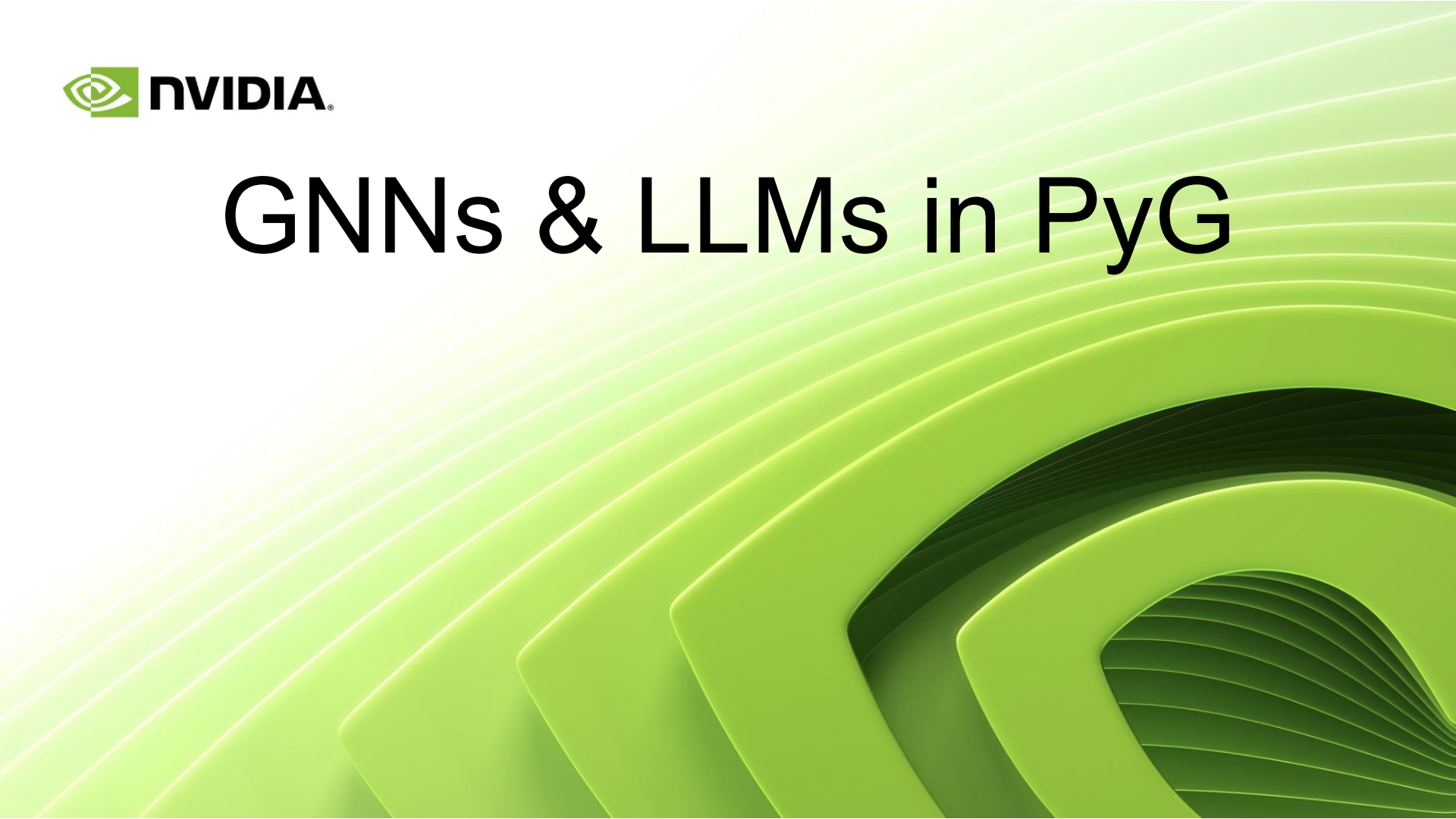
Stanford CS224W: Large Language Models and GNNs

