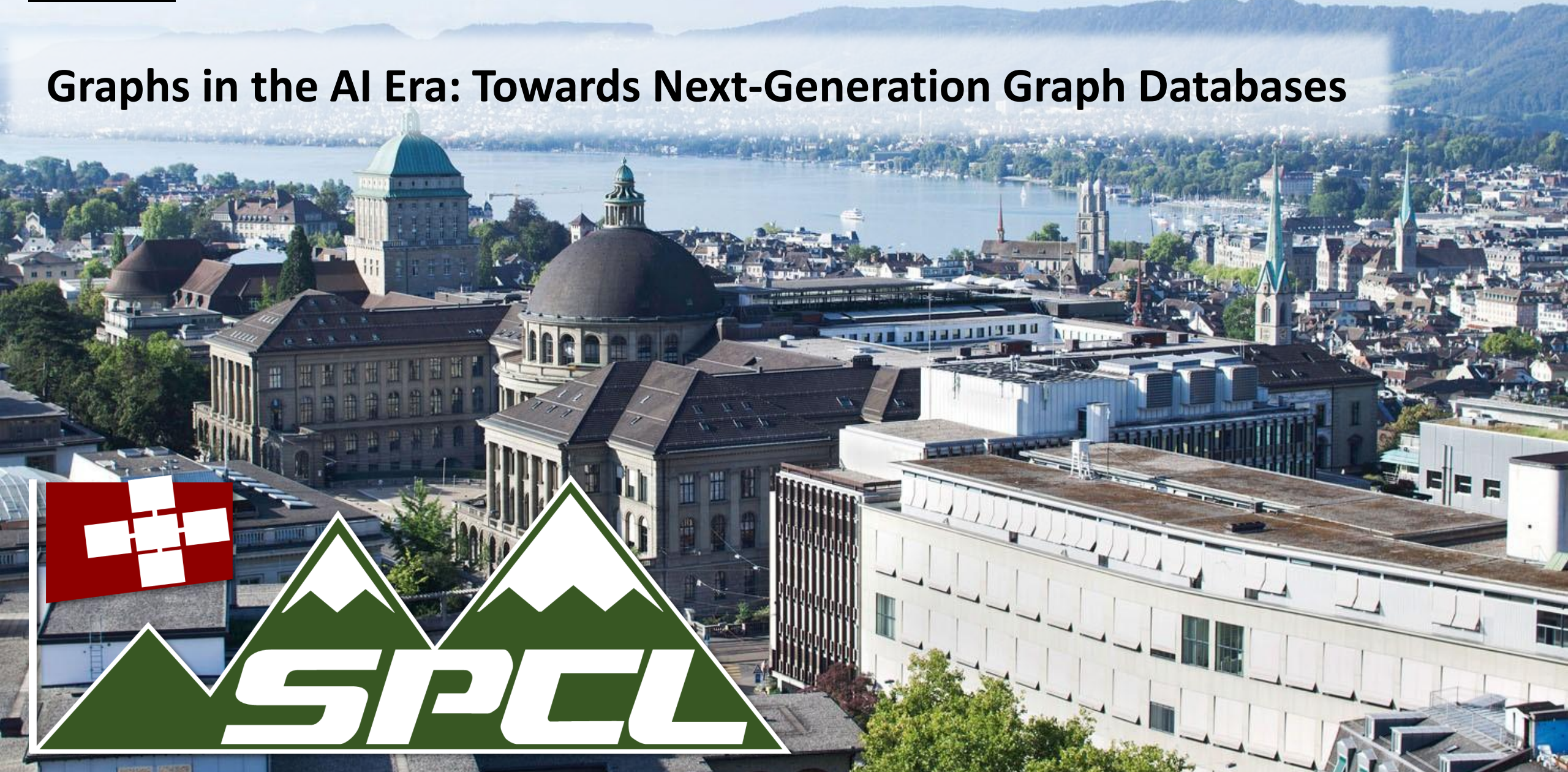


MACIEJ BESTA

WITH TORSTEN HOEFLER & MANY MEMBERS OF SPCL

# Graphs in the AI Era: Towards Next-Generation Graph Databases



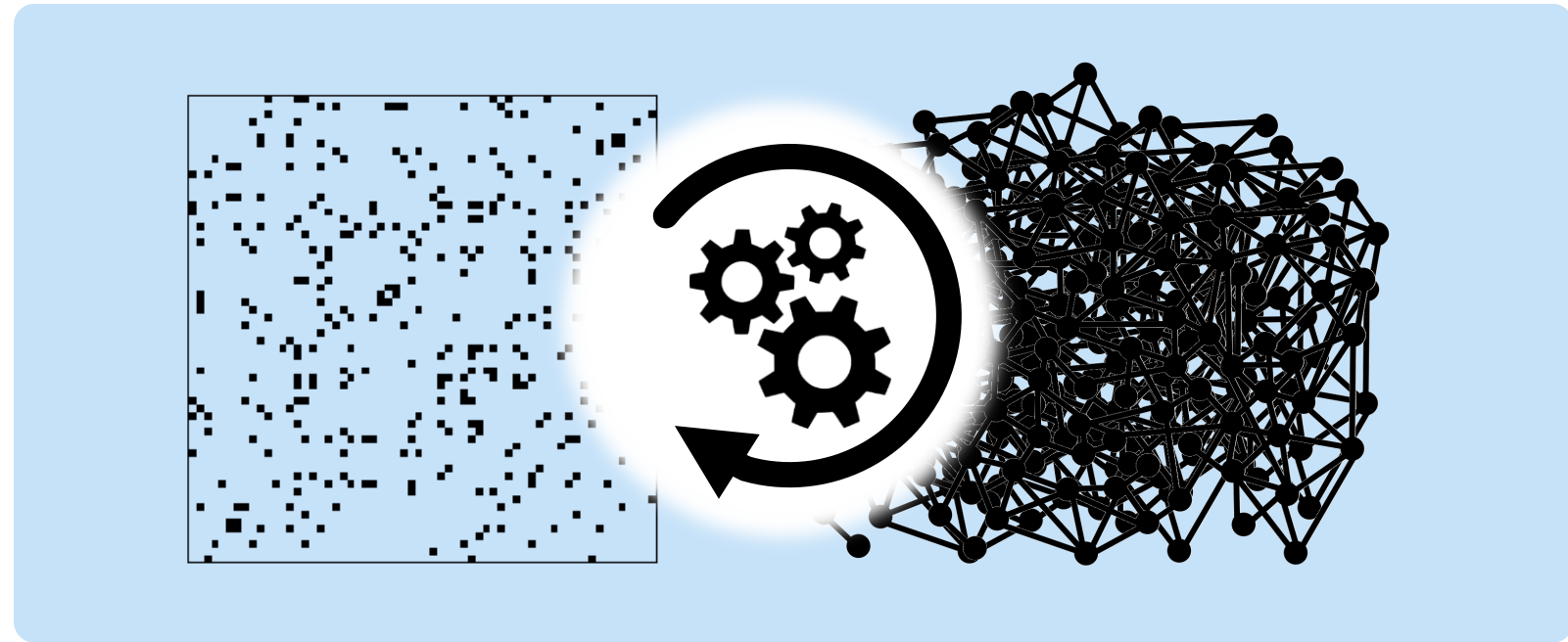
# My Research Overview

## My Research Overview

# Sparse & irregular computing

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## Sparse & irregular computing



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## Sparse & irregular computing

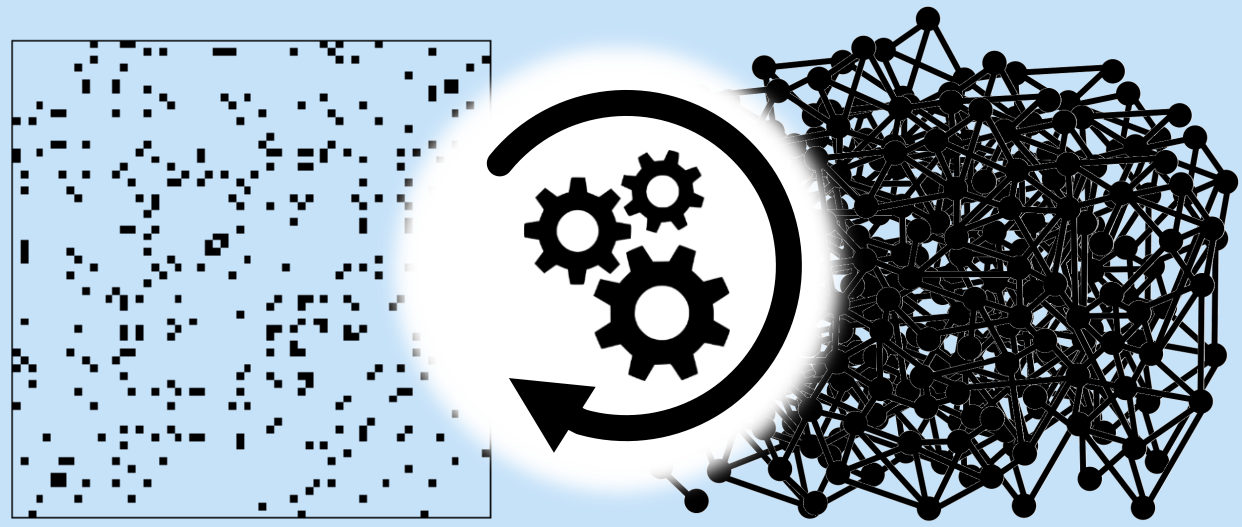
...

LLM ecosystems & agent infrastructures

Generative AI training & inference

Representation Learning & Graph Neural Networks

Graph databases



Graph compression & summarization

Graph pattern matching

[Parallel] graph algorithms

Streaming, dynamic, temporal graphs



# My Research Overview

## Sparse & irregular computing

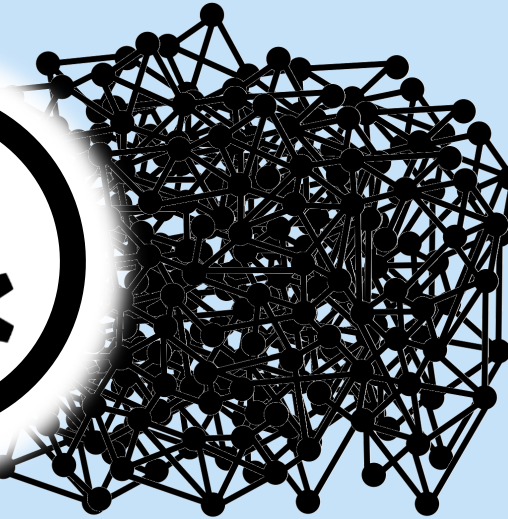
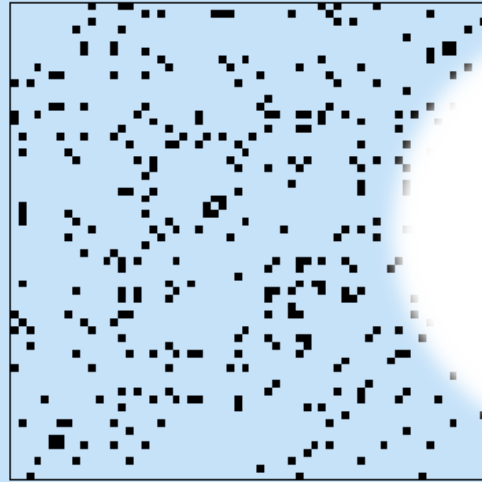
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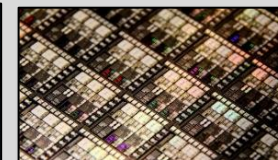
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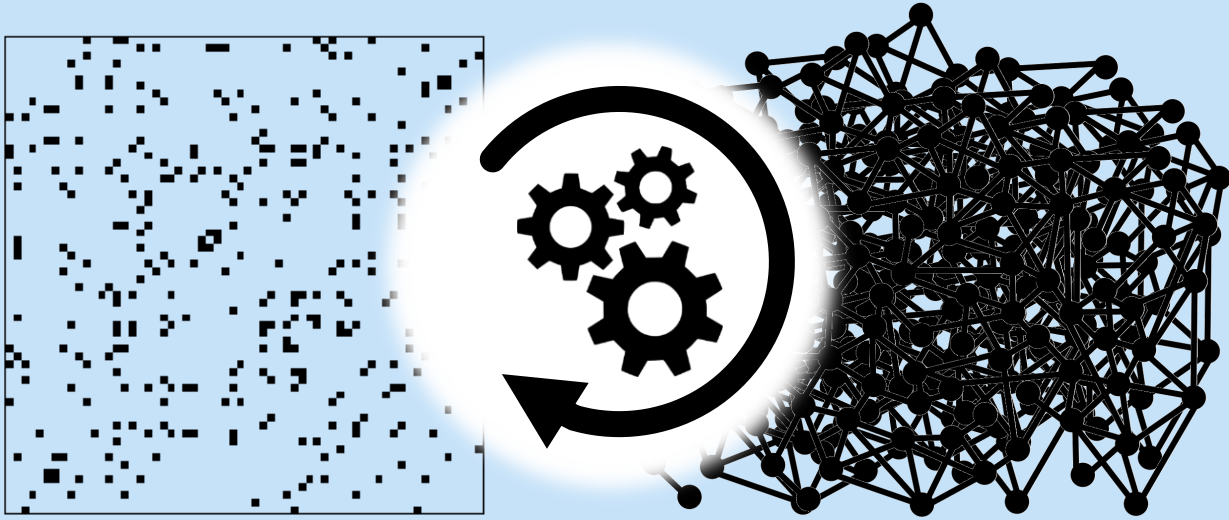
Massively parallel settings



# Sparse & irregular computing

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**Fast**

**Massively parallel settings**

# Sparse & irregular computing

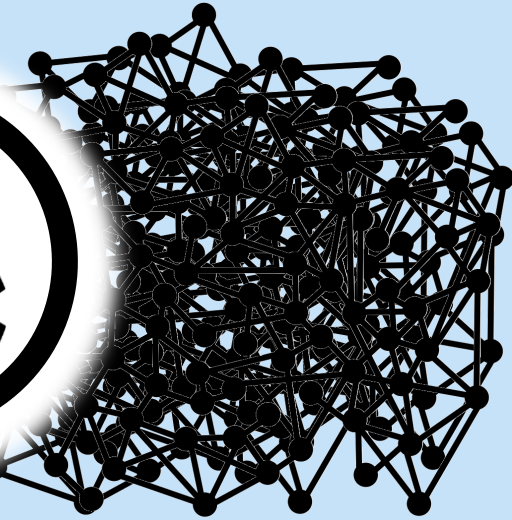
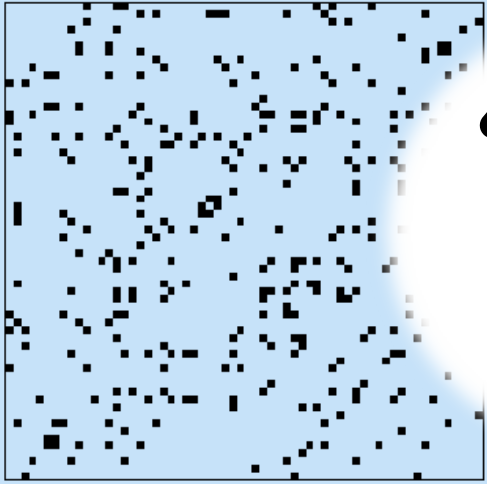
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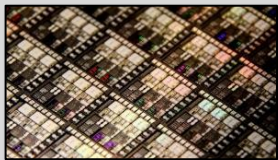


Effective



Fast

Massively parallel settings



# My Research Overview

## Sparse & irregular computing

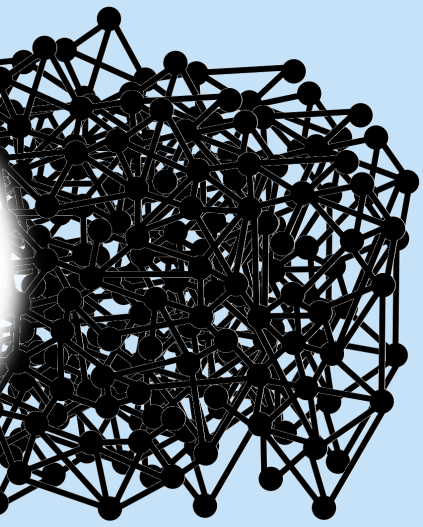
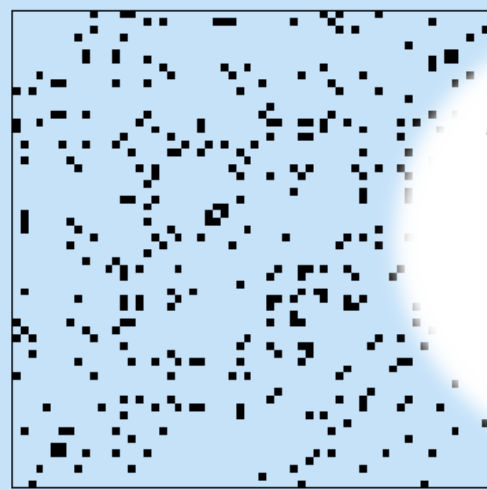
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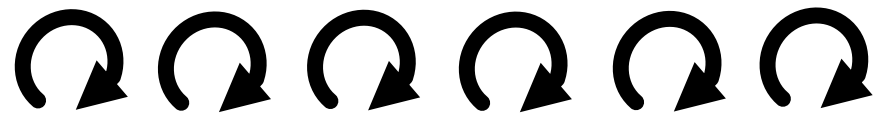
Graph pattern matching

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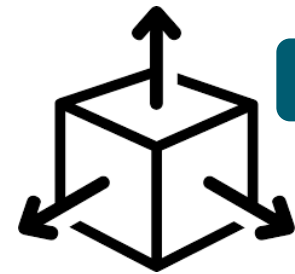
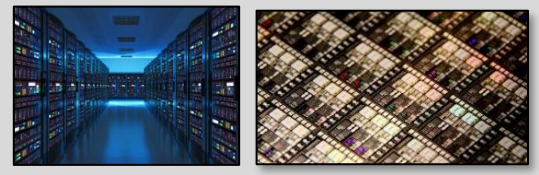


Effective



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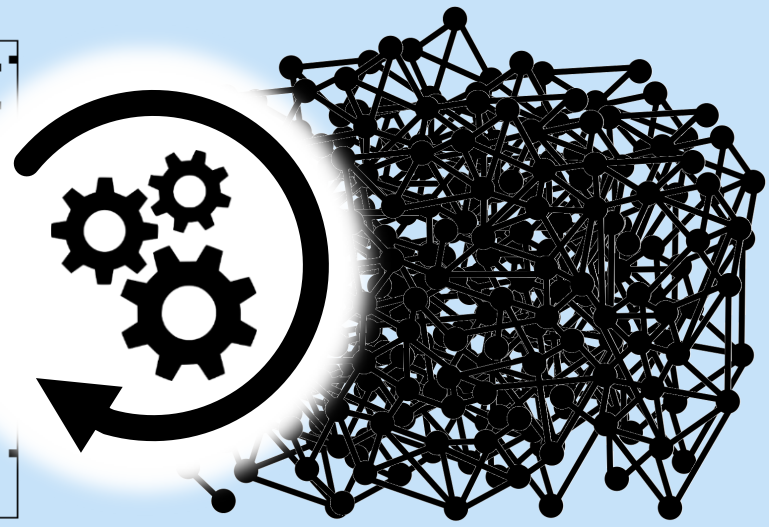
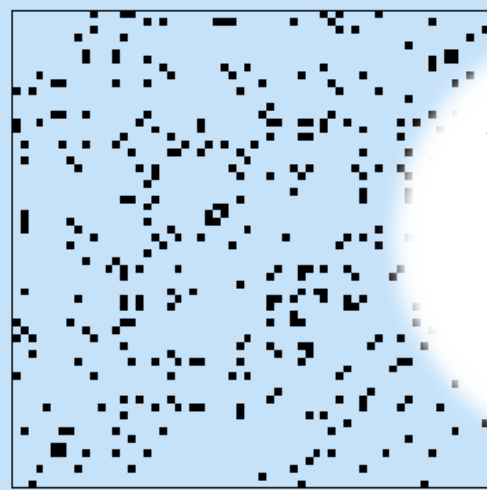
Scalable

# My Research Overview

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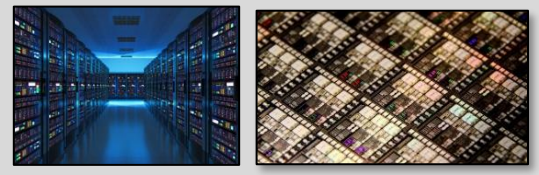
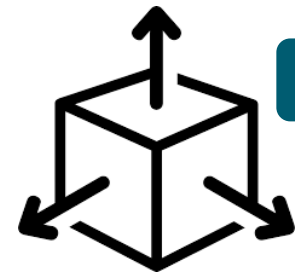


Effective



Fast

Massively parallel settings

Scalable

Simple



# My Research Overview

## Sparse & irregular computing

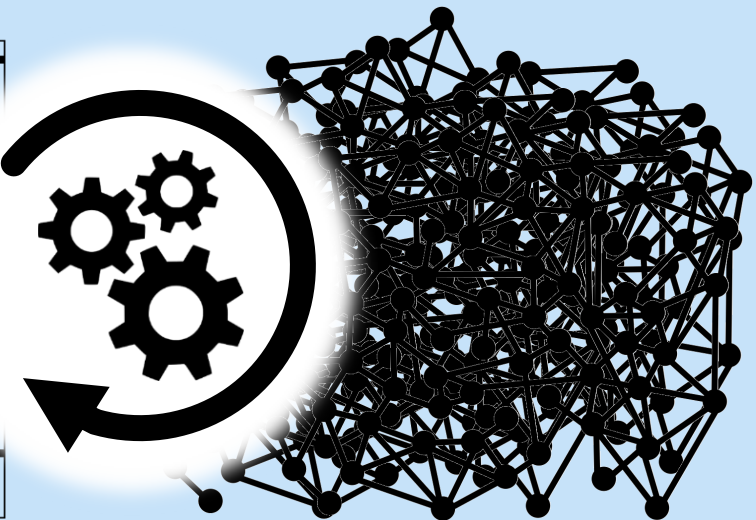
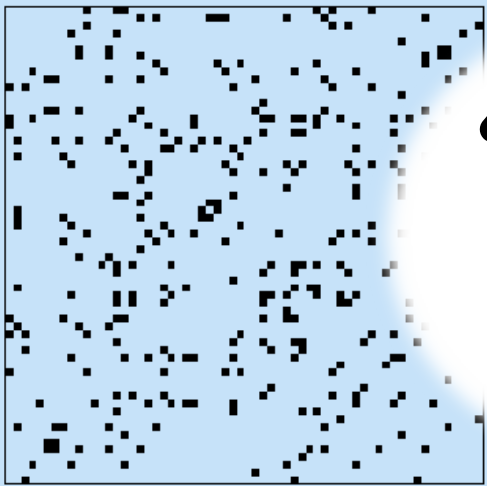
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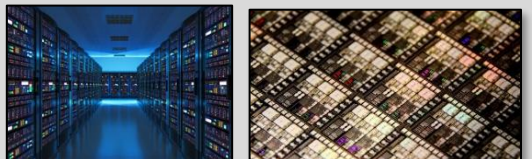
Streaming, dynamic, temporal graphs



Effective

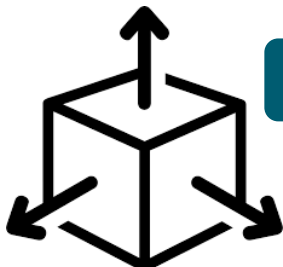


Massively parallel settings



Fast

Getting to foundations



Scalable

Simple



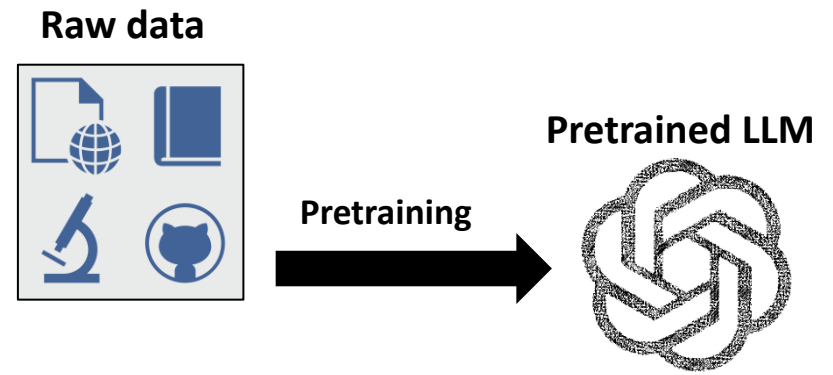
# Overview of the LLM Processing Pipeline

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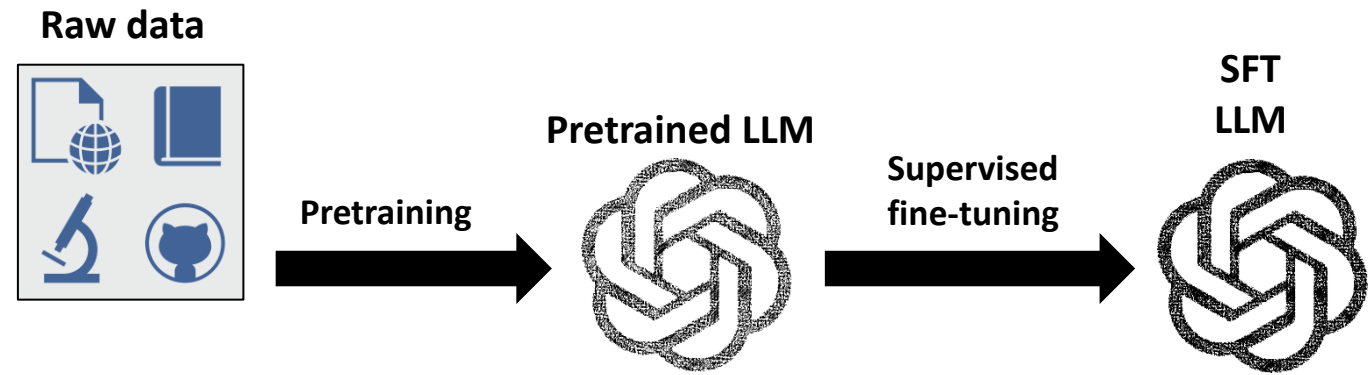
## Raw data



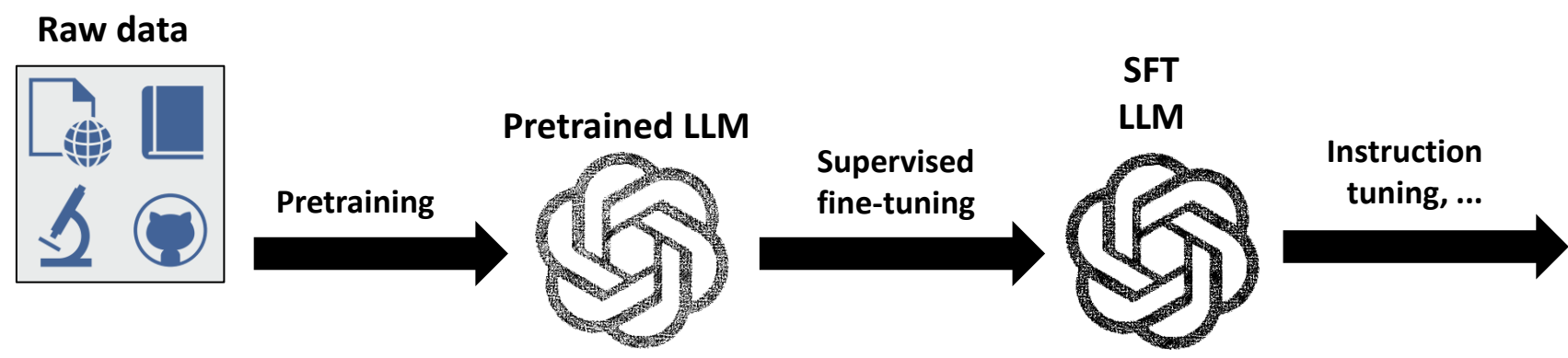
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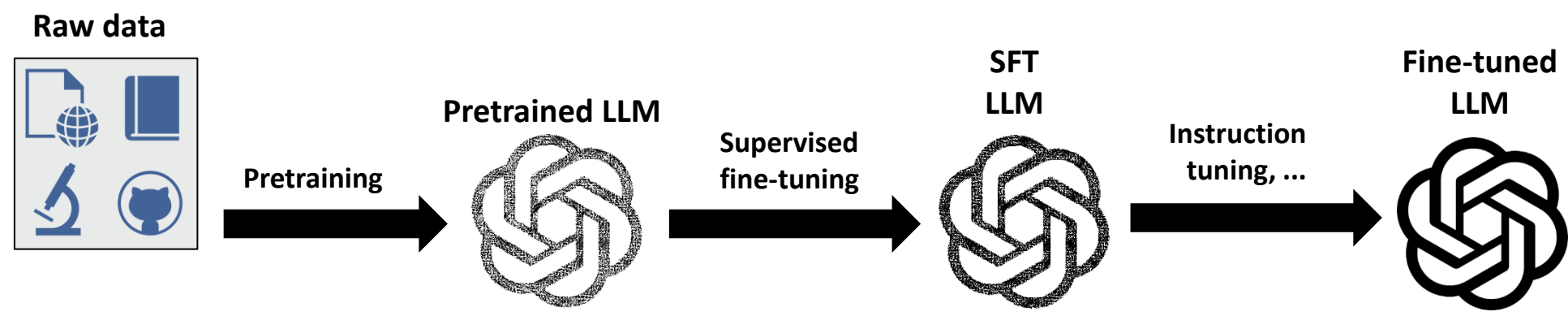
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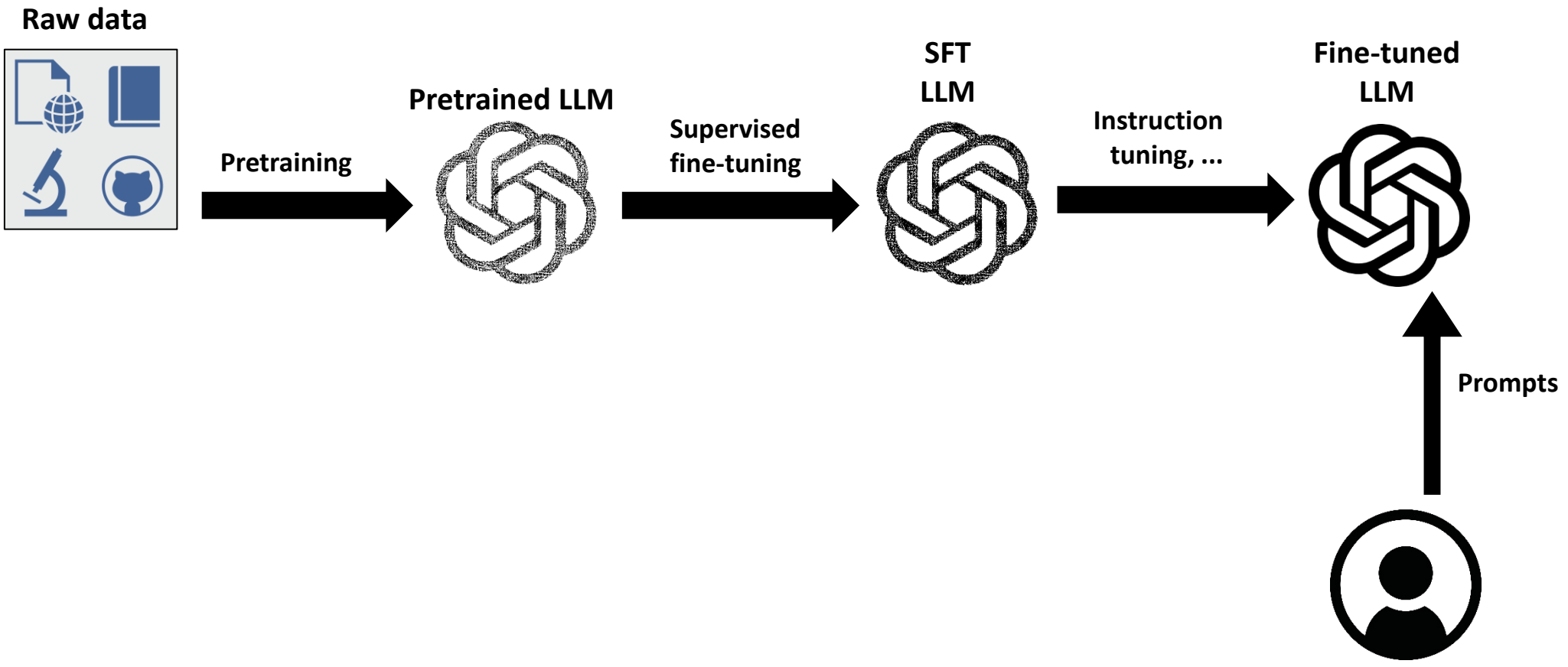
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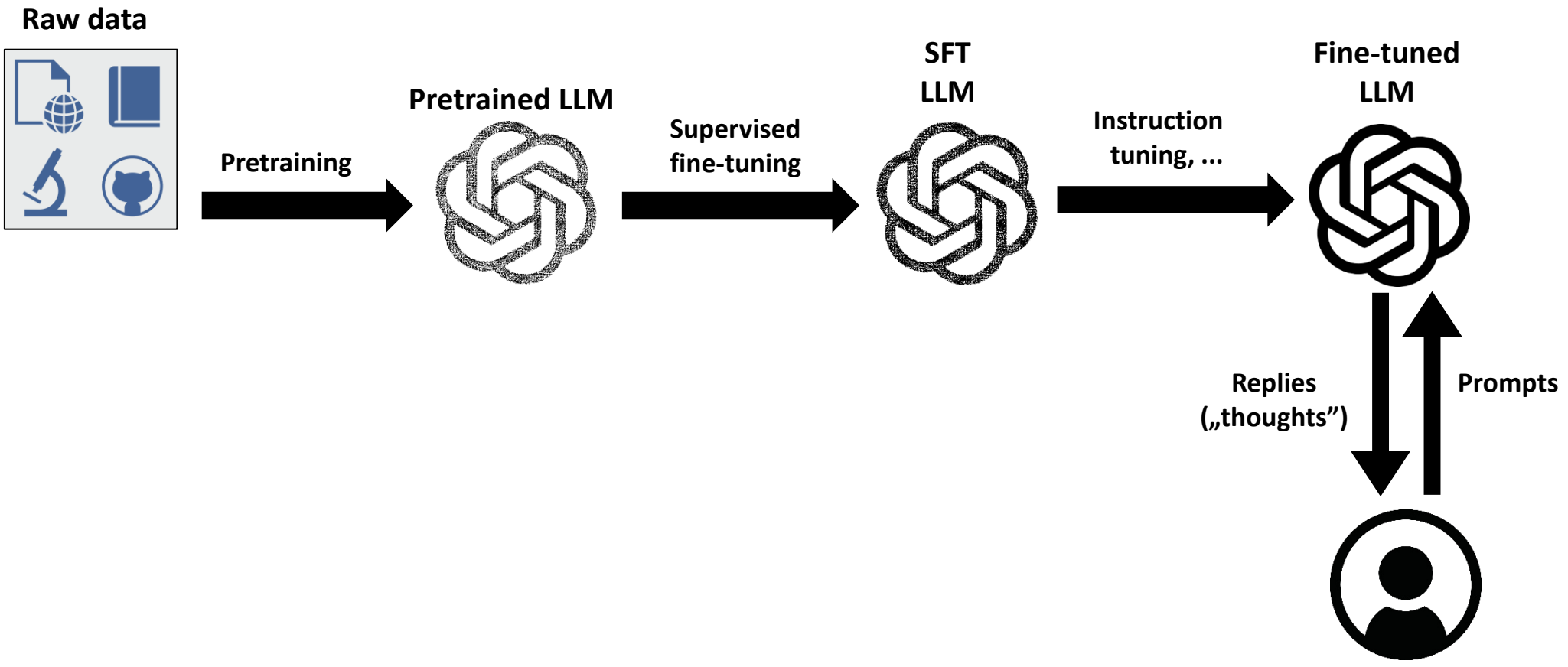
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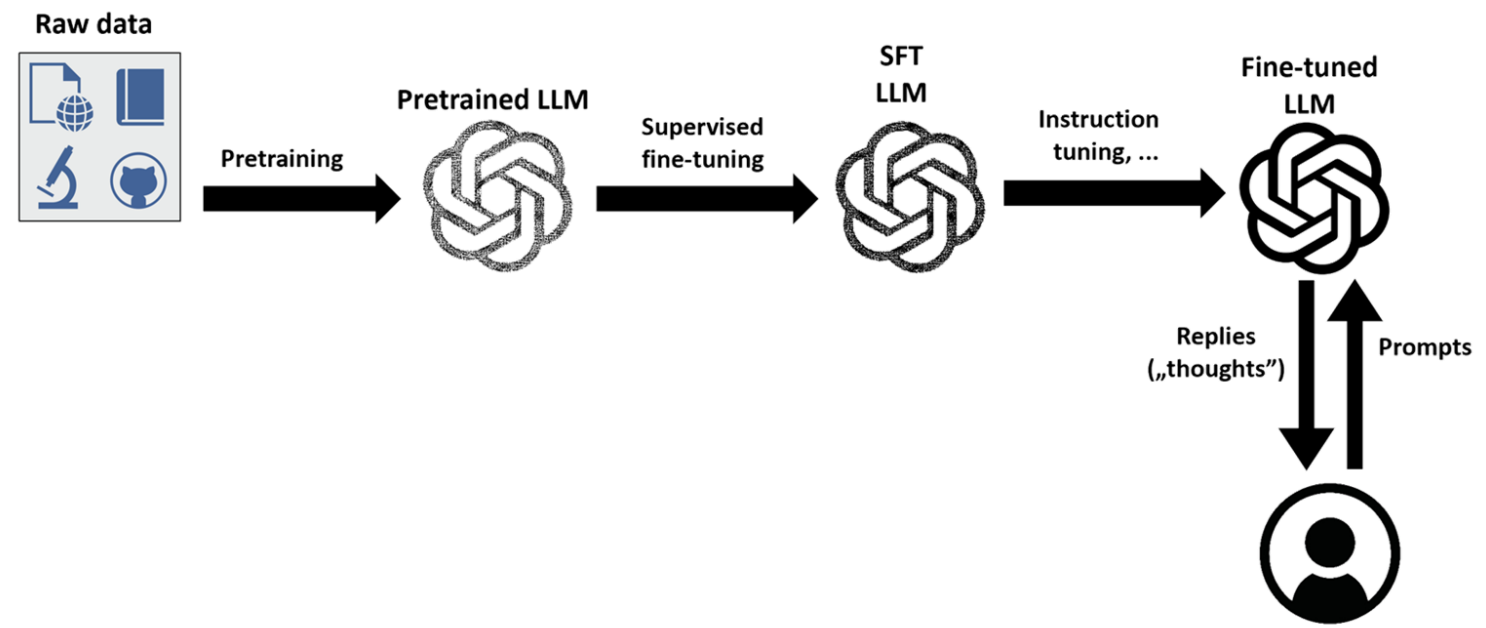
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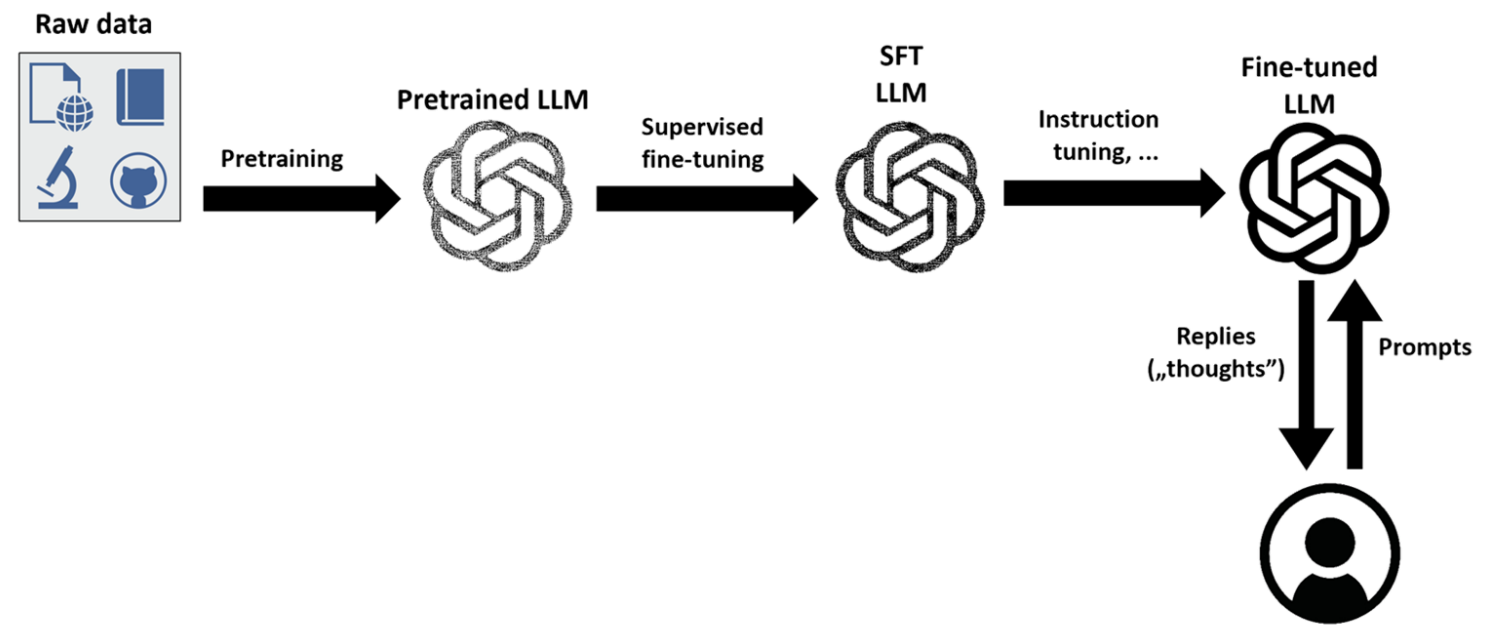
# Overview of the LLM Processing Pipeline



# The Emergence of the „Generative AI Ecosystem”

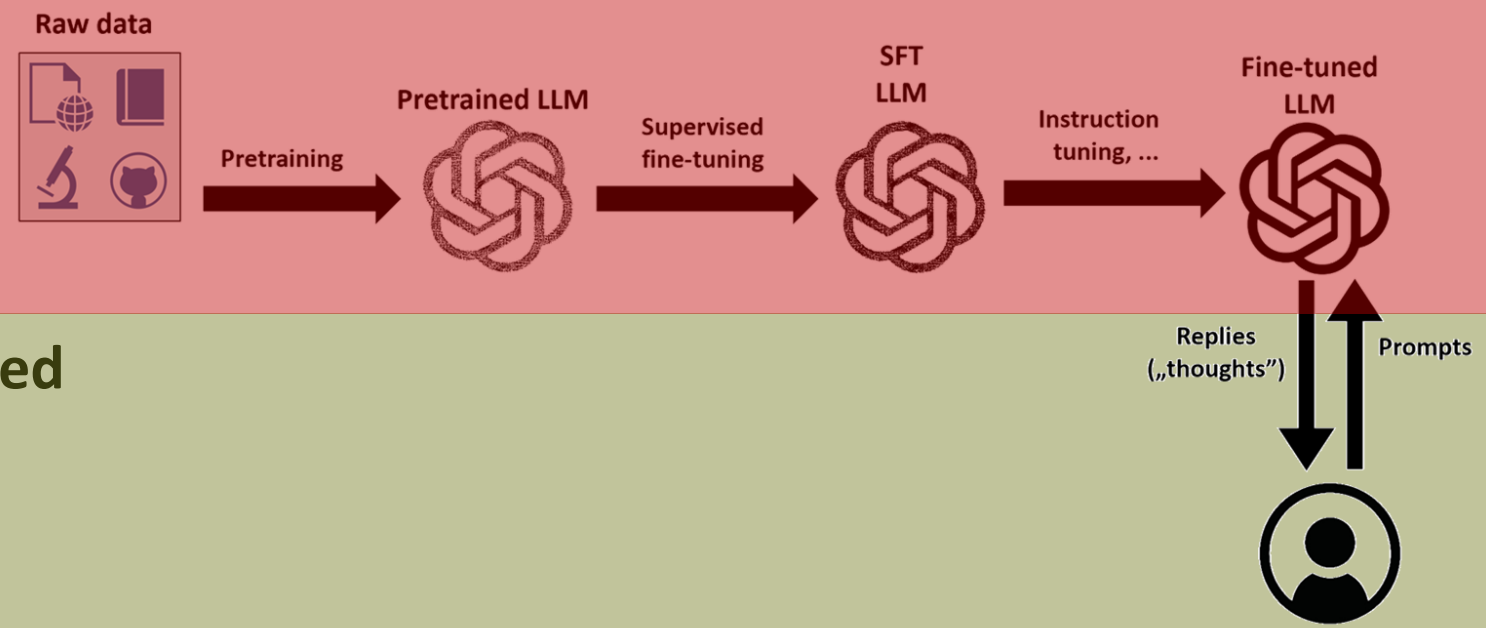


# The „Generative AI Ecosystem”



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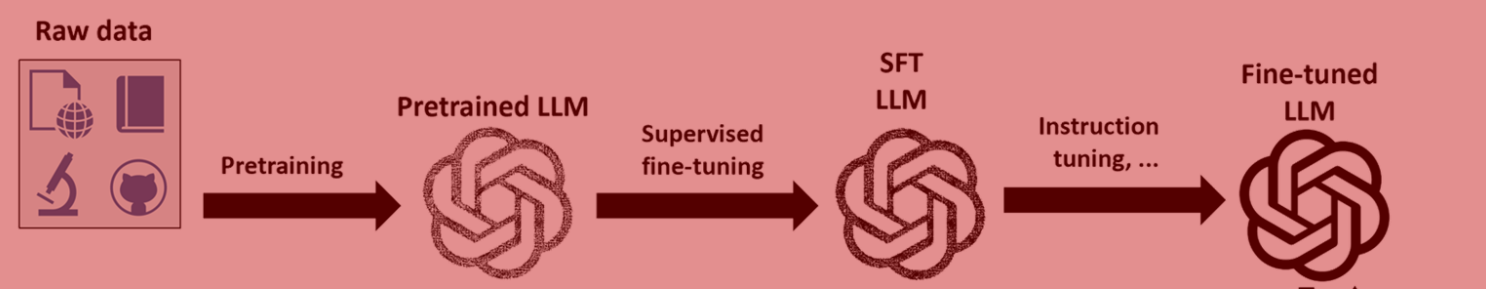
## Training related



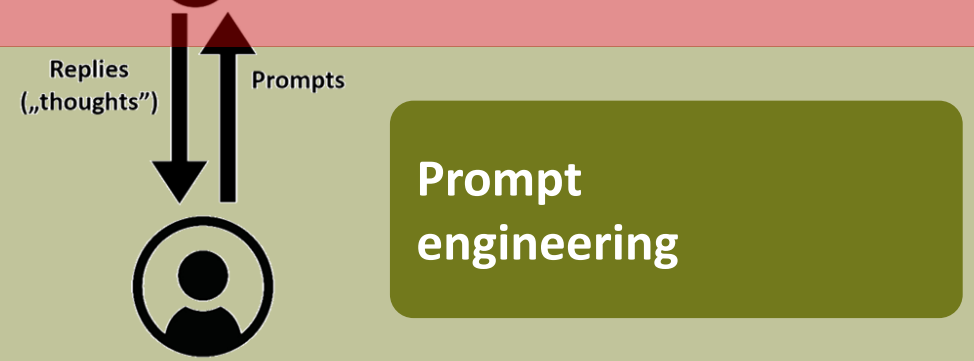
## Inference related

# The „Generative AI Ecosystem”

## Training related

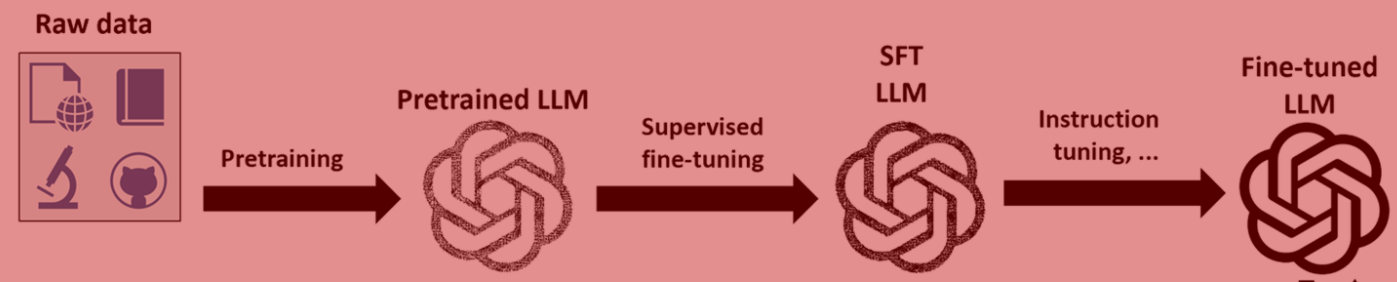


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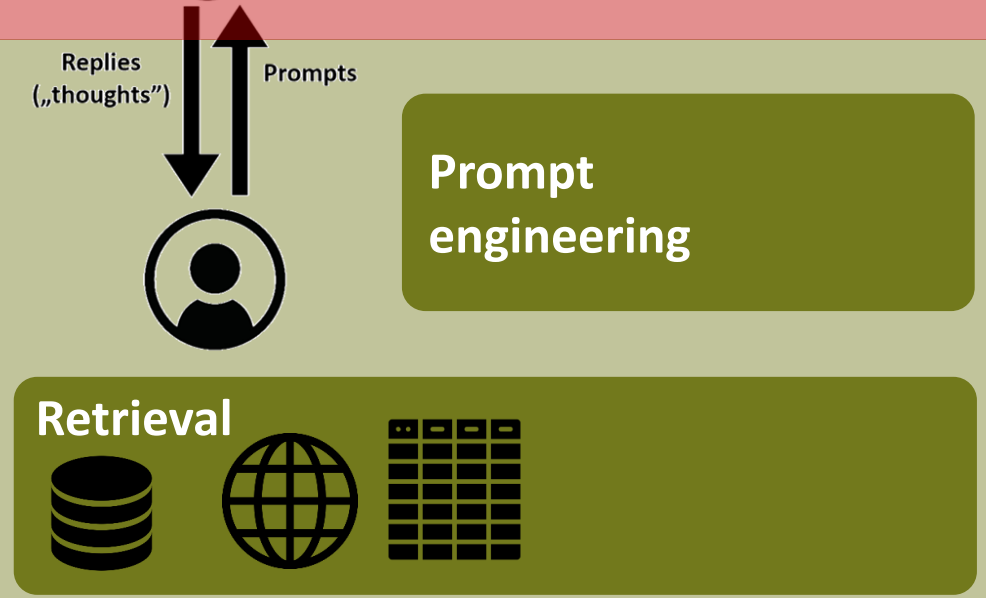


# The „Generative AI Ecosystem”

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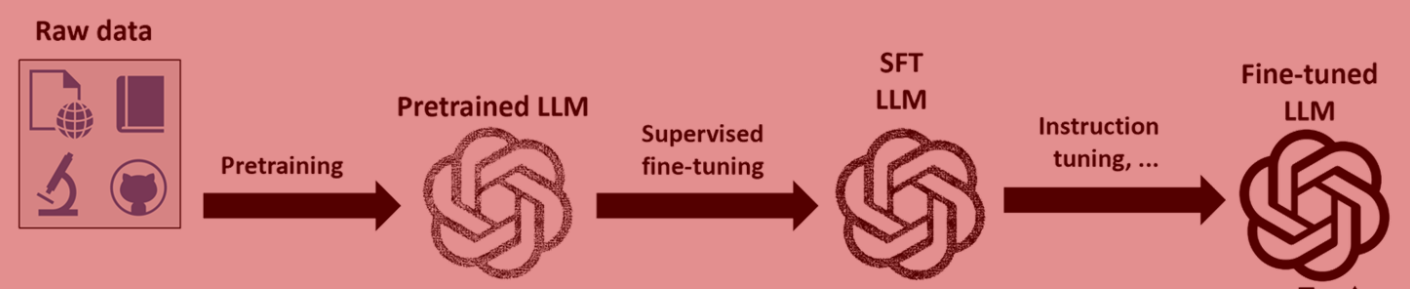


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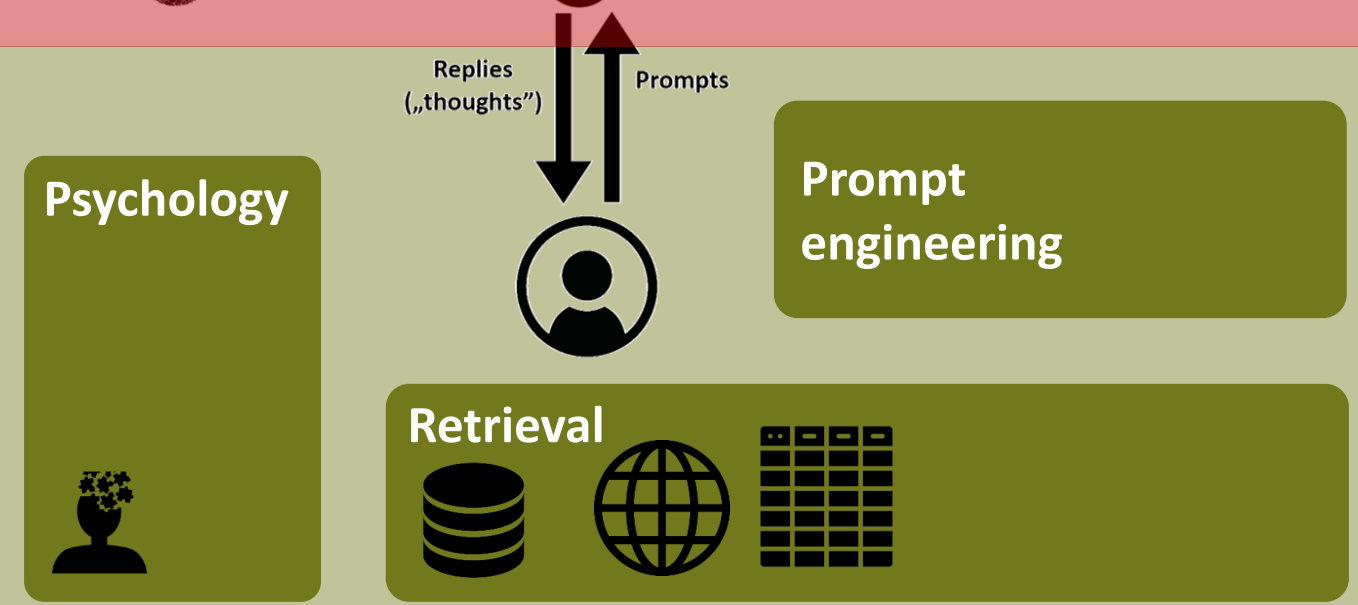


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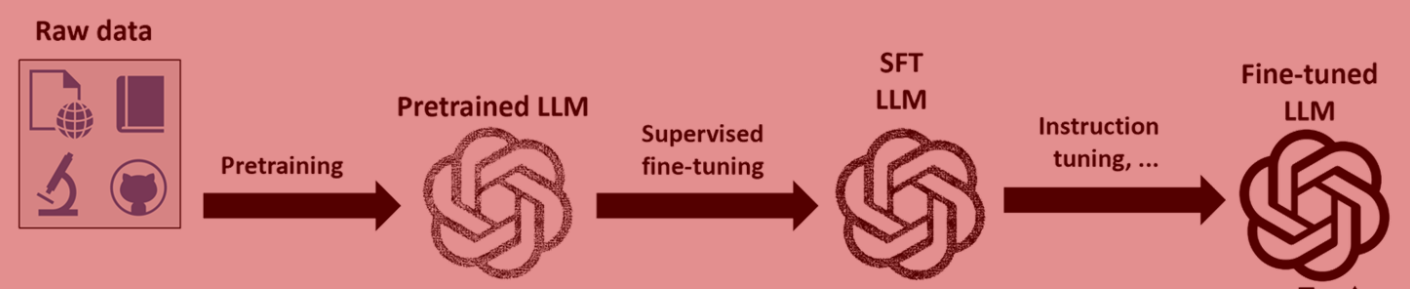


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## Training related



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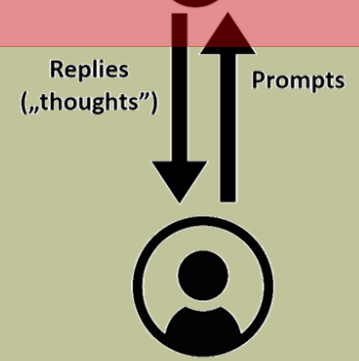

**Agents, Tools**



**Psychology**



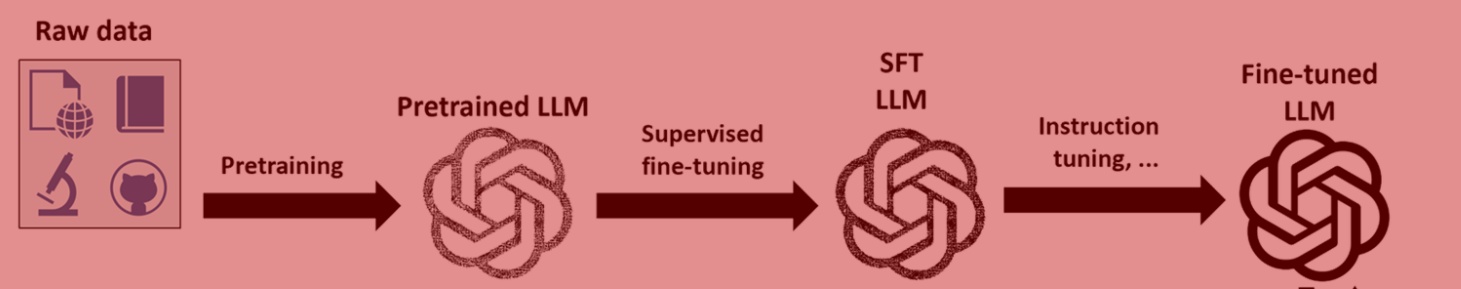
**Retrieval**



**Prompt engineering**

# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

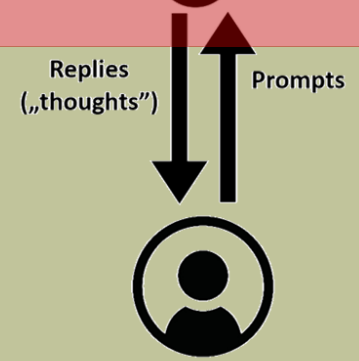
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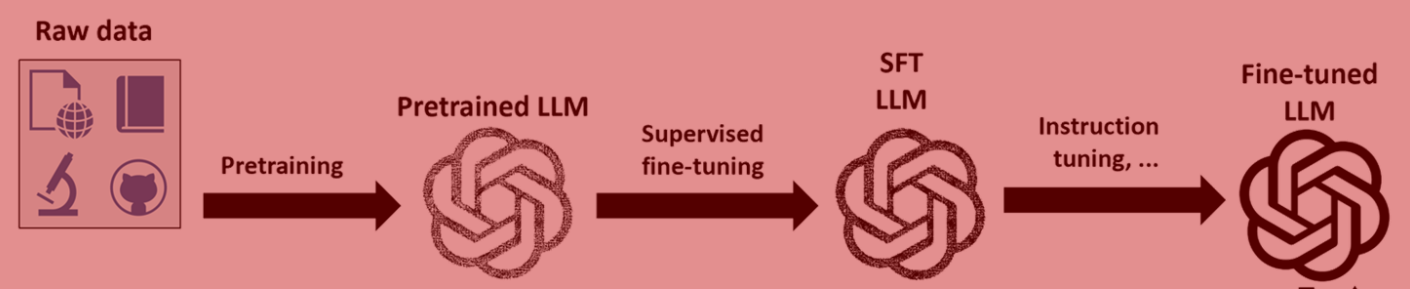
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# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

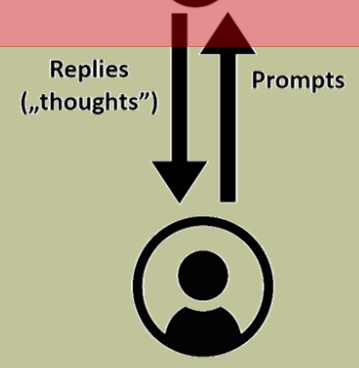

**Agents, Tools**



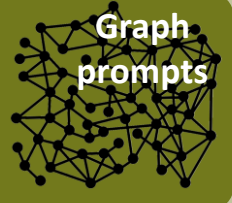
**Psychology**



**Retrieval**

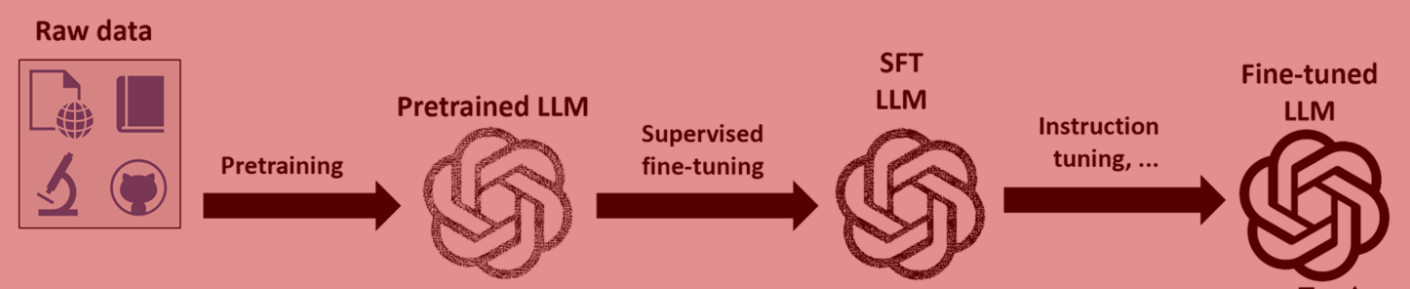


**Prompt engineering**



# Graphs in the LLM Pipeline: Overview

## Training related



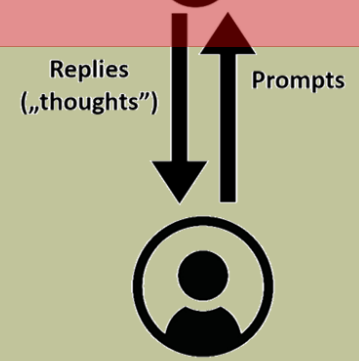
## Inference related

**Agents, Tools**

**Psychology**

**Retrieval**

Graph database  
 Knowledge graph

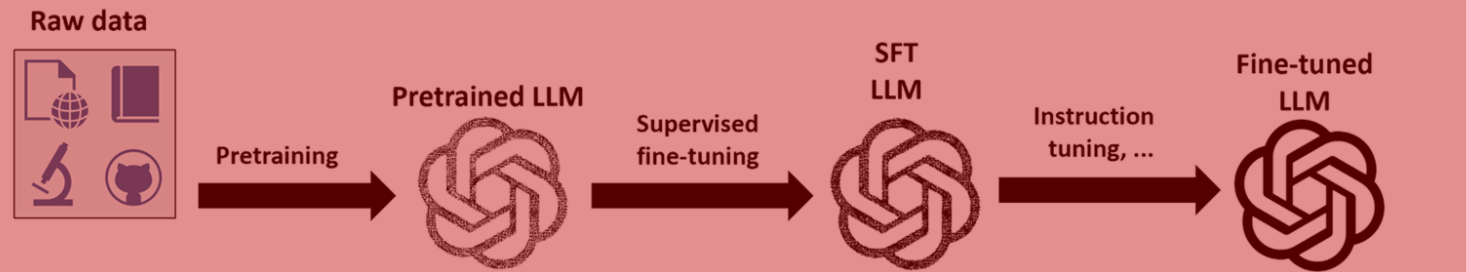


**Prompt engineering**

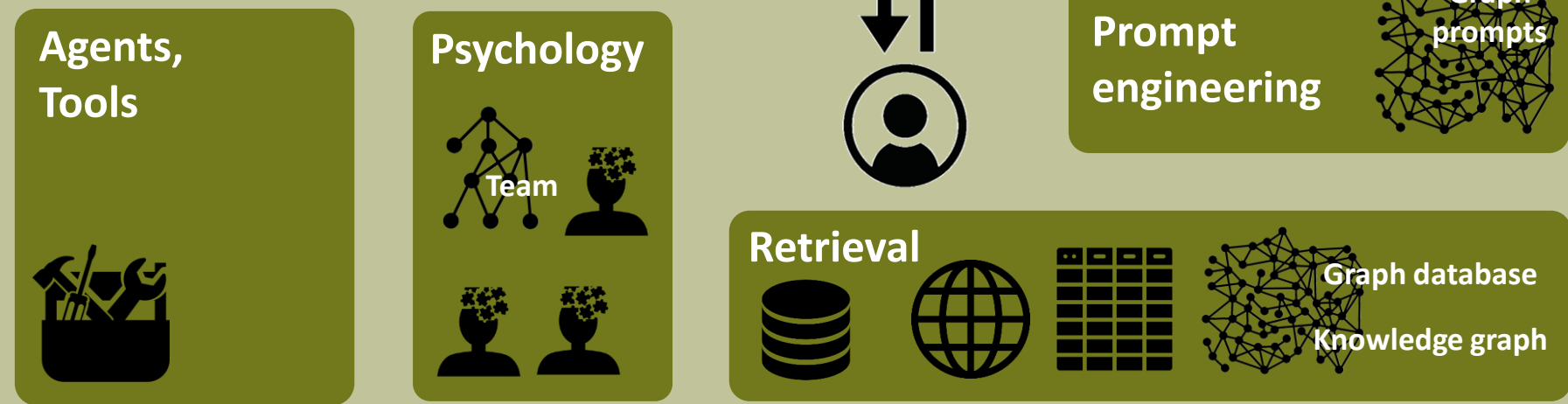
Graph prompts

# Graphs in the LLM Pipeline: Overview

## Training related

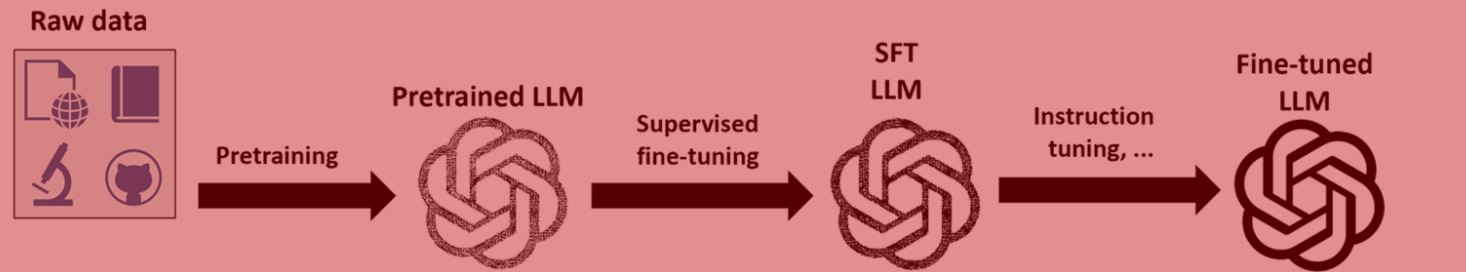


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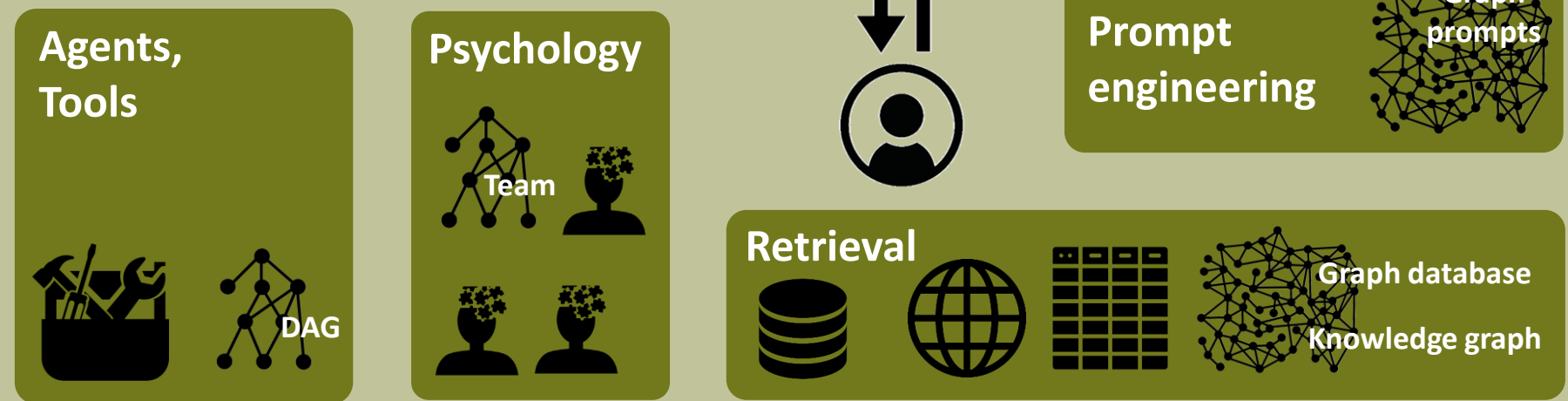


