Schema Discovery

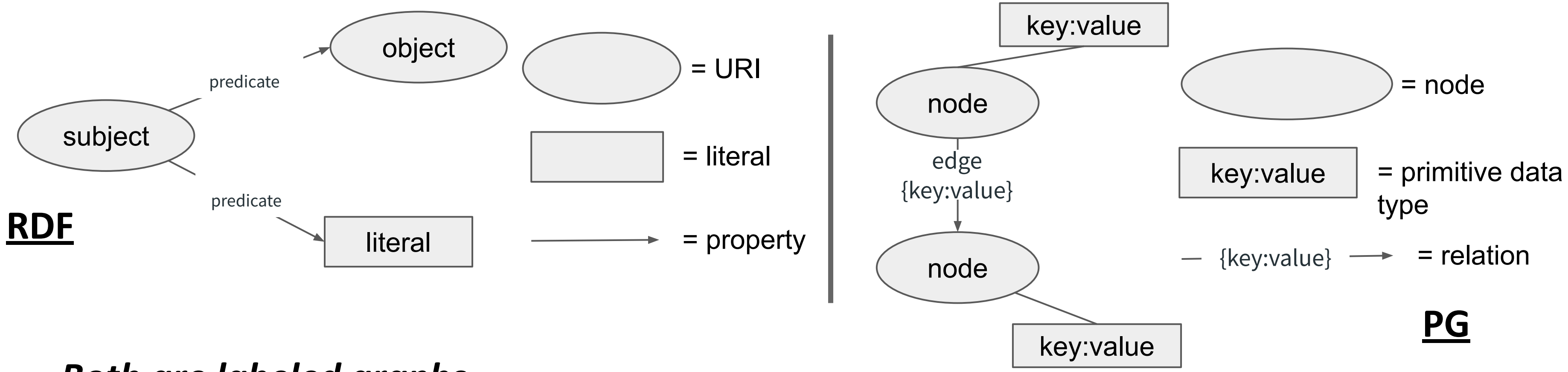
CS-562 Lab 5

Sophia Sideri

Preliminaries

RDF & Property Graphs:

- **RDF**: subject–predicate–object triples, semantic interoperability via ontologies.
- **PGs**: nodes/edges with labels and key–value properties; flexible, used in industry.



Both are labeled graphs.

Key difference: RDF edges (triples) can't hold properties; PG edges can.

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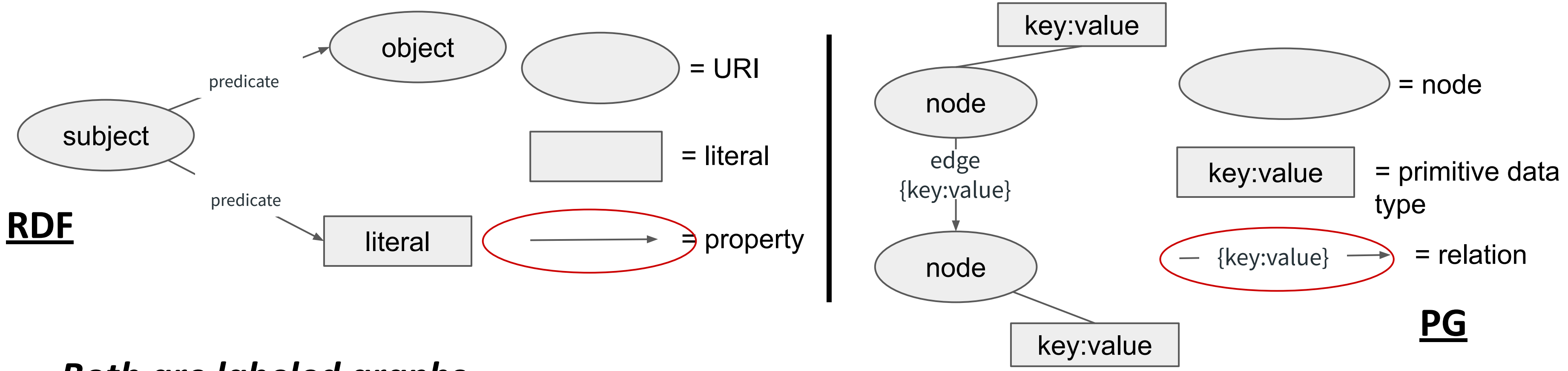

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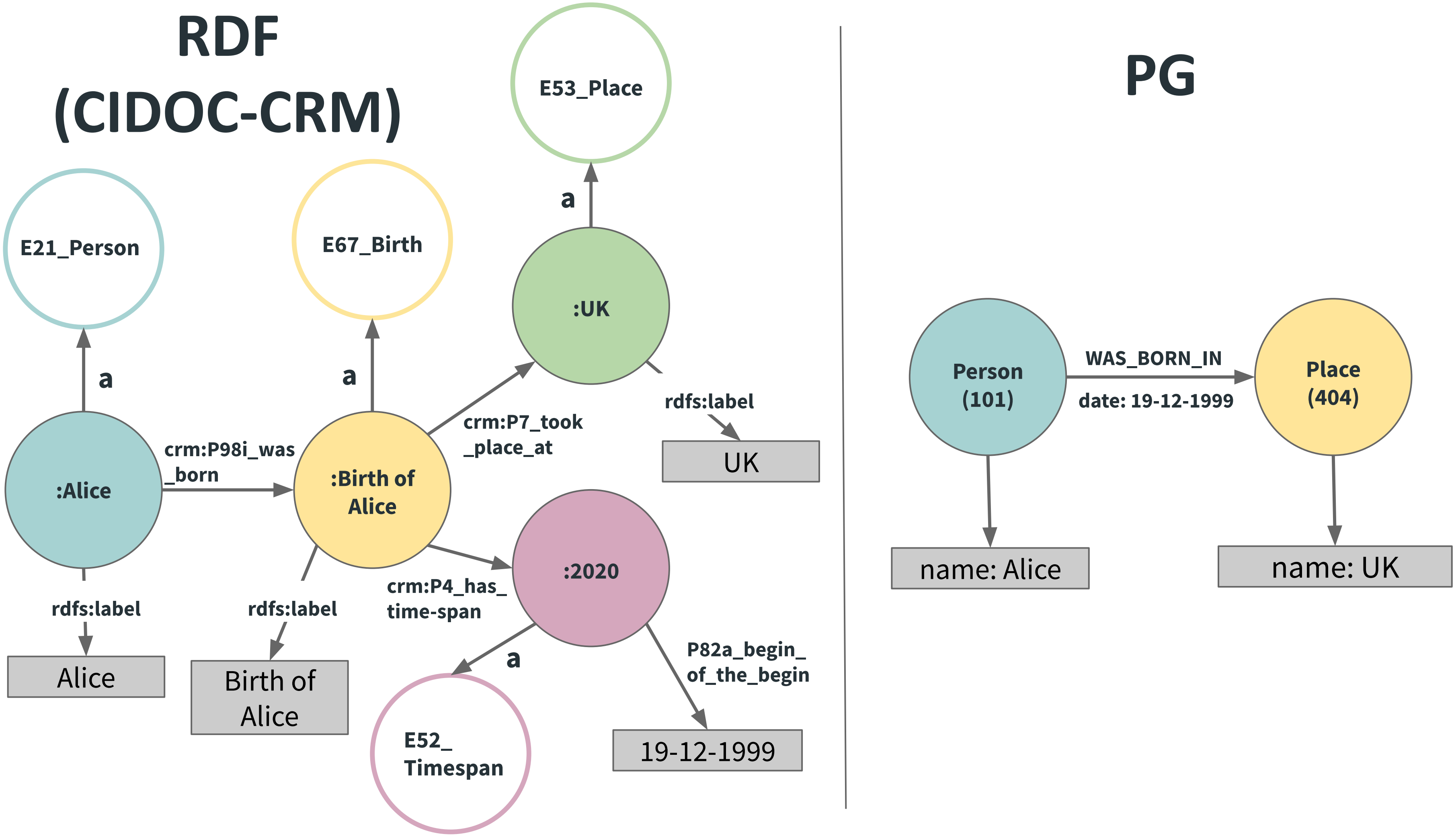

RDF
(CIDOC-CRM)
E53_Place
a
E21_Person
E67_Birth
:UK
a
a
rdfs:label
crm:P7_took
_place_at
UK
crm:P98i_was
_born
:Alice
:Birth of
Alice
:2020
crm:P4_has_
time-span
rdfs:label
rdfs:label
Alice
Birth of
Alice
a
P82a_begin_
of_the_begin
E52_
Timespan
19-12-1999
PG
Person
(101)
WAS_BORN_IN
date: 19-12-1999
Place
(404)
name: Alice
name: UK

Schema Discovery Problem in PGs

*"Given a property graph of **arbitrary size and structure**, with **missing type** information, **heterogeneous properties**, and **frequent updates**, infer the schema graph efficiently and accurately."*

Challenges:

Label heterogeneity and ambiguity	Evolving datasets
Efficiency	Schema constraint level

Ambiguities in Schema Discovery in PGs

In real datasets we might have several difficult cases to identify types:

Case 1: Many labels assigned to each instance

Case 2: Different labels referring to the semantically same entity

Case 3: Missing labels to some instances

Case 4: No labels to all instances and inconsistent properties

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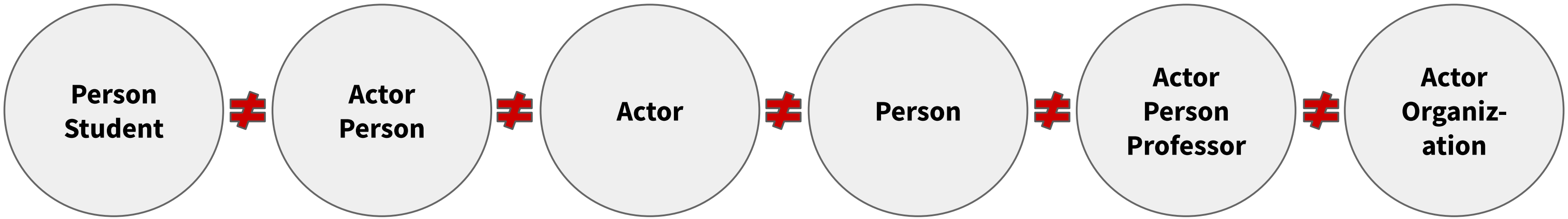

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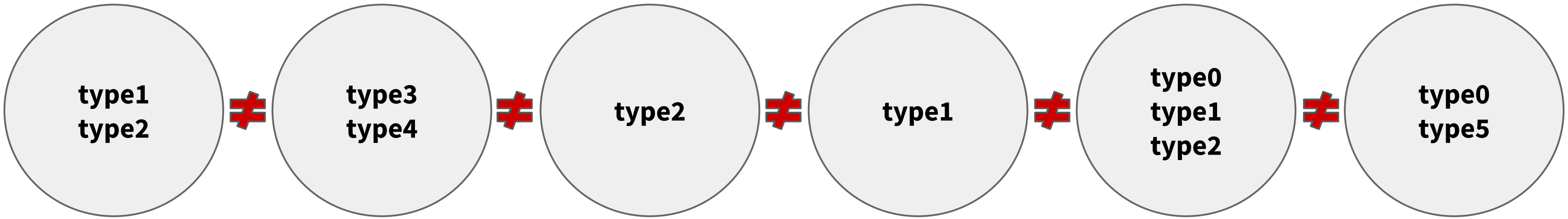

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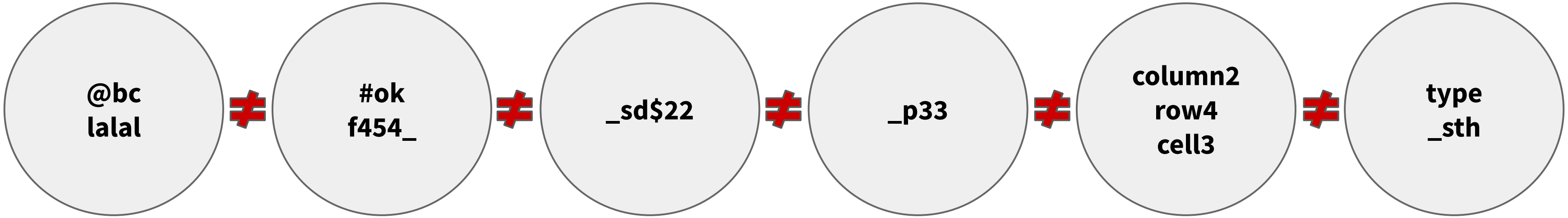
These are usually the types you are going to find in ***real noisy*** datasets



