Faithful Rule Learning and Extraction with Applications

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UNIVERSITY OF OXFORD

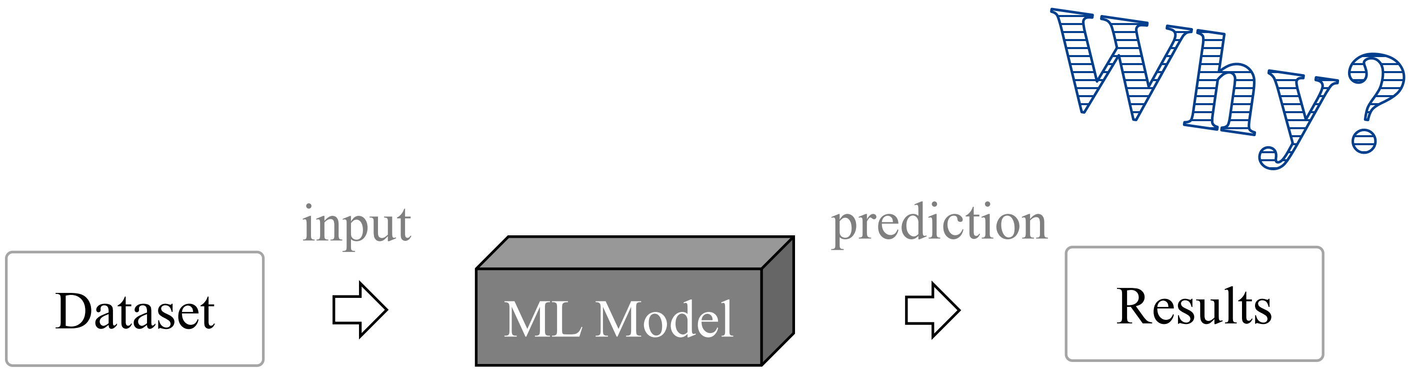
DEPARTMENT OF COMPUTER SCIENCE

Outline

1. Background
2. Motivation
3. Faithful Rule Learning for Knowledge Graph Completion
4. Faithful Rule Learning over Databases
5. Future Directions

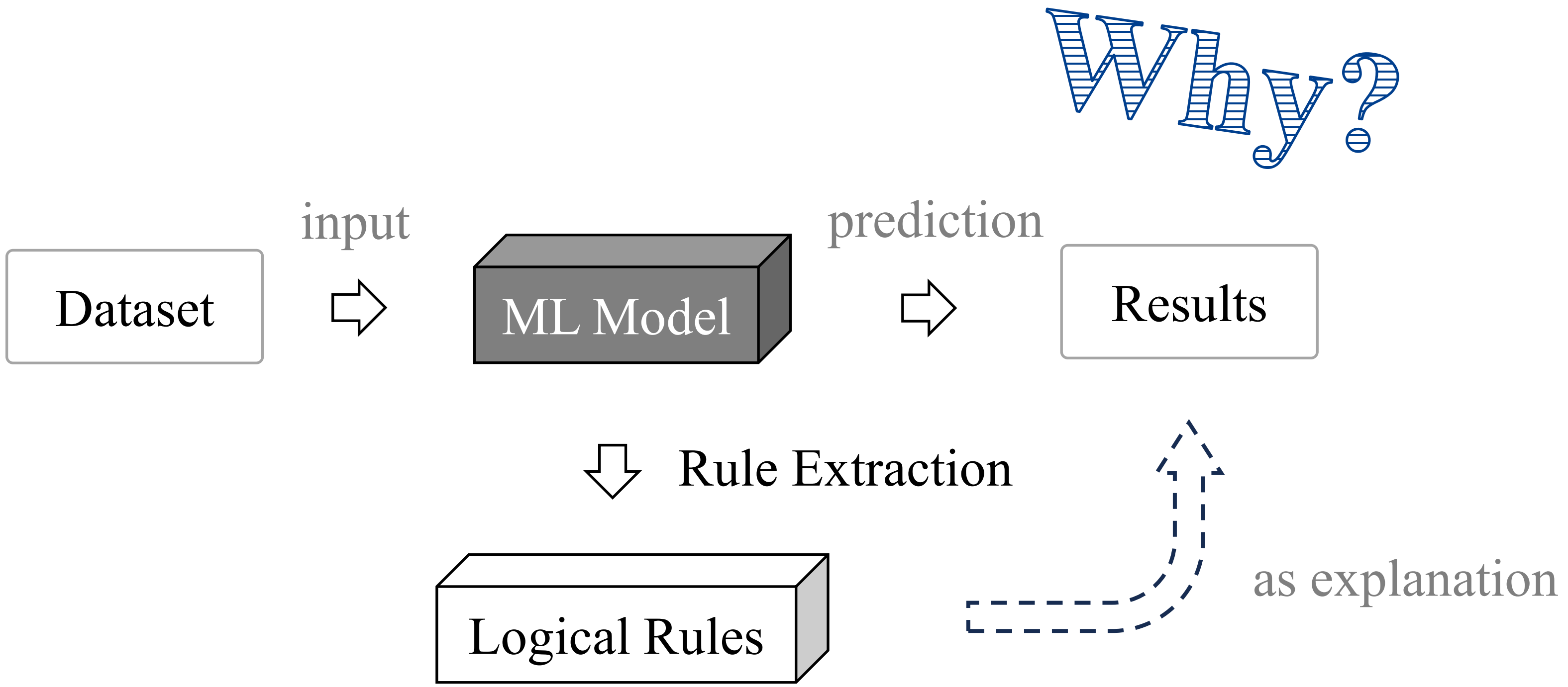
Background

- Machine Learning (ML) models are used in various domains, but they lack explainability



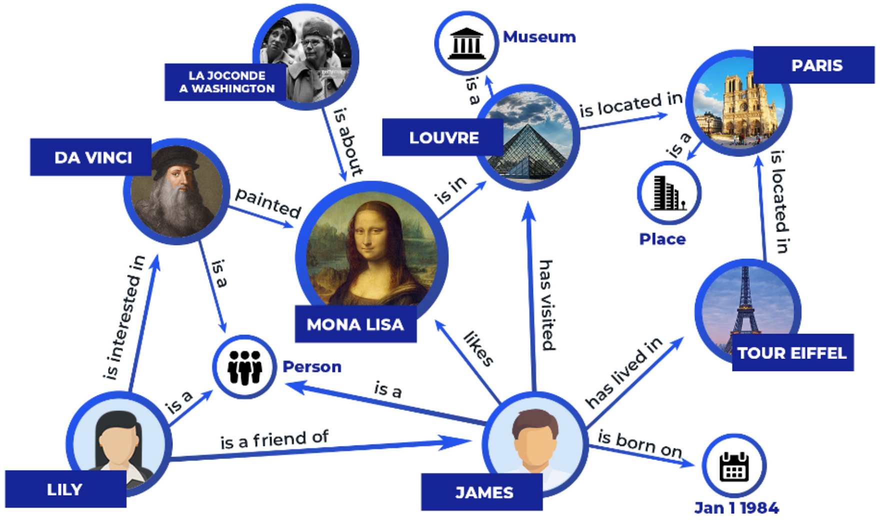
Background

- Machine Learning (ML) models are used in various domains, but they lack explainability
- Rule extraction improves the explainability of ML models