# Graphs in the LLM Pipeline: Overview

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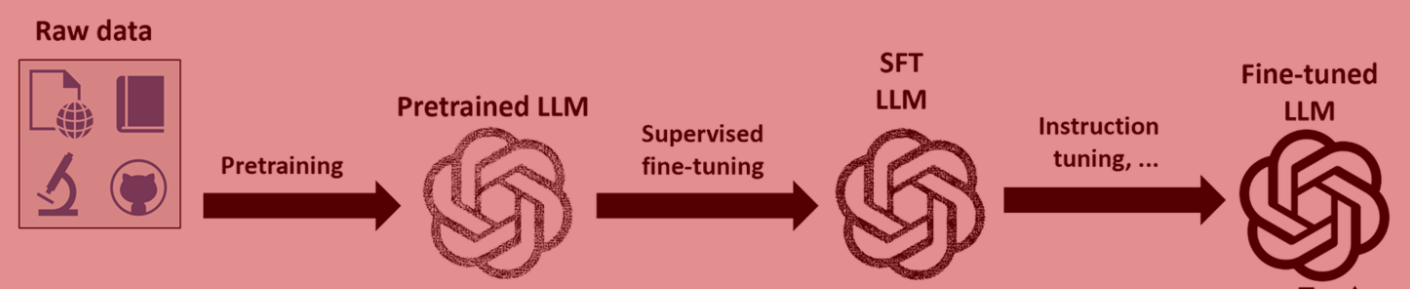


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

**Agents, Tools**

GNN  
Heuristic  
DAG

**Psychology**

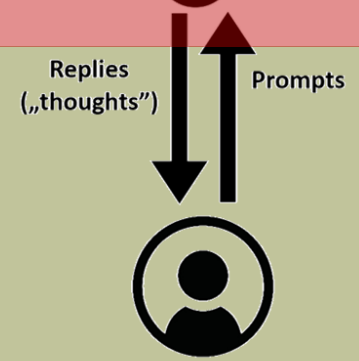
Team

**Retrieval**

Graph database  
Knowledge graph

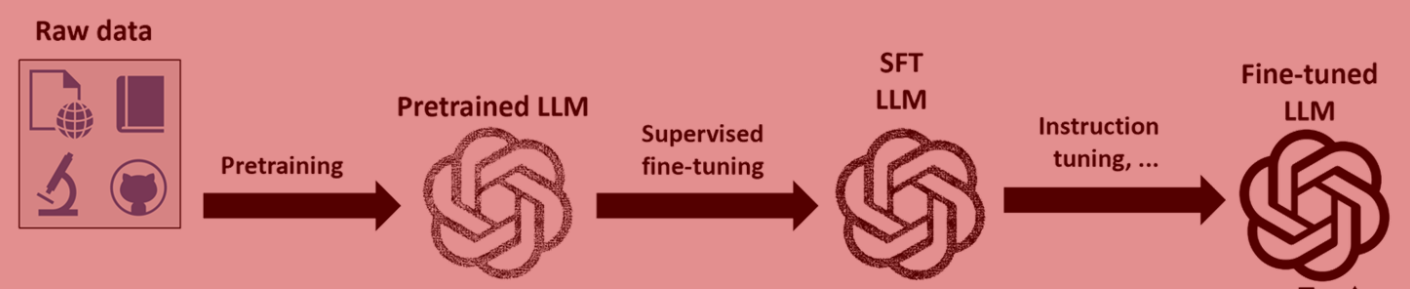
**Prompt engineering**

Graph prompts



# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

**Reasoning Structures**

**Agents, Tools**

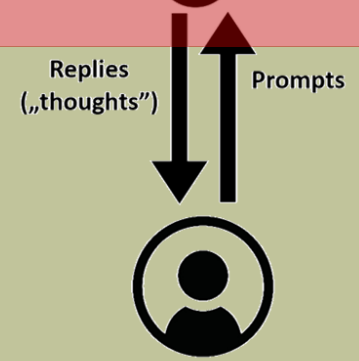
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**Psychology**

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- Graph database
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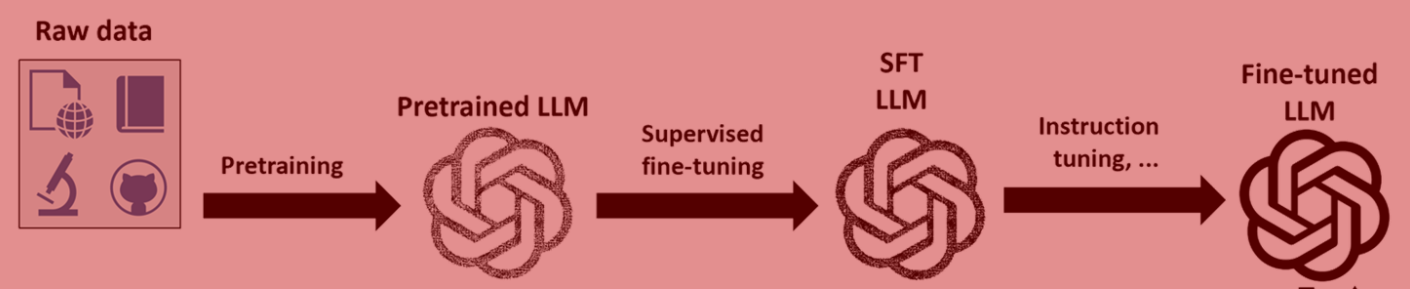


**Prompt engineering**

- Graph prompts


# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

**Reasoning Structures**



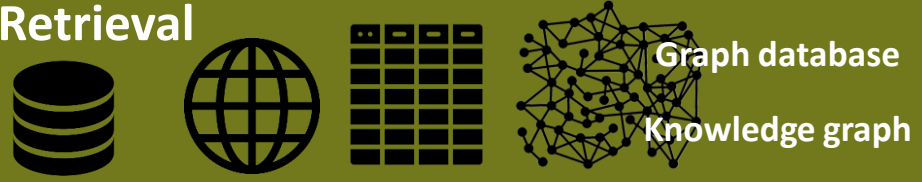
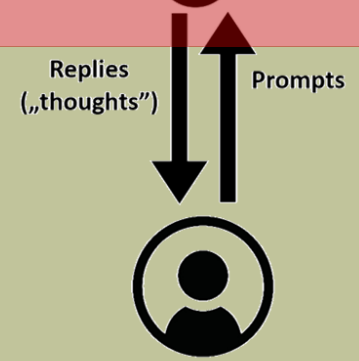
**Agents, Tools**



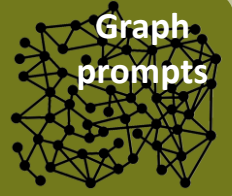
**Psychology**



**Retrieval**

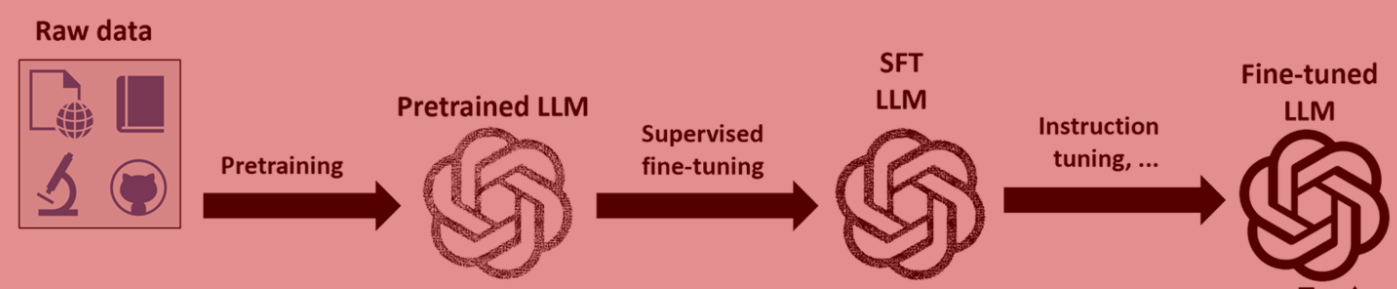



**Prompt engineering**



# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

**Reasoning Structures**

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GNN  
Heuristic  
DAG

**Psychology**

Team

Replies („thoughts“)  
 Prompts

**Prompt engineering**

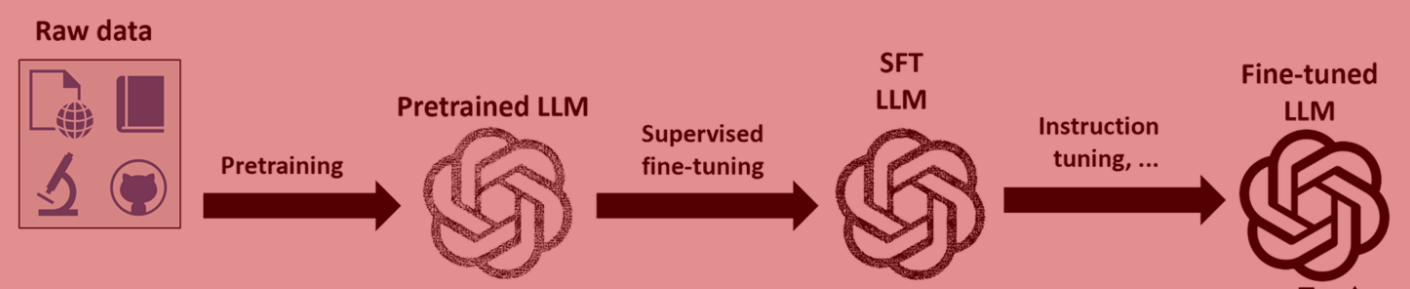
Graph prompts

**Retrieval**

Graph database  
Knowledge graph

# Graphs in the LLM Pipeline: Overview

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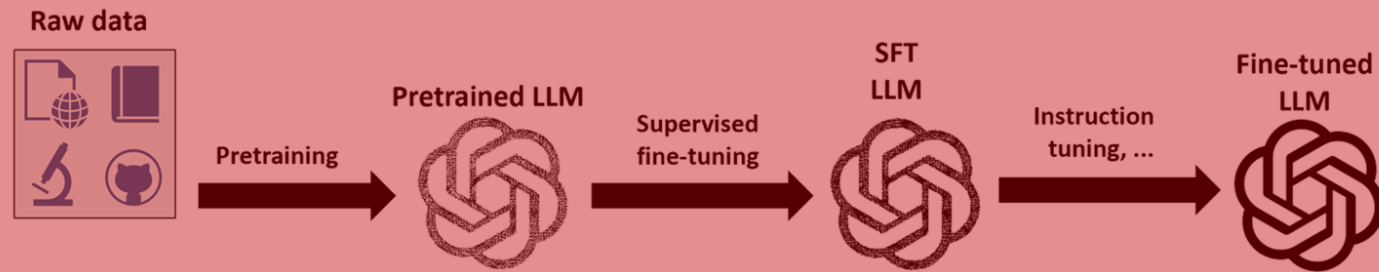
**Prompt engineering**

Graph prompts

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# Graphs in the LLM Pipeline: Overview

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## Inference related

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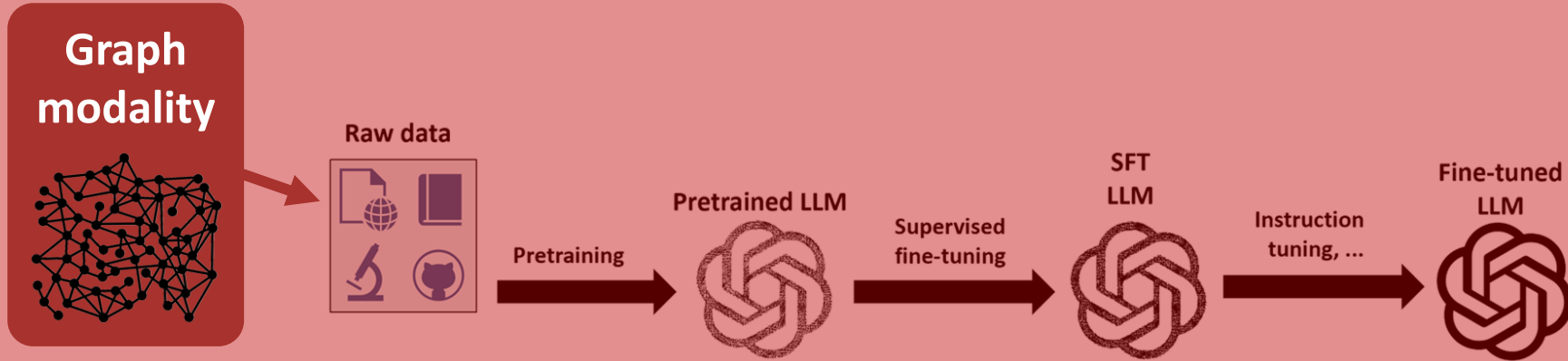
Graph prompts

**Retrieval**

Graph database  
Knowledge graph

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## Training related

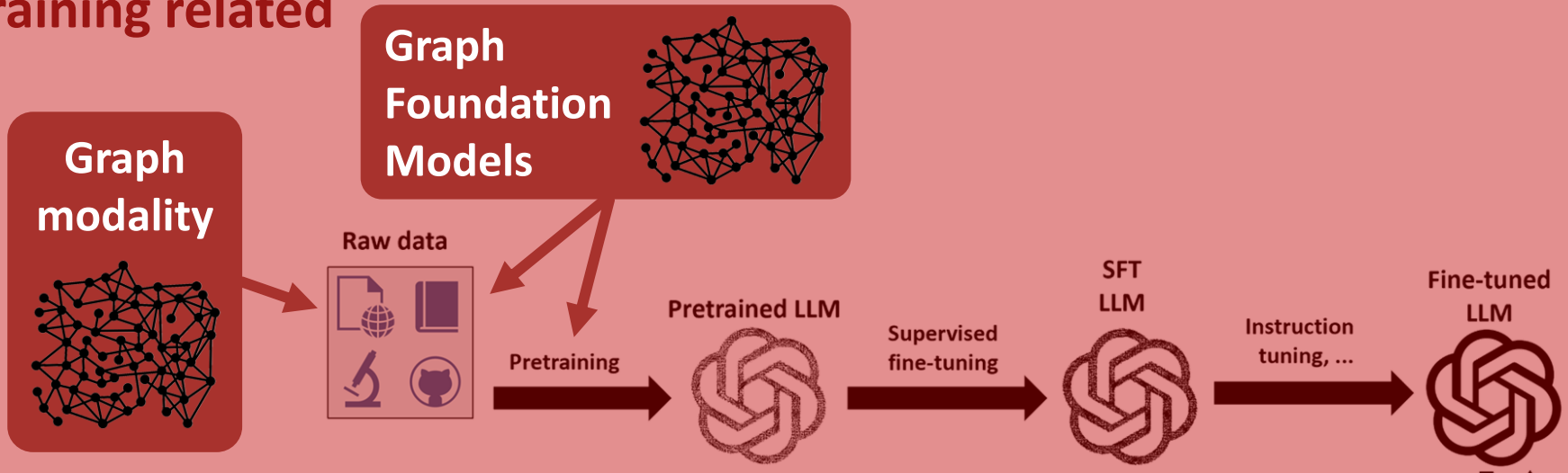


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related

**Reasoning Structures**

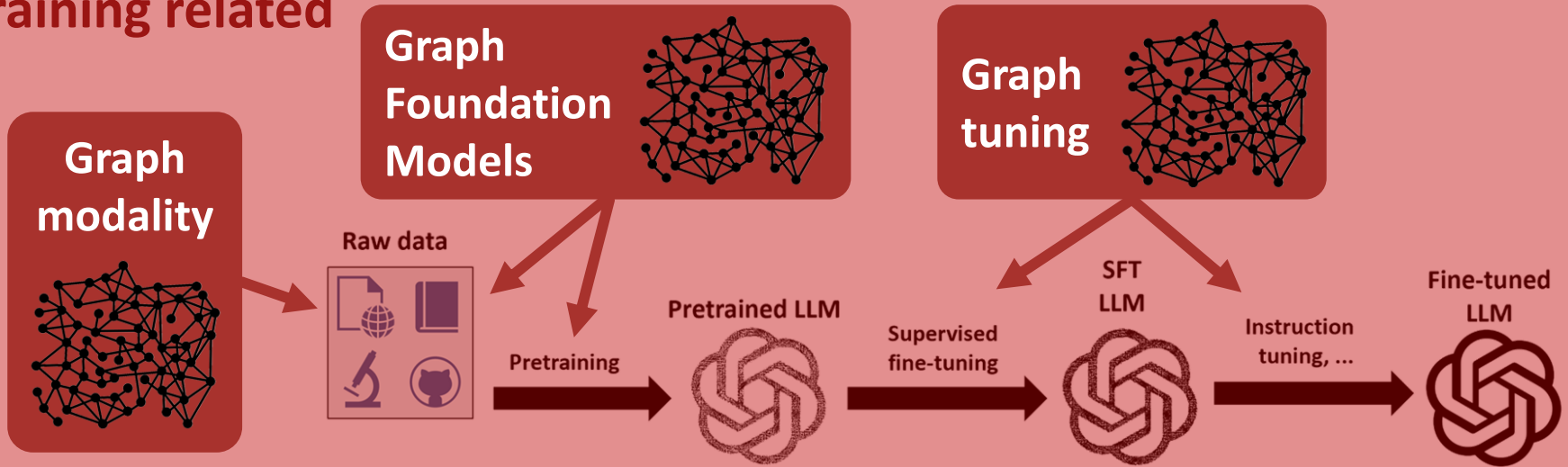
**Agents, Tools**

**Psychology**

**Prompt engineering**

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## Training related

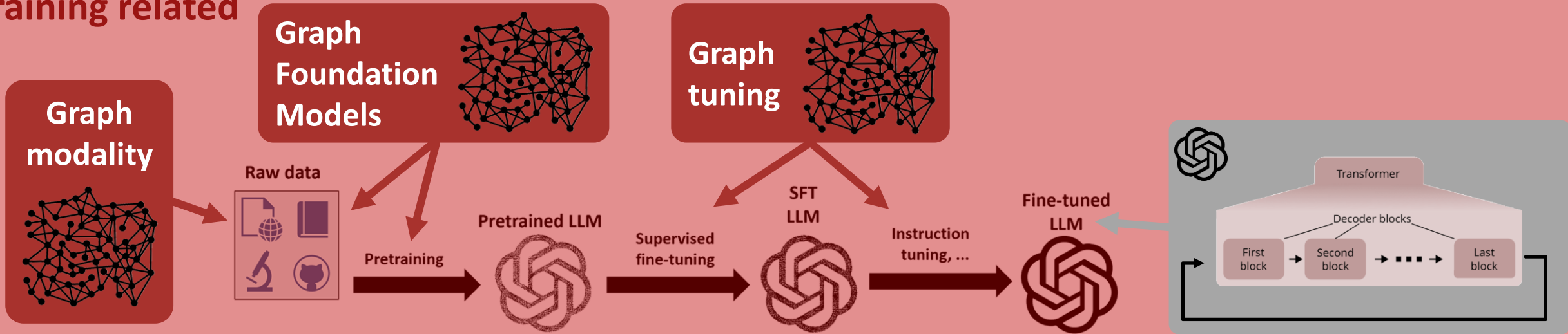


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related

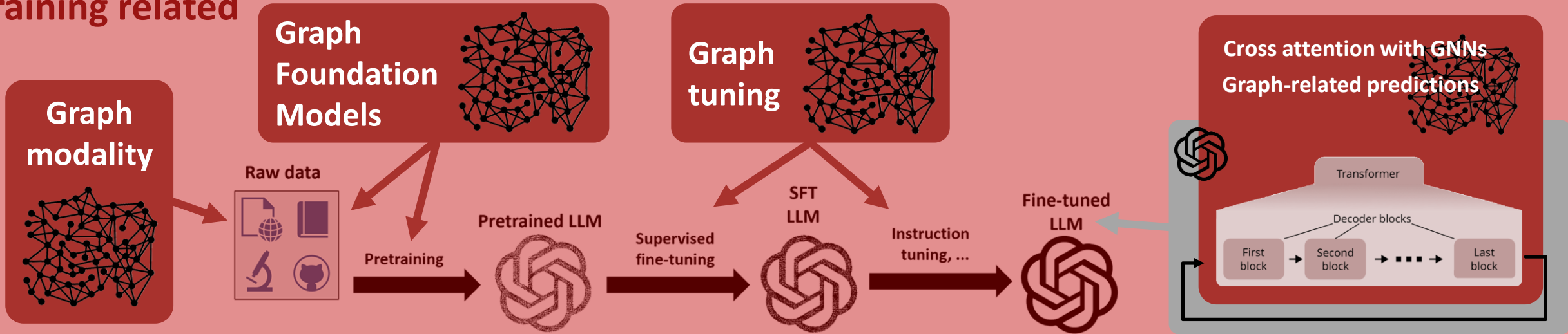


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related

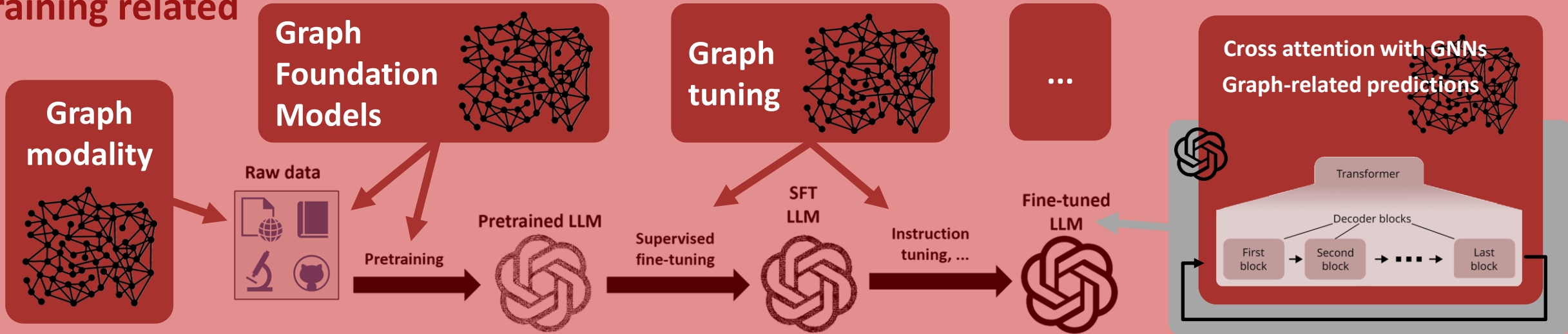


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related

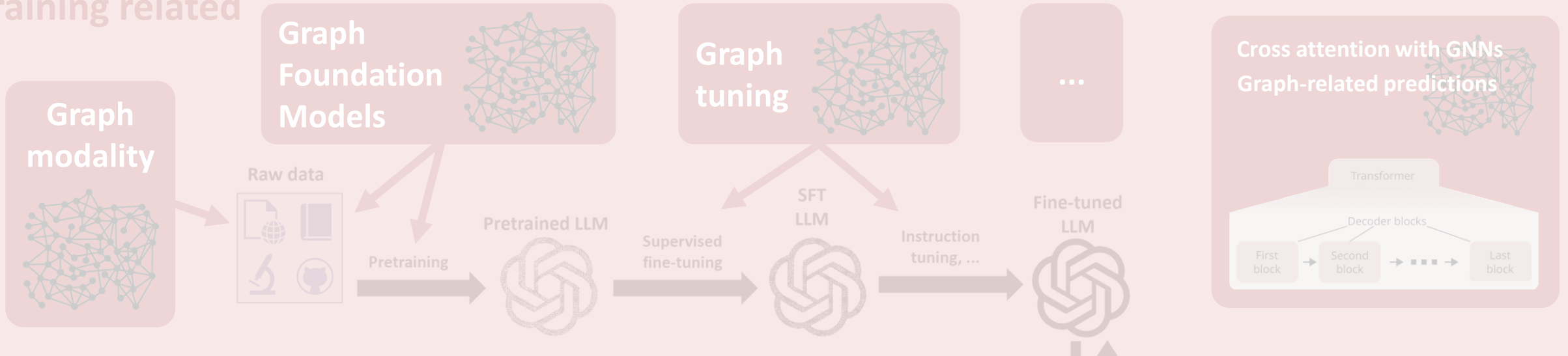


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related



## Inference related



# Graphs in the LLM Pipeline: Overview

<https://github.com/spcl/graph-of-thoughts>, @AAAI'24

## Graph of Thoughts: Solving Elaborate Problems with Large Language Models

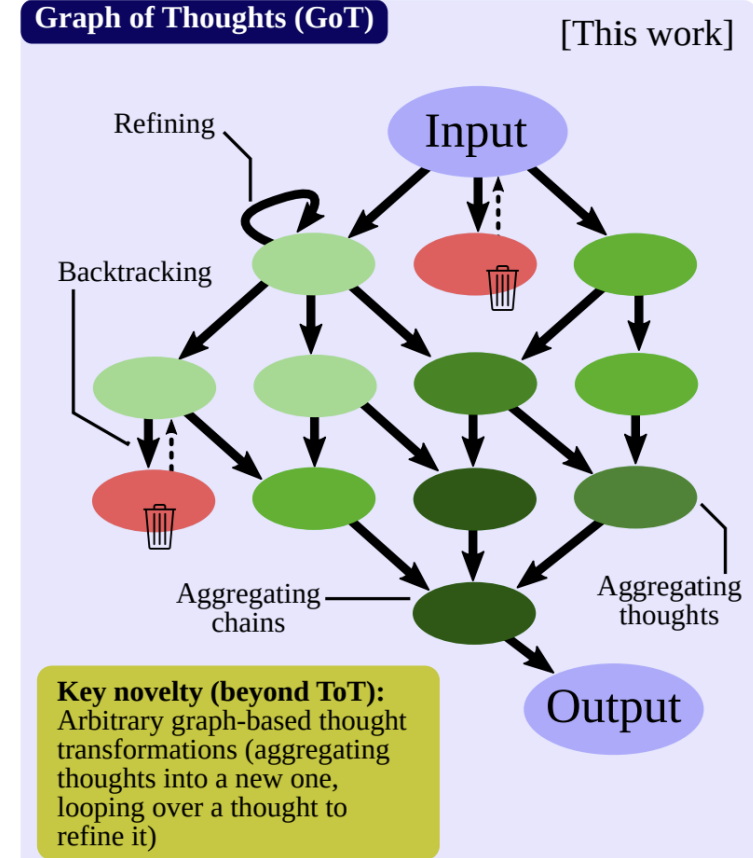
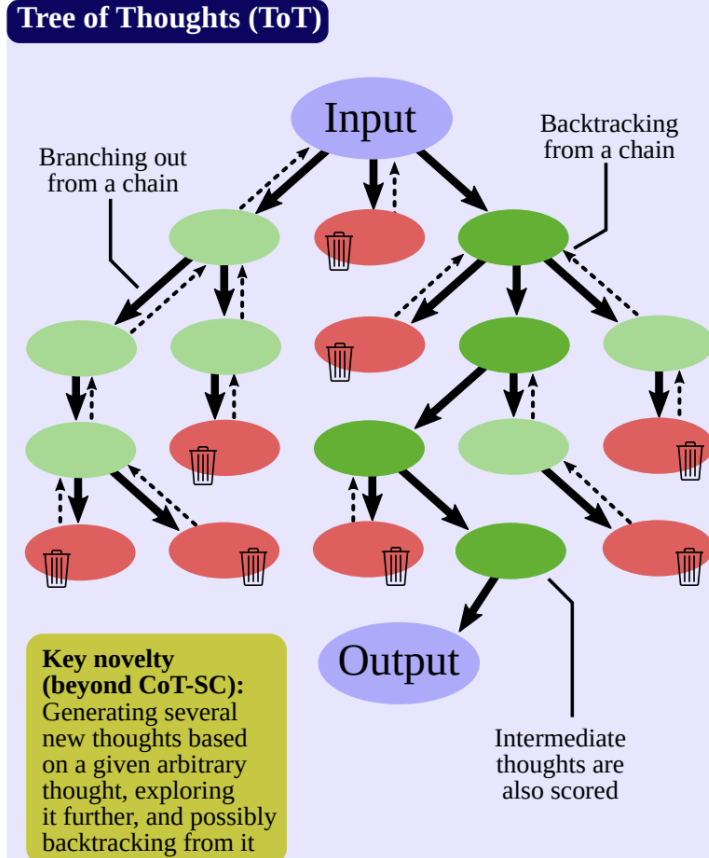
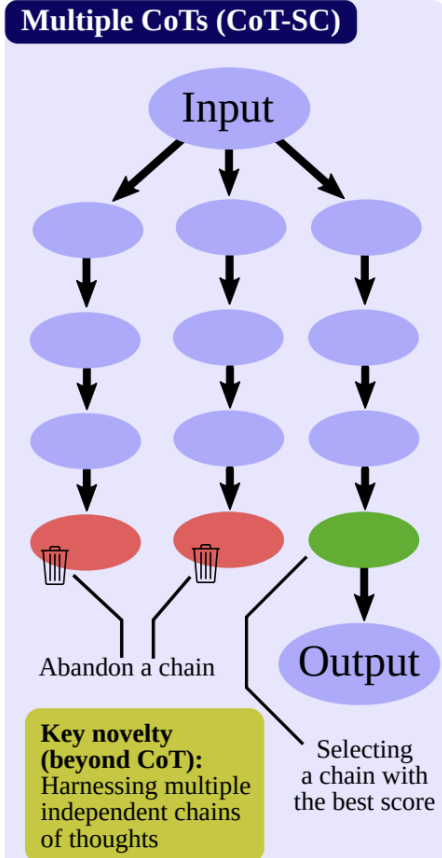
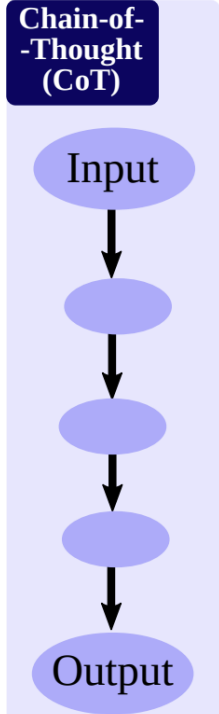
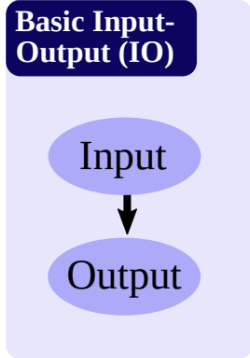
Maciej Besta<sup>1\*</sup>, Nils Blach<sup>1\*</sup>, Ales Kubicek<sup>1</sup>, Robert Gerstenberger<sup>1</sup>,  
 Lukas Gianinazzi<sup>1</sup>, Joanna Gajda<sup>2</sup>, Tomasz Lehmann<sup>2</sup>, Michał Podstawski<sup>3</sup>,  
 Hubert Niewiadomski<sup>2</sup>, Piotr Nyczyk<sup>2</sup>, Torsten Hoefler<sup>1</sup>

<sup>1</sup>ETH Zurich, <sup>2</sup>Cledar, <sup>3</sup>Warsaw University of Technology  
 bestam@inf.ethz.ch, nils.blach@inf.ethz.ch, htor@inf.ethz.ch

### Inference related



# Reasoning Paradigms



**Legend**

Thoughts:

- Unscored
- Positive score
- Negative score

↓ Dependencies between thoughts

🗑️ Abandon thought

↶ Backtrack



# Graphs in the LLM Pipeline: Overview

<https://github.com/spcl/graph-of-thoughts>, @AAAI'24

## Graph of Thoughts: Solving Elaborate Problems with Large Language Models

Maciej Besta<sup>1\*</sup>, Nils Blach<sup>1\*</sup>, Ales Kubicek<sup>1</sup>, Robert Gerstenberger<sup>1</sup>,  
 Lukas Gianinazzi<sup>1</sup>, Joanna Gajda<sup>2</sup>, Tomasz Lehmann<sup>2</sup>, Michał Podstawski<sup>3</sup>,  
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<sup>1</sup>ETH Zurich, <sup>2</sup>Cledar, <sup>3</sup>Warsaw University of Technology  
 bestam@inf.ethz.ch, nils.blach@inf.ethz.ch, htor@inf.ethz.ch

### Inference related




**Graphs in the**  
 Training related

# Topologies of Reasoning: Demystifying Chains, Trees, and Graphs of Thoughts

Maciej Besta<sup>1†</sup>, Florim Memedi<sup>1</sup>, Zhenyu Zhang<sup>1</sup>, Robert Gerstenberger<sup>1</sup>, Nils Blach<sup>1</sup>,  
 Piotr Nyczyk<sup>2</sup>, Marcin Copik<sup>1</sup>, Grzegorz Kwaśniewski<sup>1</sup>, Jürgen Müller<sup>3</sup>, Lukas Gianinazzi<sup>1</sup>,  
 Ales Kubicek<sup>1</sup>, Hubert Niewiadomski<sup>2</sup>, Onur Mutlu<sup>1</sup>, Torsten Hoefler<sup>1</sup>

<sup>1</sup>ETH Zurich   <sup>2</sup>Cledar   <sup>3</sup>BASF SE

**Graph modality**

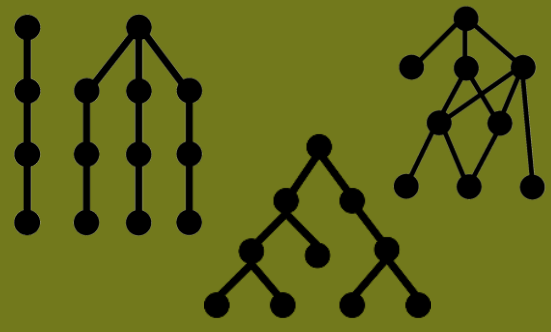


n with GNNs  
 predictions



**Inference related**

**Reasoning Structures**




**Agents, Tools**



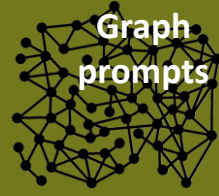
**Psychology**



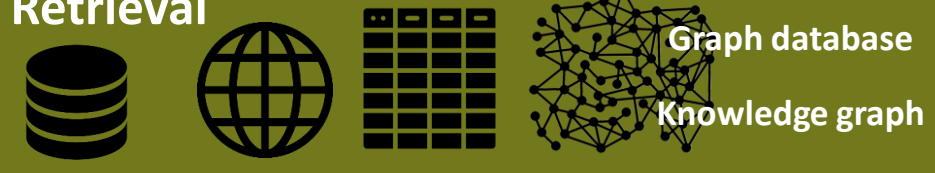
Replies („thoughts“)  
 Prompts



**Prompt engineering**



**Retrieval**




# Graphs in the LLM Pipeline: Overview

## Affordable AI Assistants with Knowledge Graph of Thoughts

Maciej Besta<sup>† 1</sup> Lorenzo Paleari<sup>1</sup> Jia Hao Andrea Jiang<sup>1</sup> Robert Gerstenberger<sup>1</sup> You Wu<sup>1</sup> Patrick Iff<sup>1</sup>  
 Ales Kubicek<sup>1</sup> Piotr Nyczyk<sup>2</sup> Diana Khimey<sup>1</sup> Jón Gunnar Hannesson<sup>1</sup> Grzegorz Kwaśniewski<sup>1</sup>  
 Marcin Copik<sup>1</sup> Hubert Niewiadomski<sup>2</sup> Torsten Hoefler<sup>1</sup>

Inference related

**Reasoning Structures**



**Agents, Tools**



**Psychology**

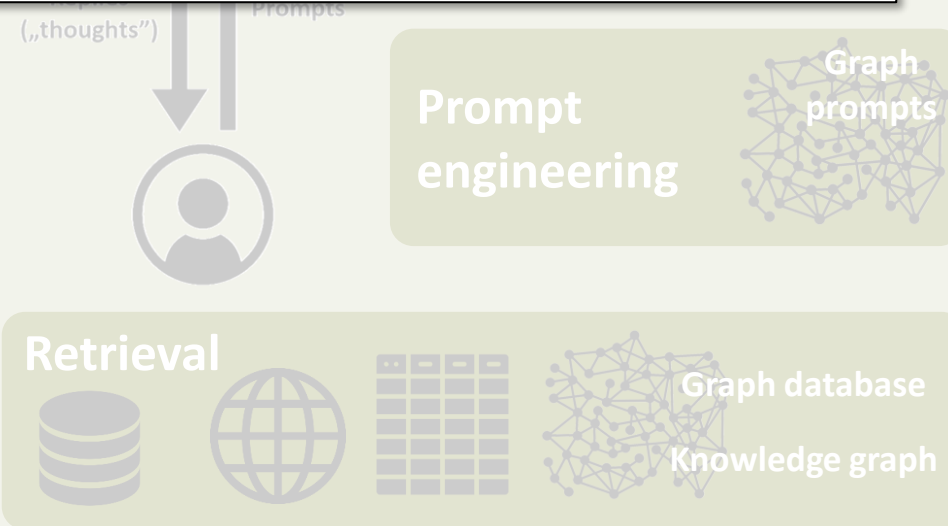


**Prompt engineering**

Graph prompts

Retrieval

Graph database  
Knowledge graph



# Agents, Tools

# Agents, Tools

Graph as a model of the agent's task and its state

# Agents, Tools

## Graph as a model of the agent's task and its state

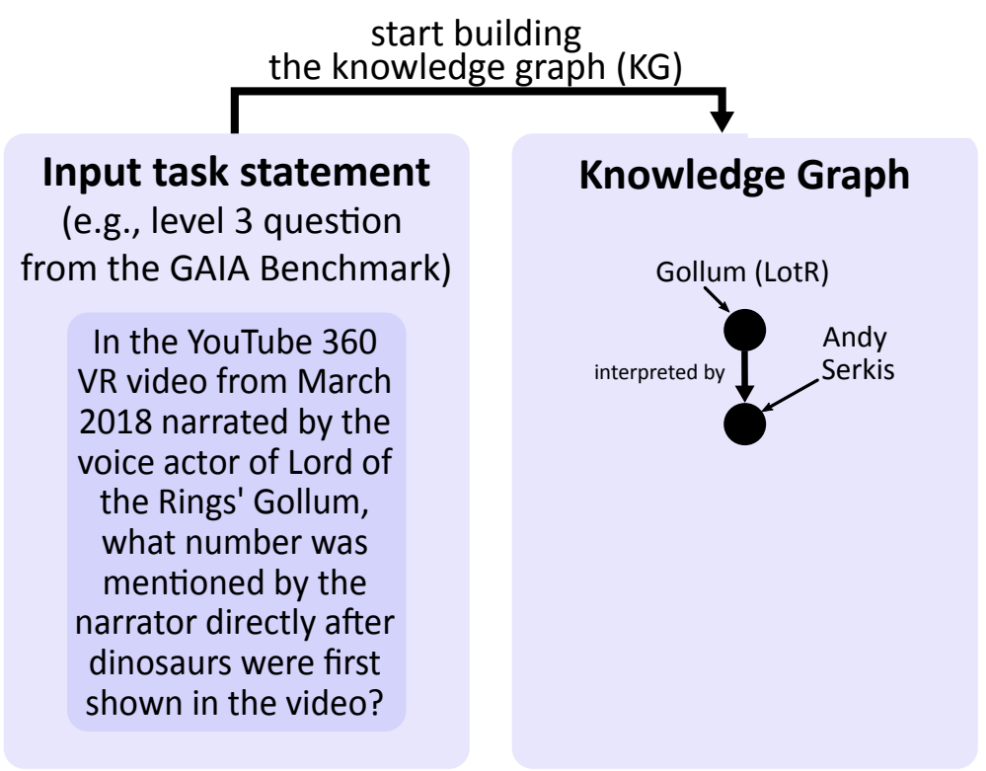
### Input task statement

(e.g., level 3 question from the GAIA Benchmark)

In the YouTube 360 VR video from March 2018 narrated by the voice actor of Lord of the Rings' Gollum, what number was mentioned by the narrator directly after dinosaurs were first shown in the video?

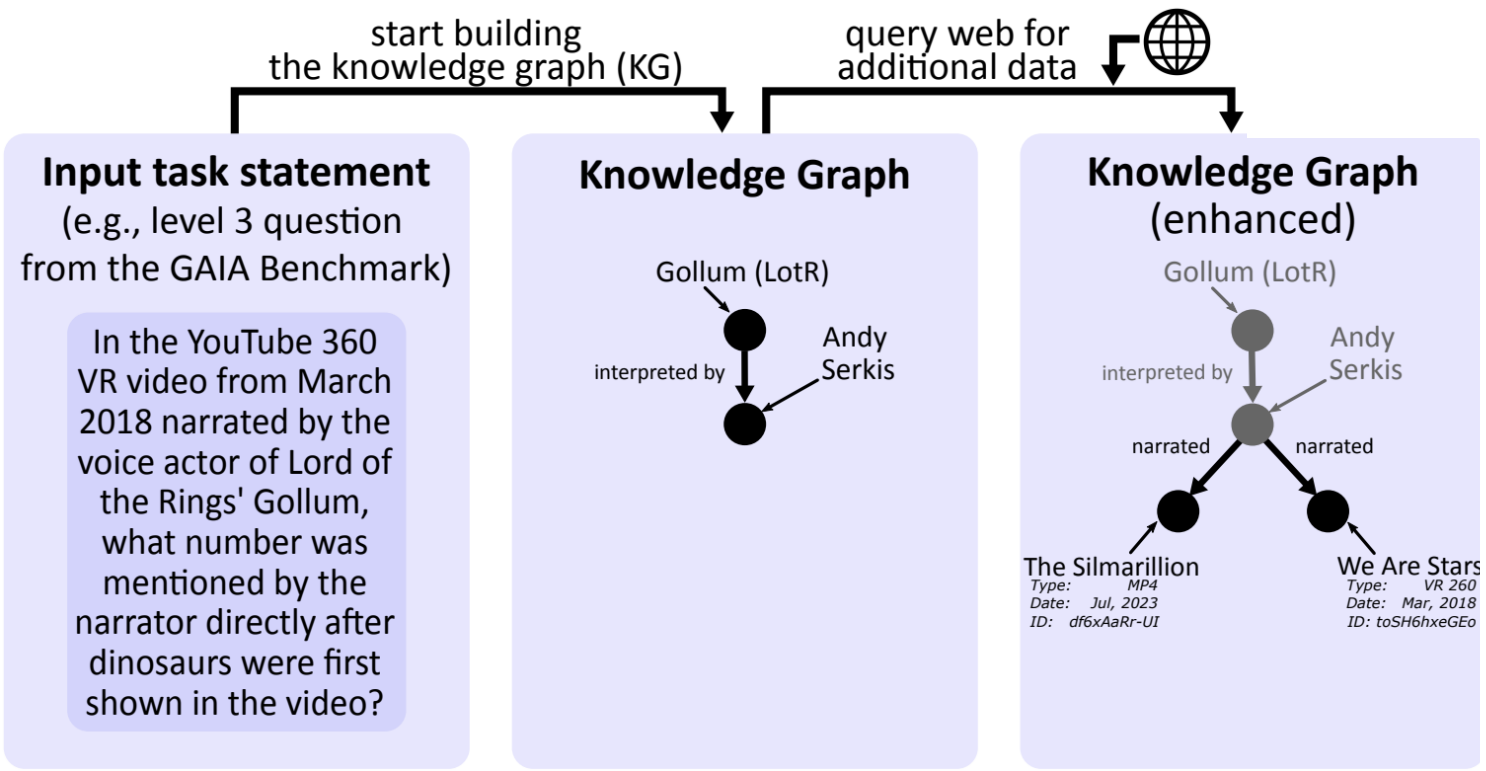
# Agents, Tools

## Graph as a model of the agent's task and its state



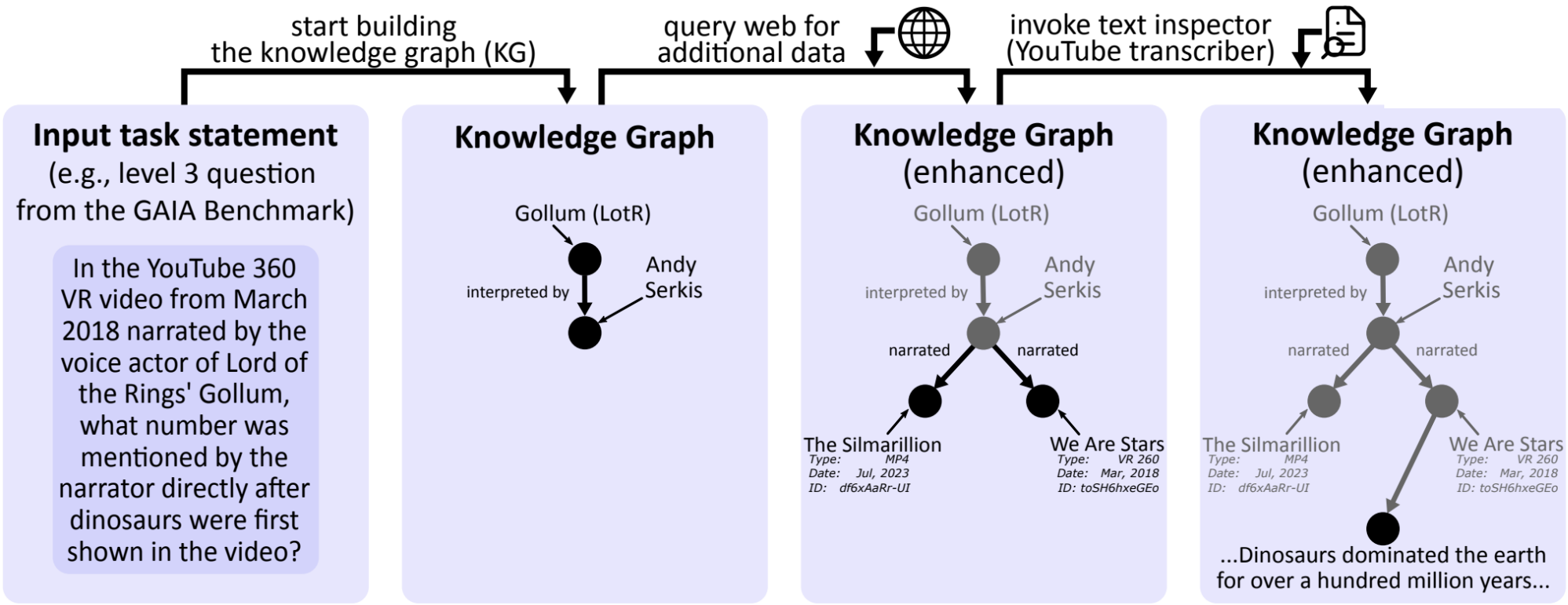
# Agents, Tools

## Graph as a model of the agent's task and its state



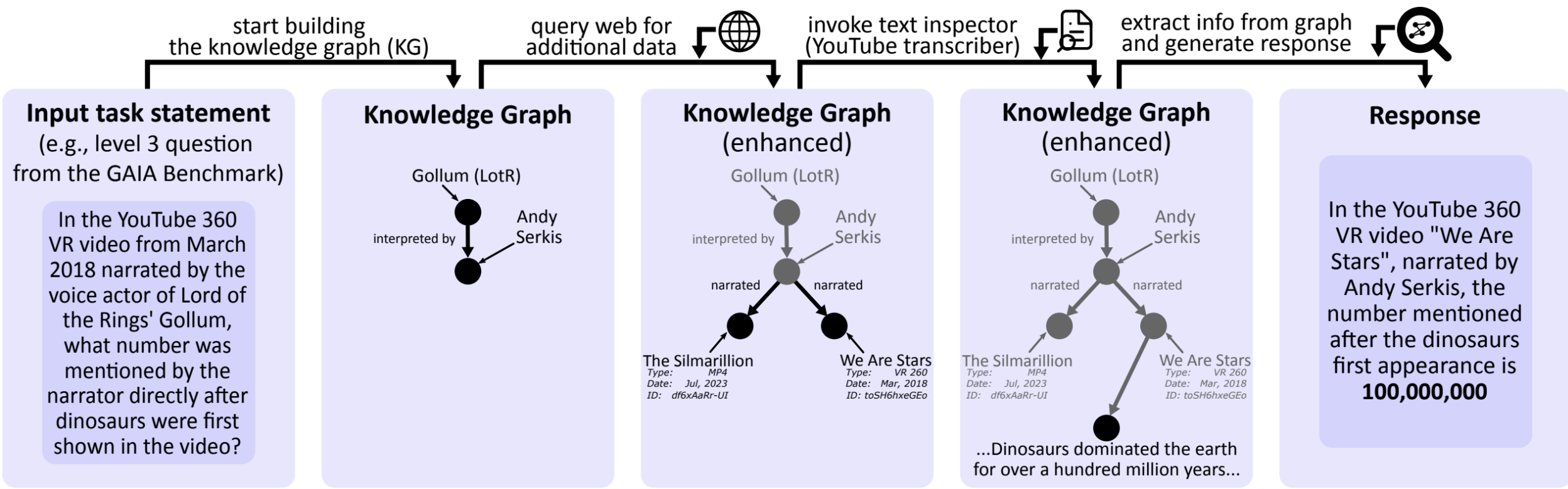
# Agents, Tools

## Graph as a model of the agent's task and its state



# Agents, Tools

## Graph as a model of the agent's task and its state




# Graphs in the LLM Pipeline: Overview

## Affordable AI Assistants with Knowledge Graph of Thoughts

Maciej Besta<sup>† 1</sup> Lorenzo Paleari<sup>1</sup> Jia Hao Andrea Jiang<sup>1</sup> Robert Gerstenberger<sup>1</sup> You Wu<sup>1</sup> Patrick Iff<sup>1</sup>  
 Ales Kubicek<sup>1</sup> Piotr Nyczyk<sup>2</sup> Diana Khimey<sup>1</sup> Jón Gunnar Hannesson<sup>1</sup> Grzegorz Kwaśniewski<sup>1</sup>  
 Marcin Copik<sup>1</sup> Hubert Niewiadomski<sup>2</sup> Torsten Hoefler<sup>1</sup>

Inference related

**Reasoning Structures**




**Agents, Tools**




GNN  
Heuristic  
DAG

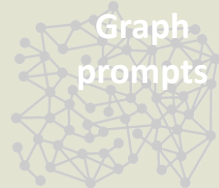
**Psychology**




Team

(„thoughts“) Prompts  


**Prompt engineering**



**Retrieval**



Graph database  
Knowledge graph

# Graphs in the LLM Pipeline: Overview


## Psychologically Enhanced AI Agents

**Maciej Besta<sup>1†</sup>, Shriram Chandran<sup>1</sup>, Robert Gerstenberger<sup>1</sup>, Mathis Lindner<sup>1</sup>,  
 Marcin Chrapek<sup>1</sup>, Sebastian Hermann Martschat<sup>2</sup>, Taraneh Ghandi<sup>2\*</sup>, Patrick Iff<sup>1</sup>,  
 Hubert Niewiadomski<sup>3,4</sup>, Piotr Nyczyk<sup>3,4</sup>, Jürgen Müller<sup>2</sup>, Torsten Hoefler<sup>1</sup>**


<sup>1</sup>ETH Zurich   <sup>2</sup>BASF SE   <sup>3</sup>Cledar   <sup>4</sup>IDEAS Research Institute  
 † *Corresponding author*

Inference related

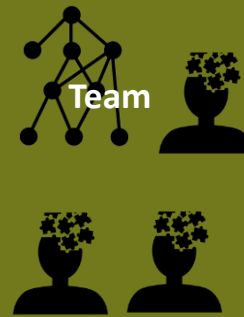
**Reasoning Structures**




**Agents, Tools**

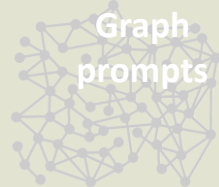






**Psychology**



(„thoughts“) Prompts  


**Prompt engineering**

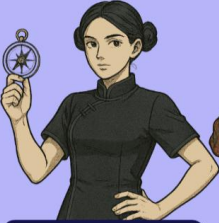





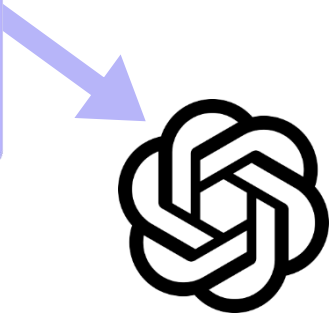
**Retrieval**  




 Graph database  
 Knowledge graph

# Psychology of Agents

# Psychology of Agents





**Analysts (...NT...)**

<b>INTJ ("Architect")</b>	<b>INTP ("Logician")</b>	<b>ENTJ ("Commander")</b>	<b>ENTP ("Debater")</b>
			
Master strategist, excels at complex, long-term planning	Analytical thinker ideal for abstract problem-solving and system design	Effective leader, great at high-stakes decision-making & coordination	Innovative challenger, thrives in brainstorming & rapid ideation







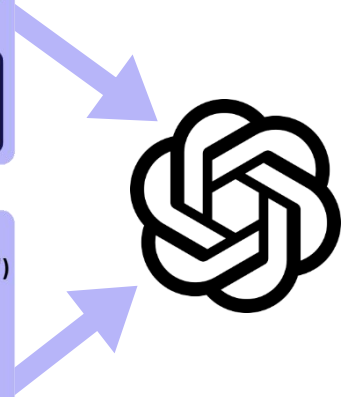
# Psychology of Agents

**Analysts (...NT...)**

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**Diplomats (...NF...)**

<b>INFJ ("Advocate")</b>	<b>INFP ("Mediator")</b>	<b>ENFJ ("Protagonist")</b>	<b>ENFP ("Campaigner")</b>
			
Visionary guide, great at counseling, ethics, and mission-driven tasks	Empathic creator, excels at emotional support and storytelling	Inspirational motivator, ideal for team leadership and persuasion	Energetic connector, great for creative outreach and exploration







# Psychology of Agents

**Analysts (...NT...)**

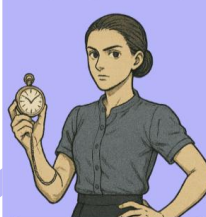



<b>INTJ ("Architect")</b>  Master strategist, excels at complex, long-term planning	<b>INTP ("Logician")</b>  Analytical thinker, ideal for abstract problem-solving and system design	<b>ENTJ ("Commander")</b>  Effective leader, great at high-stakes decision-making & coordination	<b>ENTP ("Debater")</b>  Innovative challenger, thrives in brainstorming & rapid ideation
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**Diplomats (...NF...)**

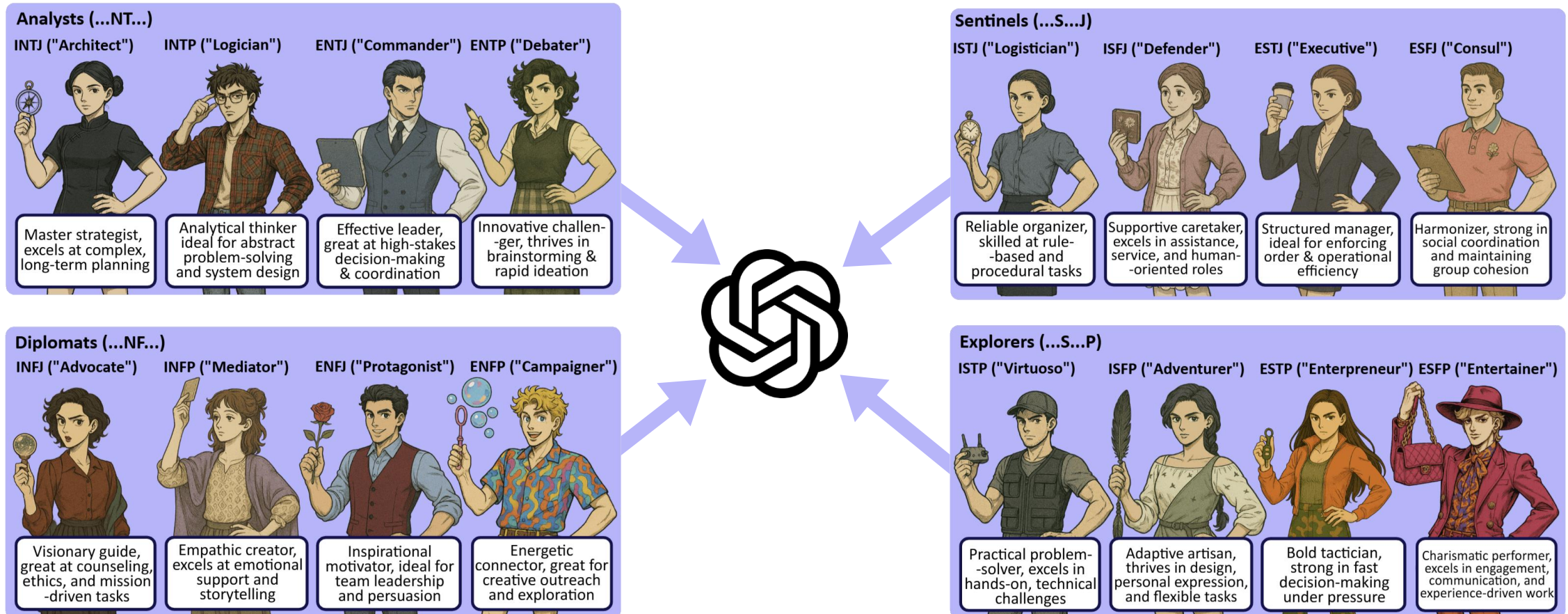
<b>INFJ ("Advocate")</b>  Visionary guide, great at counseling, ethics, and mission-driven tasks	<b>INFP ("Mediator")</b>  Empathic creator, excels at emotional support and storytelling	<b>ENFJ ("Protagonist")</b>  Inspirational motivator, ideal for team leadership and persuasion	<b>ENFP ("Campaigner")</b>  Energetic connector, great for creative outreach and exploration
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**Sentinels (...S...J)**

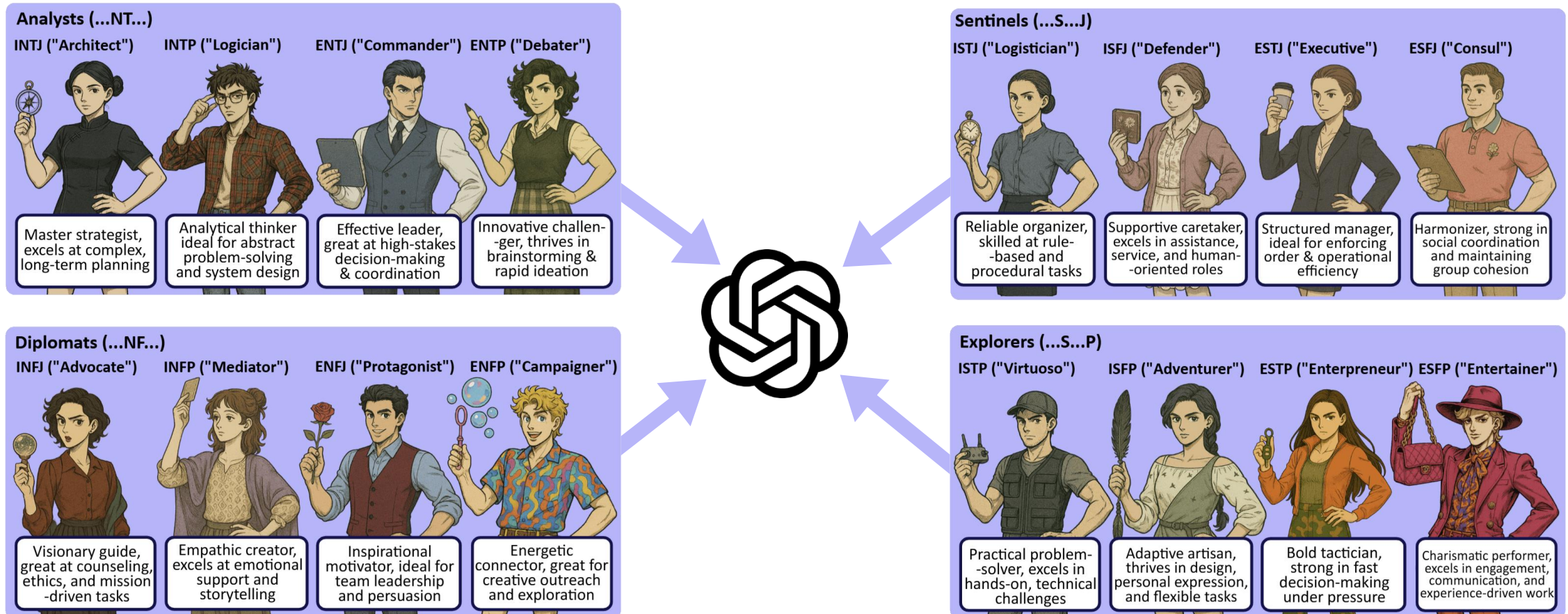
<b>ISTJ ("Logistician")</b>  Reliable organizer, skilled at rule-based and procedural tasks	<b>ISFJ ("Defender")</b>  Supportive caretaker, excels in assistance, service, and human-oriented roles	<b>ESTJ ("Executive")</b>  Structured manager, ideal for enforcing order & operational efficiency	<b>ESFJ ("Consul")</b>  Harmonizer, strong in social coordination and maintaining group cohesion
--	--	--	---

# Psychology of Agents



# Psychology of Agents

## Graph as a model of the inter-agent communication pattern



# Psychology of Agents

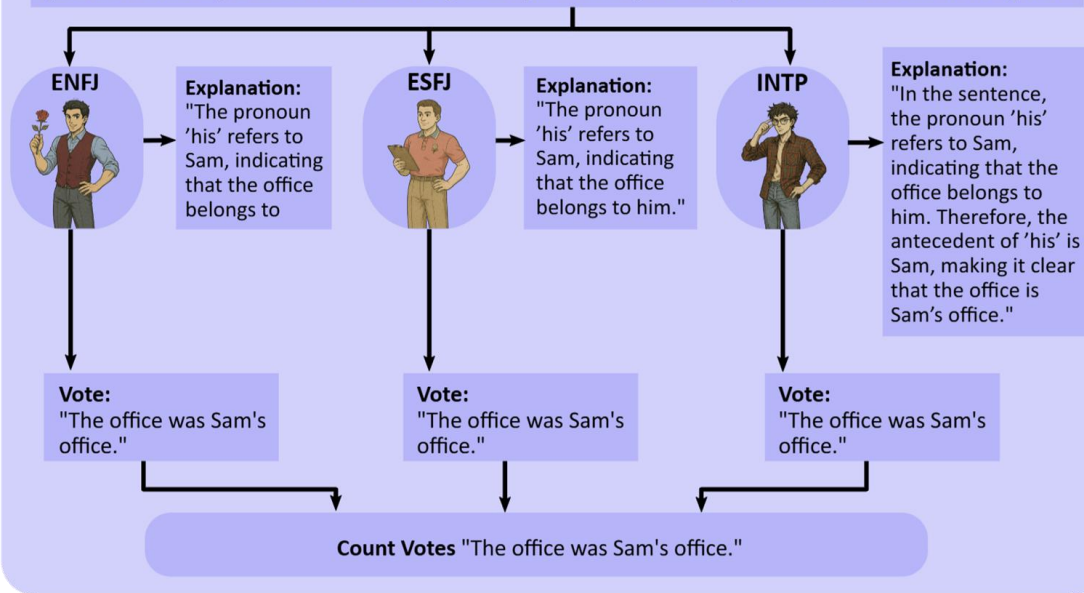
Graph as a model of the inter-agent communication pattern

# Psychology of Agents

## Graph as a model of the inter-agent communication pattern

### Majority Voting

**Task Description:** "In the following sentences, explain the antecedent of the pronoun (which thing the pronoun refers to), or state that it is ambiguous. *After meeting with the producers, Sam went to his office.*"

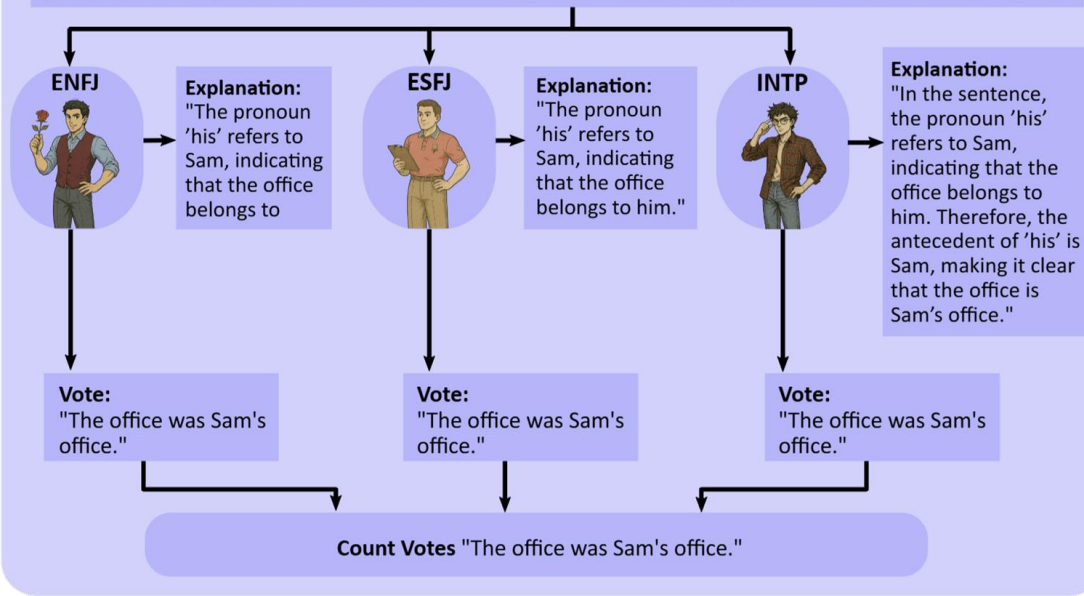


# Psychology of Agents

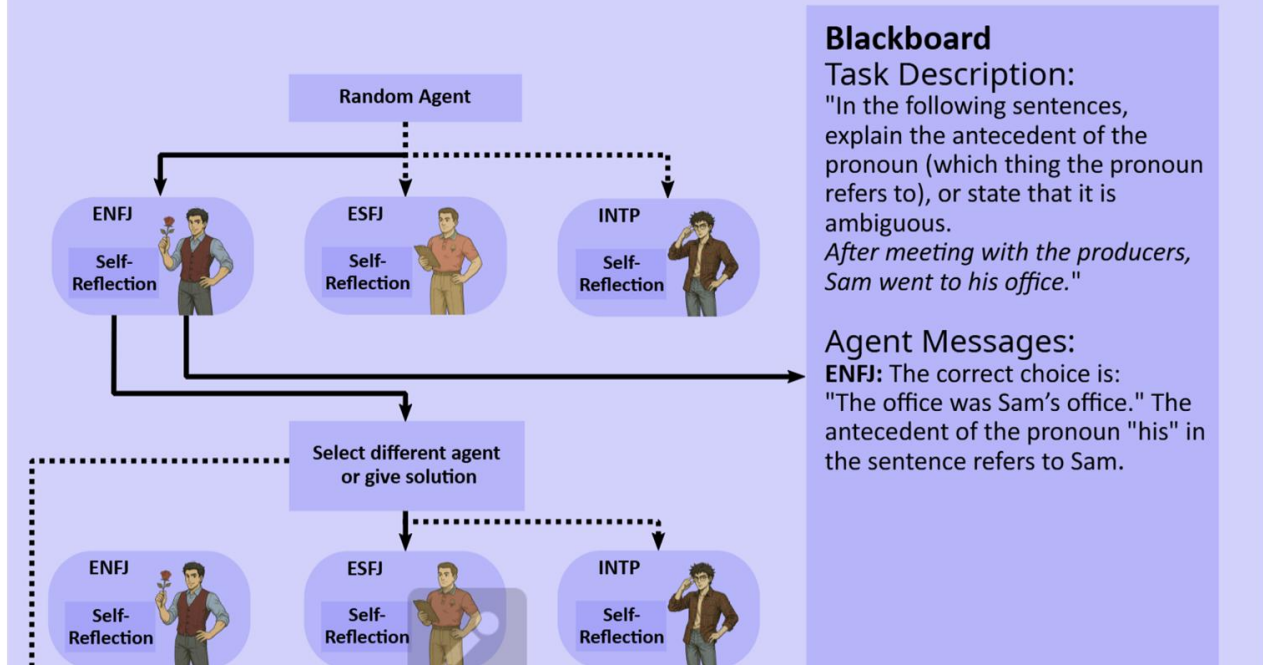
## Graph as a model of the inter-agent communication pattern