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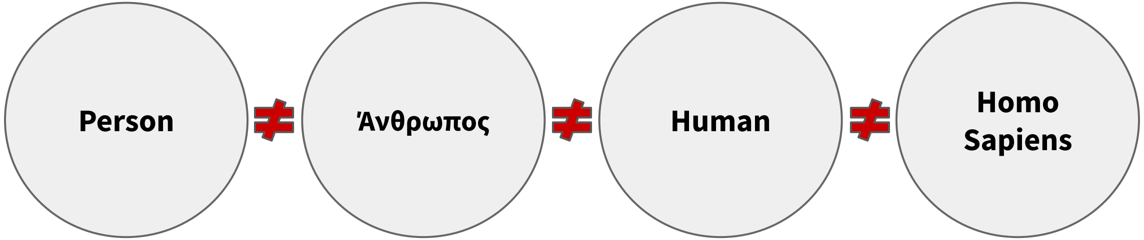

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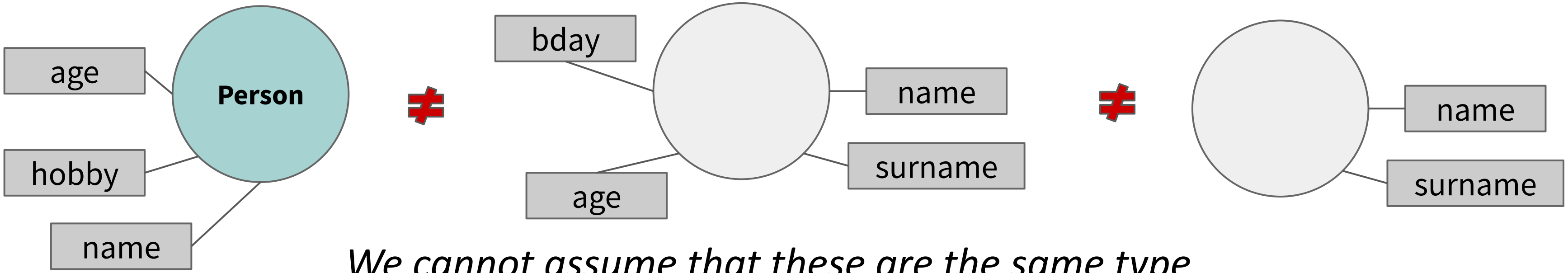

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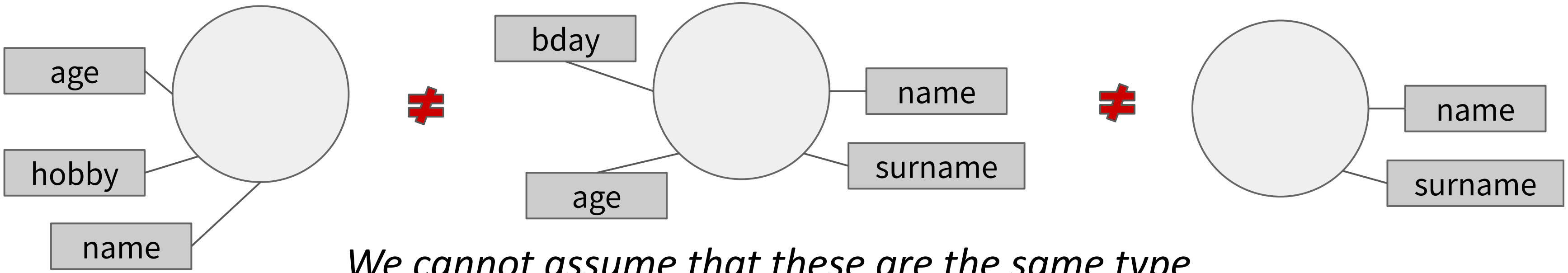

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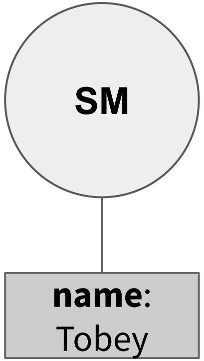
Ambiguities in Integrated Datasets

Dataset: Spider-Man



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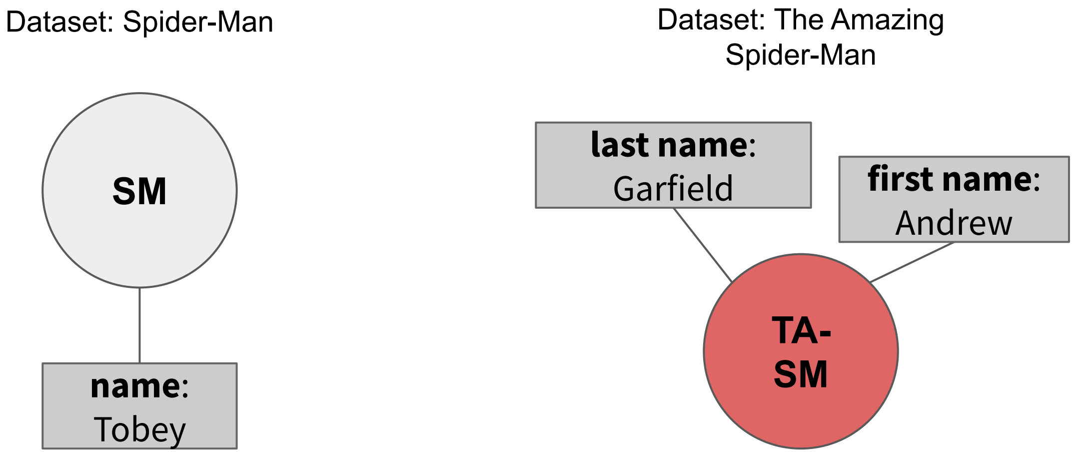

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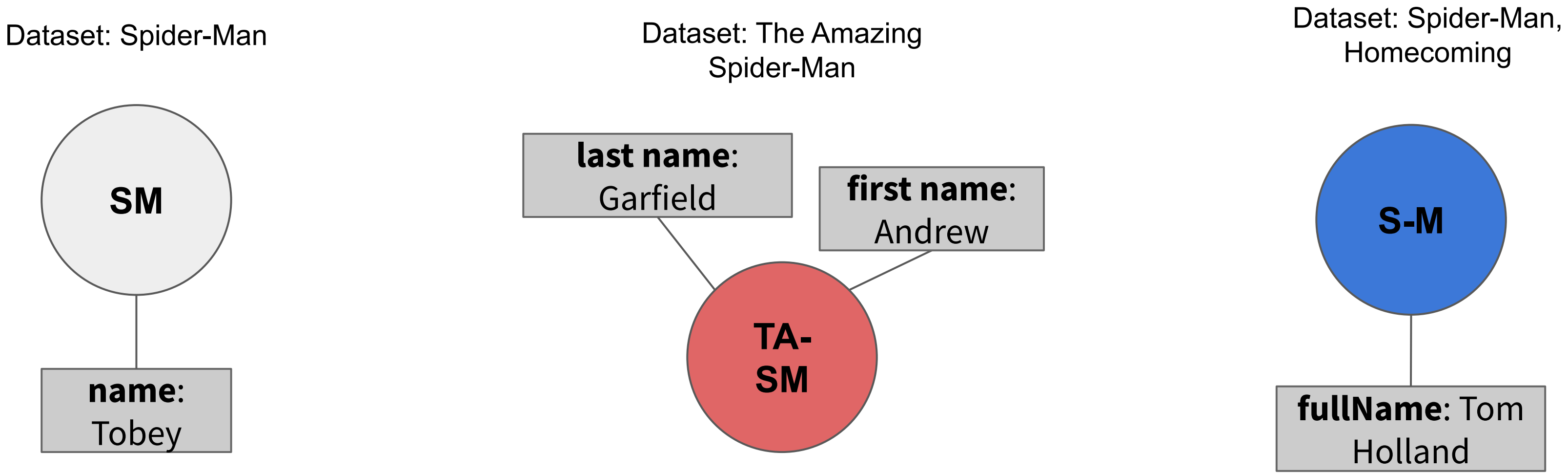

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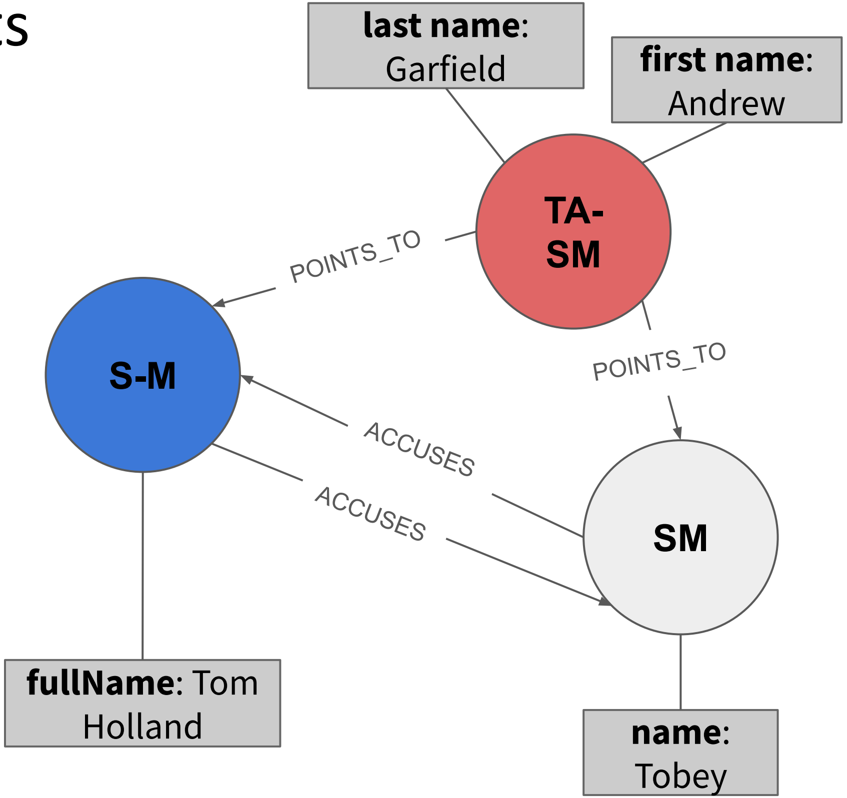


Is anyone the imposter? 👀

Ambiguities in Integrated Datasets

Spider-Man: No Way Home (2021)

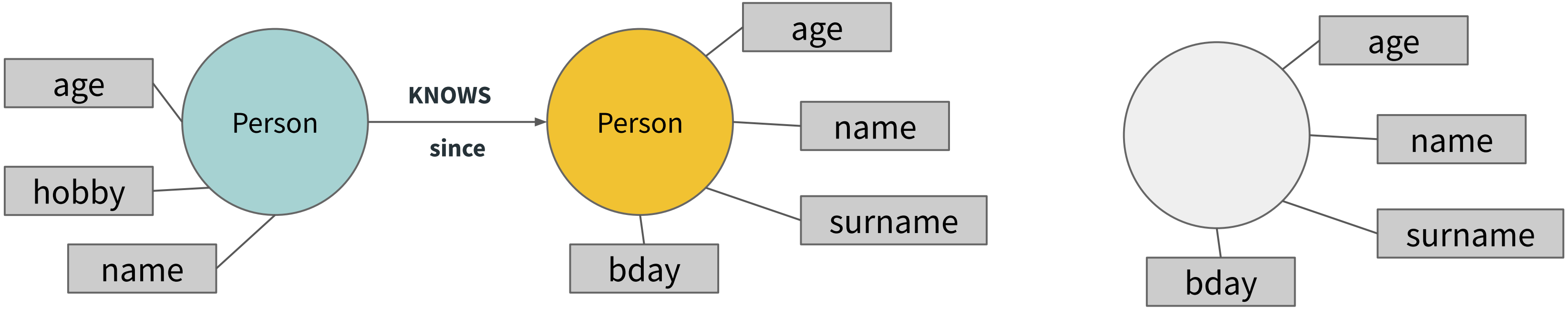
No one was an imposter, but how could we know? 🤔

The data **had different type labels, and different properties.**

What is a *type*?