CS224W: Machine Learning with Graphs
Jure Leskovec and Charilaos Kanatsoulis, Stanford University

http://cs224w.stanford.edu

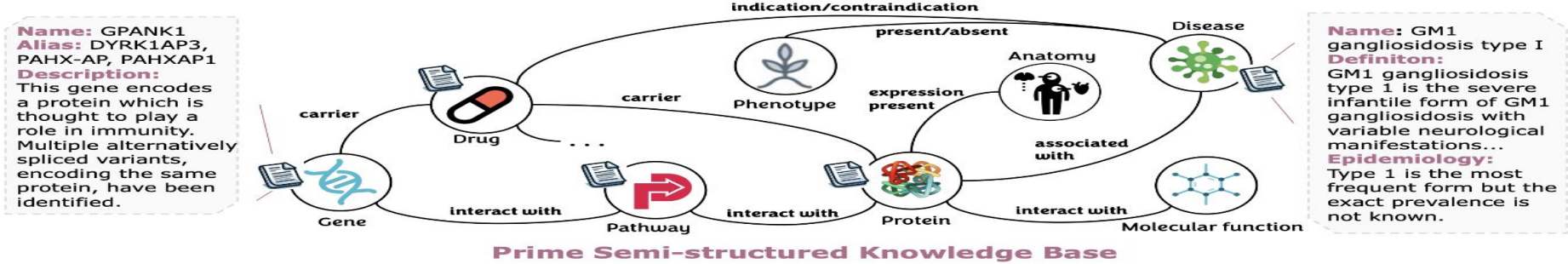
Announcements

- **Exam** is tomorrow! (11/19, 6-8PM)
  - See Ed for your assigned room
  - If taking an OAE or makeup exam, you should have received details by email already
- **Colab 4** due Tuesday 12/2
- **Colab 5** due Thursday 12/4
- **Project Report** due Thursday 12/11


NVIDIA
GNNs & LLMs in PyG

Neo4j Case Study

- Neo4j* Cyphers w/ PyG 2.6 G-retriever on Stark Prime (https://stark.stanford.edu/)
- 2x hit@1!
  - (.16->.32) (7B LLM Agentic GraphRAG vs PyG GNN+LLM)
  - PyG GNN+LLM Solution: LLAMA3.1-8B w/ LoRA + 10M param GAT
  - Even outperforms agentic GraphRAG w/ much larger frontier models:
    - claude-3-opus (.18) and gpt-4-turbo (.2) (Agentic GraphRAGs)
- https://github.com/neo4j-product-examples/neo4j-gnn-llm-example
- https://developer.nvidia.com/blog/boosting-qa-accuracy-with-graphrag-using-pyg-and-graph-databases/



Neo4j (Graph Database and Analytics): https://neo4j.com/

LLM/Transformer Intro

- LLMs (Transformer) excel at predicting the next token in sequences
- “Attention is all you need” is plateauing
- LLM’s pretrained for single hop logic:
  - Given context tokens, predict next tokens
- Single hop logic -> **associative memory**
  - Fails out of distribution
- Infinite out of distribution tasks in NLP, robotics, medicine, etc

