

- Comments are highly predictable
 - 47% of characters predicted
- Un-intuitively: Shallow statistical method performed best
 - 3-gram: Train a named-entity extractor
 - link-LDA: Train a named-entity extractor
- Intuitively: Domain encoding improves performance
 - Link-LDA > LDA

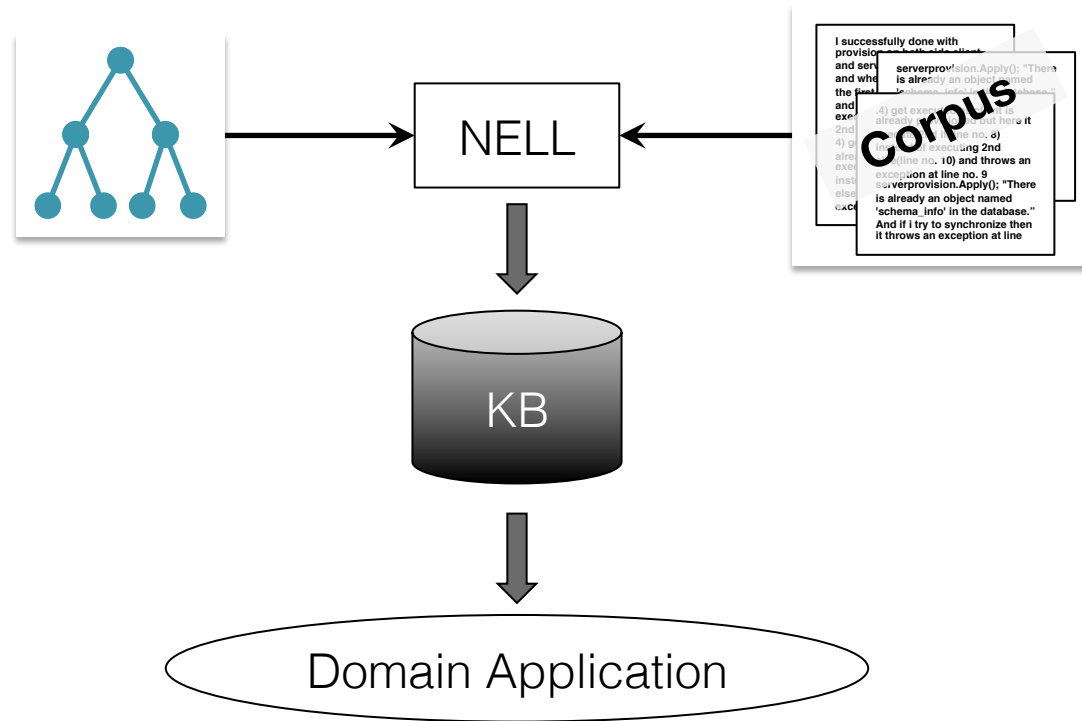
We Need Deeper Understanding of Domain Entities

```
/* This method reads the next double from stdin */  
float  
long  
int
```



Semantics and **categorical understanding** contribute to language modeling task

We Need Deeper Understanding of Domain Entities

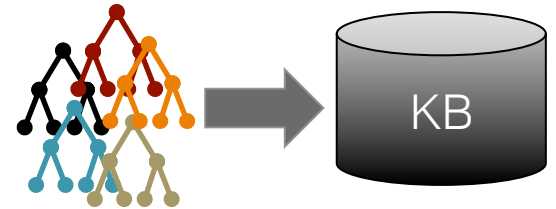


Semantics and ***categorical understanding*** contribute to language modeling task

Roadmap

Statistical Language Model for
Software Domain Application

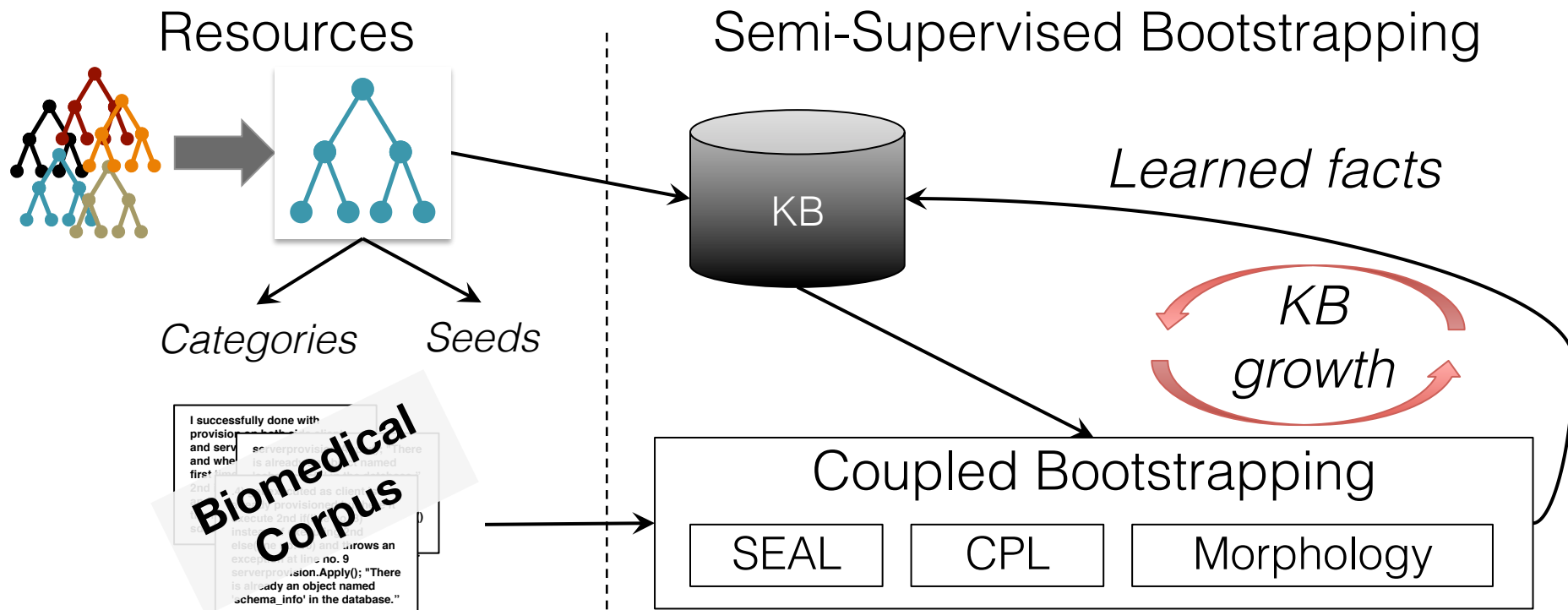
```
/* comment prediction */
```



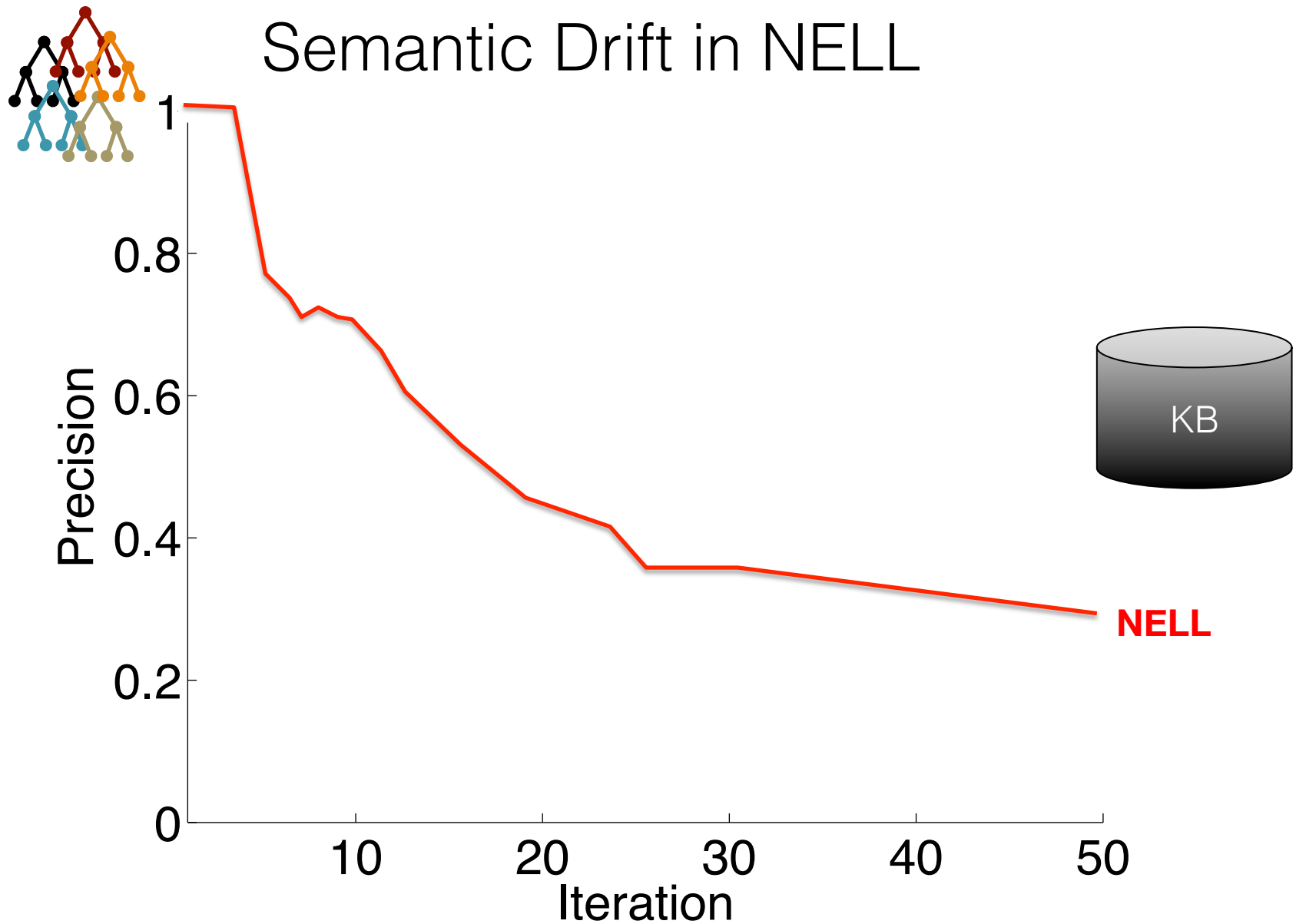
Bootstrap KB Learning for
the Biomedical Domain

Bootstrap KB Learning for the Biomedical Domain

- Modify KB learning system (NELL) for biomedical domain



Semantic Drift in NELL

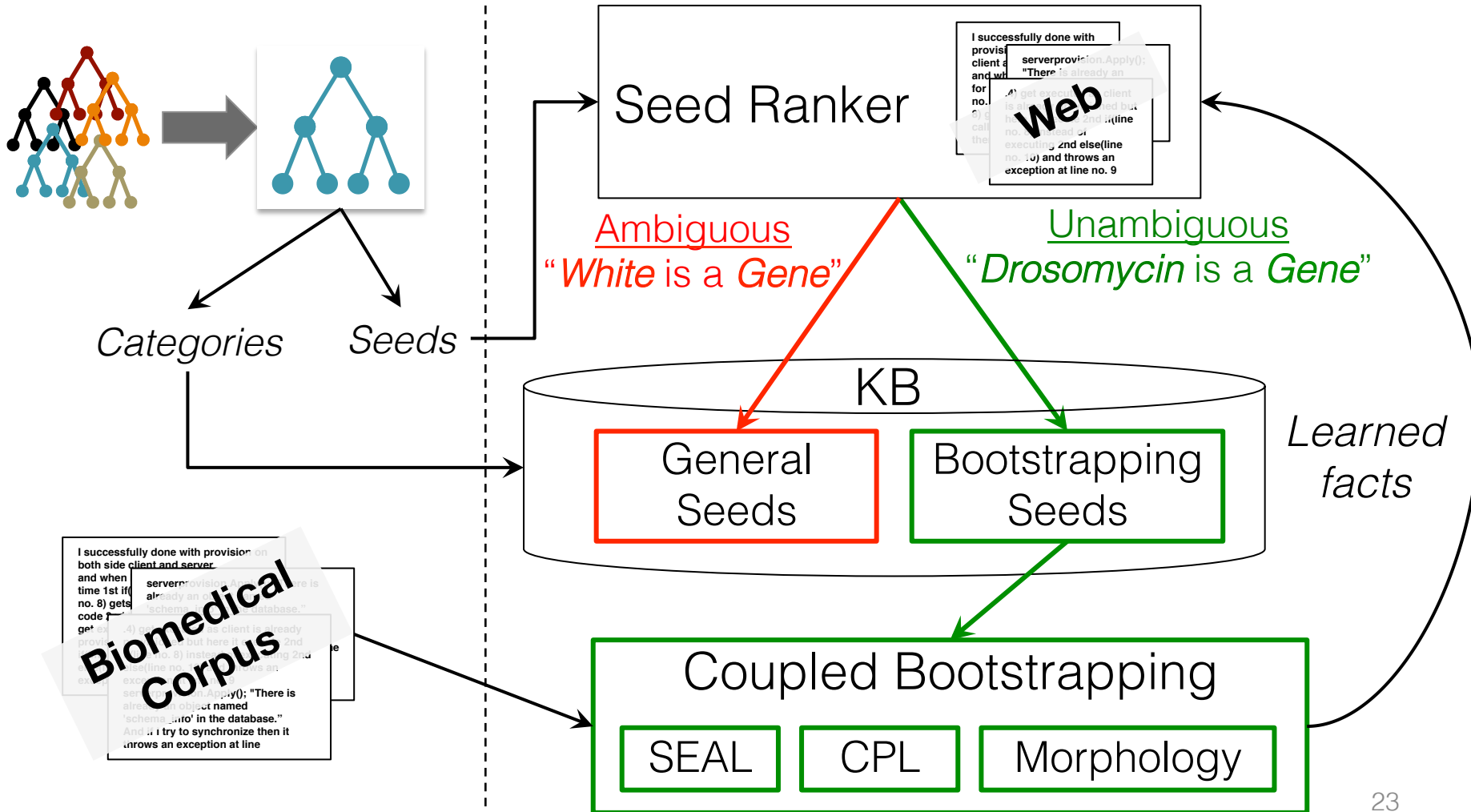


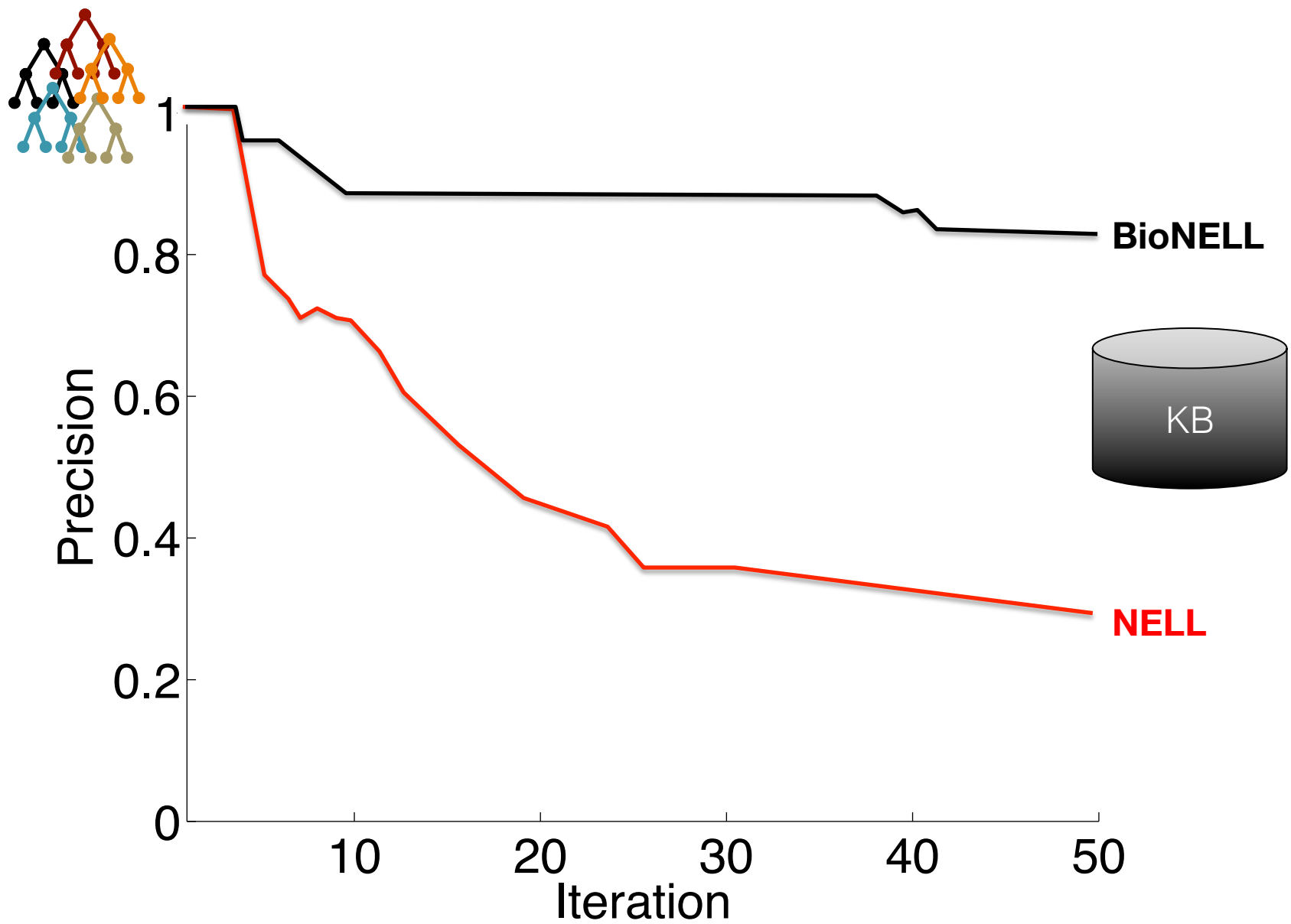
BioNELL



Biomedical Resources

Modified Bootstrapping

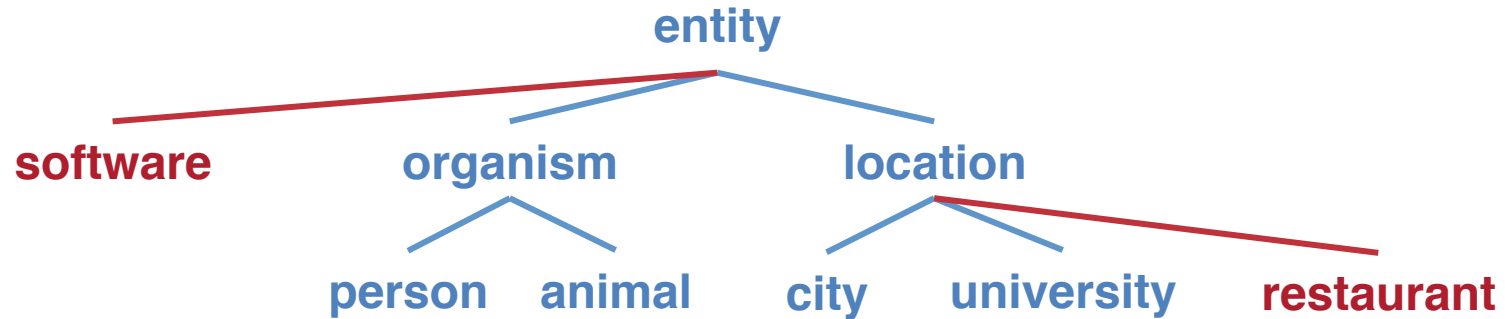




BioNELL: Lessons

- Biomedical ontologies + filtering bootstrapping seeds lead to:
 - High-precision biomedical KB
 - Improves domain applications (NER)
- Disadvantage: Relies on input ontologies
 - No existing Software ontologies

Reasoning with Ontologies



- ✓ Ontologies give information context
- ✓ Easy to extract domain-specific information
- ✗ Ontologies are
 - expensive
 - require prior knowledge
- ✗ Manual ontology does not reflect language statistics
- ✗ **Ontology and facts are often drawn from different sources**

Roadmap

Statistical Language Model for
Software Domain Application

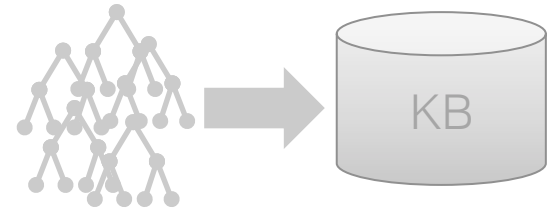
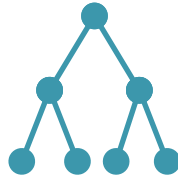
```
/* comment prediction */
```