Patterns & Types

We identify patterns in the data in order to extract our types.



Pattern 1: {Person}, {age, hobby, name}
Pattern 2: {Person}, {age, name, surname, bday}
Pattern 3: {∅}, {age, name, surname, bday}
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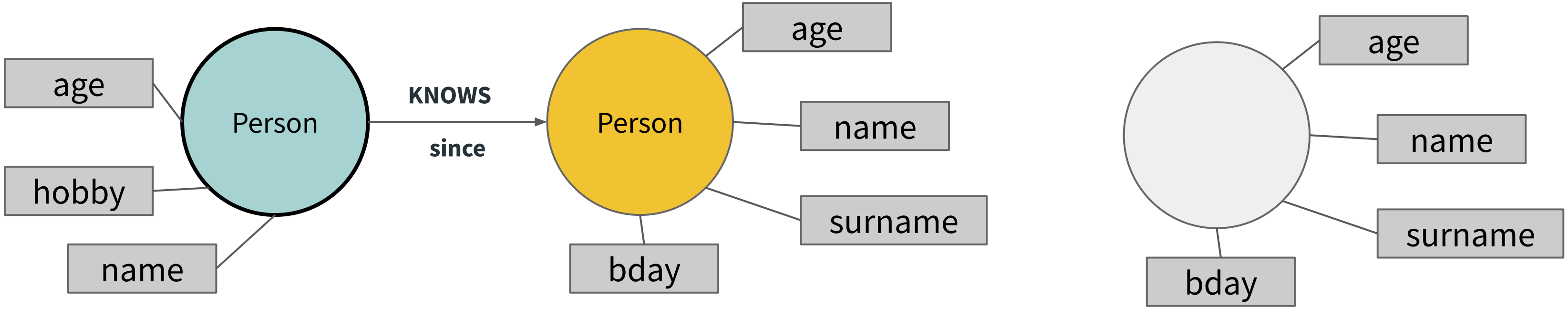

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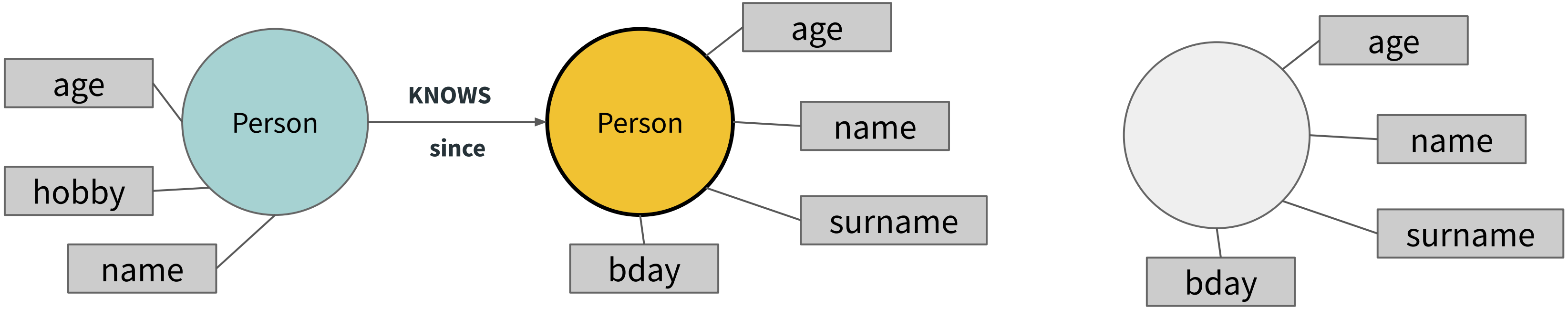

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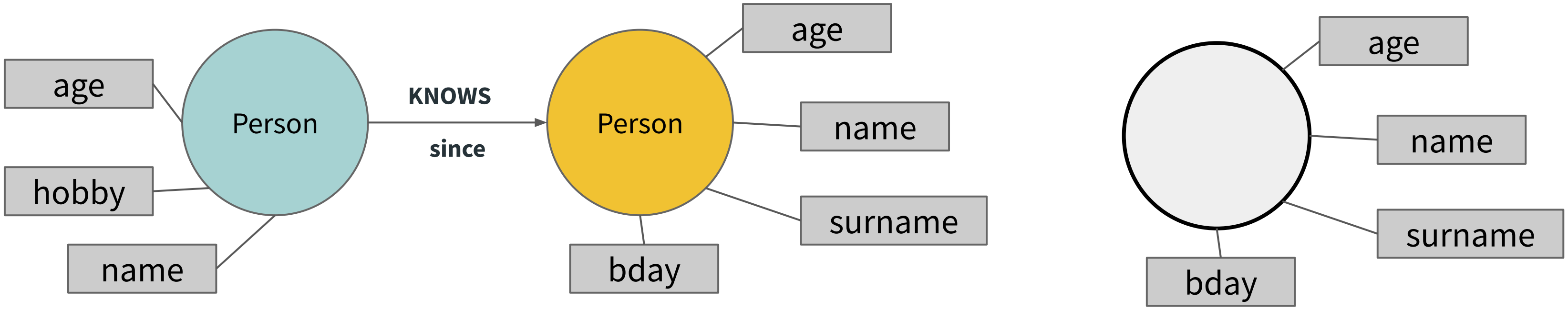

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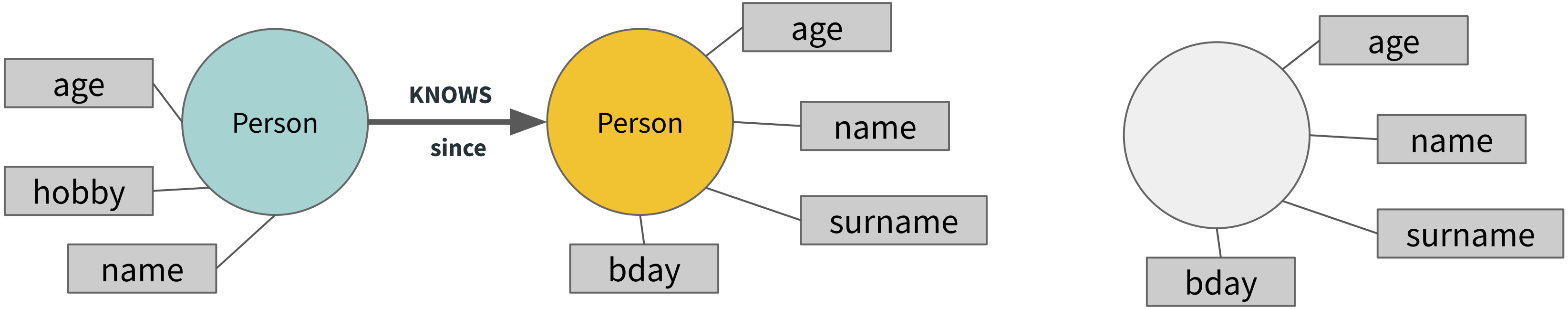

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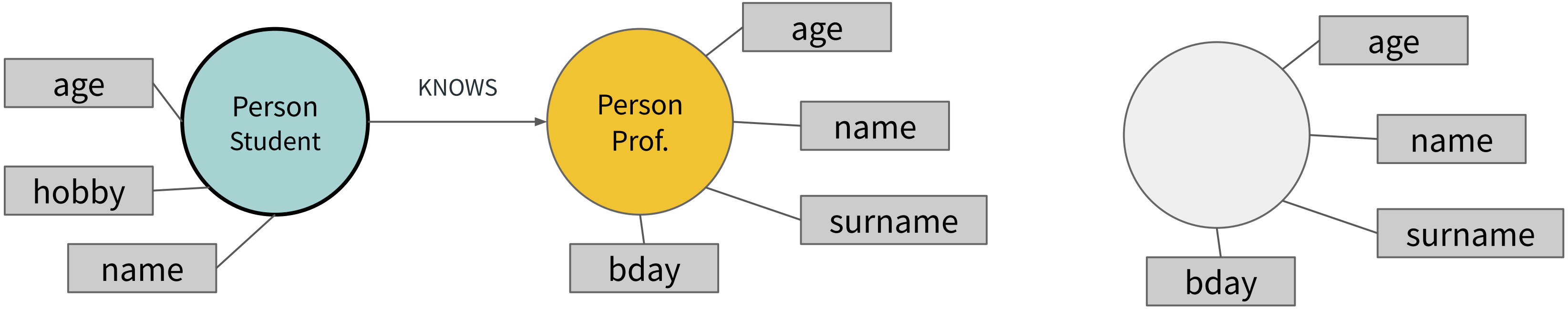

Pattern 5: {Person,Student}, {age, hobby, name}
Pattern 6: {Person,Prof.}, {age, name, surname, bday}
Pattern 7: {KNOWS}, {Person}, {Person}, {∅}

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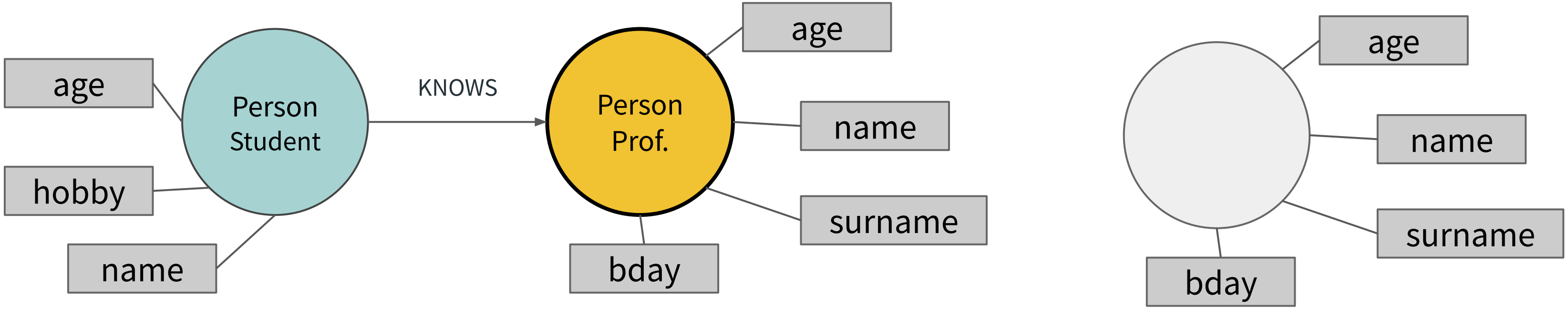

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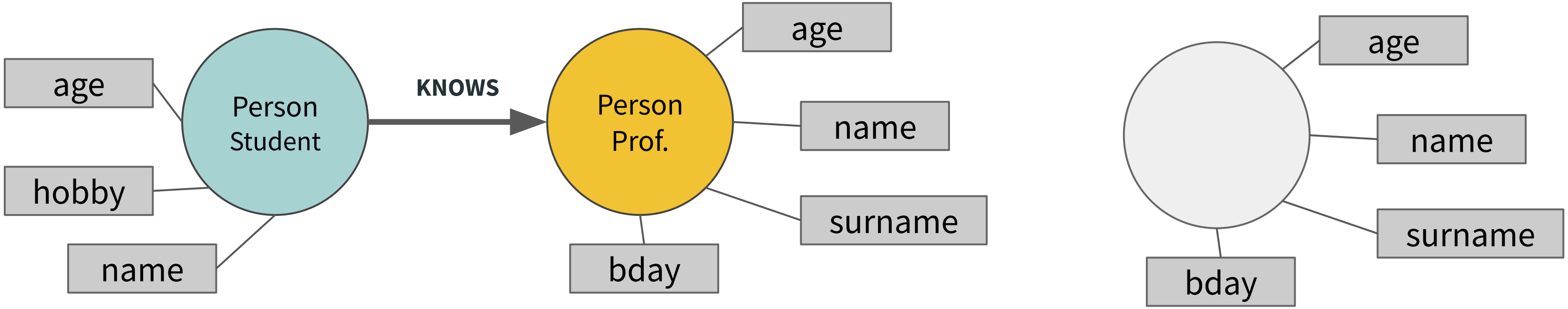