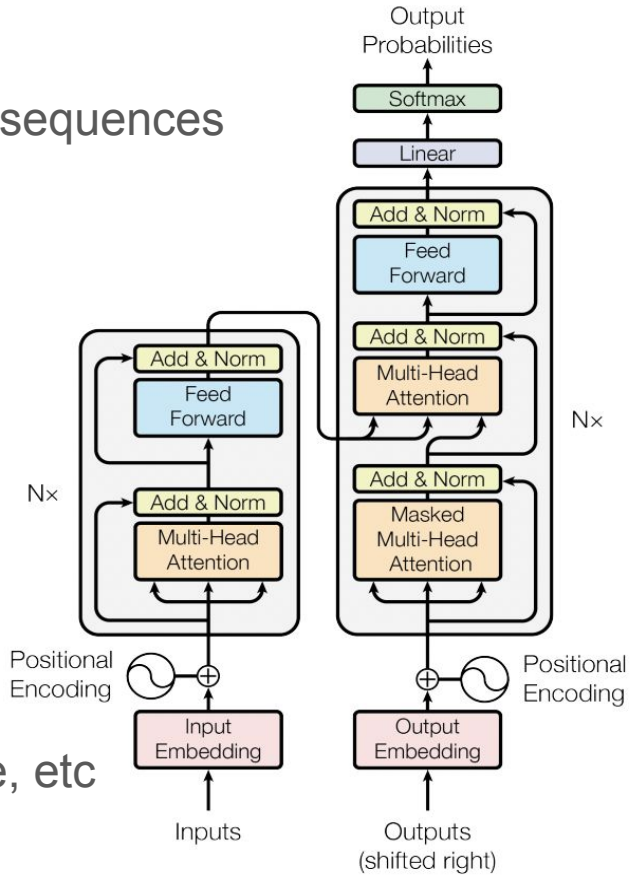


Figure 1: The Transformer - model architecture.

Today's LLMs = Associative Memory

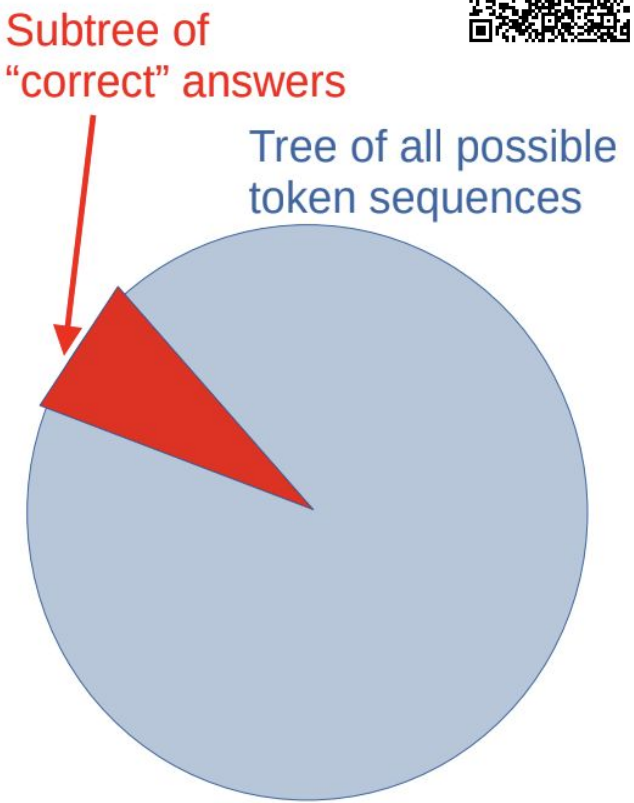
- Imagine: Goal is learn "2, 4, 6, 8, 10, 12, 14, …"
- General Human Intelligence (Won't Fail out of Distribution):
  - Given a number, return that number + 2
- Associative Memory Model (Will Fail out of Distribution)
  - Training: For 500GB worth of numbers, store the next token in the sequence
    - 2->4, 4->6, 6->8, …
  - Testing: passes within distribution, fails out of distribution
    - output undefined -> hallucinate
- LLMs close to associative memory than human intelligence

Auto-Regressive Generative Models Suck!