Background

- Machine Learning (ML) models are used in various domains, but they lack explainability
- Rule extraction improves the explainability of ML models
- We focus on ML models for graph data, e.g., knowledge graphs (KGs)



https://deeppavlov.ai/research/tpost/bn15u1y4v1-improving-knowledge-graph-completion-wit

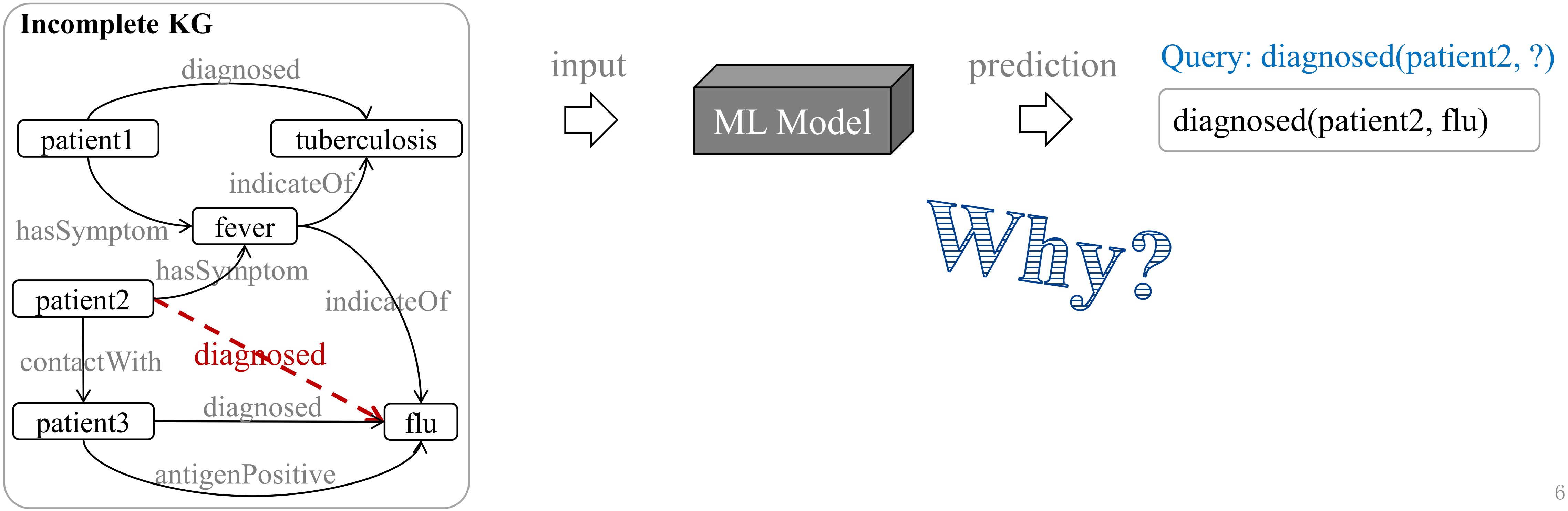
An example KG

Knowledge graph: a structured data representation

- each node: a real-world entity
- each directed edge: a relationship between entities, expressed as a fact *relation(subject, object)*, e.g., *painted(DA_VINCI, MONA_LISA)*
- a KG is a set of facts

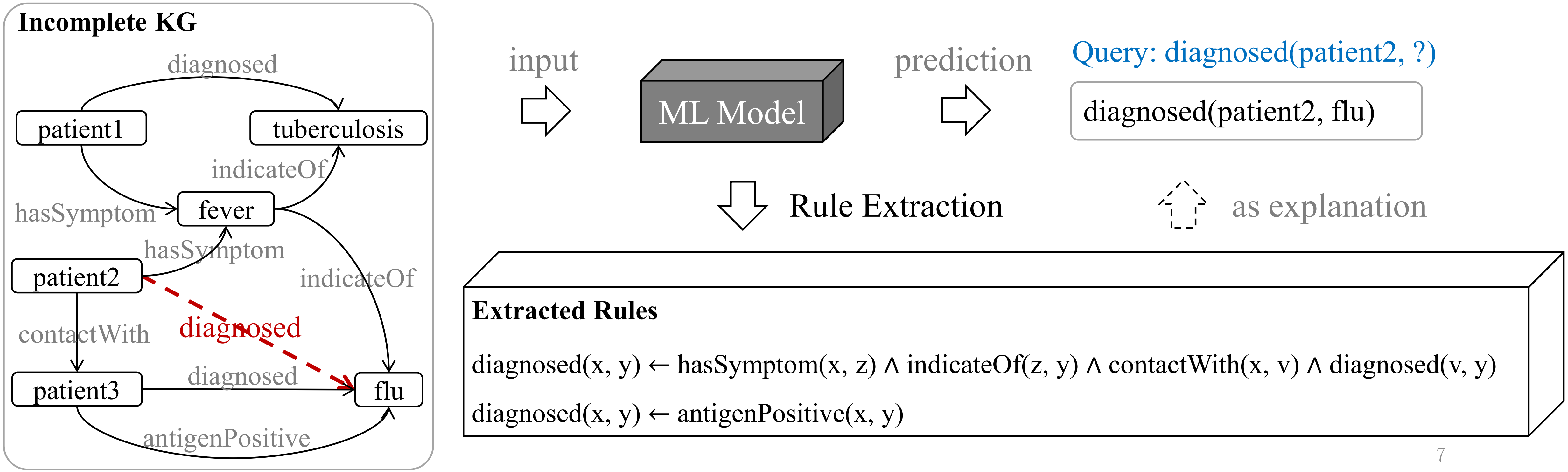
Background

- An example task: Knowledge Graph Completion (KGC)
  - real-world KGs are usually **incomplete**
  - KGC: to infer missing facts based on existing facts in the KG
  - given a query ***relation(subject, ?)***, to predict the object that matches ***?***