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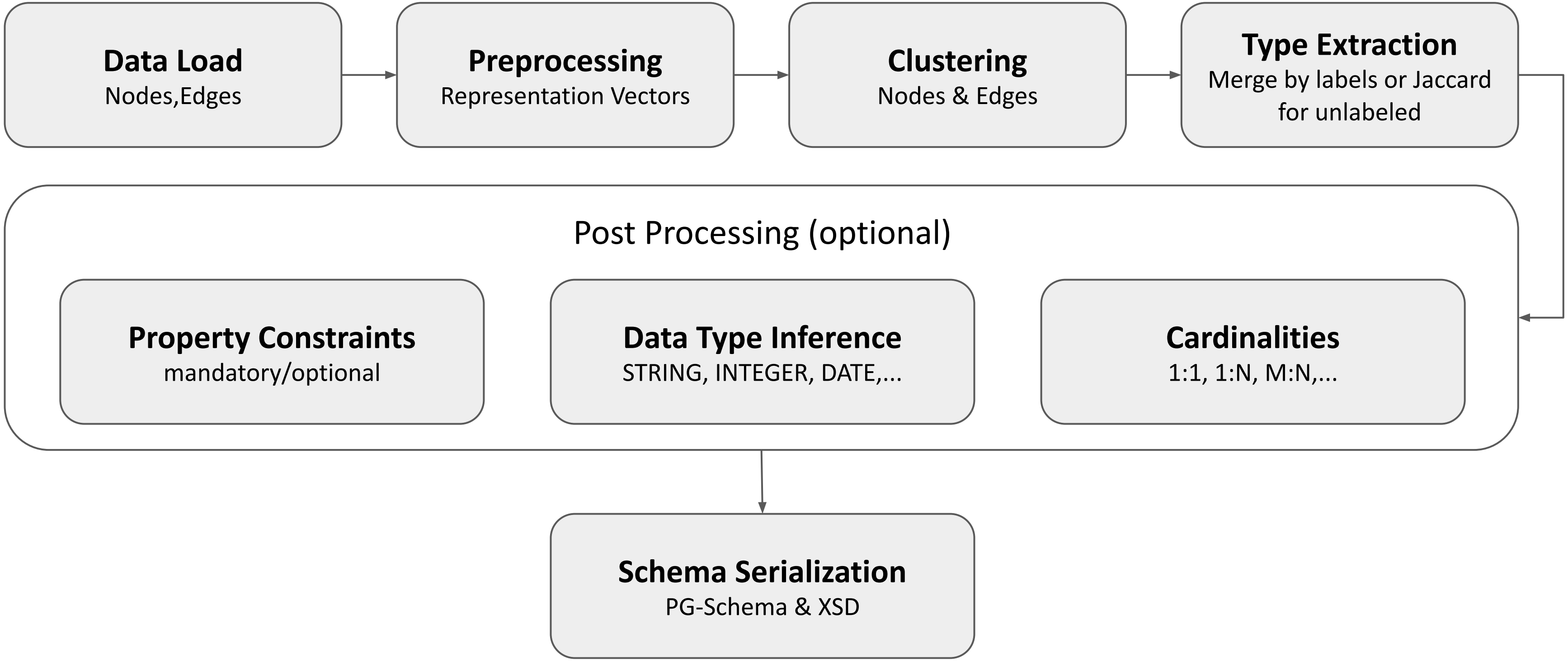
PG-HIVE

PG-HIVE: Hybrid Incremental Schema Discovery for PGs

HYBRID	**INCREMENTAL**
Labels	**Batch processing**
Properties	**Merging schemas**
Graph characteristics	

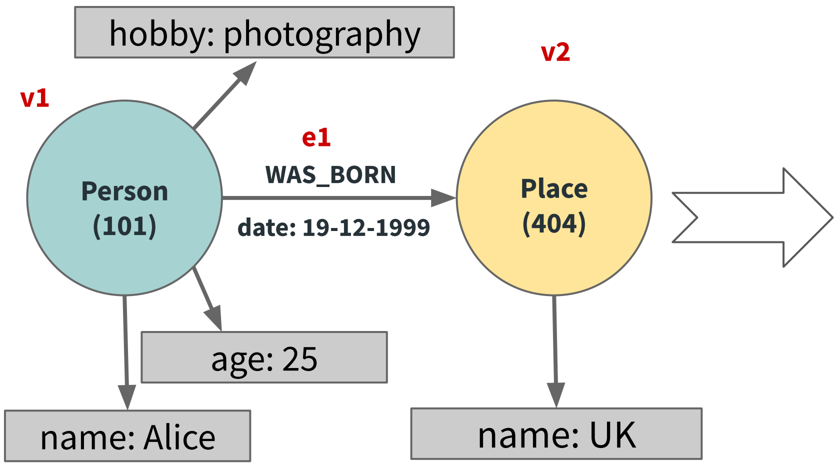
PG-HIVE: Hybrid Incremental Schema Discovery for PGs



PG-HIVE: Data Loading

We load data from PG storage (Neo4j) and transform them into vectors:

vi={{Word2Vec_label},{one-hot encoded properties}}
ei={{Word2Vec_src},{Word2Vec_tgt},{Word2Vec_label},{one-hot encoded properties}}



v1={w2v{Person},{0-1{name,age,hobby}}}
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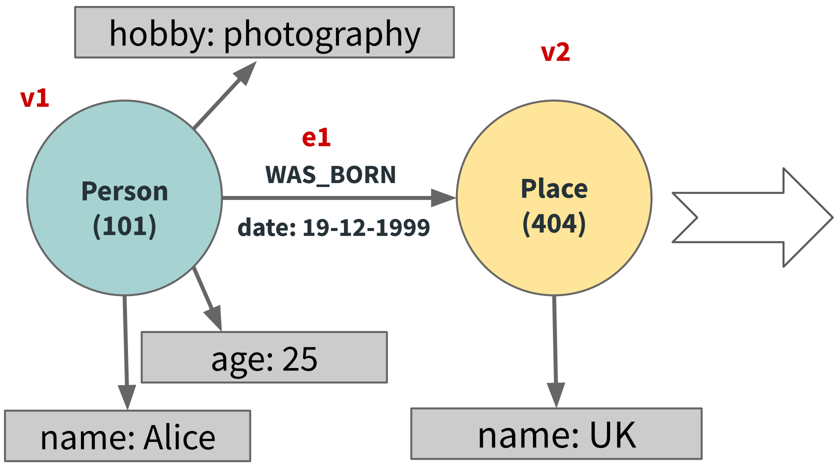

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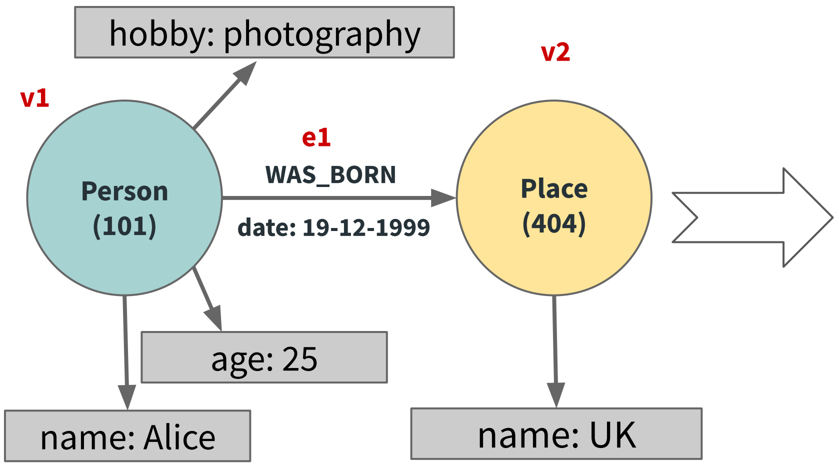

v1={w2v{2,1,4},{0-1{1,1,1}}}
v2={w2v{1,6,3},{0-1{1,0,0}}}
e1={w2v{2,1,4},w2v{1,6,3},w2v{1,1,1},{0-1{1}}}

PG-HIVE: Clustering

We use two clustering algorithms:

ELSH

Euclidean distance

Parameters: ***T, b***

T: number of hash tables

b: bucket length

Performs better in *feature vectors*

MinHash LSH

Jaccard Similarity

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Performs better in *set-like* data

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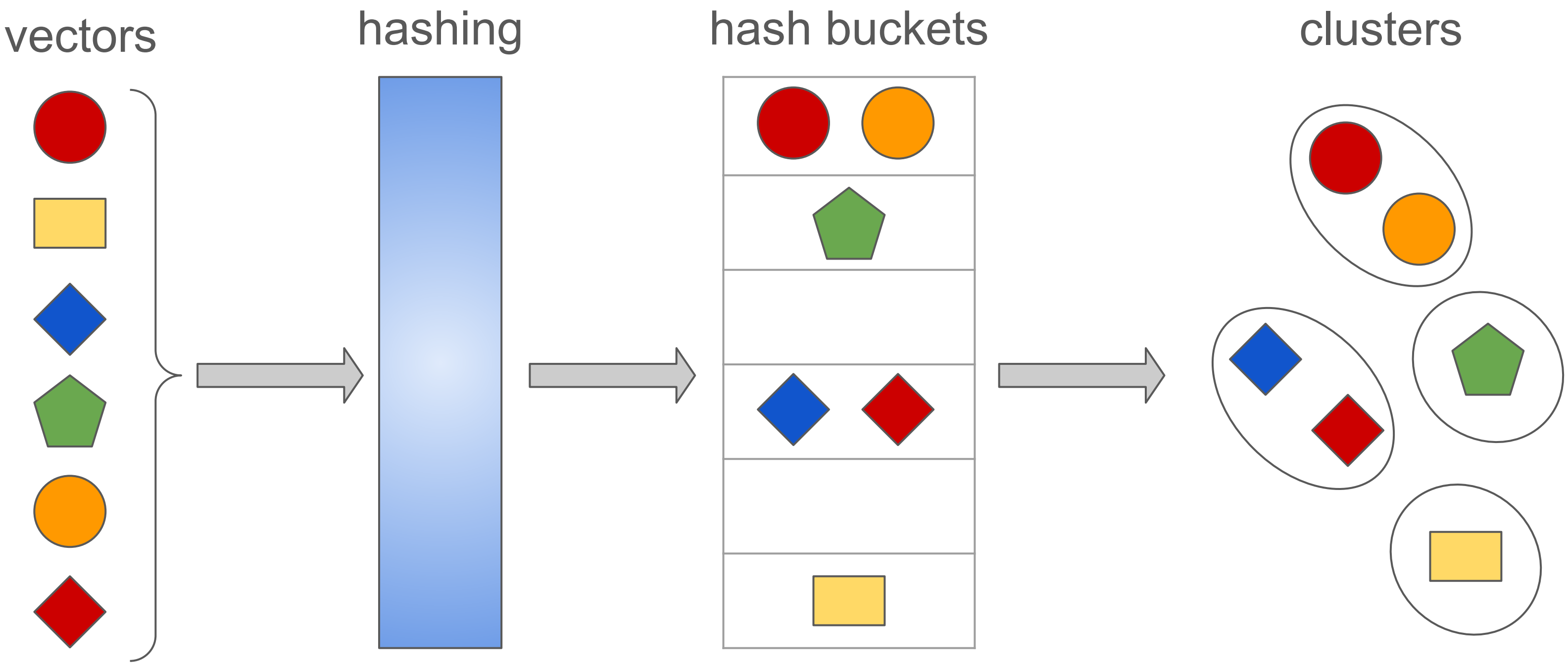
How to choose the best parameters? 🤔

PG-HIVE: LSH

How does LSH work?