**Grounded Software
Ontology Construction**

Corpus

```
I successfully done with  
provision  
and ser  
and whe  
the file  
and  
and ex-  
2nd  
4) g  
alre  
exce  
inat  
else  
exce
```

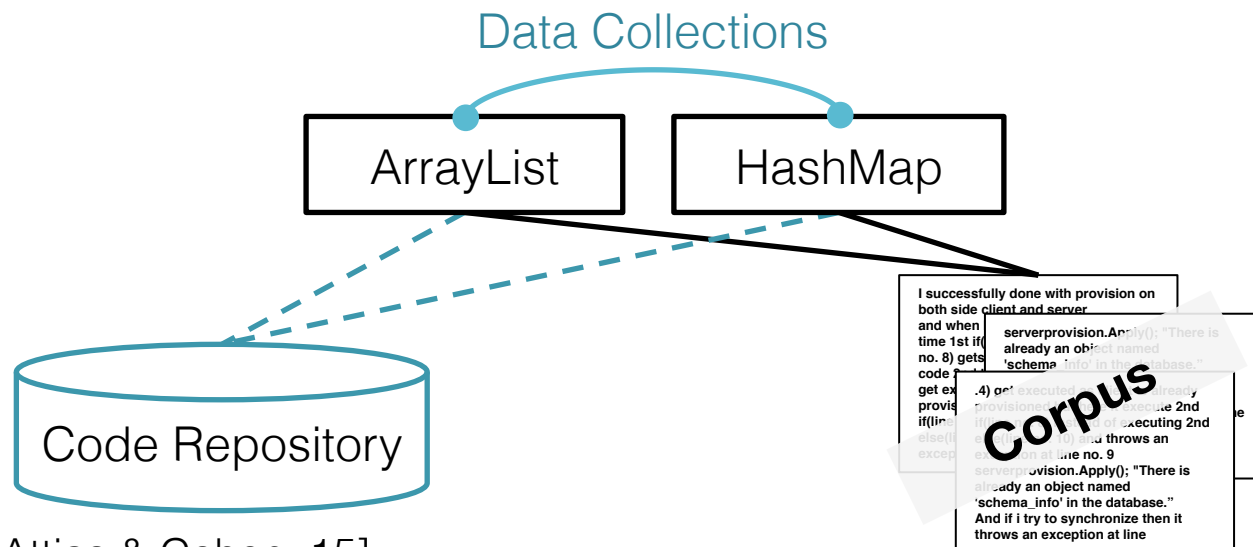
```
serverprovision.Apply(); "There  
is already an object named  
'schema_info' in the database."  
And if I try to synchronize then  
it throws an exception at line
```



Bootstrap KB Learning for
the Biomedical Domain

Grounded Software Ontology Construction

- We detect coordinate relations (similarity) between Java classes
 - “This method iterates over ArrayLists **and** HashMaps”



Grounding

I successfully done with provision on both side client and server and when time 1st if already an object named no. 8) gets code get ex provi if(line else(excep

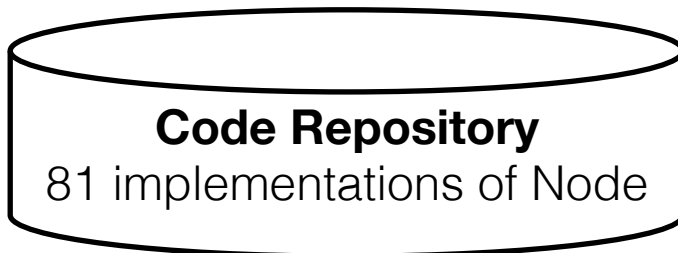
serverprovision.Apply(); "There is already an object named 'schema_info' in the database."

4) or executed provision already executing 2nd if(line else(excep

serverprovision.Apply(); "There is already an object named 'schema_info' in the database." And if i try to synchronize then it throws an exception at line

Corpus

“...Is a root node an internal node?...”



```
public interface TreeNode
{
    /**
     * Returns the child <code>TreeNode</code> at index
     * <code>childIndex</code>.
     */
    TreeNode getChildAt(int childIndex);

    /**
     * Returns the number of children <code>TreeNode</code>s the receiver
     * contains.
     */
    int getChildCount();

    /**
     * Returns the parent <code>TreeNode</code> of the receiver.
     */
    TreeNode getParent();

    /**
     * Returns the index of <code>node</code> in the receivers children.
     * If the receiver does not contain <code>node</code>, -1 will be
     * returned.
     */
    int getIndex(TreeNode node);

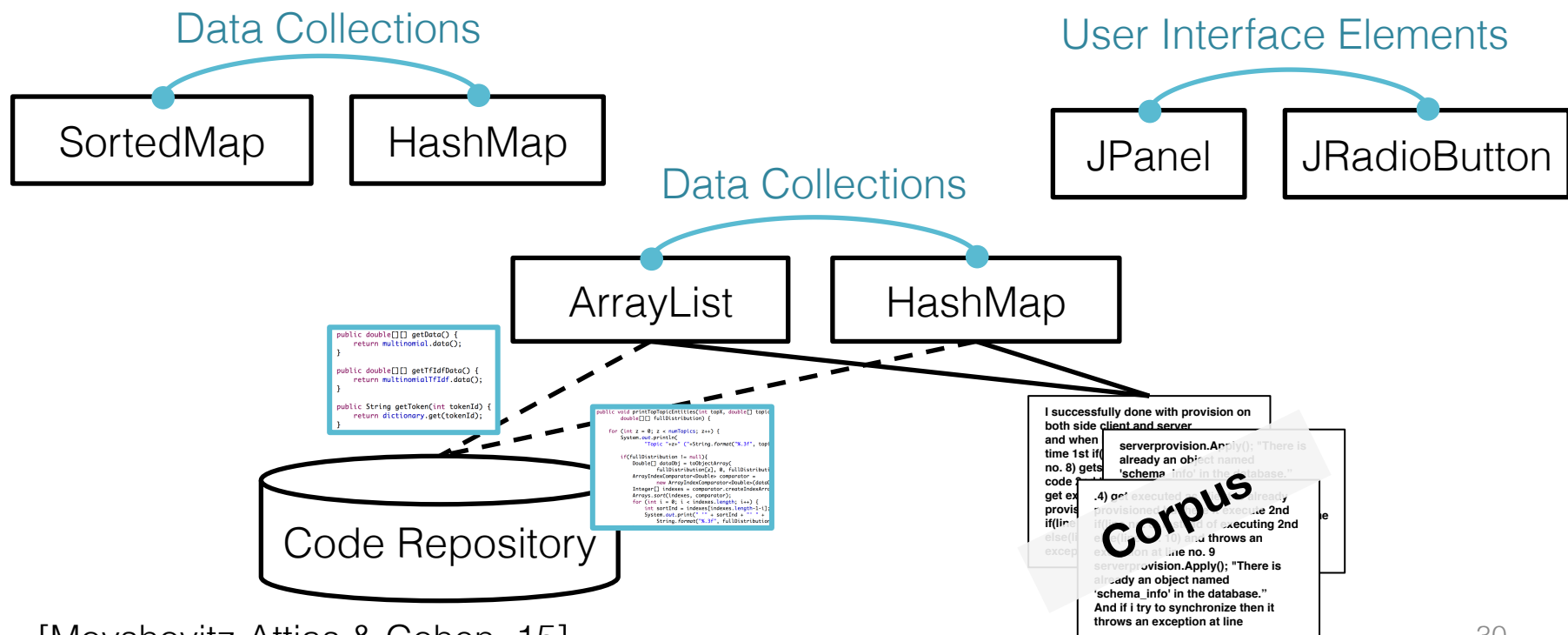
    /**
     * Returns true if the receiver allows children.
     */
    boolean getAllowsChildren();

    /**
     * Returns true if the receiver is a leaf.
     */
}
```

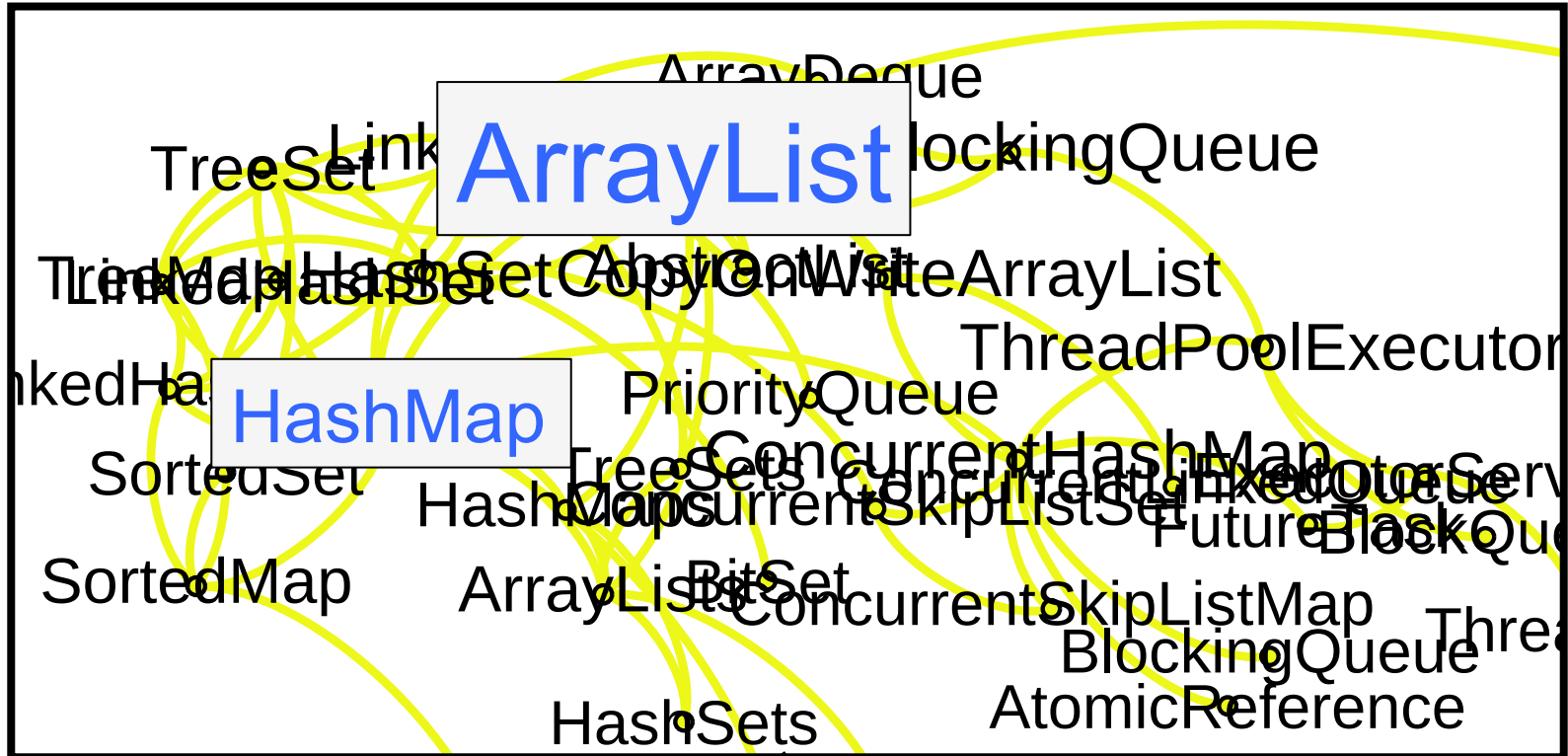
javax.xml.soap.**Node**
javax.imageio.spi.Digraph**Node**
javax.swing.tree.TreeNode
javax.swing.tree.MutableTree**Node**
com.sun.org.apache.xerces.internal.dom.**NodeImpl**

Grounded Software Ontology Construction

- We detect coordinate relations (similarity) between Java classes
 - “This method iterates over ArrayLists **and** HashMaps”



Utility Classes



- TreeSet
- SortedMap
- SortedSet
- HashSet
- BitSet
- ArrayDeque
- PriorityQueue
- BlockingQueue
- ArrayBlockingQueue
- LinkedHashMap

Nodes: Classes
Edges: Coordinate relations
Edge color: community detection (Louvain method)
Label size: betweenness centrality

Utilities

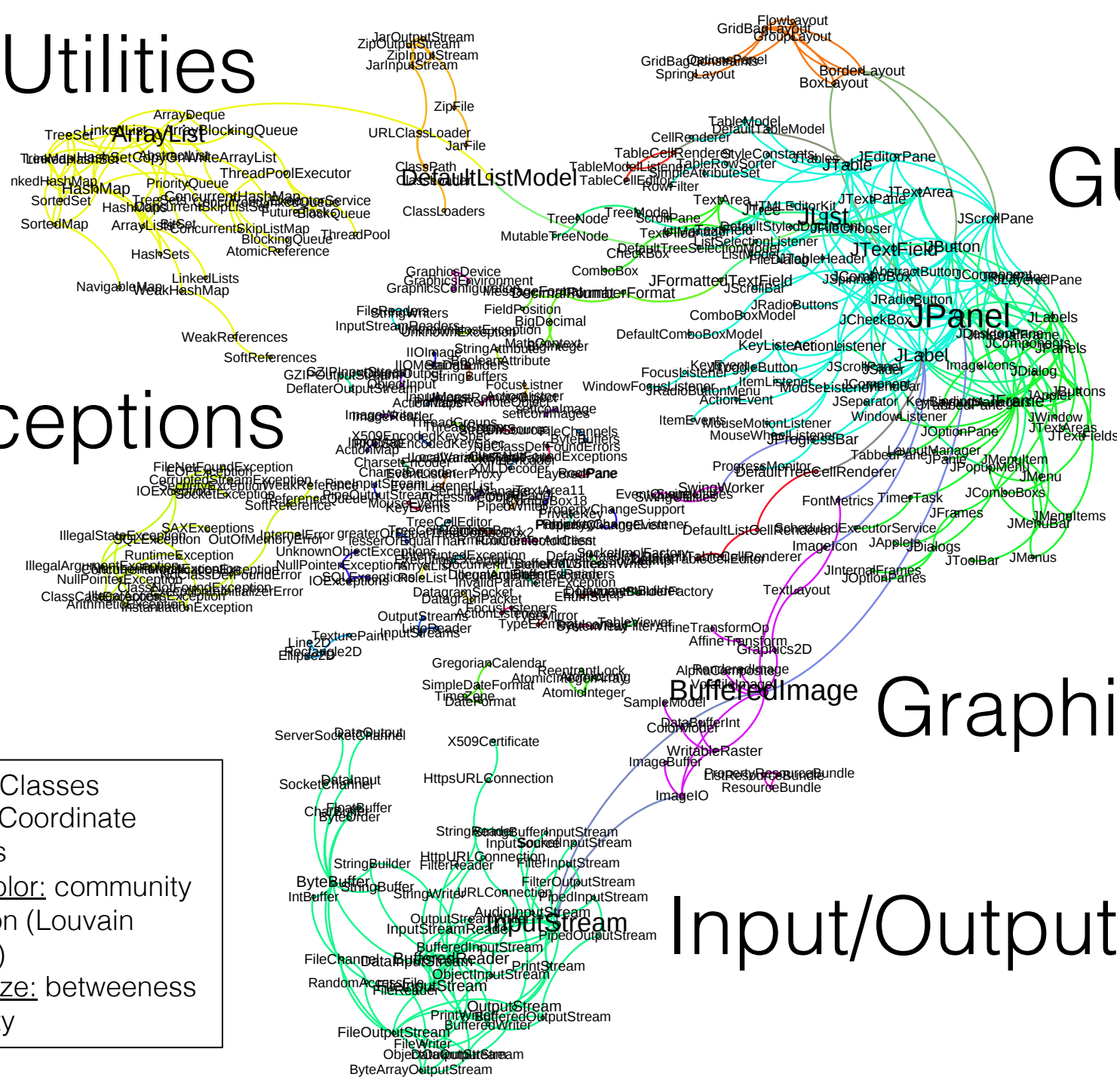
GUI

Exceptions

Graphics

Input/Output

- Nodes: Classes
- Edges: Coordinate relations
- Edge color: community detection (Louvain method)
- Label size: betweenness centrality



Contributions & Lessons

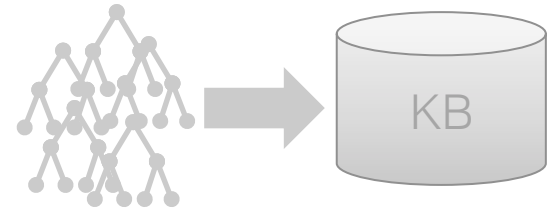
- Linked class entities to code implementation
- Defined distributional similarity for code
- By combining code and text similarities we learned relations (and ontology)
- Advantage: This ontology reflects statistics in language and code
 - In contrast to manually built ontologies
- Grounding to code limits scope of learned ontology to code entities
 - What's missing?

Users
Computer resources
Design patterns

Roadmap

Statistical Language Model for
Software Domain Application

```
/* comment prediction */
```



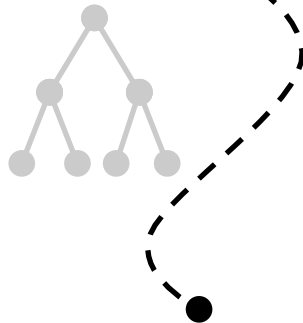
Bootstrap KB Learning for
the Biomedical Domain

Grounded Software
Ontology Construction

Corpus

```
I successfully done with  
provisio  
and ser  
and whe  
the first  
and ex  
2nd  
4) g  
alre  
exa  
inst  
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```

serverprovision.Apply(); "There
is already an object named
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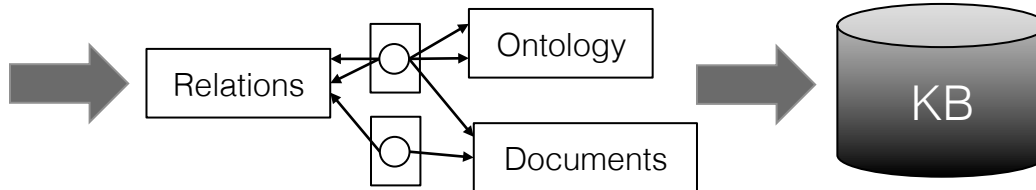


Topic-Model KB Learning

Corpus

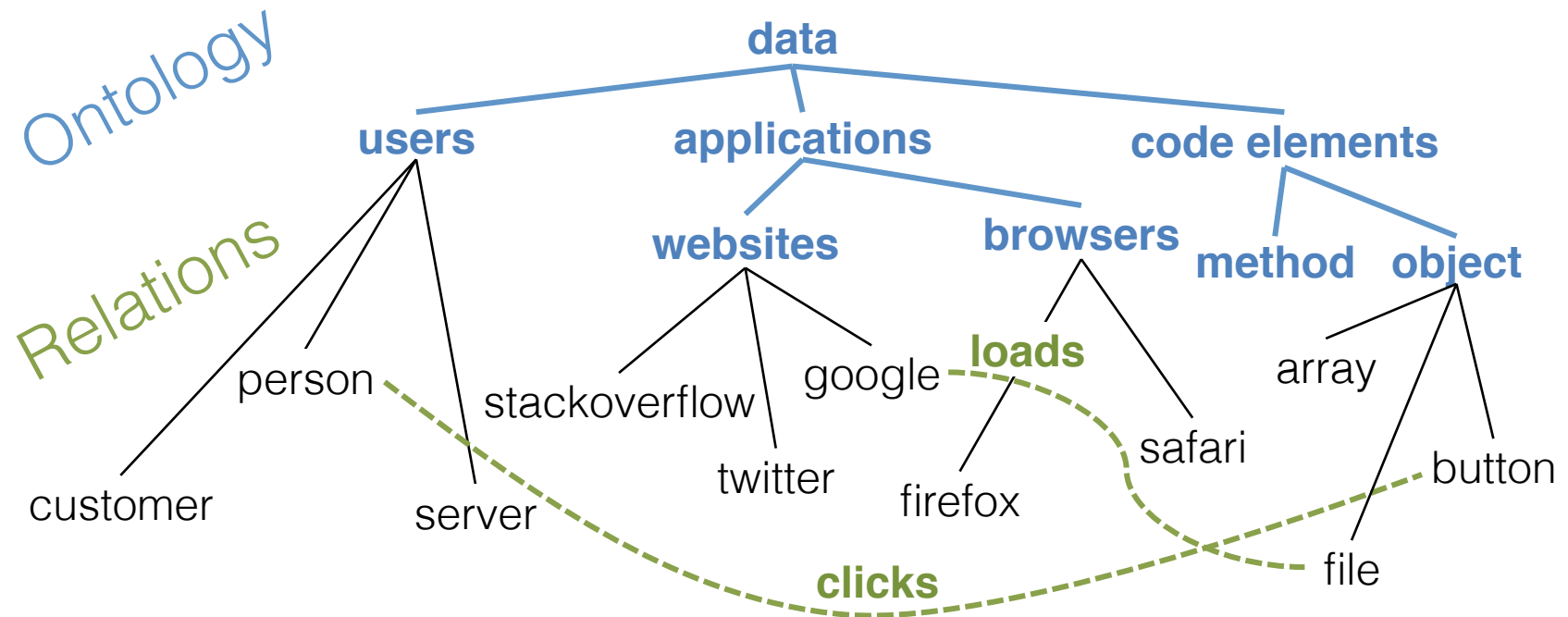
```
I successfully done with  
provisio  
and ser  
and whe  
the first  
and ex  
2nd  
4) g  
alre  
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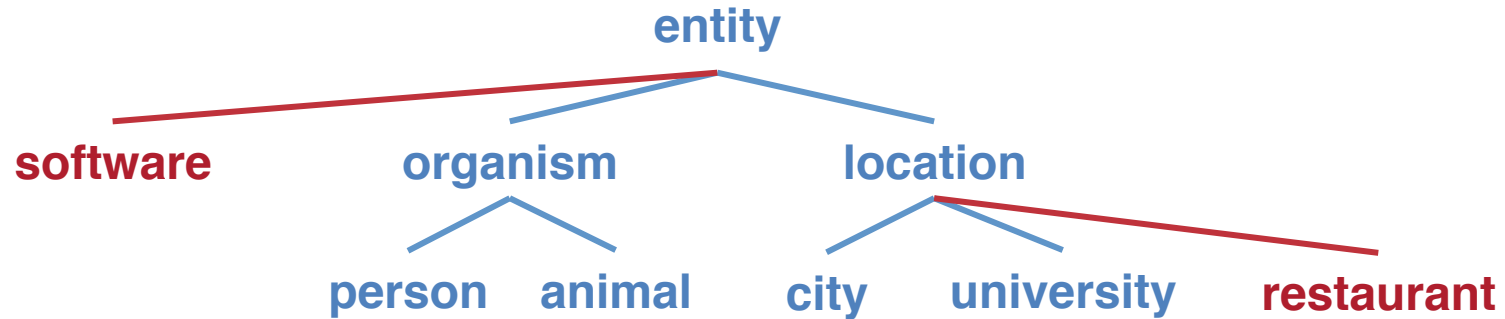