### Majority Voting

**Task Description:** "In the following sentences, explain the antecedent of the pronoun (which thing the pronoun refers to), or state that it is ambiguous. *After meeting with the producers, Sam went to his office.*"



### Interactive Communication



# Graphs in the LLM Pipeline: Overview


## Psychologically Enhanced AI Agents

**Maciej Besta<sup>1†</sup>, Shriram Chandran<sup>1</sup>, Robert Gerstenberger<sup>1</sup>, Mathis Lindner<sup>1</sup>,  
 Marcin Chrapek<sup>1</sup>, Sebastian Hermann Martschat<sup>2</sup>, Taraneh Ghandi<sup>2\*</sup>, Patrick Iff<sup>1</sup>,  
 Hubert Niewiadomski<sup>3,4</sup>, Piotr Nyczyk<sup>3,4</sup>, Jürgen Müller<sup>2</sup>, Torsten Hoefler<sup>1</sup>**

<sup>1</sup>ETH Zurich   <sup>2</sup>BASF SE   <sup>3</sup>Cledar   <sup>4</sup>IDEAS Research Institute  
 † *Corresponding author*

Inference related

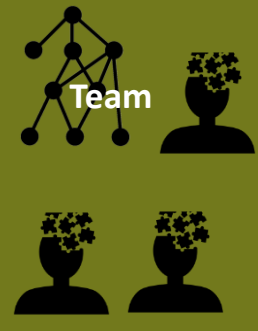
**Reasoning Structures**




**Agents, Tools**

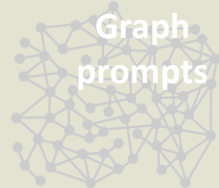


**Psychology**




(„thoughts“) Prompts  


**Prompt engineering**



**Retrieval**



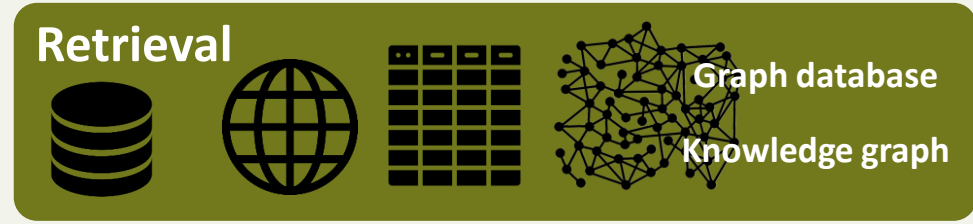
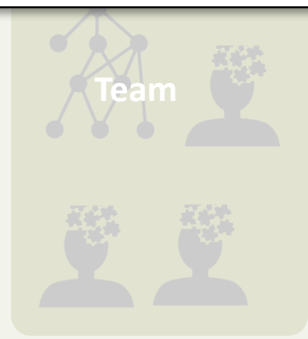
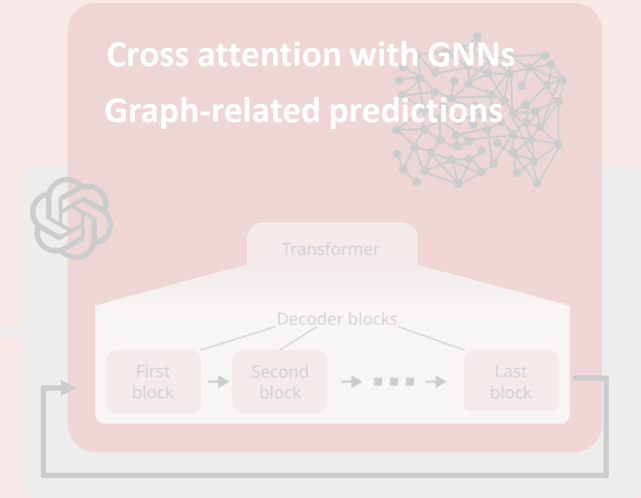
Graph database  
Knowledge graph

# Graphs in the LLM Pipeline: Overview

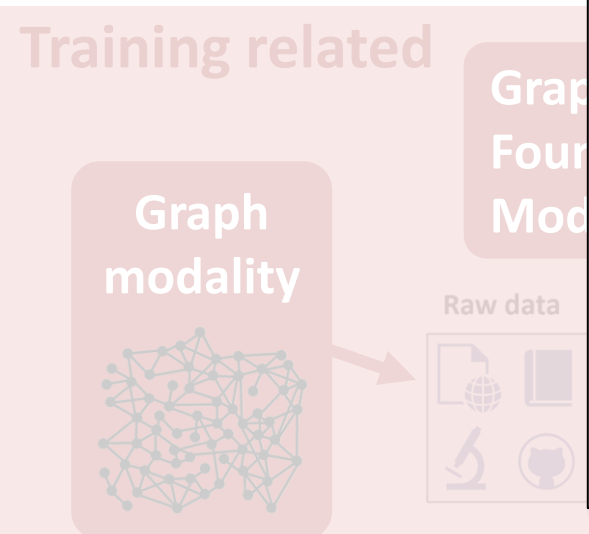
## Multi-Head RAG: Solving Multi-Aspect Problems with LLMs

Maciej Besta<sup>1\*</sup> Ales Kubicek<sup>1</sup> Roman Niggli<sup>1</sup> Robert Gerstenberger<sup>1</sup>  
 Lucas Weitzendorf<sup>1</sup> Mingyuan Chi<sup>1</sup> Patrick Iff<sup>1</sup> Joanna Gajda<sup>2</sup>  
 Piotr Nyczyk<sup>2</sup> Jürgen Müller<sup>3</sup> Hubert Niewiadomski<sup>2</sup> Marcin Chrapek<sup>1</sup>  
 Michał Podstawski<sup>4</sup> Torsten Hoeffler<sup>1</sup>

<sup>1</sup>ETH Zurich <sup>2</sup>Cledar <sup>3</sup>BASF SE <sup>4</sup>Warsaw University of Technology

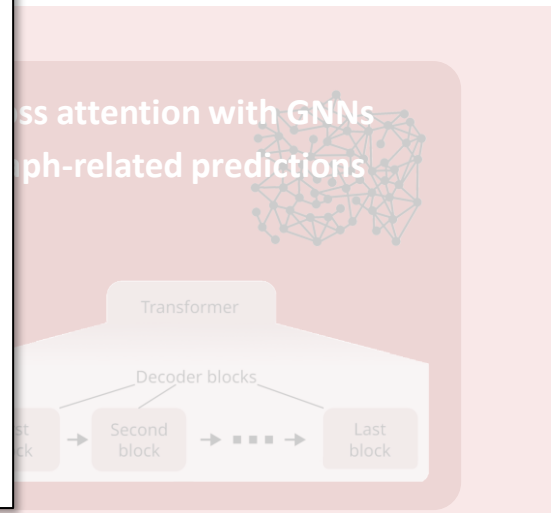


# Graphs in the LLM



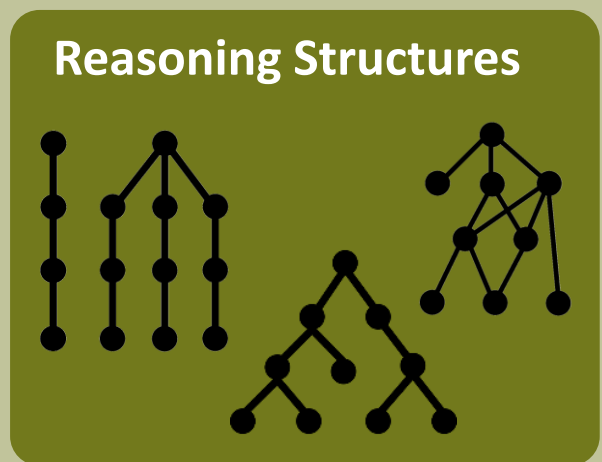
## CHECKEMBED: Effective Verification of LLM Solutions to Open-Ended Tasks

<b>Maciej Besta*</b> ETH Zurich	<b>Lorenzo Paleari</b> ETH Zurich	<b>Marcin Copik</b> ETH Zurich	<b>Robert Gerstenberger</b> ETH Zurich	<b>Ales Kubicek</b> ETH Zurich
<b>Piotr Nyczyk</b> Cledar	<b>Patrick Iff</b> ETH Zurich	<b>Eric Schreiber</b> ETH Zurich	<b>Tanja Srin dran</b> ETH Zurich	
<b>Tomasz Lehmann</b> Cledar Warsaw University of Technology	<b>Hubert Niewiadomski</b> Cledar IDEAS Research Institute	<b>Torsten Hoeffler</b> ETH Zurich		



## Inference related

**Reasoning Structures**



**Agents, Tools**

GNN  
Heuristic  
DAG



**Psychology**

Team



Replies („thoughts“)

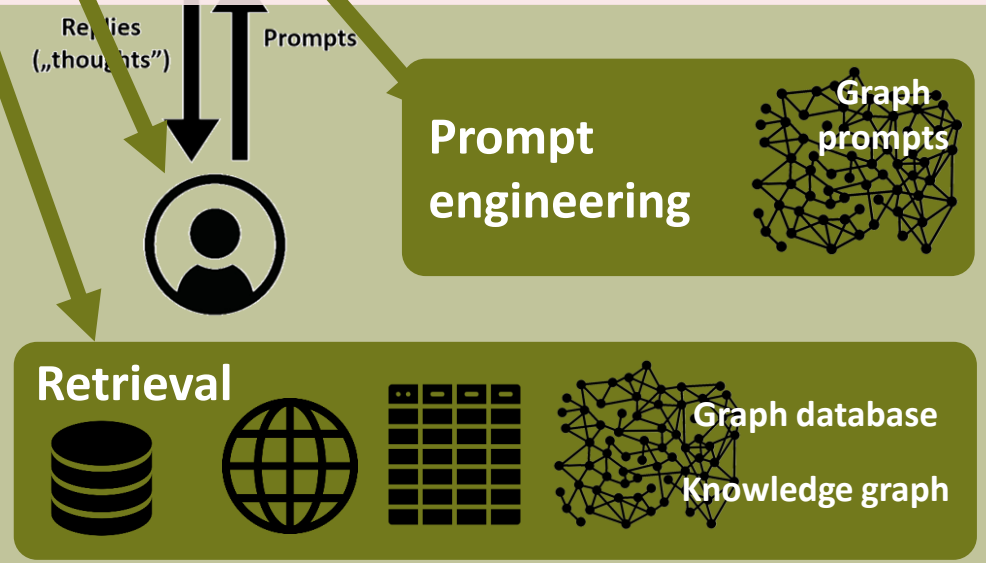
Prompts

**Prompt engineering**

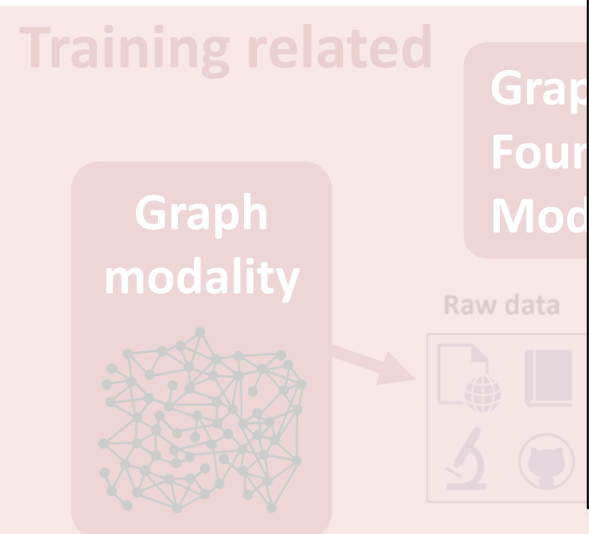
Graph prompts

**Retrieval**

Graph database  
Knowledge graph

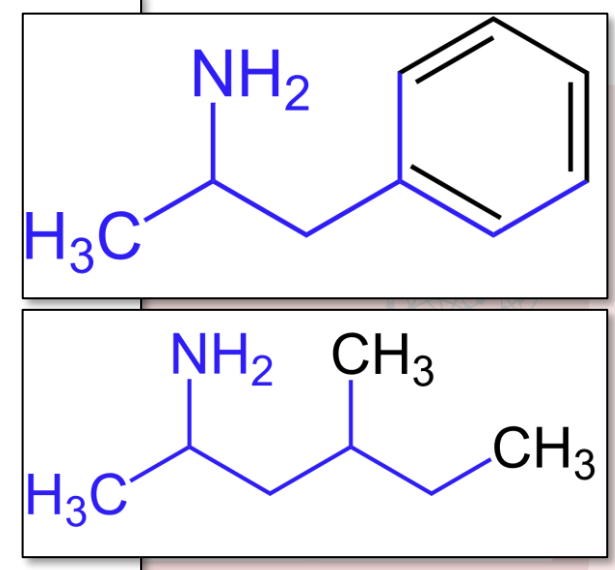


# Graphs in the LLM



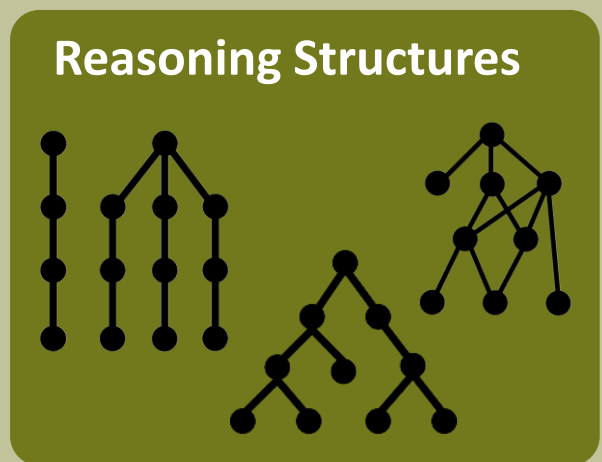
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<b>Piotr Nyczyk</b> Cledar	<b>Patrick Iff</b> ETH Zurich	<b>Eric Schreiber</b> ETH Zurich	<b>Tanja Srin dran</b> ETH Zurich	
<b>Tomasz Lehmann</b> Cledar Warsaw University of Technology	<b>Hubert Niewiadomski</b> Cledar IDEAS Research Institute	<b>Torsten Hoeffler</b> ETH Zurich		



## Inference related

**Reasoning Structures**



**Agents, Tools**

GNN  
Heuristic  
DAG



**Psychology**

Team



Replies („thoughts“)

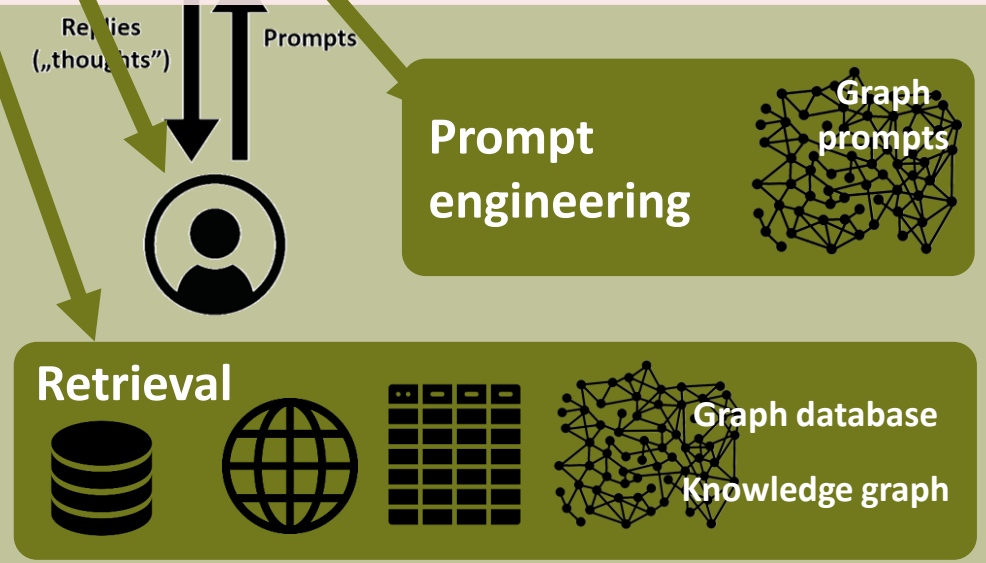
Prompts

**Prompt engineering**

Graph prompts

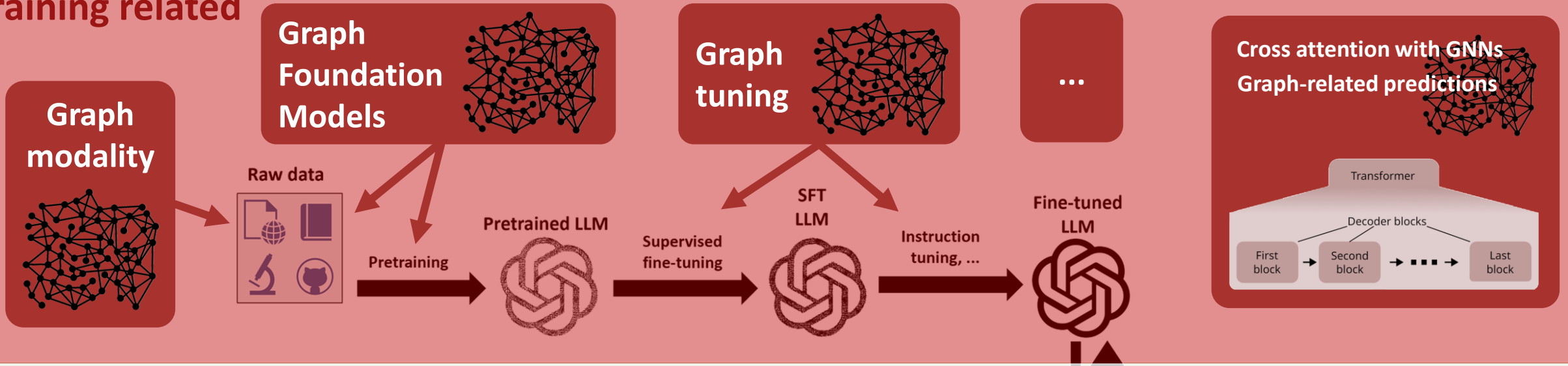
**Retrieval**

Graph database  
Knowledge graph



# Graphs in the LLM Pipeline: Overview

## Training related

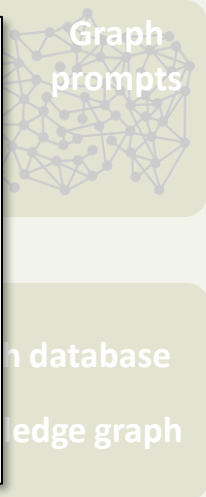
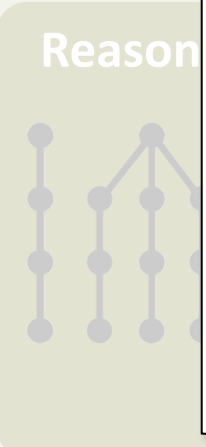


## Inference related

## Reasoning Language Models: A Blueprint

Maciej Besta<sup>1†</sup>, Julia Barth<sup>1</sup>, Eric Schreiber<sup>1</sup>, Ales Kubicek<sup>1</sup>, Afonso Catarino<sup>1</sup>, Robert Gerstenberger<sup>1</sup>,  
 Piotr Nyczyk<sup>2</sup>, Patrick Iff<sup>1</sup>, Yueling Li<sup>3</sup>, Sam Houlston<sup>1</sup>, Tomasz Sternal<sup>1</sup>, Marcin Copik<sup>1</sup>, Grzegorz  
 Kwaśniewski<sup>1</sup>, Jürgen Müller<sup>3</sup>, Łukasz Flis<sup>4</sup>, Hannes Eberhard<sup>1</sup>, Hubert Niewiadomski<sup>2</sup>, Torsten Hoefler<sup>1</sup>

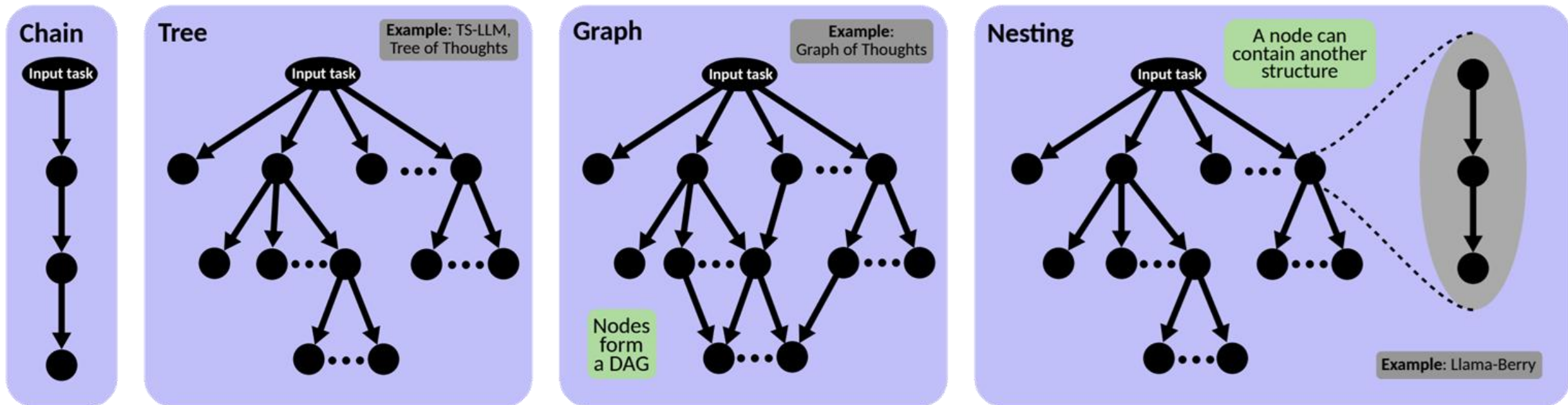
<sup>†</sup>Corresponding author    <sup>1</sup>ETH Zurich    <sup>2</sup>Cledar    <sup>3</sup>BASF SE    <sup>4</sup>Cyfronet AGH



Replies („thoughts“)  
Prompts

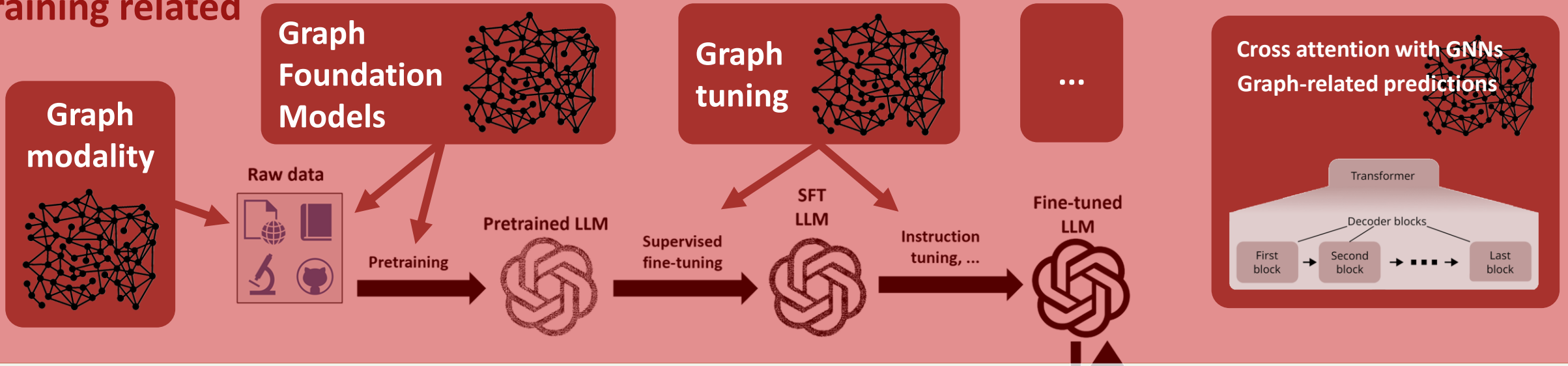
# Reasoning Paradigms

## Graph as a model of the reasoning process (training)



# Graphs in the LLM Pipeline: Overview

## Training related

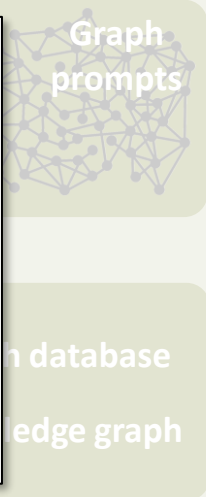
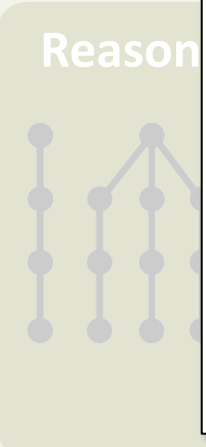


## Inference related

## Reasoning Language Models: A Blueprint

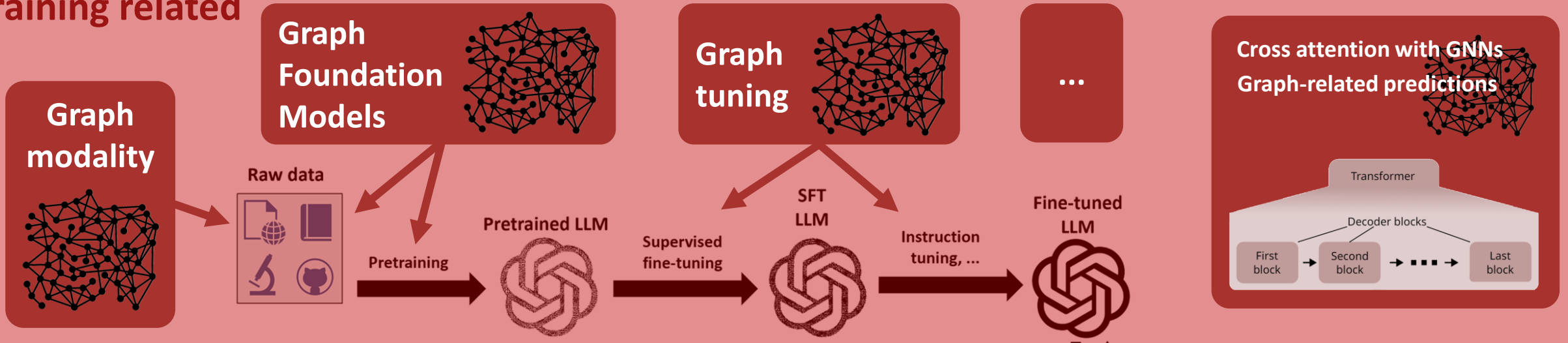
Maciej Besta<sup>1†</sup>, Julia Barth<sup>1</sup>, Eric Schreiber<sup>1</sup>, Ales Kubicek<sup>1</sup>, Afonso Catarino<sup>1</sup>, Robert Gerstenberger<sup>1</sup>,  
 Piotr Nyczyk<sup>2</sup>, Patrick Iff<sup>1</sup>, Yueling Li<sup>3</sup>, Sam Houlston<sup>1</sup>, Tomasz Sternal<sup>1</sup>, Marcin Copik<sup>1</sup>, Grzegorz  
 Kwaśniewski<sup>1</sup>, Jürgen Müller<sup>3</sup>, Łukasz Flis<sup>4</sup>, Hannes Eberhard<sup>1</sup>, Hubert Niewiadomski<sup>2</sup>, Torsten Hoefler<sup>1</sup>

<sup>†</sup>Corresponding author    <sup>1</sup>ETH Zurich    <sup>2</sup>Cledar    <sup>3</sup>BASF SE    <sup>4</sup>Cyfronet AGH



# Graphs in the LLM Pipeline: Overview

## Training related

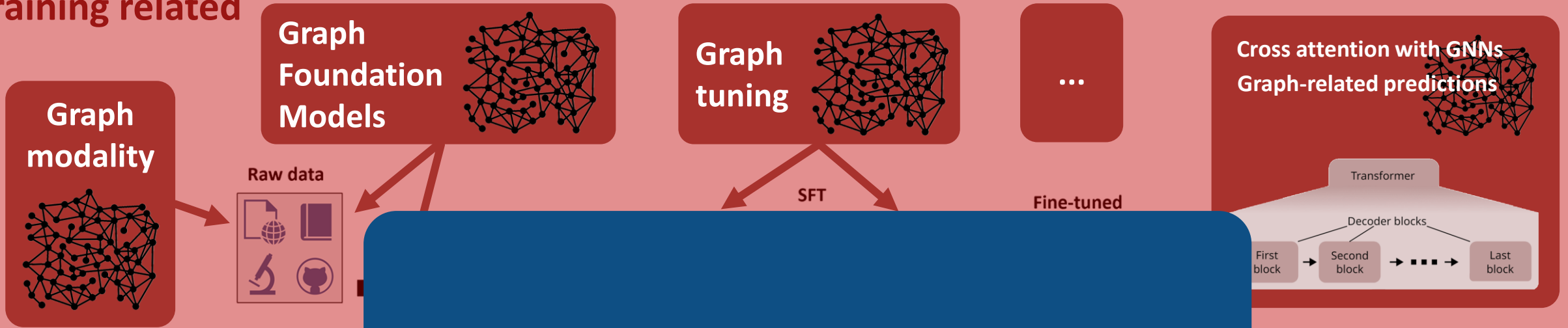


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related

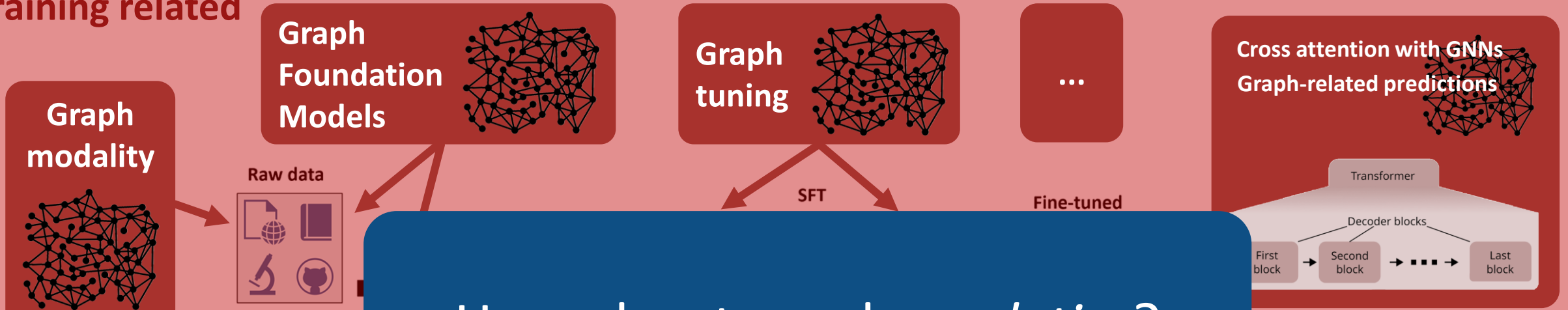


## Inference related



# Graphs in the LLM Pipeline: Overview

## Training related



How about graph *analytics*?

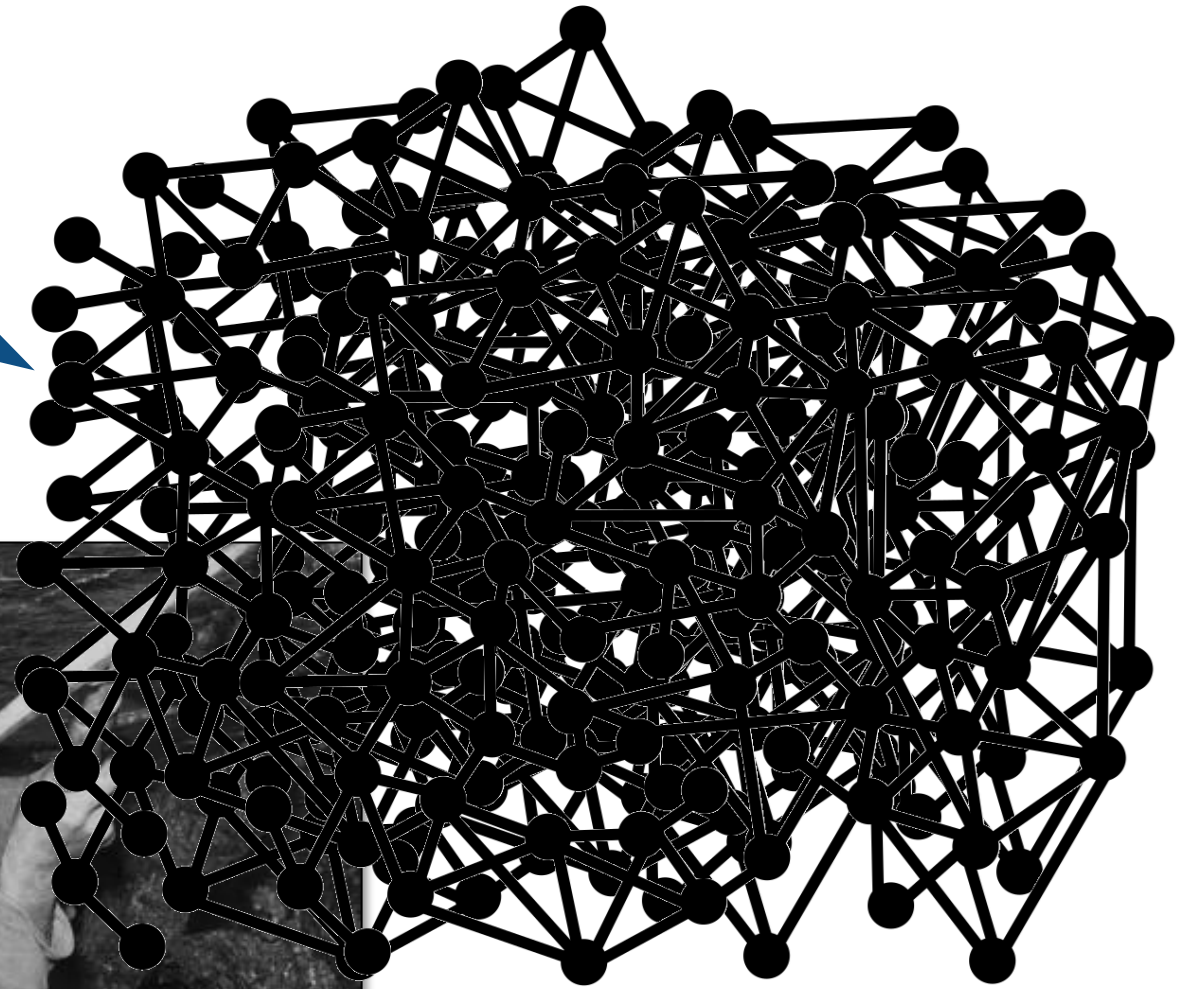
## Inference related



# Graph Analytics

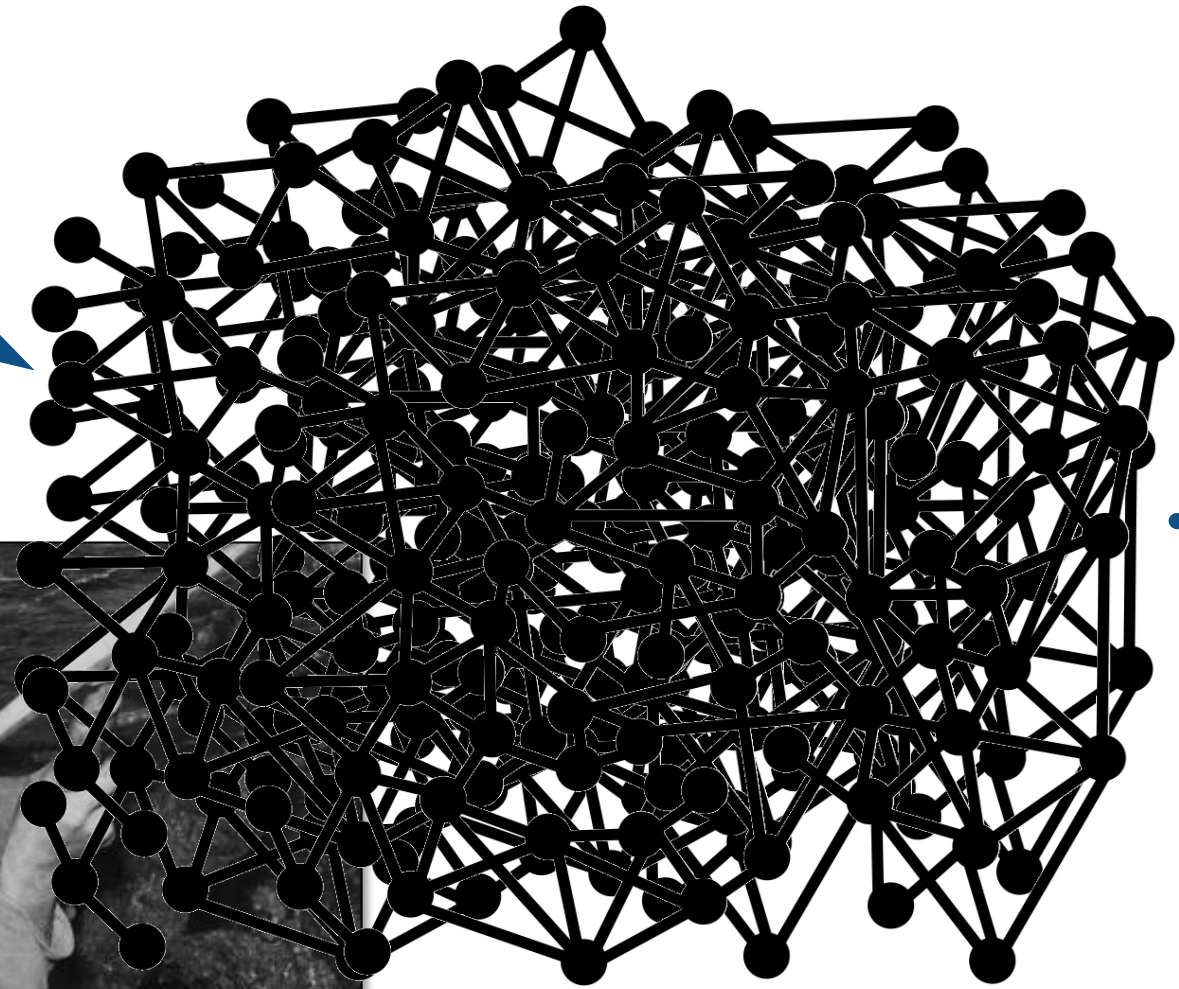
# Graph Analytics

A huge & complex graph dataset

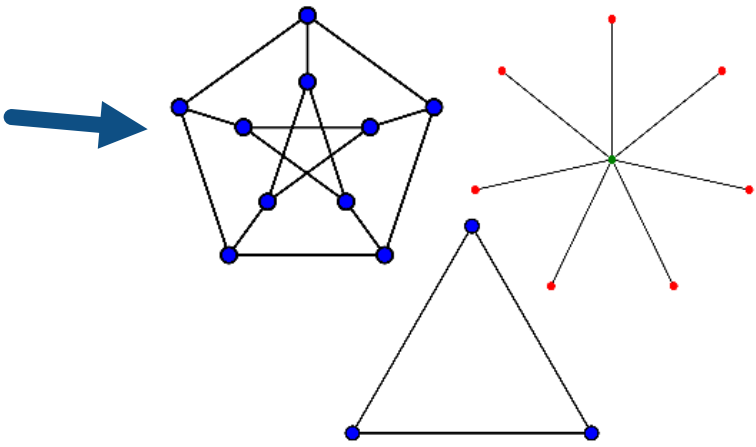


# Graph Analytics

A huge & complex graph dataset



Pattern counting (triangles, higher-order cliques, dense subgraphs, ...)

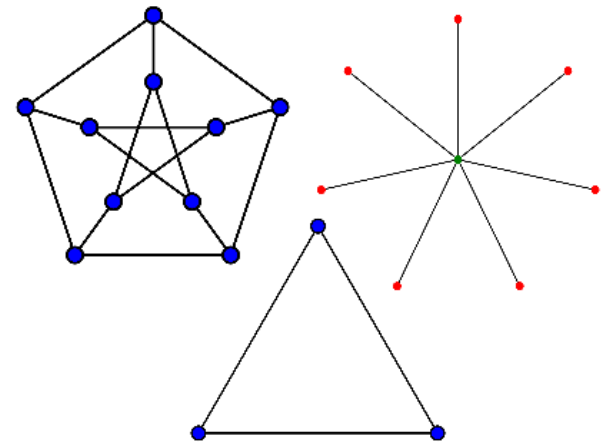


# Graph Analytics

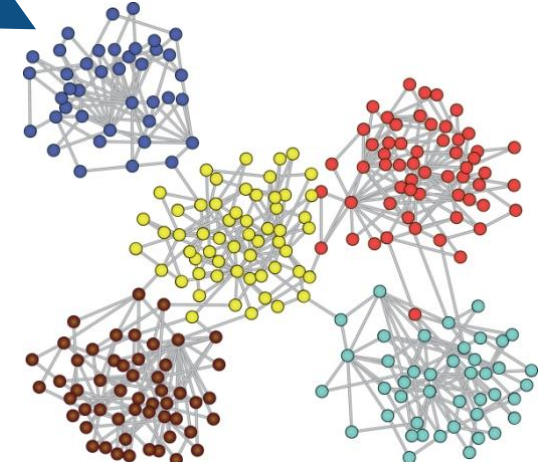
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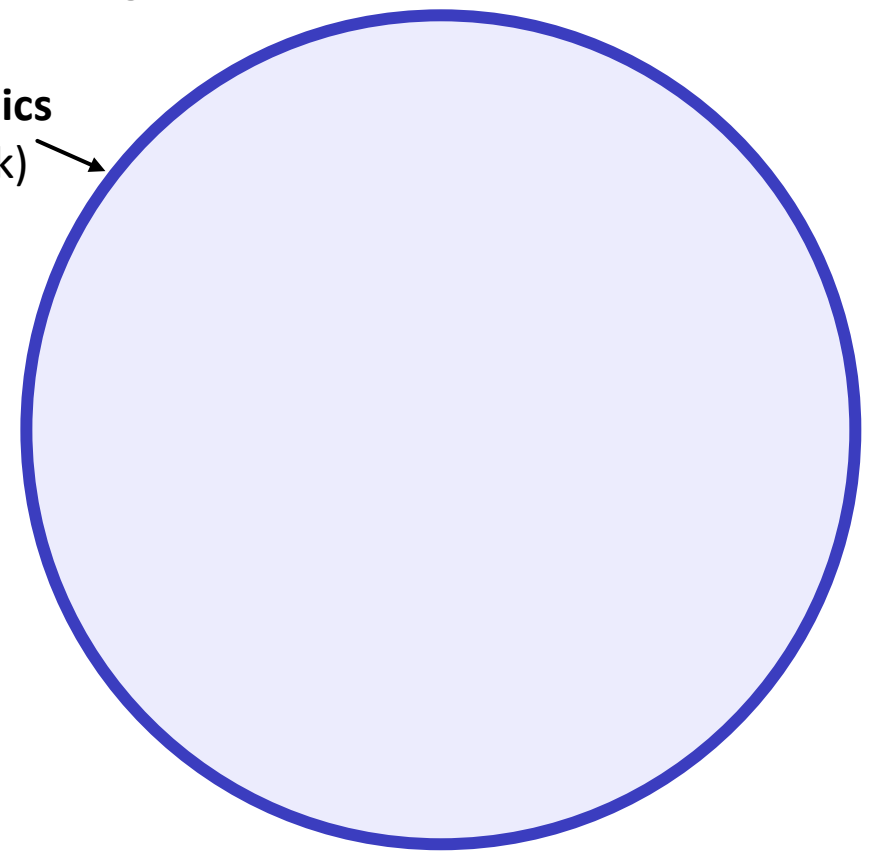
Clustering, Link Prediction, Vertex Similarity, ...



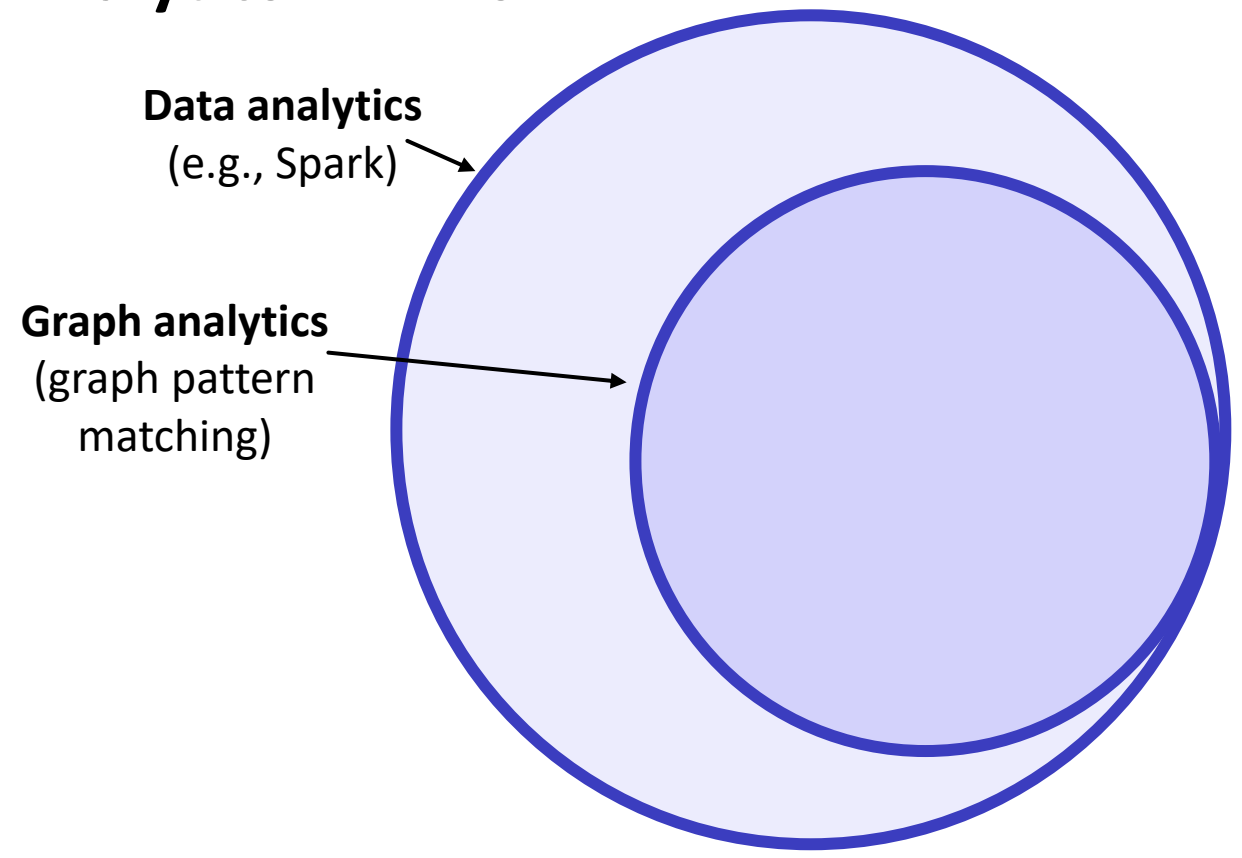
# Graph Analytics + LLMs

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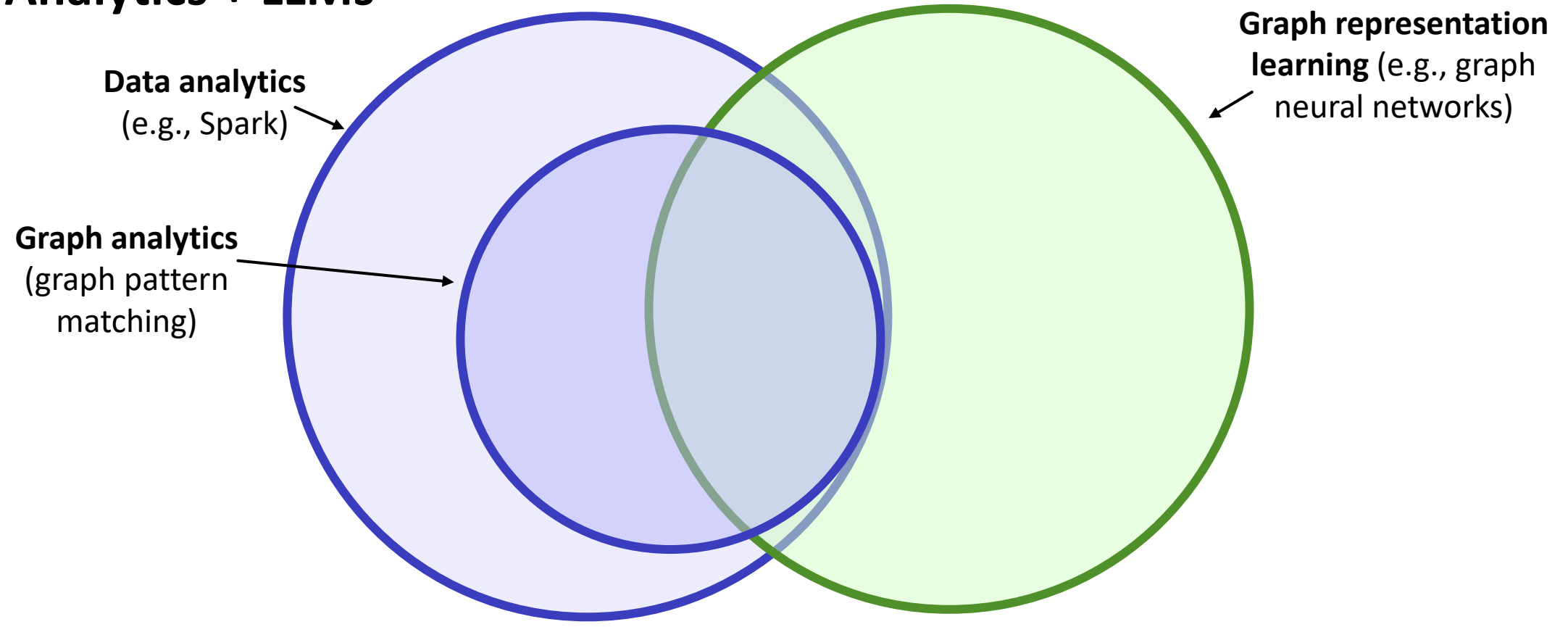
Data analytics  
(e.g., Spark) →



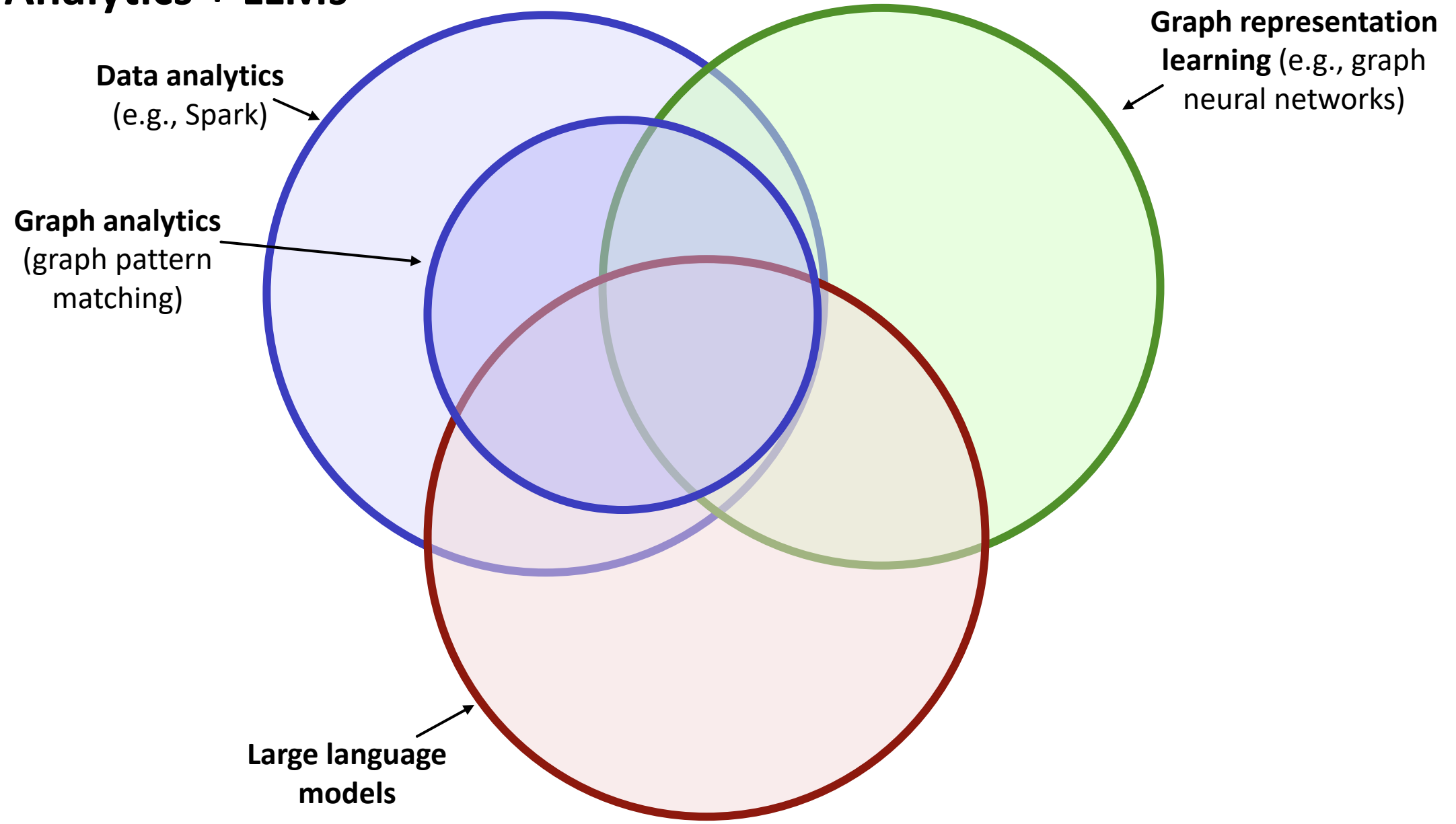
# Graph Analytics + LLMs



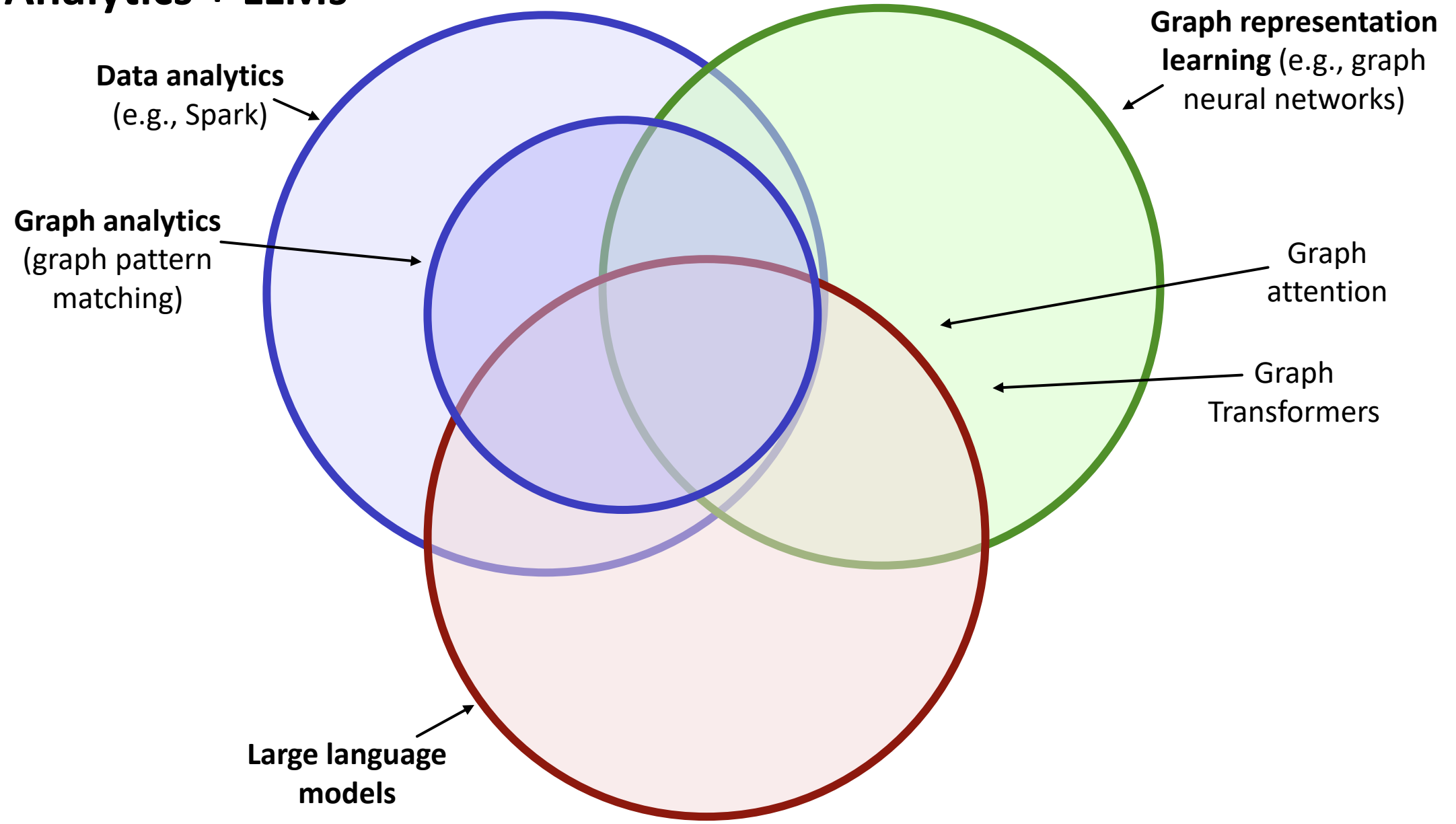
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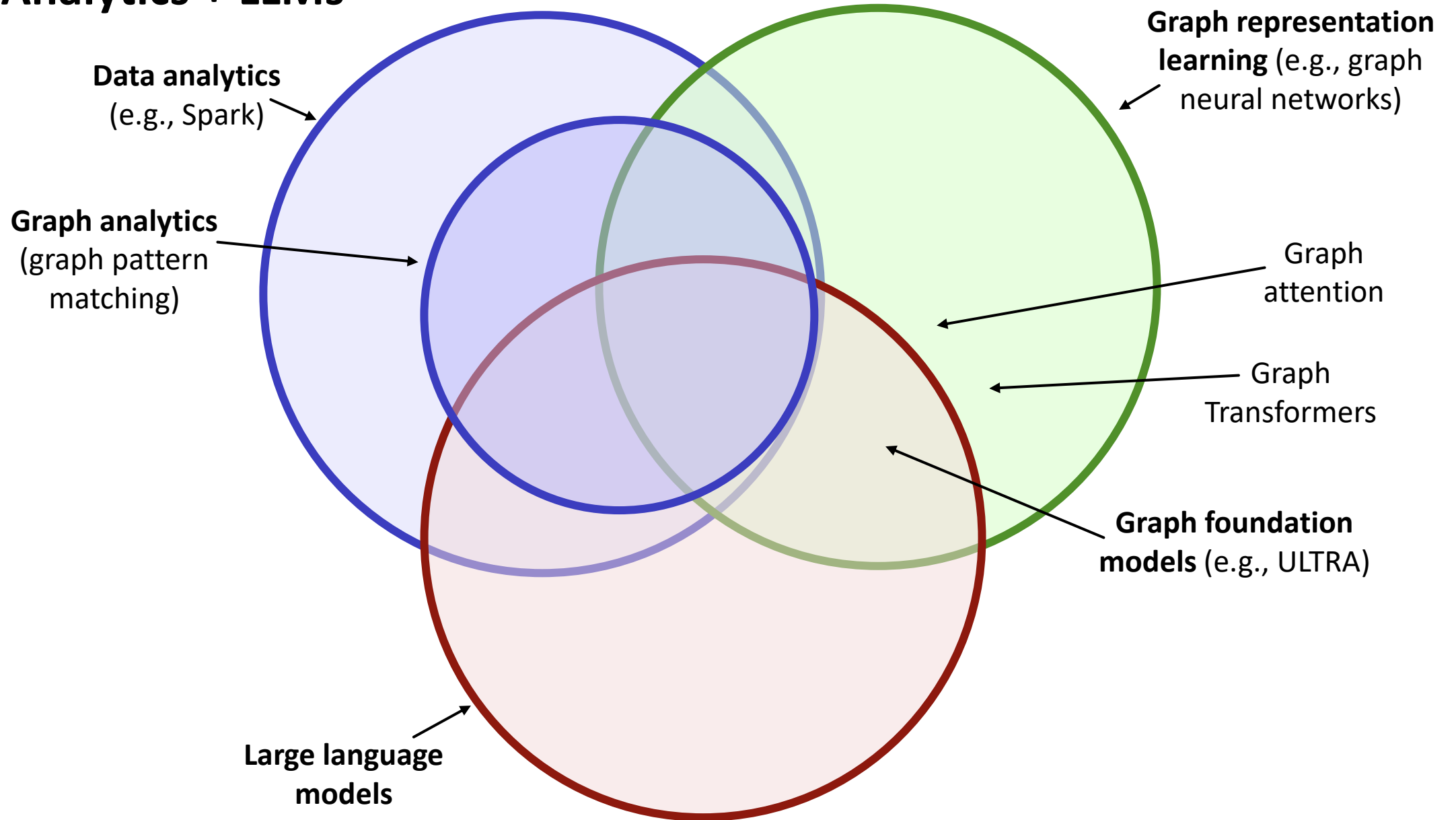
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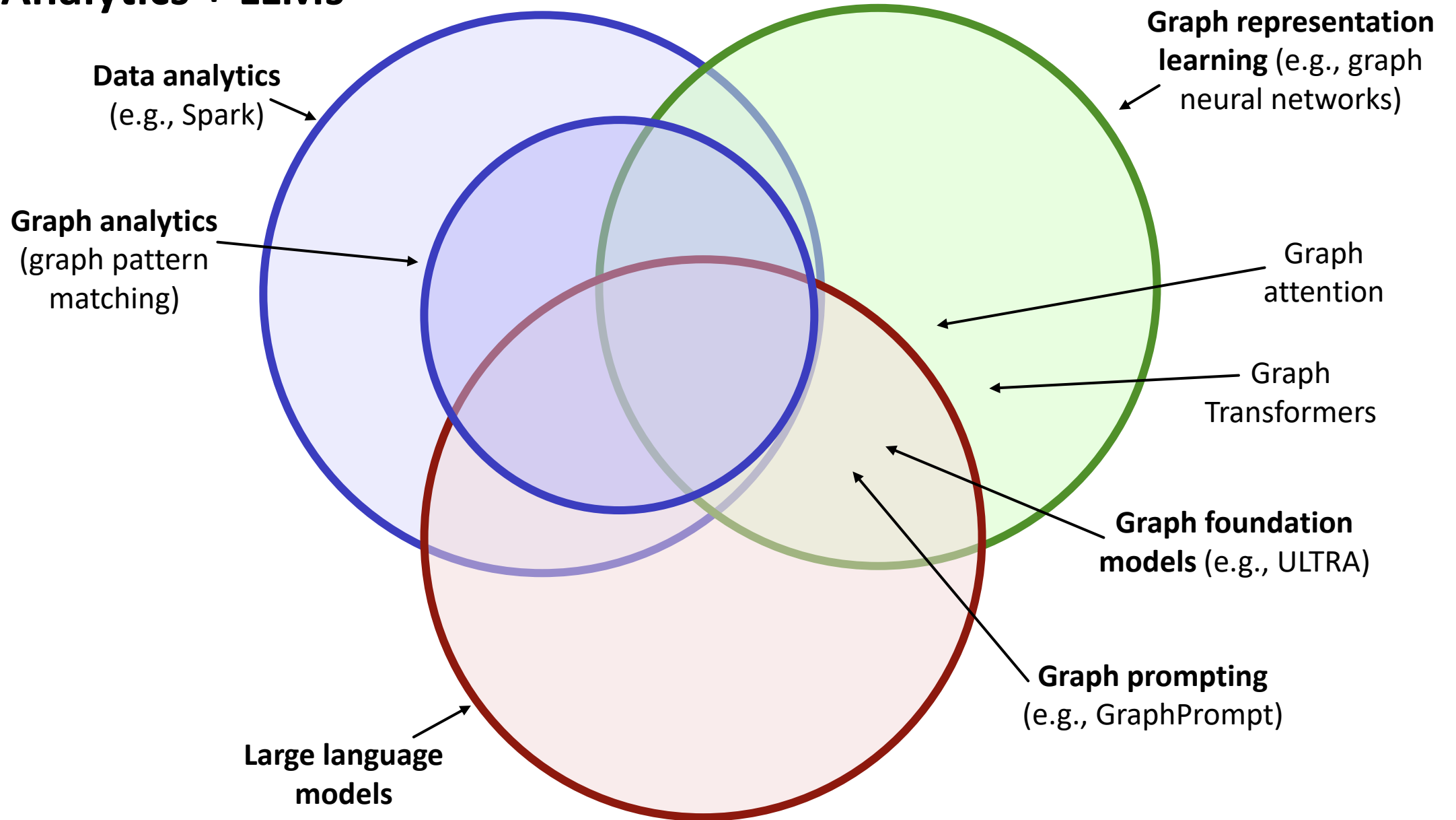
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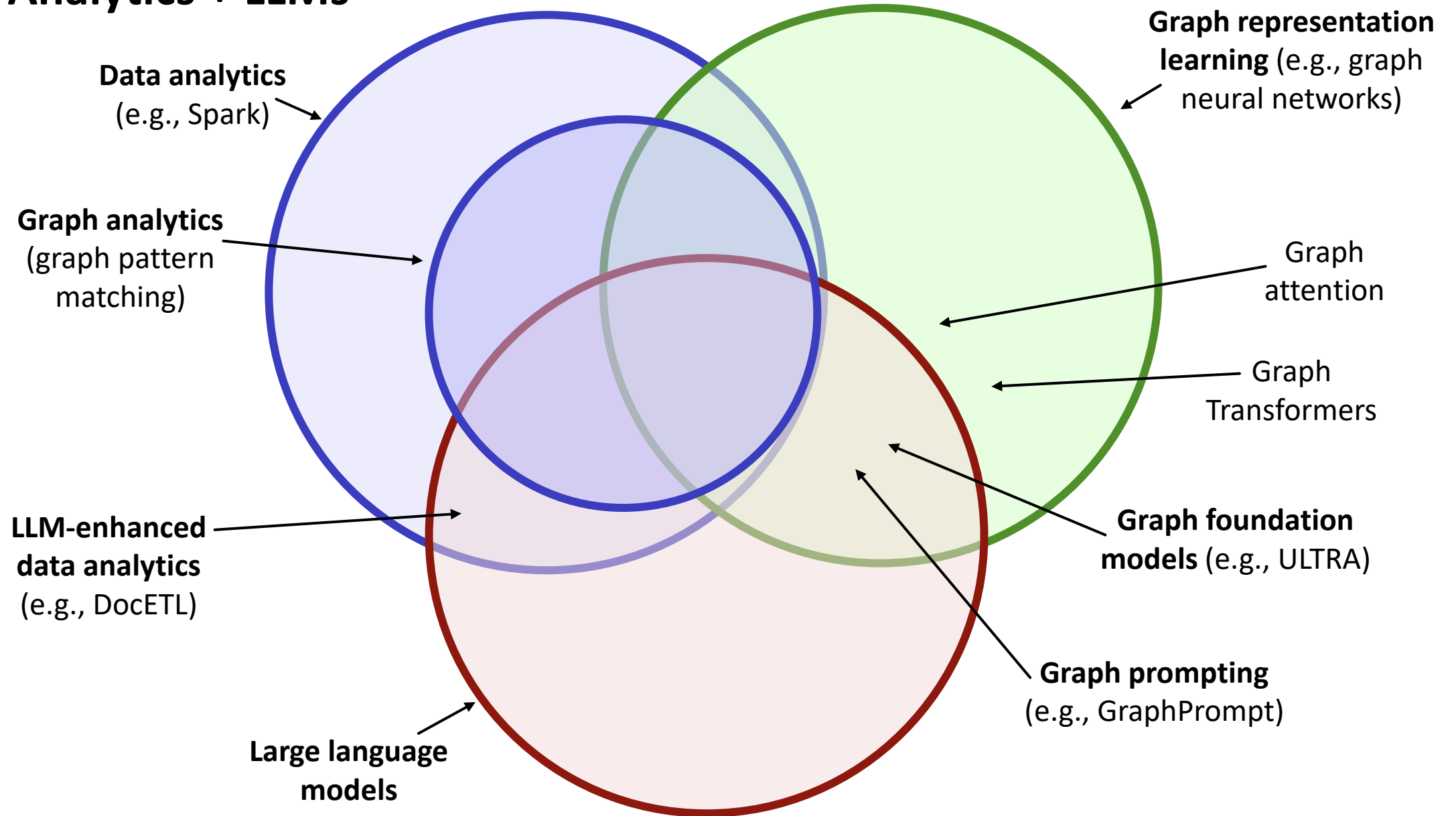
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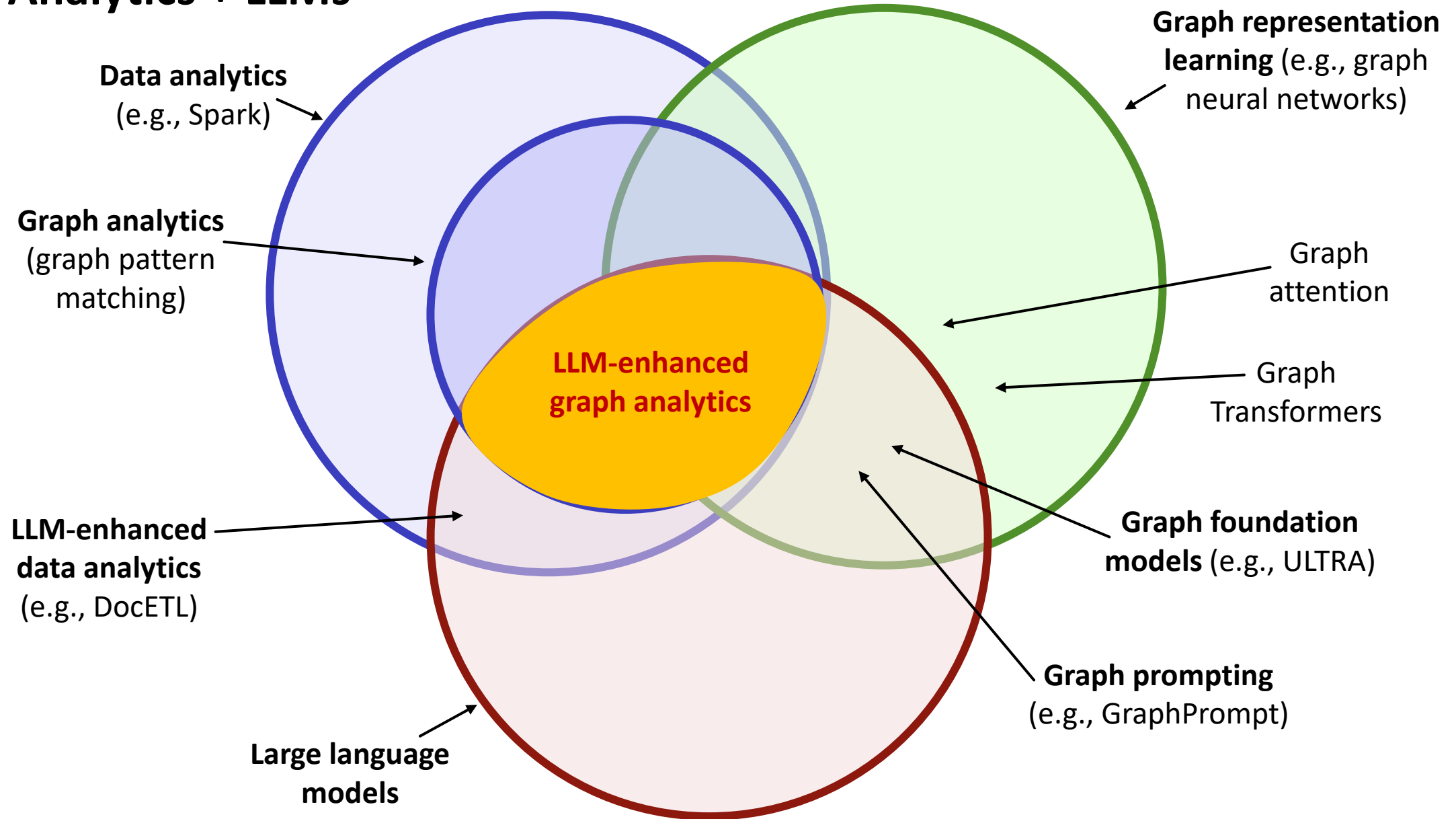
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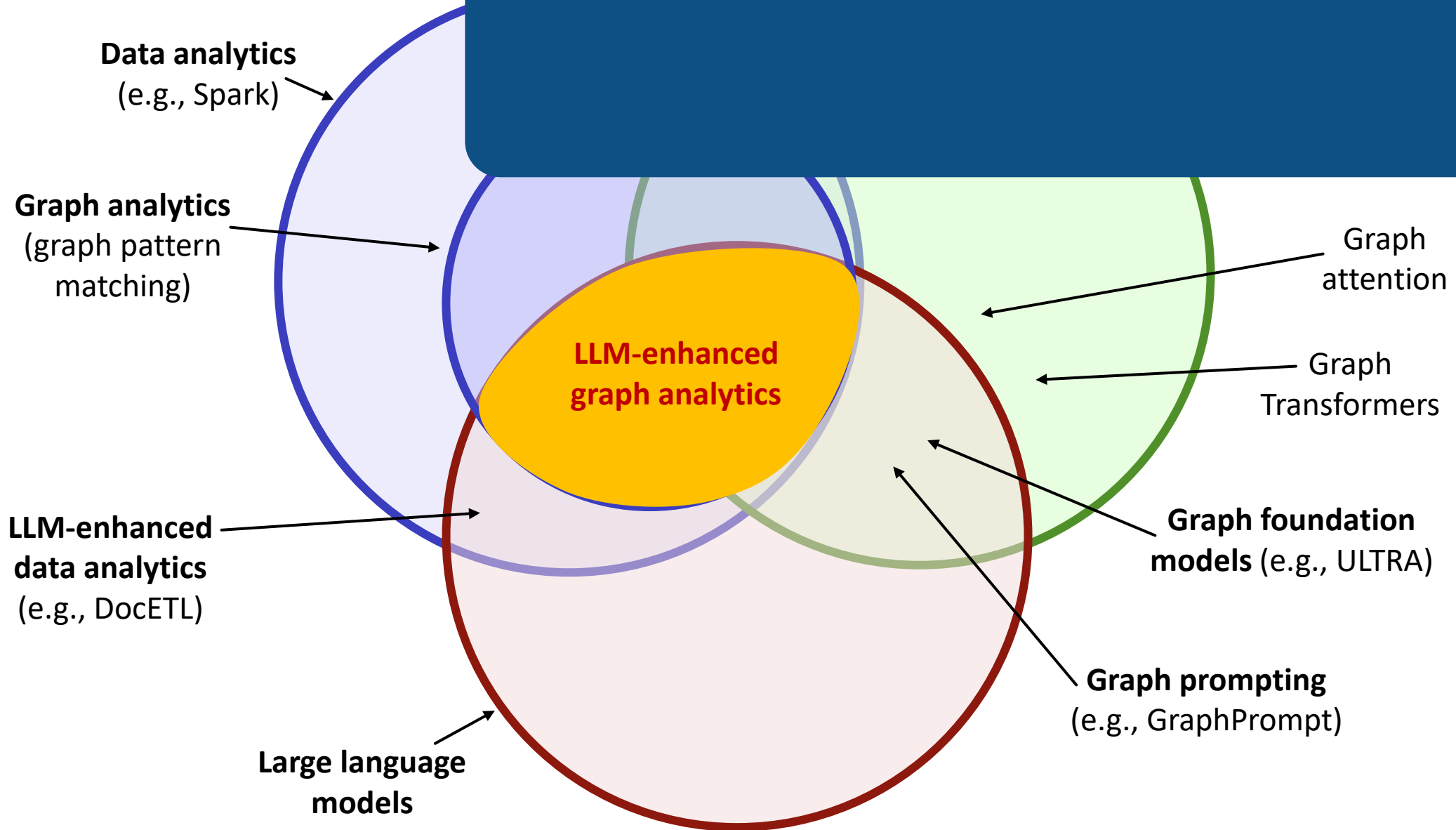