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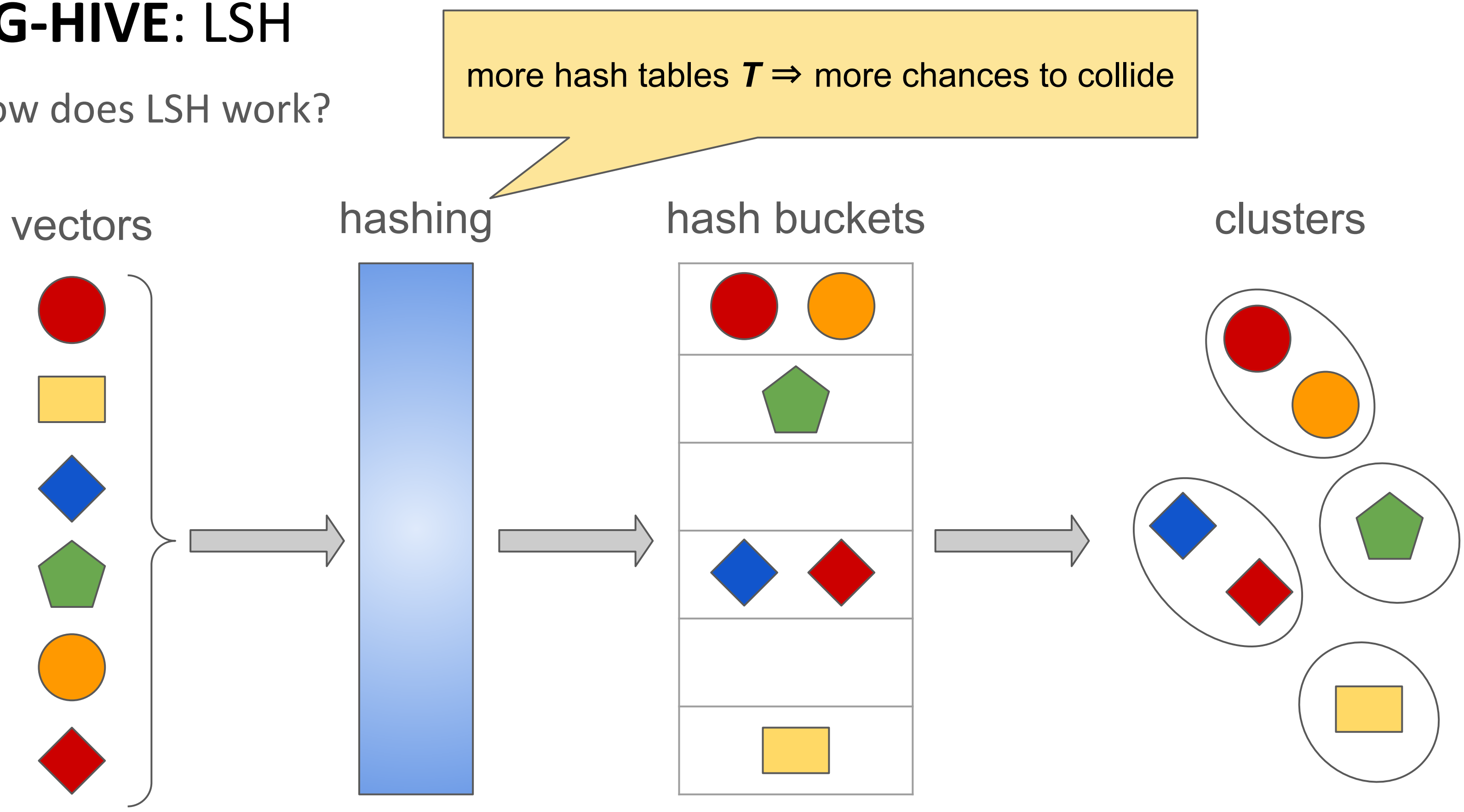

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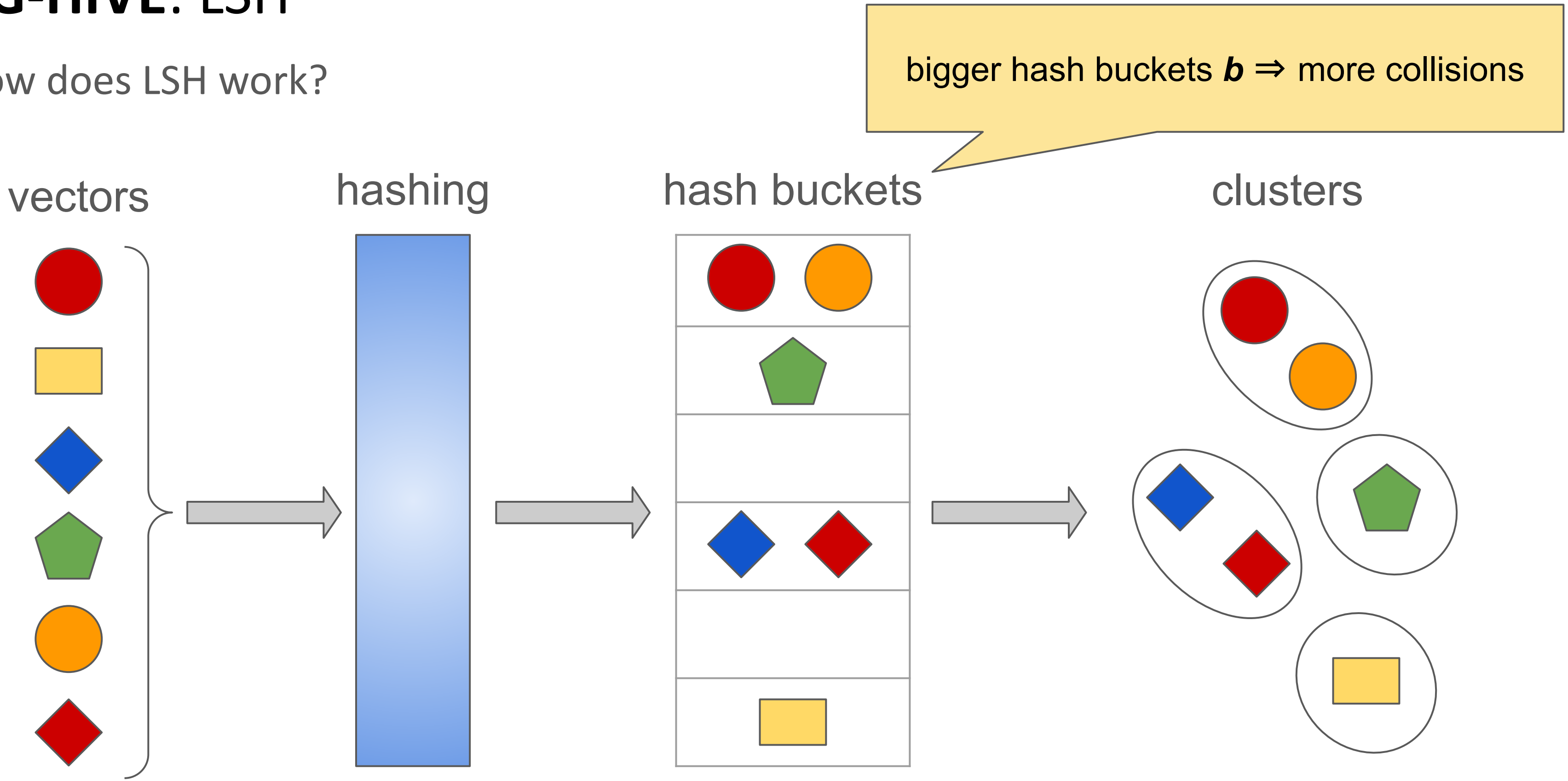
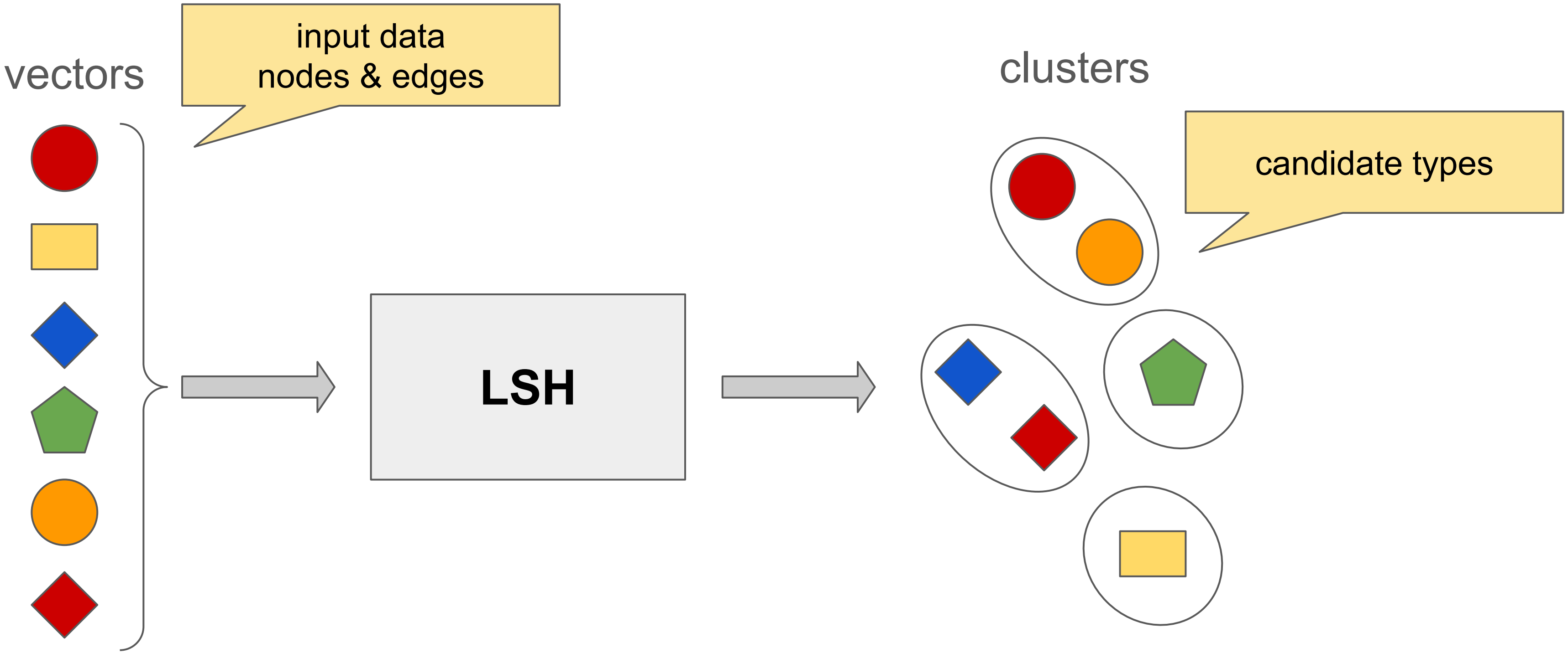


PG-HIVE: LSH

In our case



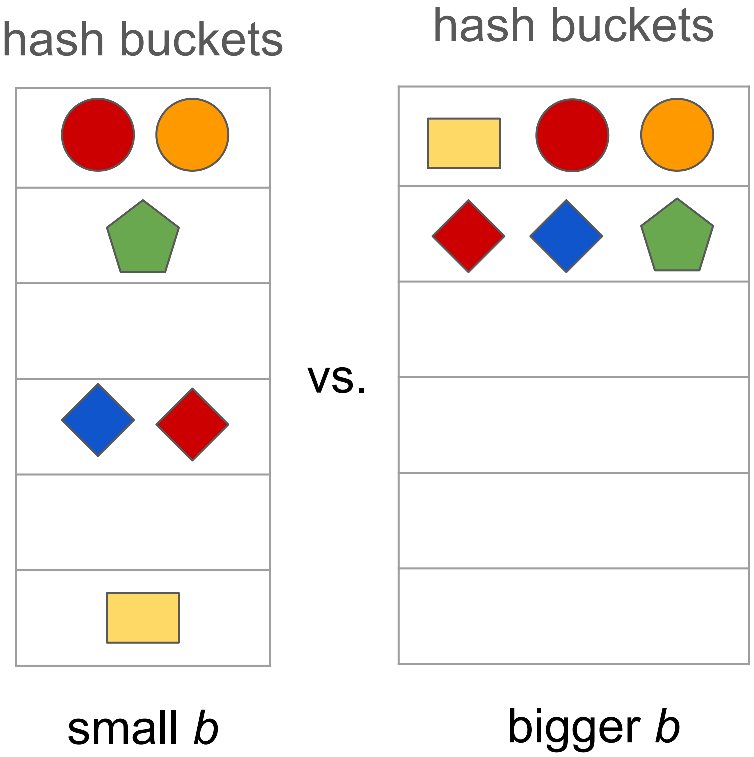
PG-HIVE: Adaptive parameterization

To avoid manual tuning of LSH, we introduce an adaptive selection of b and T.