Goal: Corpus-Driven Knowledge Base

- Schema and facts are drawn from corpus
- Unsupervised: learn optimal latent corpus structure together with best-matching facts



Reasoning with Ontologies



- ✓ Ontologies give information context
- ✓ Easy to extract domain-specific information

- 😊 Ontologies are
 - expensive
 - require prior knowledge
- 😊 Manual ontology does not reflect language statistics
- 😊 Ontology and facts are often drawn from different sources

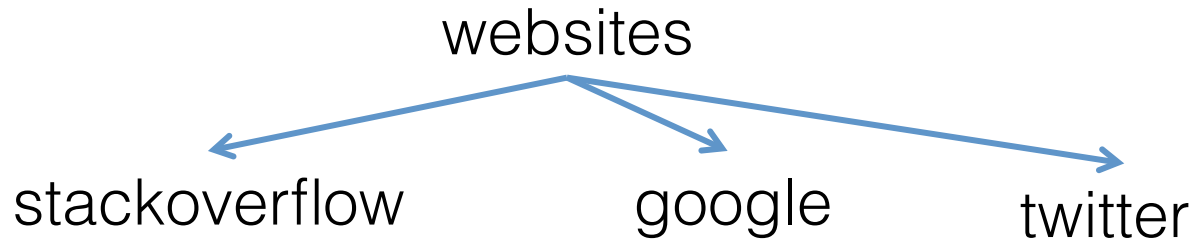
Pattern-based Relation Extraction

1. Hypernym-hyponym

“**websites** such as **stackoverflow**”

“**websites** including **google** and **twitter**”

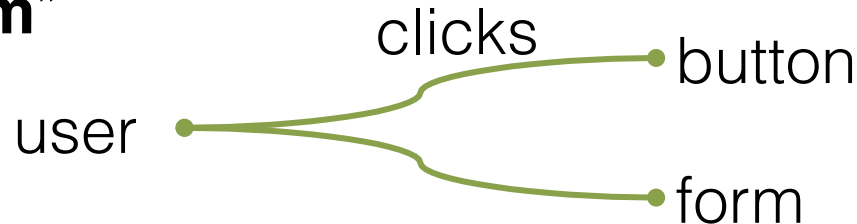
Y such as **X**
X is a **Y**
Y including **X**



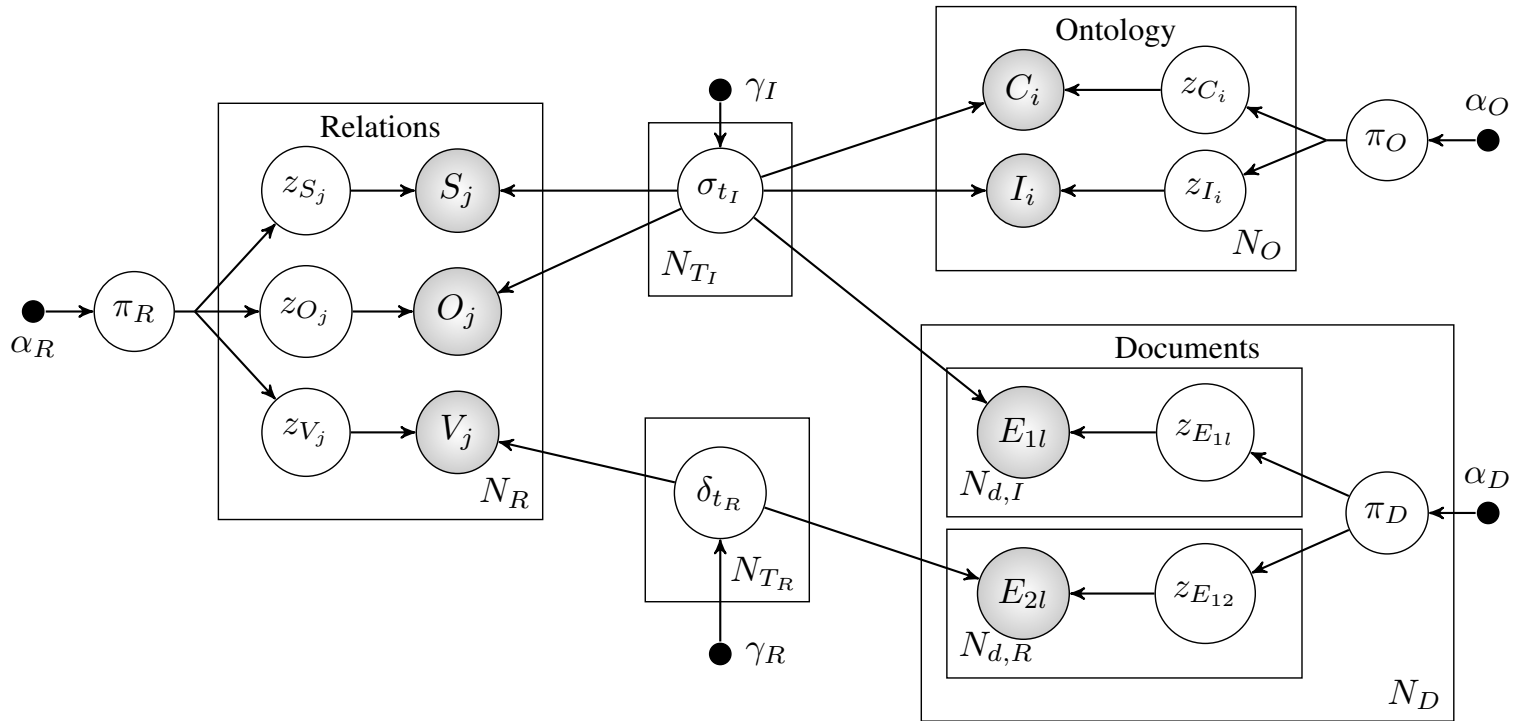
2. Subject-Verb-Object

“**user** clicks **button**”

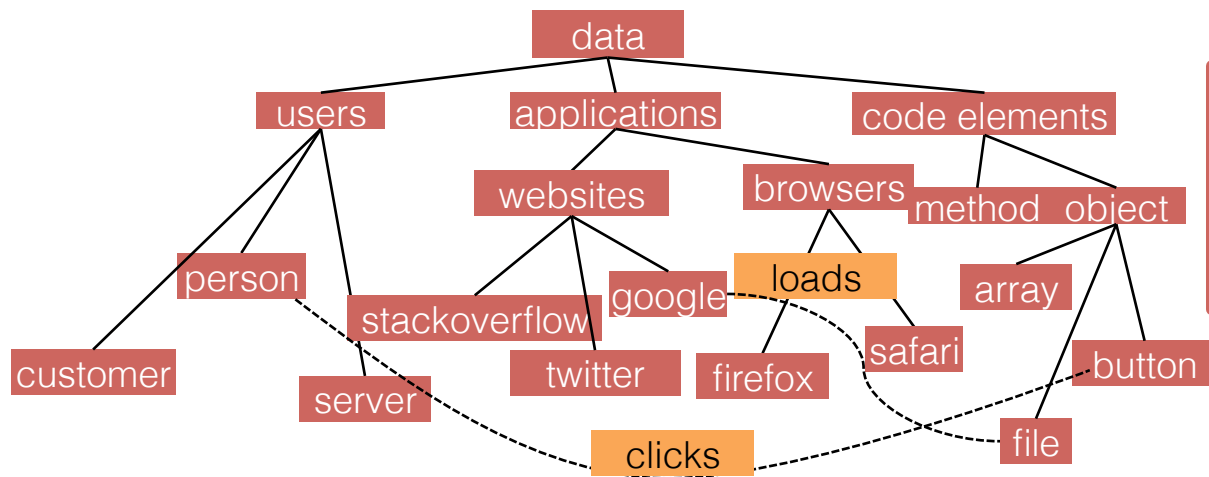
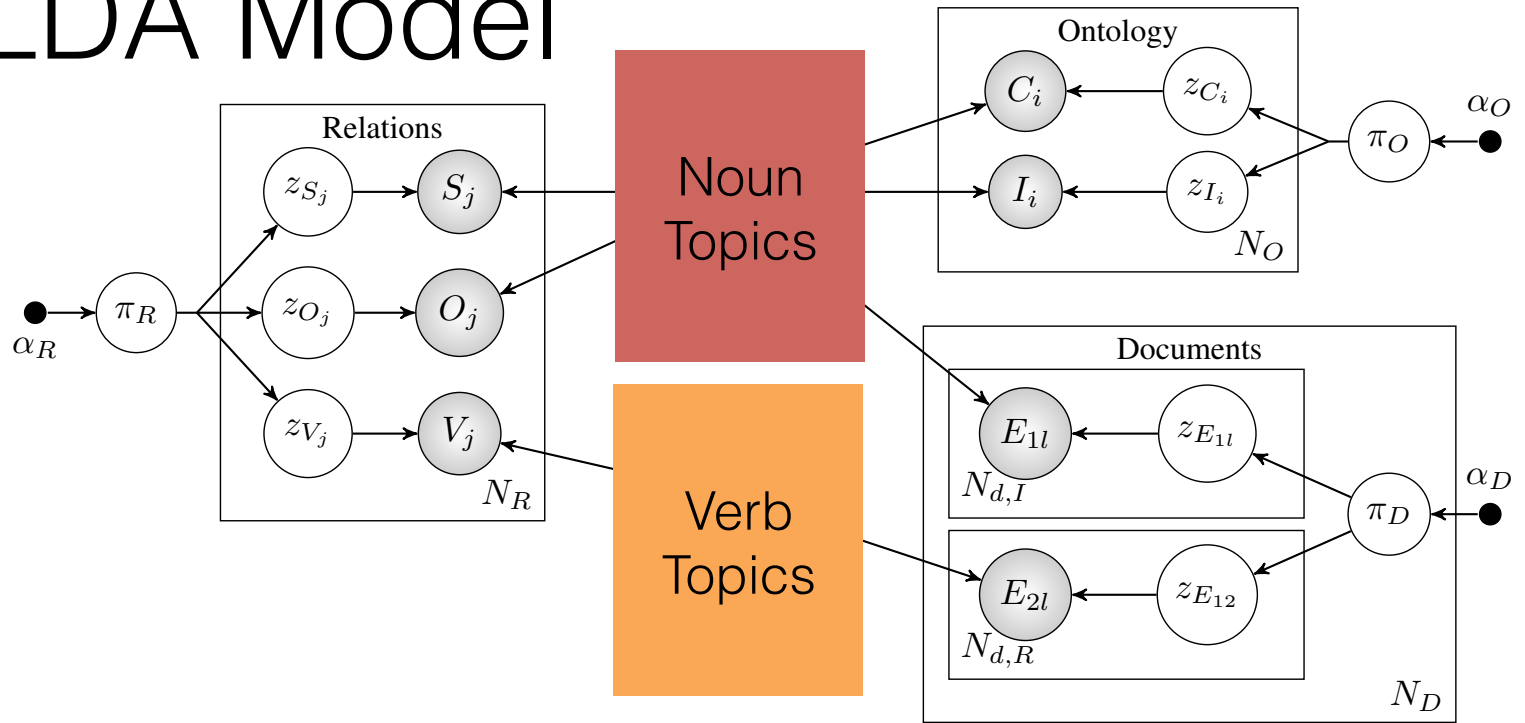
“**user** clicks **form**”



KB-LDA Model



KB-LDA Model

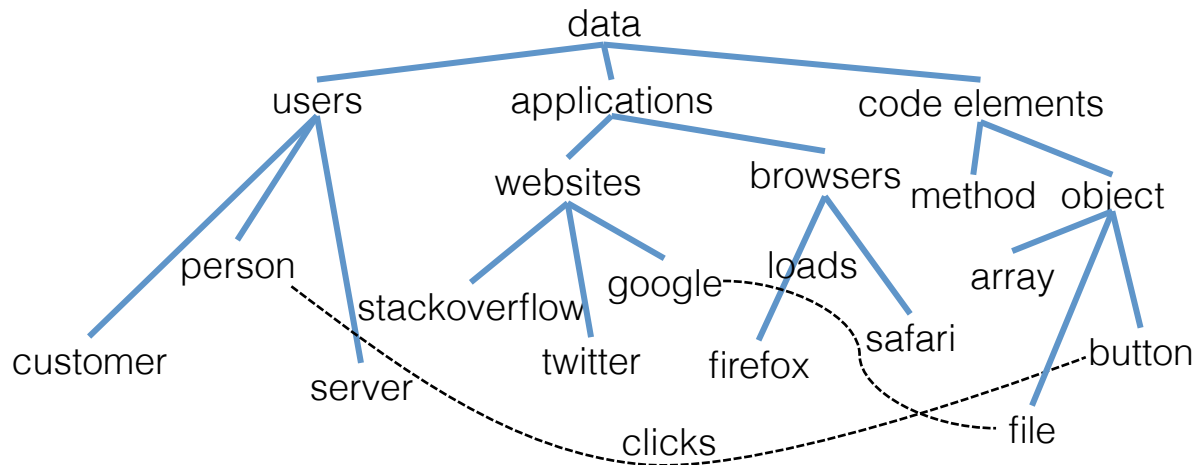
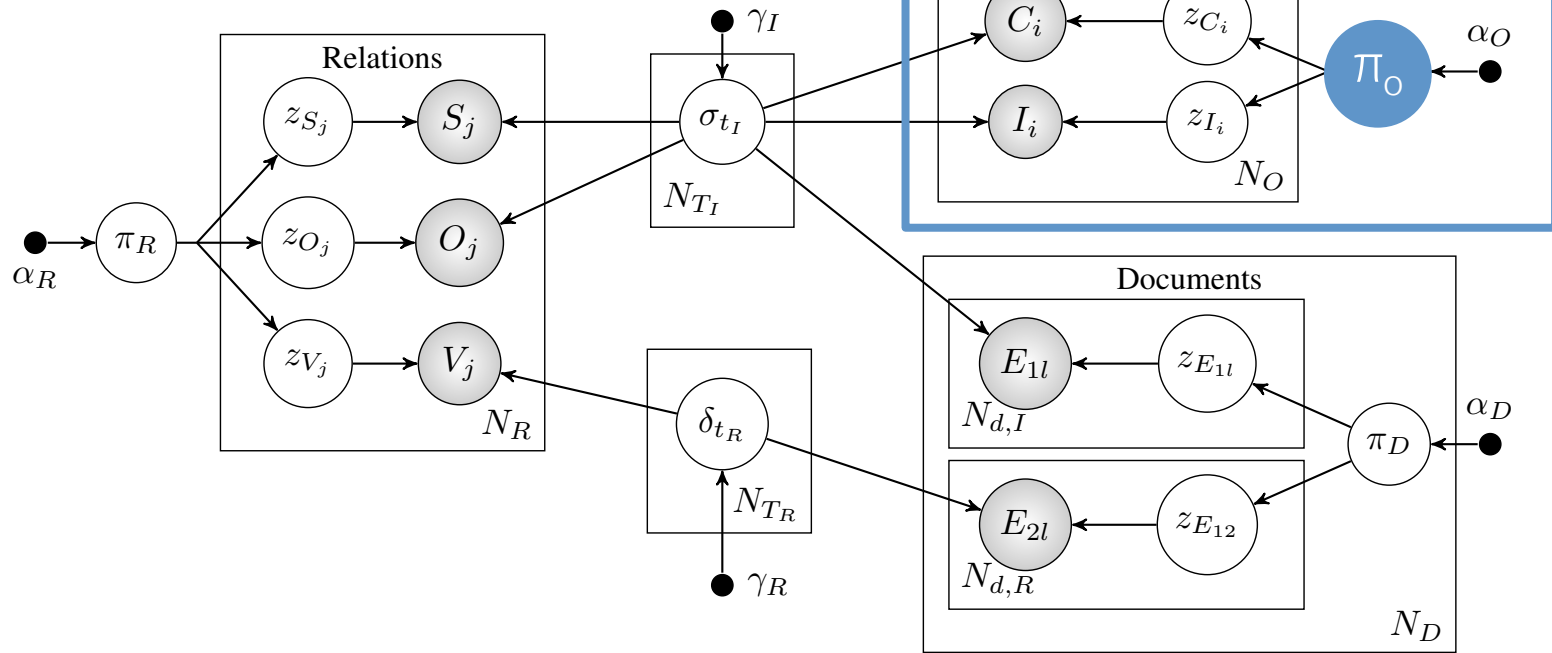