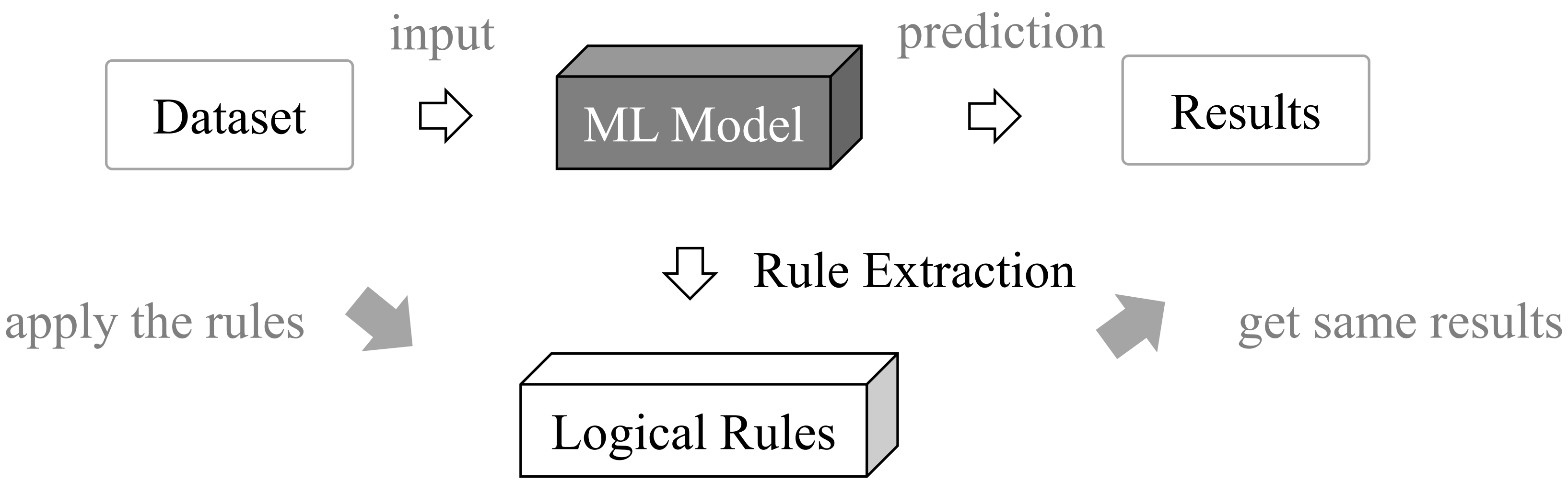
Background

- An example task: Knowledge Graph Completion (KGC)
- Rule extraction improves the explainability of ML models
  - by providing human-readable rules as explanation



Motivation

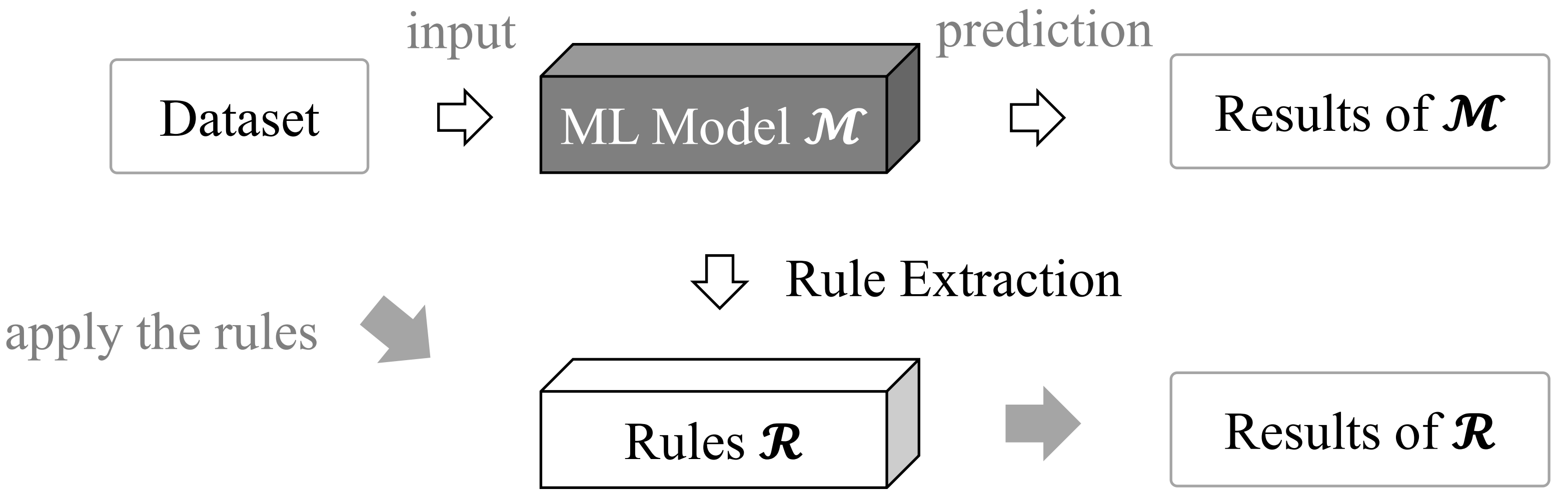
- Requirement: The extracted rules **must be “equivalent”** to the ML model
  - produce the same result on the same input
- Why is this important? — Otherwise, we cannot trust the rules to be explanation



*apply rules to a dataset: the fact (as a grounded rule head) is derived, if the rule body is grounded on the dataset

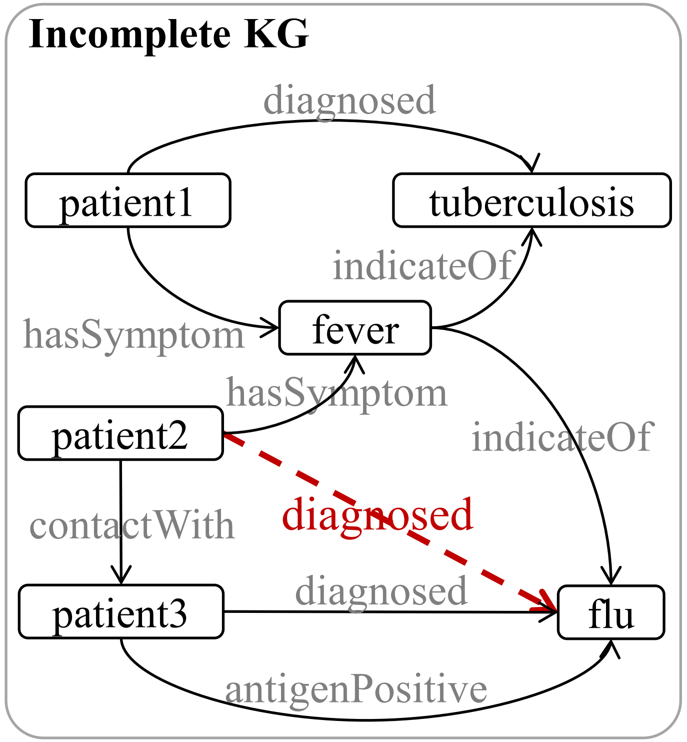
Motivation

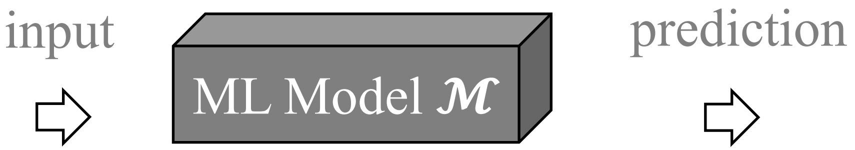
- Requirement: The extracted rules **must be "equivalent"** to the ML model
  - produce the same result on the same input
- Formally, let $\mathcal{M}$ and $\mathcal{R}$ denote the model and the set of extracted rules
  - $\mathcal{R}$ is sound for $\mathcal{M}$ if for any input dataset, {result of $\mathcal{R}$} $\subseteq$ {result of $\mathcal{M}$}
  - $\mathcal{R}$ is complete for $\mathcal{M}$ if for any input dataset, {result of $\mathcal{R}$} $\supseteq$ {result of $\mathcal{M}$}
  - $\mathcal{R}$ is faithful to $\mathcal{M}$ if both sound and complete