# Graph Analytics + LLMs

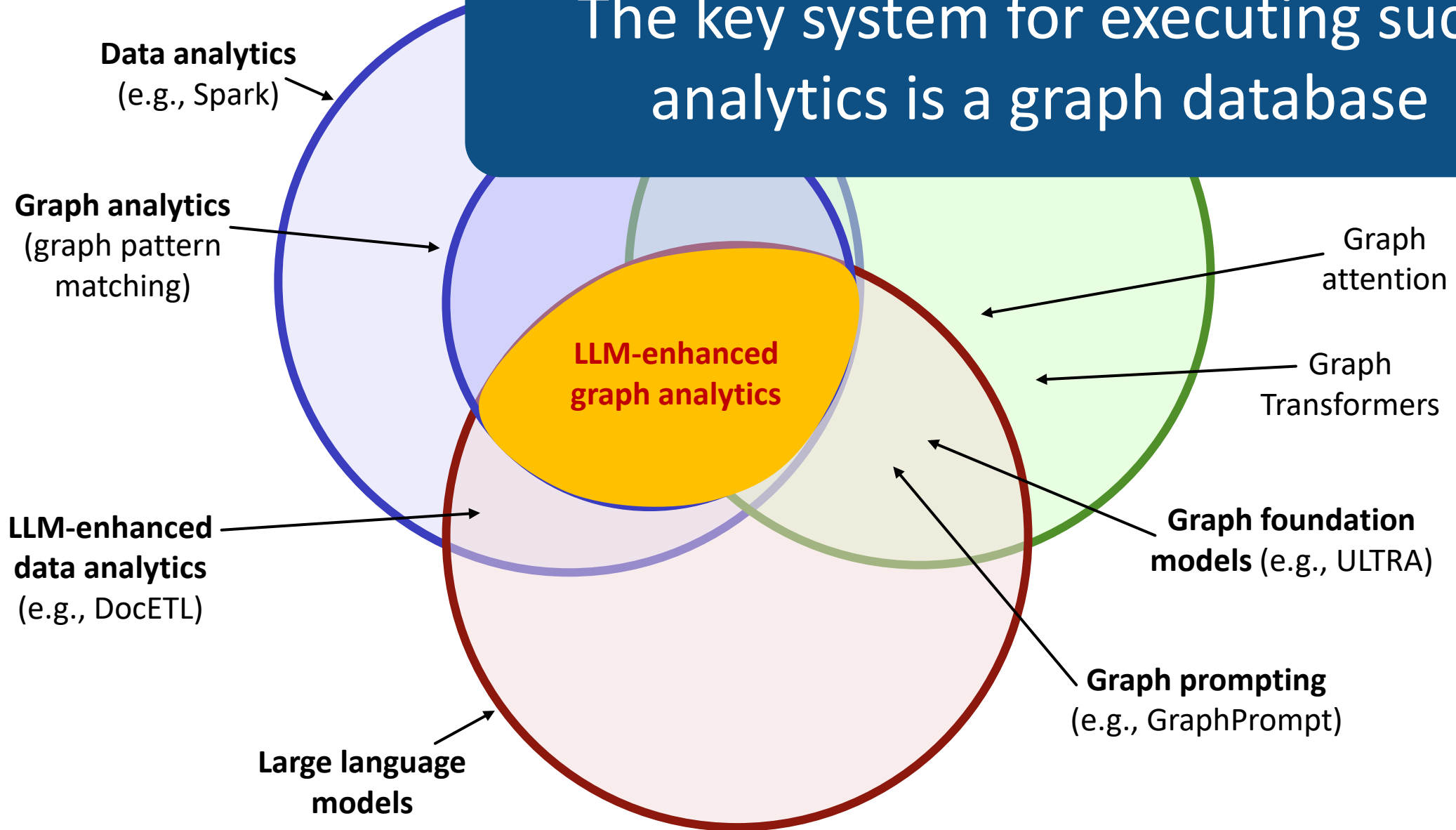




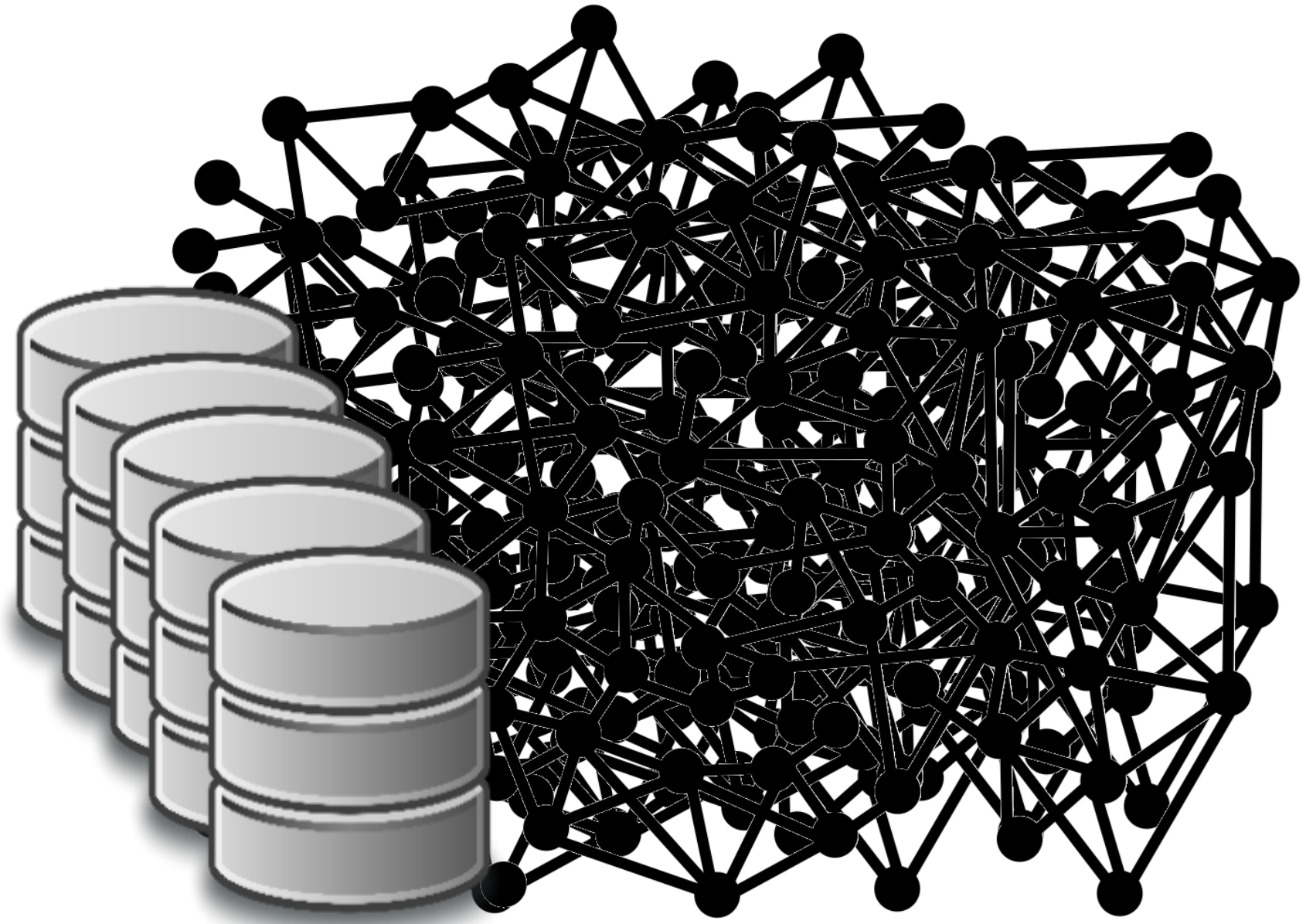
# Graph Analytics + LLMs



The key system for executing such analytics is a graph database

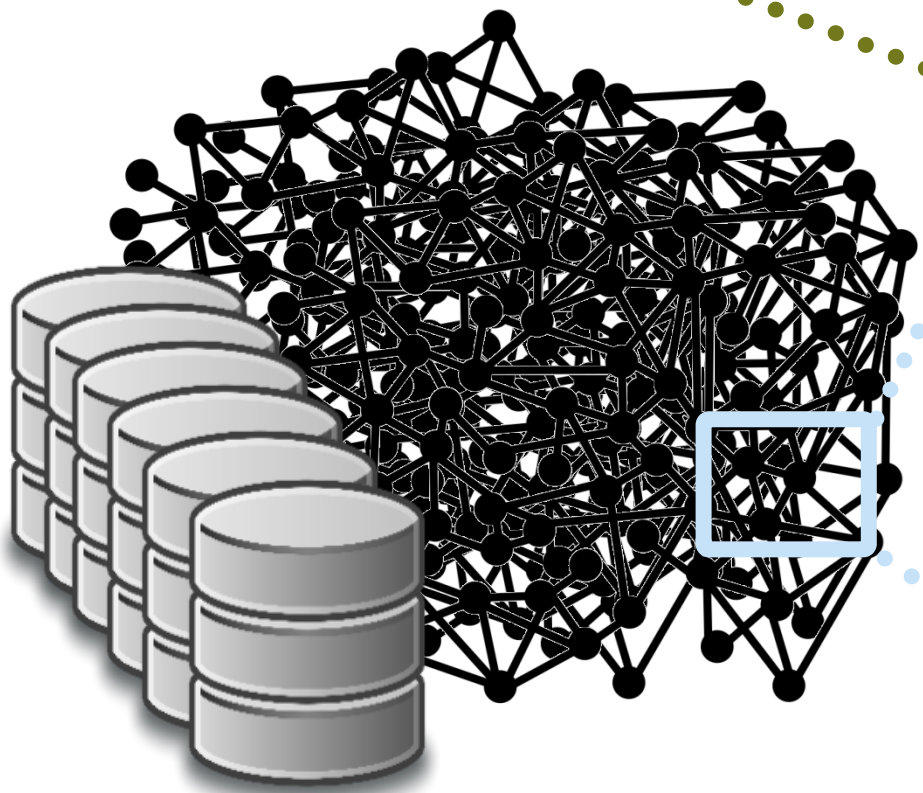


# Graph Databases (GDBs): A Very Brief Introduction





# Graph Databases: The Labeled Property Graph Data Model

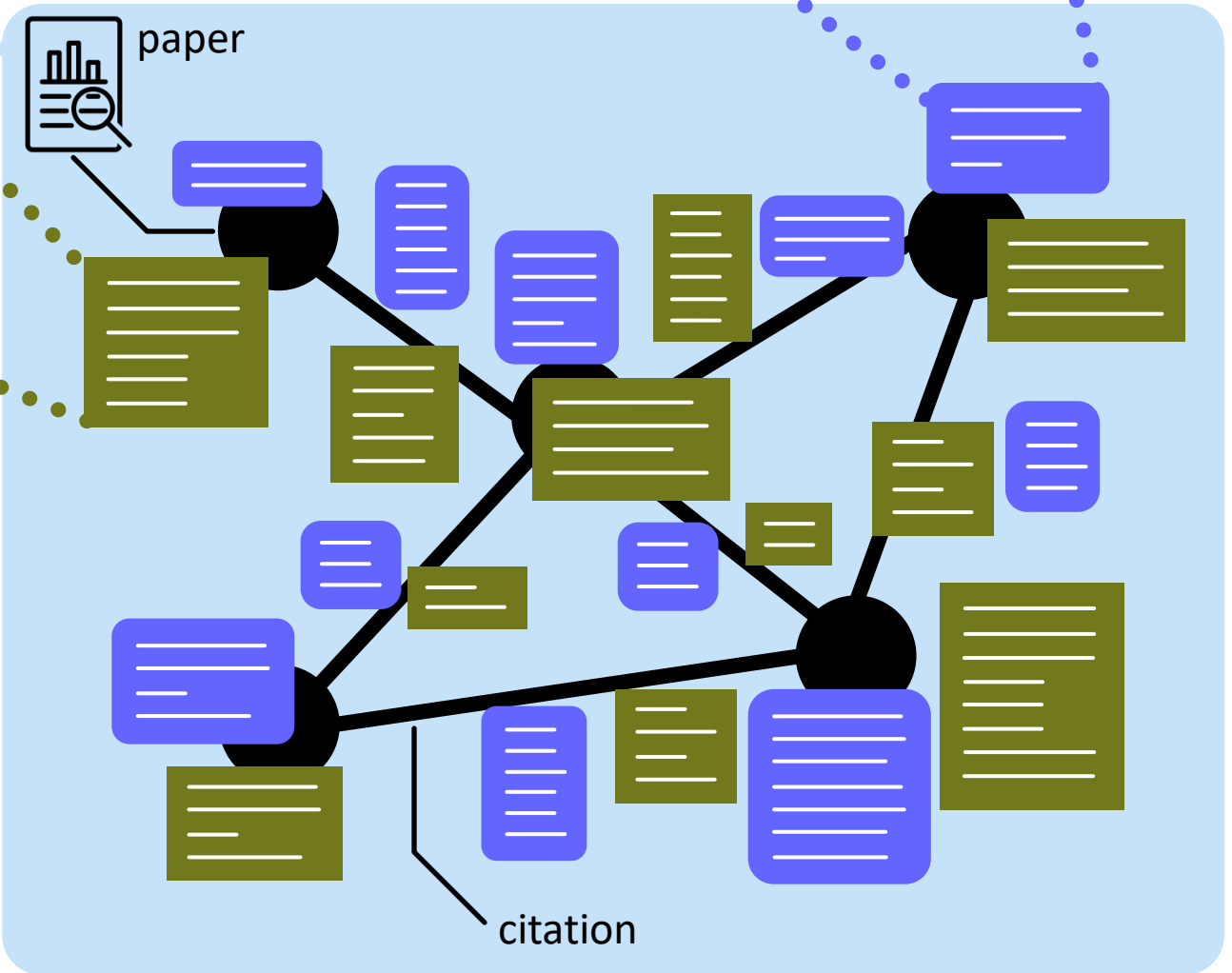


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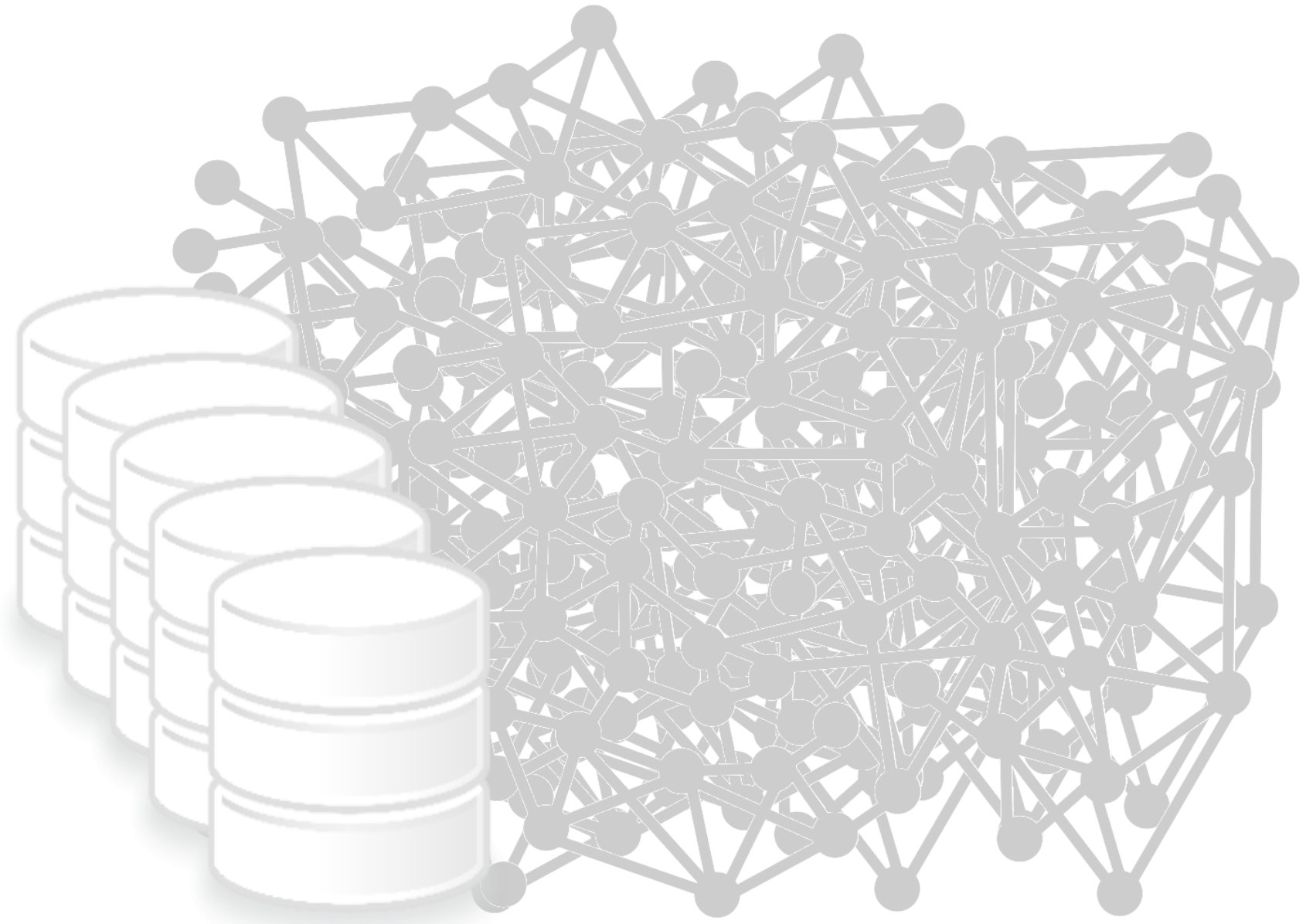
Labels

Properties

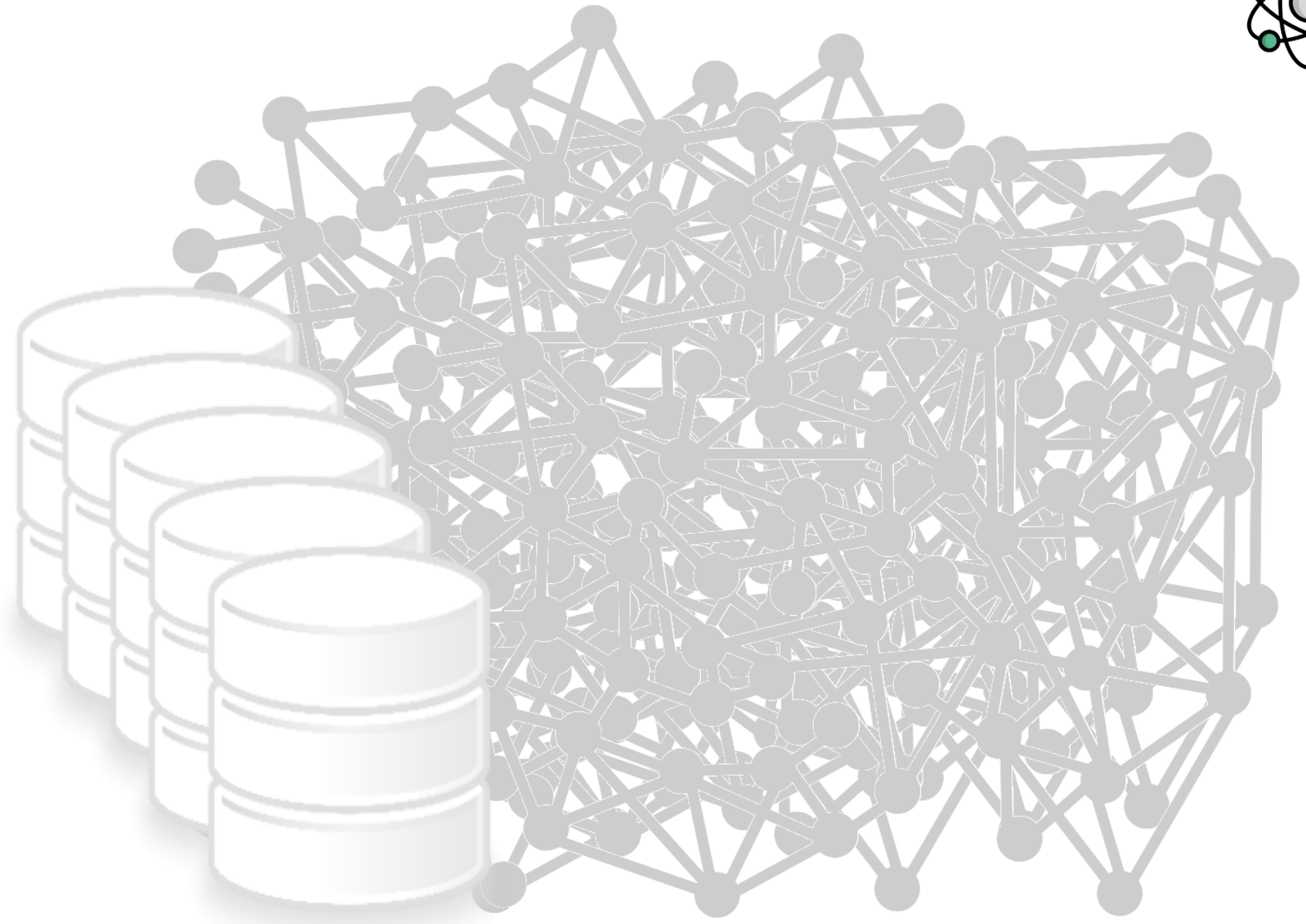
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:TechReport  
:PaperHighlights



# Graph Databases: Where Do We Use Them?



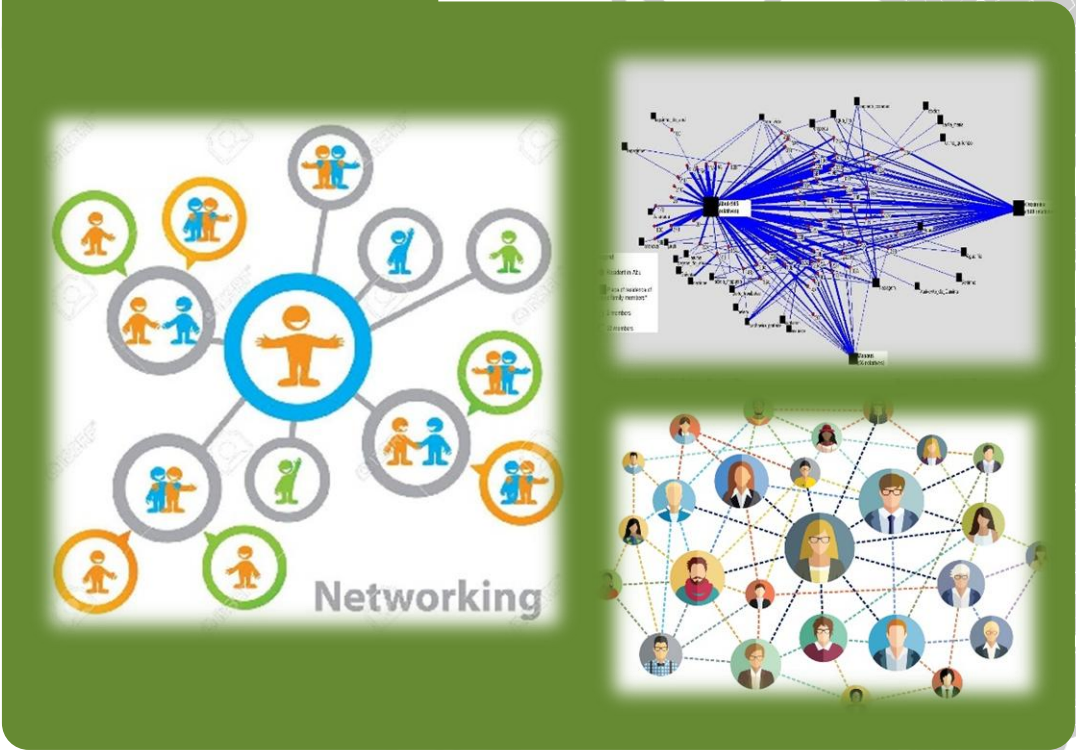
# Graph Databases: Where Do We Use Them?



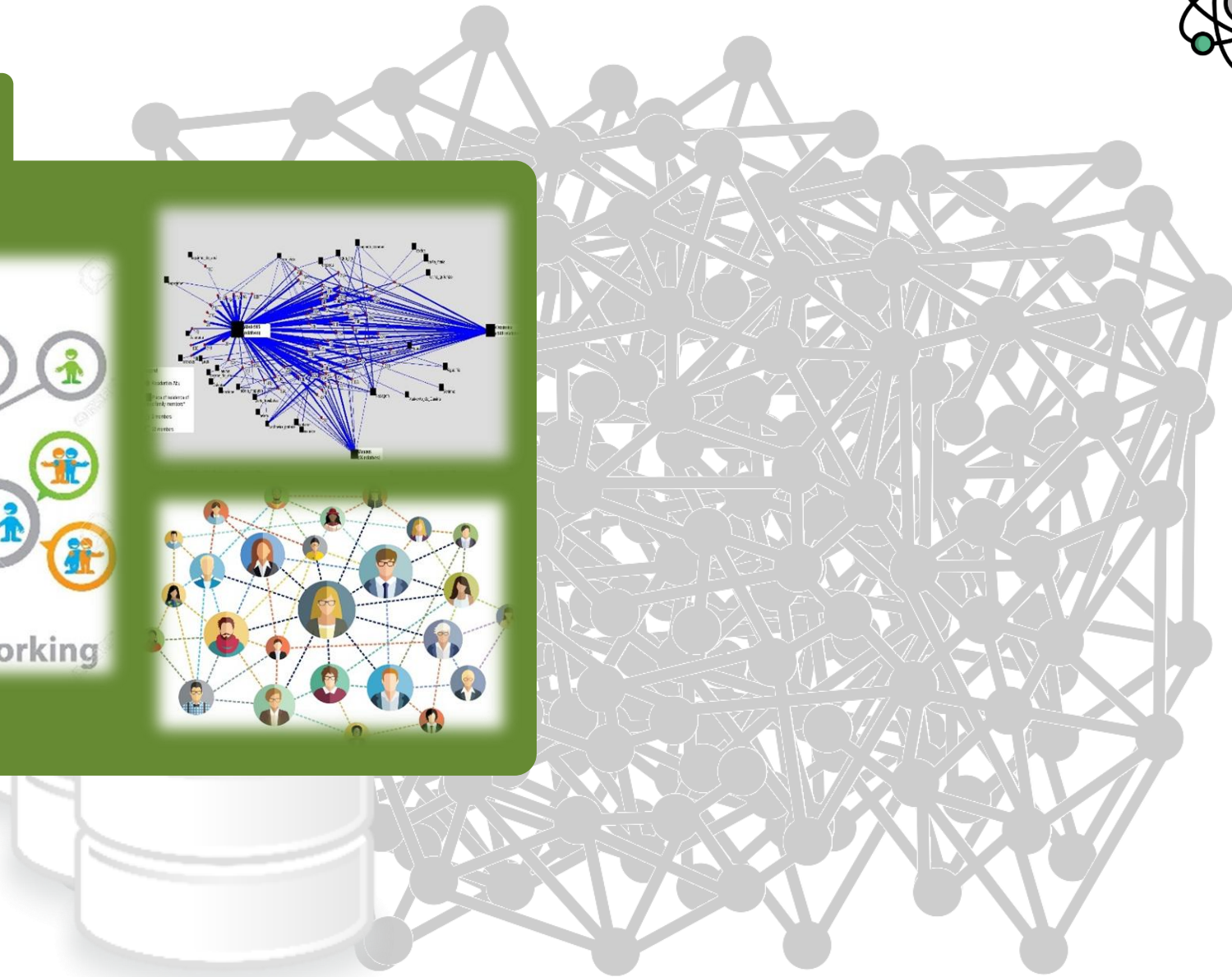
# Graph Databases: Where Do We Use Them?



## Social sciences



Networking

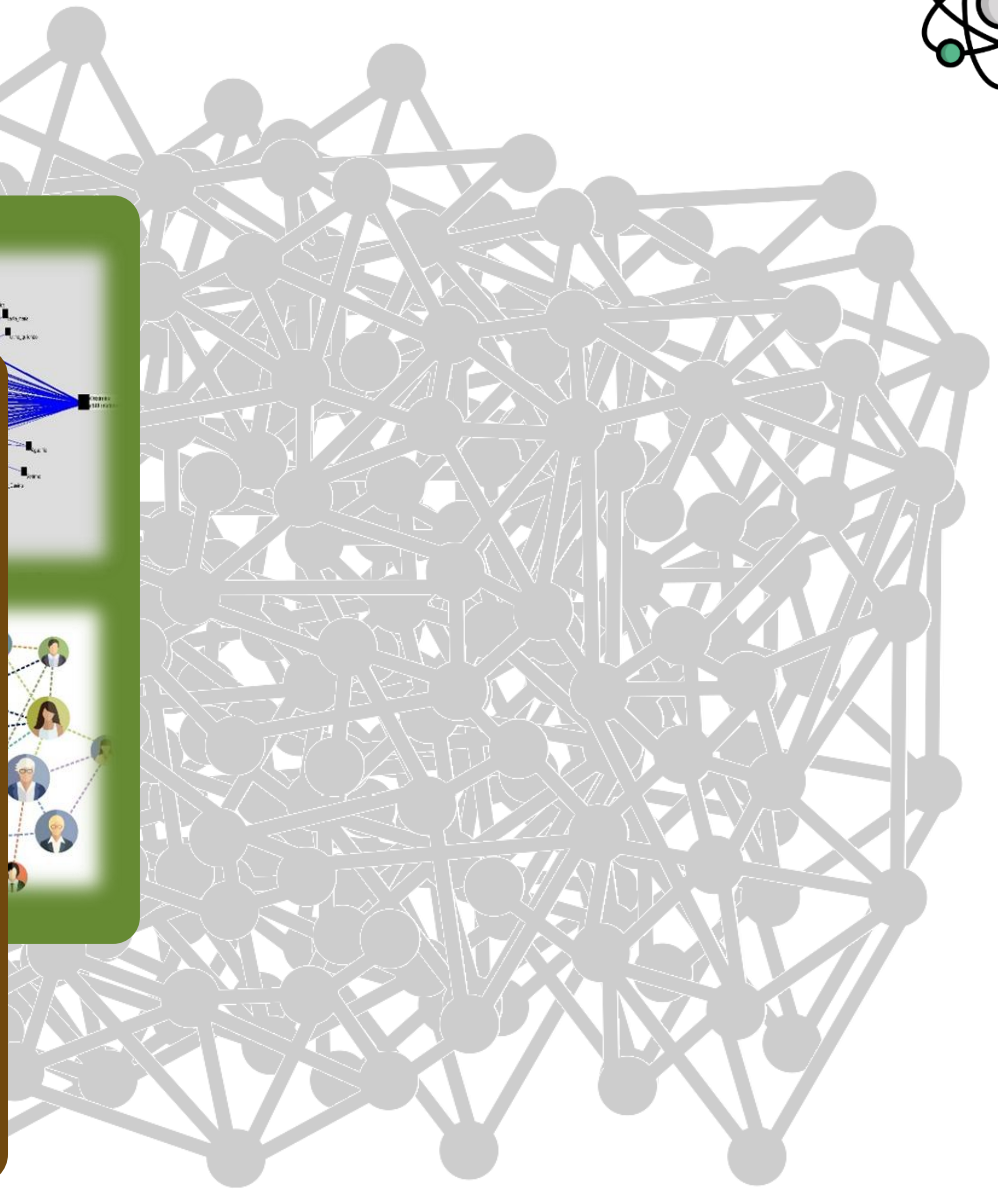


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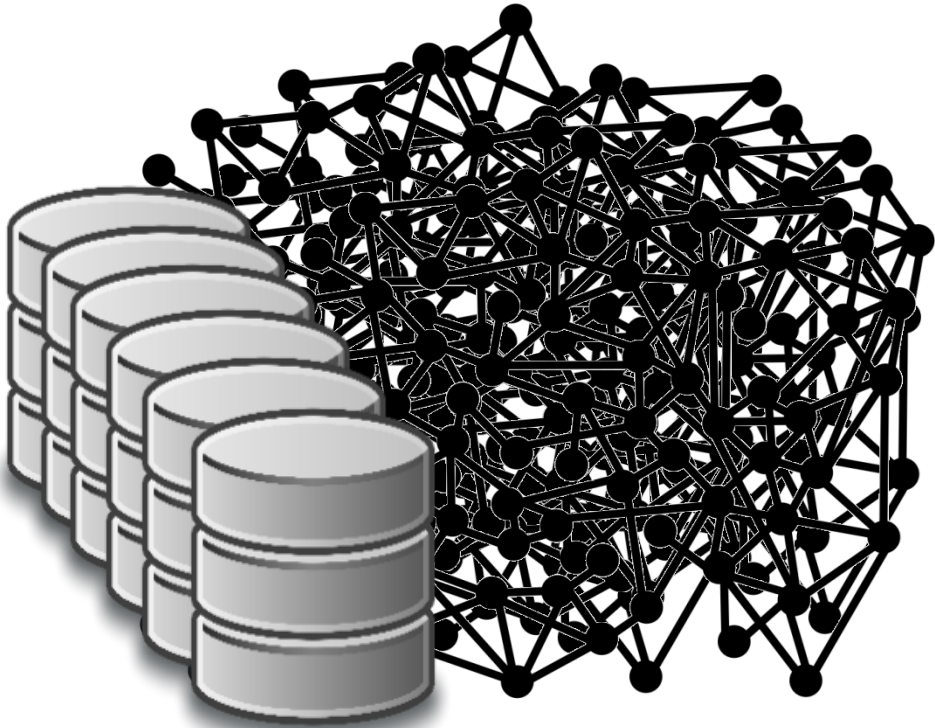
Social sciences

Engineering





That's why there are lots of them!



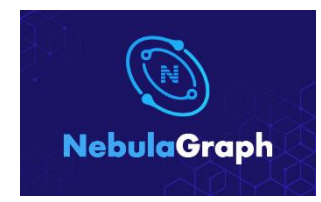
That's why there are lots of them!

VelocityDB 



InfiniteGraph 

Dgraph 



ArangoDB 



GALAXYBASE 

AGENS  
Graph Database 

HugeGraph 

ANZO 

Amazon Neptune 

fauna 



graphbase.ai 

BangDB 

neo4j 

ULTiPa 

Vaticle TypeDB 

blazegraph 

GraphDB

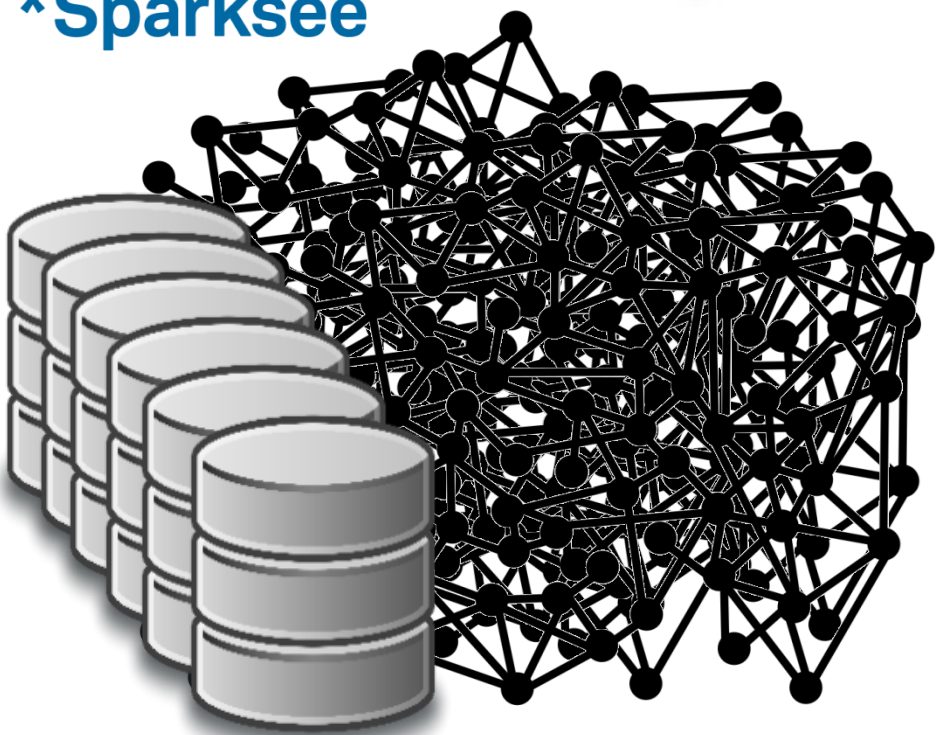
\*Sparksee

rcadeDB 



OrientDB 

TITAN 



FlockDB

MEM GRAPH 

KATANA GRAPH 

TerminusDB 

JanusGraph 

Franz Inc. AllegroGraph 

TigerGraph 



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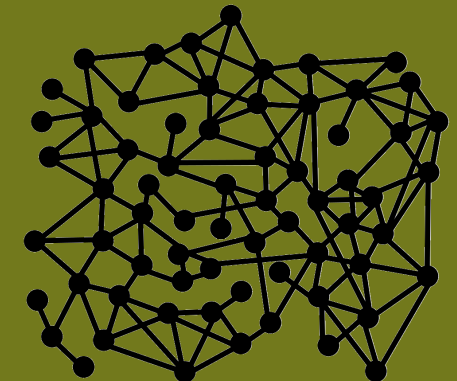
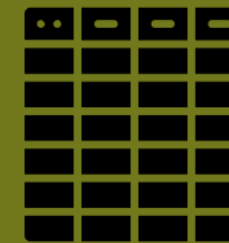
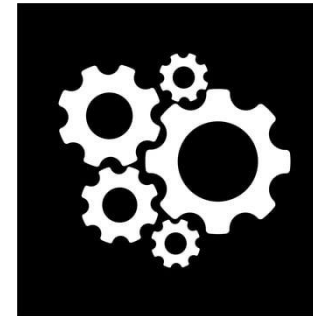
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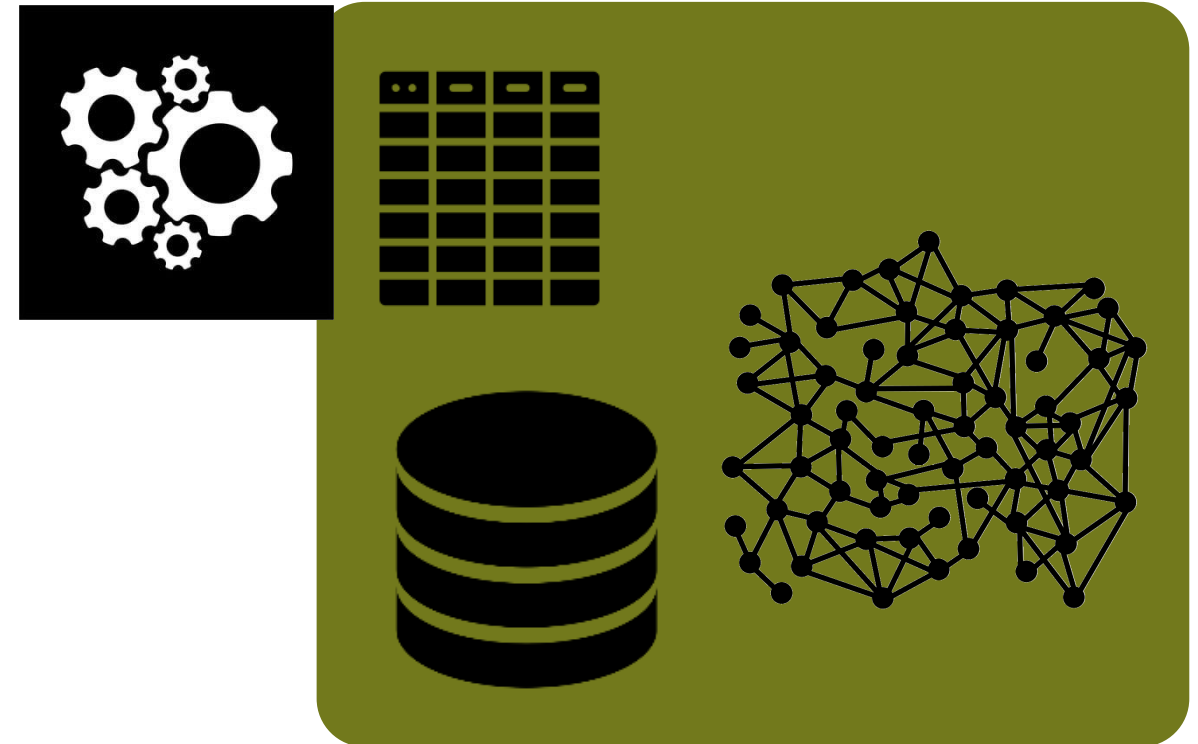
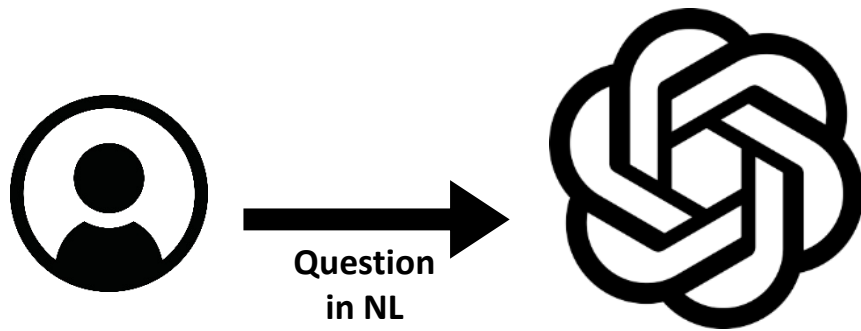
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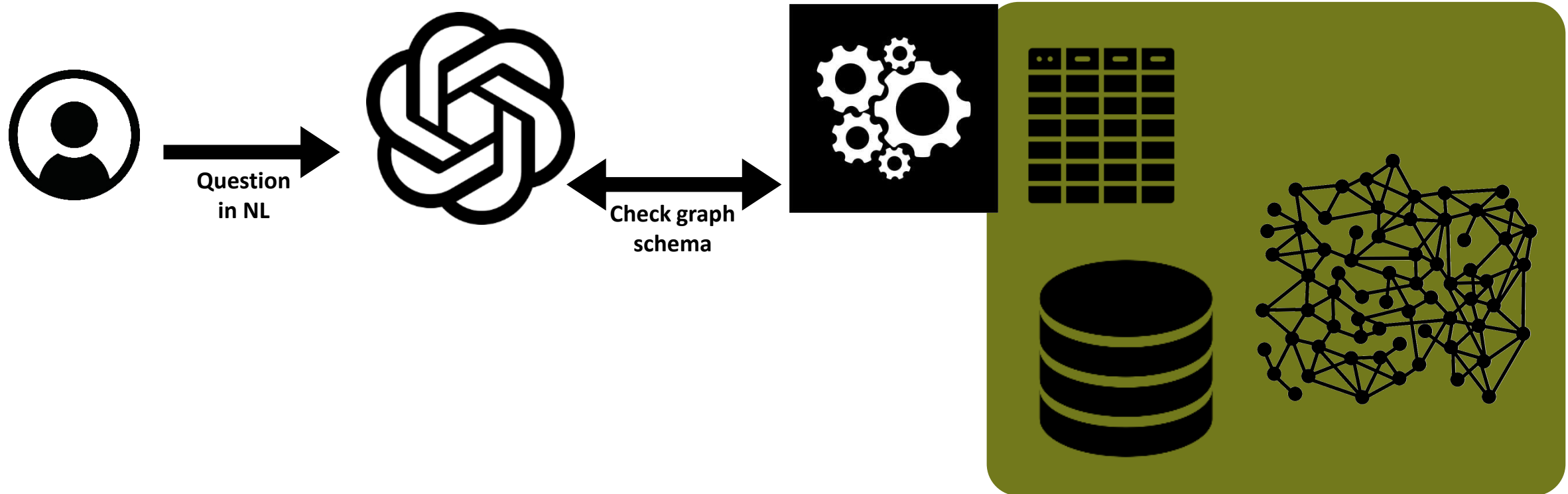
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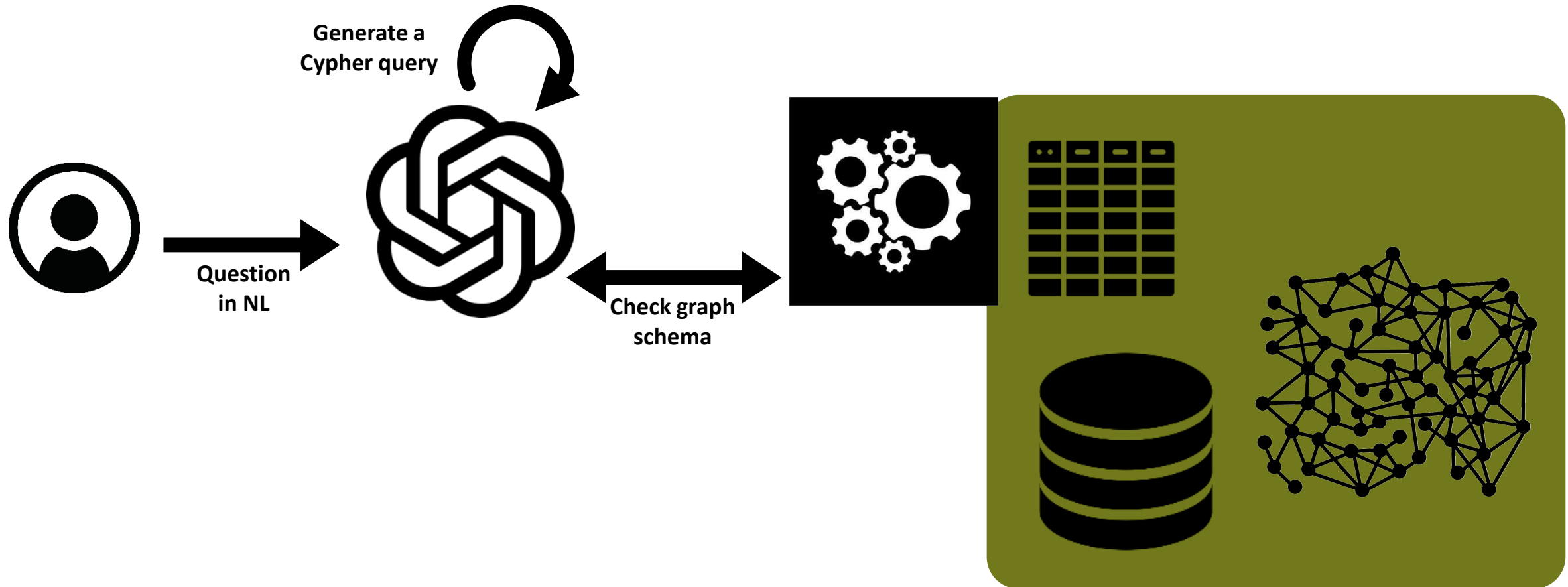
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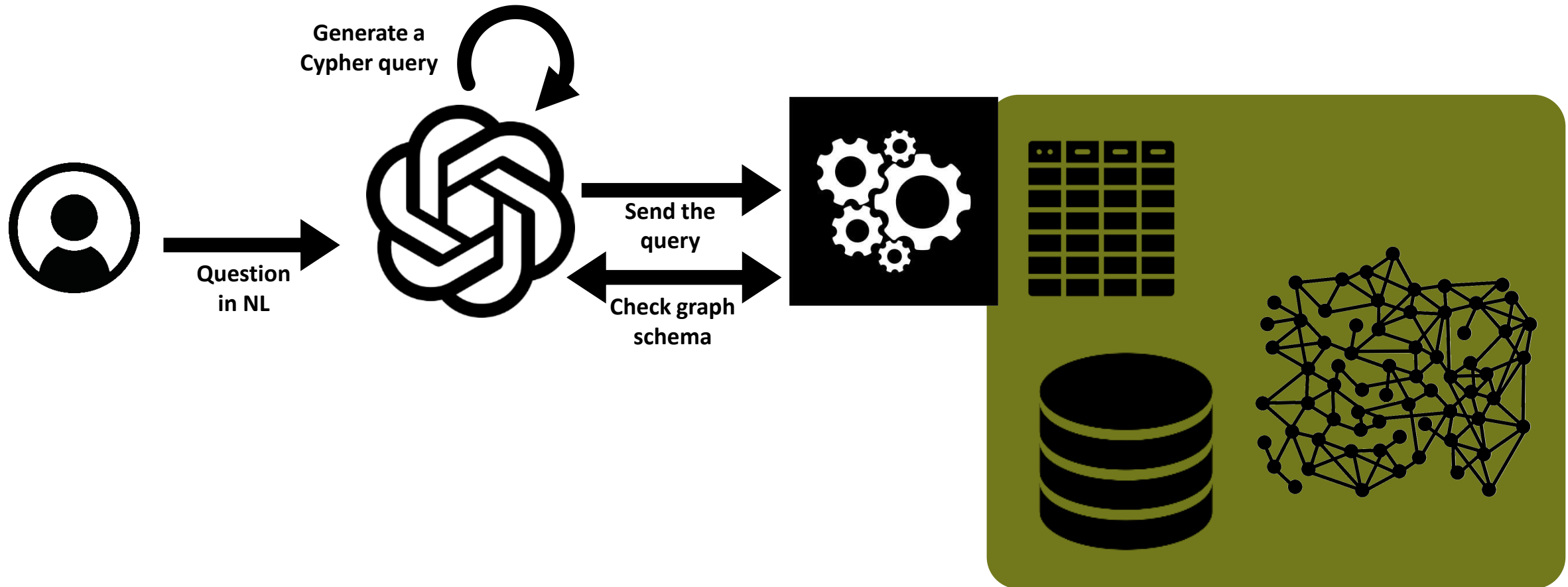
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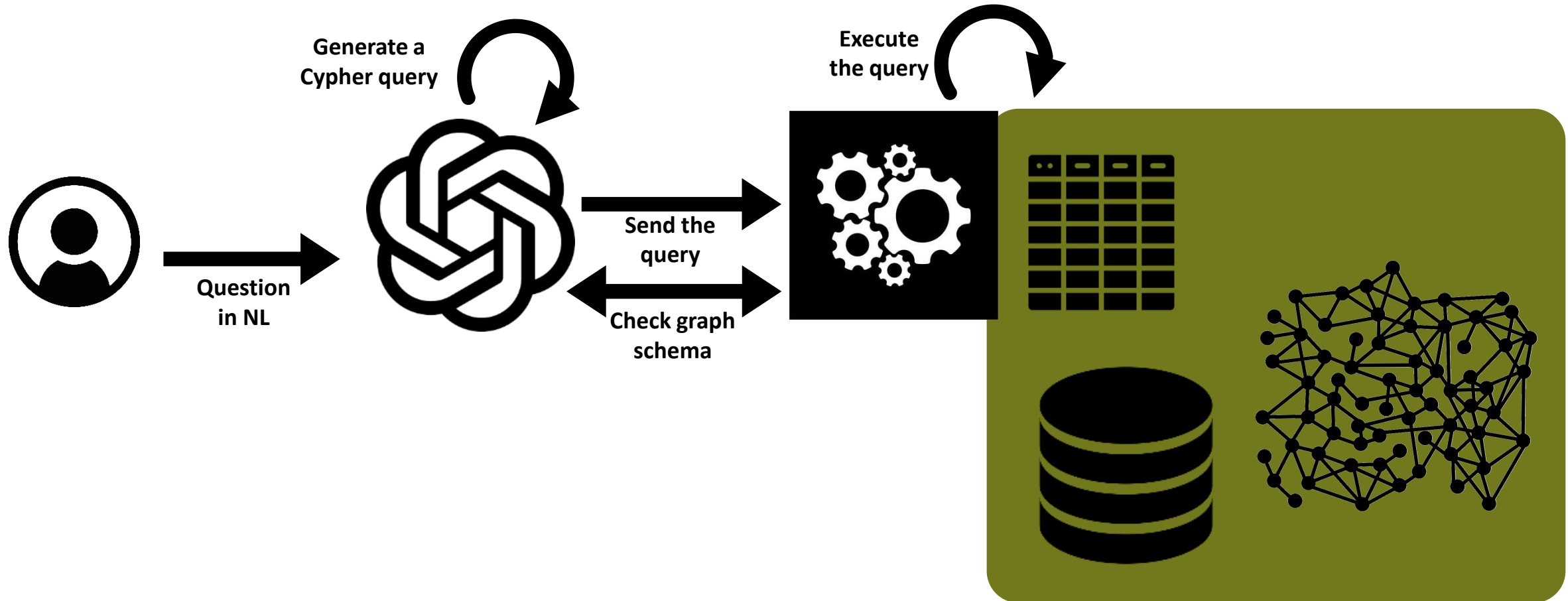
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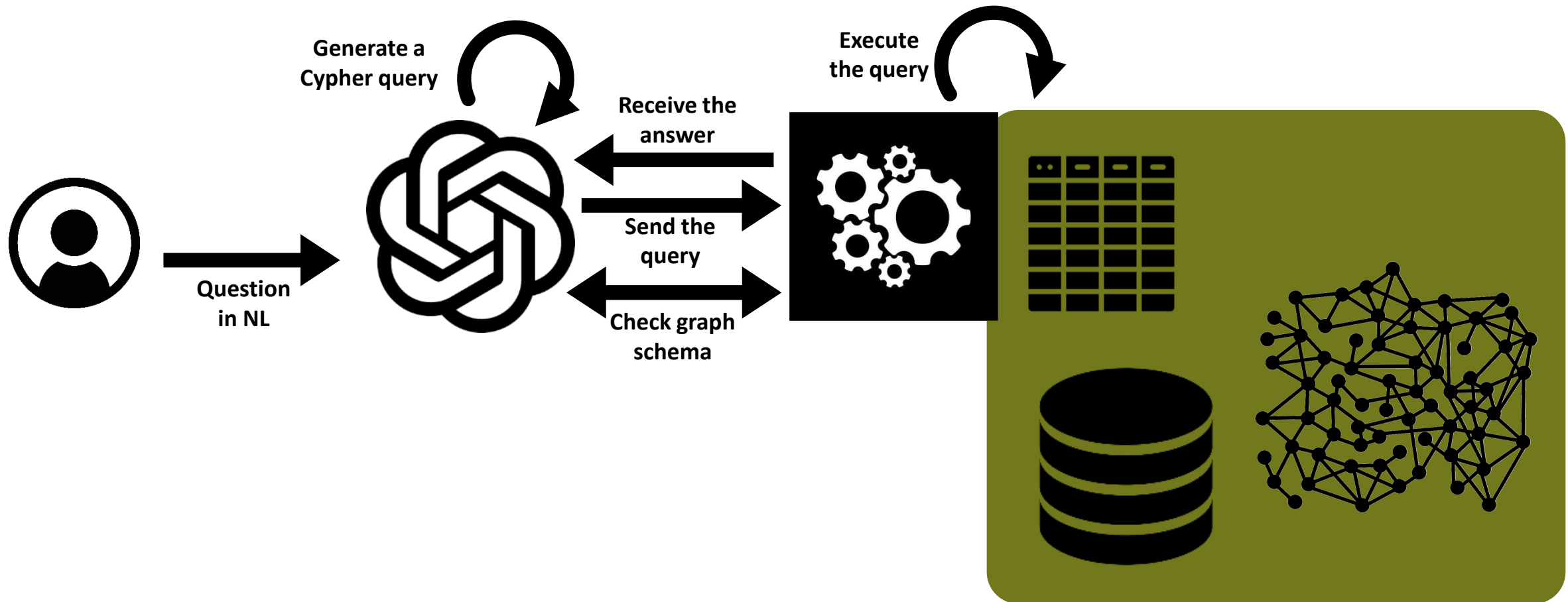
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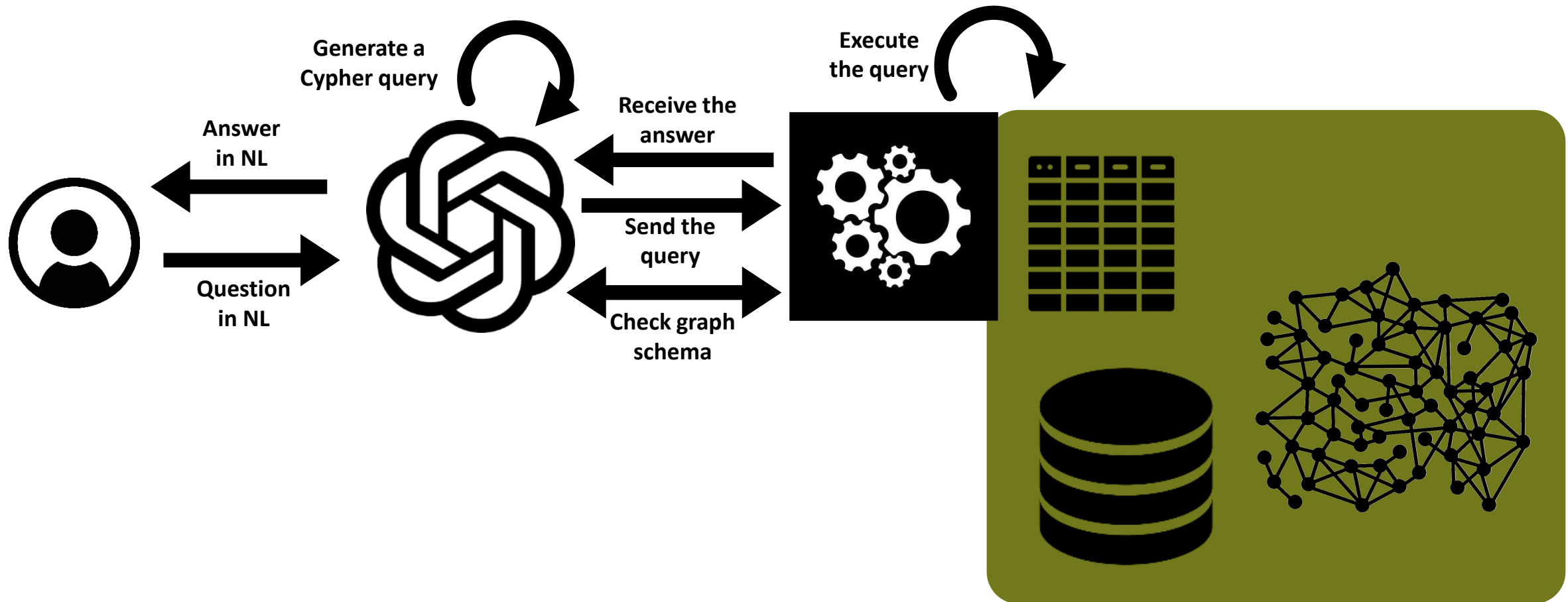
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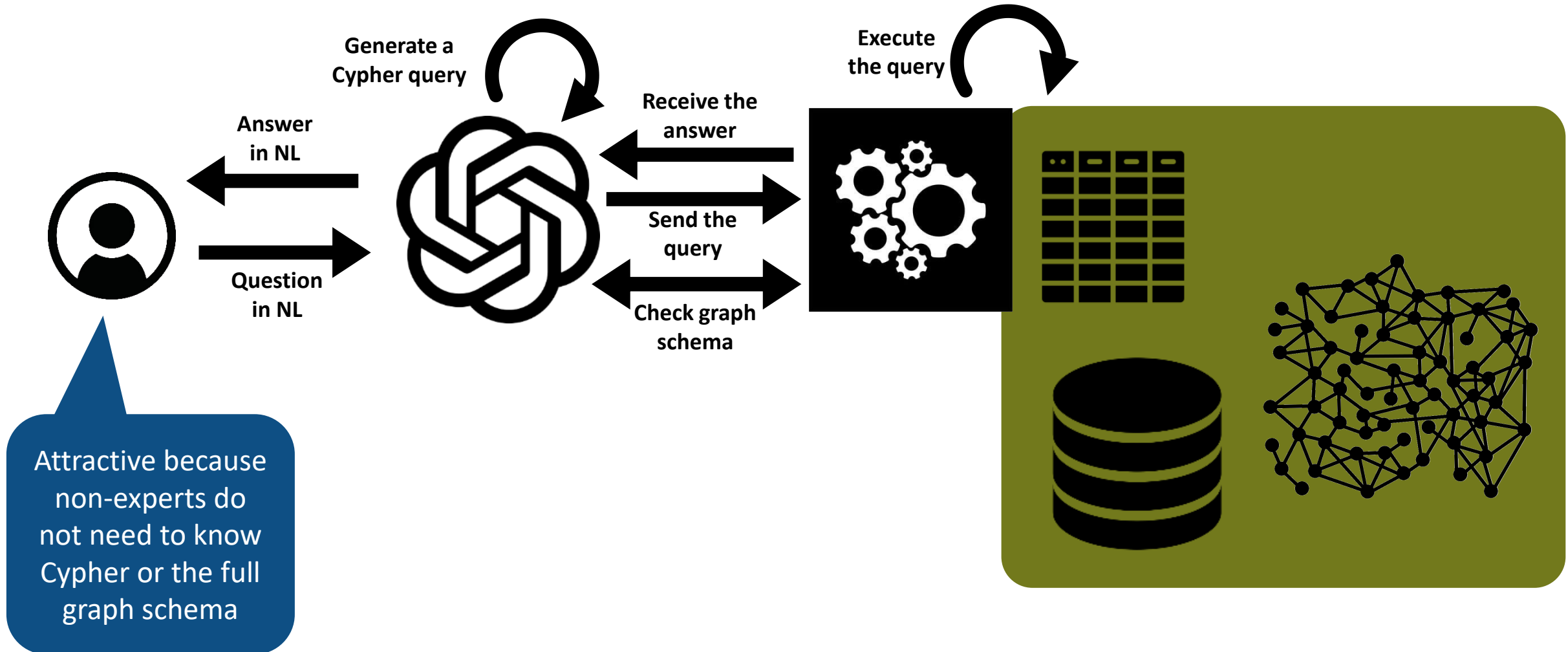
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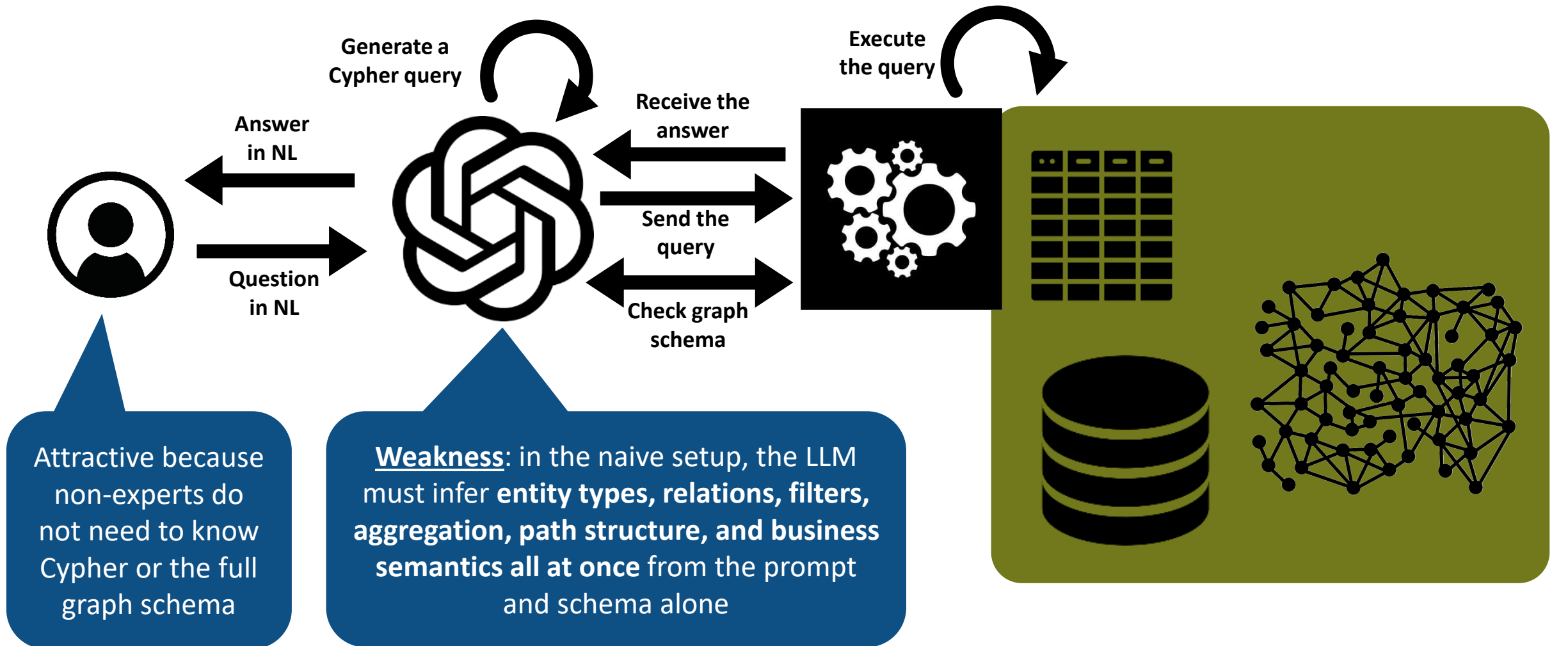
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Attractive because non-experts do not need to know Cypher or the full graph schema