For sparse graph we increase the bucket length and hash tables

For less sparse graphs we decrease them

increasing $T \Rightarrow$ more chances to collide
increasing $b \Rightarrow$ more collisions, higher recall but lower precision



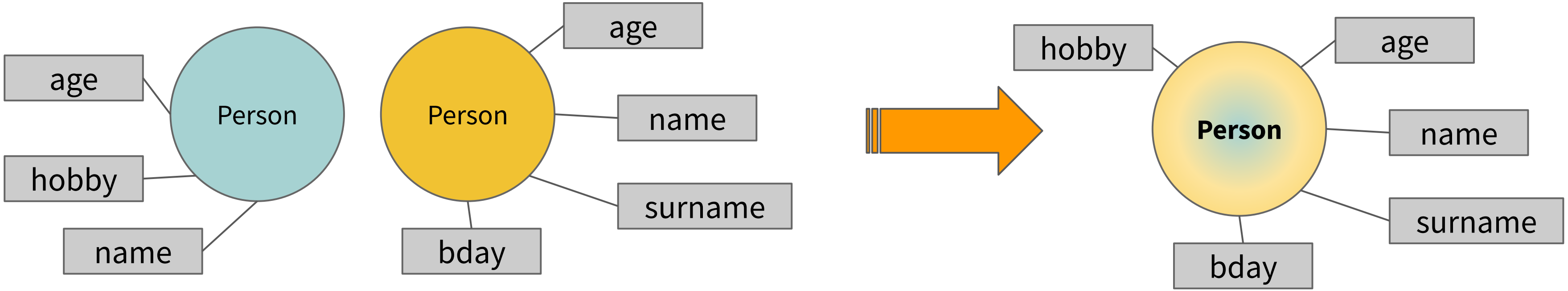
PG-HIVE: Extracting Types

After the clustering step, we refine the candidate node/edge types by merging the ones that correspond to the same schema type

Step 1: Same label

Step 2: Unlabeled clusters with Labeled ones (*iff* Jaccard > 0.9)

Step 3: Unlabeled clusters with the remaining unlabeled (*iff* Jaccard > 0.9)



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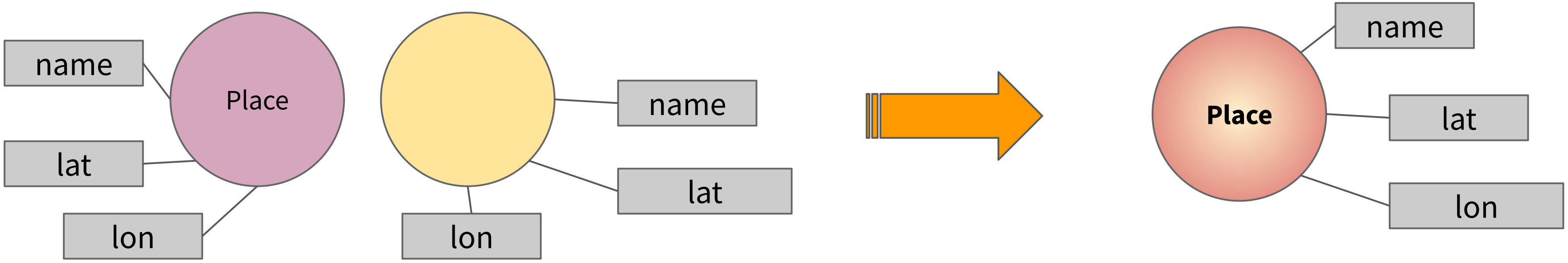

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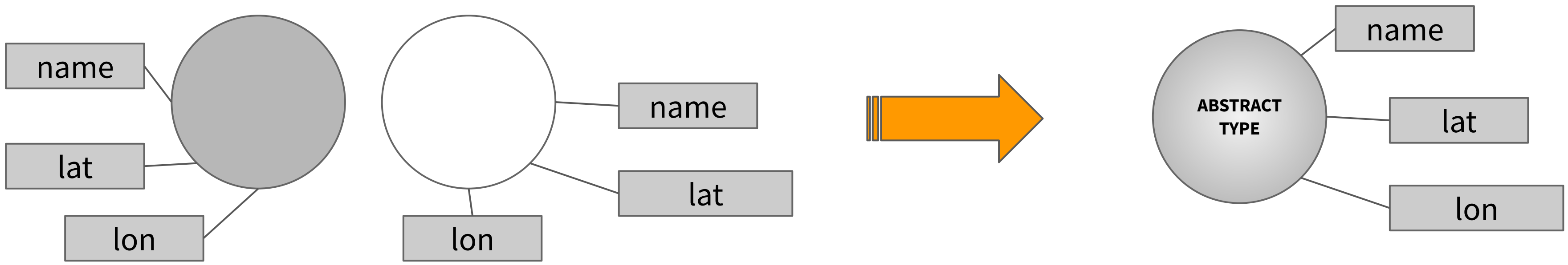


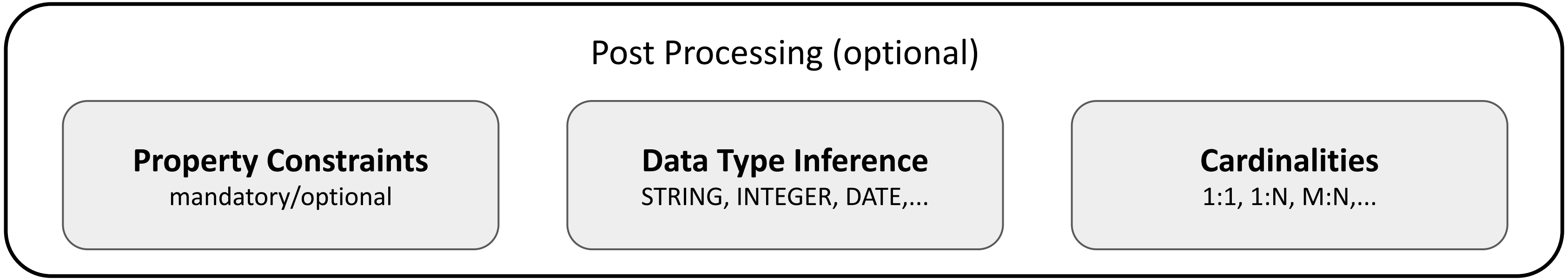
PG-HIVE: Post Processing

The post processing step is optional infers:

(i) property constraints

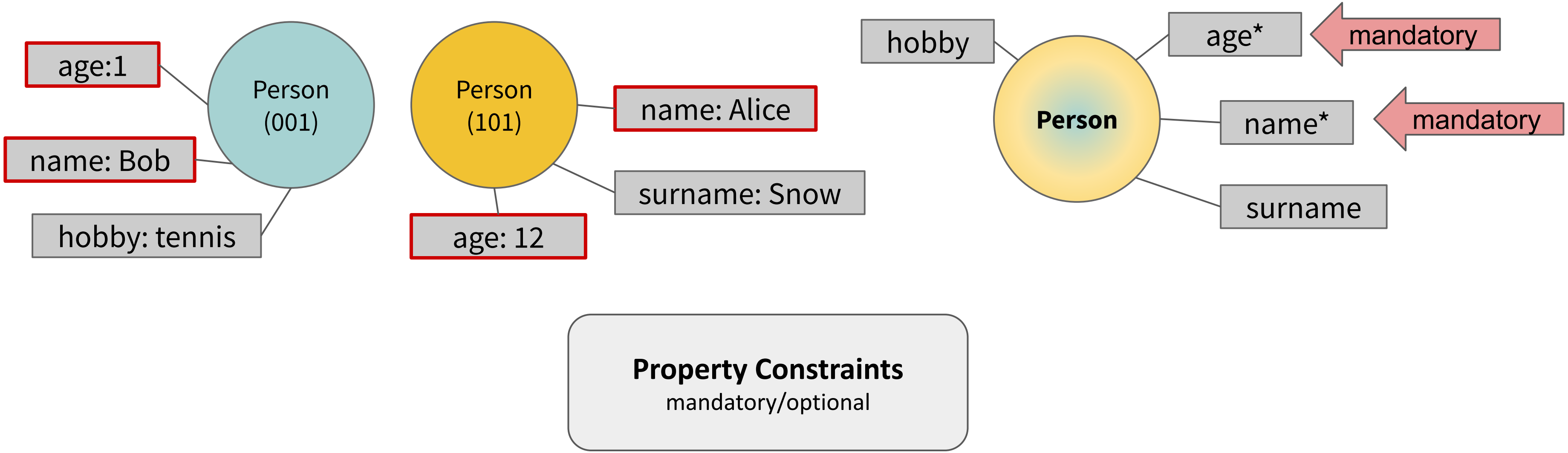
(ii) data type inference

(iii) cardinalities



PG-HIVE: Post Processing - Property Constraints

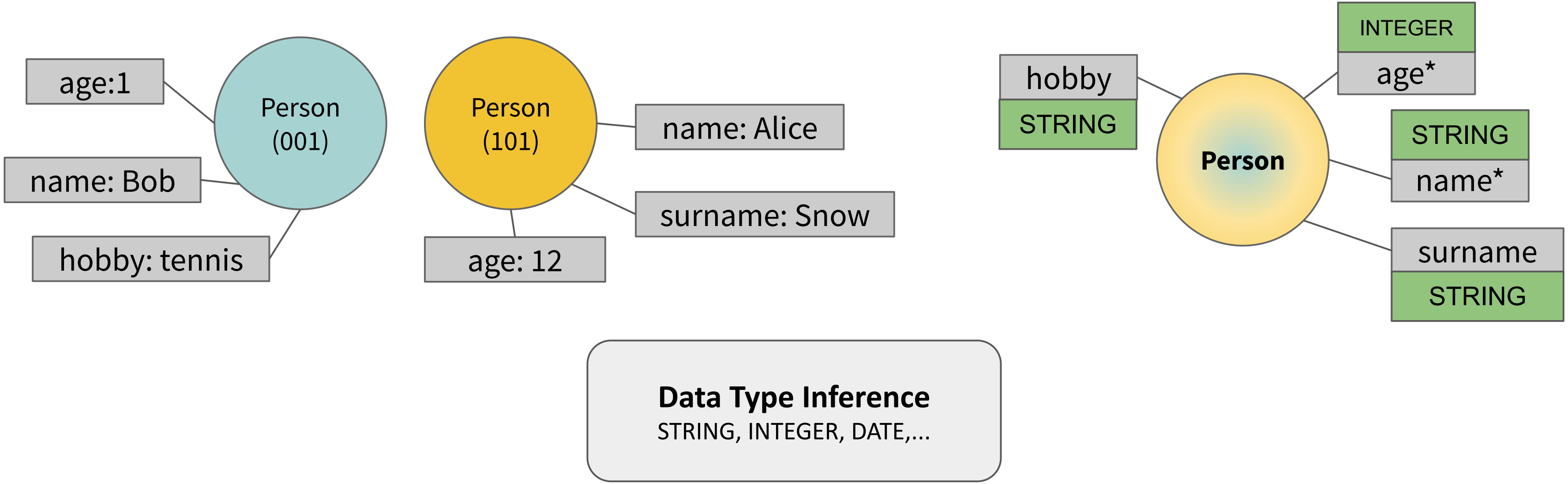
A property is characterized as **mandatory** for a given type if it appears in every instance of that type, otherwise, it is considered **optional**.



PG-HIVE: Post Processing - Data Types

We use heuristics to find the data type of each property:

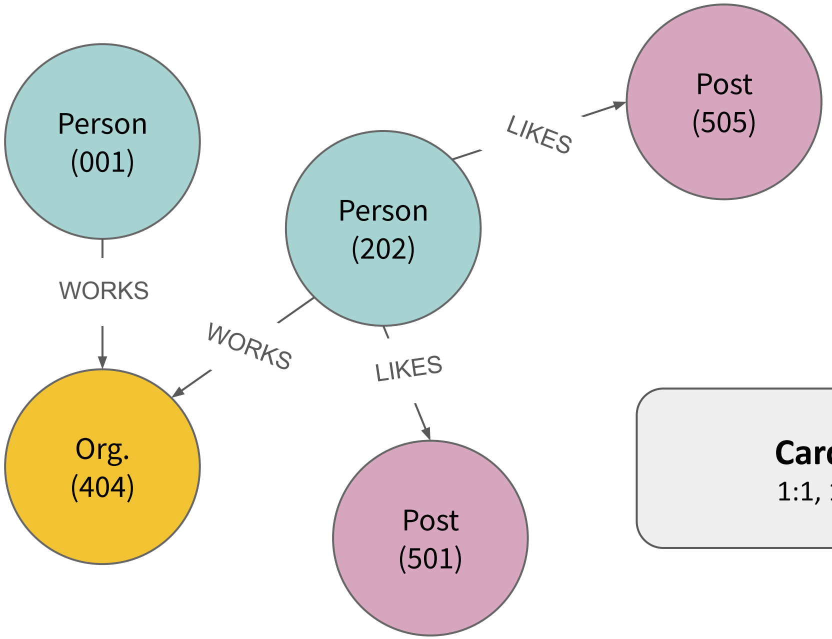
INTEGER ⟶ FLOAT ⟶ BOOLEAN ⟶ DATE ⟶ STRING (fallback)



**using sampling*

PG-HIVE: Post Processing - Cardinalities

To find the cardinalities of edge types, we query how many distinct targets each source connects to, for each edge type, and vice versa.