Motivation

- Requirement: The extracted rules **must be "equivalent"** to the ML model
  - produce the same result on the same input
- Issues with unsound or incomplete rules





Query: *diagnosed(patient2, ?)*

diagnosed(patient2, flu)

faithful rules $\mathcal{R}_1$

diagnosed(x, y) ← hasSymptom(x, z) ∧ indicateOf(z, y) ∧ contactWith(x, v) ∧ diagnosed(v, y)
diagnosed(x, y) ← antigenPositive(x, y)

Unsound rules $\mathcal{R}_2$

diagnosed(x, y) ← hasSymptom(x, z) ∧ indicateOf(z, y)

Wrong results

diagnosed(patient_2, flu)
diagnosed(patient_2, tuberculosis)

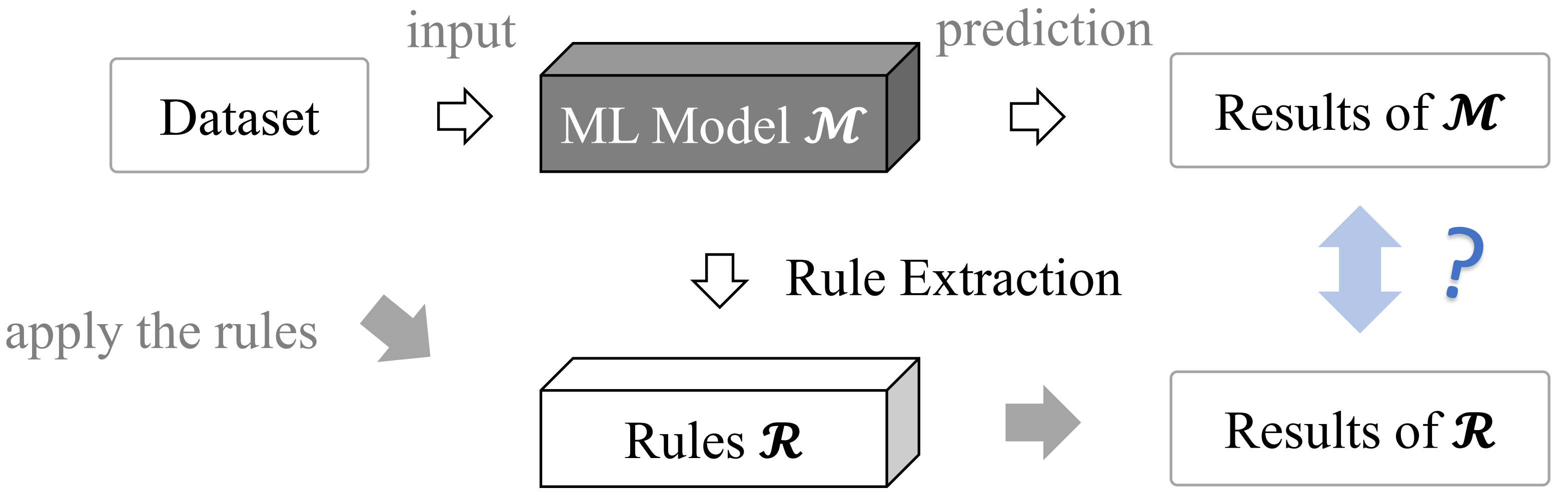
Incomplete rules $\mathcal{R}_3$

diagnosed(x, y) ← antigenPositive(x, y)

Missing results

Motivation

- Requirement: The extracted rules **must be "equivalent"** to the ML model
  - produce the same result on the same input
- Issues with unsound or incomplete rules
- Prior works[1—4] on rule extraction have **NO** formal guarantee of faithfulness

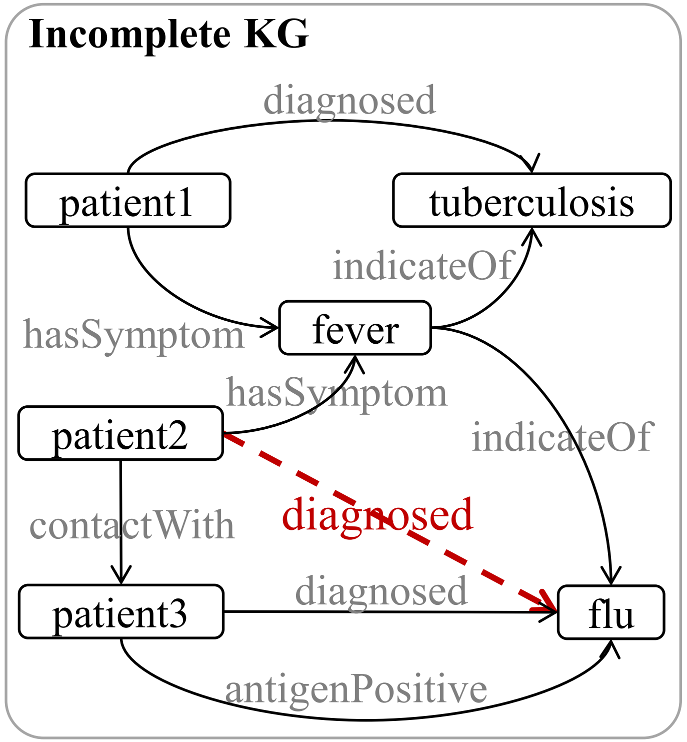


[1] Yang et al. Differentiable Learning of Logical Rules for Knowledge Base Reasoning. NeurIPS 2017
[2] Sadeghian et al. DRUM: End-To-End Differentiable Rule Mining On Knowledge Graphs. NeurIPS 2019
[3] Xiong et al. TILP: Differentiable Learning of Temporal Logical Rules on Knowledge Graphs. ICLR 2023
[4] Han et al. Logical Entity Representation in Knowledge-Graphs for Differentiable Rule Learning. ICLR 2023