Weakness: in the naive setup, the LLM must infer **entity types, relations, filters, aggregation, path structure, and business semantics all at once** from the prompt and schema alone

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Generate a Cypher query

Execute the query

**Solution: separate semantics („LLM part”) from execution („Non-LLM part”)**

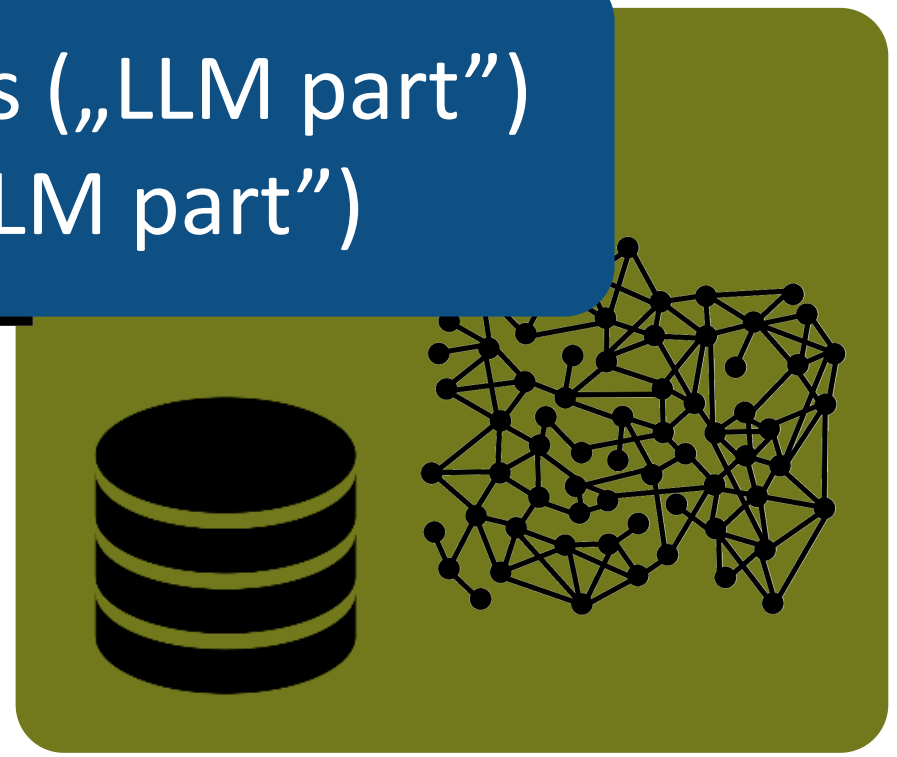


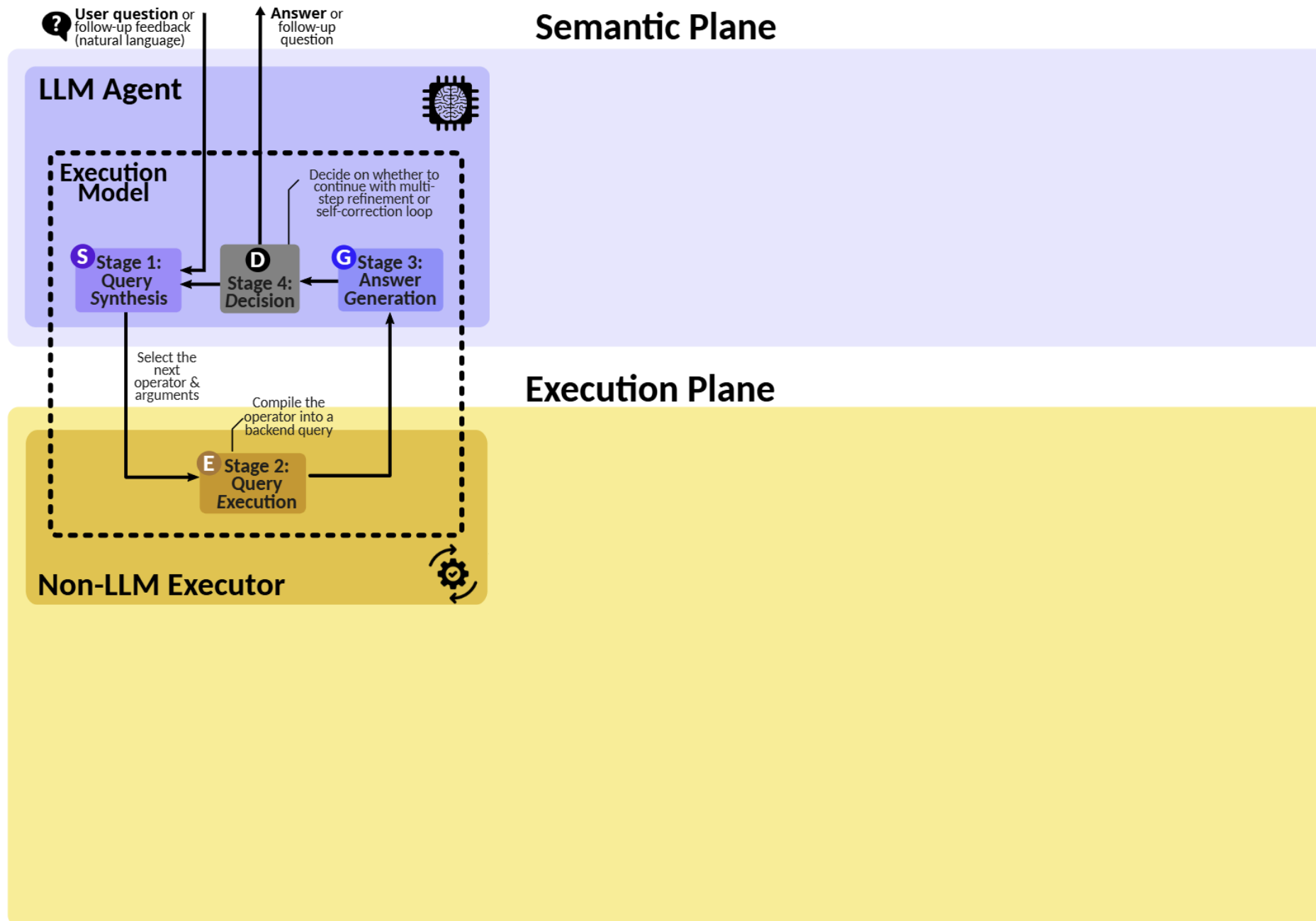
In NL

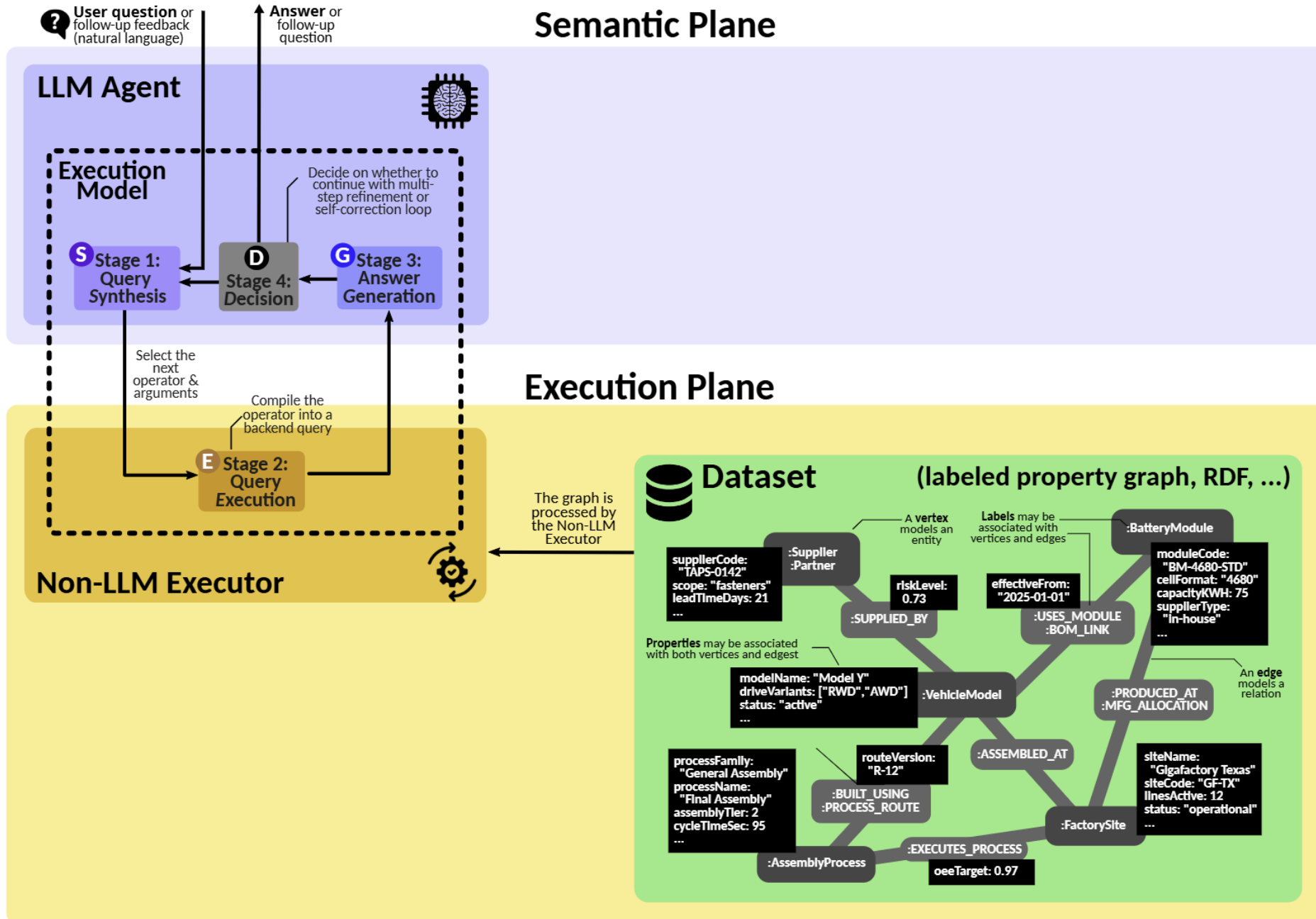
Check graph schema

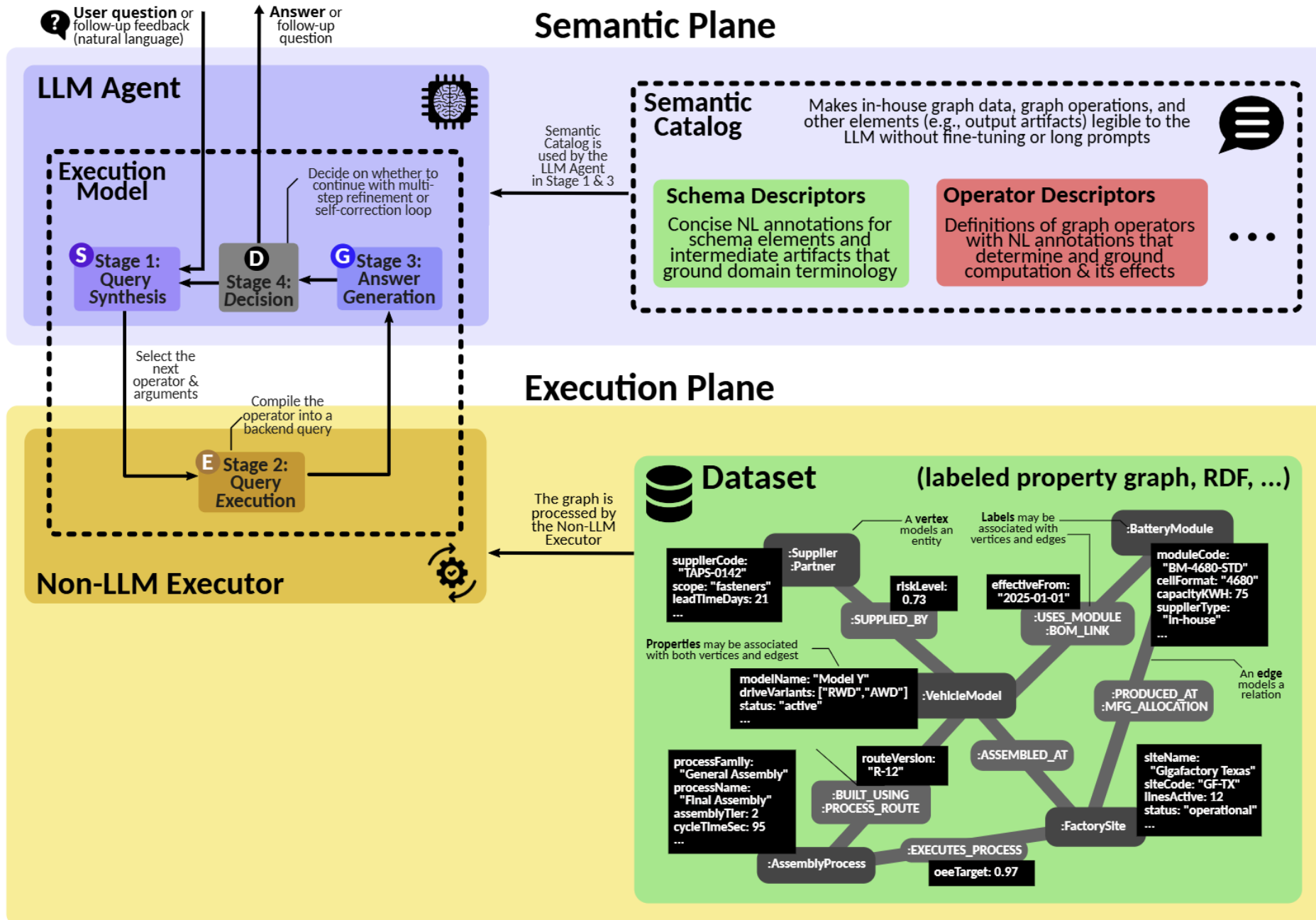
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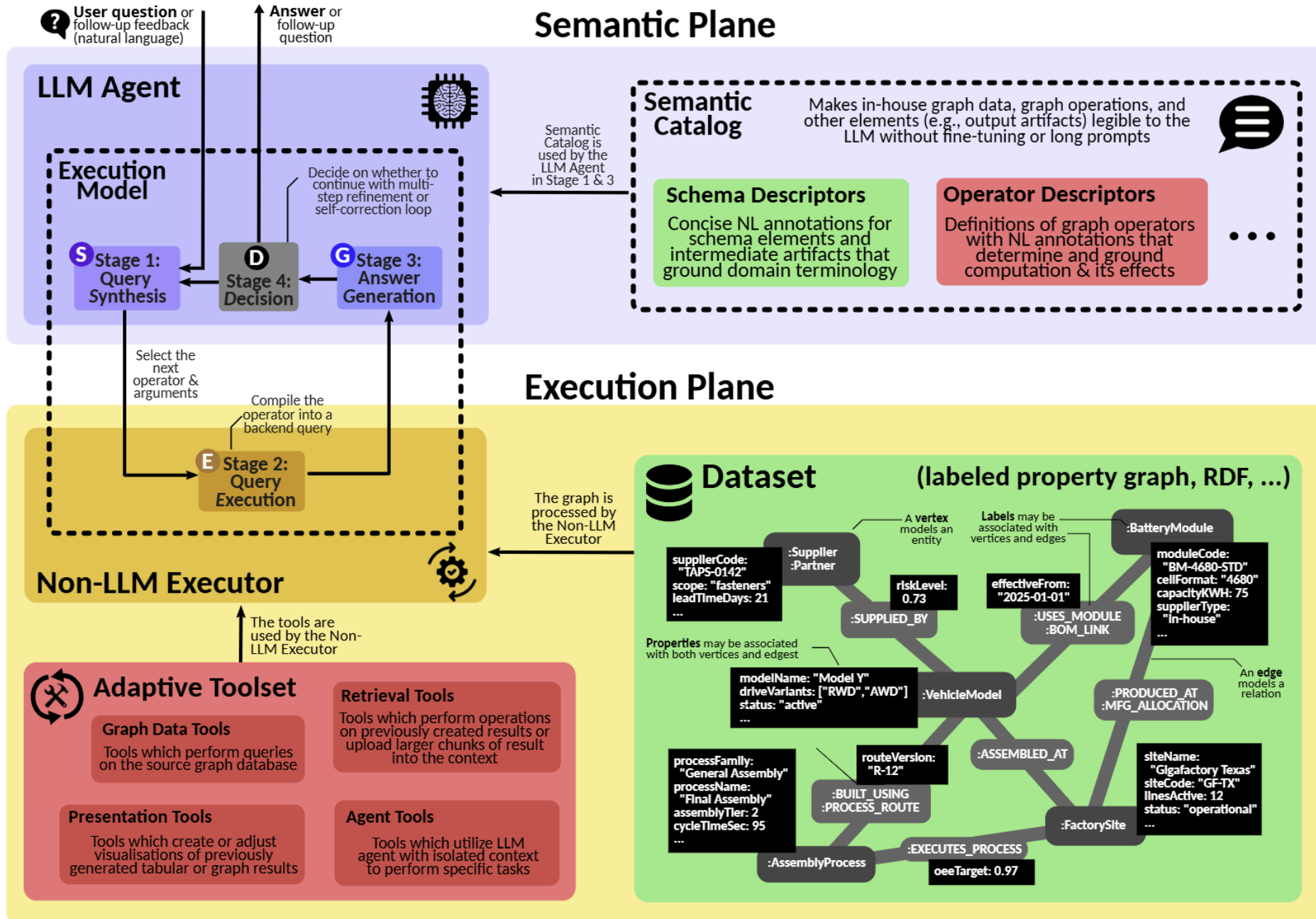
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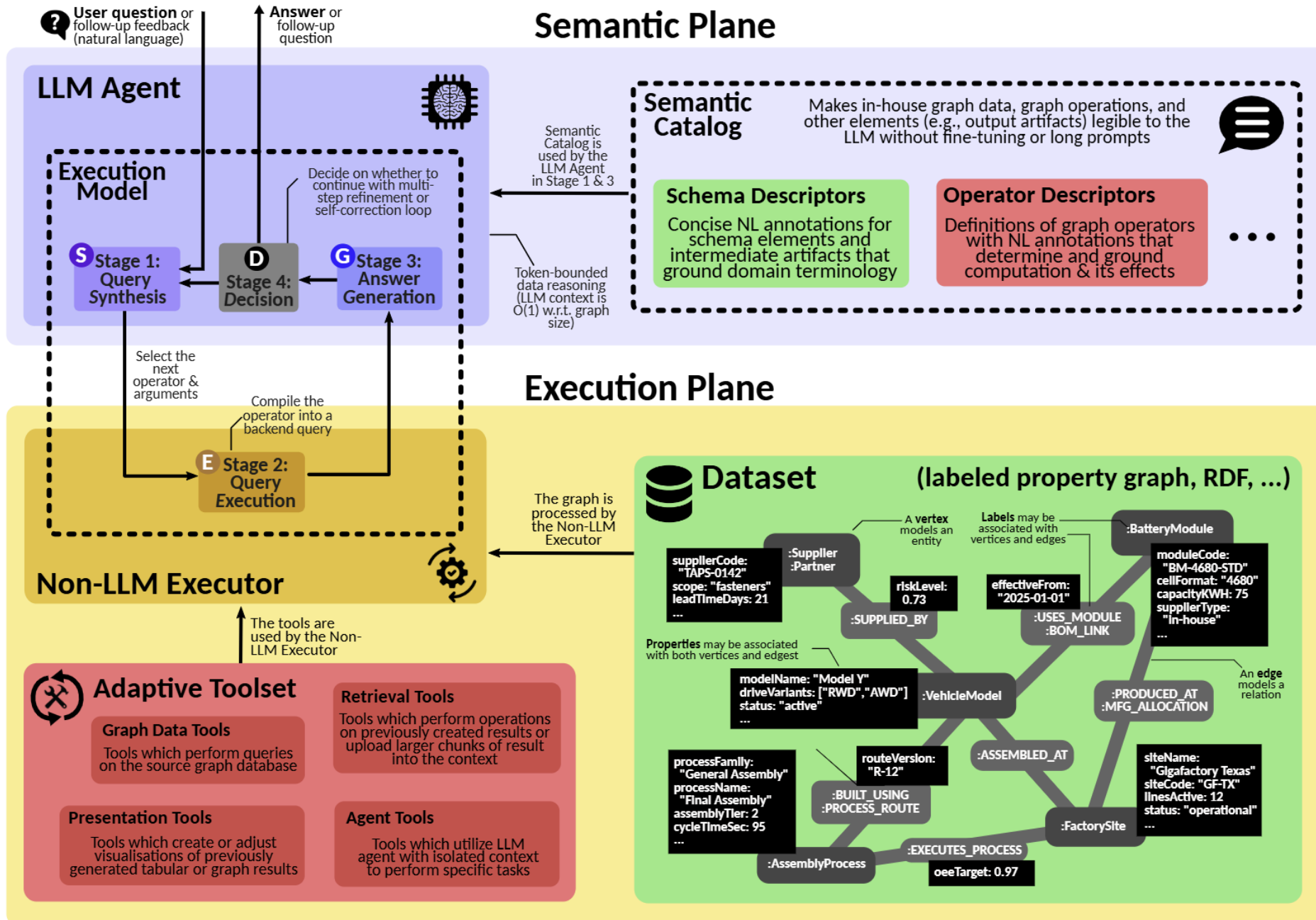




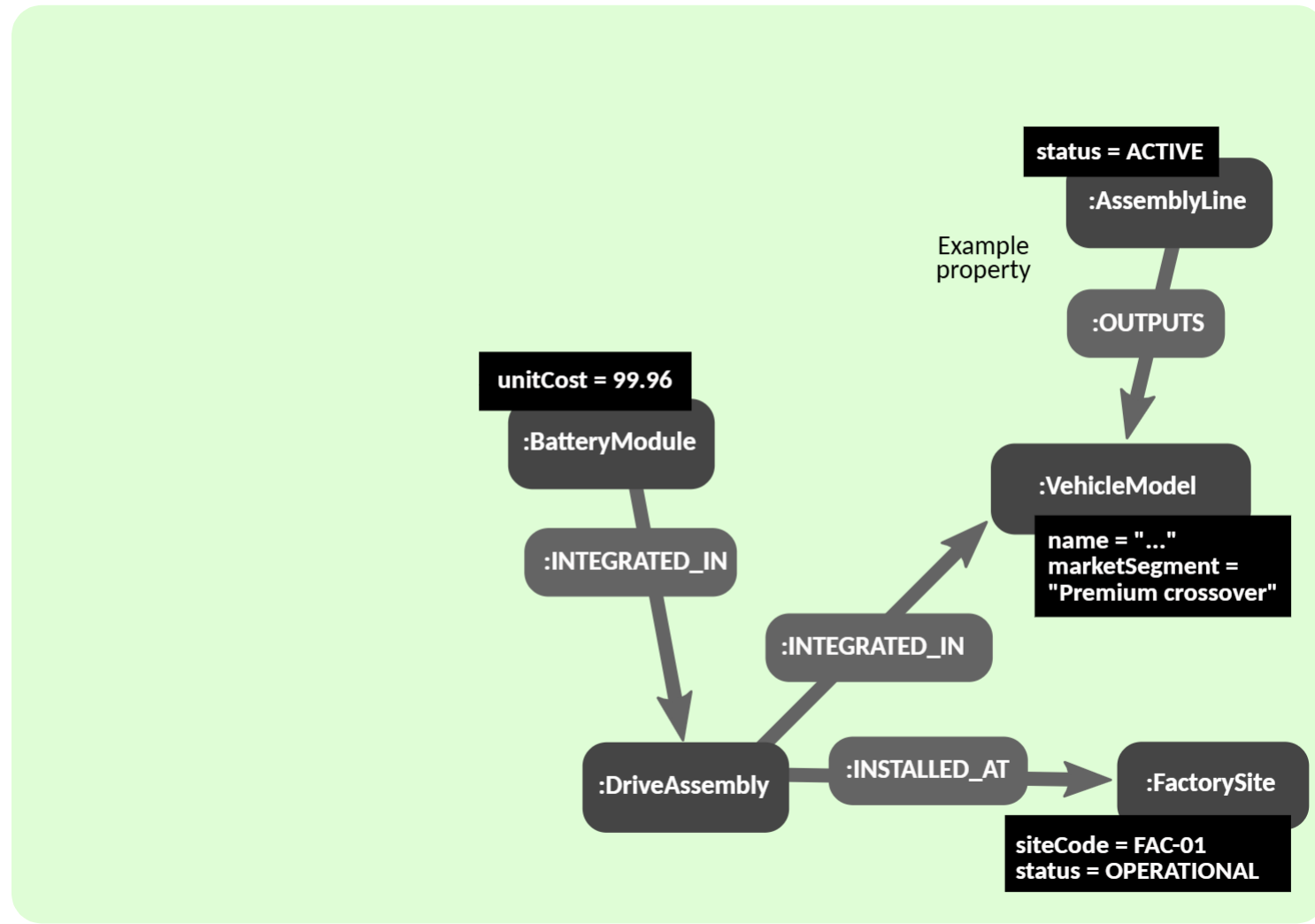




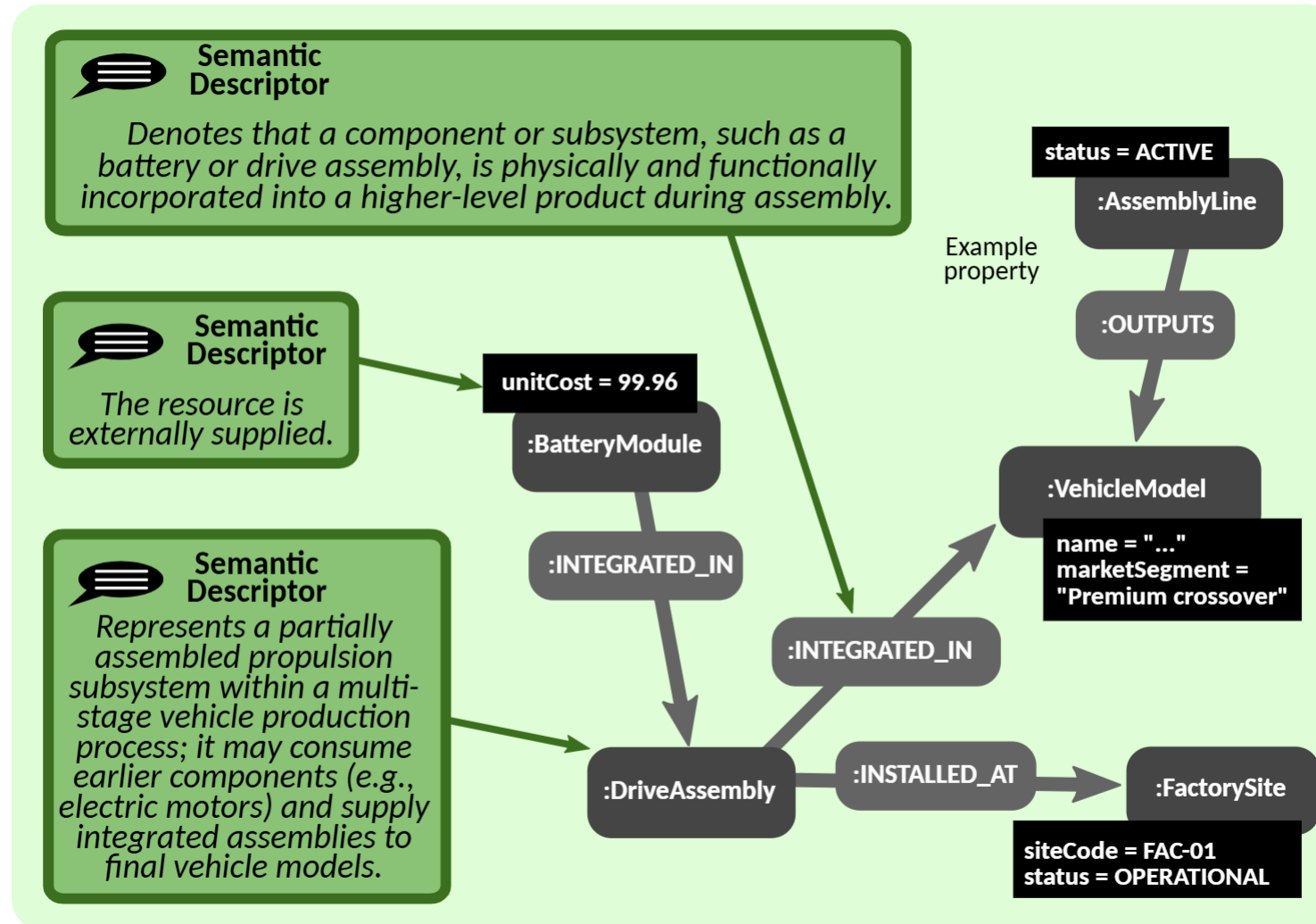




# Example Semantic Descriptors



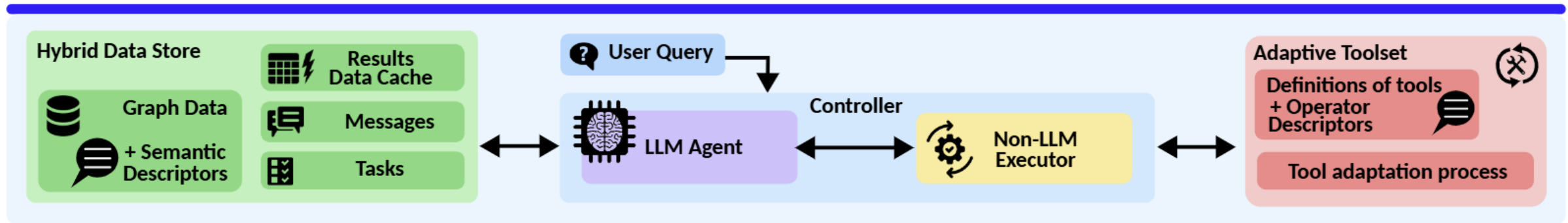
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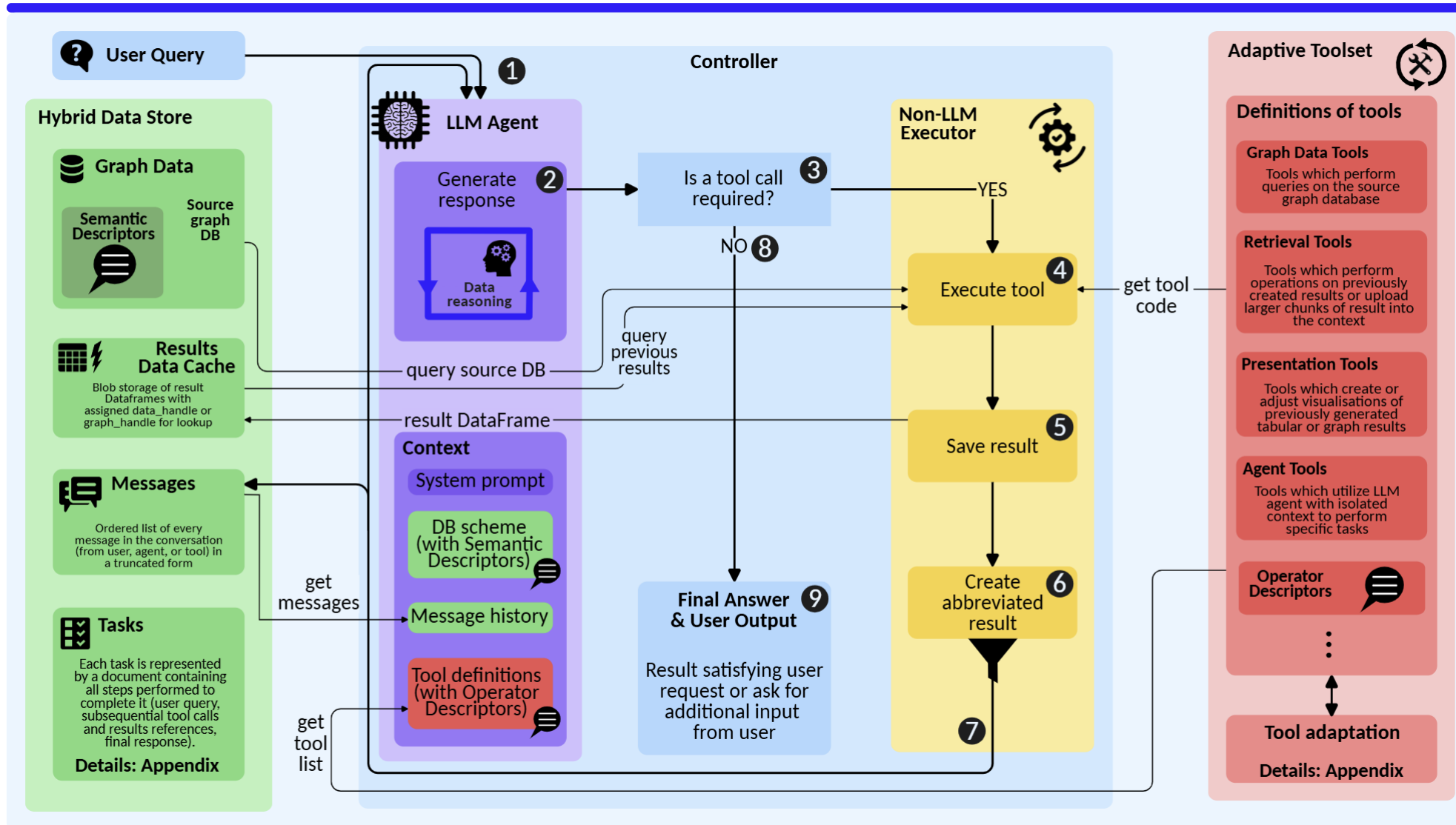
# GraphSeek Design & Implementation

## GraphSeek (high-level overview)

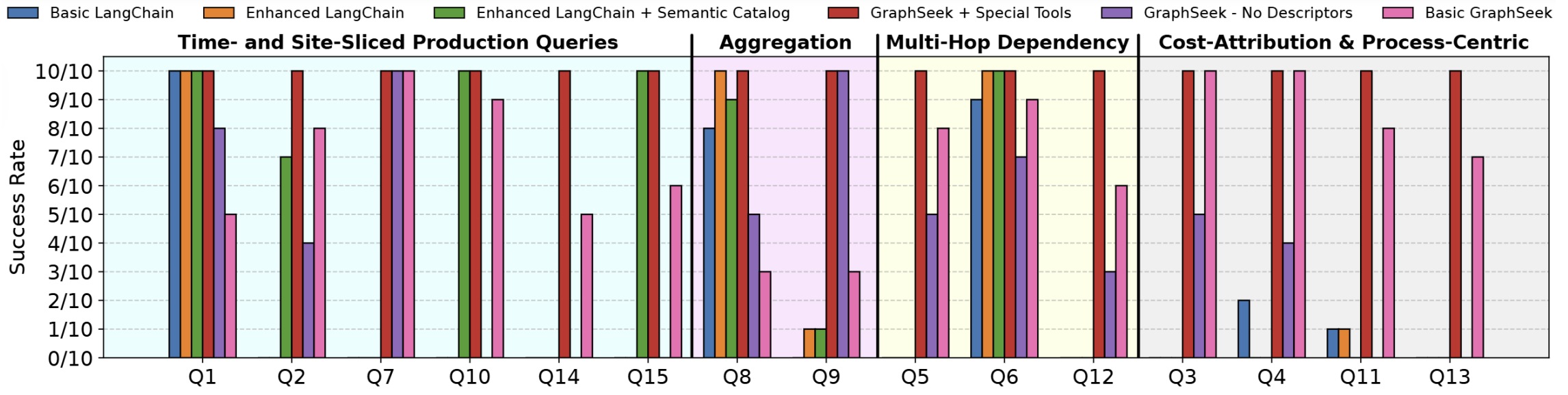
Legend: Green: data-related Blue: general workflow (Non-LLM) related Violet: executed by the LLM Red: Tool definitions Yellow: Non-LLM tool execution



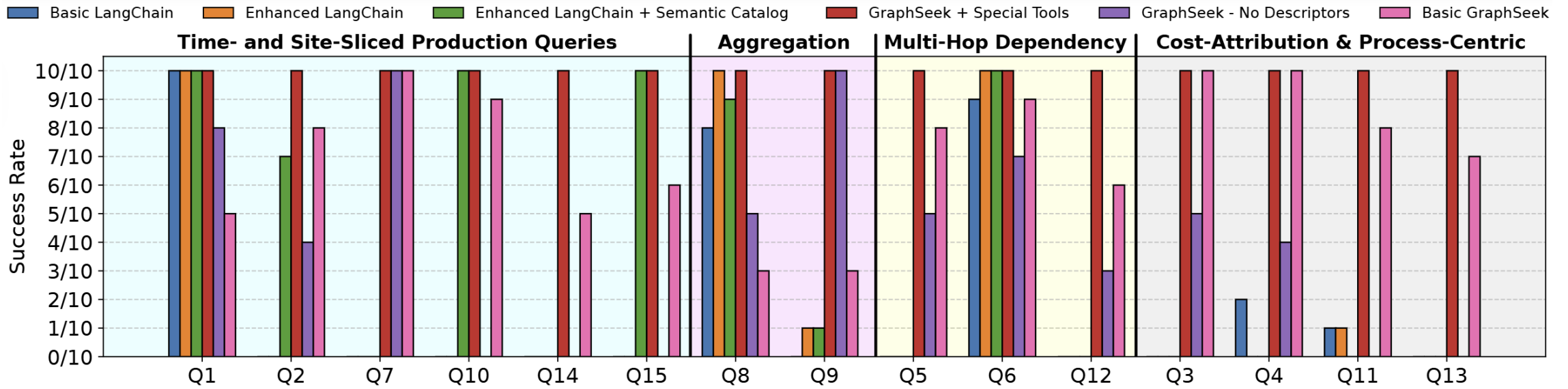
# GraphSeek Design & Implementation



# Evaluation

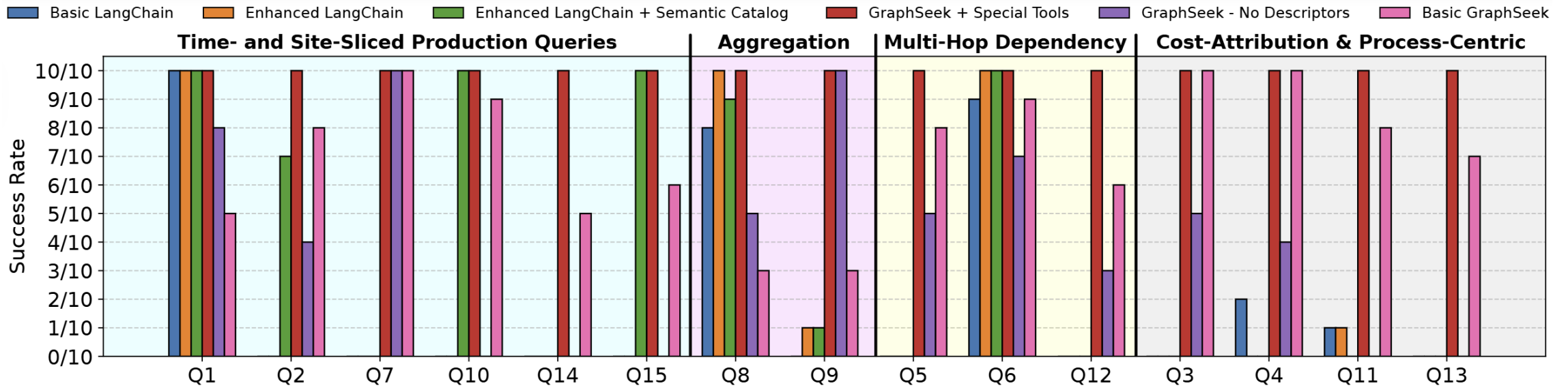


# Evaluation



How many base-tier drive assemblies do we produce at each factory site?

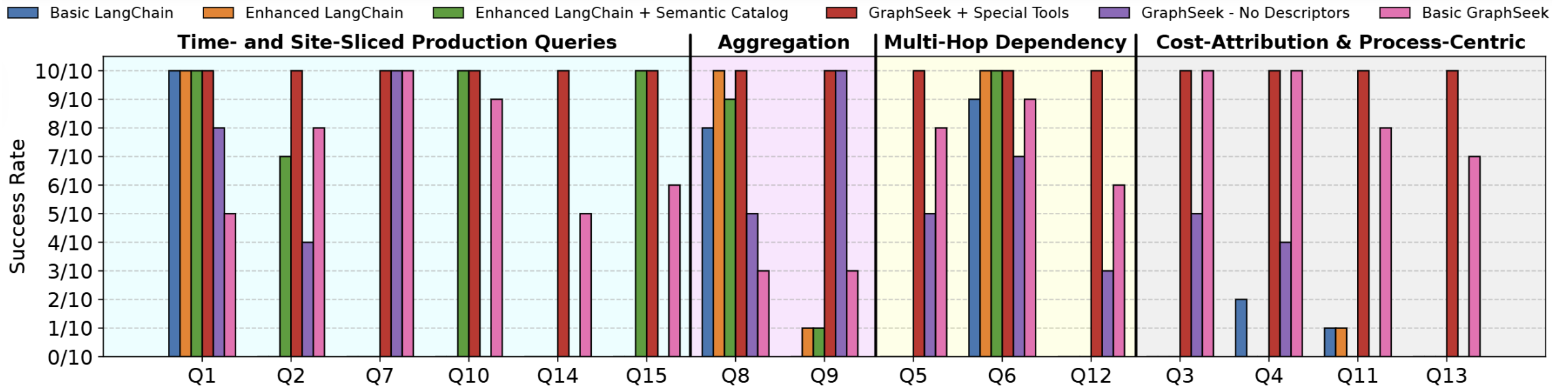
# Evaluation



How many base-tier drive assemblies do we produce at each factory site?

Show me the unique manufacturing blueprint for vehicle model EV-X7

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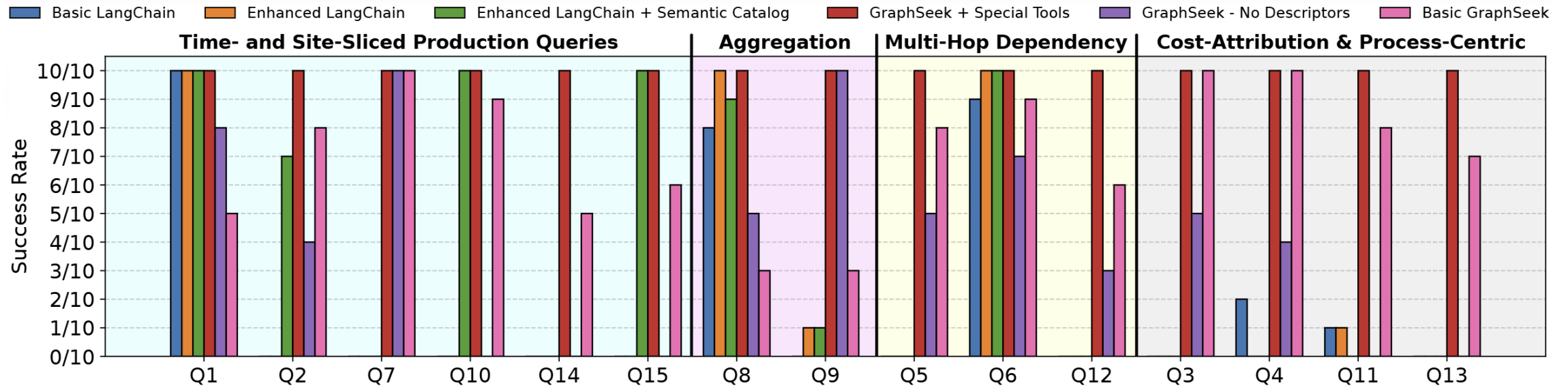


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# Evaluation



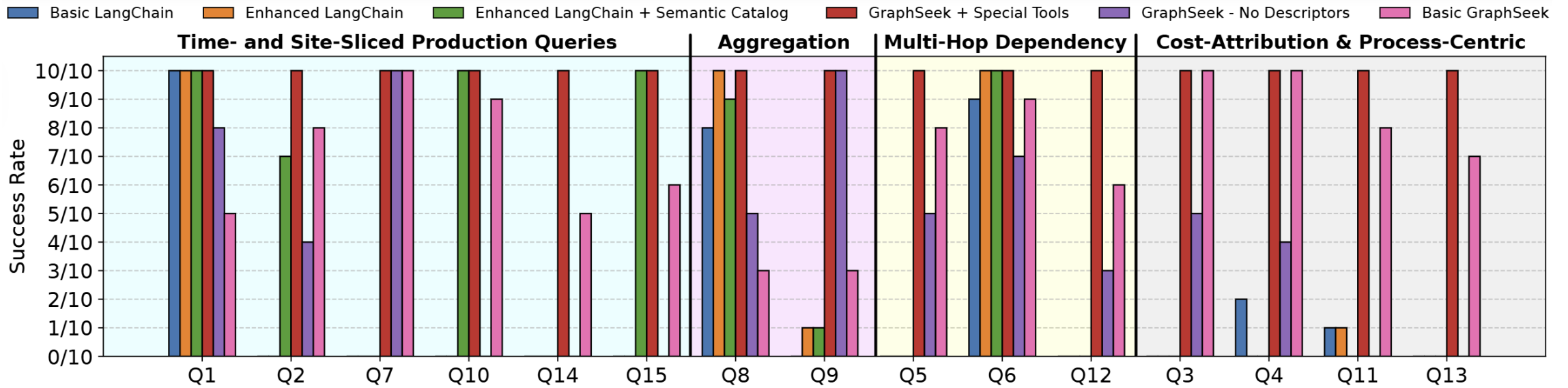
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Show me the unique manufacturing blueprint for vehicle model EV-X7

At which factory site is the component with the highest market price manufactured?

Check unique production plans for three vehicle models whose names start with 'B', and tell me which one uses the largest number of modules.

# Evaluation



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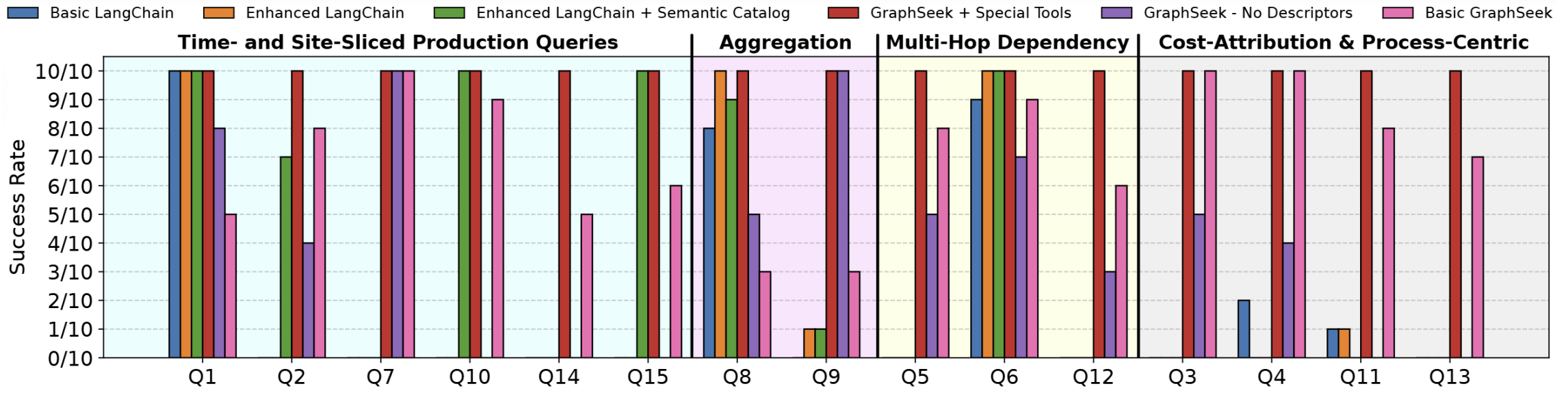
Show me the unique manufacturing blueprint for vehicle model EV-X7

At which factory site is the component with the highest market price manufactured?

What is the highest module cost?

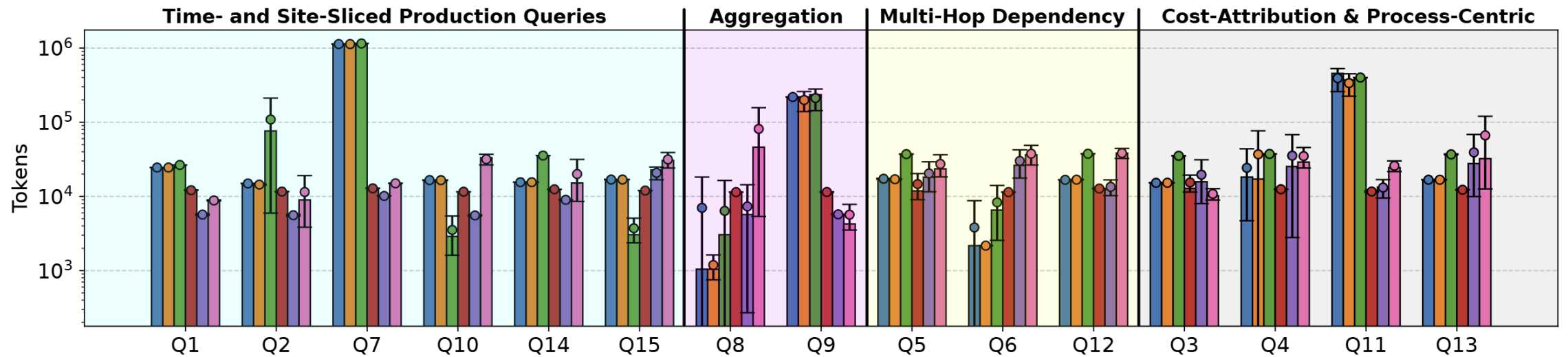
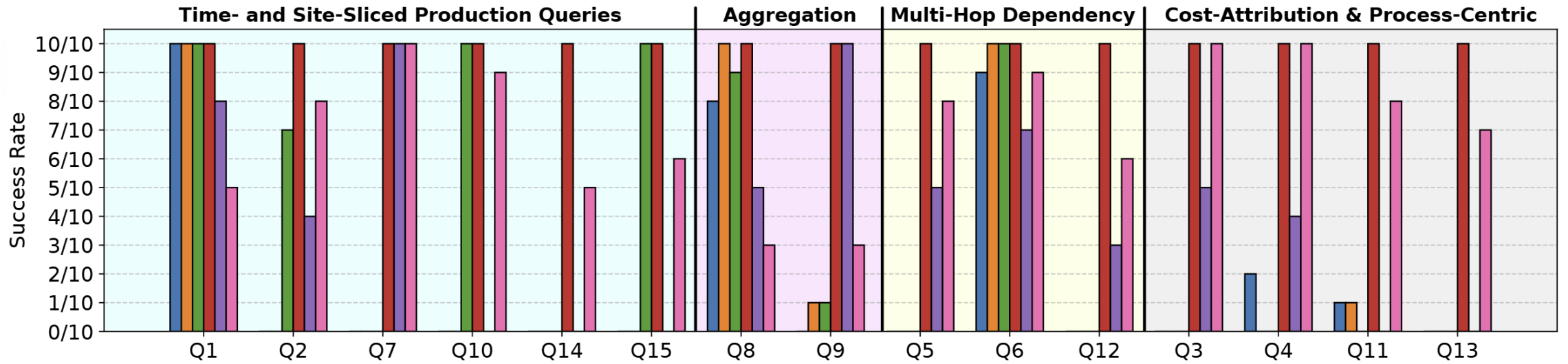
Check unique production plans for three vehicle models whose names start with 'B', and tell me which one uses the largest number of modules.