- Auto-Regressive LLMs are **doomed**.
- They cannot be made factual, non-toxic, etc.
- They are not controllable
- Probability e that any produced token takes us outside of the set of correct answers
- Probability that answer of length n is correct (assuming independence of errors):
  - $P(\text{correct}) = (1-e)^n$
- **This diverges exponentially.**
- **It's not fixable (without a major redesign).**

- See also [Dziri...Choi, ArXiv:2305.18654]

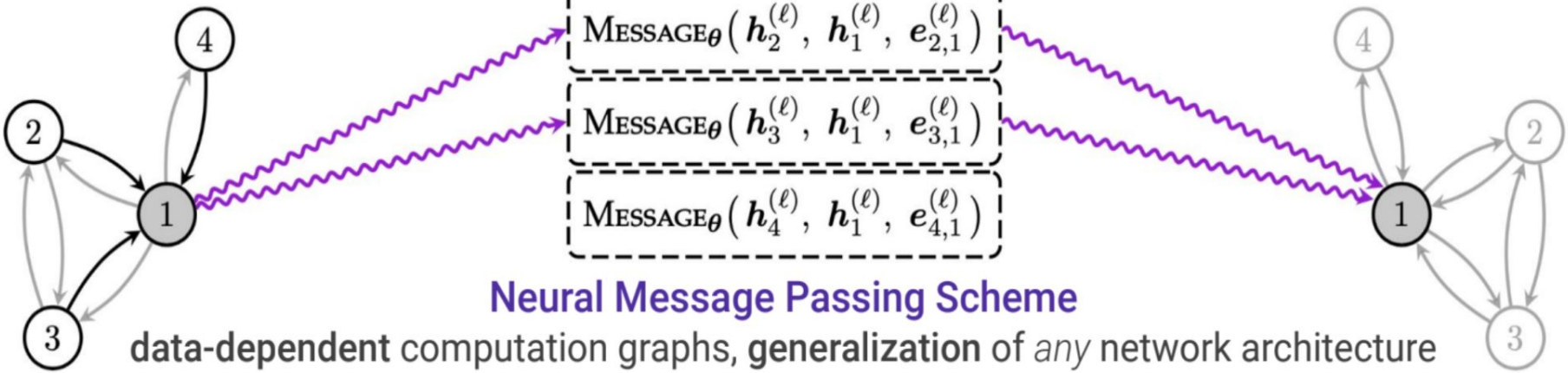
Full Lecture:



GNN Visualizer (GNN 101 University of Minnesota):

GNN Intro

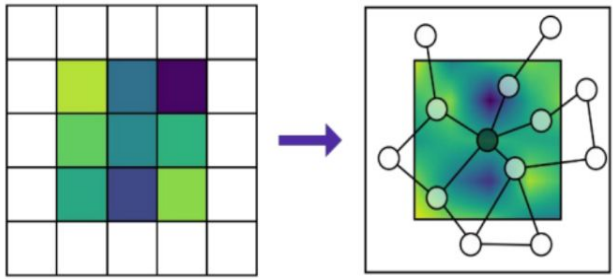
Graph Neural Networks (GNNs) update **node representations** by *repeatedly* **transforming** *and* **aggregating** representations *of* **direct neighbors**

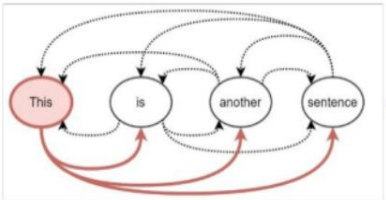


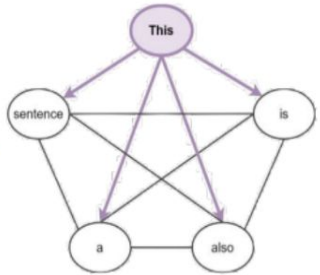
Neural Message Passing Scheme

data-dependent computation graphs, **generalization** of *any* network architecture