Faithful Rule Learning for Knowledge Graph Completion

- **Question 1**: Do existing approaches hold faithfulness?
- We consider DRUM[2], a representative rule learning approach for KGC
  - model: predict "missing" facts based on existing facts
  - rule extraction algorithm: obtain a set of chain-like rules

    e.g., *diagnosed(x, y)* ← *contactWith(x, z)* ∧ *diagnosed(z, y)*



Faithful Rule Learning for Knowledge Graph Completion

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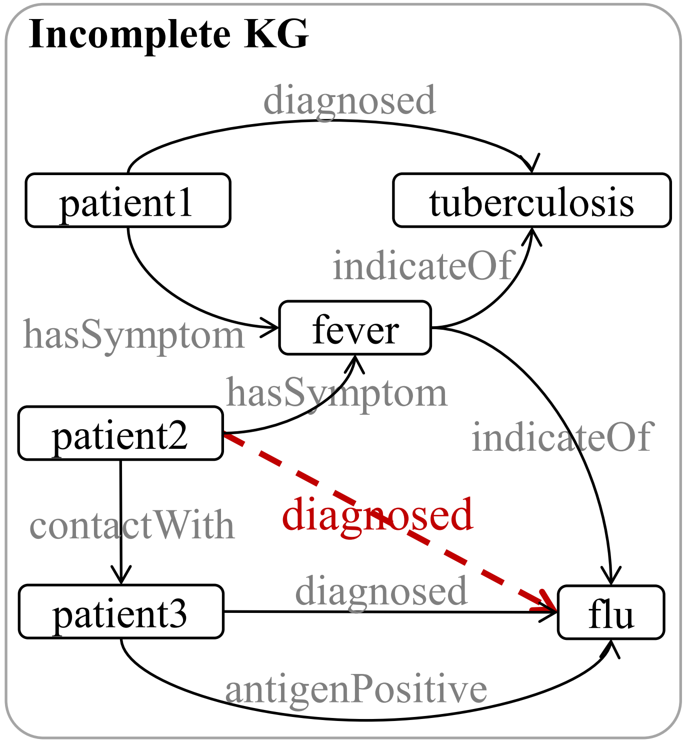
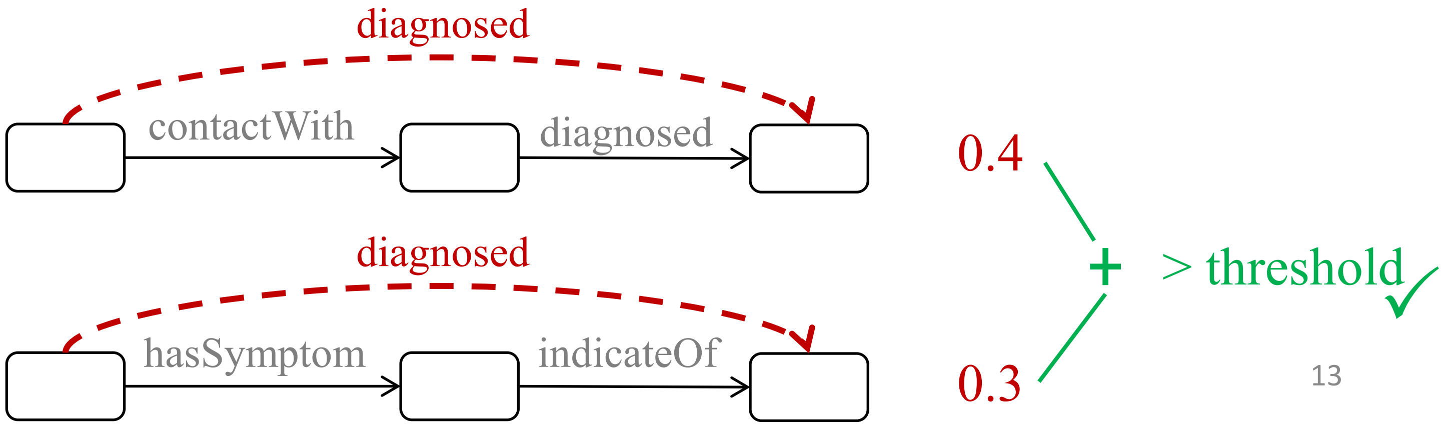


How does the model work?

- for each relation, e.g., *diagnosed*
- it learns a weight for each “chain pattern”
- given a query *diagnosed(s, ?)*, it **sums up** all paths from *s* to the target node



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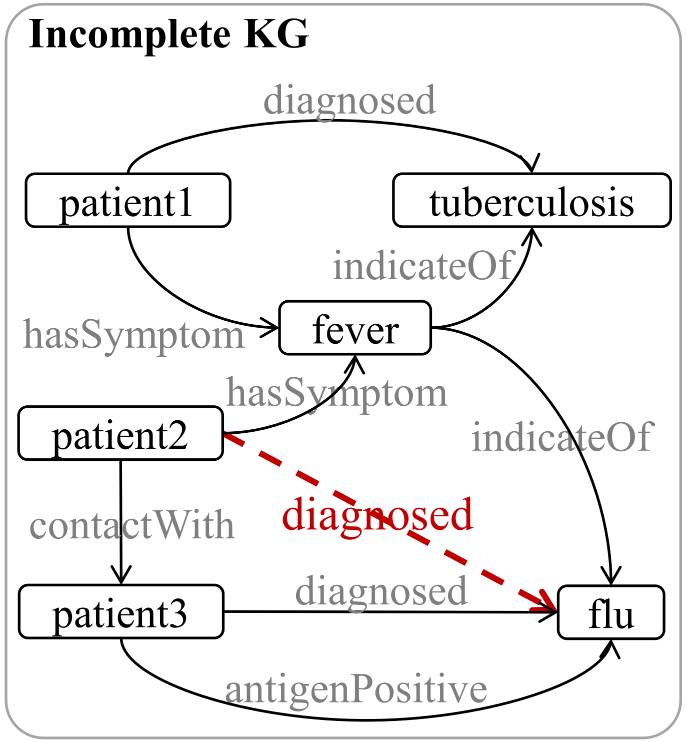
    e.g., *diagnosed(x, y)* ← *contactWith(x, z)* ∧ *diagnosed(z, y)*
  - **a single chain-like rule body cannot capture the "sum up" behavior**