# Evaluation

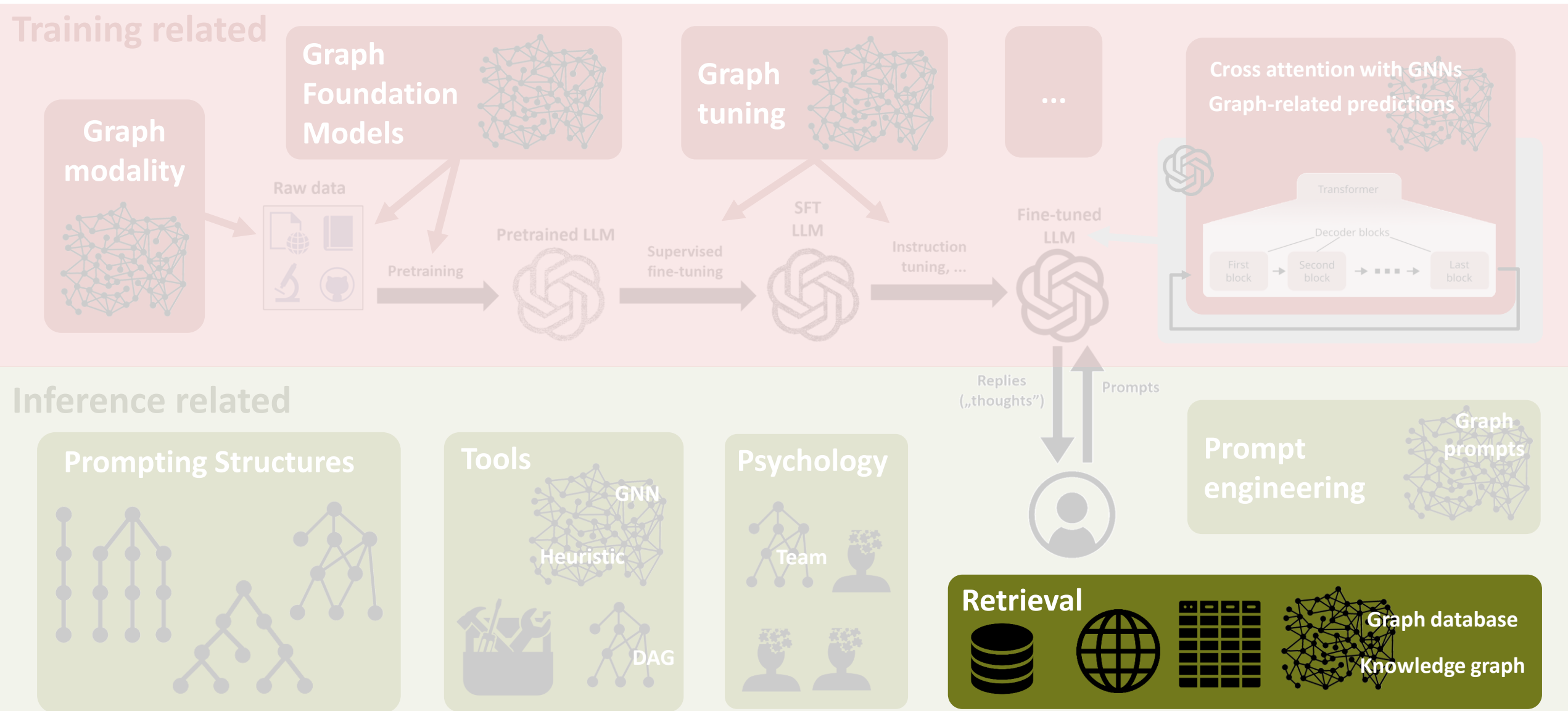


# Evaluation

■ Basic LangChain  
 ■ Enhanced LangChain  
 ■ Enhanced LangChain + Semantic Catalog  
 ■ GraphSeek + Special Tools  
 ■ GraphSeek - No Descriptors  
 ■ Basic GraphSeek



# Graphs in the LLM Pipeline: Overview



# Graphs in the LLM Pipeline: Overview



# Graphs + Deep Learning = Graphs Neural Networks (GNNs)

# Graphs + Deep Learning = Graphs Neural Networks (GNNs)

## Article


# A graph placement methodology for fast chip design



<https://doi.org/10.1038/s41586-021-03544-w>

Received: 3 November 2020

Accepted: 13 April 2021

Published online: 9 June 2021

 Check for updates

Azalia Mirhoseini<sup>1,4</sup>, Anna Goldie<sup>1,3,4</sup>, Mustafa Yazgan<sup>2</sup>, Joe Wenjie Jiang<sup>1</sup>,  
Ebrahim Songhori<sup>1</sup>, Shen Wang<sup>1</sup>, Young-Joon Lee<sup>2</sup>, Eric Johnson<sup>1</sup>, Omkar Pathak<sup>2</sup>,  
Azade Nazi<sup>1</sup>, Jiwoo Pak<sup>2</sup>, Andy Tong<sup>2</sup>, Kavya Srinivasa<sup>2</sup>, William Hang<sup>3</sup>, Emre Tuncer<sup>2</sup>,  
Quoc V. Le<sup>1</sup>, James Laudon<sup>1</sup>, Richard Ho<sup>2</sup>, Roger Carpenter<sup>2</sup> & Jeff Dean<sup>1</sup>

Chip floorplanning is the engineering task of designing the physical layout of a computer chip. Despite five decades of research<sup>1</sup>, chip floorplanning has defied

# Graphs + Deep Learning = Graphs Neural Networks (GNNs)

## Article


### A graph placement methodology for fast chip design

<https://doi.org/10.1038/s41586-021-03>

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## Article

### Advancing mathematics by guiding human intuition with AI

<https://doi.org/10.1038/s41586-021-04086-x>

Received: 10 July 2021

Accepted: 30 September 2021

Published online: 1 December 2021

Open access

Alex Davies<sup>1✉</sup>, Petar Veličković<sup>1</sup>, Lars Buesing<sup>1</sup>, Sam Blackwell<sup>1</sup>, Daniel Zheng<sup>1</sup>, Nenad Tomašev<sup>1</sup>, Richard Tanburn<sup>1</sup>, Peter Battaglia<sup>1</sup>, Charles Blundell<sup>1</sup>, András Juhász<sup>2</sup>, Marc Lackenby<sup>2</sup>, Geordie Williamson<sup>3</sup>, Demis Hassabis<sup>1</sup> & Pushmeet Kohli<sup>1✉</sup>

The practice of mathematics involves discovering patterns and using these to formulate and prove conjectures, resulting in theorems. Since the 1960s

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formul

## Article

### Highly accurate protein structure prediction with AlphaFold


<https://doi.org/10.1038/s41586-021-03819-2>

Received: 11 May 2021

Accepted: 12 July 2021

Published online: 15 July 2021

Open access

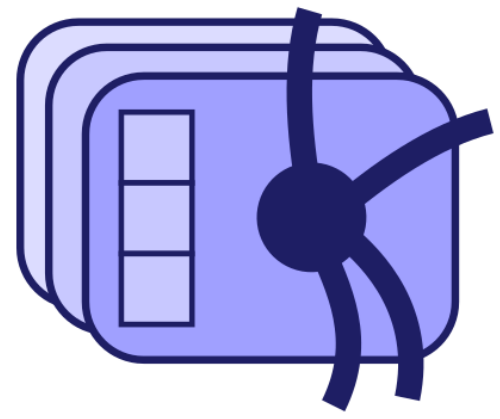
 Check for updates

John Jumper<sup>1,4</sup>, Richard Evans<sup>1,4</sup>, Alexander Pritzel<sup>1,4</sup>, Tim Green<sup>1,4</sup>, Michael Figurnov<sup>1,4</sup>, Olaf Ronneberger<sup>1,4</sup>, Kathryn Tunyasuvunakool<sup>1,4</sup>, Russ Bates<sup>1,4</sup>, Augustin Židek<sup>1,4</sup>, Anna Potapenko<sup>1,4</sup>, Alex Bridgland<sup>1,4</sup>, Clemens Meyer<sup>1,4</sup>, Simon A. A. Kohl<sup>1,4</sup>, Andrew J. Ballard<sup>1,4</sup>, Andrew Cowie<sup>1,4</sup>, Bernardino Romera-Paredes<sup>1,4</sup>, Stanislav Nikolov<sup>1,4</sup>, Rishub Jain<sup>1,4</sup>, Jonas Adler<sup>1</sup>, Trevor Back<sup>1</sup>, Stig Petersen<sup>1</sup>, David Reiman<sup>1</sup>, Ellen Clancy<sup>1</sup>, Michal Zielinski<sup>1</sup>, Martin Steinegger<sup>2,3</sup>, Michalina Pacholska<sup>1</sup>, Tamas Berghammer<sup>1</sup>, Sebastian Bodenstein<sup>1</sup>, David Silver<sup>1</sup>, Oriol Vinyals<sup>1</sup>, Andrew W. Senior<sup>1</sup>, Koray Kavukcuoglu<sup>1</sup>, Pushmeet Kohli<sup>1</sup> & Demis Hassabis<sup>1,4</sup>

Proteins are essential to life, and understanding their structure can facilitate a

# A Single GNN Layer

Input  
samples

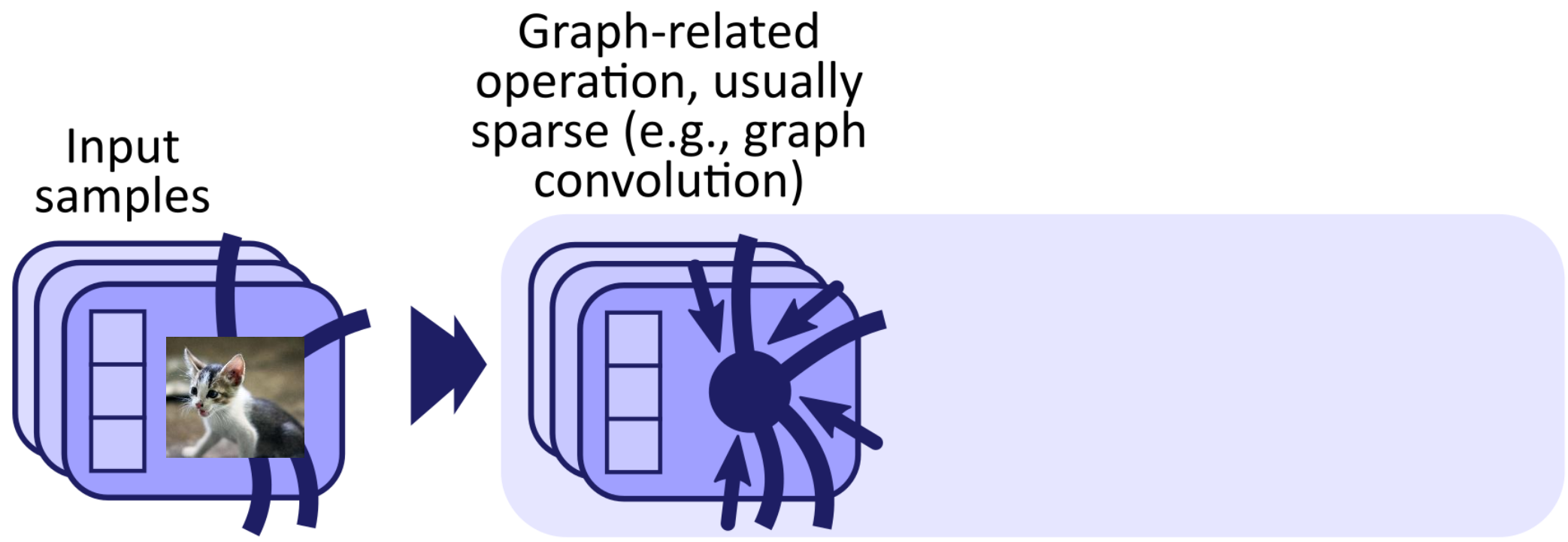


# A Single GNN Layer

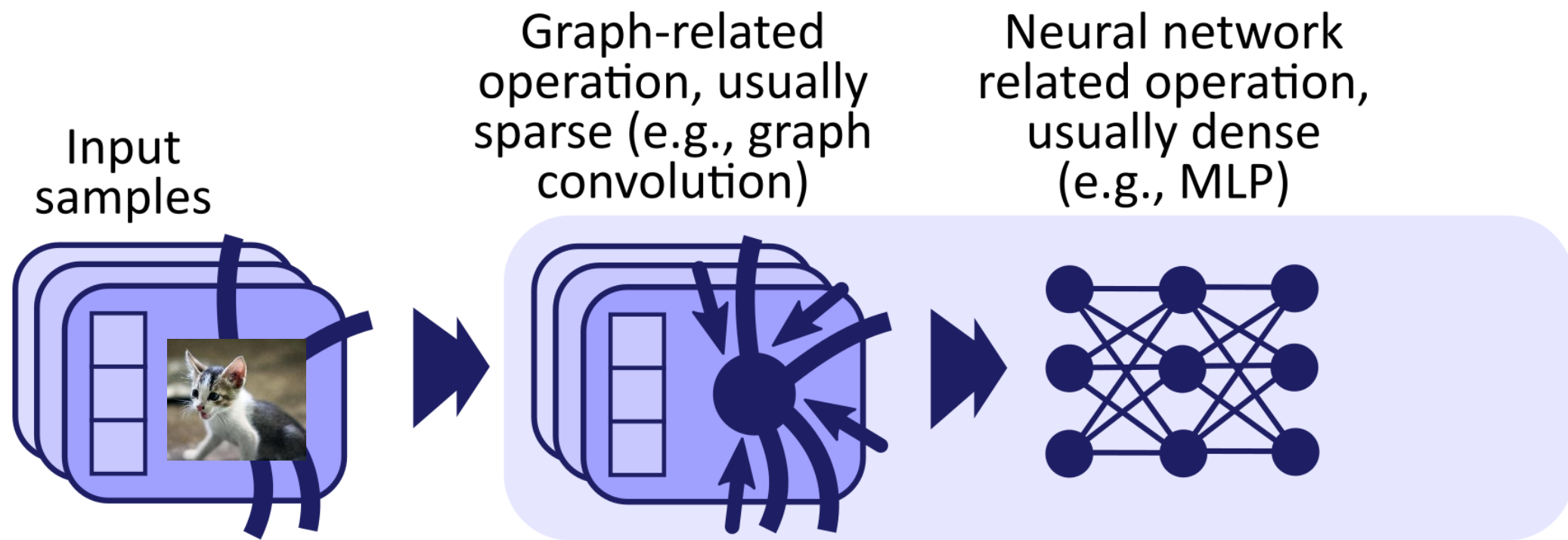
Input samples



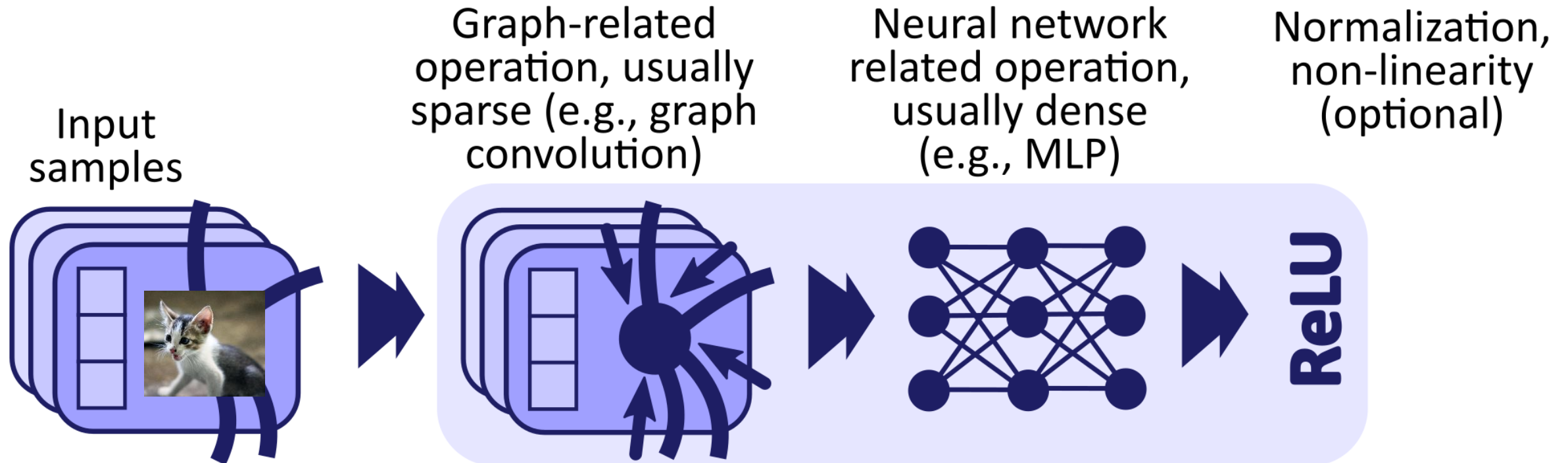
# A Single GNN Layer



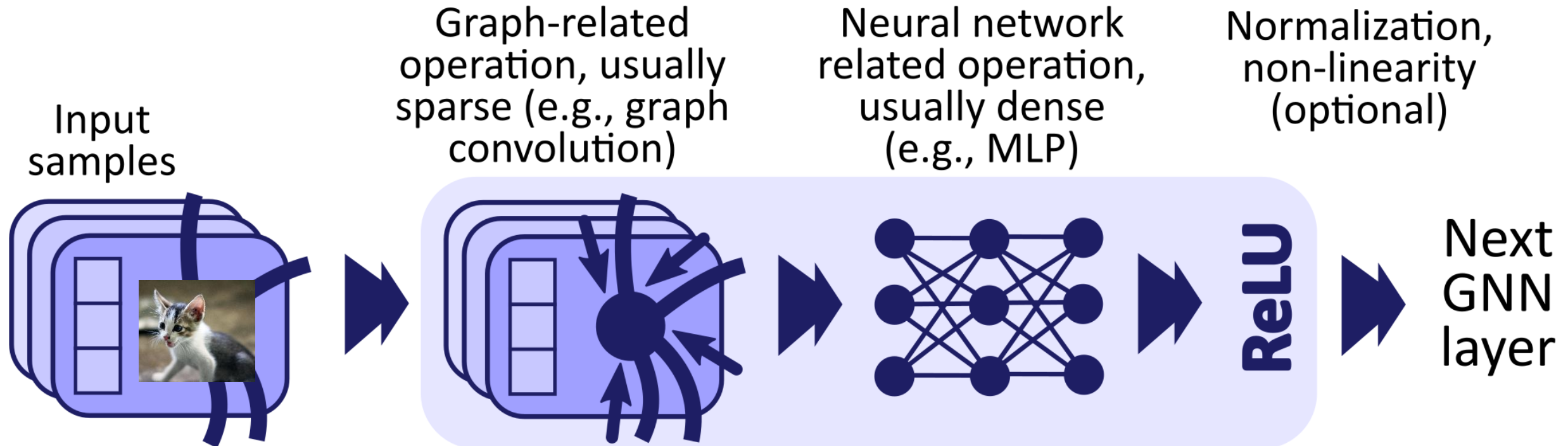
# A Single GNN Layer



# A Single GNN Layer

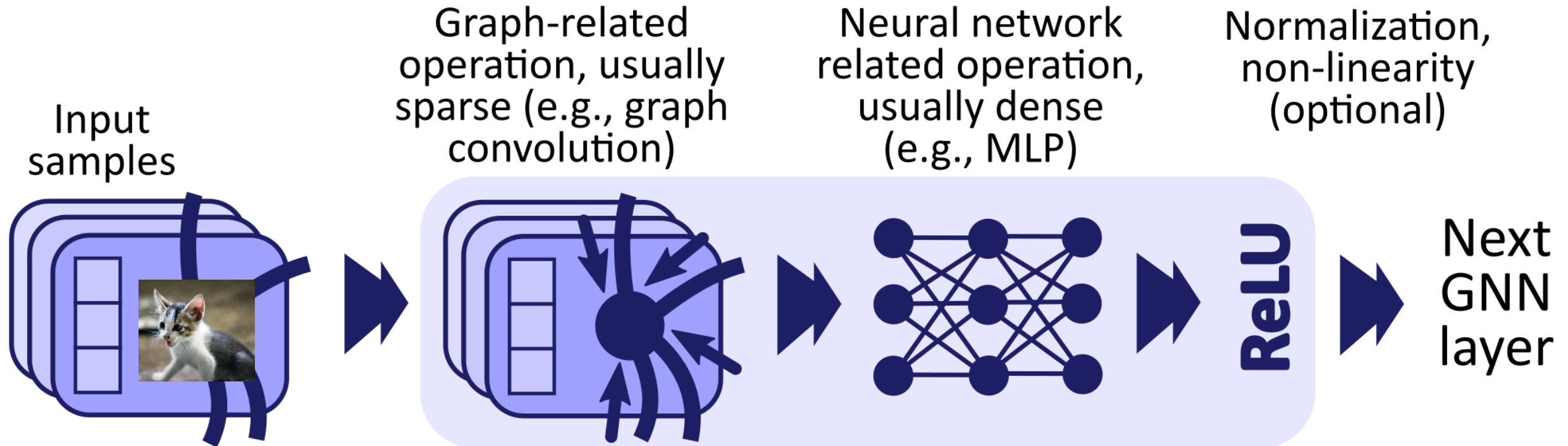


# A Single GNN Layer



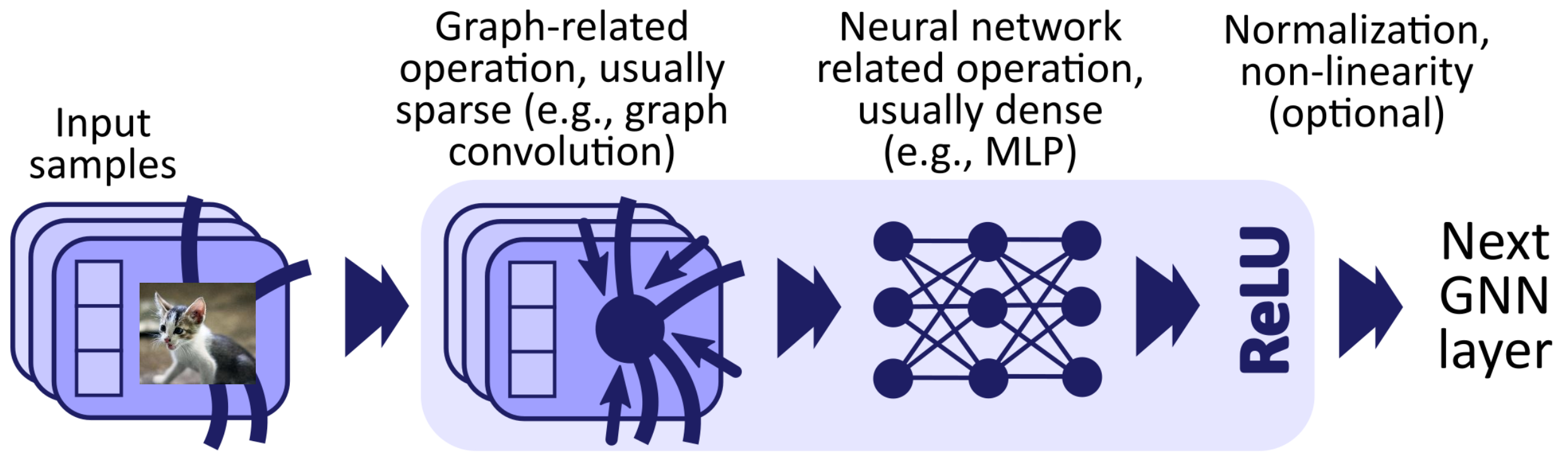
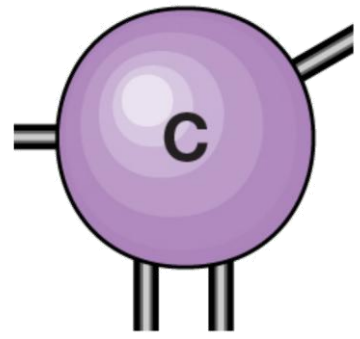
# A Single GNN Layer

Classification or regression of nodes

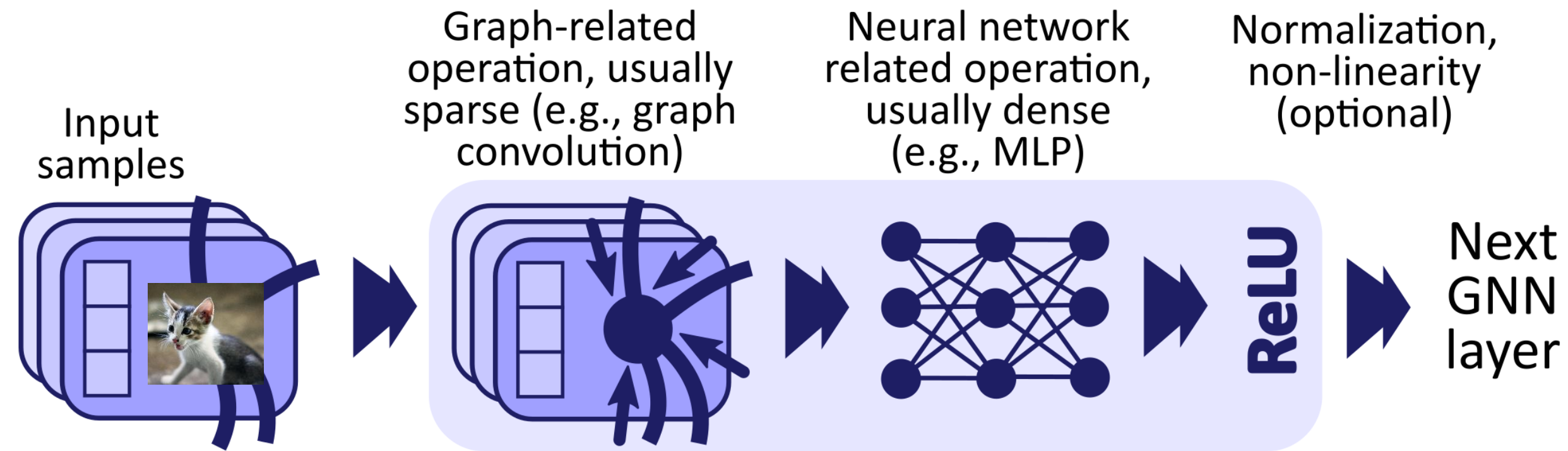
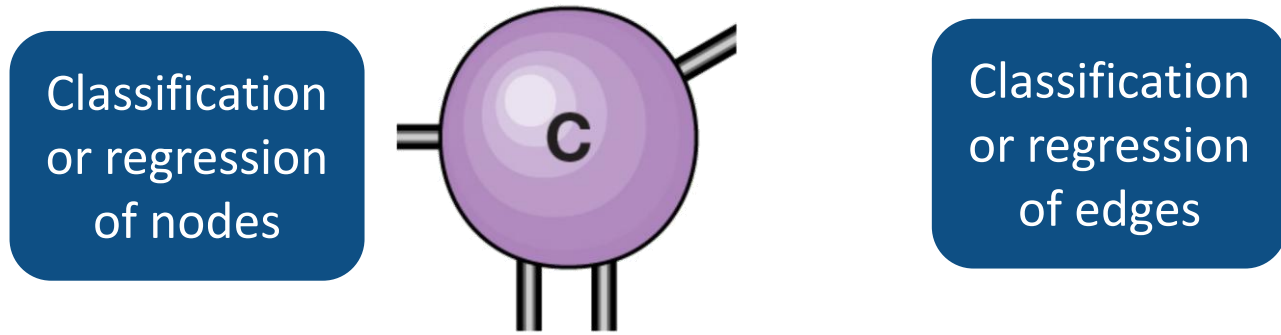


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Classification or regression of nodes

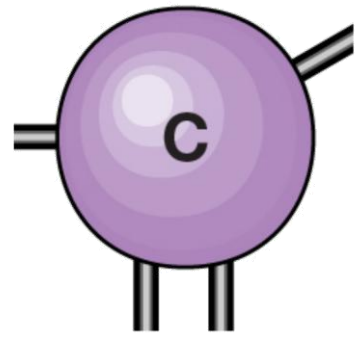


# A Single GNN Layer

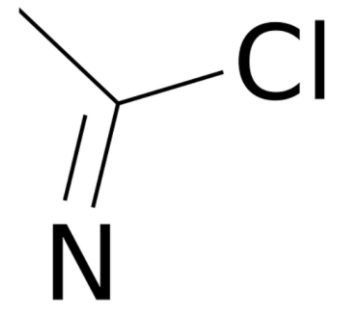


# A Single GNN Layer

Classification or regression of nodes



Classification or regression of edges



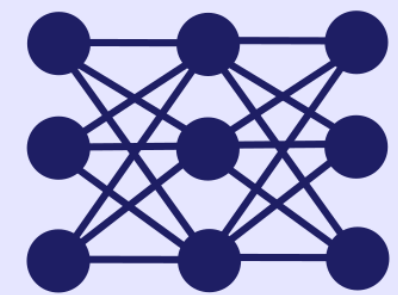
Input samples



Graph-related operation, usually sparse (e.g., graph convolution)



Neural network related operation, usually dense (e.g., MLP)

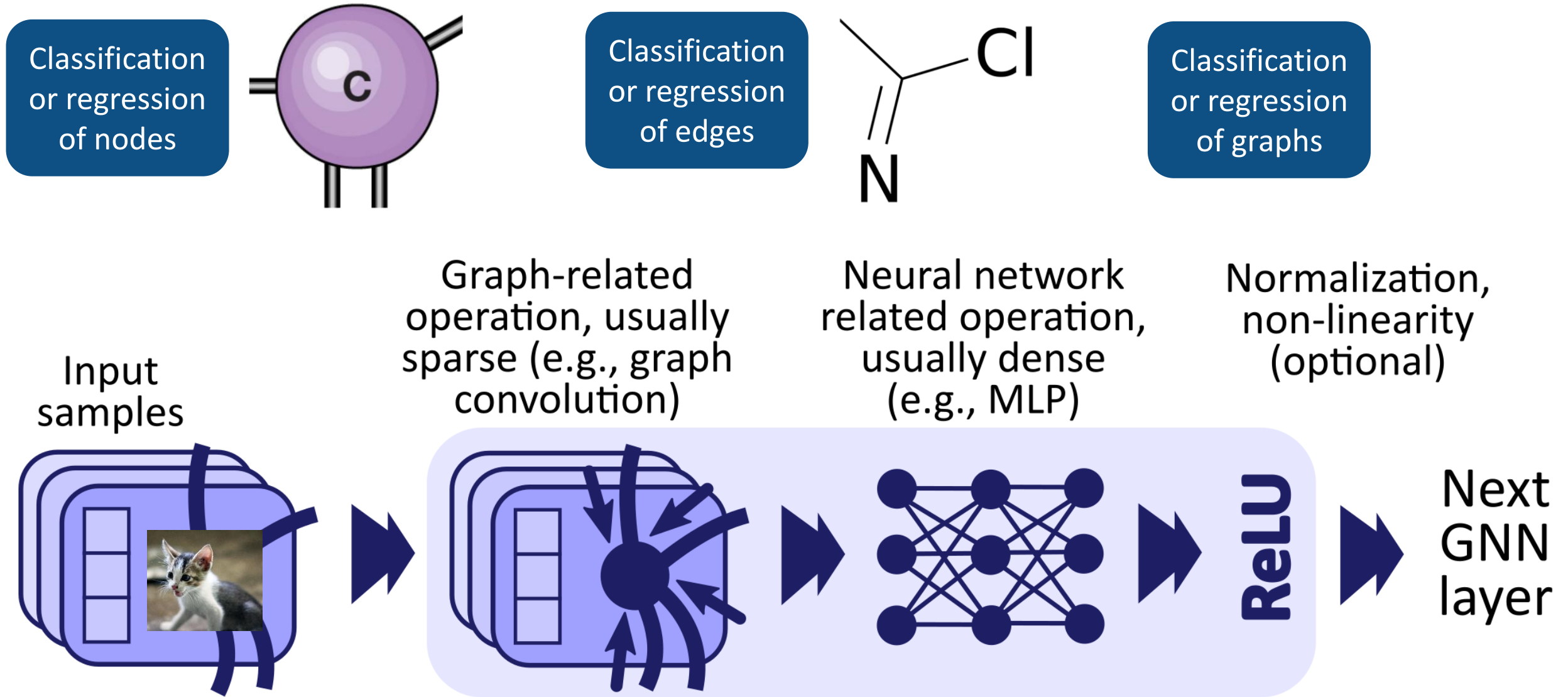


Normalization, non-linearity (optional)

**ReLU**

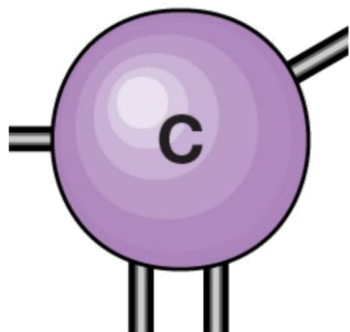
Next GNN layer

# A Single GNN Layer

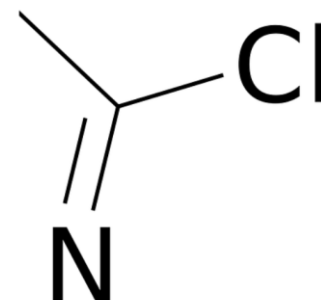


# A Single GNN Layer

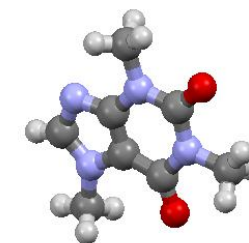
Classification or regression of nodes



Classification or regression of edges



Classification or regression of graphs



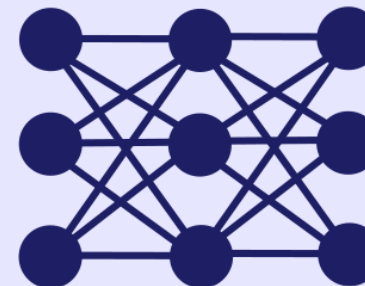
Input samples



Graph-related operation, usually sparse (e.g., graph convolution)



Neural network related operation, usually dense (e.g., MLP)

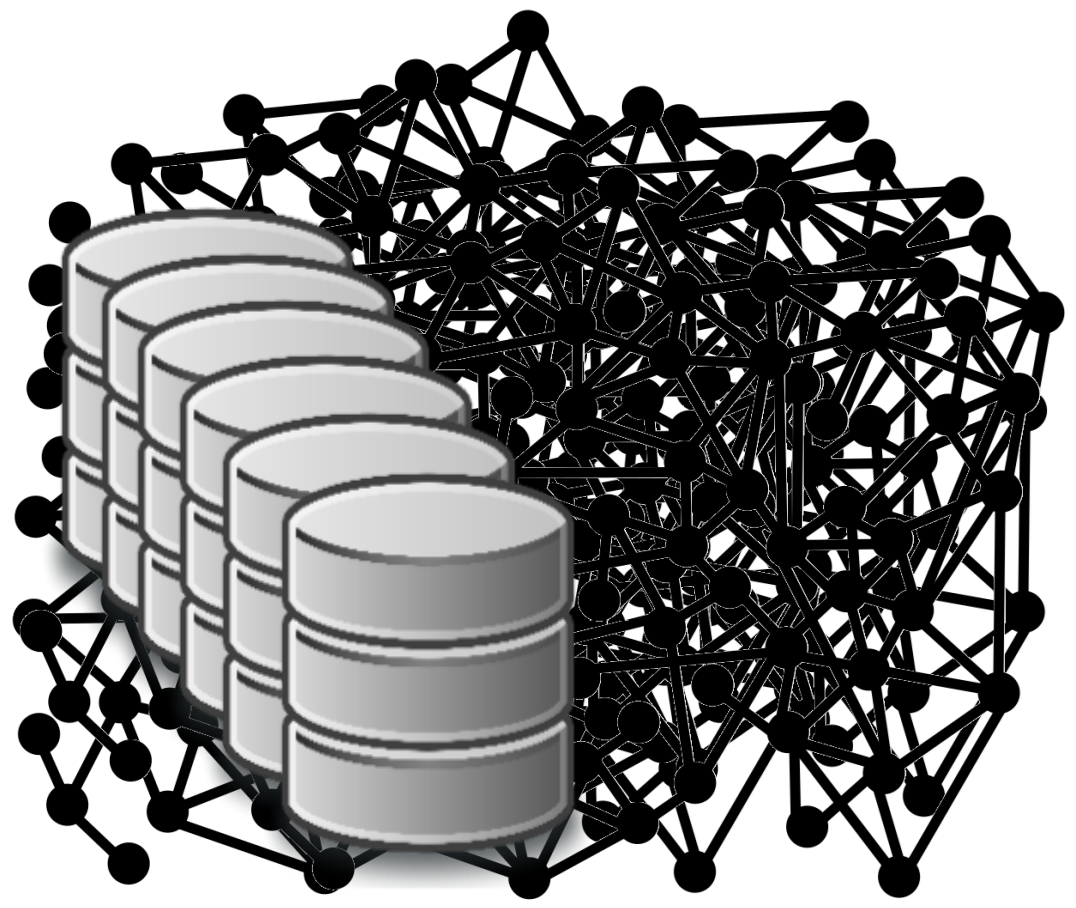


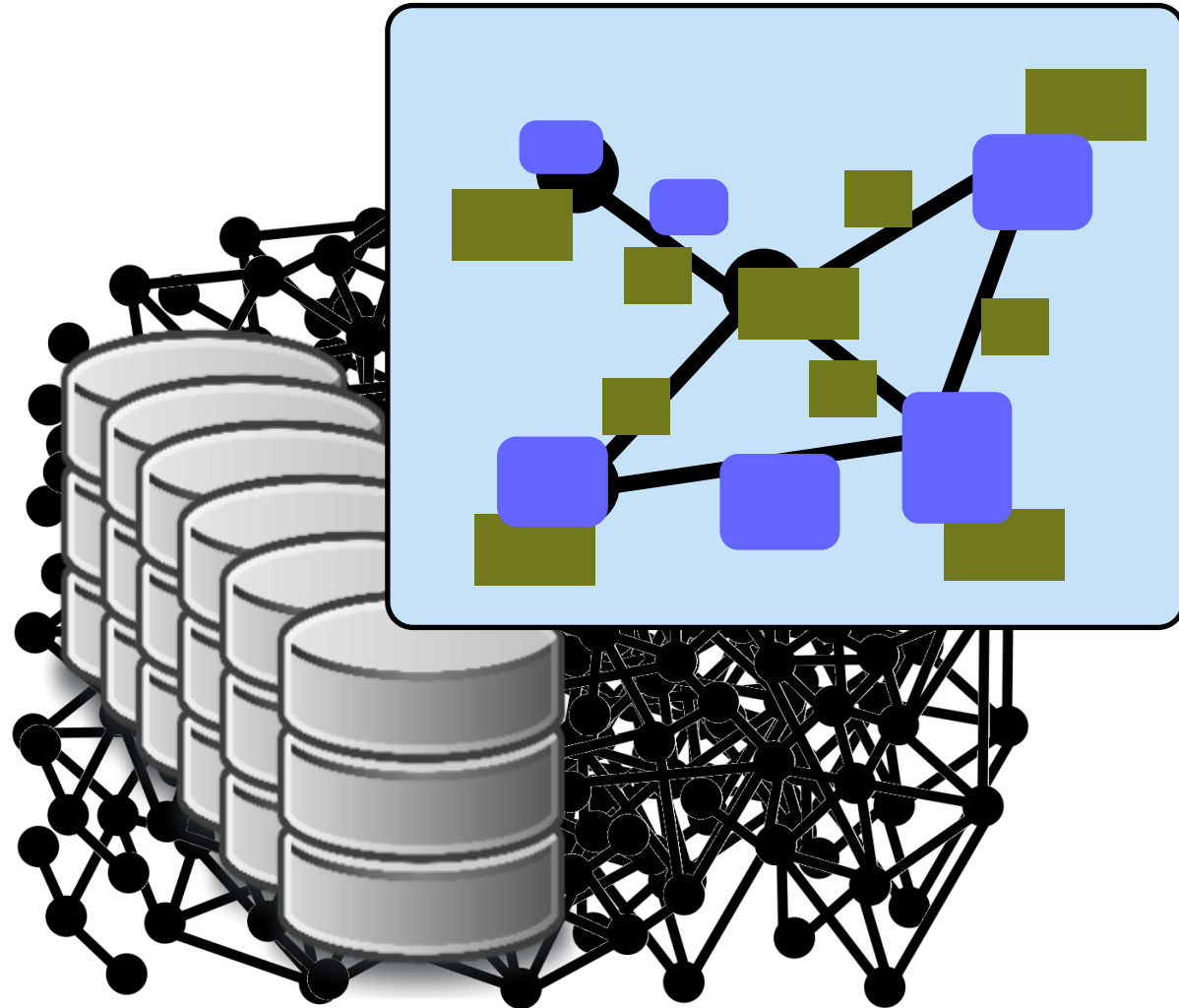
Normalization, non-linearity (optional)

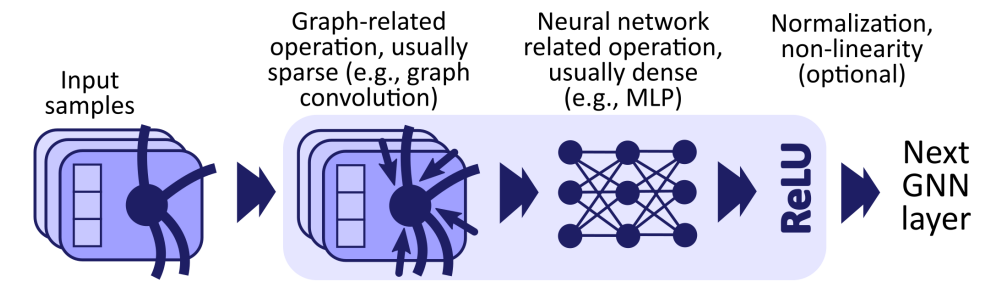
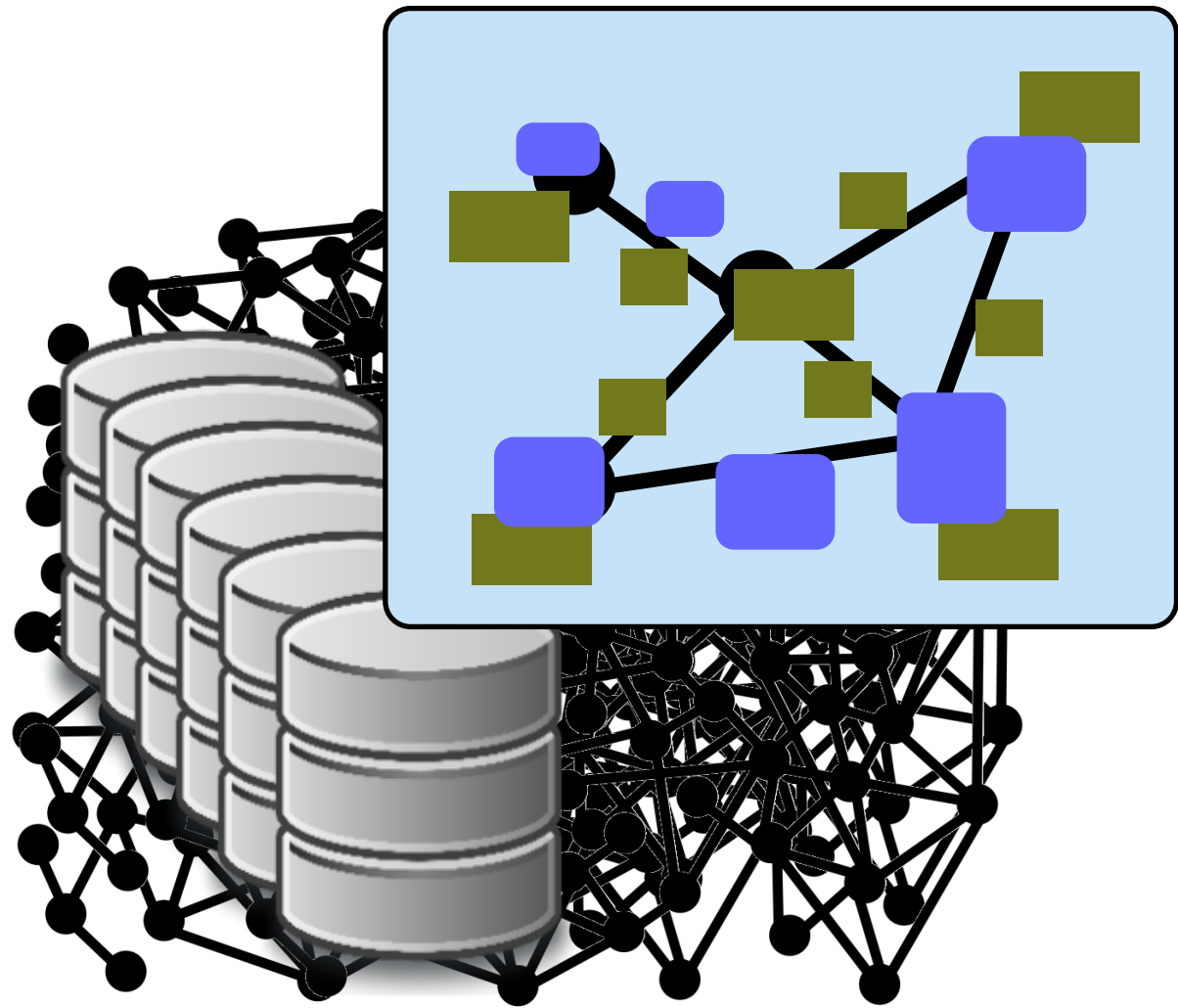
**ReLU**

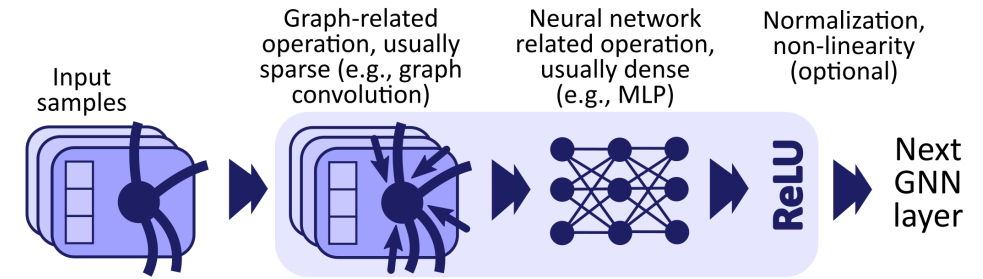
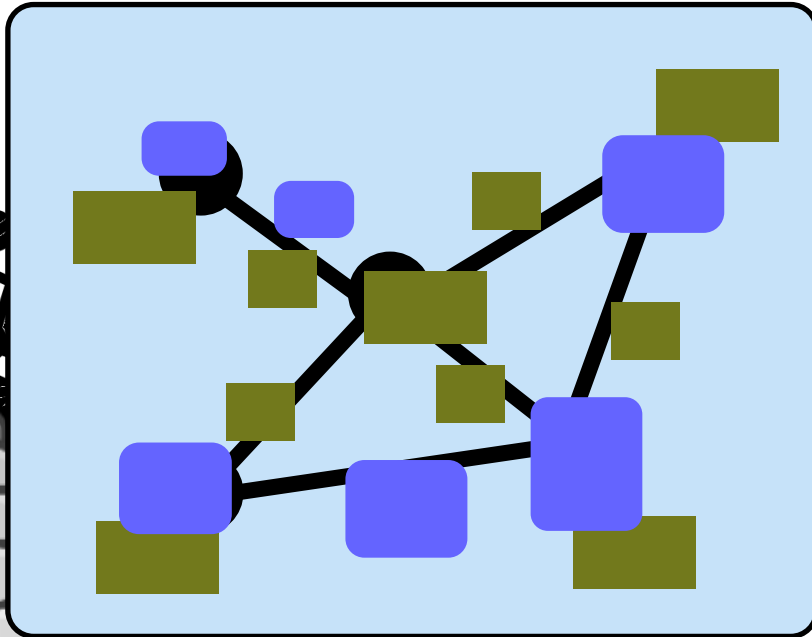
Next GNN layer



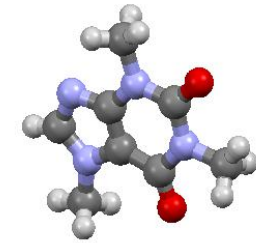


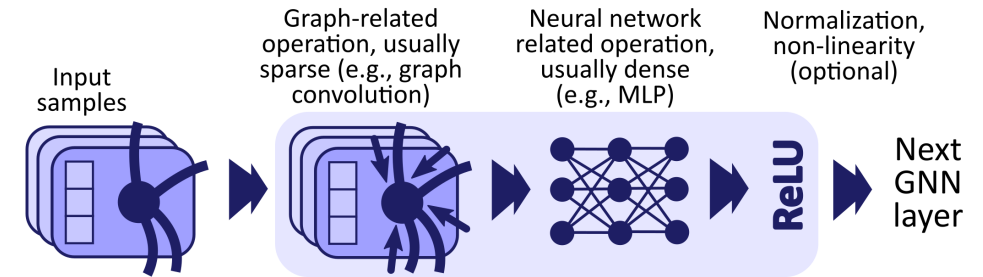
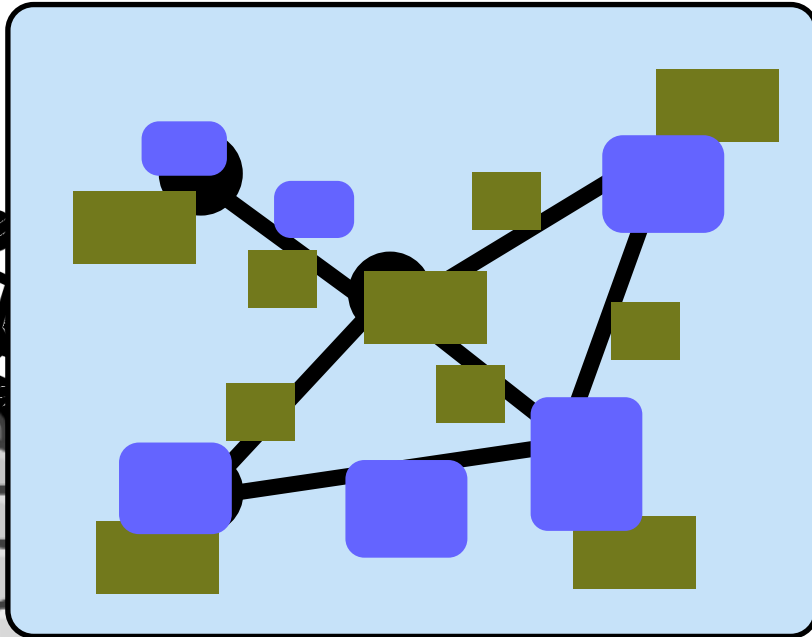




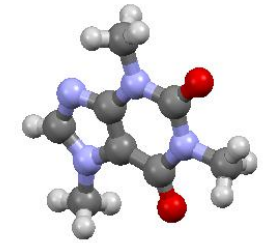


Classification  
or regression  
of graphs

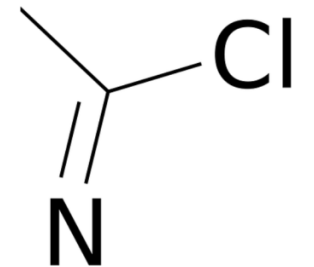


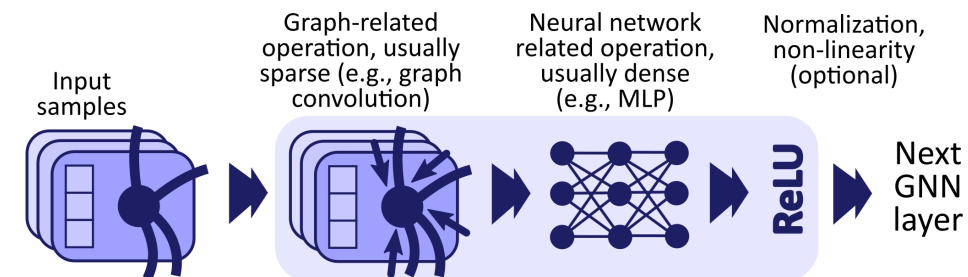
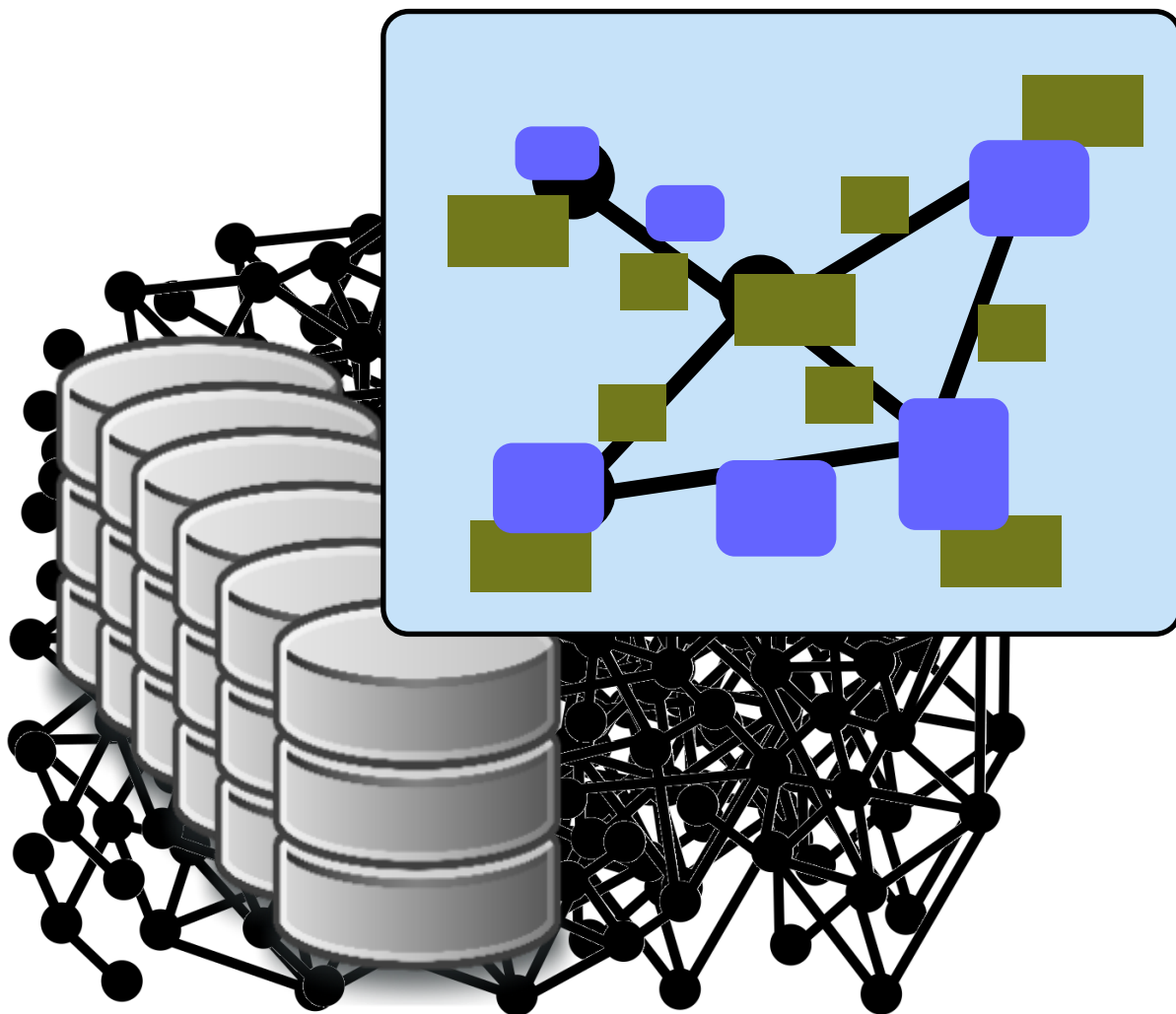


Classification  
or regression  
of graphs

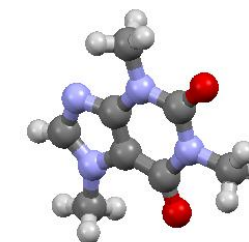


Classification  
or regression  
of edges

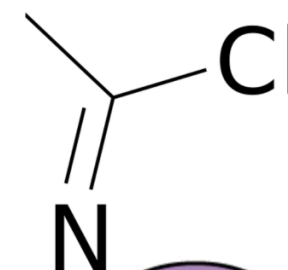




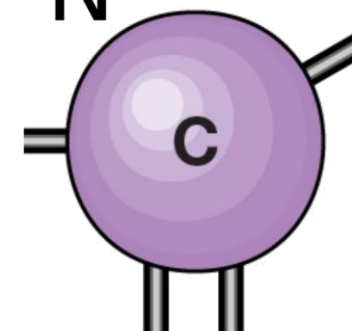
Classification  
or regression  
of graphs



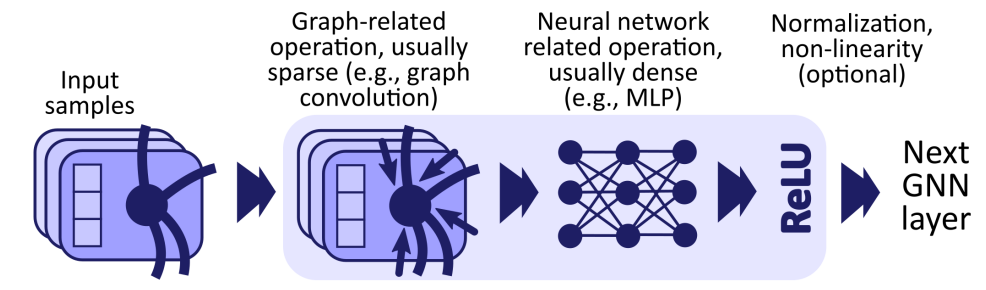
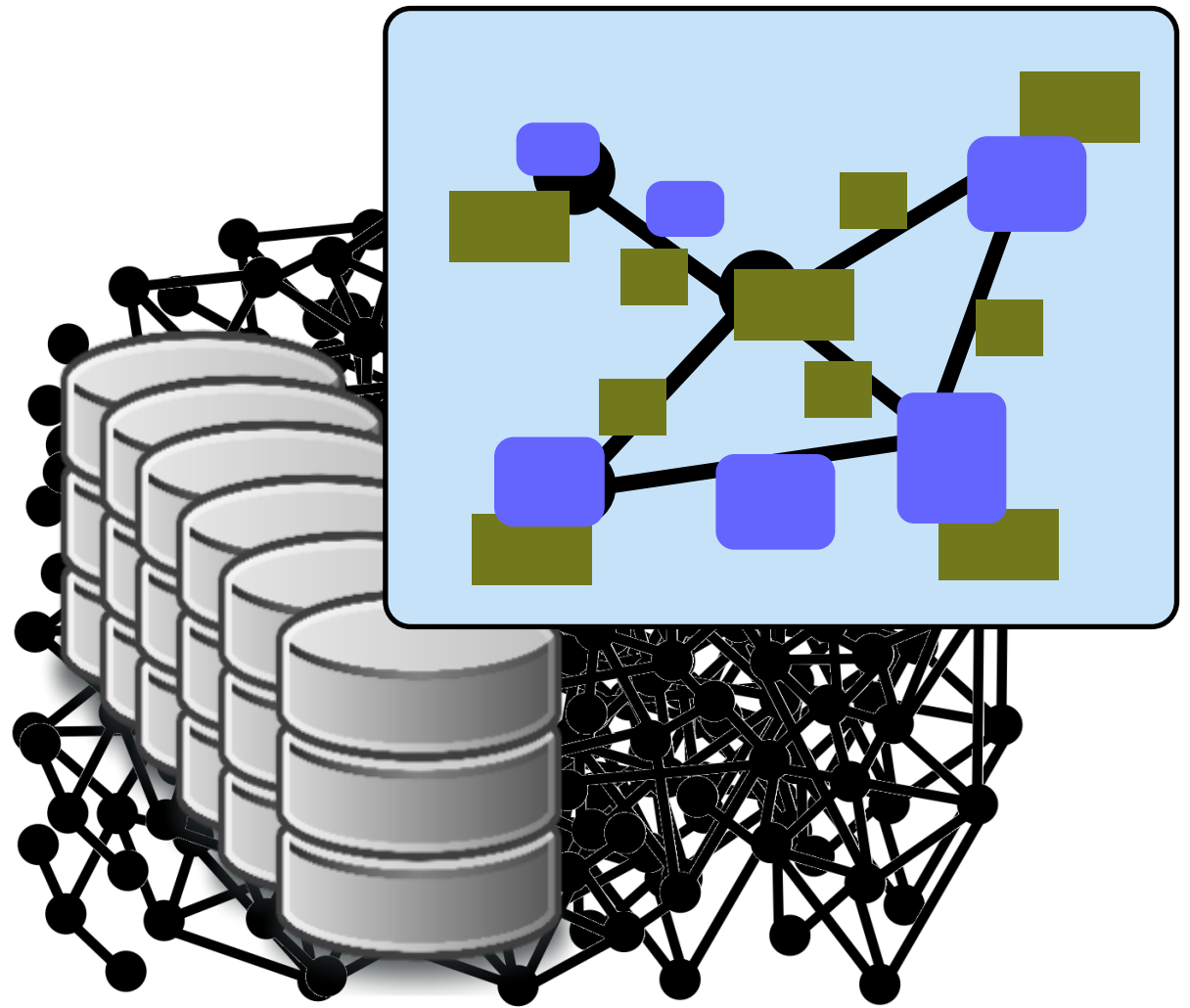
Classification  
or regression  
of edges



Classification  
or regression  
of nodes

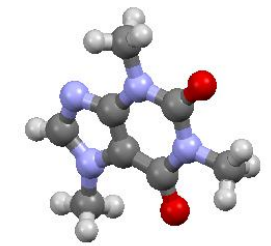


# How to marry these two?

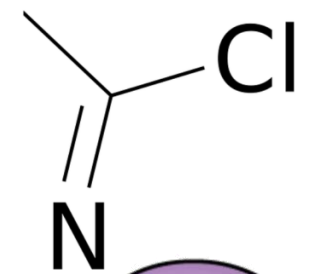


+

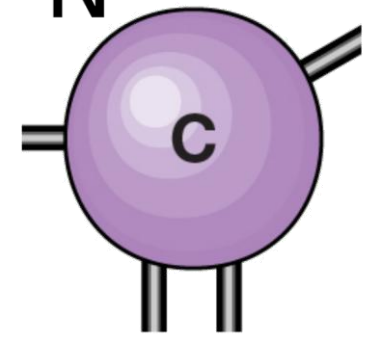
Classification or regression of graphs



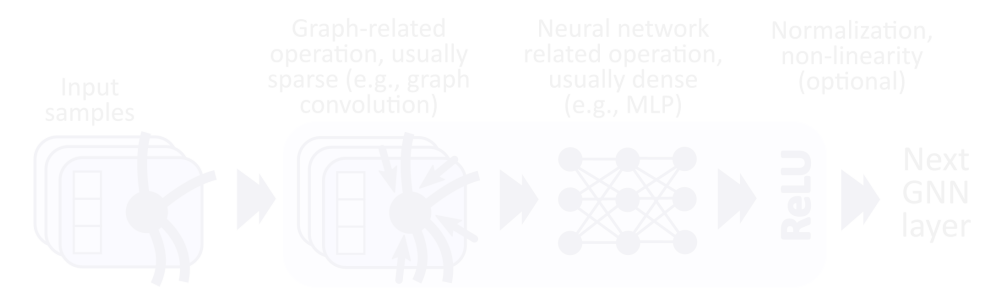
Classification or regression of edges



Classification or regression of nodes



# How to marry these two?

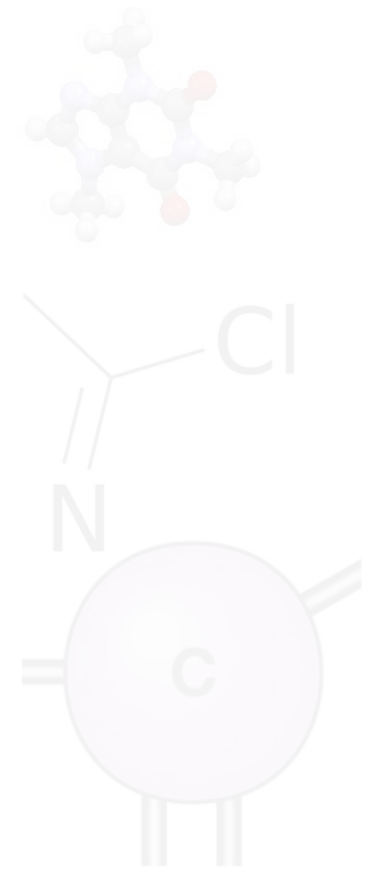


**Main challenge: understanding how to merge these two conceptually**

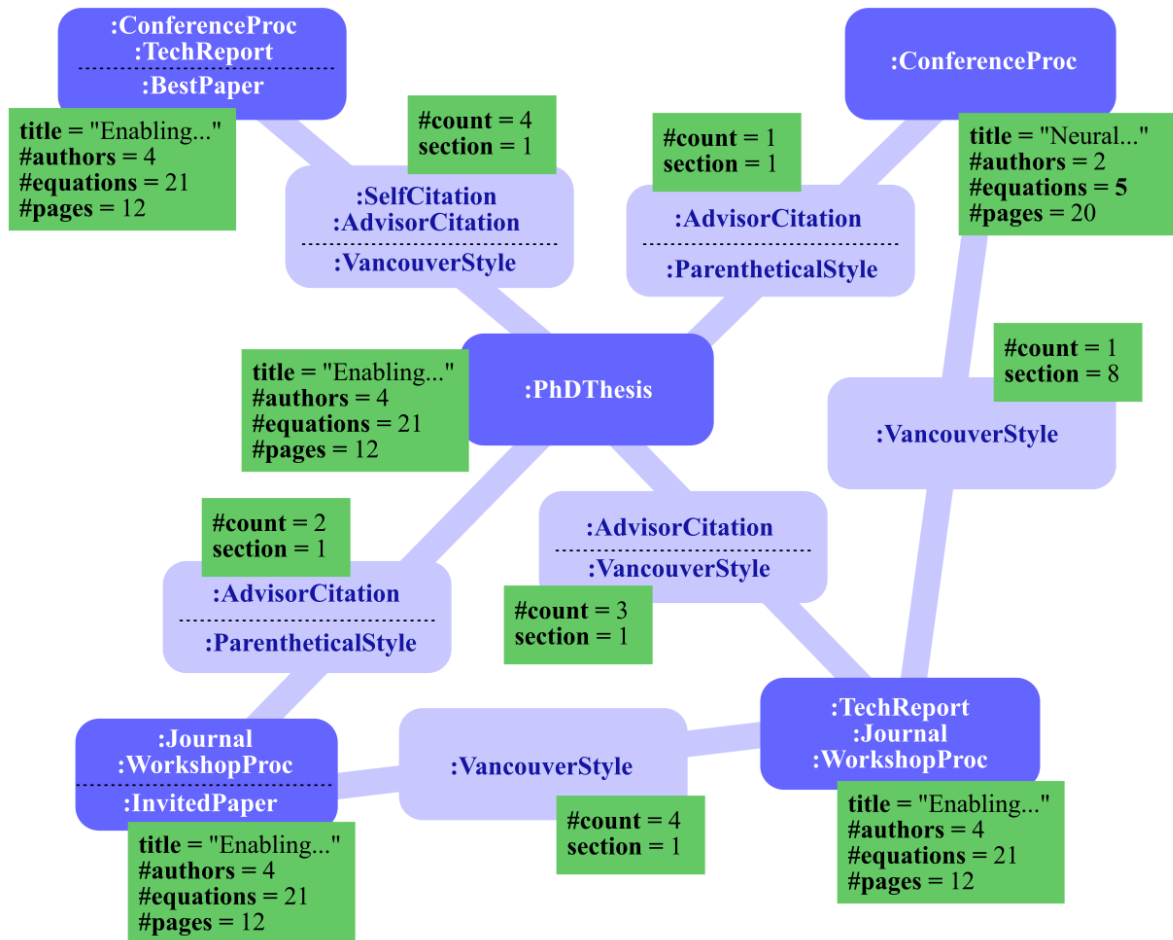
Classification of nodes

Classification or regression of edges

Classification or regression of nodes

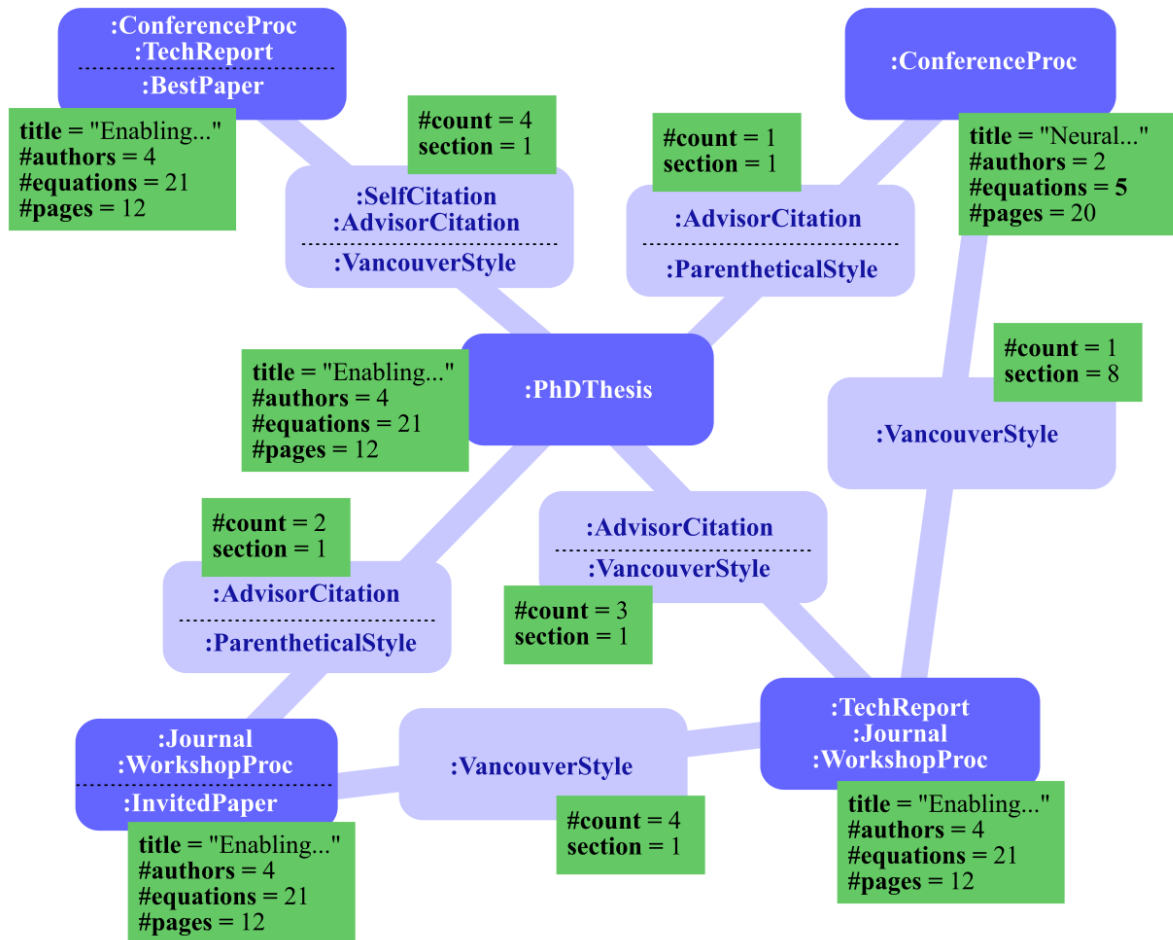


# Marrying Graph Databases and GNNs

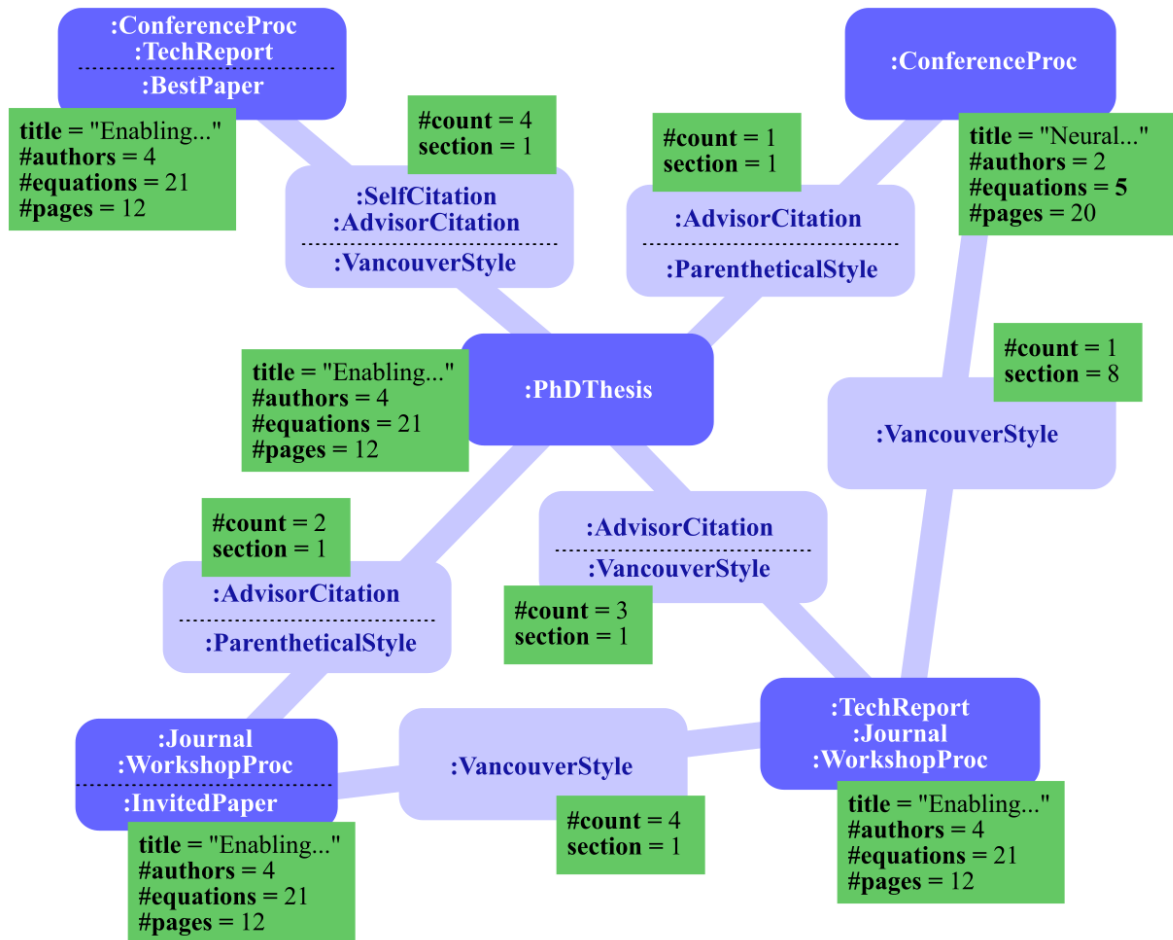


# Marrying Graph Databases and GNNs

There is a neat way to think about the GNN workloads within the LPG model



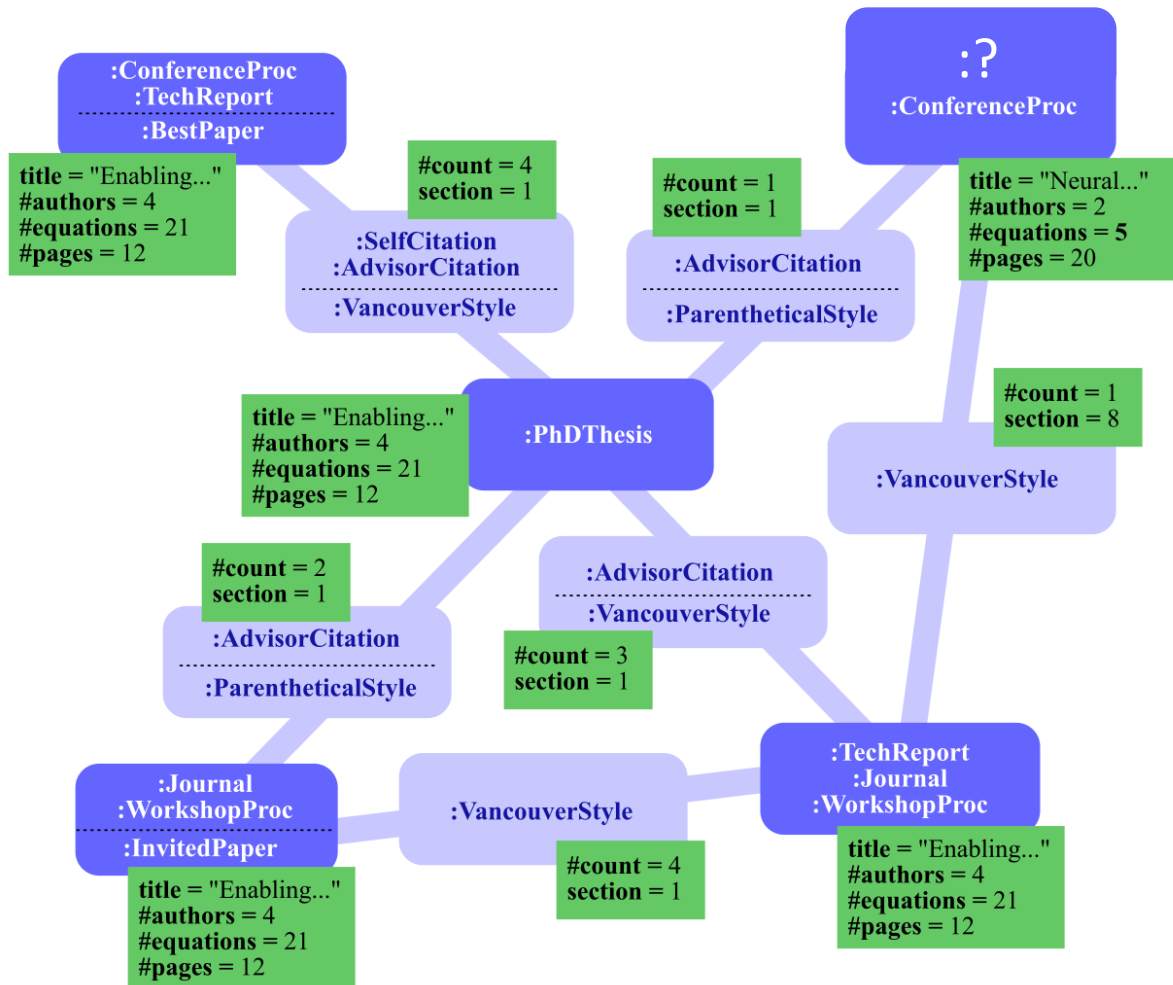
# Marrying Graph Databases and GNNs



There is a neat way to think about the GNN workloads within the LPG model

Node/edge/graph classification becomes *label prediction*

# Marrying Graph Databases and GNNs



There is a neat way to think about the GNN workloads within the LPG model

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Node/edge/graph classification becomes *label prediction*

Node/edge/graph regression becomes *property prediction*

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There is a neat way to think about the GNN workloads within the LPG model

Node/edge/graph classification becomes *label prediction*

Node/edge/graph regression becomes *property prediction*

# Marrying Graph Databases and GNNs




There is a neat way to think about the GNN workloads within the LPG model

Node/edge/graph classification becomes *label prediction*

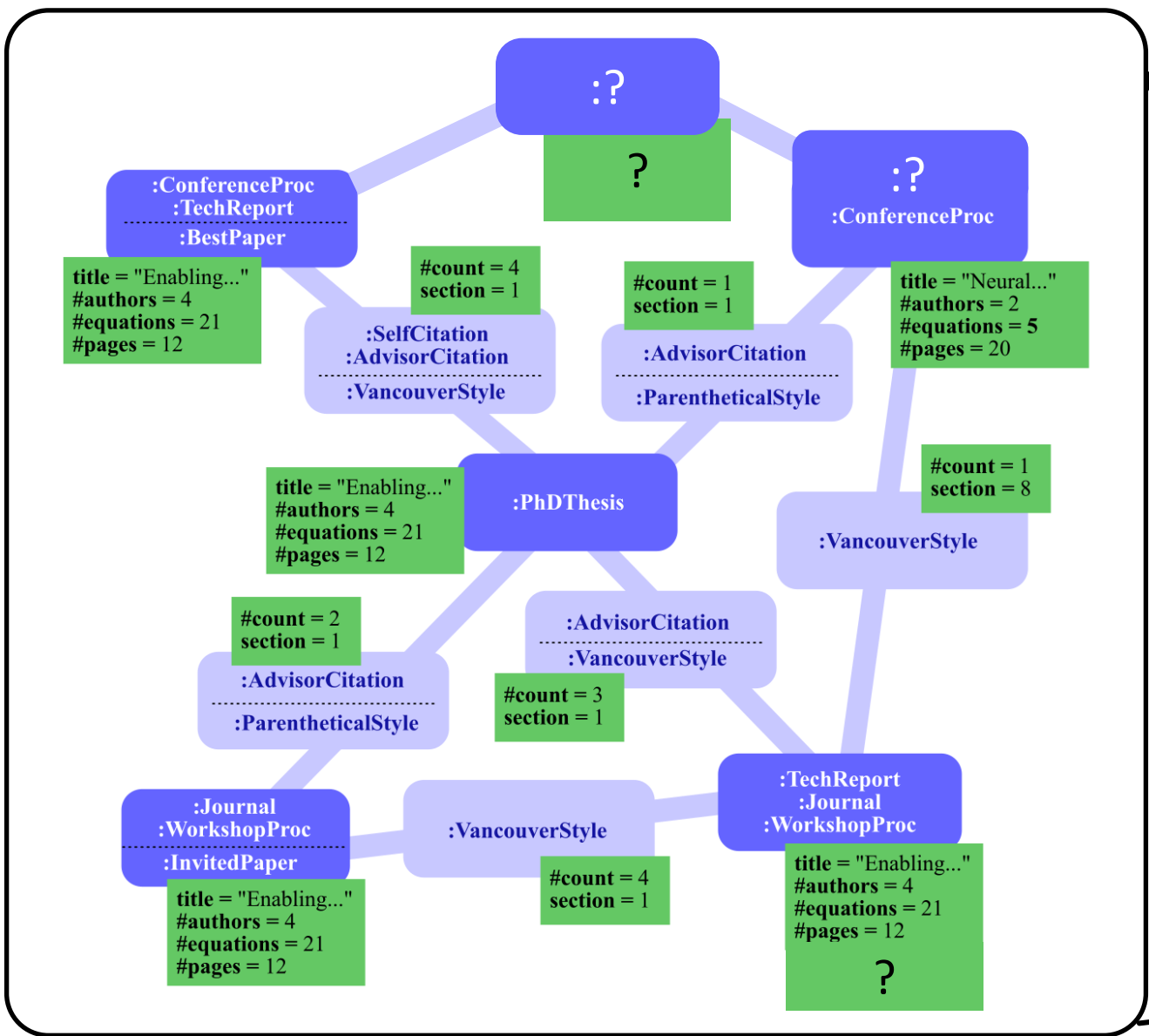
Node/edge/graph regression becomes *property prediction*

# Marrying Graph Databases and GNNs

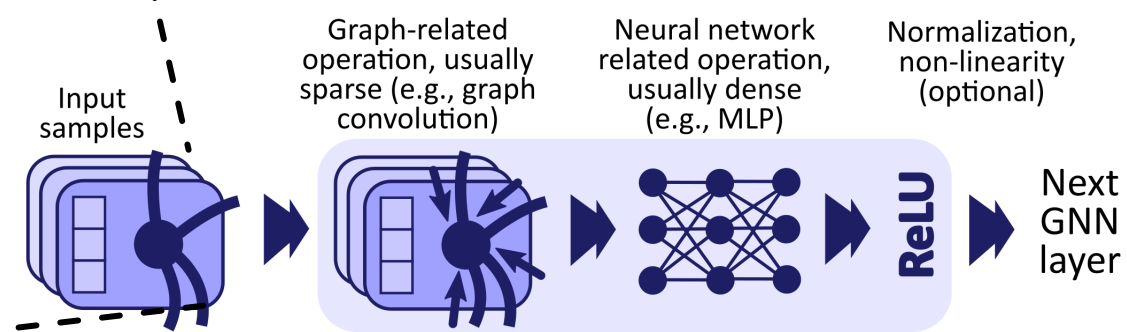



 How do we enable these GNN workloads on the LPG graph datasets while harnessing all the existing label/property information?