From **CNNs** *to* **GNNs**





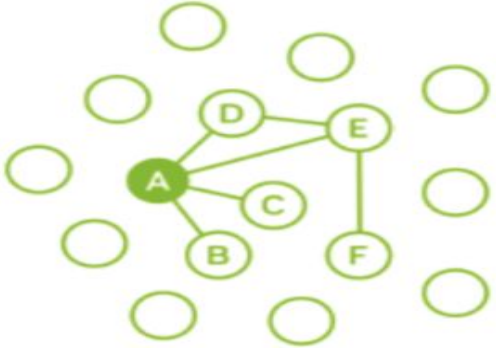


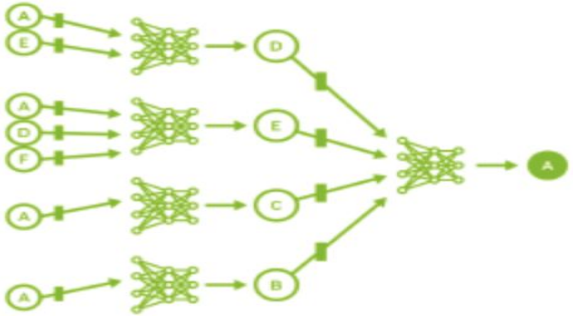
From **Transformers** *to* **GNNs**

Matthias Fey Graph Learning Conference Talk 2023

GNN Intro

- N layer GNN -> N hops of logic
- GNNs can improve LLM accuracy
  - (semi-orthogonal information)
- size(LLM) >> size(GNN)
  - “Transformer layer can be seen as a special GNN that runs on a fully connected “word” graph” - Jure Leskovec
  - -> almost no added params for adding GNN





GNNs are Deterministic, LLMs are Not!

- For any given input, output deterministic for most GNNs
- Not the case for LLMs… They are **Generative** AI
  - Learn the distribution, then randomly **generate** outputs that align with that distribution
  - 1 prompt, 2+ right answers
    - -> high chance of plausible sounding hallucination
  - Toy Example: Train LLM predict next token in 2, 4, 6, 8 and 2, 6, 18, 54
    - What does the LLM predict for 2->?

GNNs are Deterministic, LLMs are Not!

- Real World: Task + Python Solution
- Almost always multiple valid solutions
- Outcome: inference outputs that look valid but have issues
- Why: combining random chunks from correct codebases often doesn’t work
- Problem Caused:
  - Devs using AI spend substantial time debugging
  - Extremely damaging bugs can slip through -> crashes/being hacked/etc

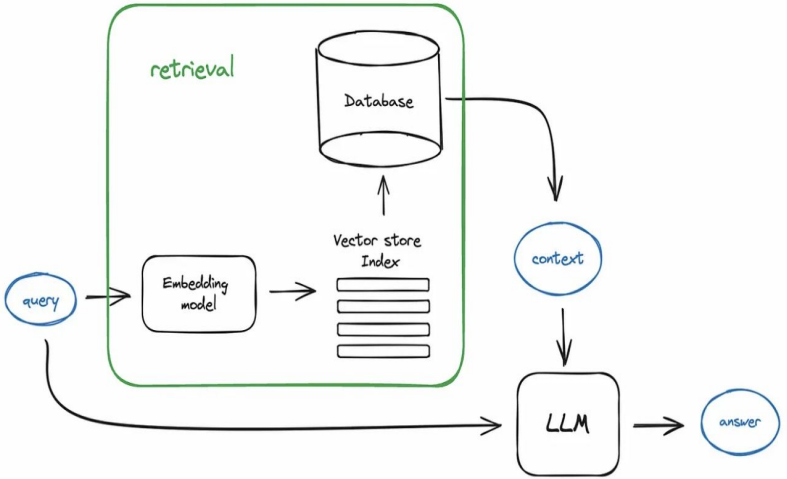
LLMs Strengths and Weaknesses

- Basic LLMs great for creative tasks that don’t need absolute precision:
  - Writing, Art, etc

- Not ideal for precise tasks like coding or making high impact decisions
- Running out of public data for LLM, GNNs enable a whole new world of data
- GNNs won’t solve all problems, but step in right direction.