Categories Typed Relations

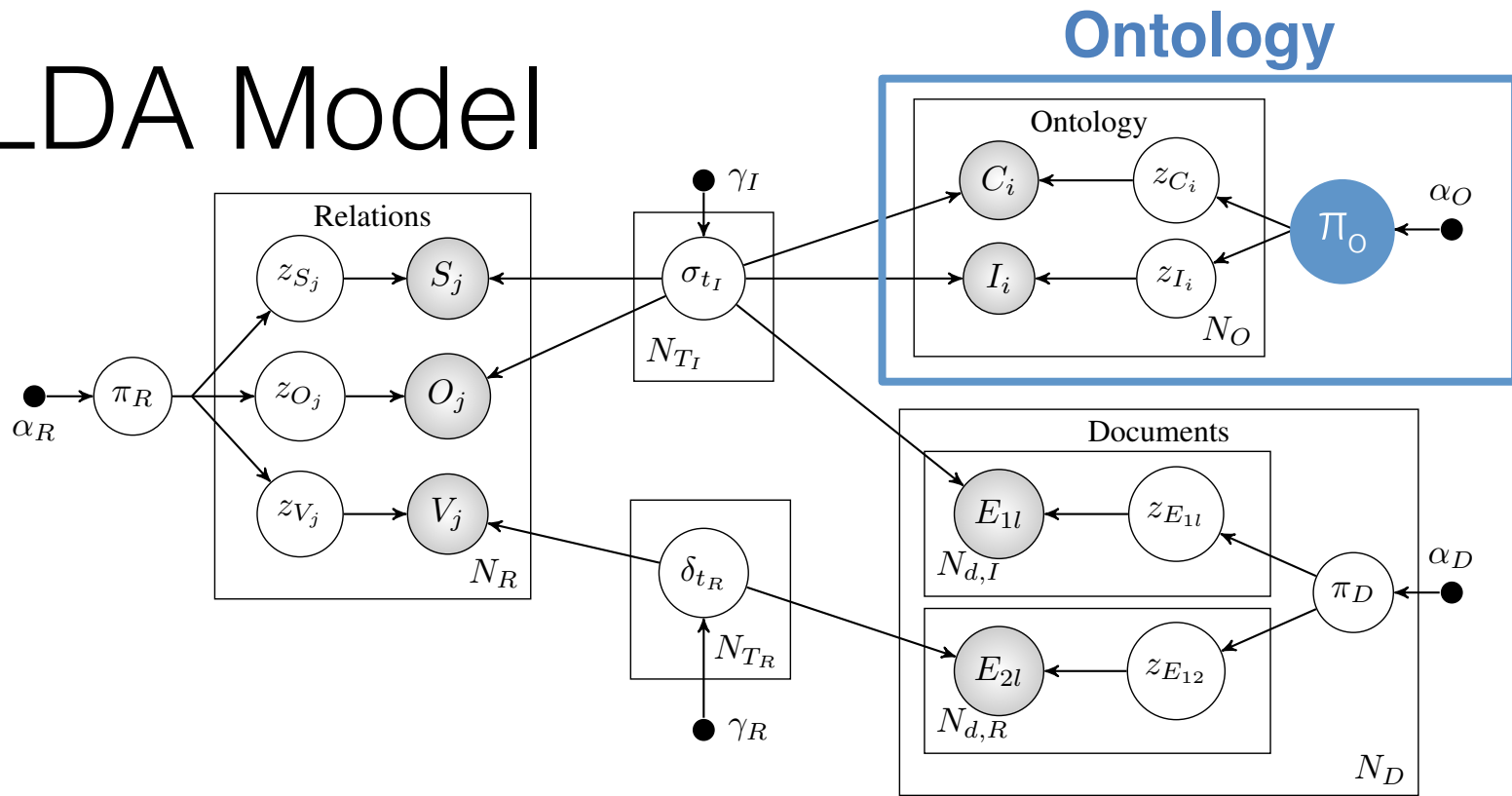
stackoverflow
google
twitter

clicks
selects
hits

KB-LDA Model

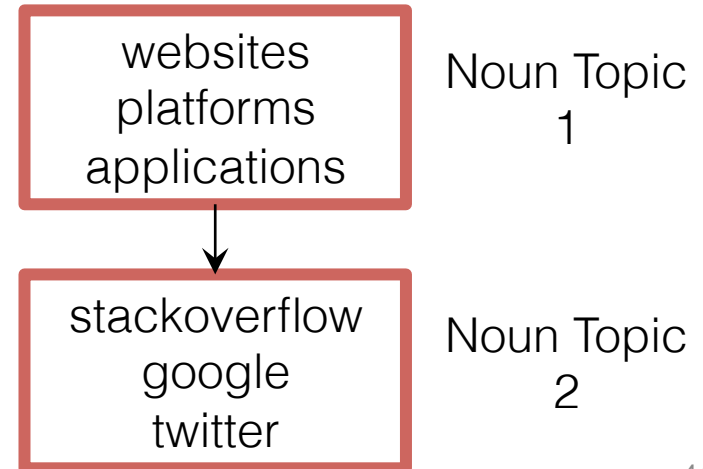


KB-LDA Model

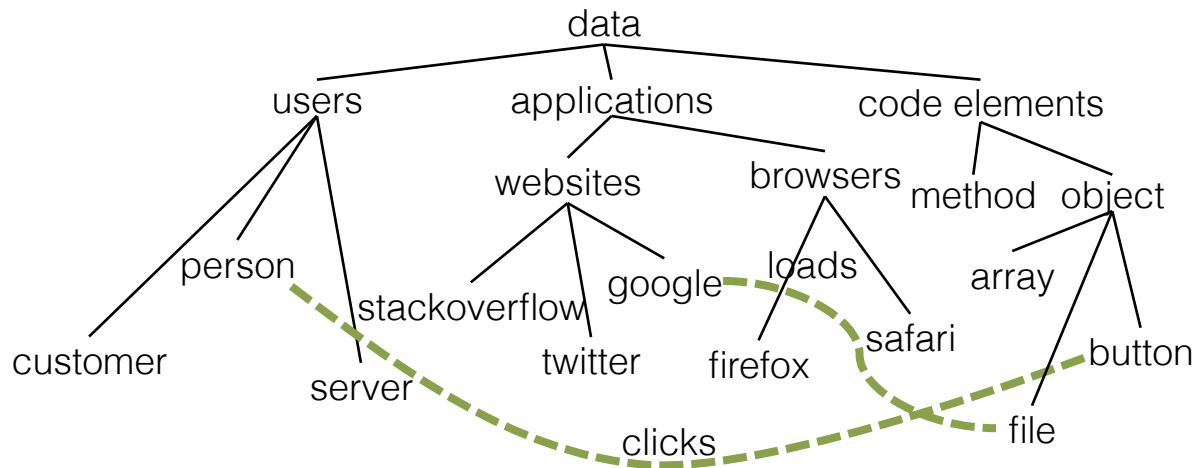
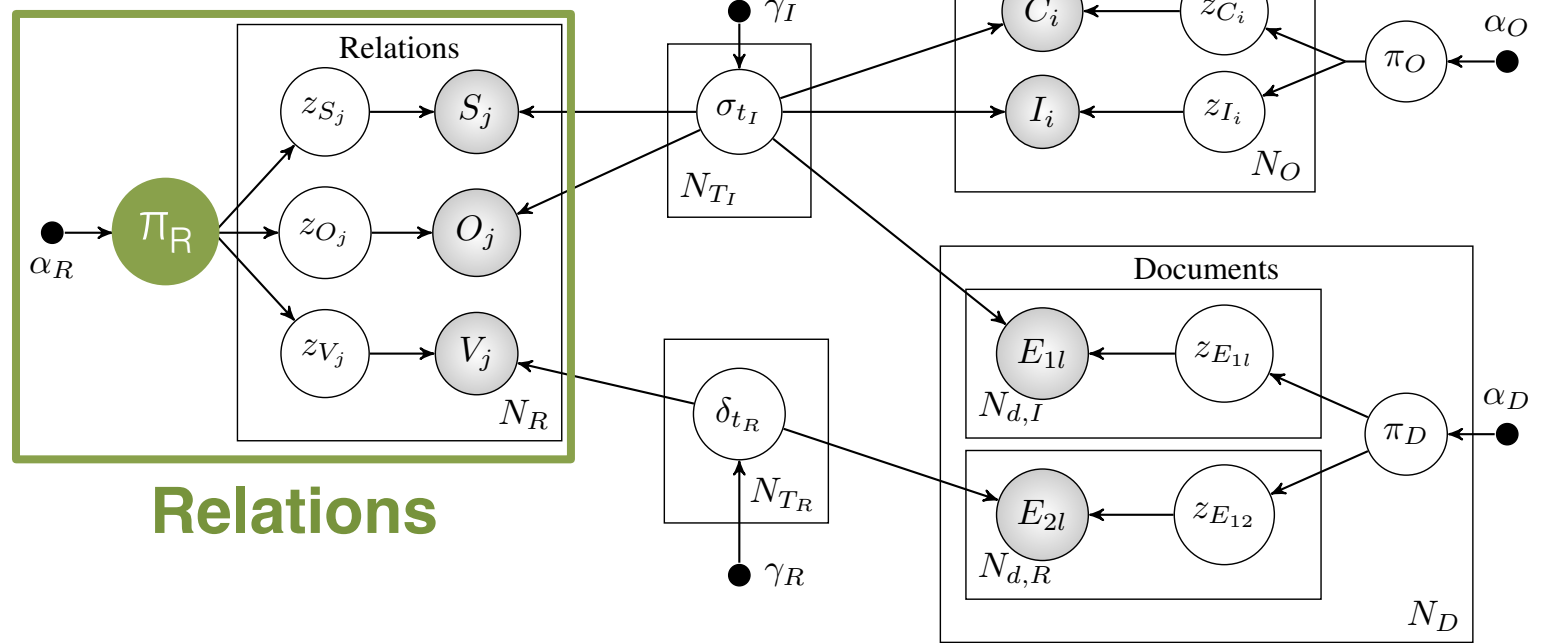


Hypernym-hyponym relations:

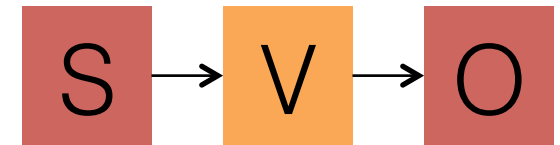
websites \rightarrow google
platforms \rightarrow stackoverflow



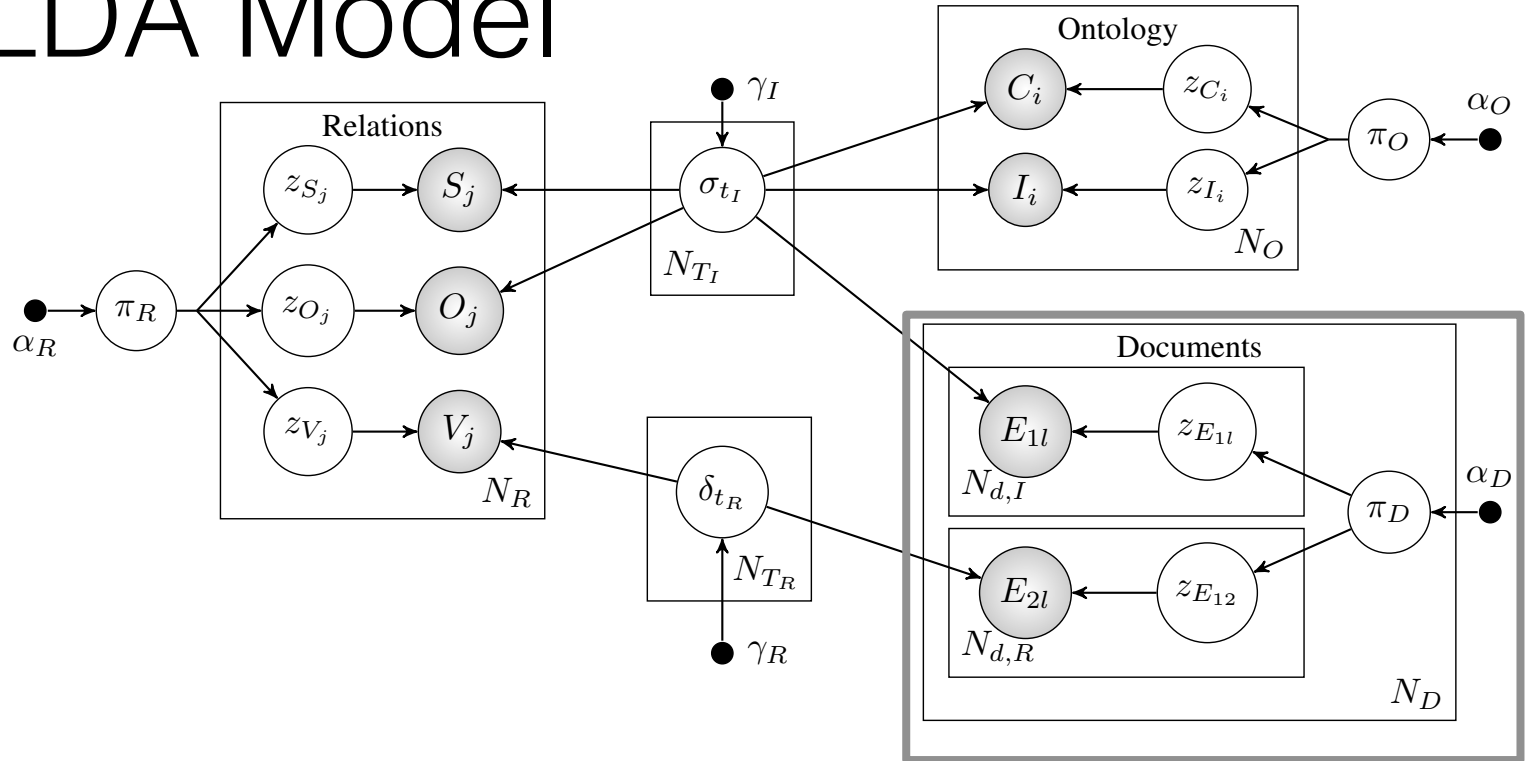
KB-LDA Model



Extracted SVO relation:
person, *clicks*, button

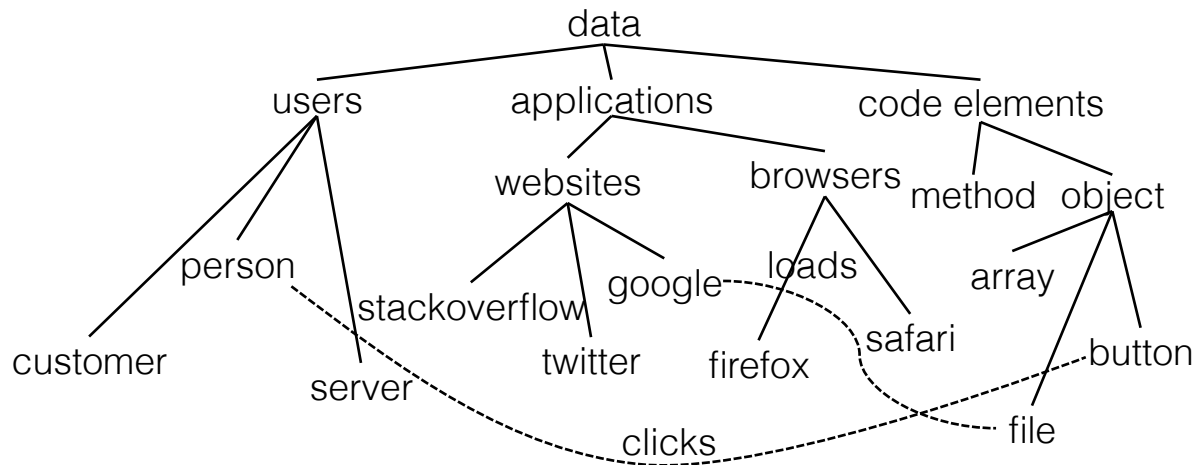


KB-LDA Model



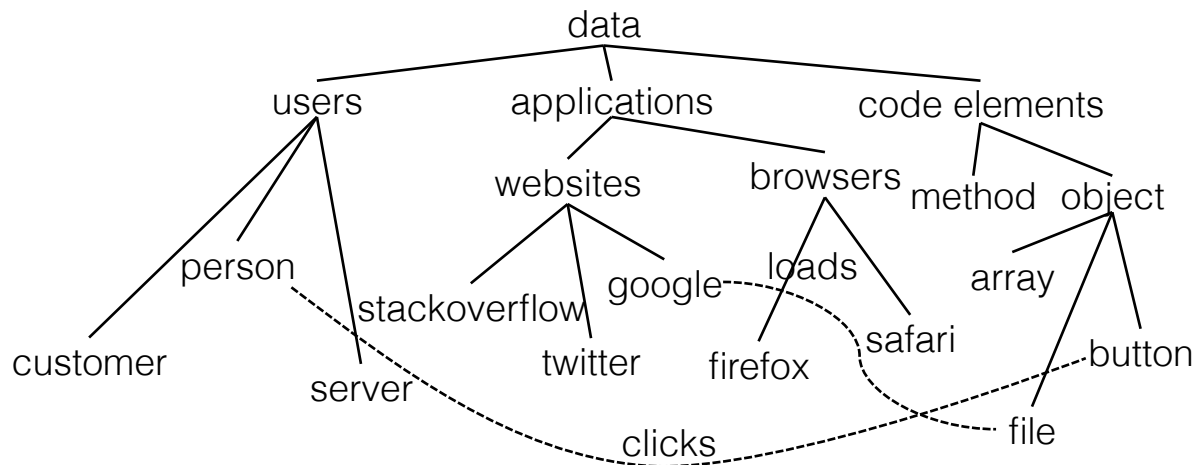
Documents

Downloads on websites sometimes have an **MD5** checksum, **allowing people** to confirm the integrity of the file. I have heard this is to allow not only corrupted files to be instantly identified before they cause a problem but also for for any **malicious changes** to be easily **detected**.



KB-LDA Model

More in thesis document:
Data-driven topic naming



Documents

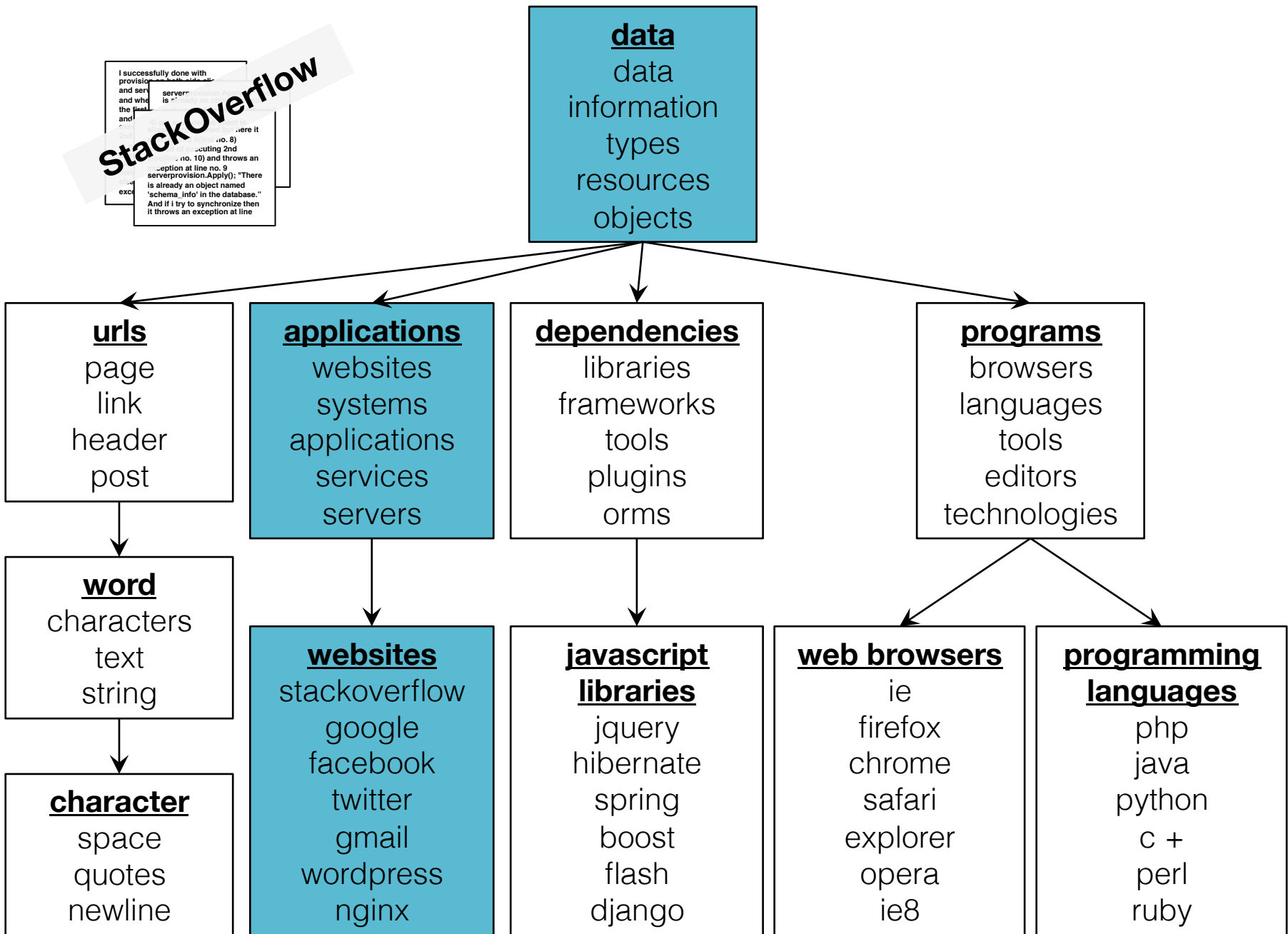
Downloads on websites sometimes have an **MD5** checksum, **allowing people** to confirm the integrity of the file. I have heard this is to allow not only corrupted files to be instantly identified before they cause a problem but also for for any **malicious changes** to be easily **detected**.