NO



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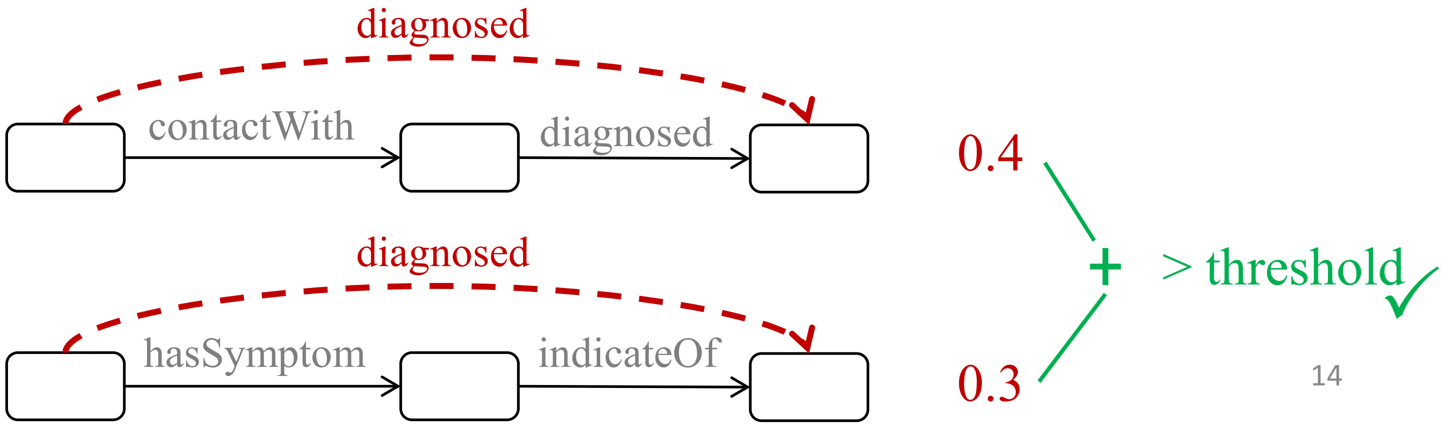
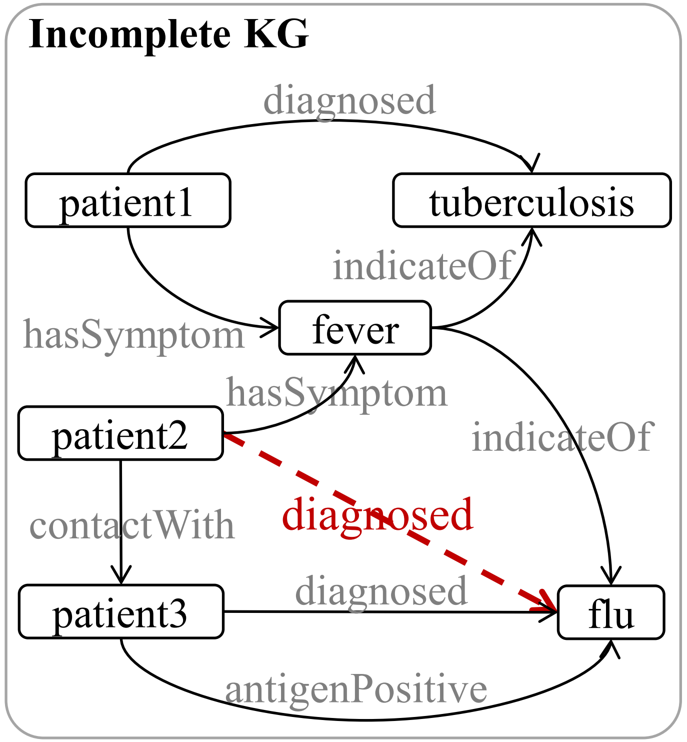


- **Question 2**: How to solve the problem and ensure faithfulness?
- We provide 2 solutions:
  1. a new rule extraction algorithm to support the "sum up" behavior
     - e.g., *diagnosed(x, y)* ← *contactWith(x, z) ∧ diagnosed(z, y)* ∧ *hasSymptom(x, v) ∧ indicateOf(v, y)*
     - by analyzing the underlying mechanism of the model, and proving the faithfulness



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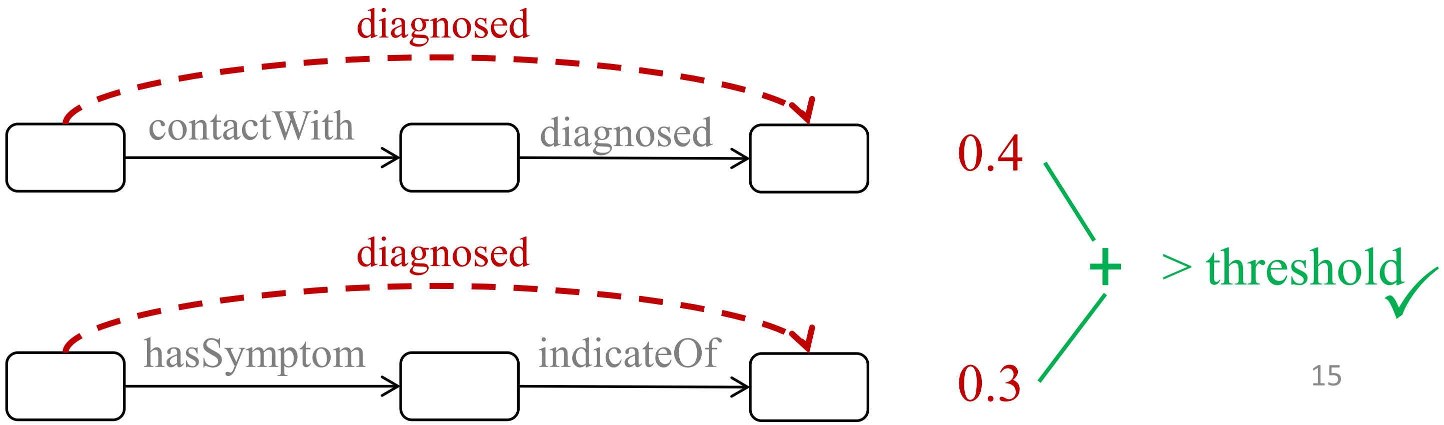

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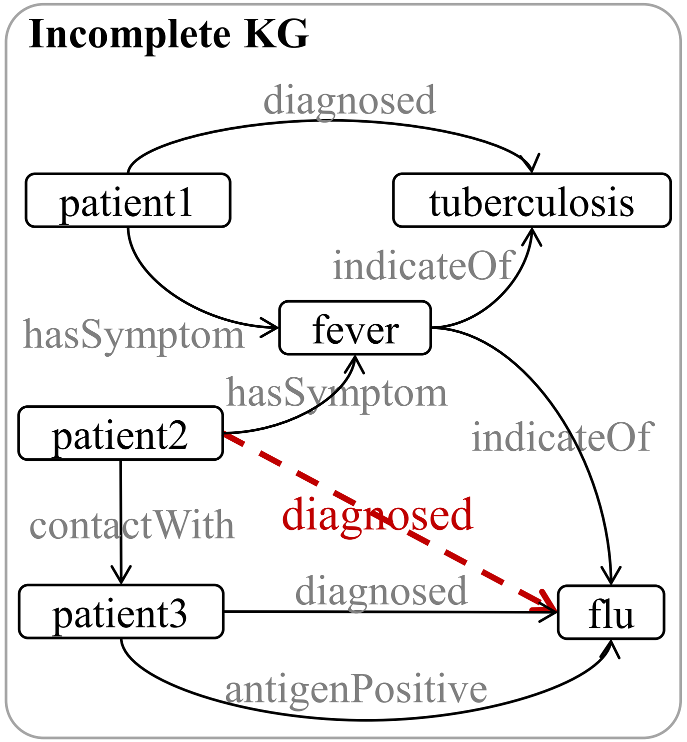
- **Question 2**: How to solve the problem and ensure faithfulness?
- We provide 2 solutions:
  1. a new rule extraction algorithm to support the "sum up" behavior
  2. a new (simplified) model with max aggregation for all paths
     - it only considers one path with max weight—can be captured by chain-like rules