# Marrying Graph Databases and GNNs



How do we enable these GNN workloads on the LPG graph datasets while harnessing all the existing label/property information?

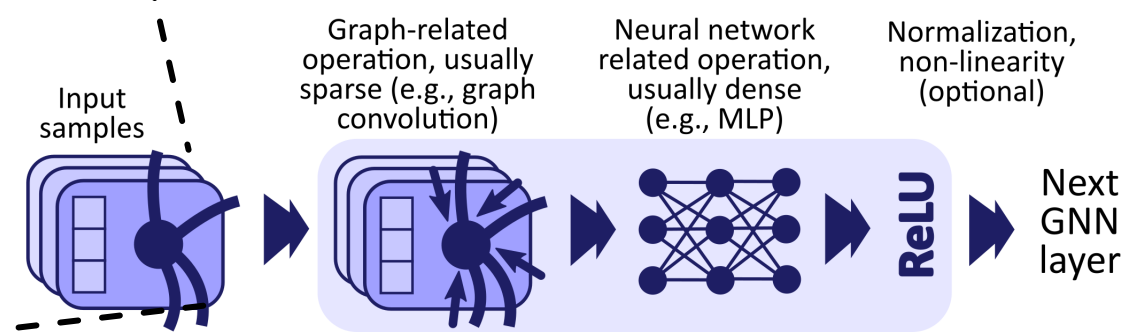


# Marrying Graph Databases and GNNs



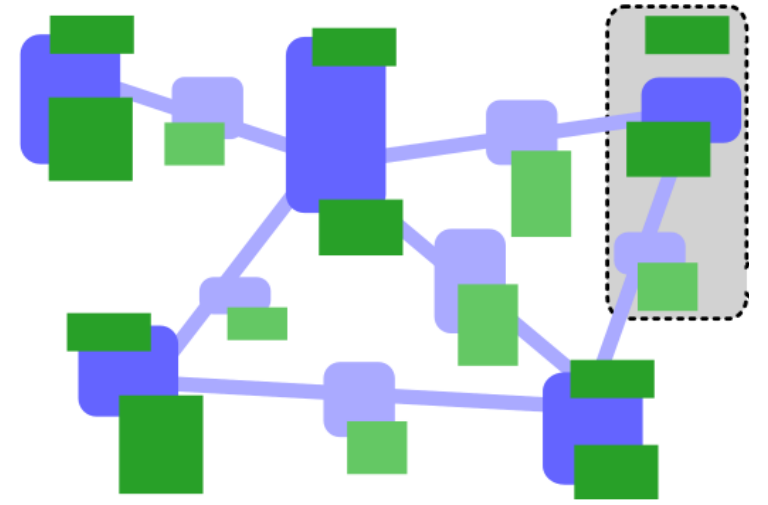
How do we enable these GNN workloads on the LPG graph datasets while harnessing all the existing label/property information?

We need the right encoder!

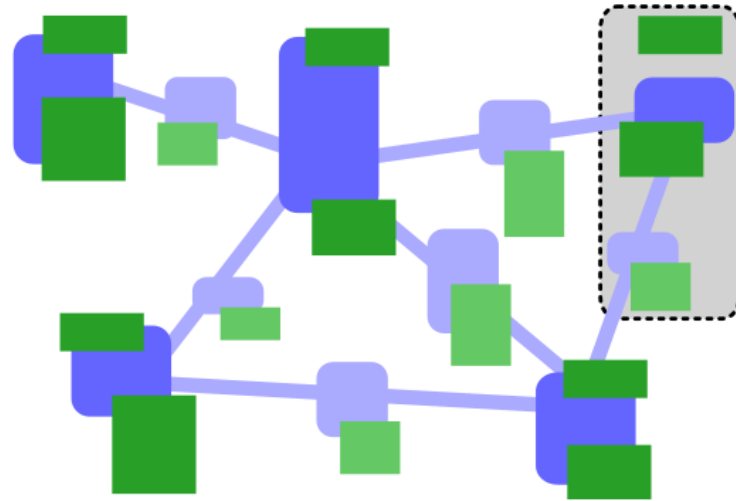


# LPG2vec: Encoding LPG Datasets into a Format Digestible by GNNs Pipelines

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# LPG2vec: Encoding LPG Datasets into a Format Digestible by GNNs Pipelines



## Encoding input LPG graphs (LPG2vec) 1

**Abstract:** We establish a general motif prediction problem and we propose...

:ConferenceProc  
 :TechReport  


---

 :BestPaper

title = "Enabling..."  
 #authors = 4  
 #equations = 21  
 #pages = 12

:SelfCitation  
 :AdvisorCitation  

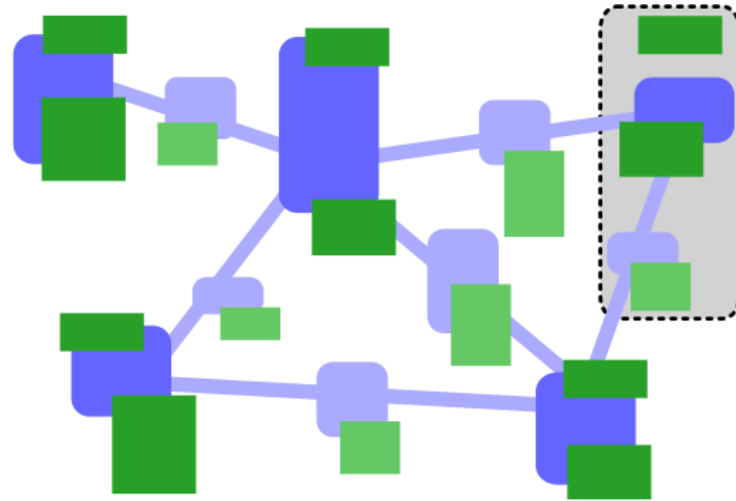

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 :VancouverStyle

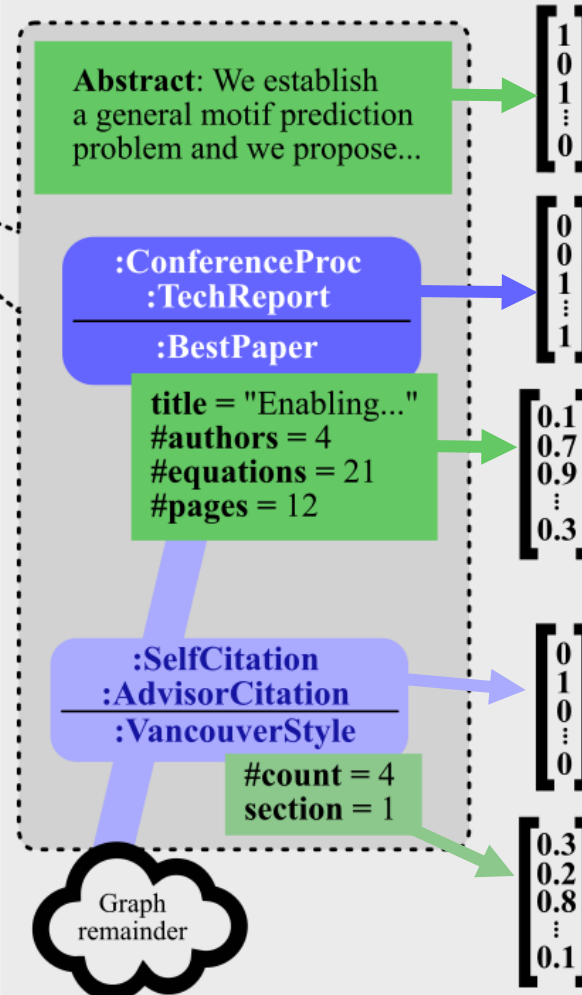
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Graph remainder

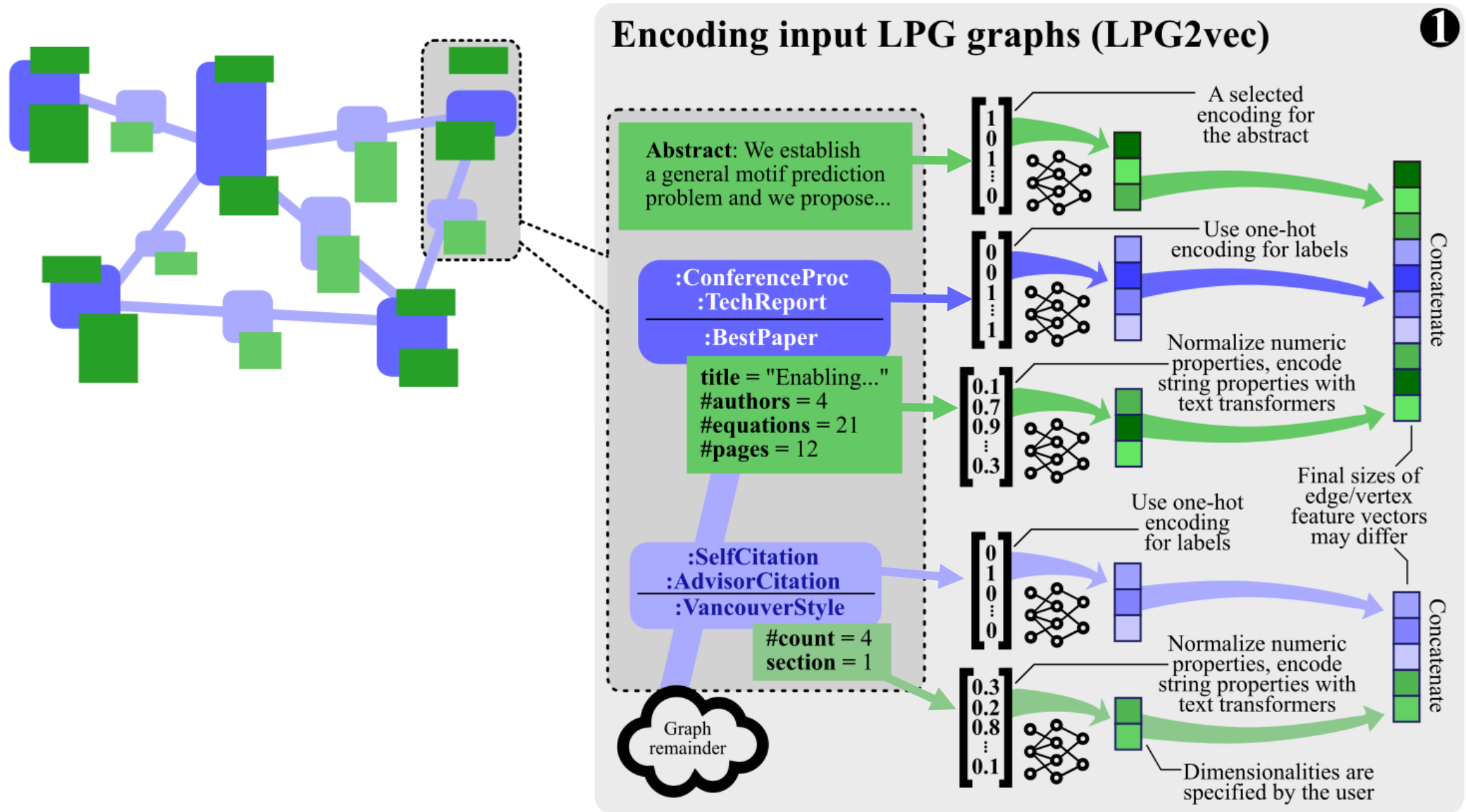
# LPG2vec: Encoding LPG Datasets into a Format Digestible by GNNs Pipelines



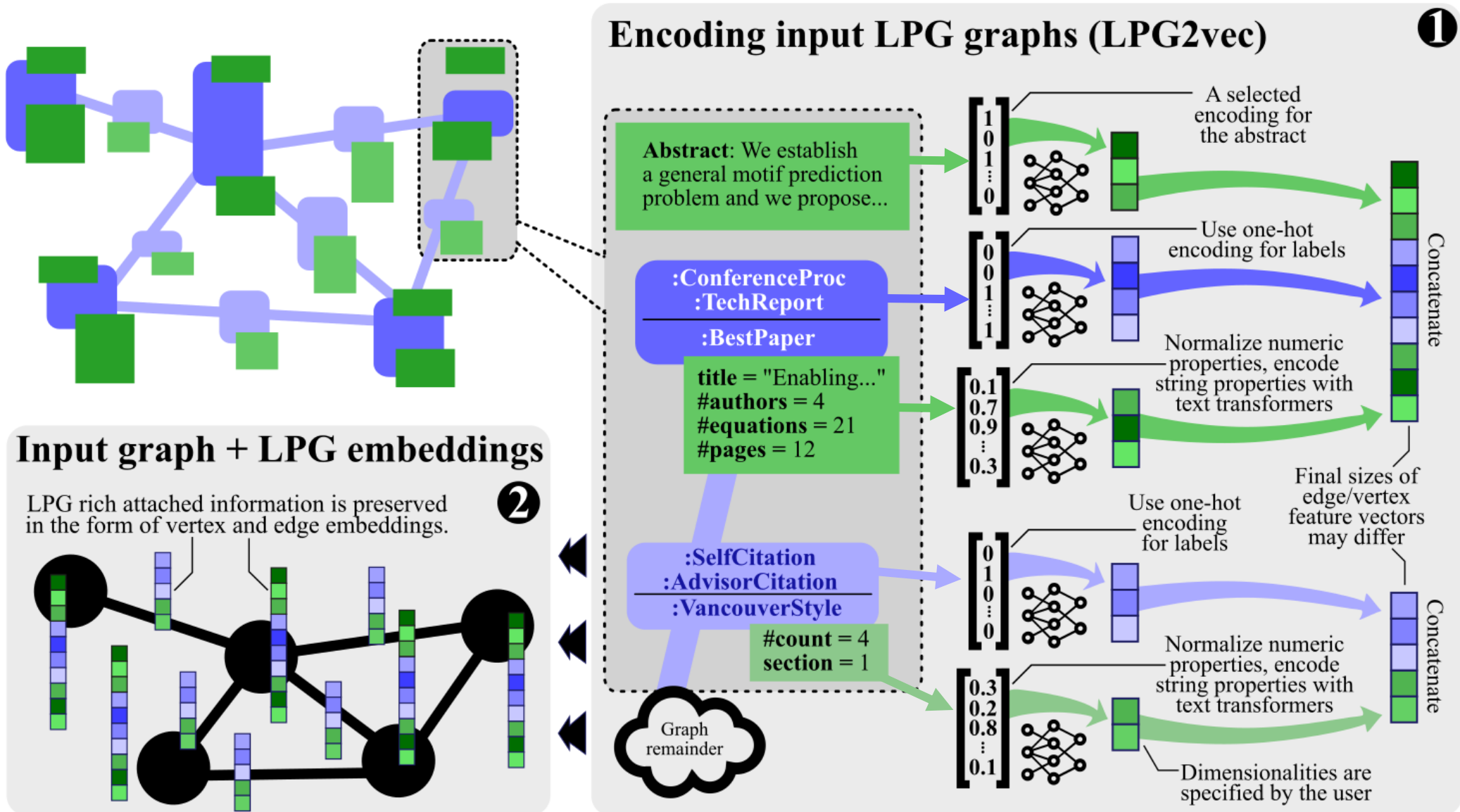
## Encoding input LPG graphs (LPG2vec) 1



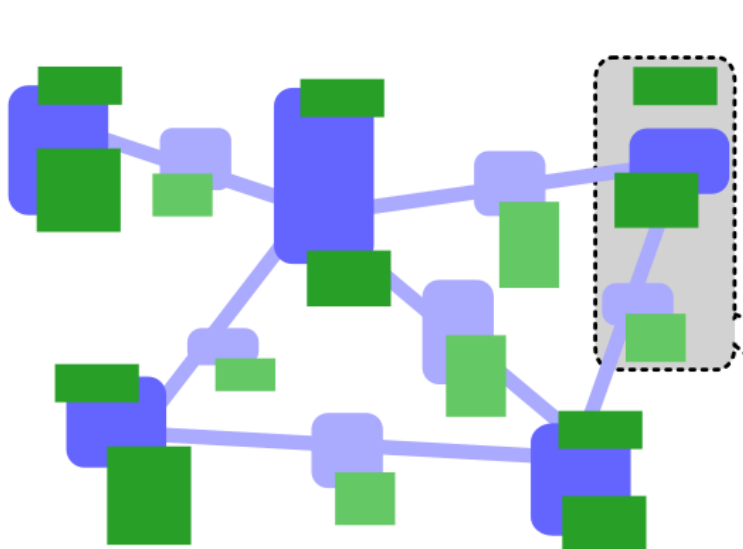
# LPG2vec: Encoding LPG Datasets into a Format Digestible by GNNs Pipelines



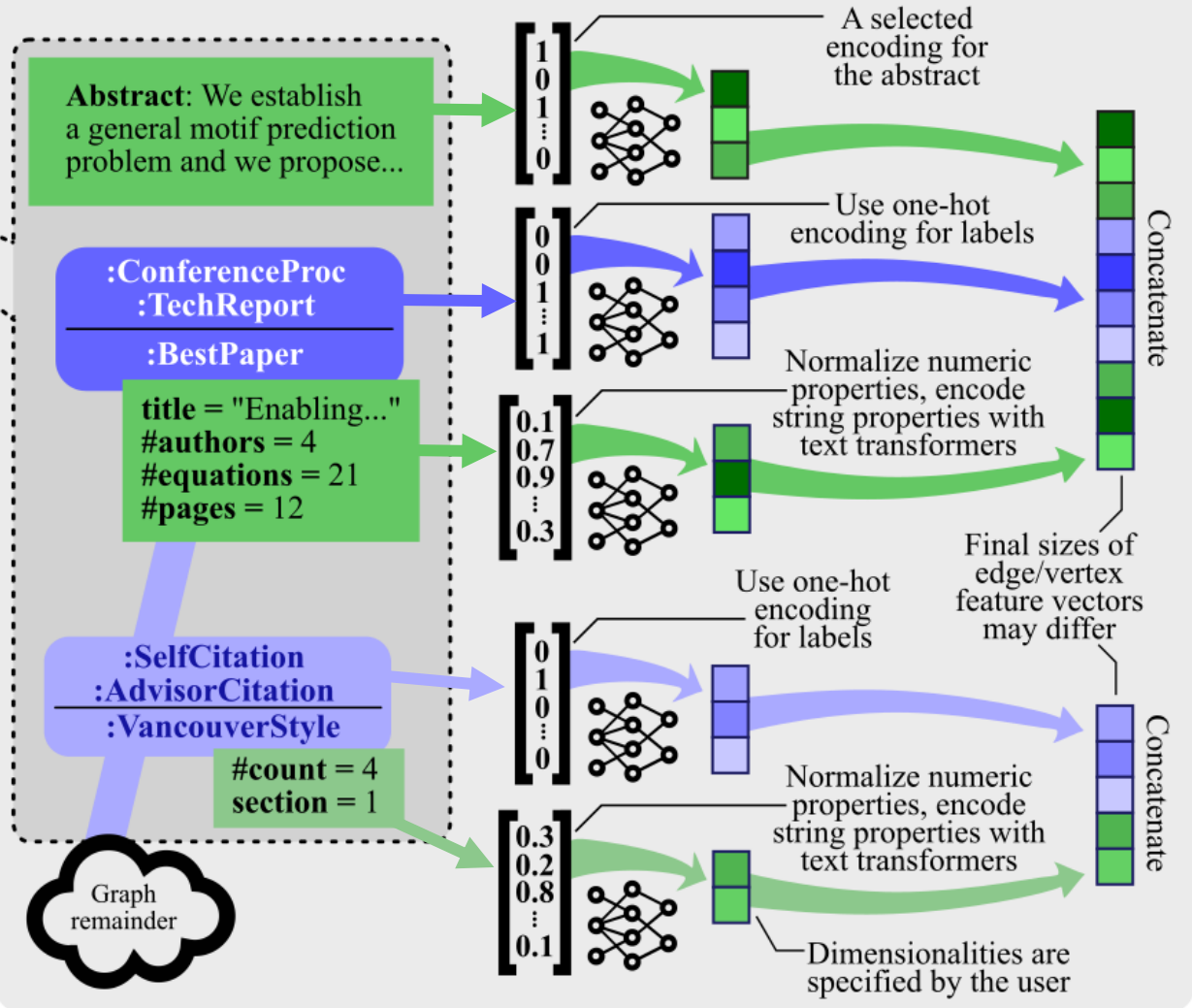
# LPG2vec: Encoding LPG Datasets into a Format Digestible by GNNs Pipelines



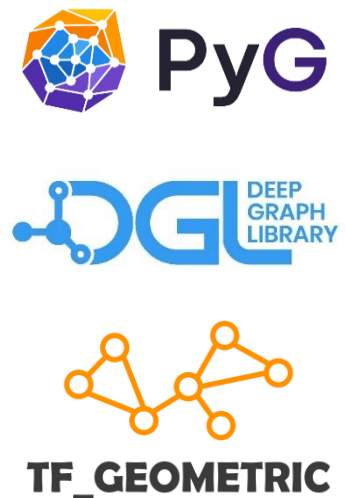
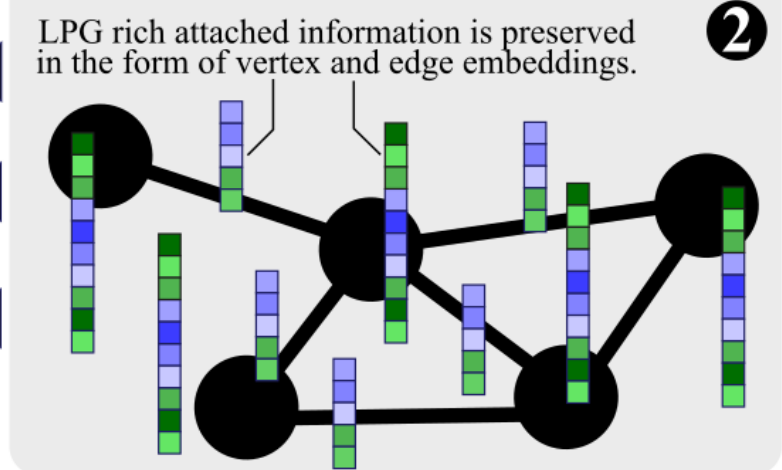
# LPG2vec: Encoding LPG Datasets into a Format Digestible by GNNs Pipelines



## Encoding input LPG graphs (LPG2vec) 1



## Input graph + LPG embeddings 2



# Evaluation: Used Machine & Objectives



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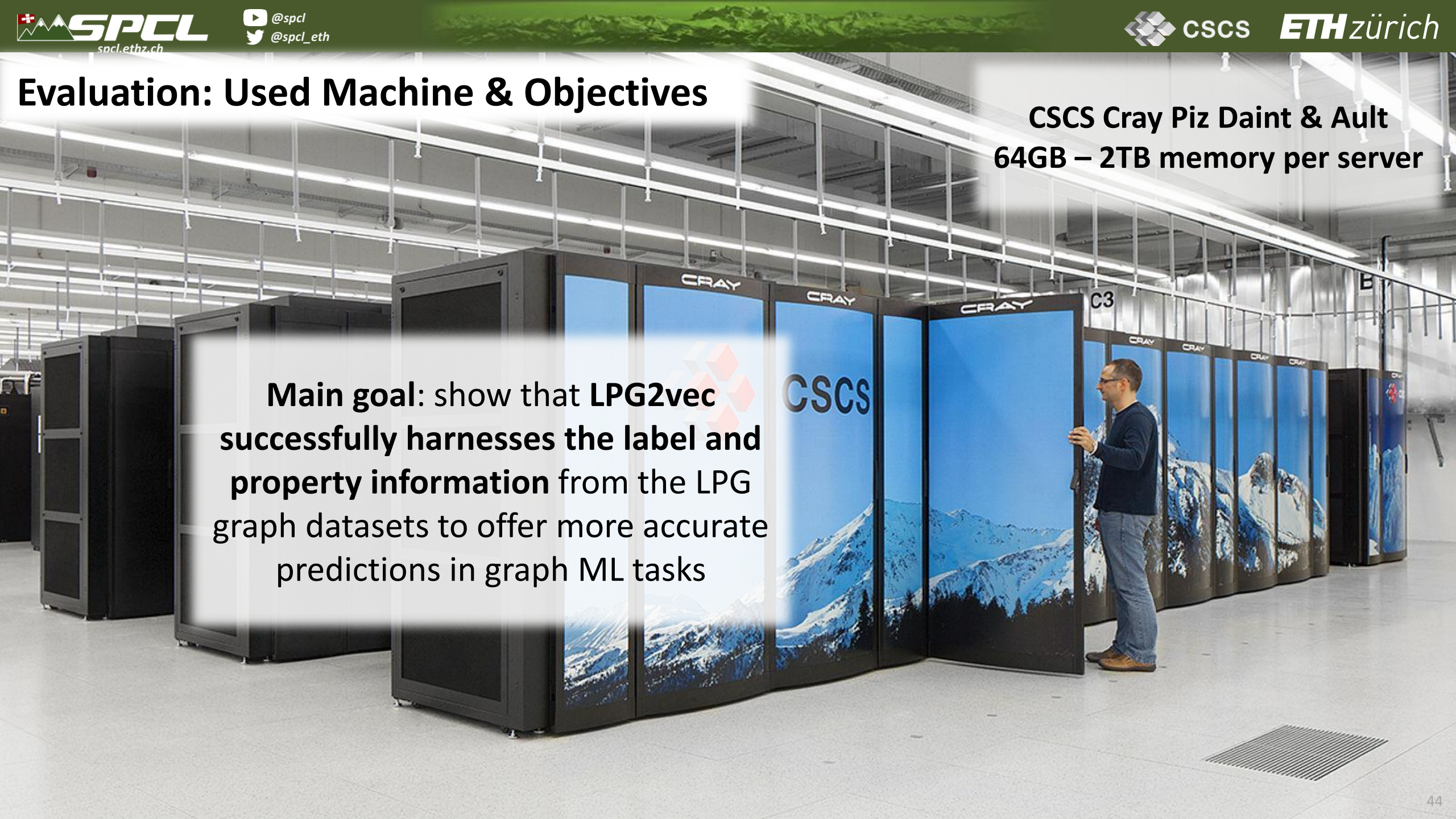
**CSCS Cray Piz Daint & Ault  
64GB – 2TB memory per server**



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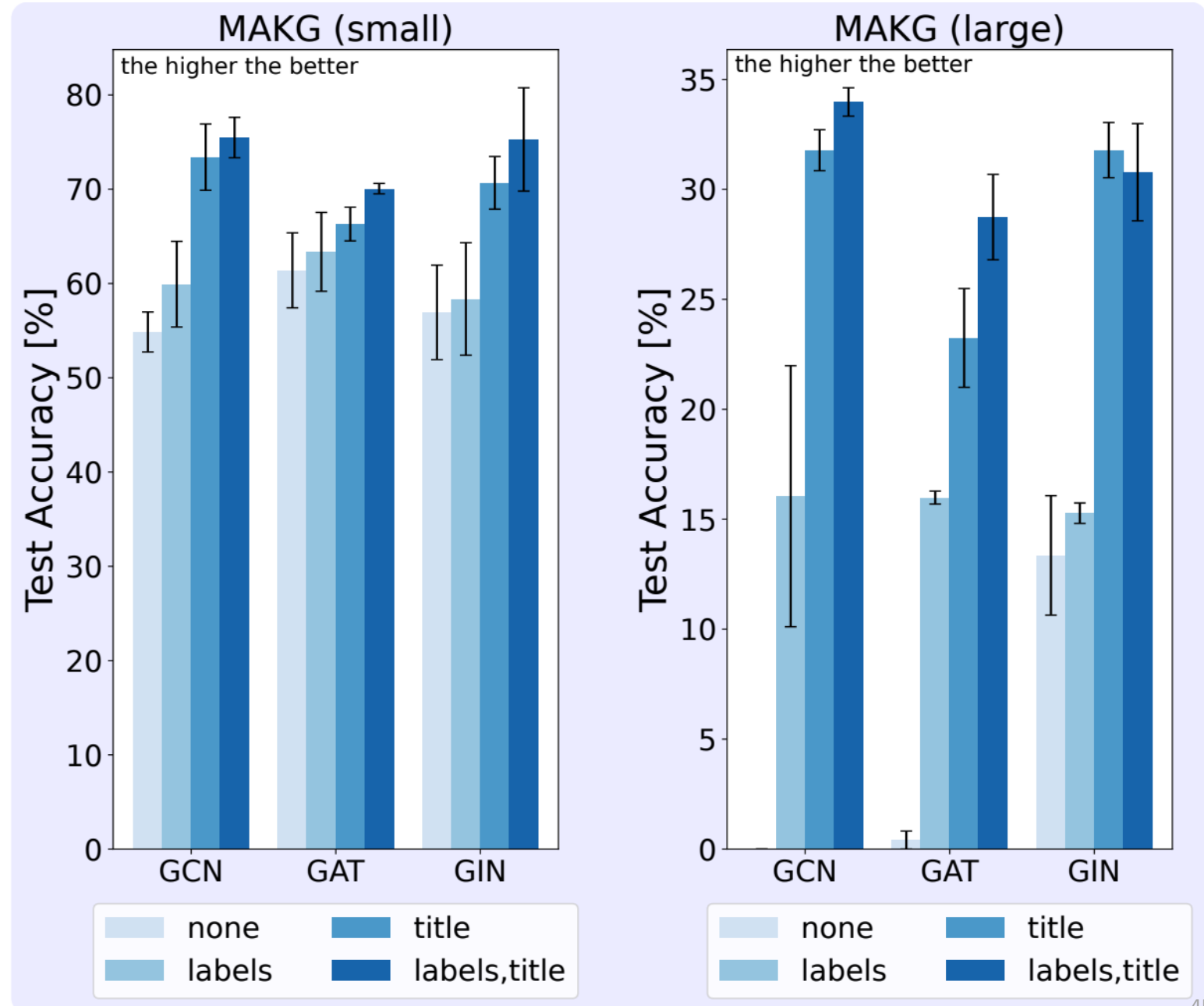
**CSCS Cray Piz Daint & Ault  
64GB – 2TB memory per server**

**Main goal: show that **LPG2vec** successfully harnesses the label and property information from the LPG graph datasets to offer more accurate predictions in graph ML tasks**



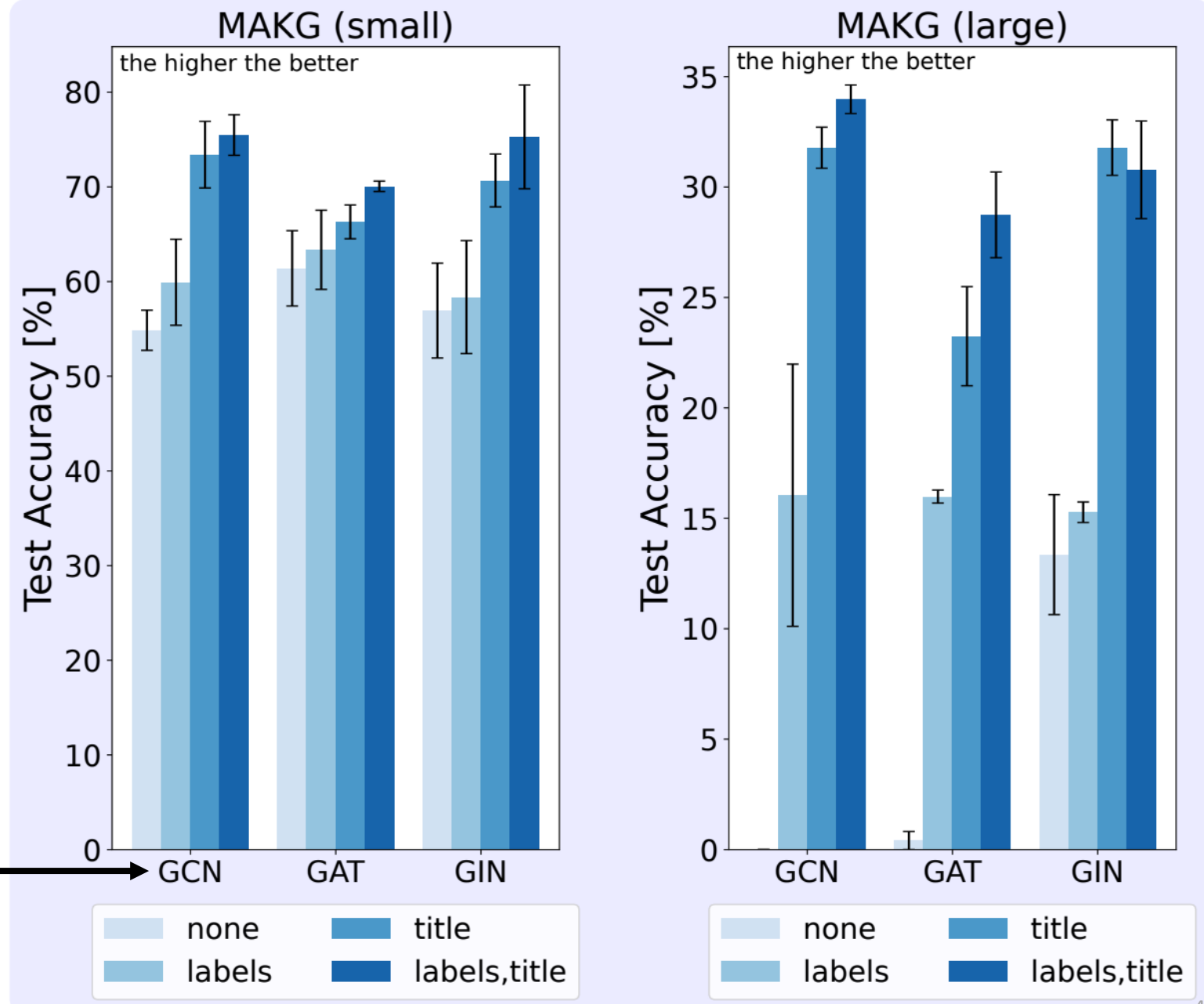
# Node Classification, aka Label Prediction

Task: predict the research area of the publication



# Node Classification, aka Label Prediction

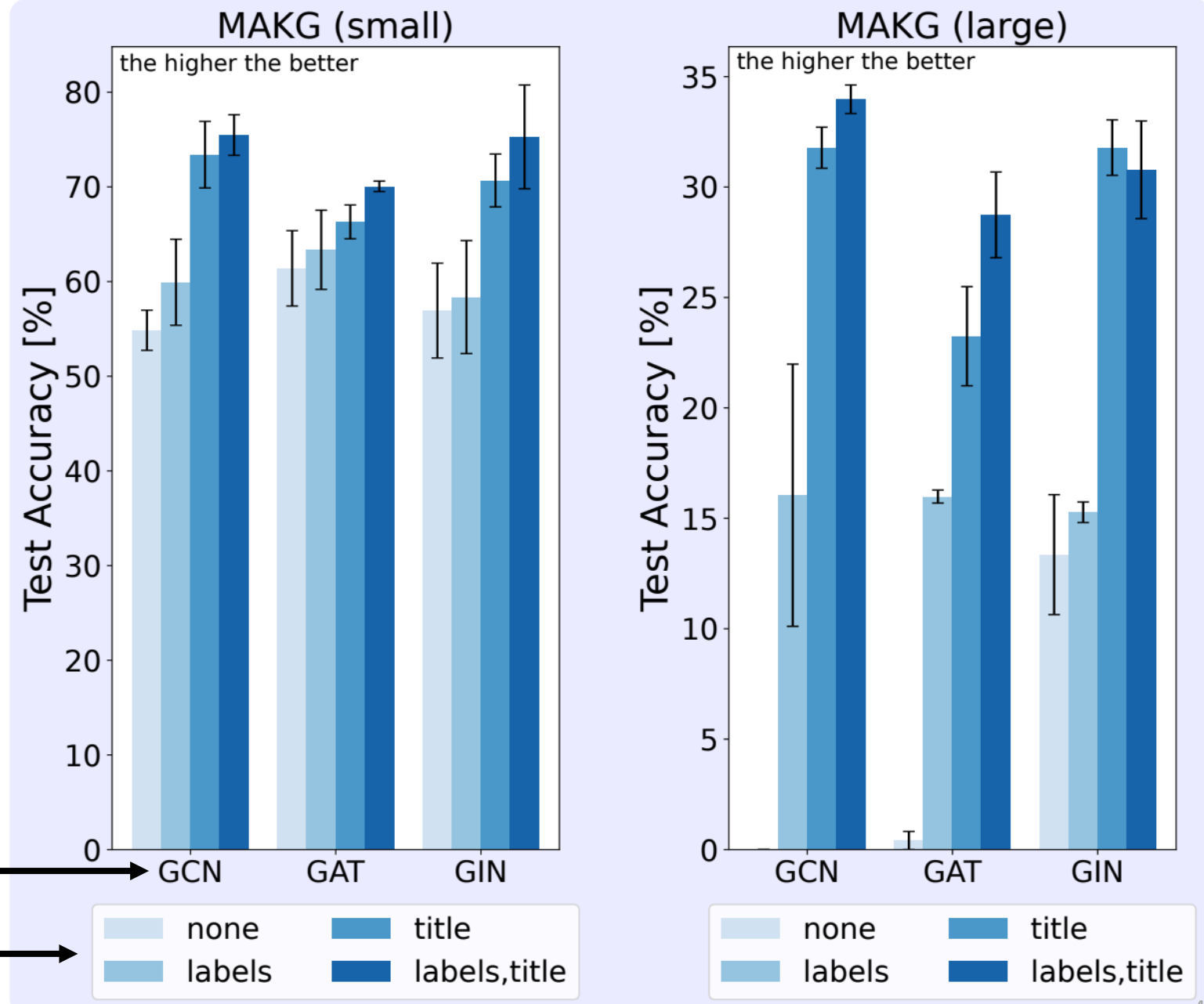
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What GNN model is considered? →

# Node Classification, aka Label Prediction

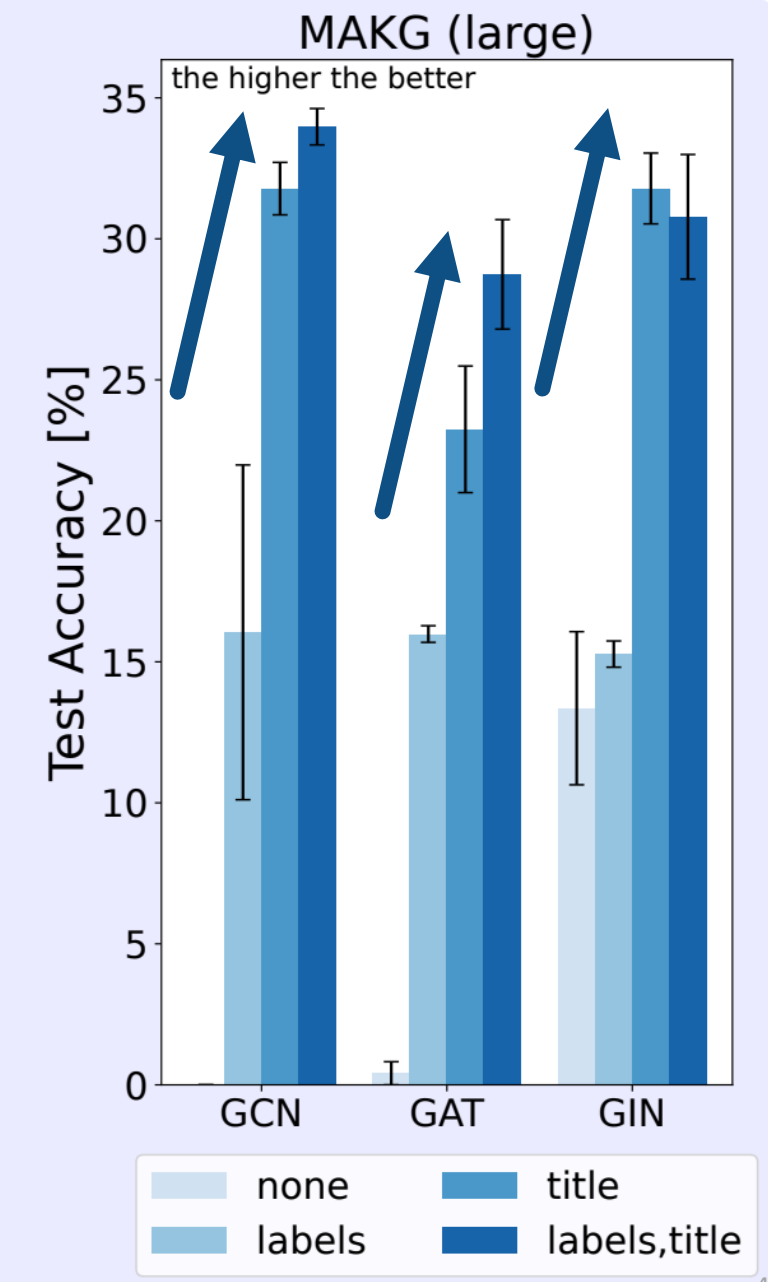
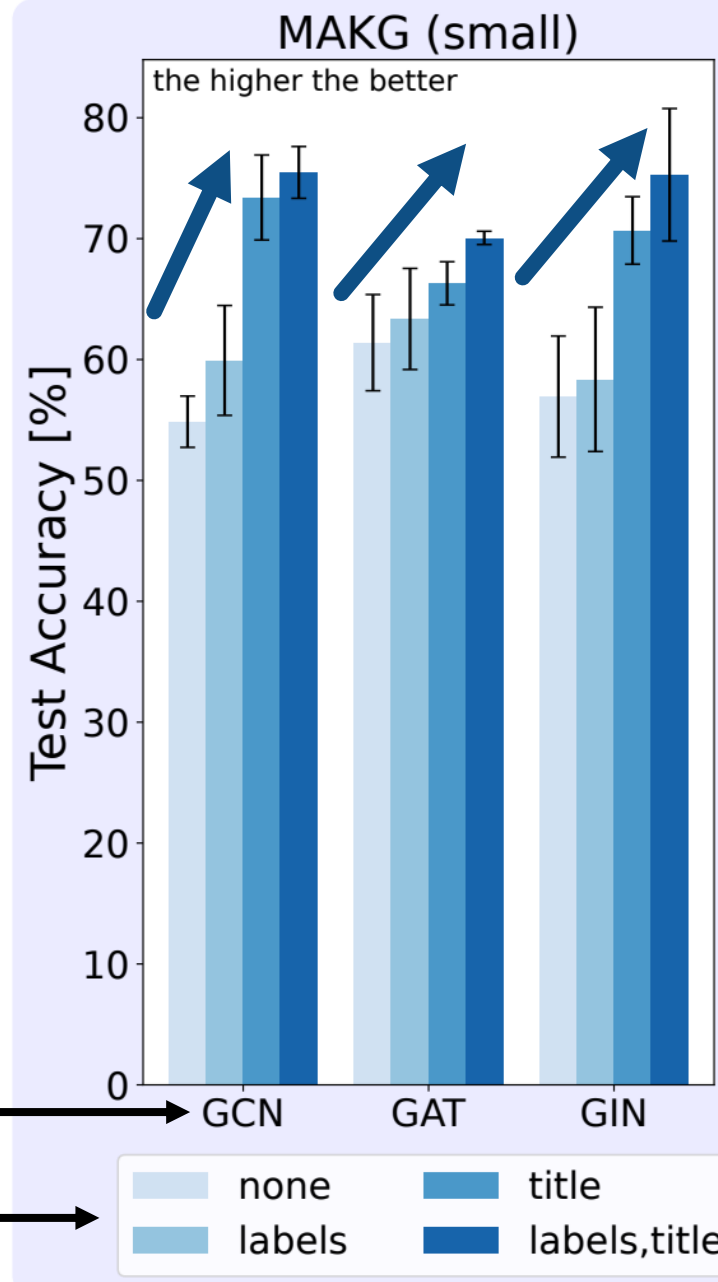
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Better accuracy with labels/properties, it is important to use them both



# Node Classification, aka Label Prediction

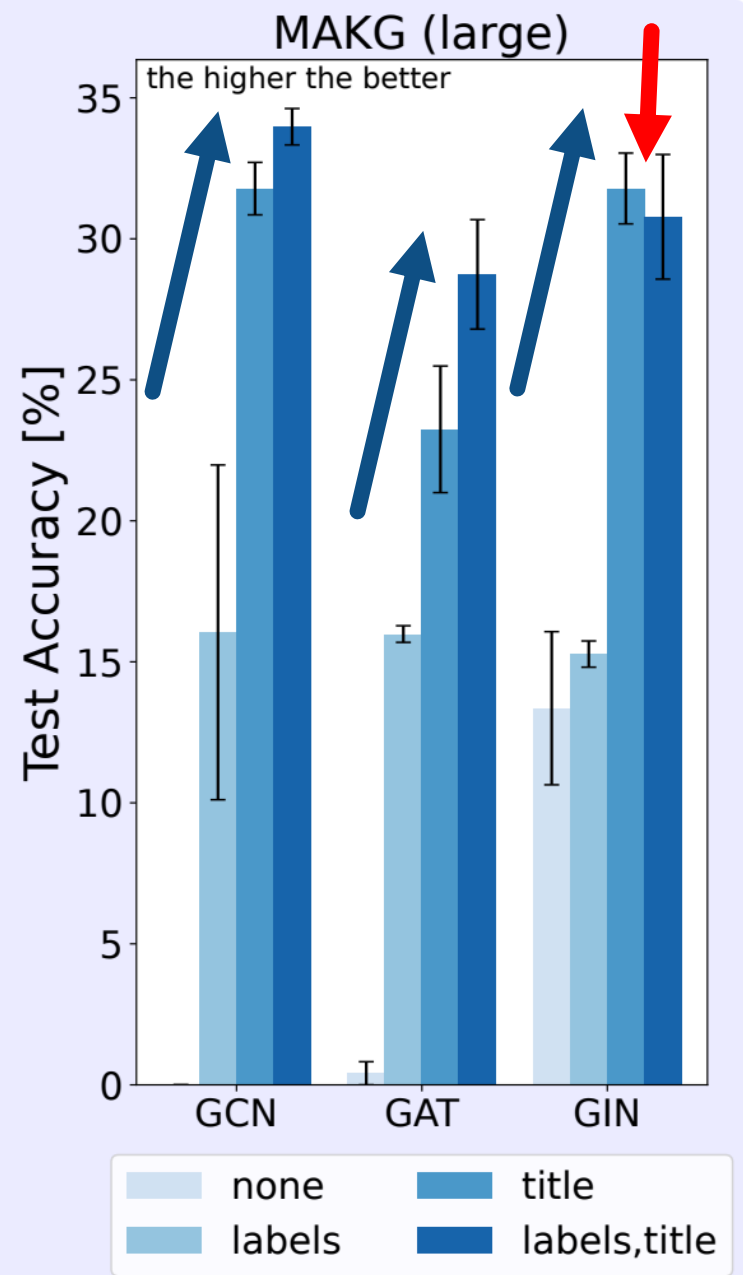
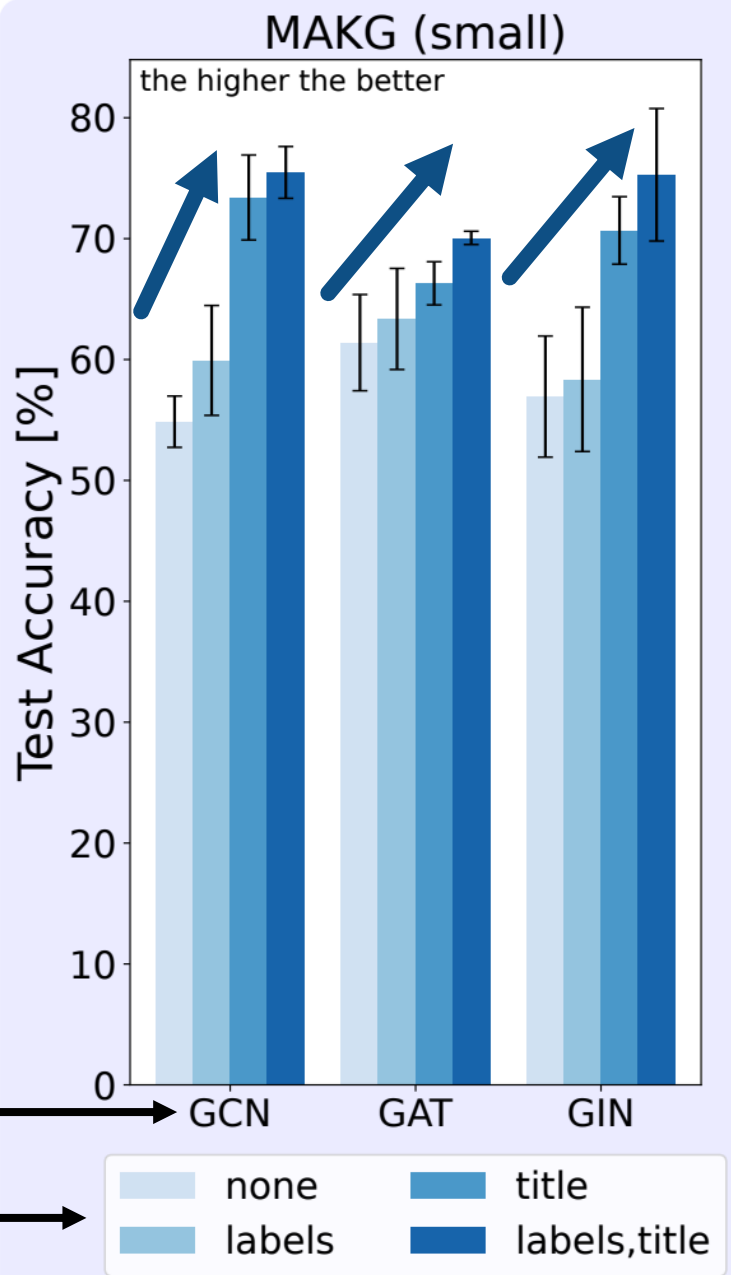
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Better accuracy with labels/properties, it is important to use them both

...not always?