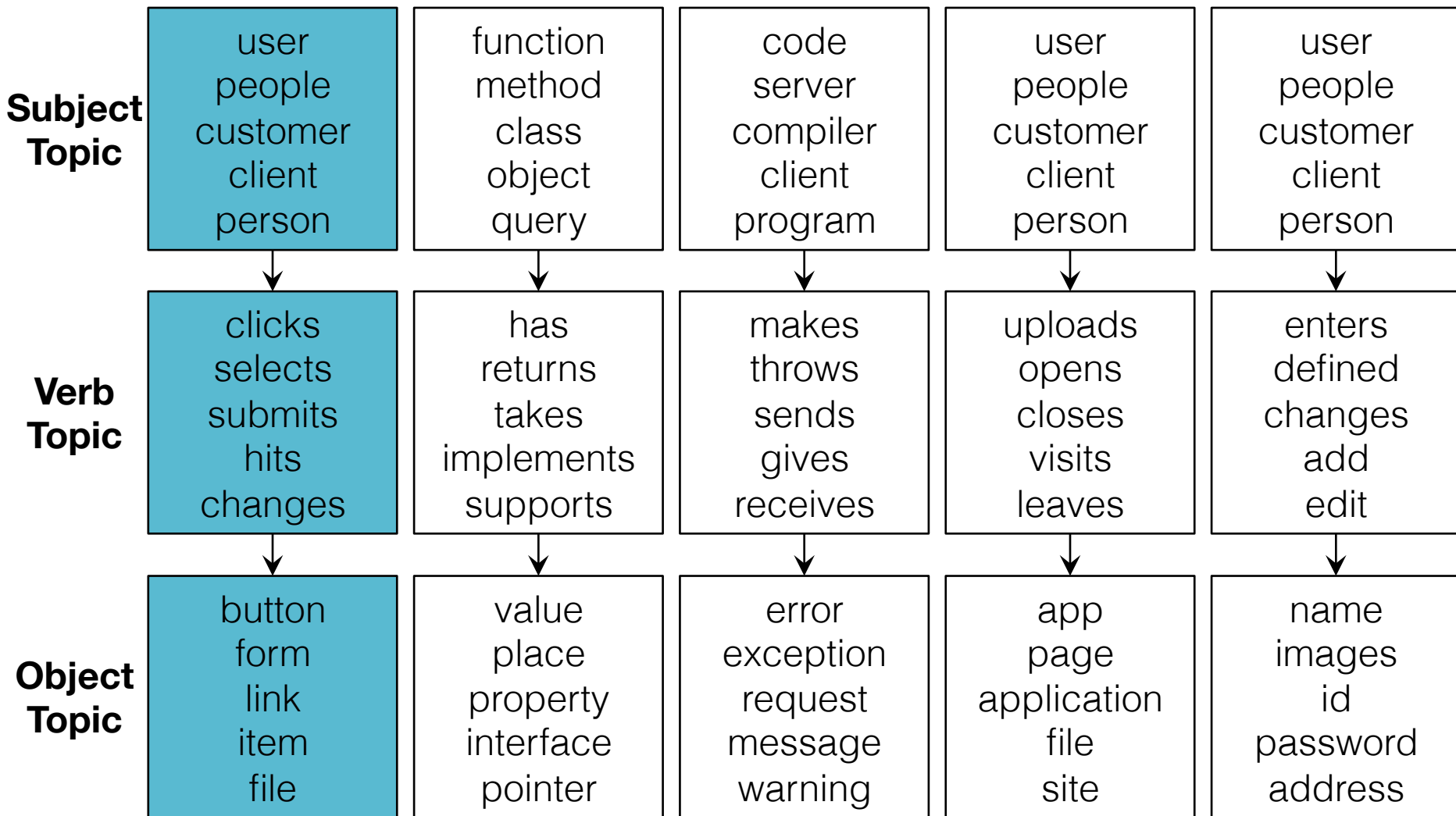
StackOverflow

```

I successfully done with
provision and sort
and who the
is "
and
...were it
...no. 8)
...cutting 2nd
...no. 10) and throws an
ception at line no. 9
serverprovision.Apply(); "There
is already an object named
'schema_info' in the database."
And if I try to synchronize then
it throws an exception at line

```



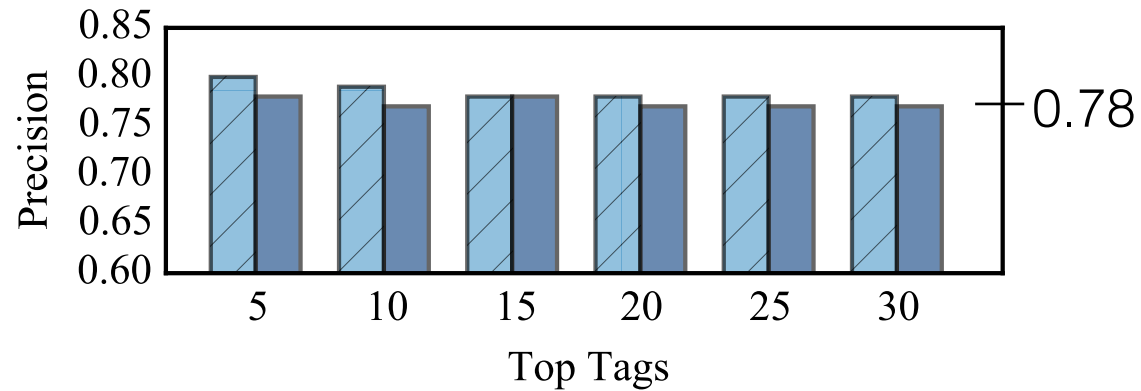


M-Turk Evaluation of Noun Topics

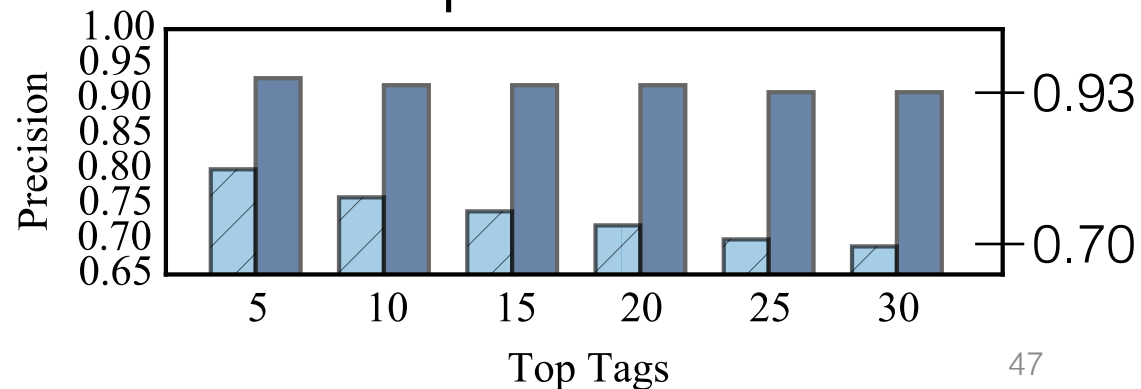
“Which words are ***not*** related to **programming languages?**”

java
python
javascript
firefox
ruby
perl

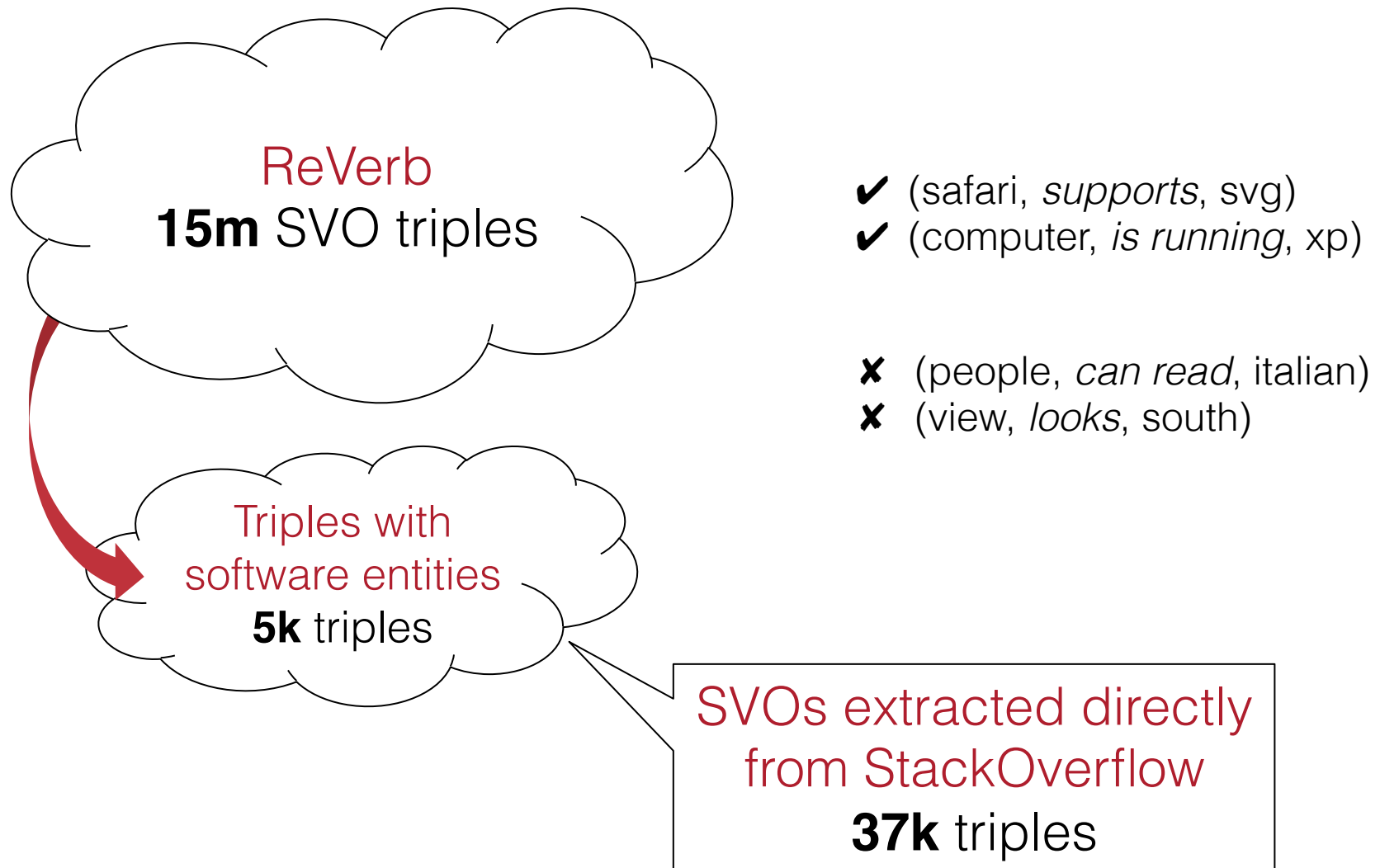
1. Word Intrusion



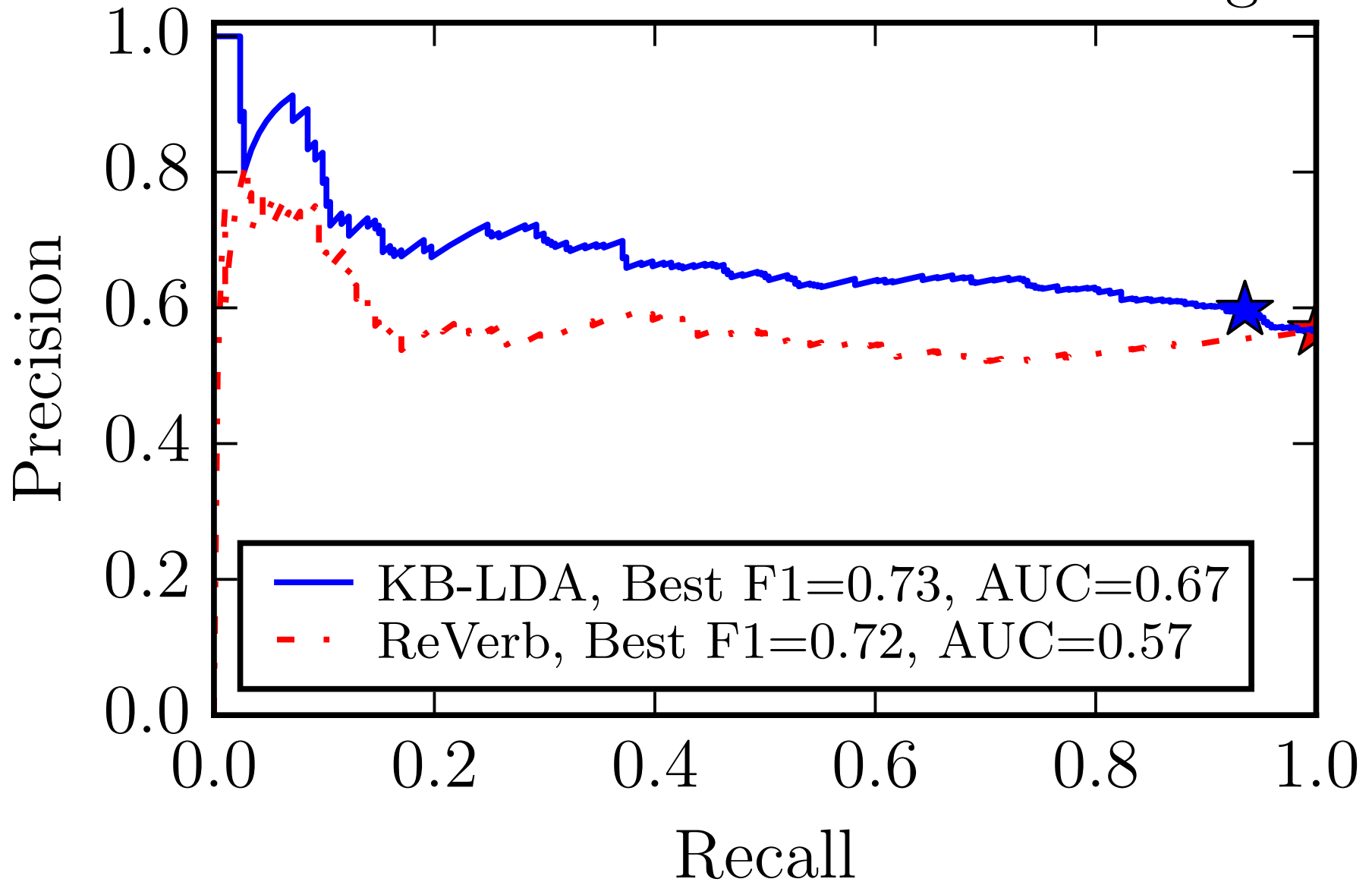
2. Group Precision



Domain-Specific Extraction from Open IE



KB-LDA versus ReVerb Ranking



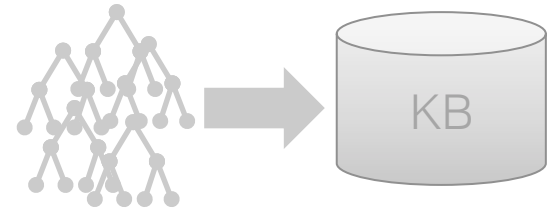
KB-LDA Lessons

- Corpus-driven KB construction: Jointly optimizes schema and facts
- Unsupervised: Useful for exploration of new domains (Software)
- Can pre-existing domain knowledge improve KB learning? How much? (Biomedical ontologies)

Roadmap

Statistical Language Model for
Software Domain Application

```
/* comment prediction */
```

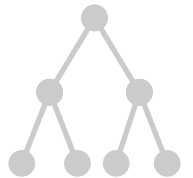


Bootstrap KB Learning for
the Biomedical Domain

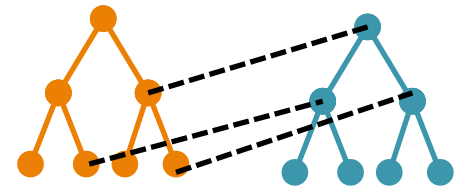
Grounded Software
Ontology Construction

Corpus

```
I successfully done with  
provisional serverprovision.Apply(); "There  
and ser is already an object named  
the first schema_info' in the database."  
and exe- 4) get exception at line no. 9  
2nd already existing 2nd  
4) get exception at line no. 10) and throws an  
exception at line no. 9  
serverprovision.Apply(); "There  
is already an object named  
'schema_info' in the database."  
And if I try to synchronize then  
it throws an exception at line
```



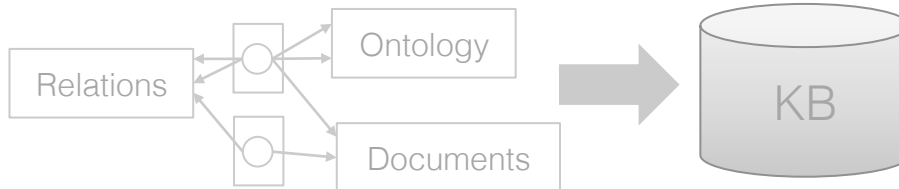
**Aligning Grounded and Learned
Biomedical Relations**