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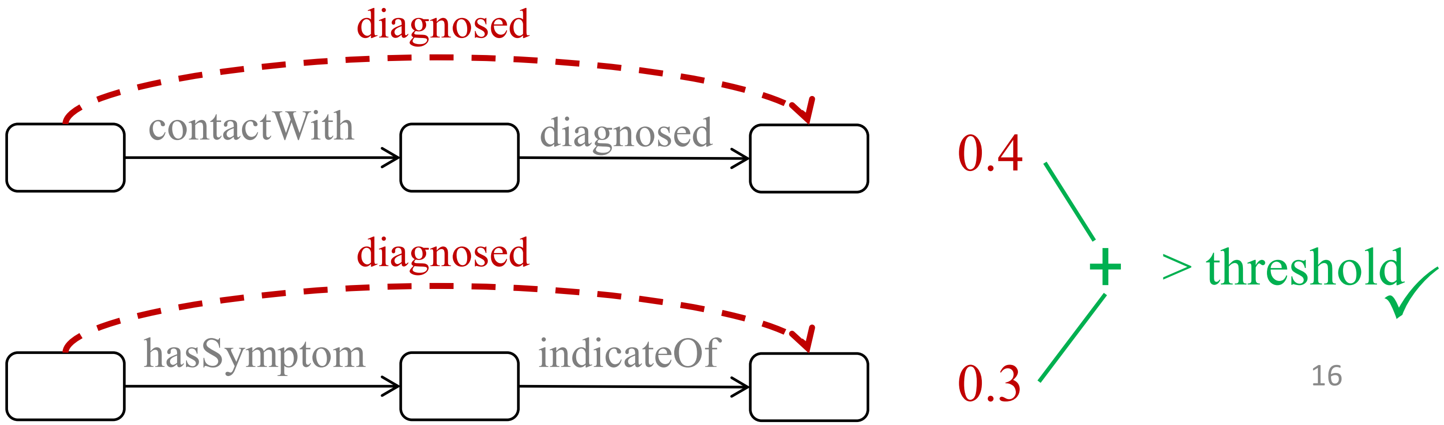

Faithful Rule Learning for Knowledge Graph Completion

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- **Question 2**: How to solve the problem and ensure faithfulness?
- We provide 2 solutions[5]:
  1. a new rule extraction algorithm to support the "sum up" behavior
  2. a new (simplified) model with max aggregation for all paths
     - it only considers one path with max weight—can be captured by chain-like rules

- **Takeaways**
  - faithful rule extraction has high computational complexity
  - the simplified model: trade-off between expressive power vs. ease of rule extraction
  - similar conclusions exist for other rule learning models, *e.g.,* NeuralILP[1,6]

[1] Yang et al. Differentiable Learning of Logical Rules for Knowledge Base Reasoning. NeurIPS 2017

[5] Wang et al. Faithful Rule Extraction for Differentiable Rule Learning Models. ICLR 2024

[6] Tena Cucala et al. Faithful Approaches to Rule Learning. KR 2022

Faithful Rule Learning over Databases

- **Question 3**: Can we extend to **more complex** graph data?
  - from knowledge graphs to databases (hypergraphs)
  - each fact contains multiple entities

Name	City	Country
Alice	*Boston*	*US*
…	…	…

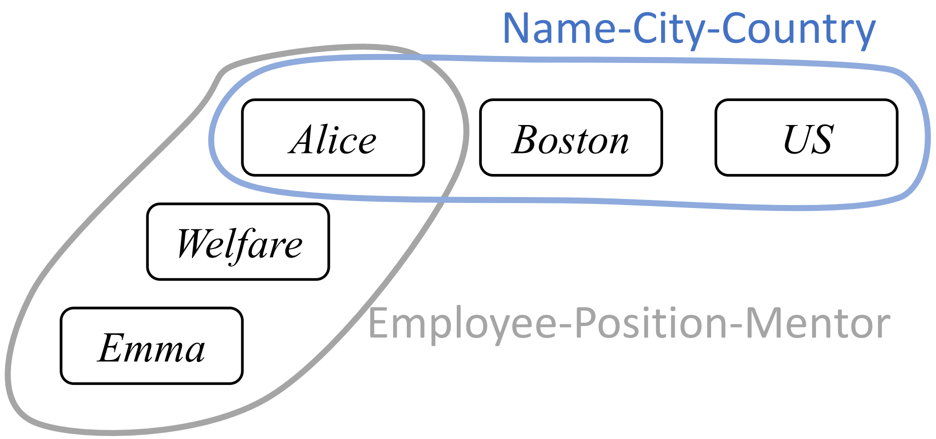
Employee	Position	Mentor
Emma	*Welfare*	*Alice*
…	…	…

Name	Org.	Country
Emma	*MIT*	*US*
…	…	…

An example database instance

Relational databases:

- each value in a row: a node (entity)
- each row (fact): a hyperedge containing multiple nodes



- **Task**: Tabular data cell completion
  - real-world tables are usually **incomplete** with missing values
  - data cell completion: to infer the missing value based on existing facts
  - given a query ***relation(a, b, ?, c, …)***, to predict the entity that matches ***?***

Name	City	Country
Alice	*Boston*	*US*
…	…	…
Emma	*Boston*	?

Employee	Position	Mentor
Emma	*Welfare*	*Alice*
…	…	…

Name	Org.	Country
Emma	*MIT*	*US*
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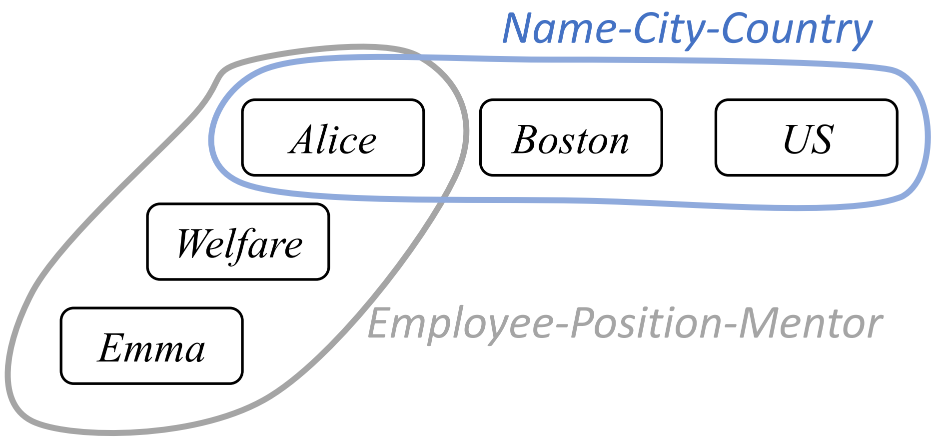