What GNN model is considered? →

What label/property data is considered? →

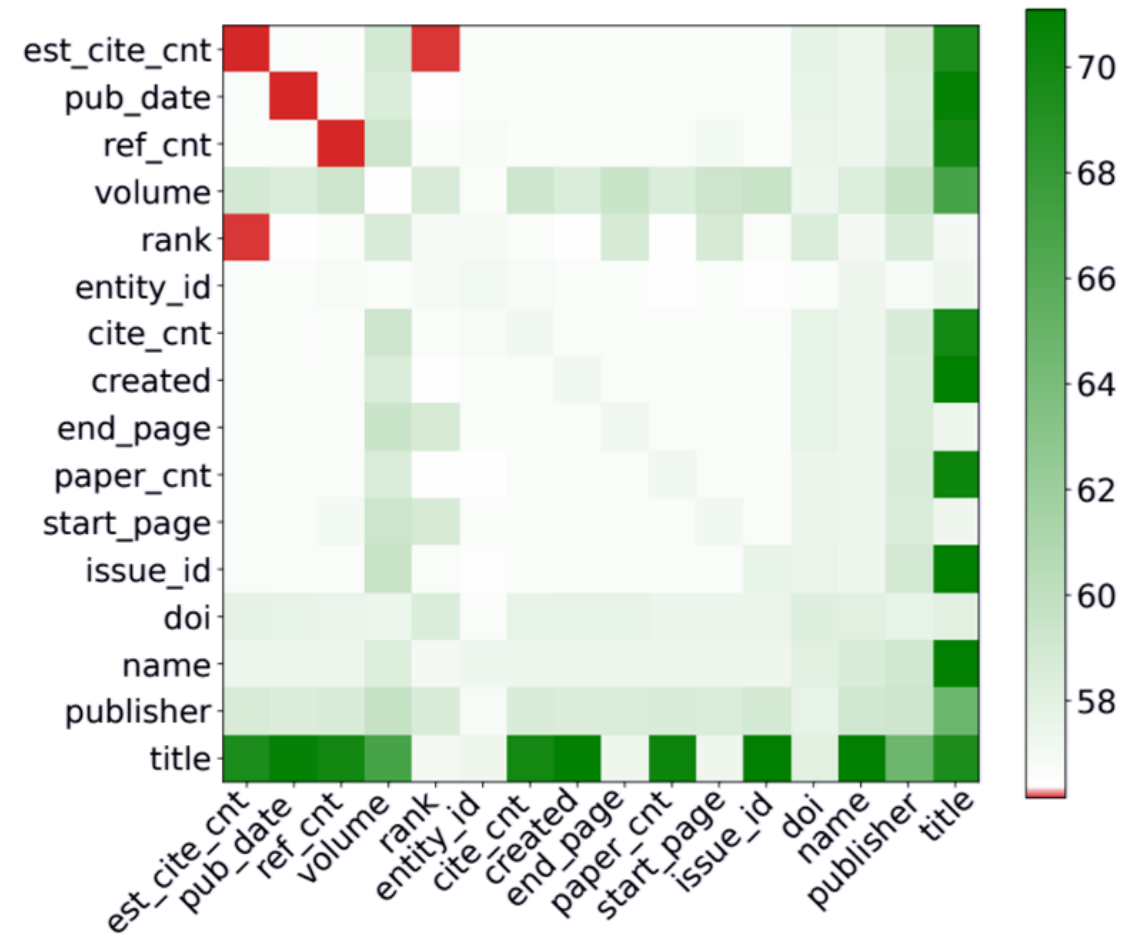
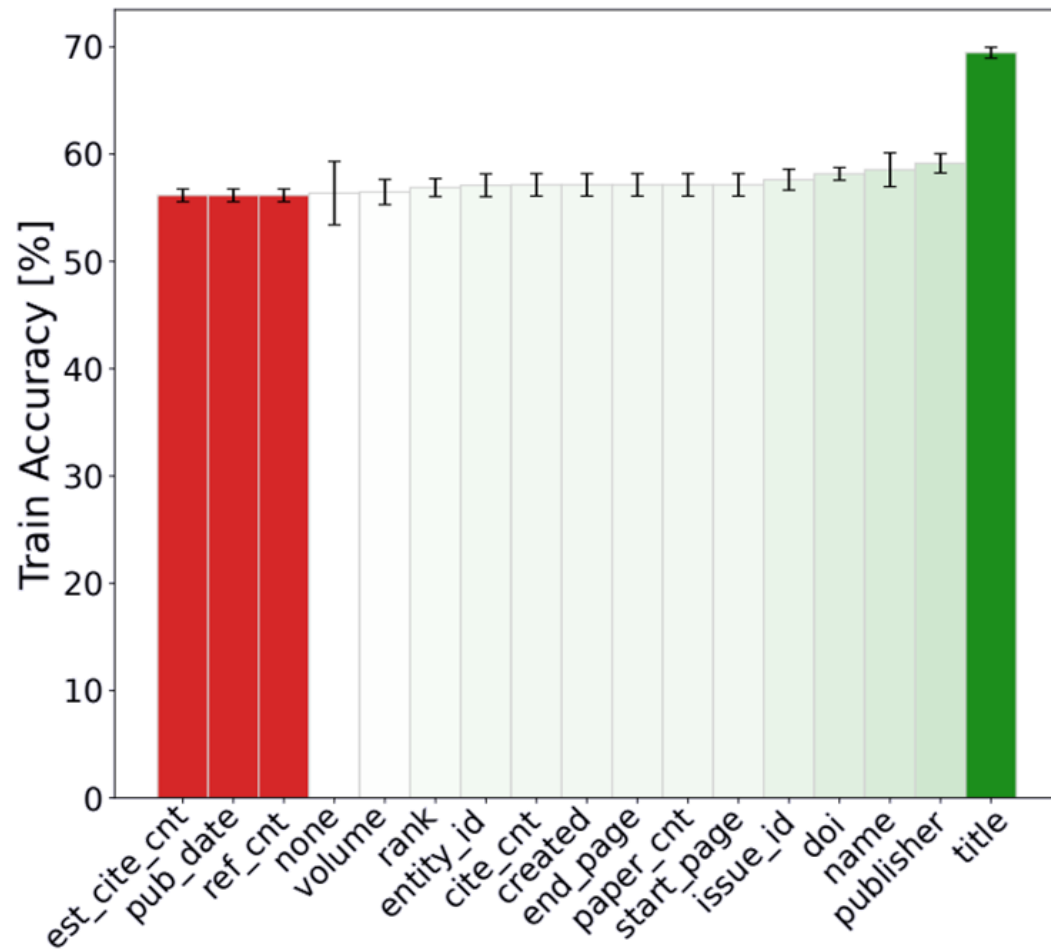


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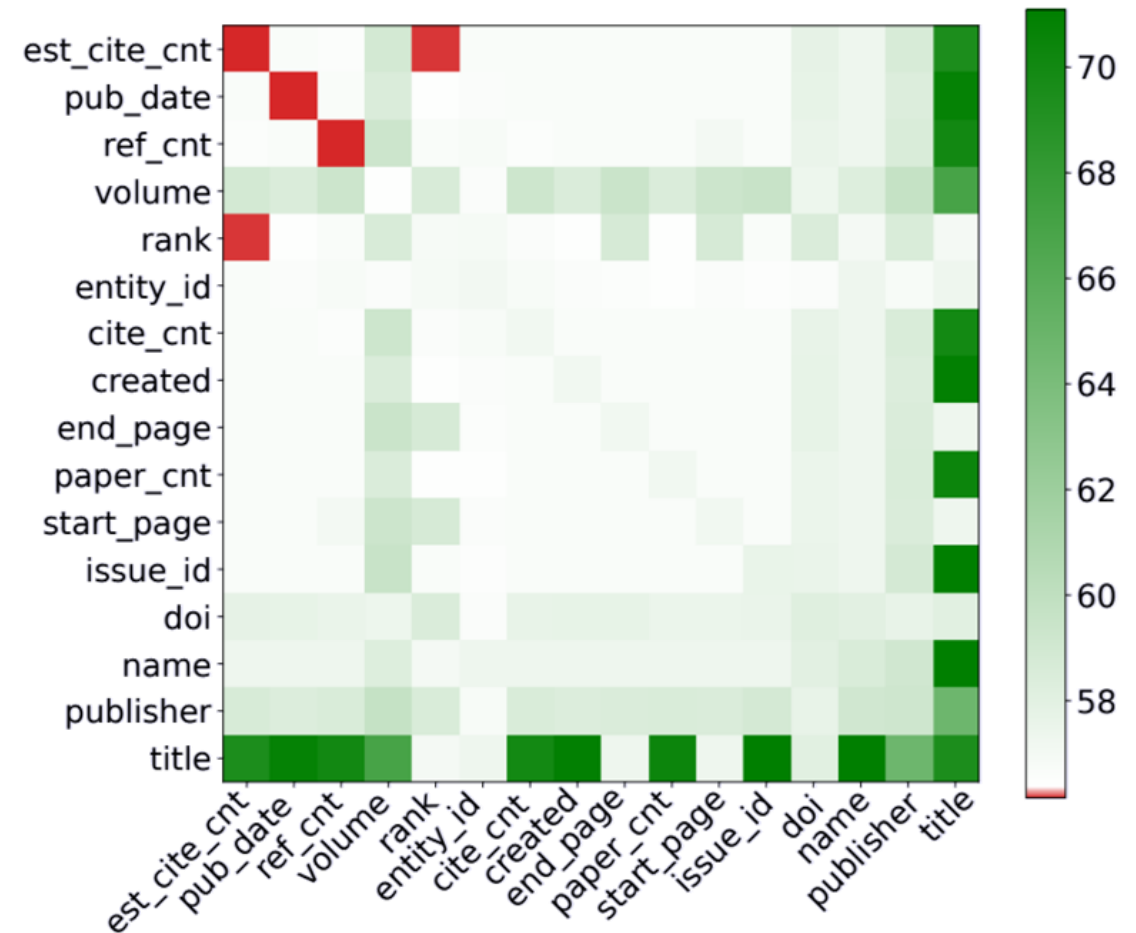
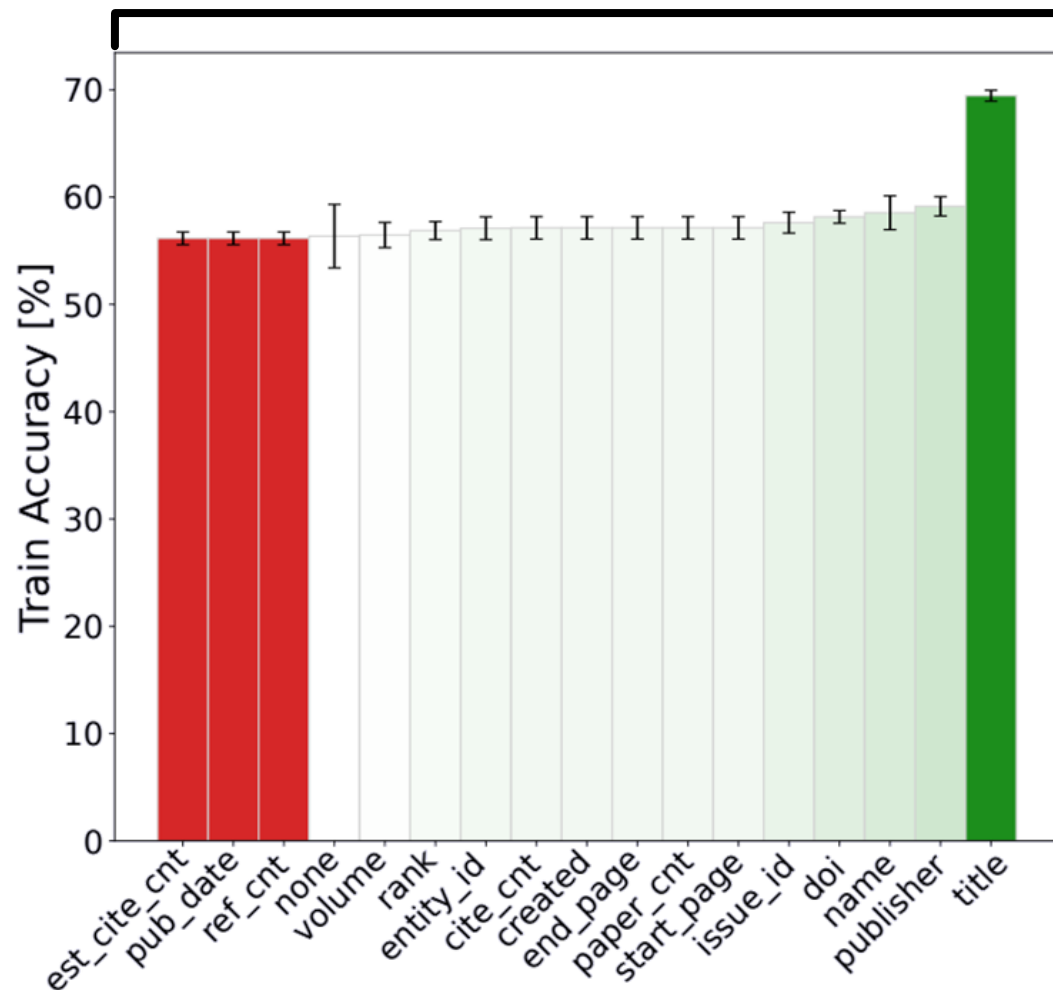
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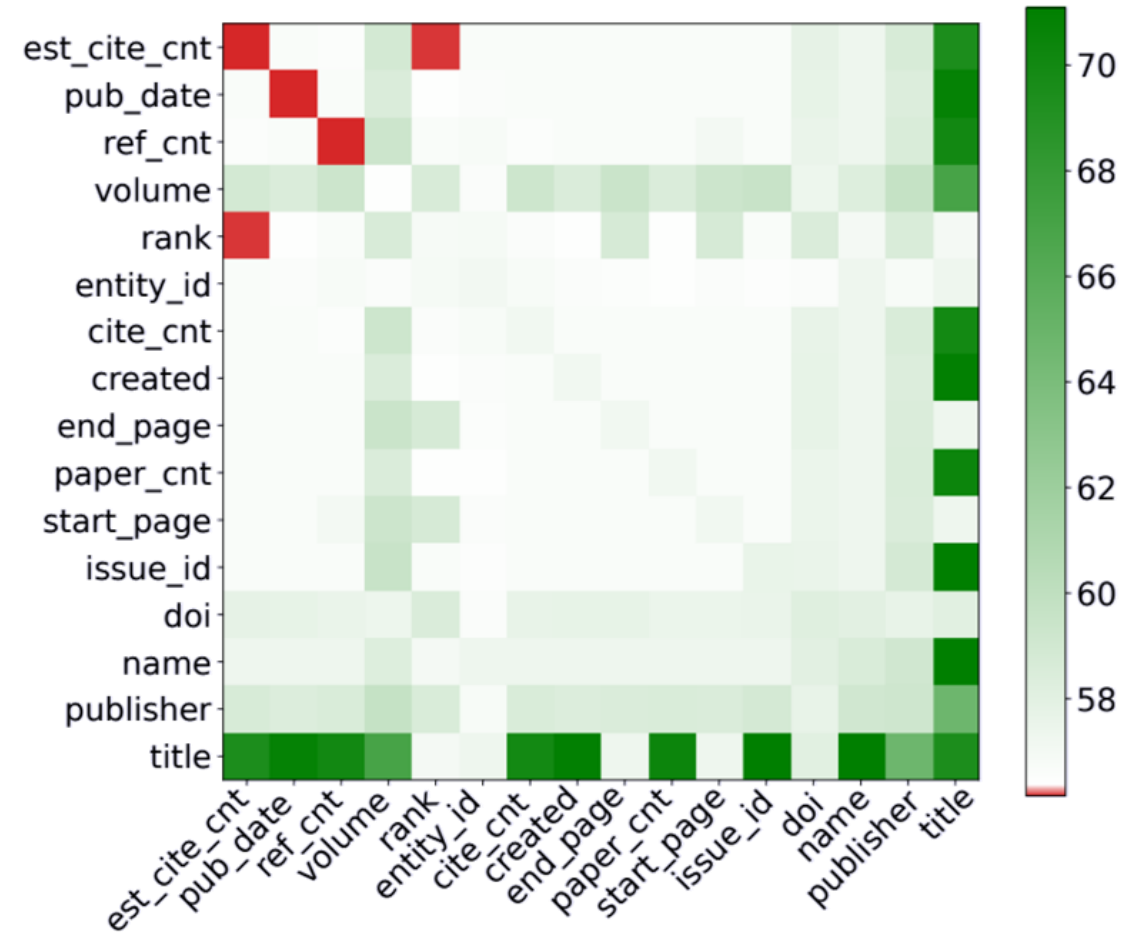
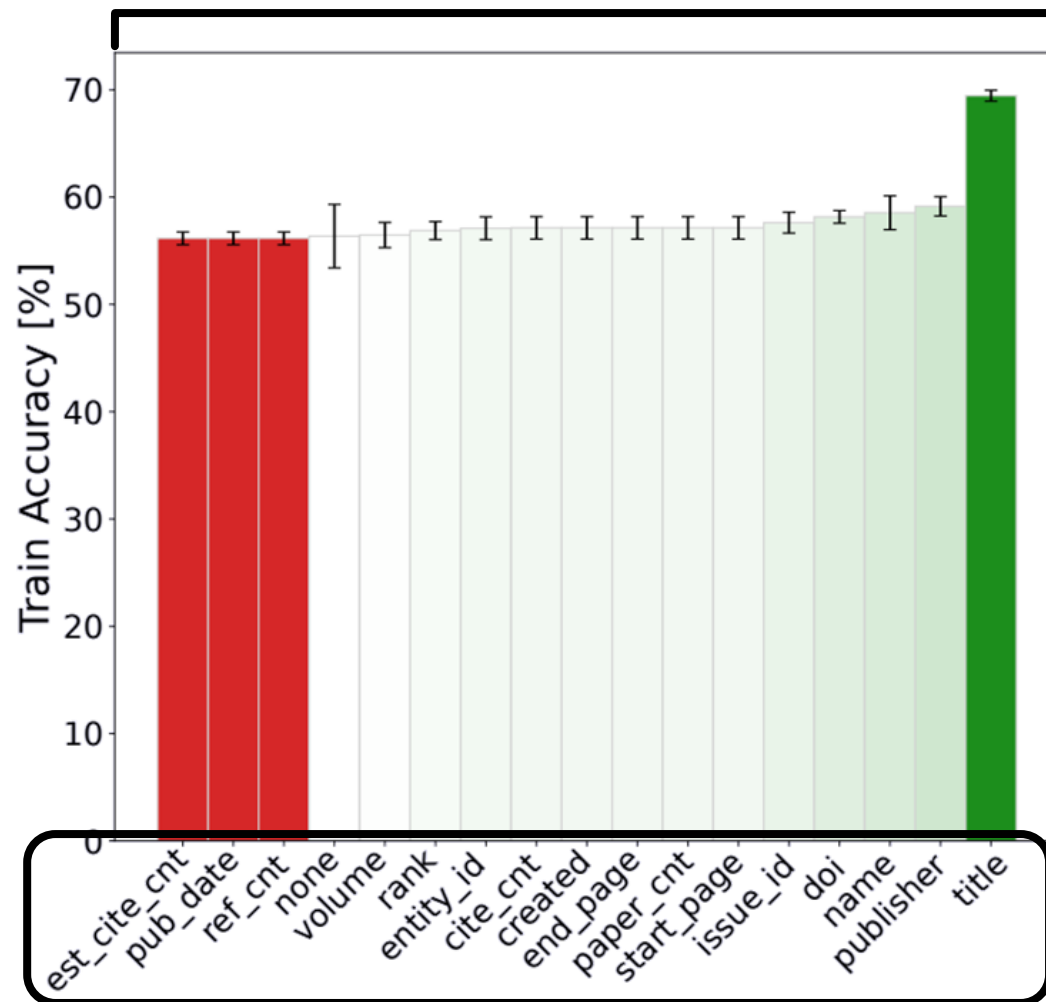
Impact from each label/property



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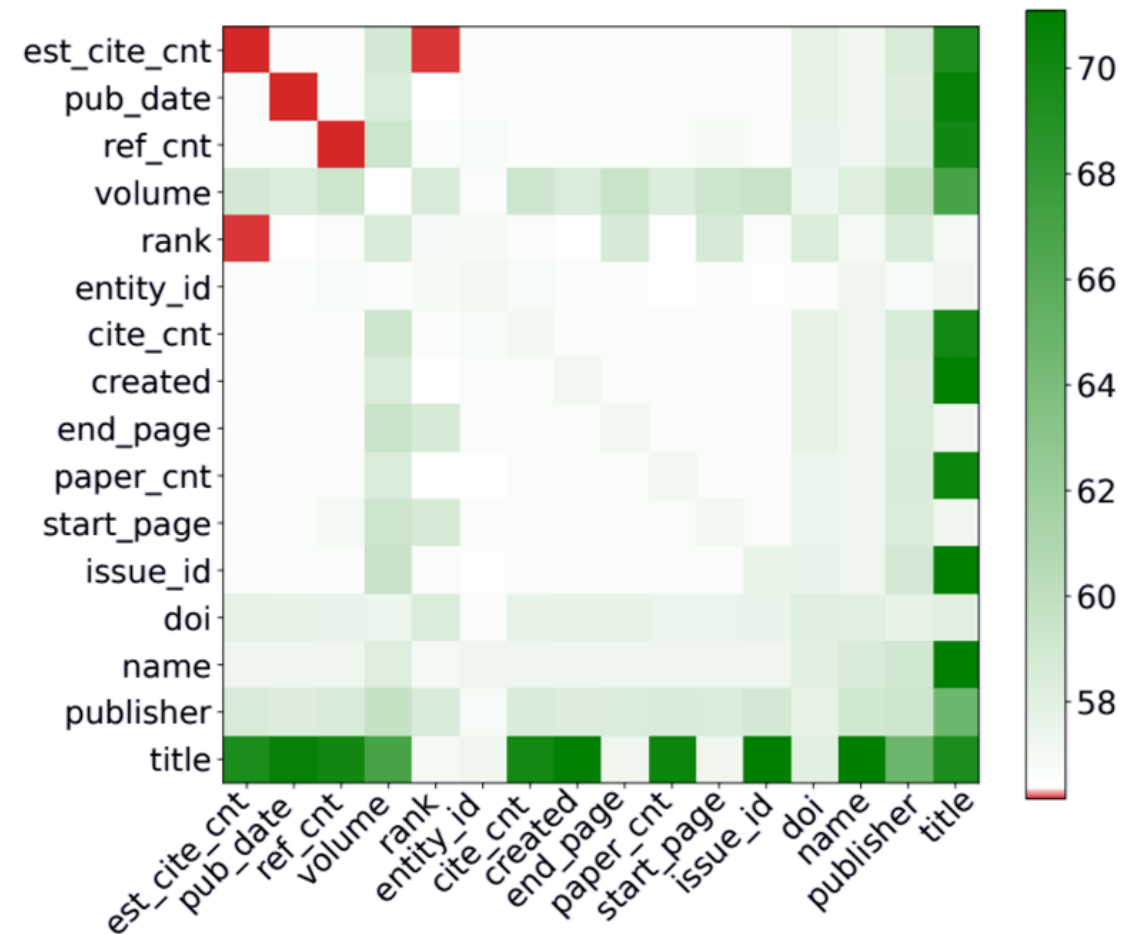
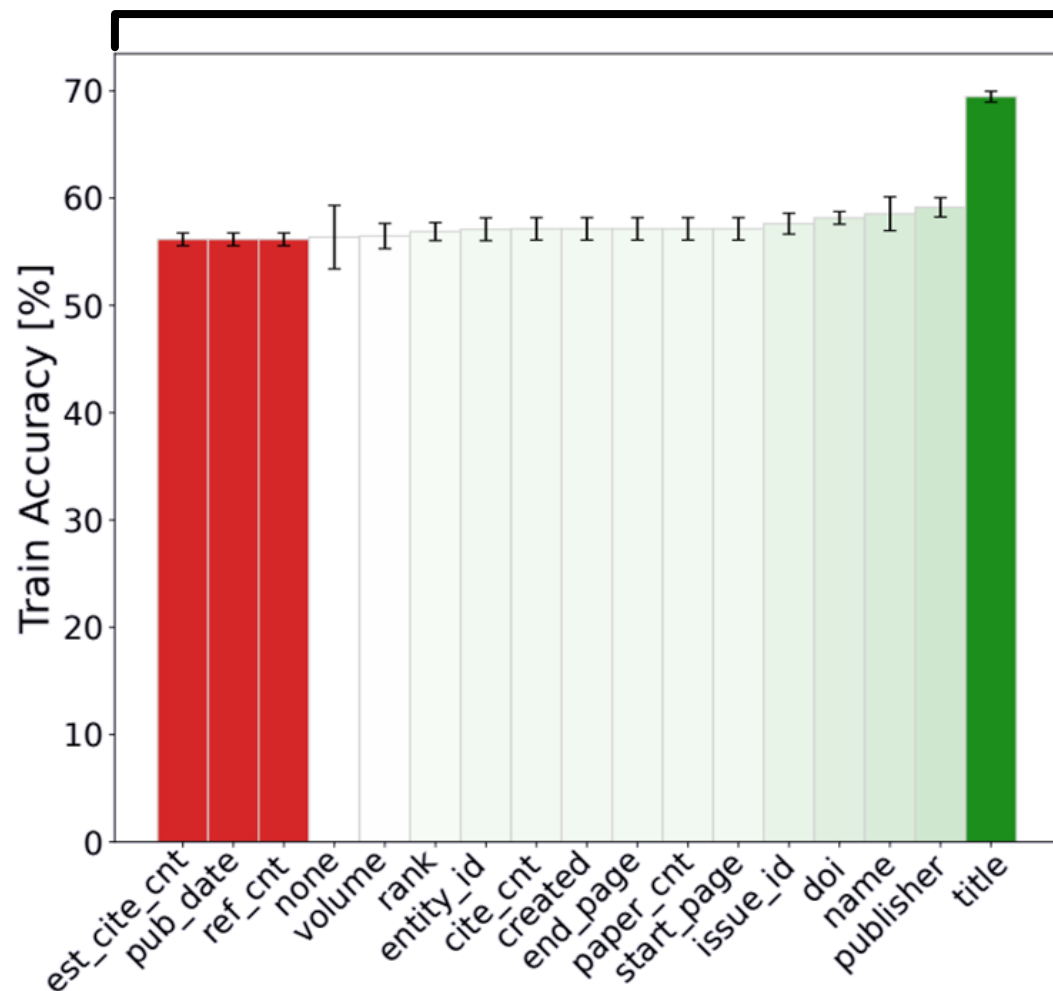
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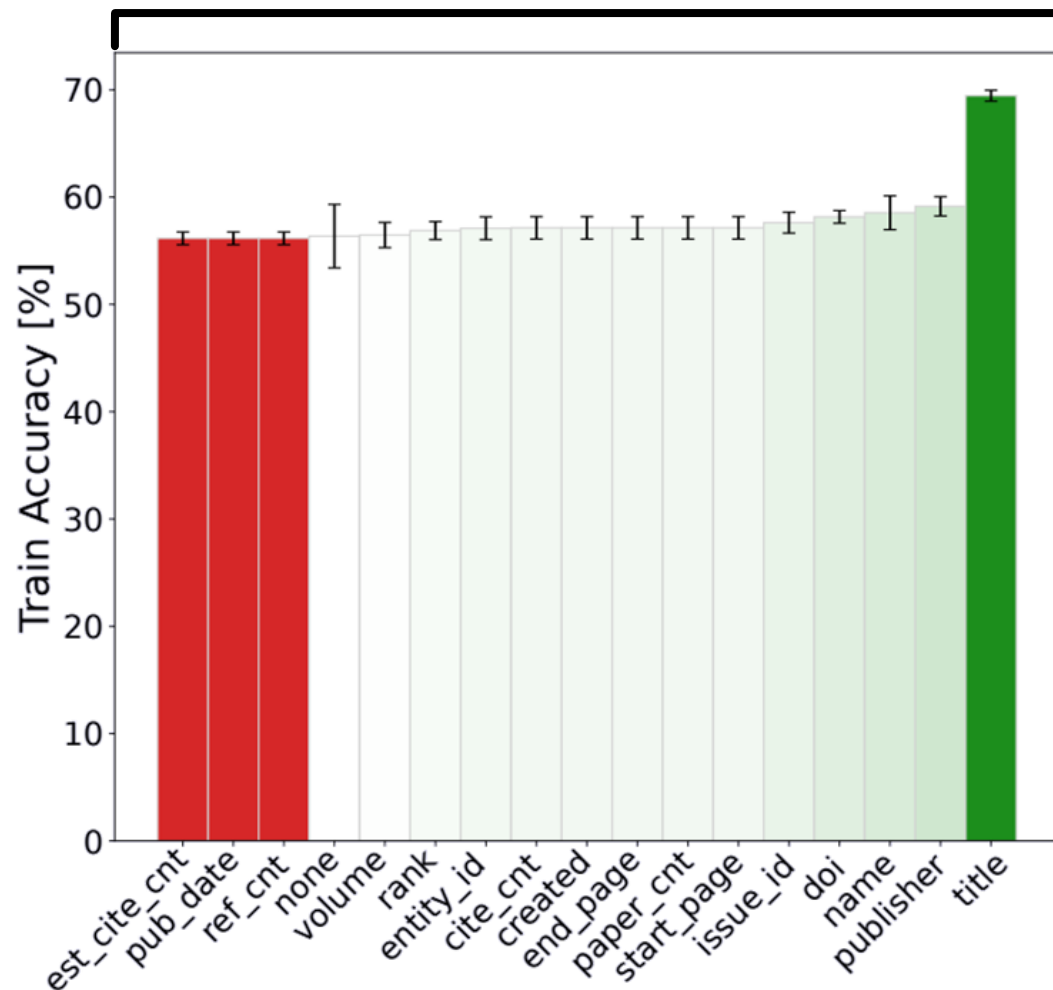
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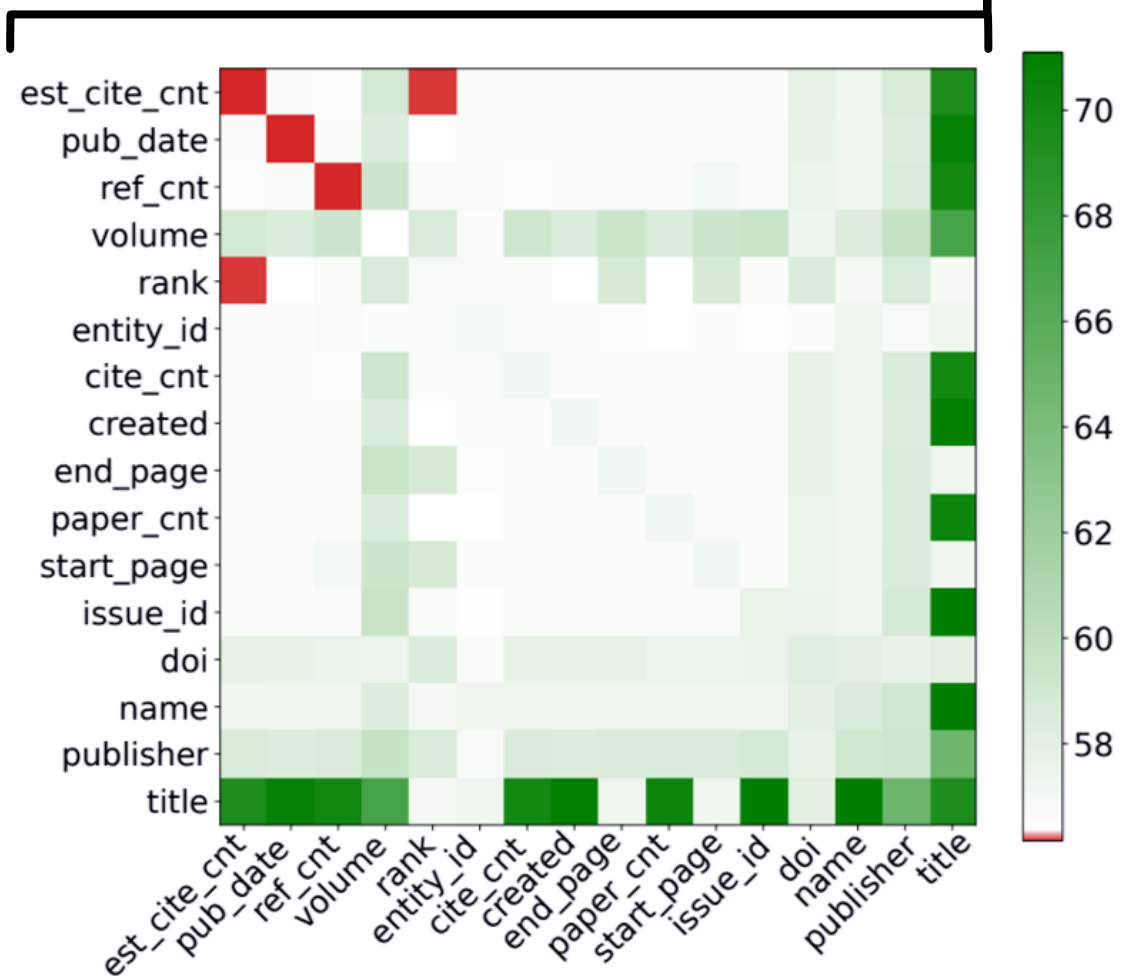
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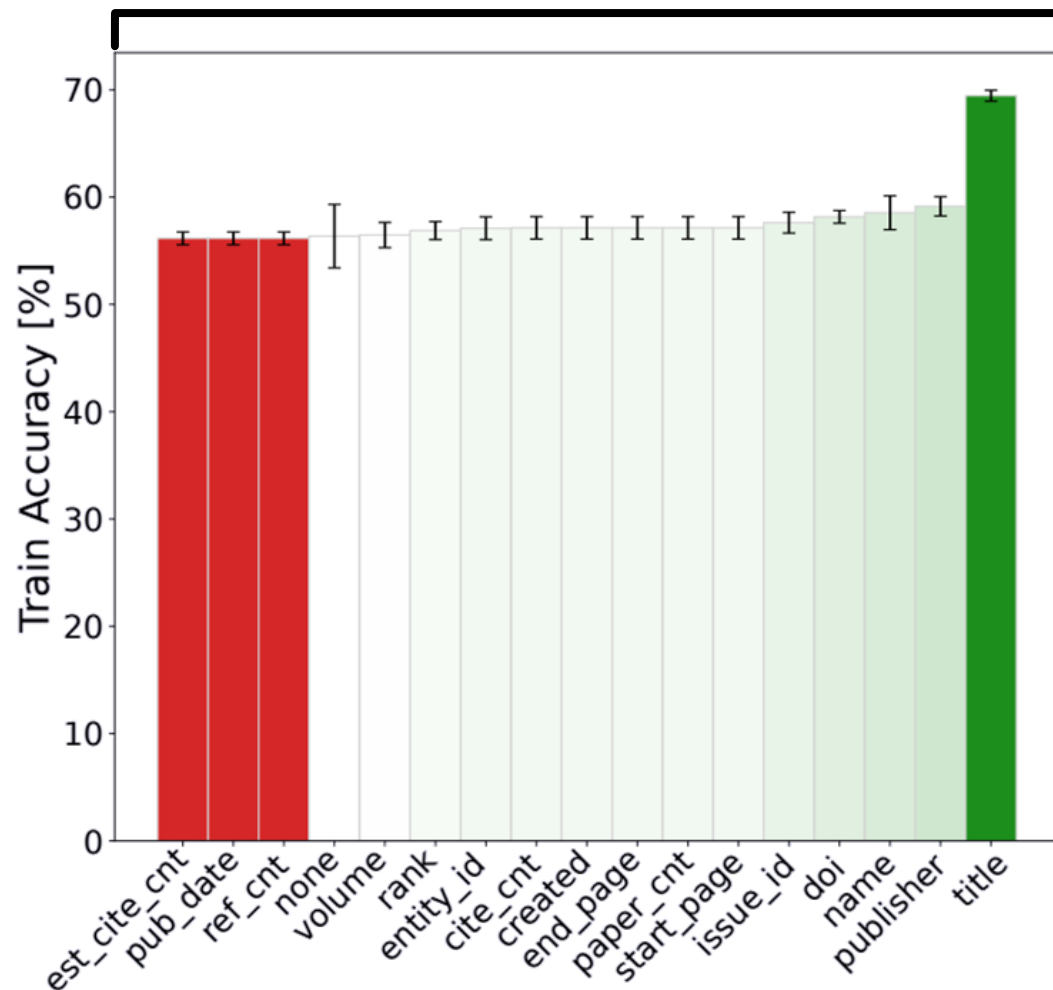
Impact from each label/property pair



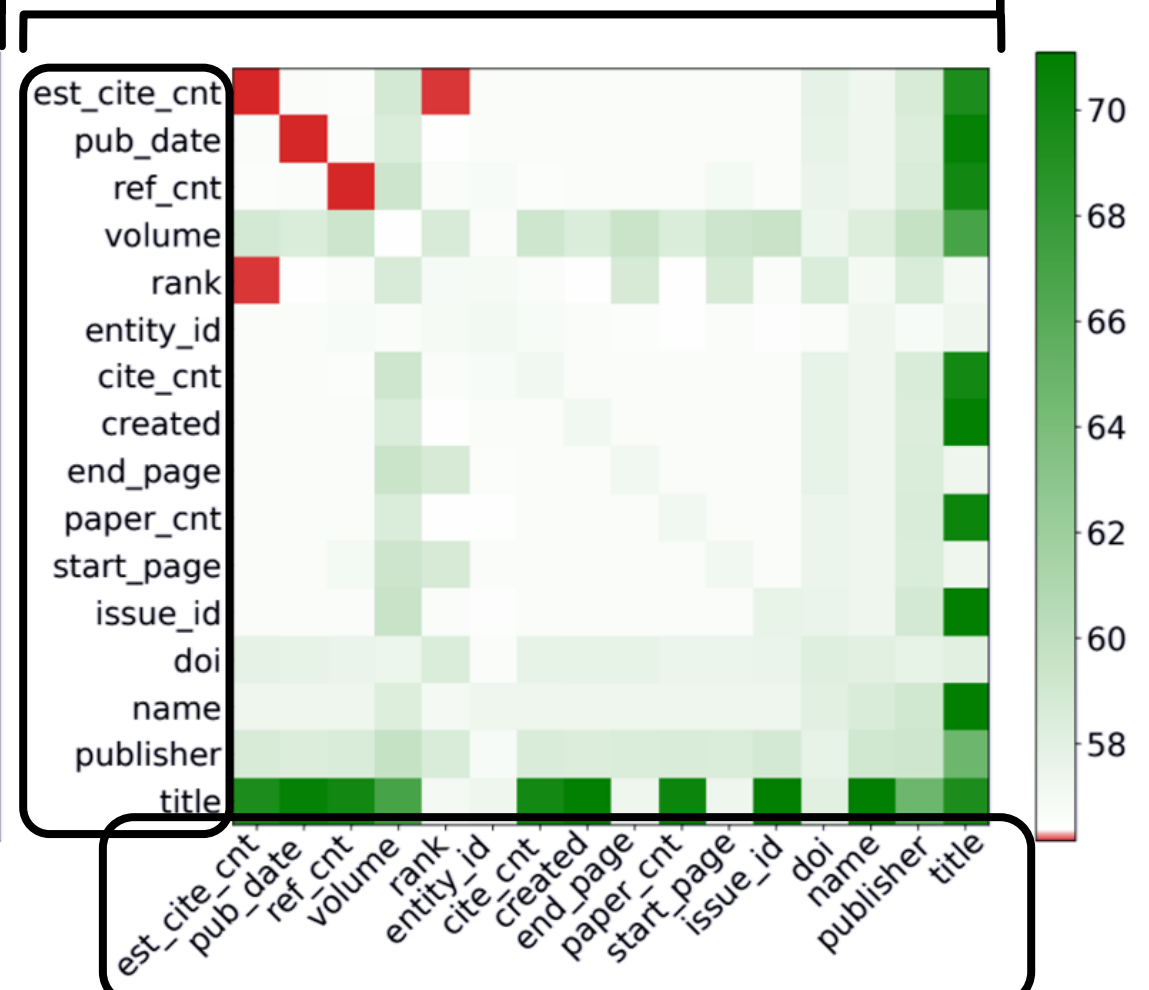
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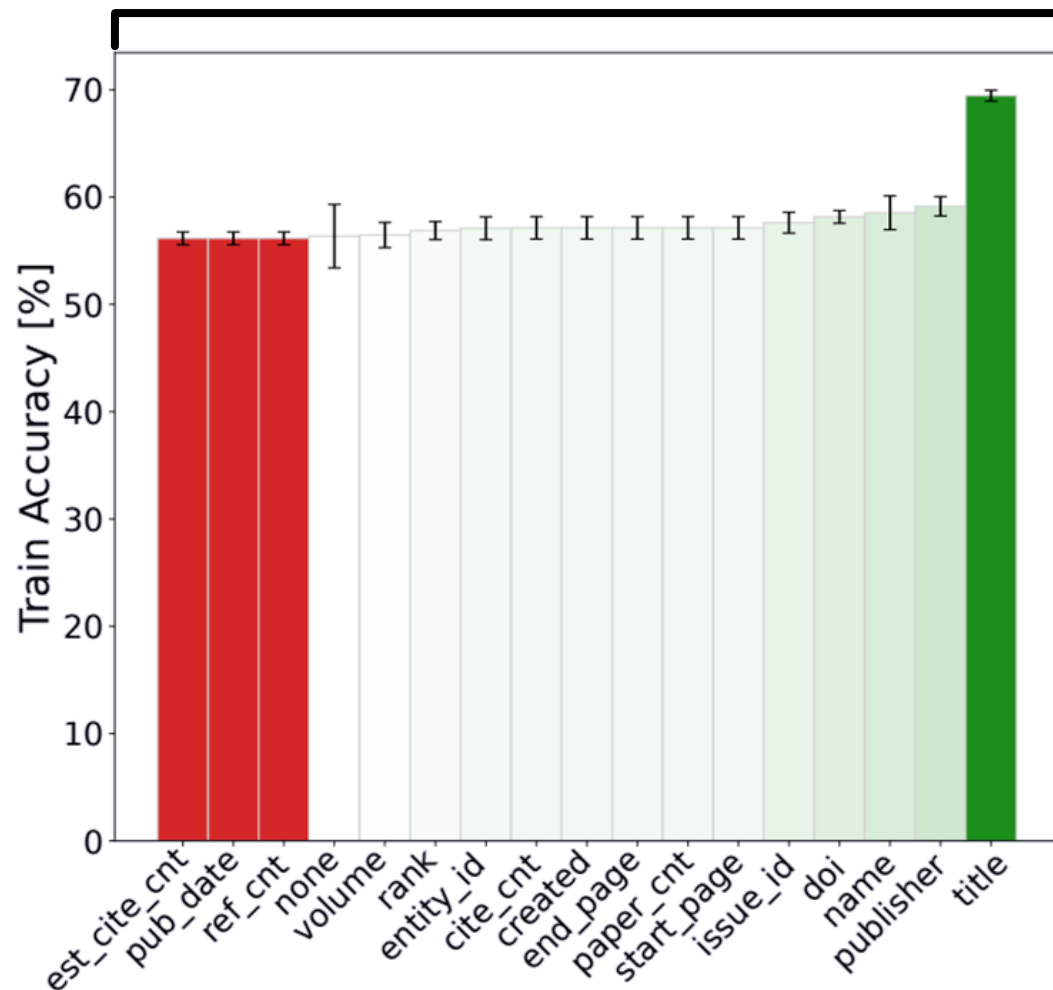
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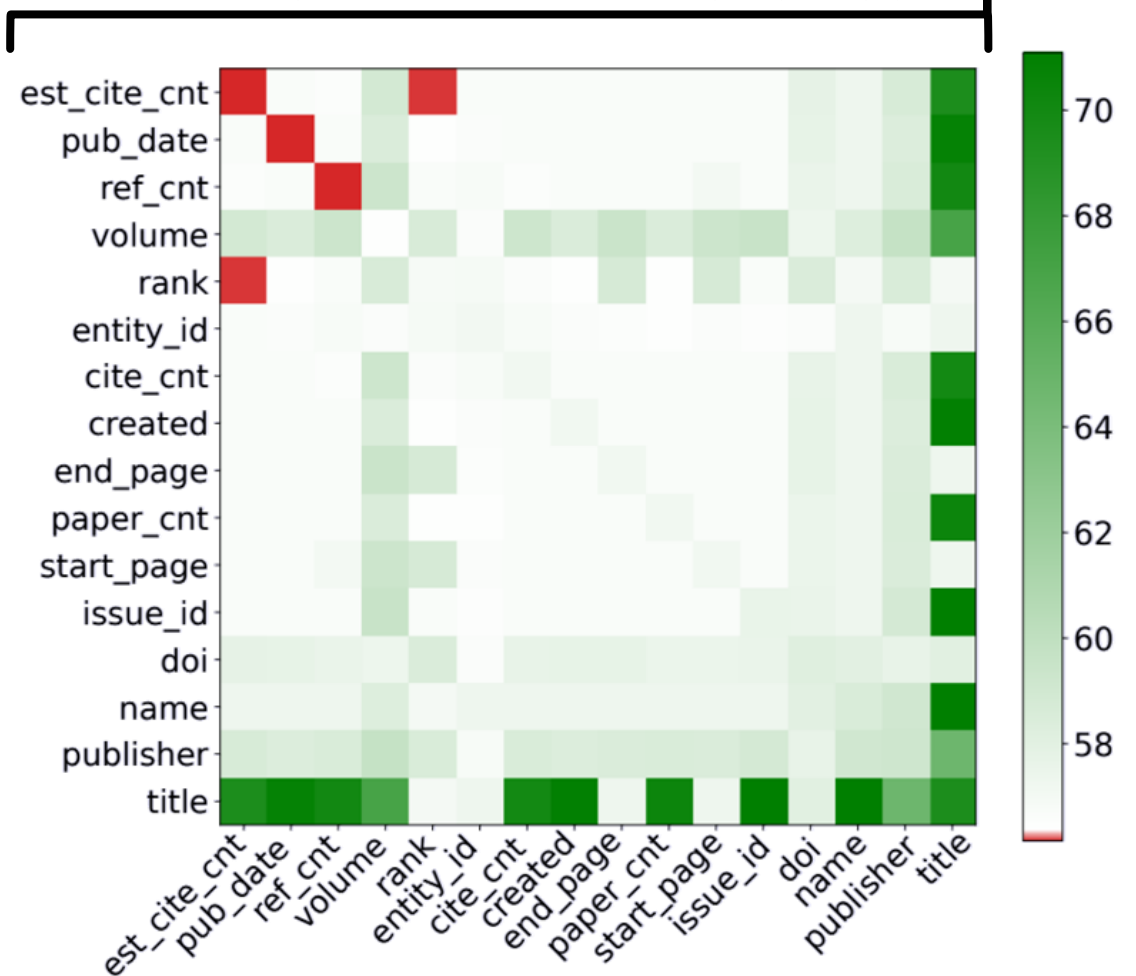
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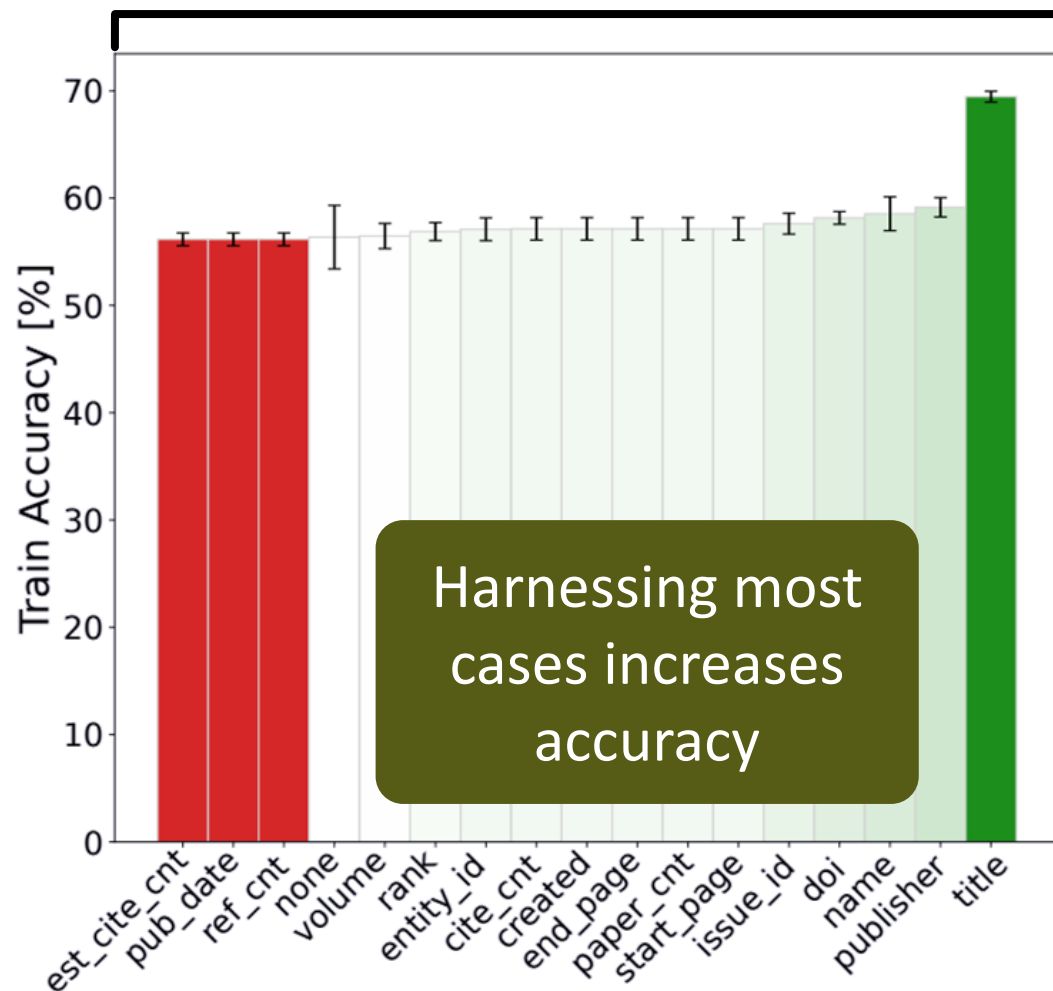
Impact from each label/property pair



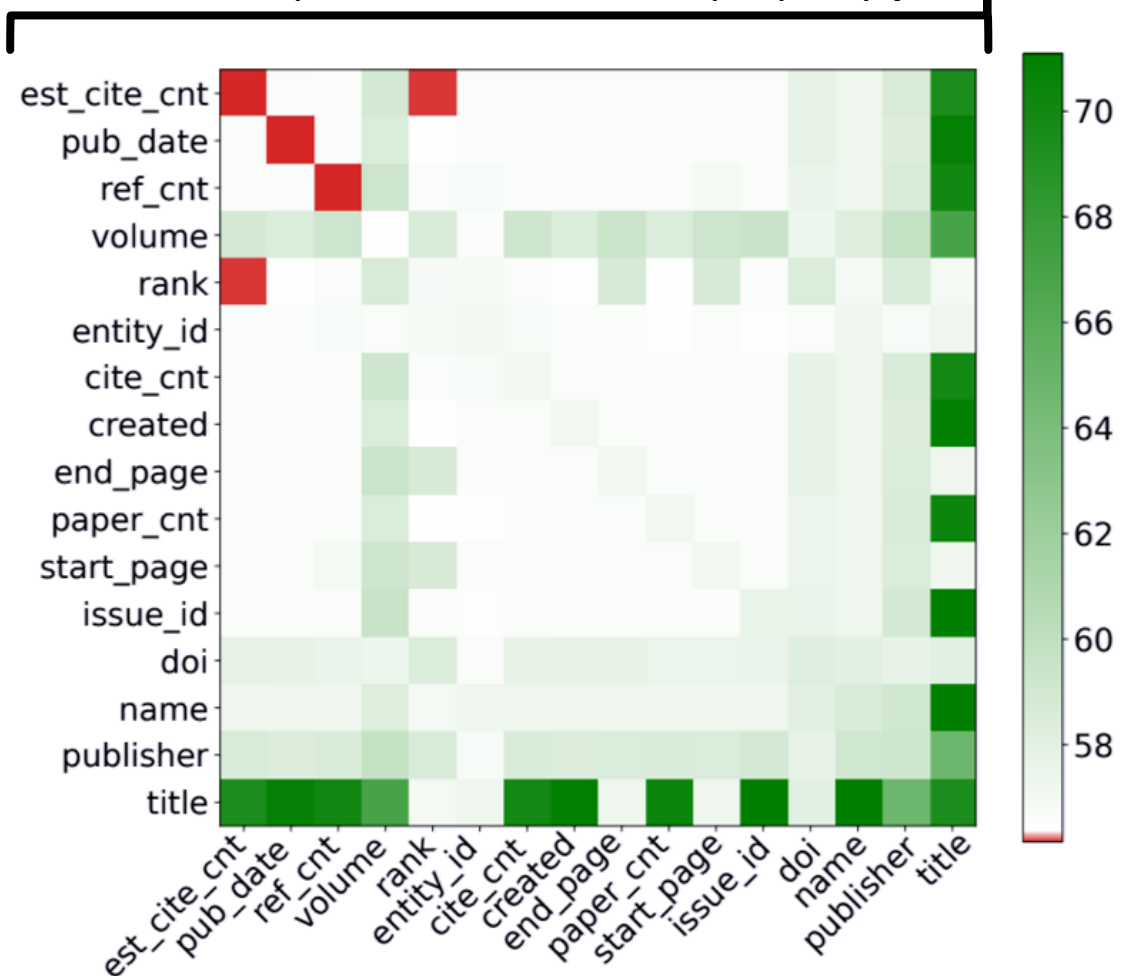
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Impact from each label/property pair

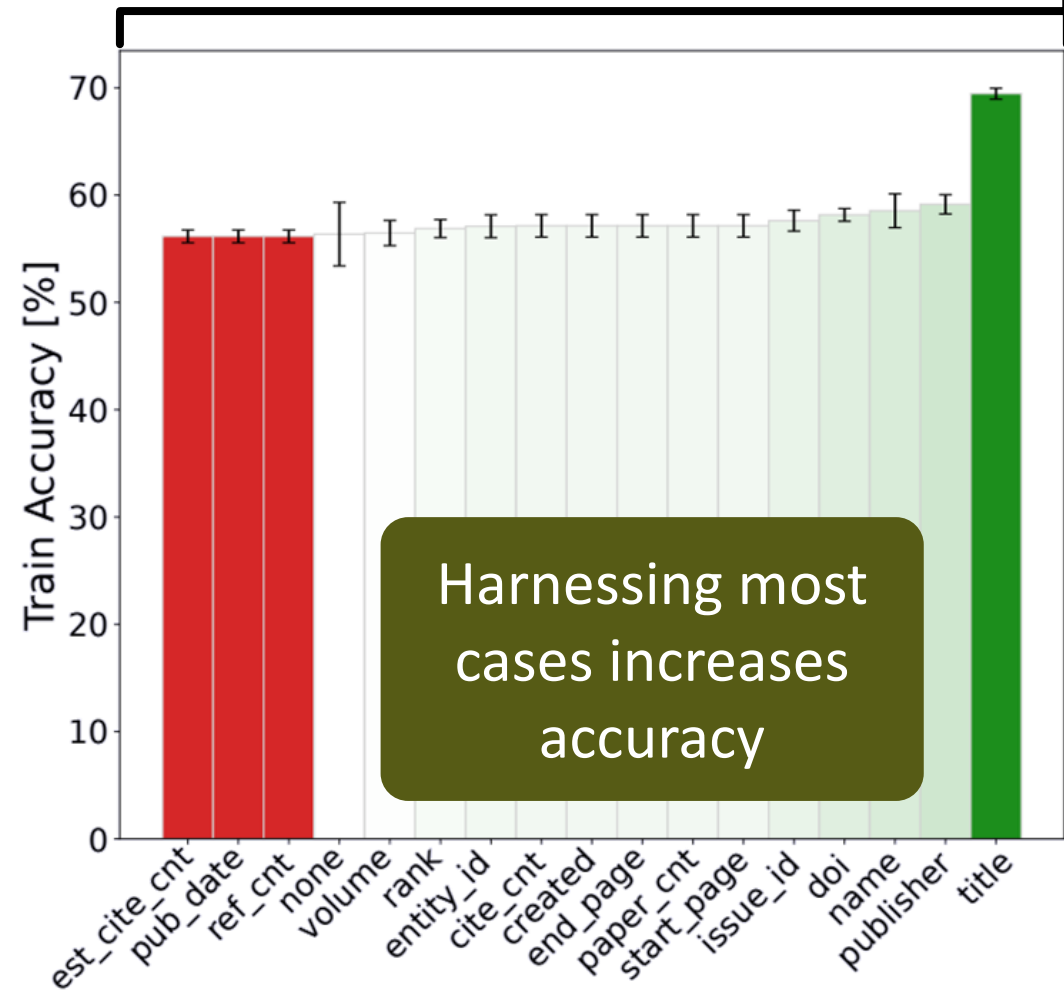


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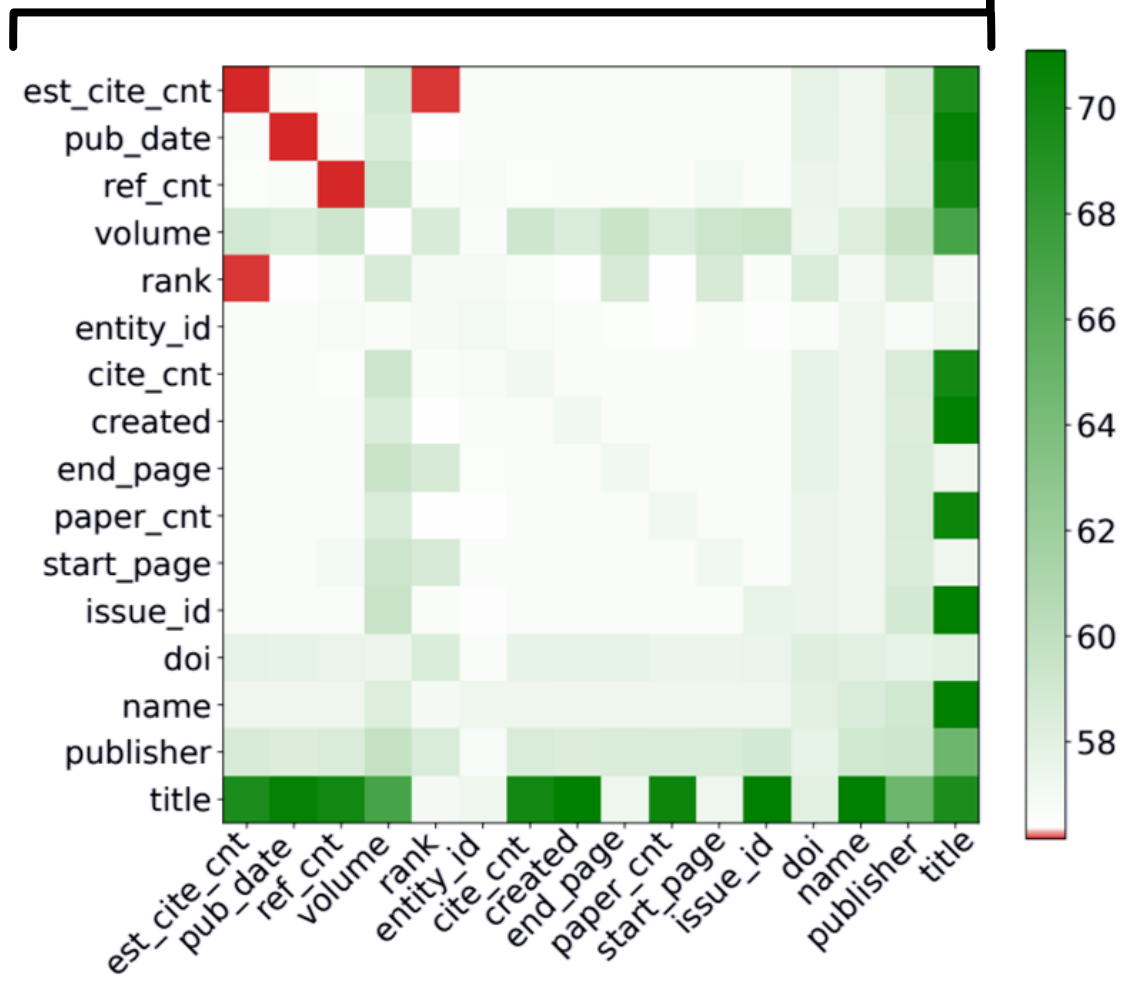
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In same cases, accuracy decreases

Impact from each label/property



Impact from each label/property pair



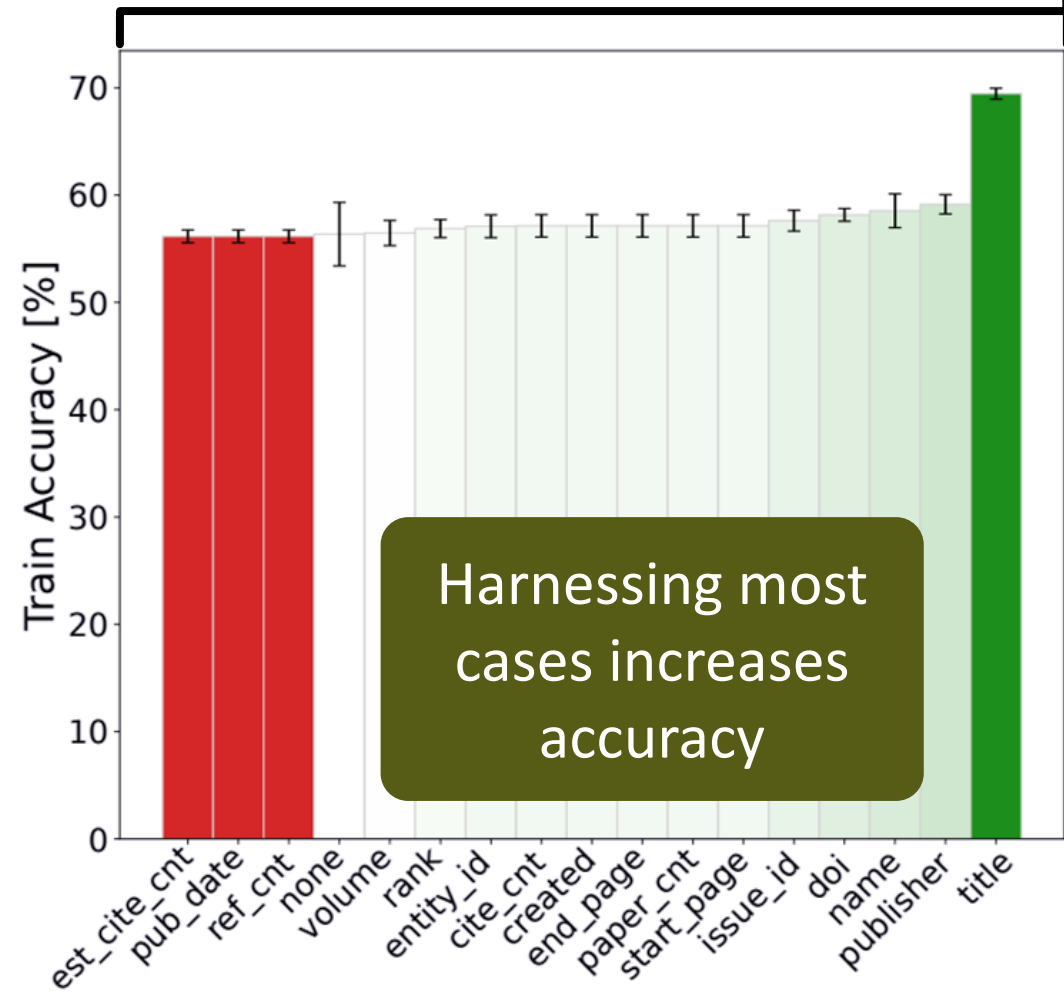
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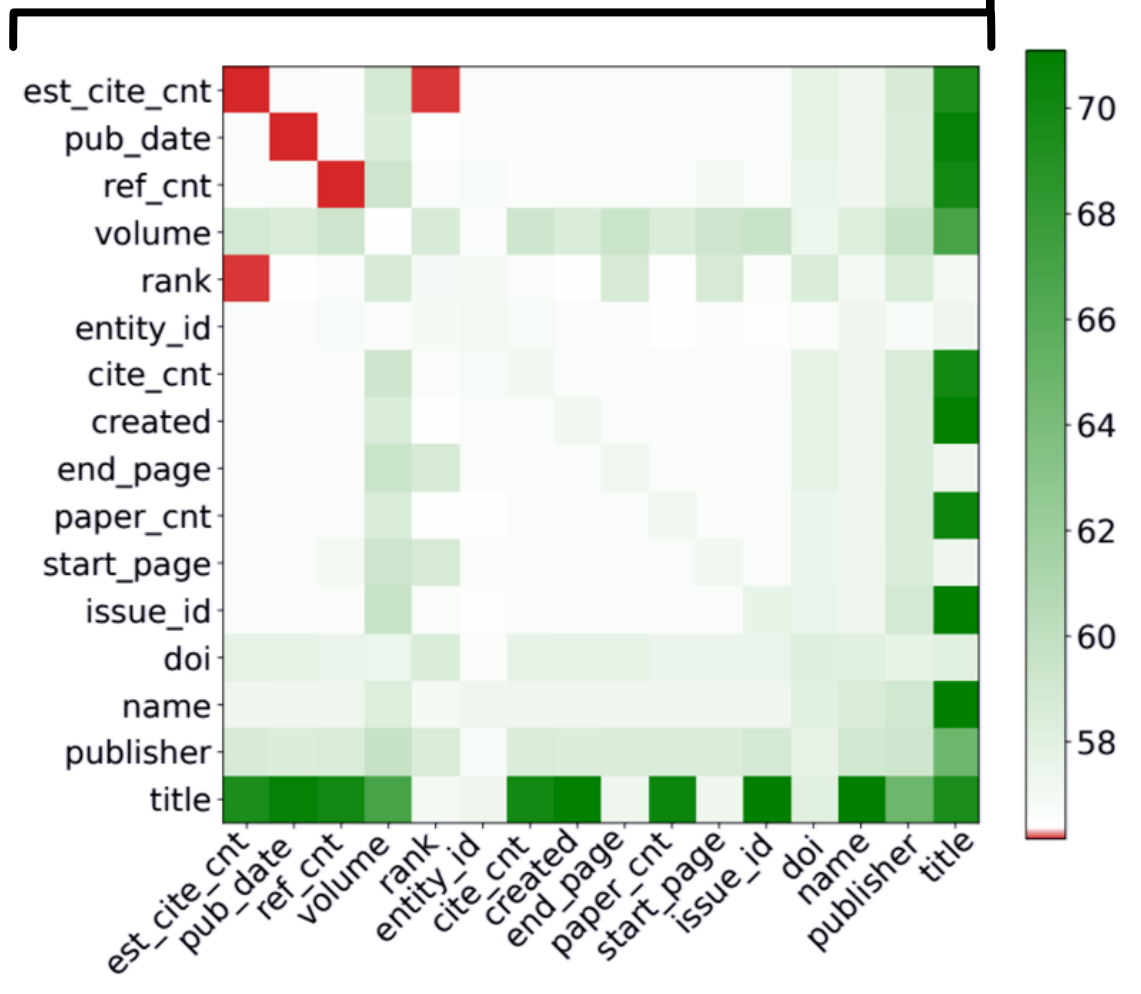
In same cases, accuracy decreases

It is important to understand the data well and select the right encoded LPG information

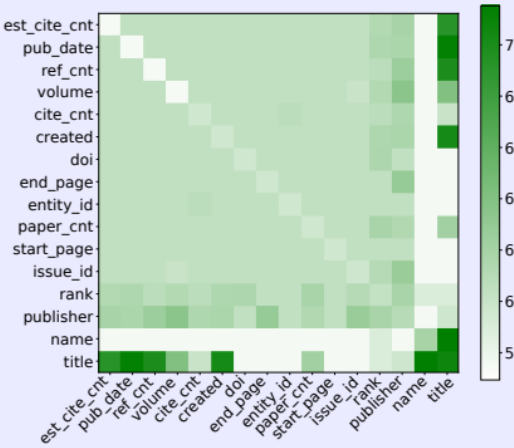
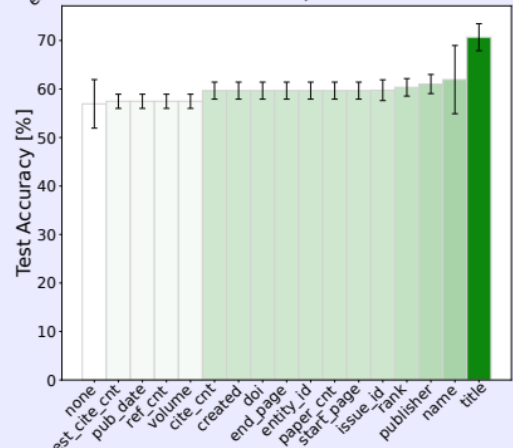
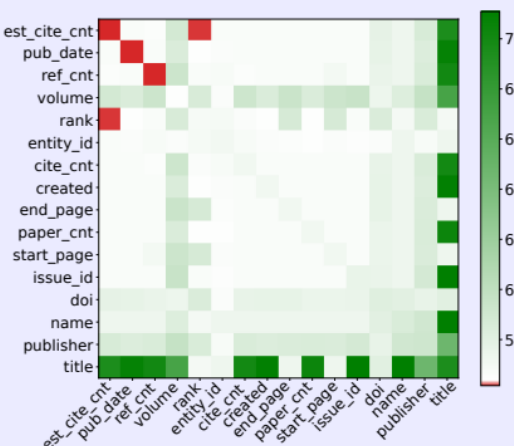
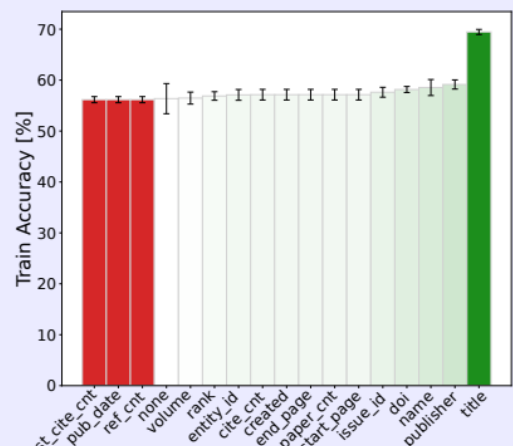
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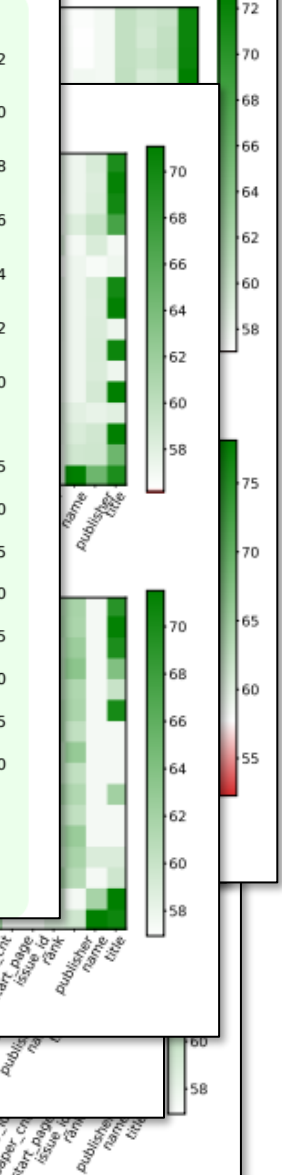
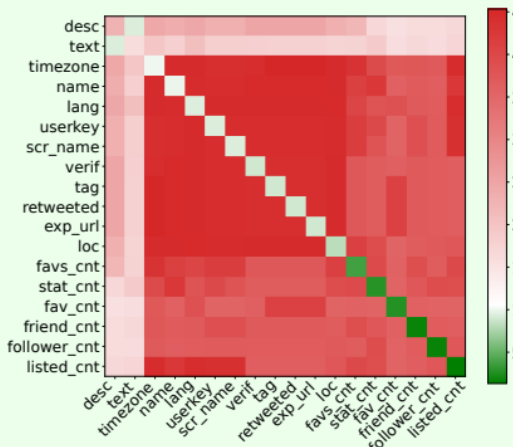
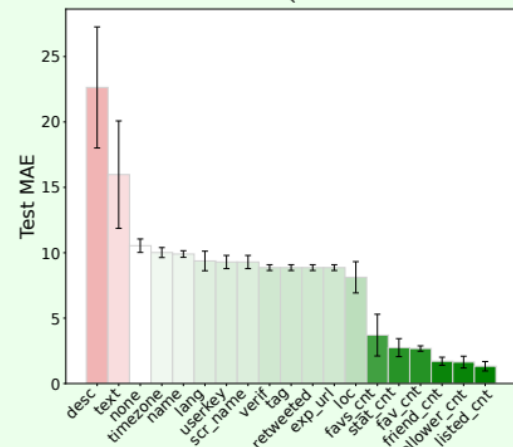
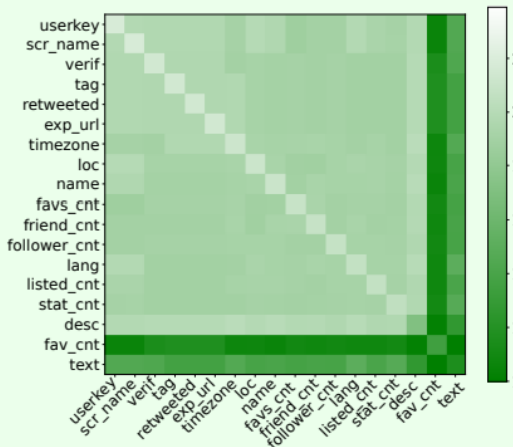
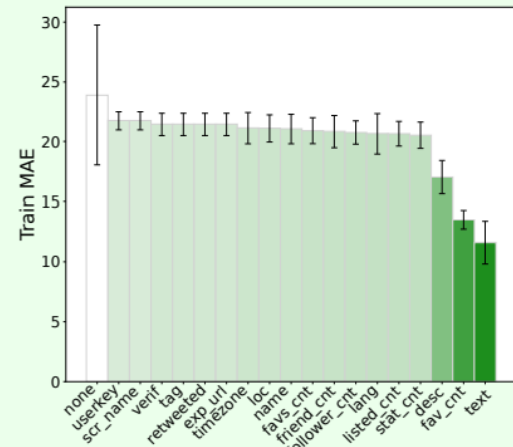
Impact from each label/property pair

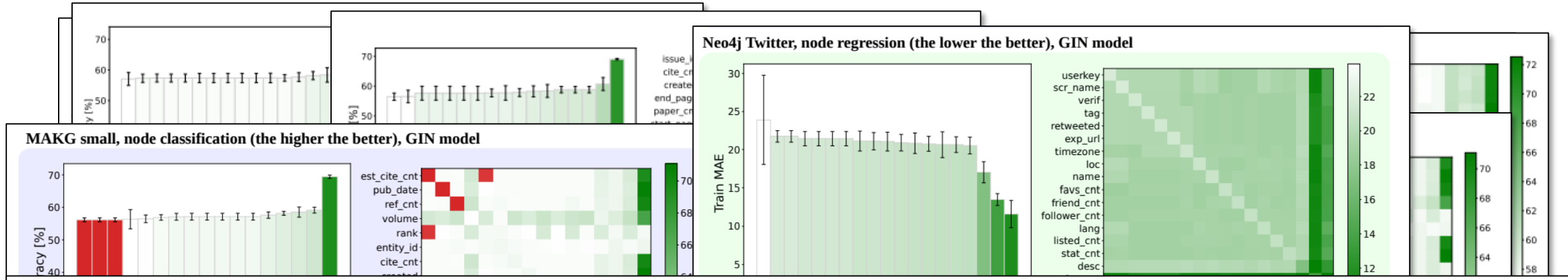


### MAKG small, node classification (the higher the better), GIN model



### Neo4j Twitter, node regression (the lower the better), GIN model





<https://arxiv.org/abs/2209.09732>

@ LoG'22 (Learning on Graphs'22)

# Neural Graph Databases

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