Topic-Model KB Learning

Corpus

```
I successfully done with  
provisional serverprovision.Apply(); "There  
and ser is already an object named  
the first schema_info' in the database."  
and exe- 4) get exception at line no. 9  
2nd already existing 2nd  
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```

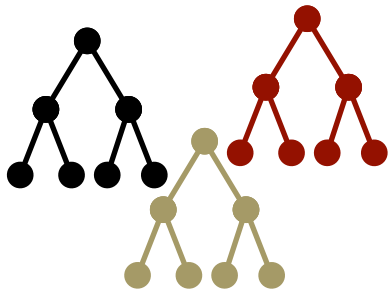


Aligning Grounded and Learned Relations

- Evaluation of KB-LDA relations compared to known relations
- Investigation of the potential of grounding

Aligning Grounded and Learned Relations

Grounded



- Proteins and Genes (PRGE)
- Chemicals (CHED)
- Diseases and disorders (DISO)
- Living Beings (LIVB)
- Unified Medical Language System (UMLS)
- ...



autoimmune
disease

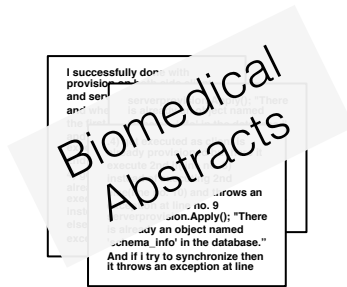
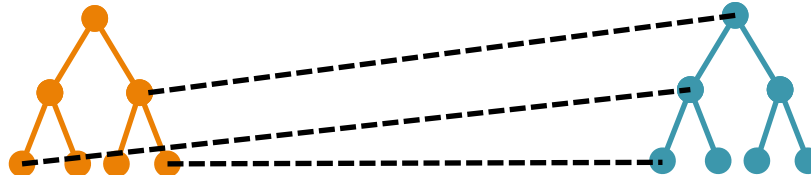
lupus

cutaneous
lupus
erythematosus

C0004364
C0442893
C0687719

C0004364
C0442893
C0024137
C0024138
C0030327

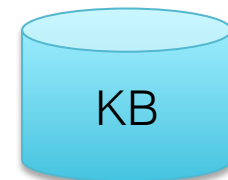
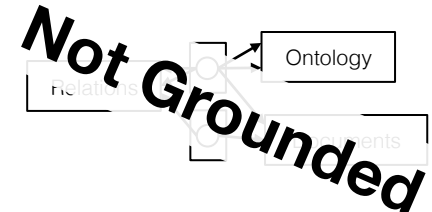
C0024137
C0024138
C1142226



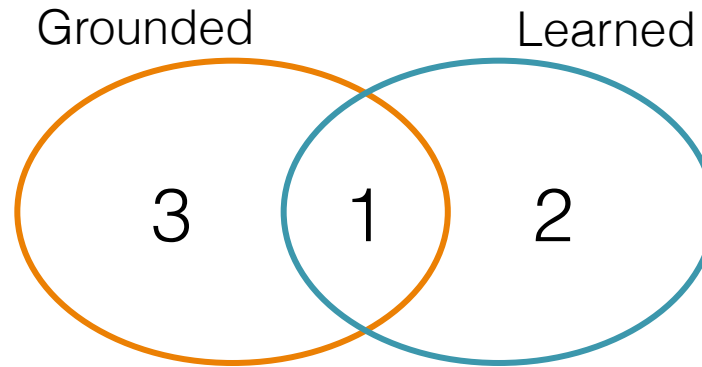
CALBC



KB-LDA



Possible Alignment Outcomes

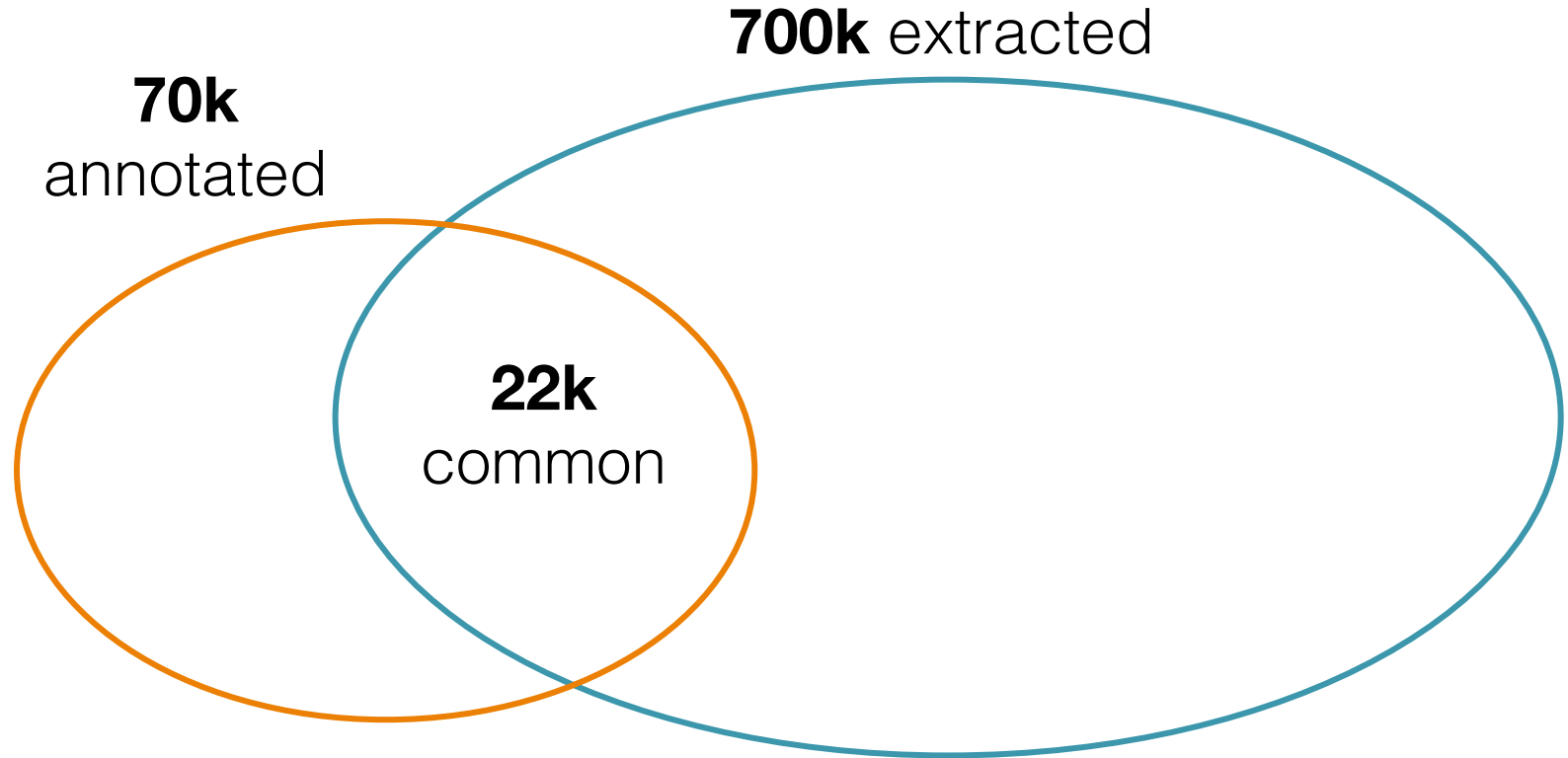


1. Does KB-LDA learn existing relations and concepts?
 - Model Validation
2. Does KB-LDA discover “new” relations and concepts?
 - Added value of language statistics
3. What is missing?
 - Can be added through grounding

Grounded and Learned Entities

Grounded

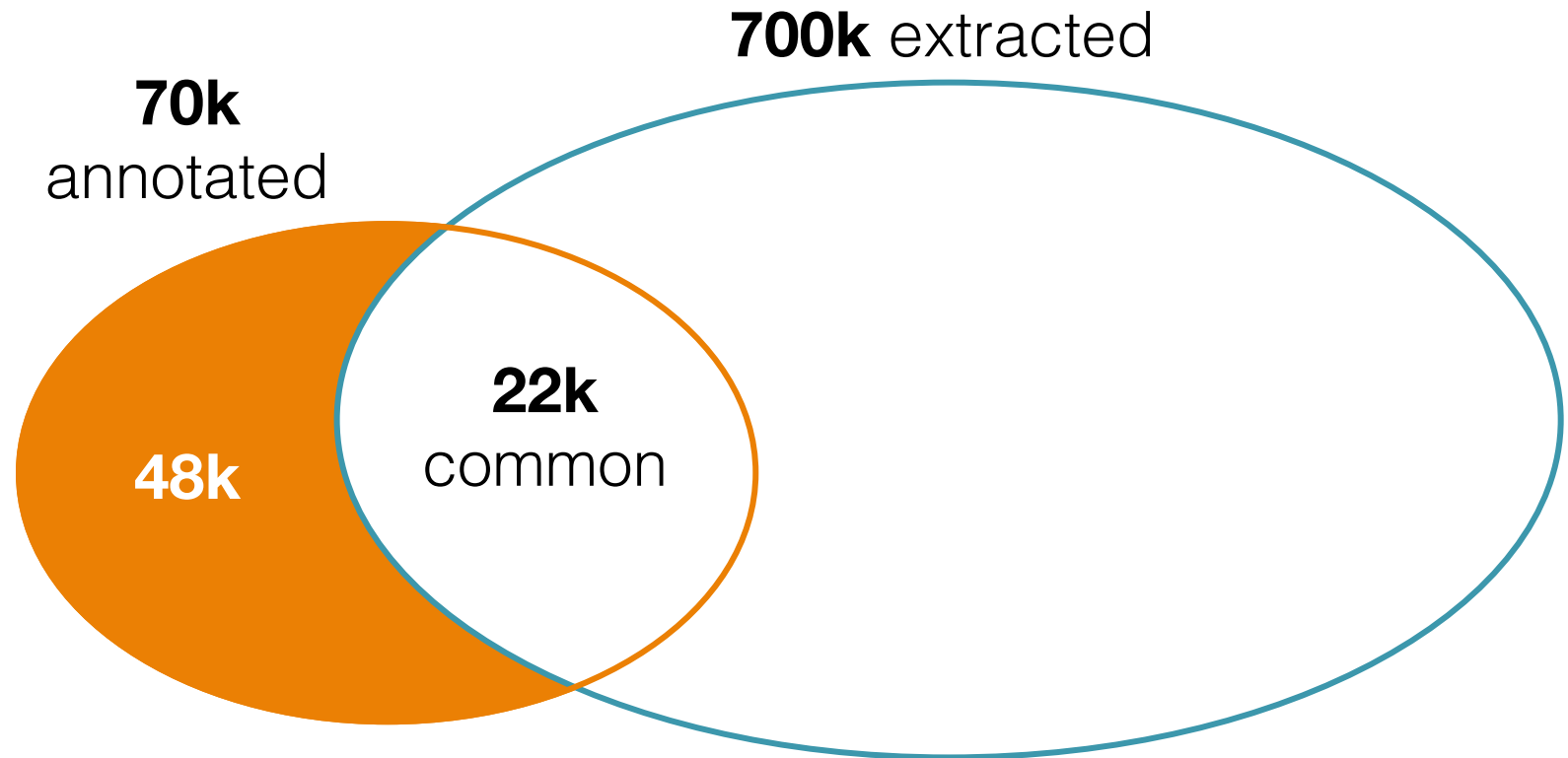
KB-LDA



Grounded and Learned Entities

Grounded

KB-LDA



Grounded Entities:

Manual evaluation of sample

Partial or incorrect
parse
35/100

Average corpus
frequency
4.87

- ✗ bronchial asthma
- ✗ pneumoniae
- ✗ beta-1,2-mannotriose

Only in incorrect
form
20/35

Frequent entities
($f > 10$)
12

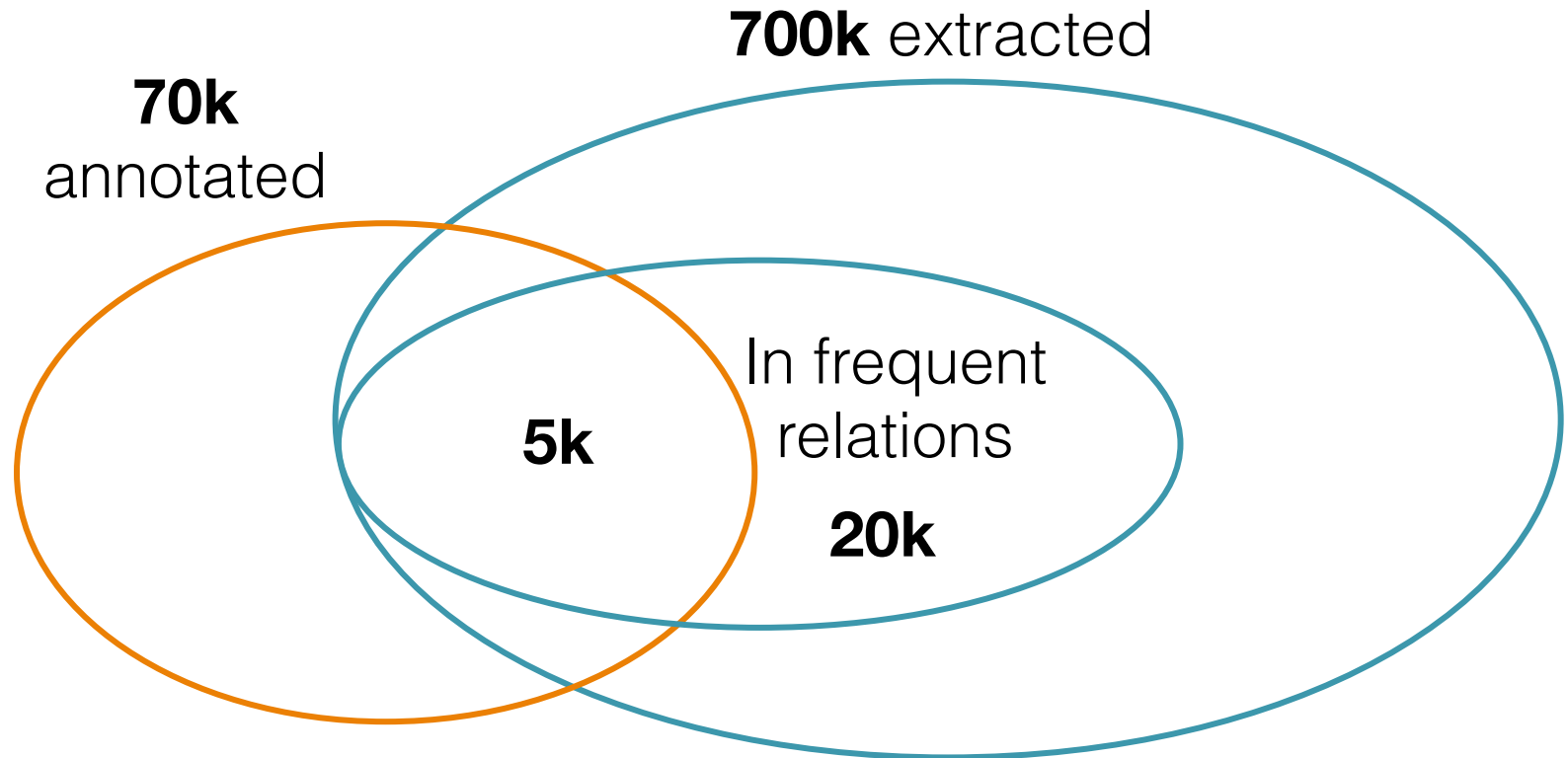
Limitation of
grounding

Potential advantage