Faithful Rule Learning over Databases

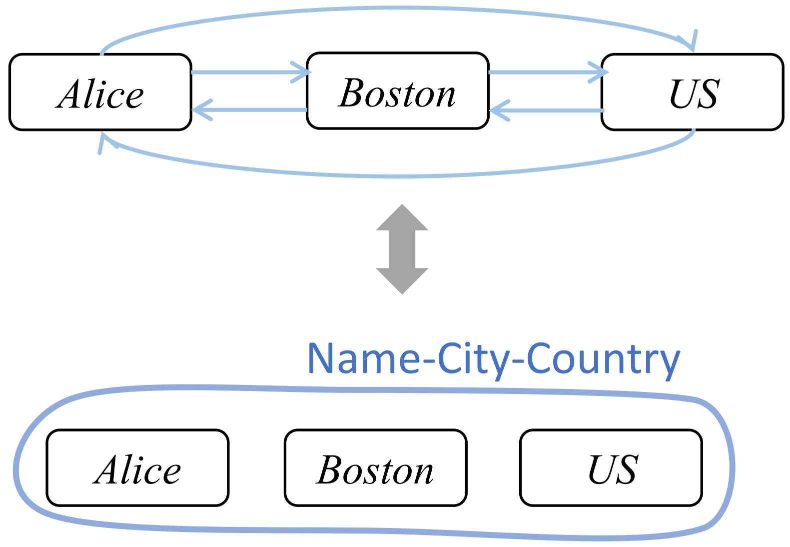
- **Task**: Tabular data cell completion
  - given a query *relation(a, b, ?, c, …)*, to predict the entity that matches *?*
- We consider binary relationships between entities

Name	City	Country
Alice	*Boston*	*US*
…	…	…
Emma	*Boston*	**?**

Employee	Position	Mentor
Emma	*Welfare*	*Alice*
…	…	…

Name	Org.	Country
Emma	*MIT*	*US*
…	…	…

An example database instance



Faithful Rule Learning over Databases

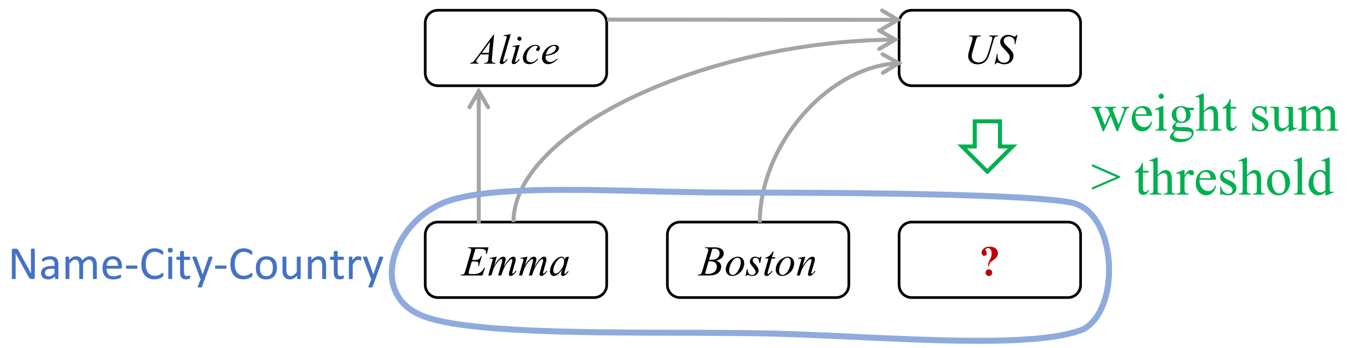
- **Task**: Tabular data cell completion
  - given a query *relation(a, b, ?, c, …)*, to predict the entity that matches *?*
- We consider binary relationships between entities
- We propose a **model**: predict missing value by aggregating paths from existing entities

Name	City	Country
Alice	*Boston*	*US*
…	…	…
Emma	*Boston*	?

Employee	Position	Mentor
Emma	*Welfare*	*Alice*
…	…	…

Name	Org.	Country
Emma	*MIT*	*US*
…	…	…

An example database instance



- aggregate paths from existing entities in the query
- weight of each path: learned by the model

Faithful Rule Learning over Databases

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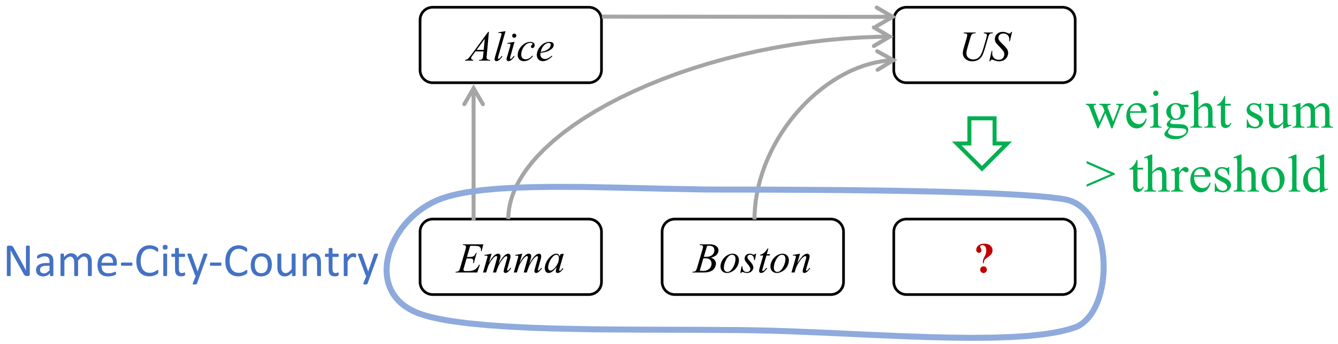
- **Task**: Tabular data cell completion
  - given a query *relation(a, b, ?, c, …)*, to predict the entity that matches *?*
- We propose a **model**: predict missing value by aggregating paths from existing entities
- We propose **faithful rule extraction** algorithms for the model

- **Evaluation results**
  - SOTA performance for the task
  - better explainability

  (compared to hypergraph neural networks)



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- weight of each path: learned by the model

Future Directions

- **We aim to**: enhance the explainability of ML models by **faithful rule extraction**

- **Future Directions**
  1. Diversified applications
     - *e.g.,* entity resolution by answer set programming[7], question answering
  2. Features of the extracted rule set
     - *e.g.,* rule multiplicity
  3. Practical & Reasonable benchmark generation
     - instead of using random splits for evaluation

[7] Xiang et al. ASPEN: ASP-Based System for Collective Entity Resolution. KR 2024

Thank You!

Q & A

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