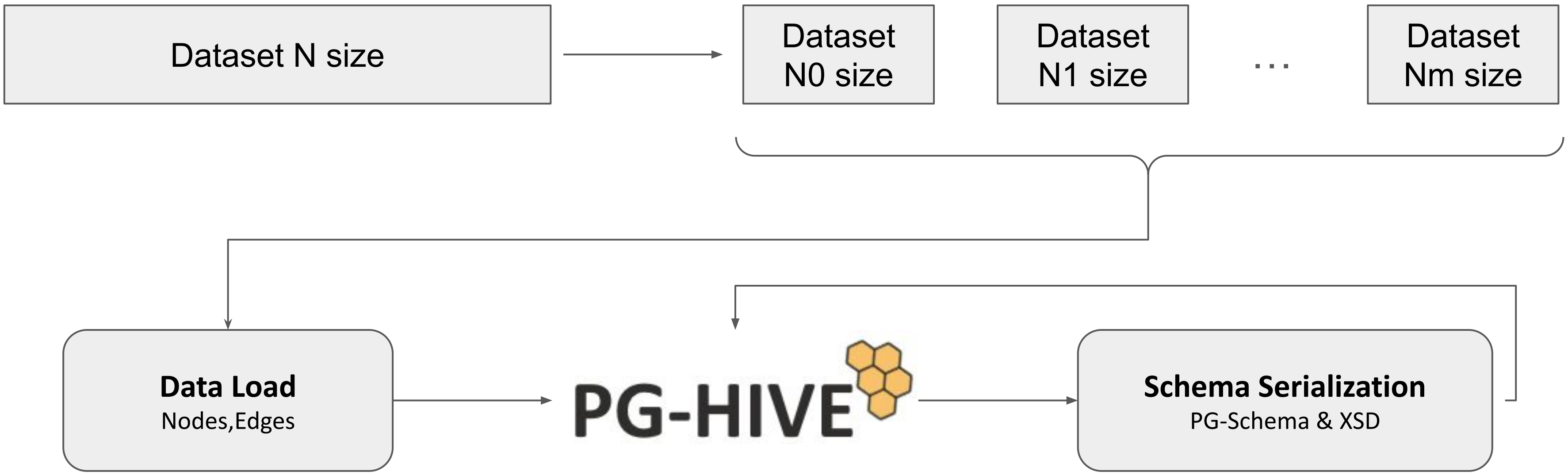


Cardinalities
1:1, 1:N, M:N,...

Person:Org ⇒N,1
Person:Post ⇒ 0,N

PG-HIVE: Incremental Module

To process big datasets in different settings we have also an incremental module



PG-HIVE: Serialization - XSD

```xml
<xs:schema name="NewGraphSchema" xmlns:xs="http://www.w3.org/2001/XMLSchema">
  <xs:complexType name="Place">
    <xs:sequence>
      <xs:element name="type" type="xs:string" minOccurs="1" maxOccurs="1"/>
      <xs:element name="name" type="xs:string" minOccurs="1" maxOccurs="1"/>
      <xs:element name="id" type="xs:double" minOccurs="1" maxOccurs="1"/>
      <xs:element name="url" type="xs:string" minOccurs="1" maxOccurs="1"/>
    </xs:sequence>
    <xs:attribute name="id" type="xs:ID" use="required"/>
    <xs:attribute name="label" type="xs:string"/>
  </xs:complexType>
  <xs:complexType name="Person">
    <xs:sequence>
      <xs:element name="lastName" type="xs:string" minOccurs="1" maxOccurs="1"/>
      <xs:element name="firstName" type="xs:string" minOccurs="1" maxOccurs="1"/>
      <xs:element name="birthday" type="xs:date" minOccurs="1" maxOccurs="1"/>
    </xs:sequence>
    <xs:attribute name="id" type="xs:ID" use="required"/>
    <xs:attribute name="label" type="xs:string"/>
  </xs:complexType>
  <xs:complexType name="IS_LOCATED_IN">
    <xs:sequence>
      <xs:element name="source" type="Person"/>
      <xs:element name="target" type="Place"/>
    </xs:sequence>
  </xs:complexType>
</xs:schema>
```

PG-HIVE: Serialization - PG-Schema

```
CREATE GRAPH TYPE NewGraphSchema LOOSE {
  (PlaceType: Place {type STRING, name STRING, id DOUBLE, url STRING}),
  (PersonType: Person {lastName STRING, firstName STRING, birthday DATE}),
  (EmailType: Email {address STRING}),
  (:PersonType)-[HAS_EMAILType: HAS_EMAIL]->(:EmailType),
  (:PersonType)-[IS_LOCATED_INType: IS_LOCATED_IN]->(:PlaceType),
}
```

LOOSE

```
CREATE NODE TYPE PlaceType : Place {type STRING, name STRING, id DOUBLE, url STRING};
CREATE NODE TYPE PersonType : Person {lastName STRING, firstName STRING, birthday DATE};
CREATE NODE TYPE EmailType : Email {address STRING};

CREATE EDGE TYPE has_emailType : HAS_EMAIL;
CREATE EDGE TYPE is_located_inType : IS_LOCATED_IN;

CREATE GRAPH TYPE NewGraphSchema STRICT {
  (PlaceType),
  (PersonType),
  (EmailType),
  (:PersonType)-[has_emailType]->(:EmailType),
  (:PersonType)-[is_located_inType]->(:PlaceType),

  FOR (x:EmailType) SINGLETON x WITHIN (:PersonType)-[y: has_emailType]->(x)
  FOR (x:PersonType) SINGLETON y WITHIN (x)-[y: is_located_inType]->(:PlaceType)
}
```

STRICT

Part 3:

Evaluation

Previous Work on Schema Discovery for PGs

	SchemI[1]	GMMSchema[2]	DiscoPG[3]	PG-HIVE (ours)
Label Independent	❌	❌	❌	✅
Multi Labeled Elements	❌	✅	✅	✅
Schema Elements	Nodes & Edges	Nodes only	Nodes & queries associated Edges	Nodes & Edges & constraints
Constraints	❌	❌	❌	✅
Incremental	❌	❌	✅	✅
Automation	✅	✅	✅ + UI	✅
Notes	Cannot handle missing labels	GMM clustering, can not handle missing labels	Demo of GMMSchema	LSH + fine tuning

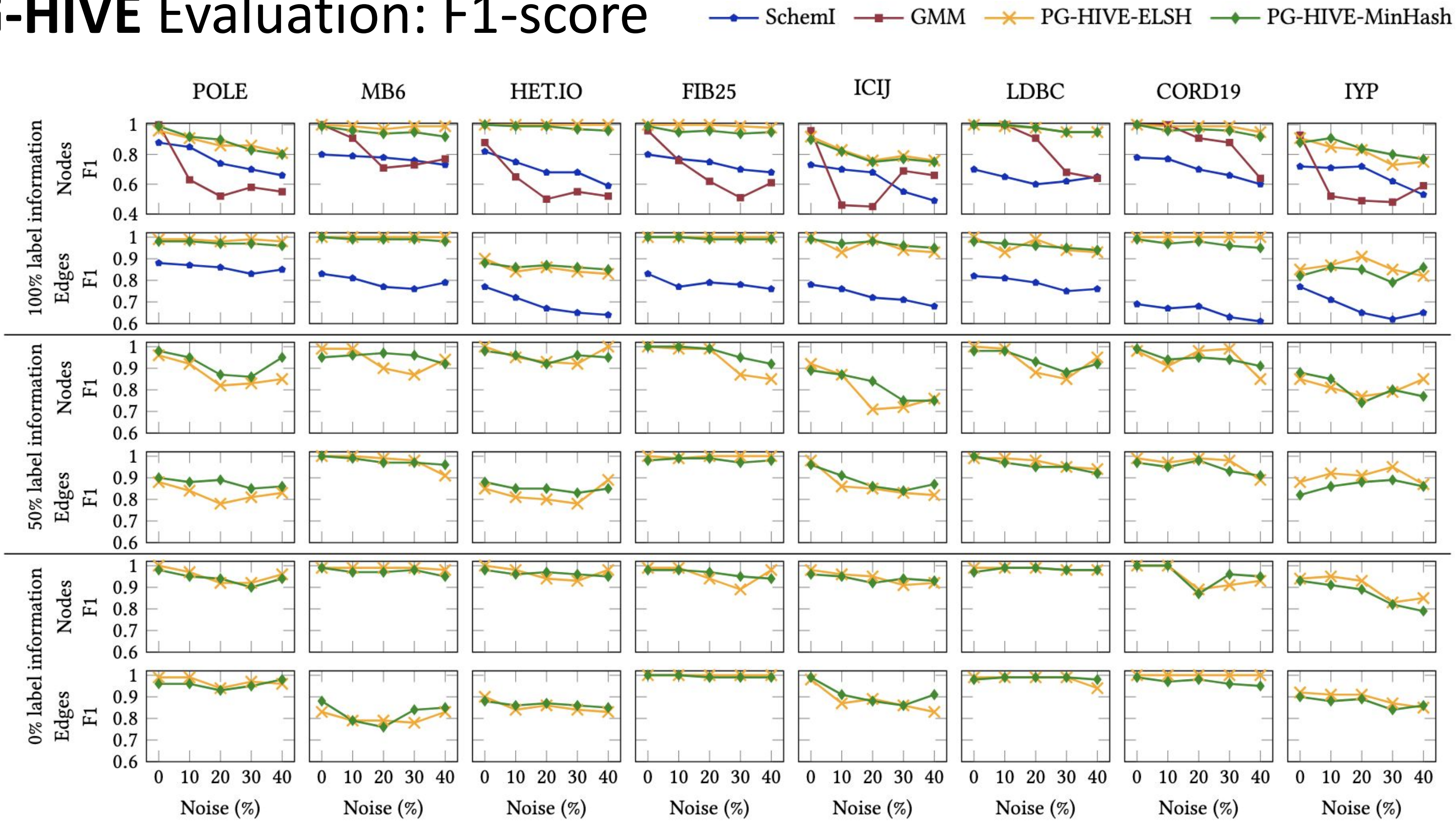
[1]SchemI:Lbath, H., Bonifati, A., Harmer, R.: Schema inference for property graphs.EDBT 2021
[2]GMMSchema: Bonifati, A., Dumbrava, S., Mir, N.: Hierarchical clustering for property graph schema discovery. EDBT 2022
[3]DiscoPG:Bonifati, A., Dumbrava, S., Martinez, E., Ghasemi, F., Jaffré, M., Luton, P., Pickles, T.: Discopg: Property graph schema discovery and exploration. Proc. VLDB 2022