of grounding

Grounded and Learned Entities

Grounded

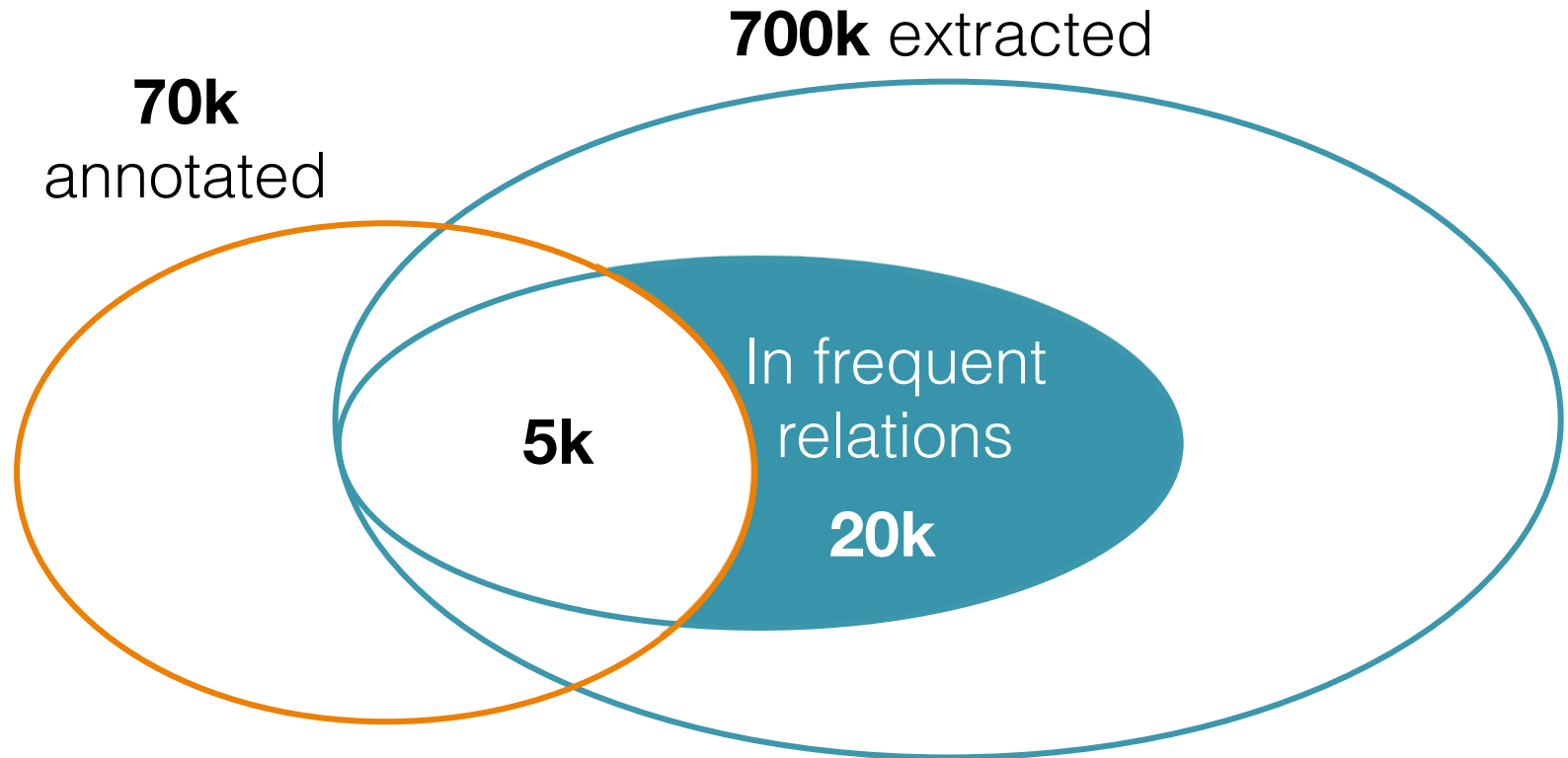
KB-LDA



Grounded and Learned Entities

Grounded

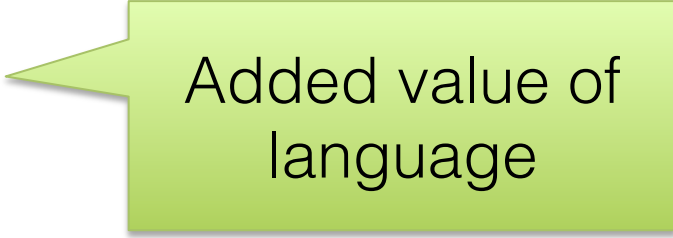
KB-LDA



KB-LDA Entities:

Manual evaluation of sample

Correct
97/100



Added value of
language

Parse errors
3/100

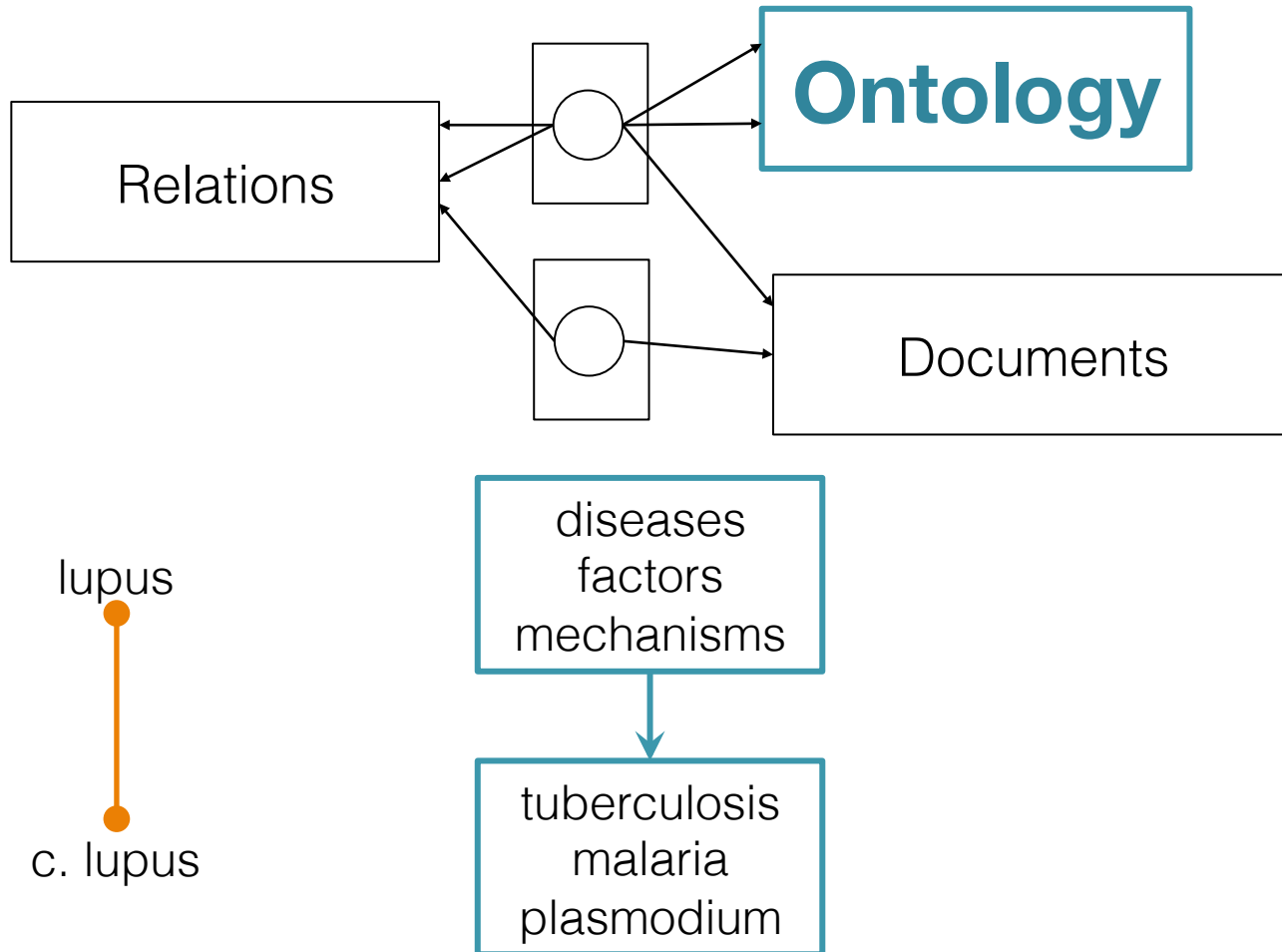
Experimental Terminology
16/100

- ✓ techniques
- ✓ samples
- ✓ hapten inhibition experiments
- ✓ sodium dodecyl sulfate-polyacrylamide gel

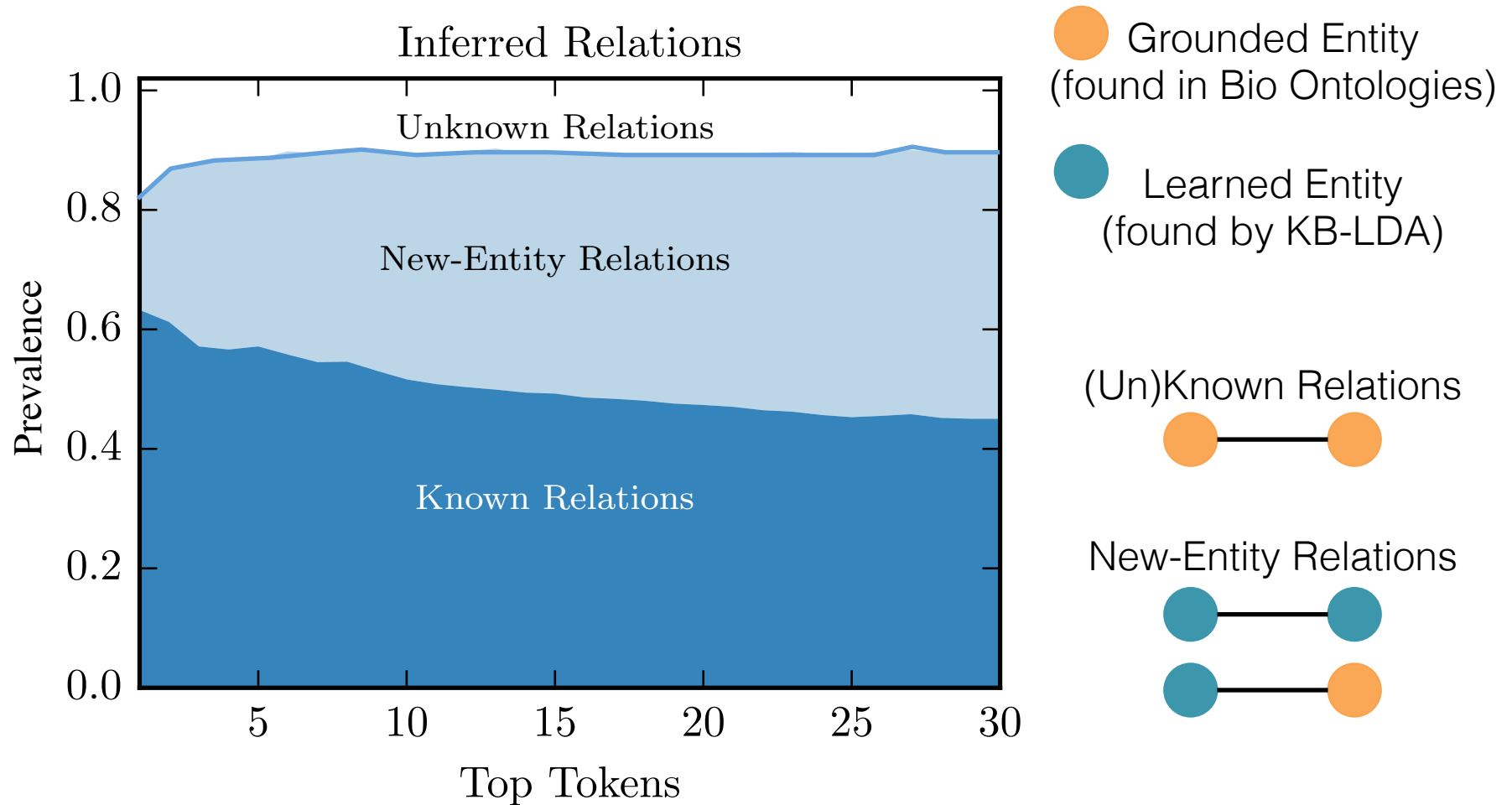
Biological Entities and
Processes
81/100

- ✓ linkage
- ✓ leukotoxin
- ✓ chemotactic response
- ✓ plasma cell-associated markers

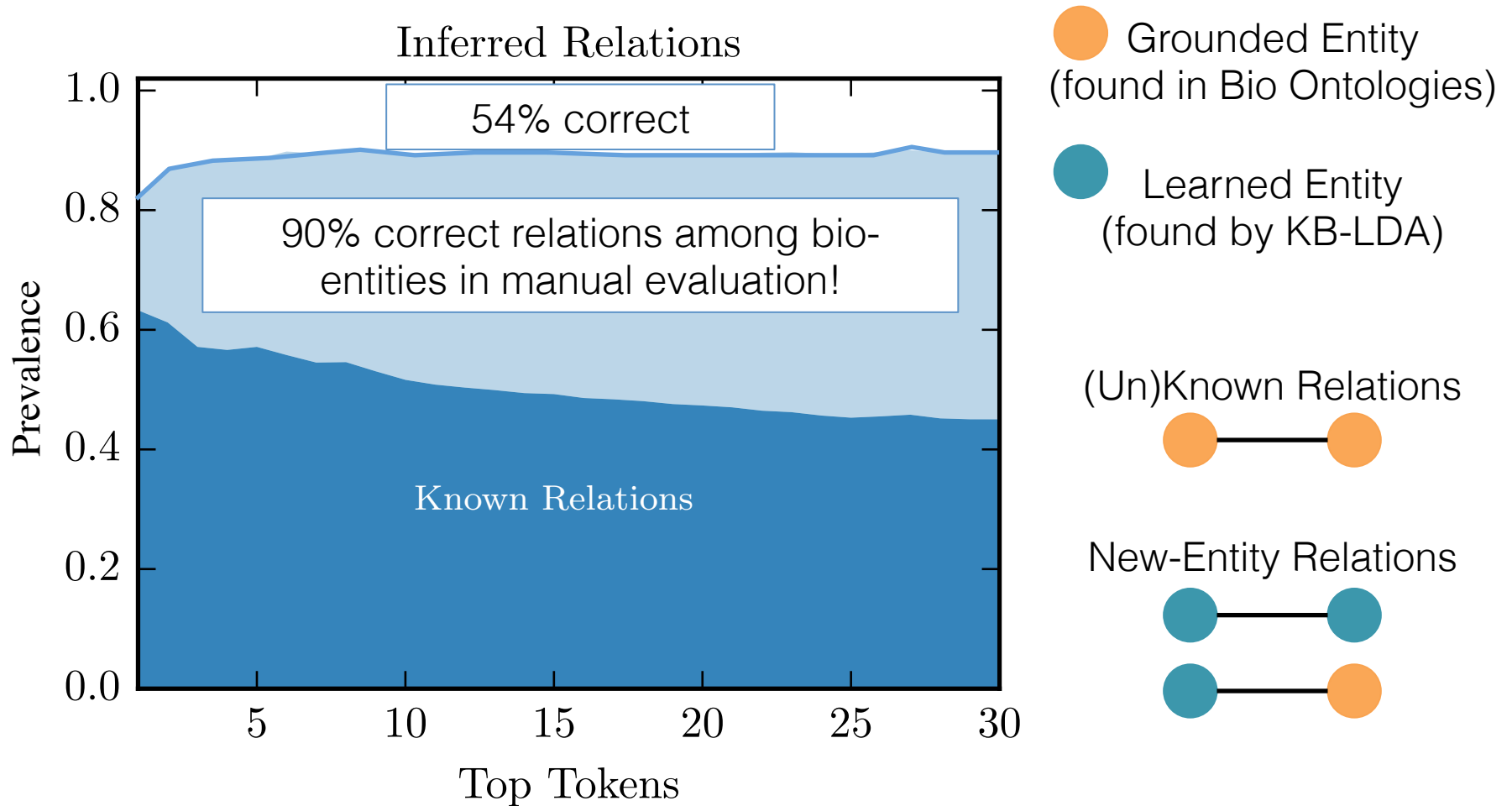
Ontology



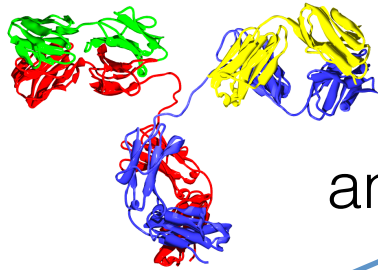
Discovered Ontology Relations



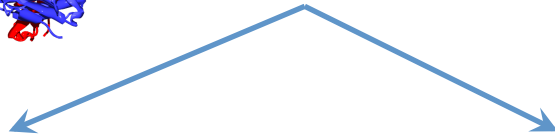
Discovered Ontology Relations



Discovered Ontology Relations

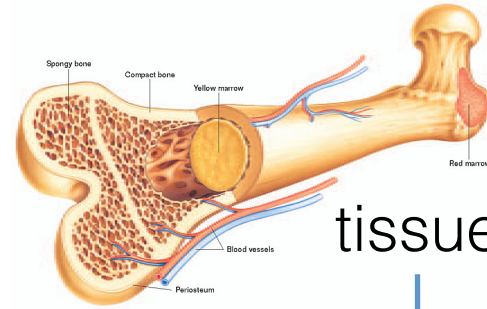


antibody



EMA (Endomysial autoantibodies)

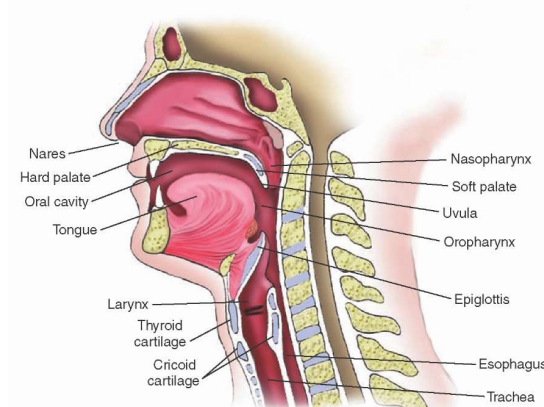
DCS-6 (Anti-Cyclin D1 antibody)



tissue



bone marrow

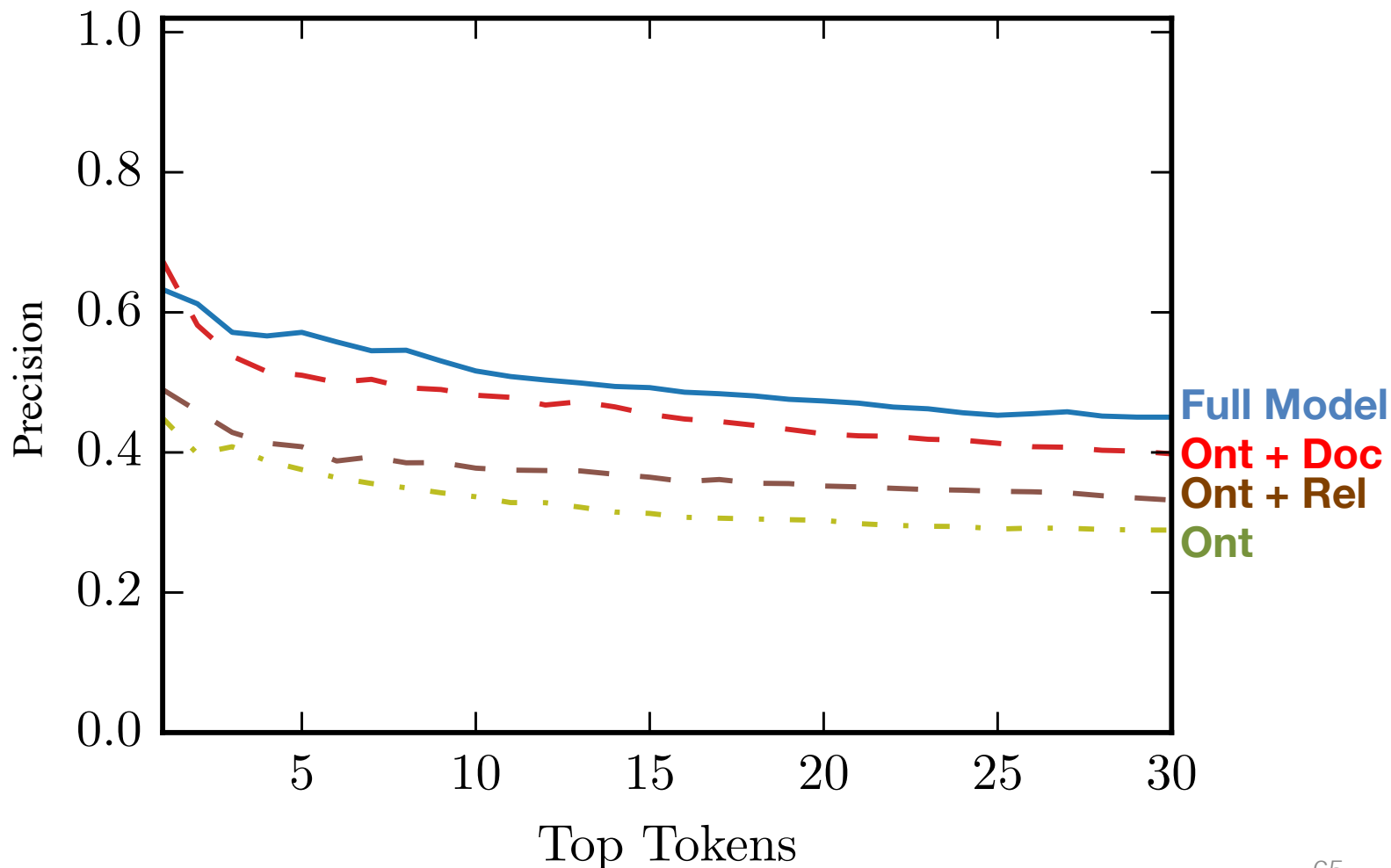


organ

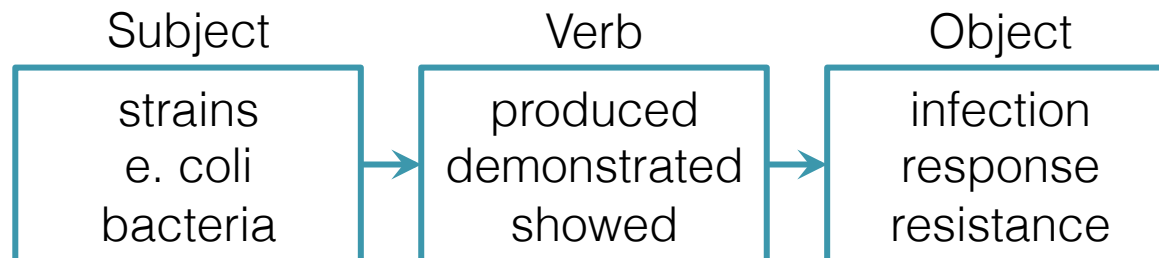
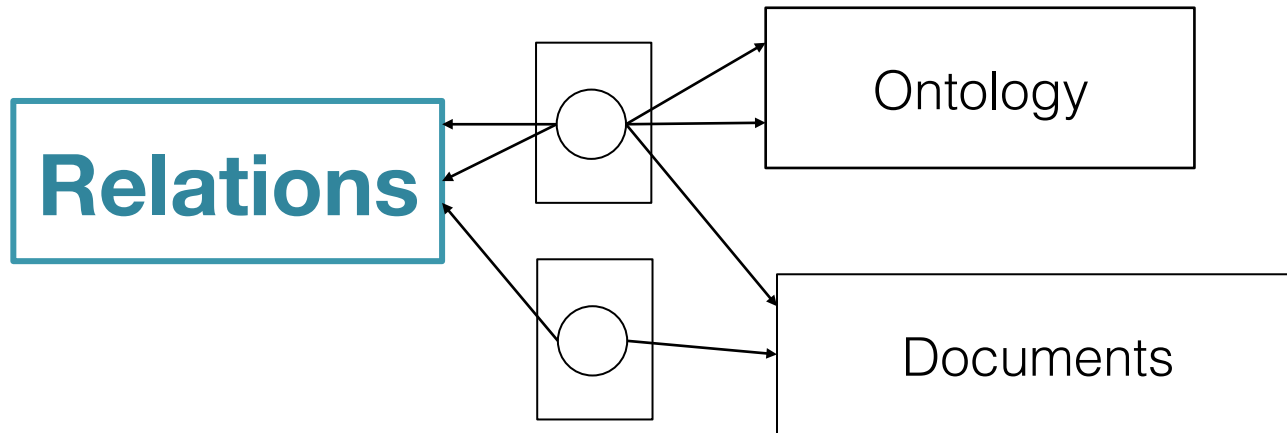


airway

Contribution of Model Components to Learning Ontology

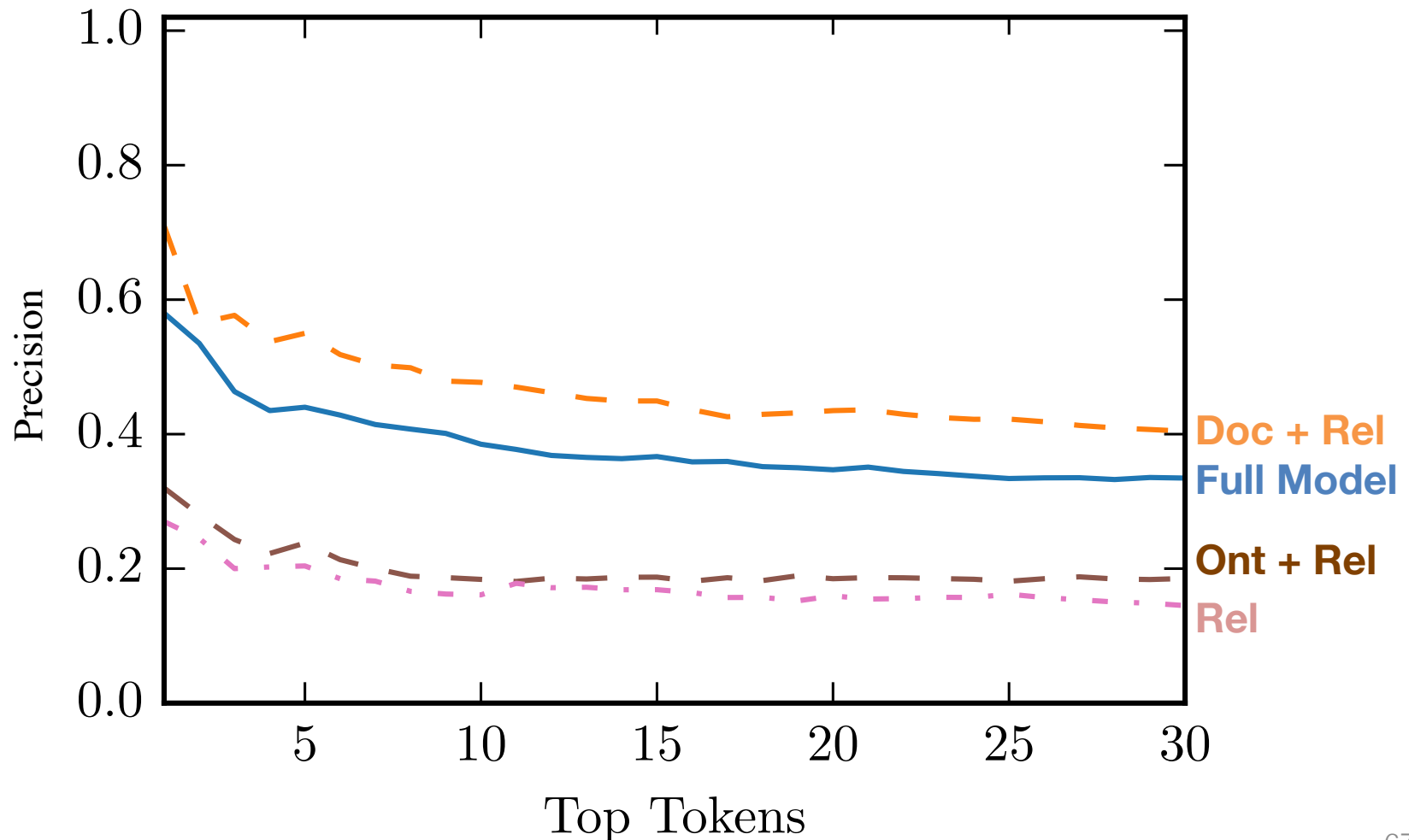


Contribution of Model Components to Learning General Relations

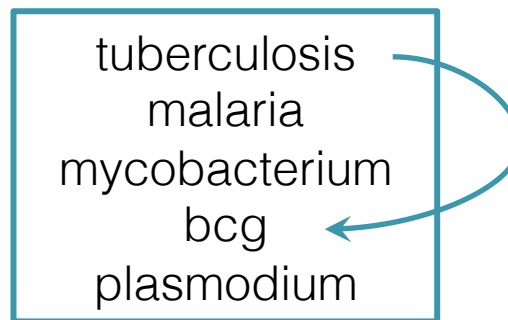
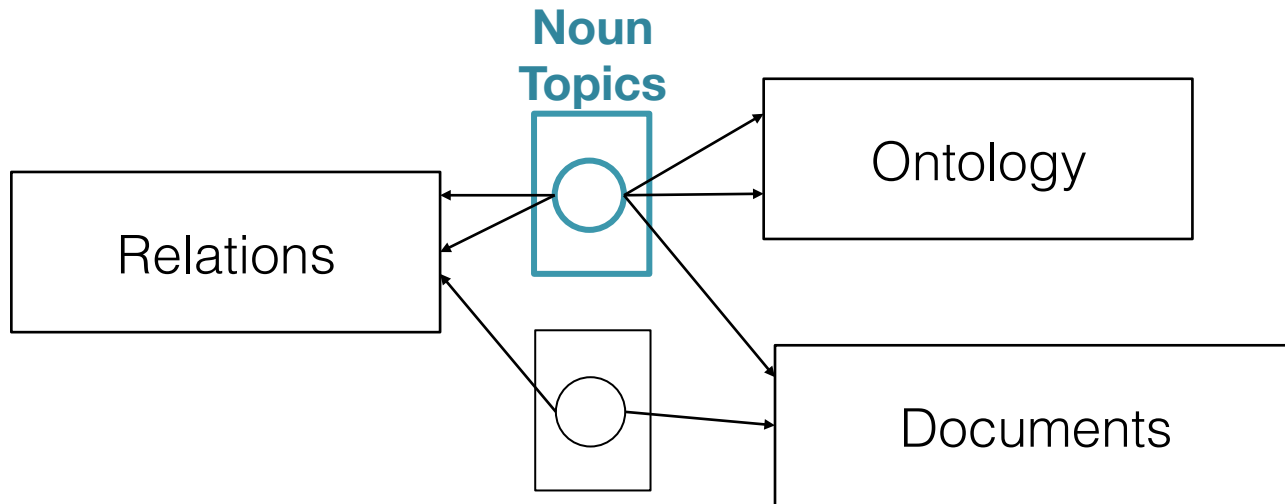


lupus ● ————— ● c. lupus

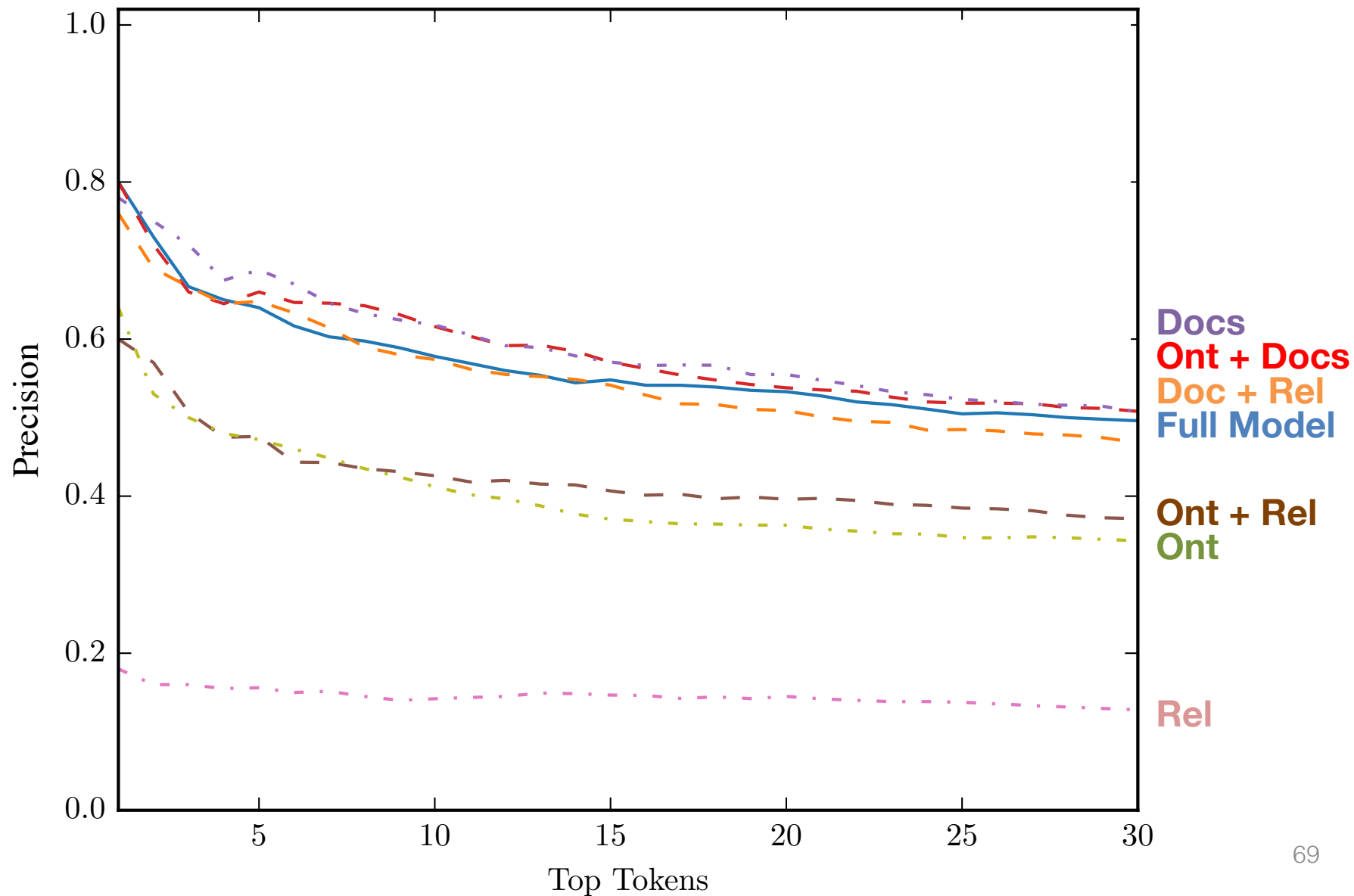
Contribution of Model Components to Learning General Relations



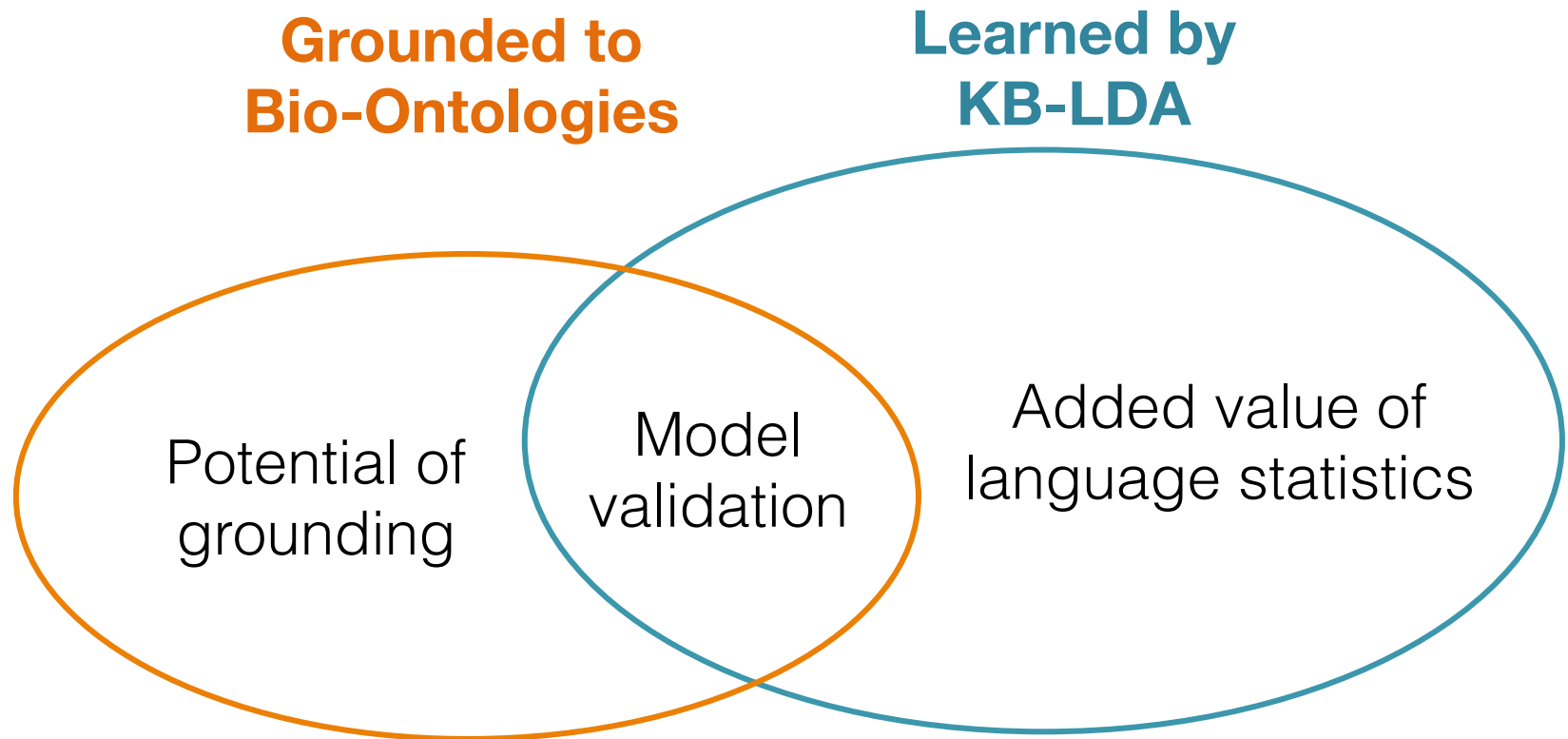
Contribution of Model Components to Learning Intra-Topic Relations



Intra-Topic Relations



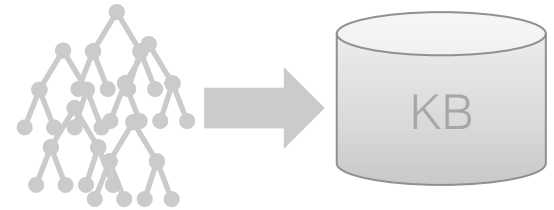
Lessons



Roadmap

Statistical Language Model for
Software Domain Application

```
/* comment prediction */
```

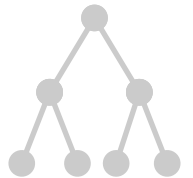


Bootstrap KB Learning for
the Biomedical Domain

Grounded Software
Ontology Construction

Corpus

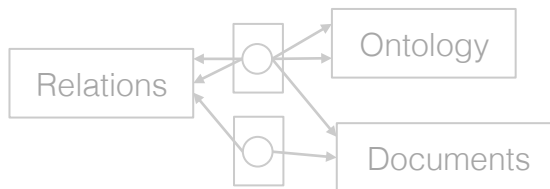
I successfully done with
provisional serverprovision.Apply(); "There
is already an object named
schema_info' in the database."
And if I try to synchronize then
it throws an exception at line
no. 9



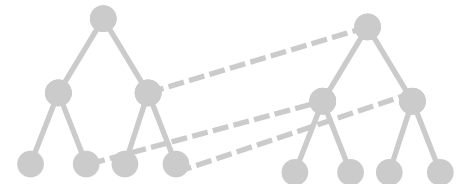
Topic-Model KB Learning

Corpus

I successfully done with
provisional serverprovision.Apply(); "There
is already an object named
schema_info' in the database."
And if I try to synchronize then
it throws an exception at line
no. 9

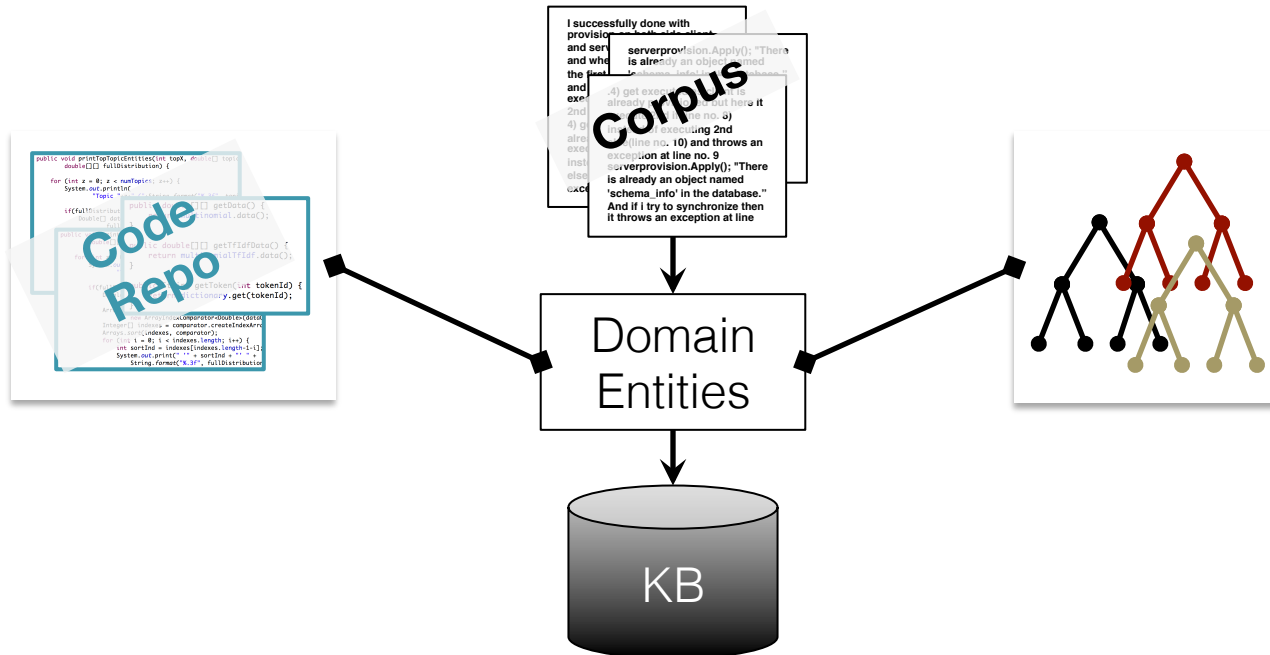


Aligning Grounded and Learned
Biomedical Relations

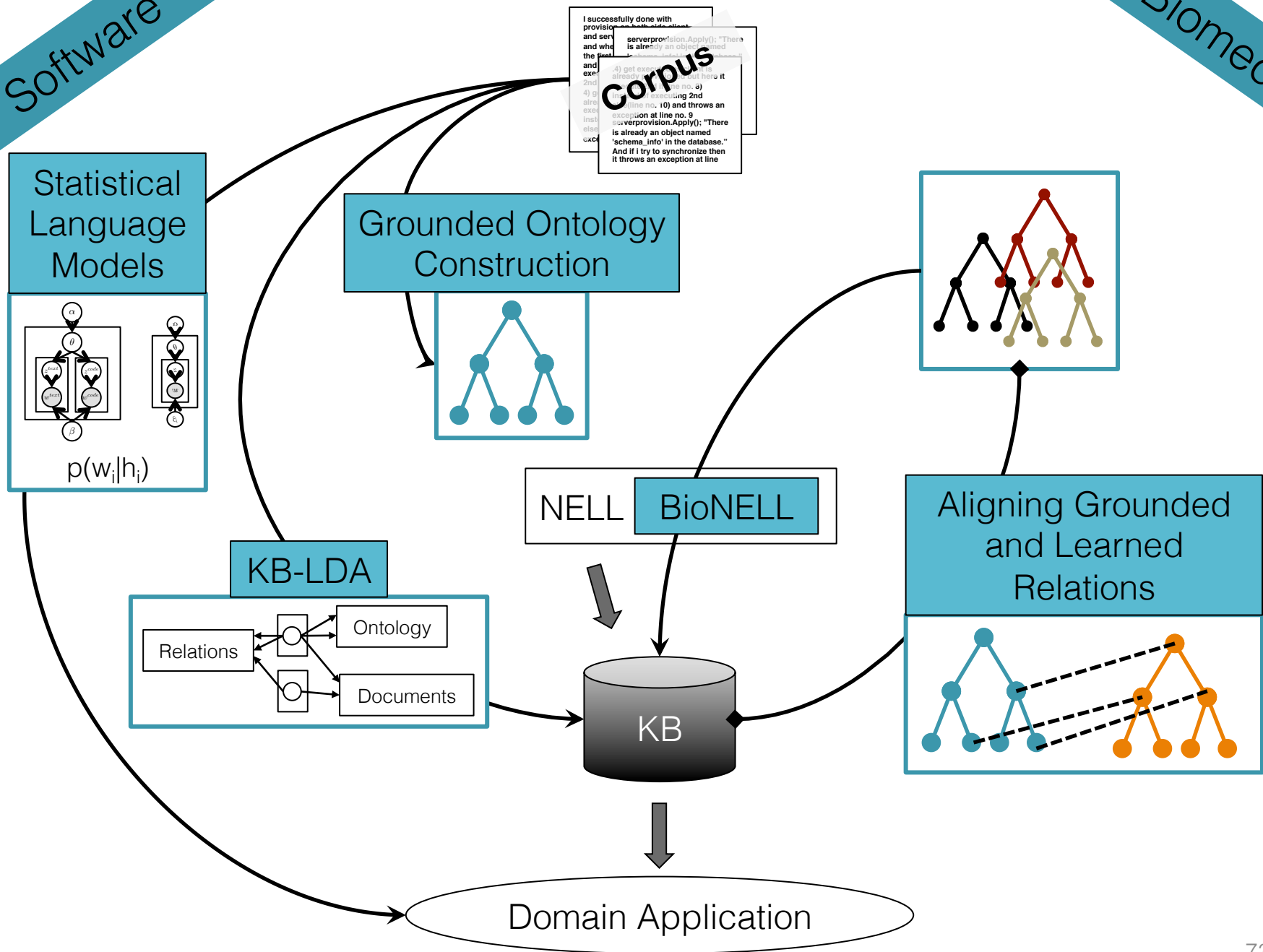


Conclusion

Key Idea

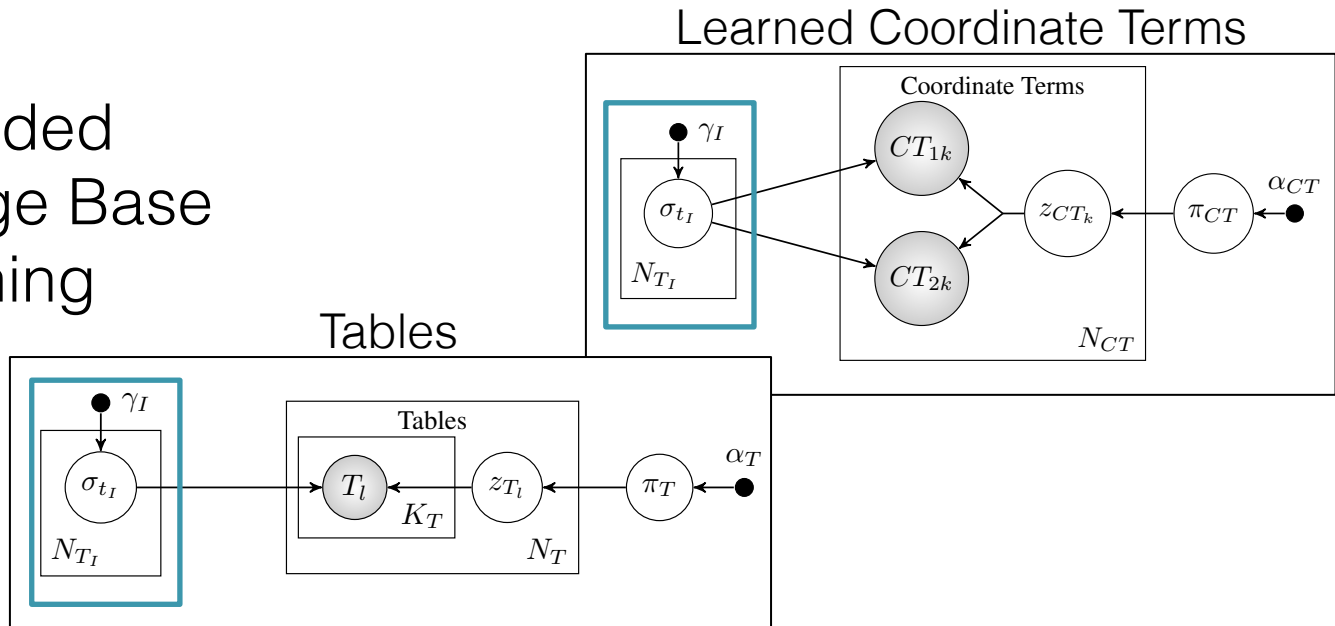


“Grounding entities to specialized data from a scientific domain facilitates improved unsupervised and semi-supervised algorithms for **Knowledge Base construction** for that domain”



What's Next?

Grounded
Knowledge Base
Learning



Revisit application
improvement using
learned KBs