PG-HIVE Evaluation: Datasets

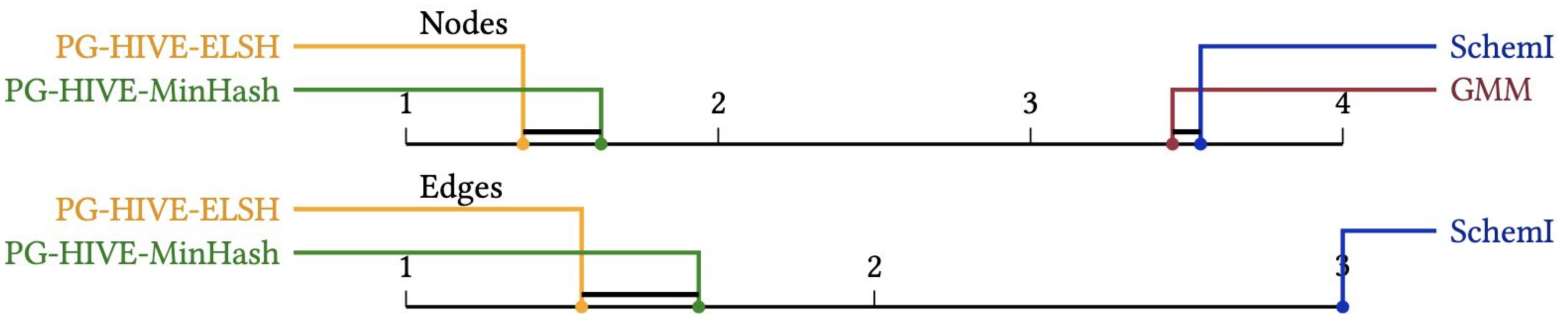
Dataset	Nodes	Edges	Node Types	Edge Types	Node Labels	Edge Labels	Node Pat.	Edge Pat.	Real Synth.
POLE	61,521	105,840	11	17	11	16	11	16	S
MB6	486,267	961,571	4	5	10	3	52	9	S
HET.IO	47,031	2,250,197	11	24	12	24	14	38	R
FIB25	802,473	1,625,428	4	5	10	3	31	9	S
ICIJ	2,016,523	3,339,267	5	14	6	14	2,263	88	R
LDBC	3,181,724	17,256,038	7	17	8	15	9	23	S
CORD19	36,025,729	59,768,373	6	5	6	5	89	6	R
IYP	44,539,999	251,432,812	32	24	33	24	25,137	790	R

Environment: Spark cluster (4 nodes × 38 cores), Scala 2.12.10, Neo4j 4.4.0

PG-HIVE Evaluation: F1-score

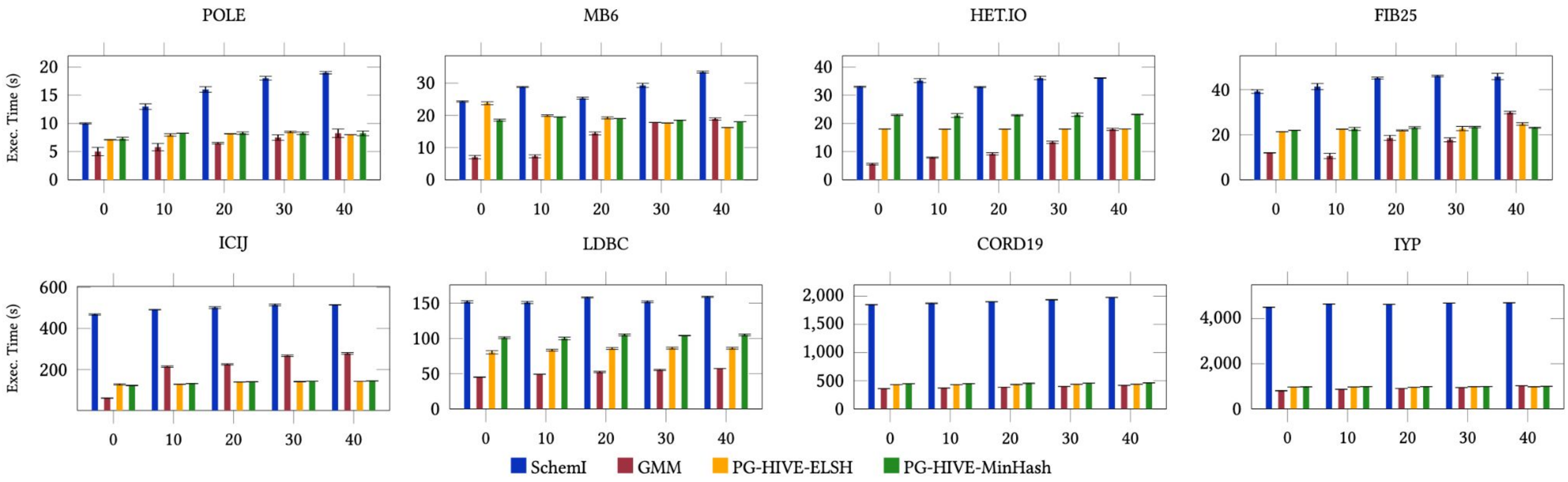


PG-HIVE Evaluation: Statistical Significance



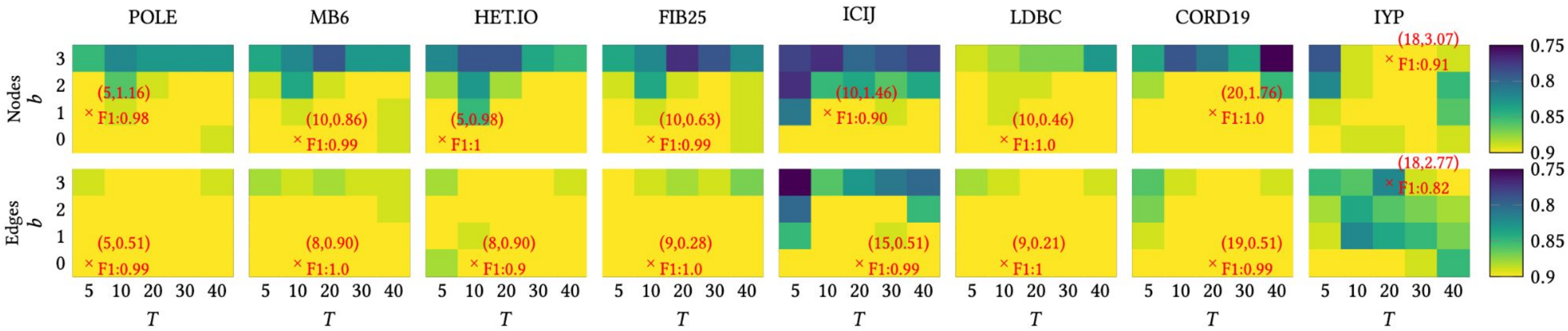
Statistical significance analysis of F1-scores across datasets for **nodes (top)** and **edges (bottom)** --GMM does not produce edge types.

PG-HIVE Evaluation: Execution Time



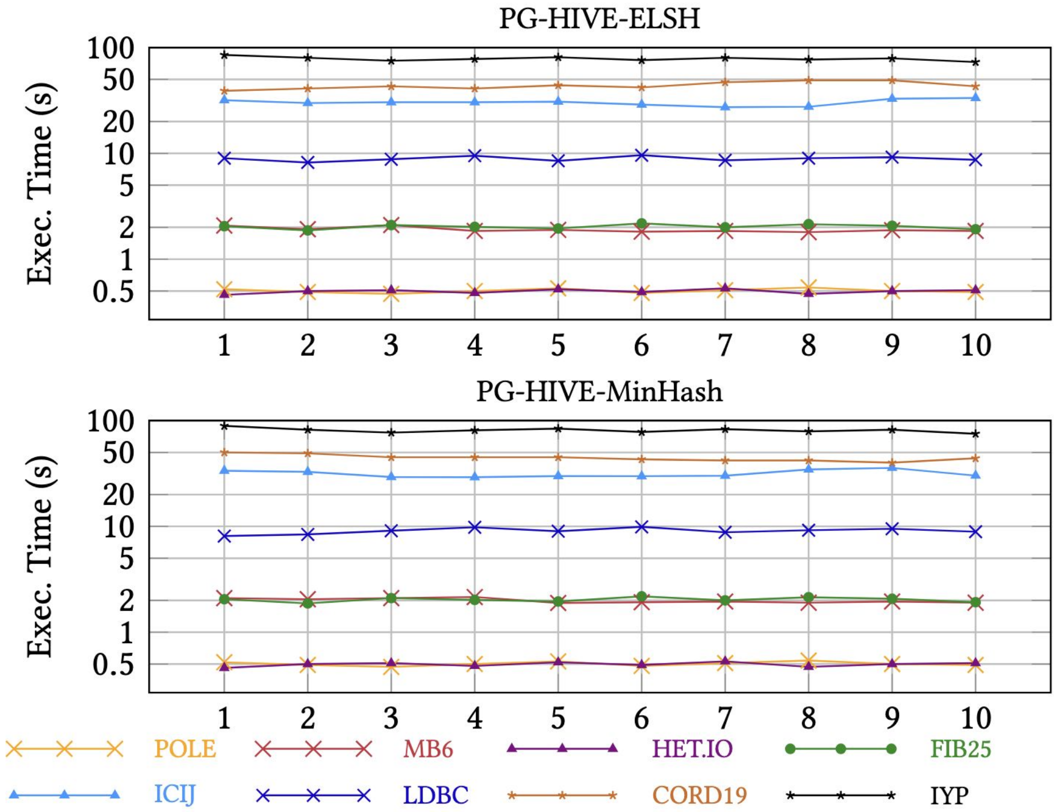
Execution time until type discovery on each dataset across different noise percentages (0% - 40%)

PG-HIVE Evaluation: Adaptive Parameterization



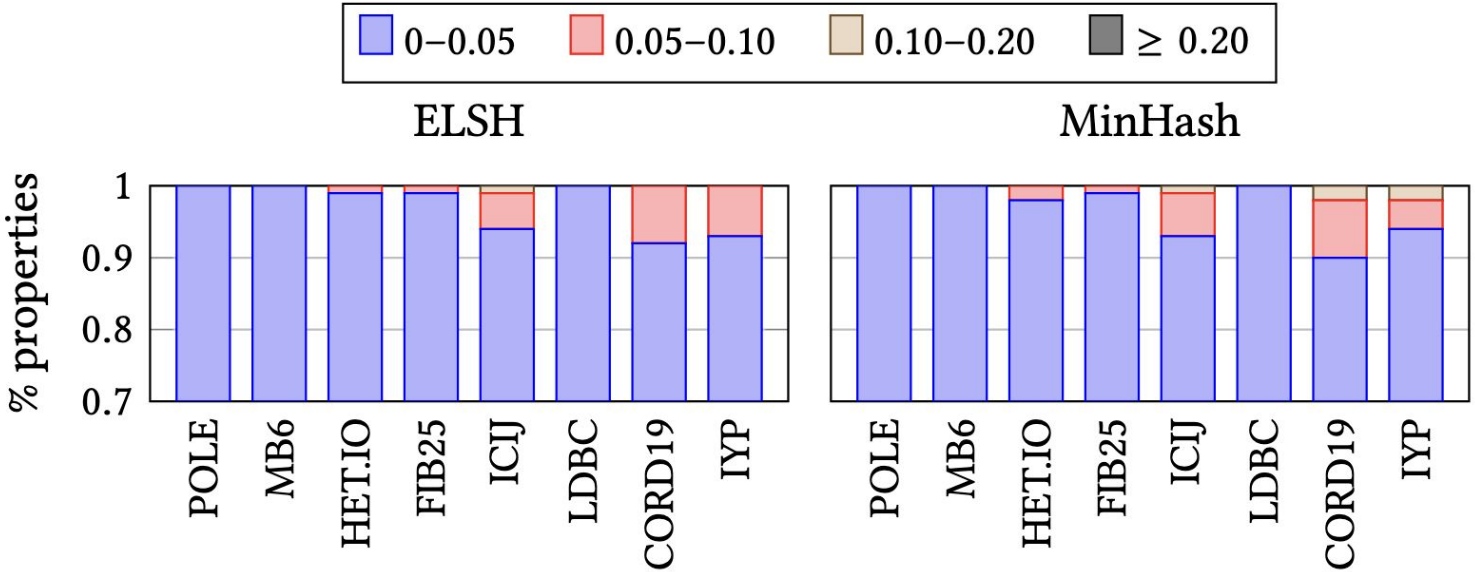
Heatmaps of F1-scores across datasets (100% label availability & 0% noise) for nodes (top) and edges (bottom) with varying T and b; red × (T , b) denotes the adaptive choice for ELSH.

PG-HIVE Evaluation: Incremental Execution



Incremental execution time per iteration. We separate each dataset in 10 equal parts.

PG-HIVE Evaluation: Data Type Inference Sampling Error



Distribution of data type inference errors using sampling, across datasets for ELSH (left) and MinHash (right).

Future Work

Schema Discovery:

- Handle unlabeled and highly sparse graphs
- Use LLMs to align and normalize labels across datasets/languages
- Support provenance, versioning, and schema evolution
- Use association rule mining to discover subtypes

Thank you

PG-HIVE github repo