RAG: VectorRAG vs GraphRAG

- RAG = Retrieval Augmented Generation
- VectorRAG: retrieve top K relevant docs based on their embedding **vector**
  - Good enough when answer requires single doc
- GraphRAG: retrieve relevant sub**graph**
  - Good when answer requires multiple docs with related entities

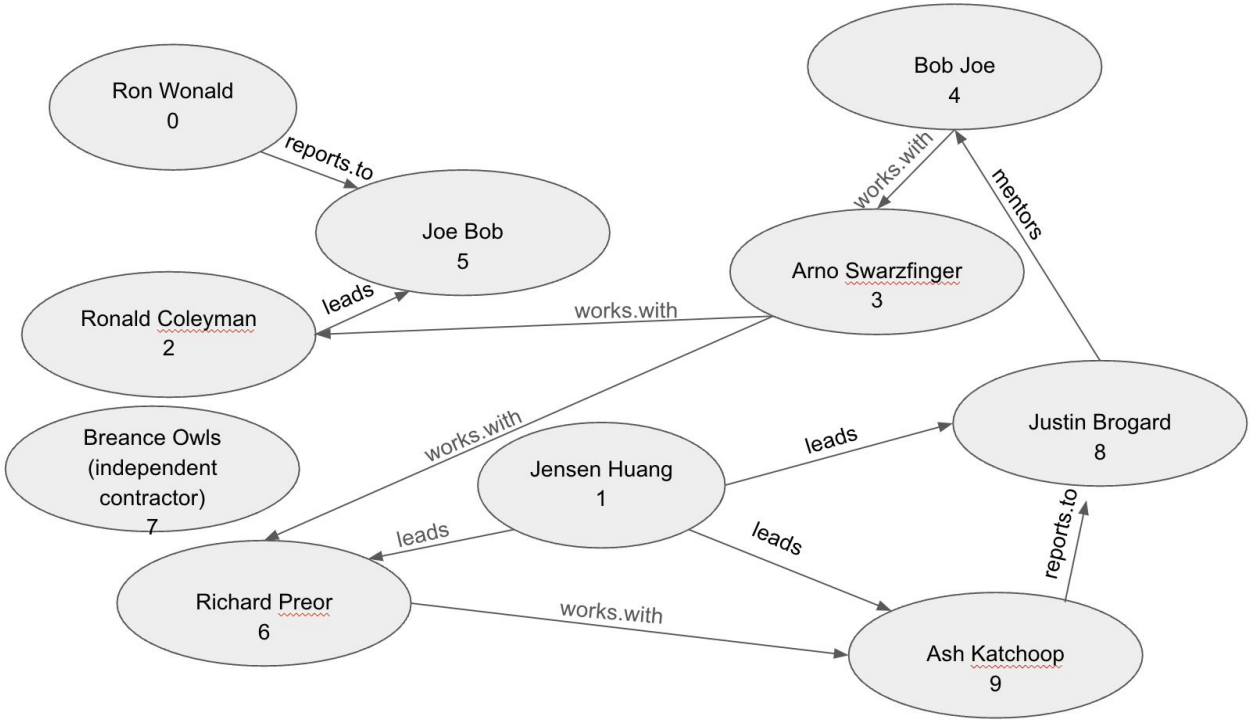


GraphRAG Example: Made Up NVIDIA Org Chart

Question:
Who is the shared coworker between **Bob Joe** and **Ronald Coleyman?**
Answer:
Arno Swarzfinger

node_id,node_attr
0,Ron Wonald
1,Jensen Huang
2,Ronald Coleyman
3,Arno Swarzfinger
4,Bob Joe
5,Joe Bob
6,Richard Preor
7,Breance Owls
8,Justin Brogard
9,Ash Katchoop
[[stop]]

src,edge_attr,dst
0,reports.to,5
9,reports.to,8
8,mentors,4
2,leads,5
1,leads,6
4,works.with,3
3,works.with,2
1,leads,9
1,leads,8
3,works.with,6
6,works.with,9
[[stop]]



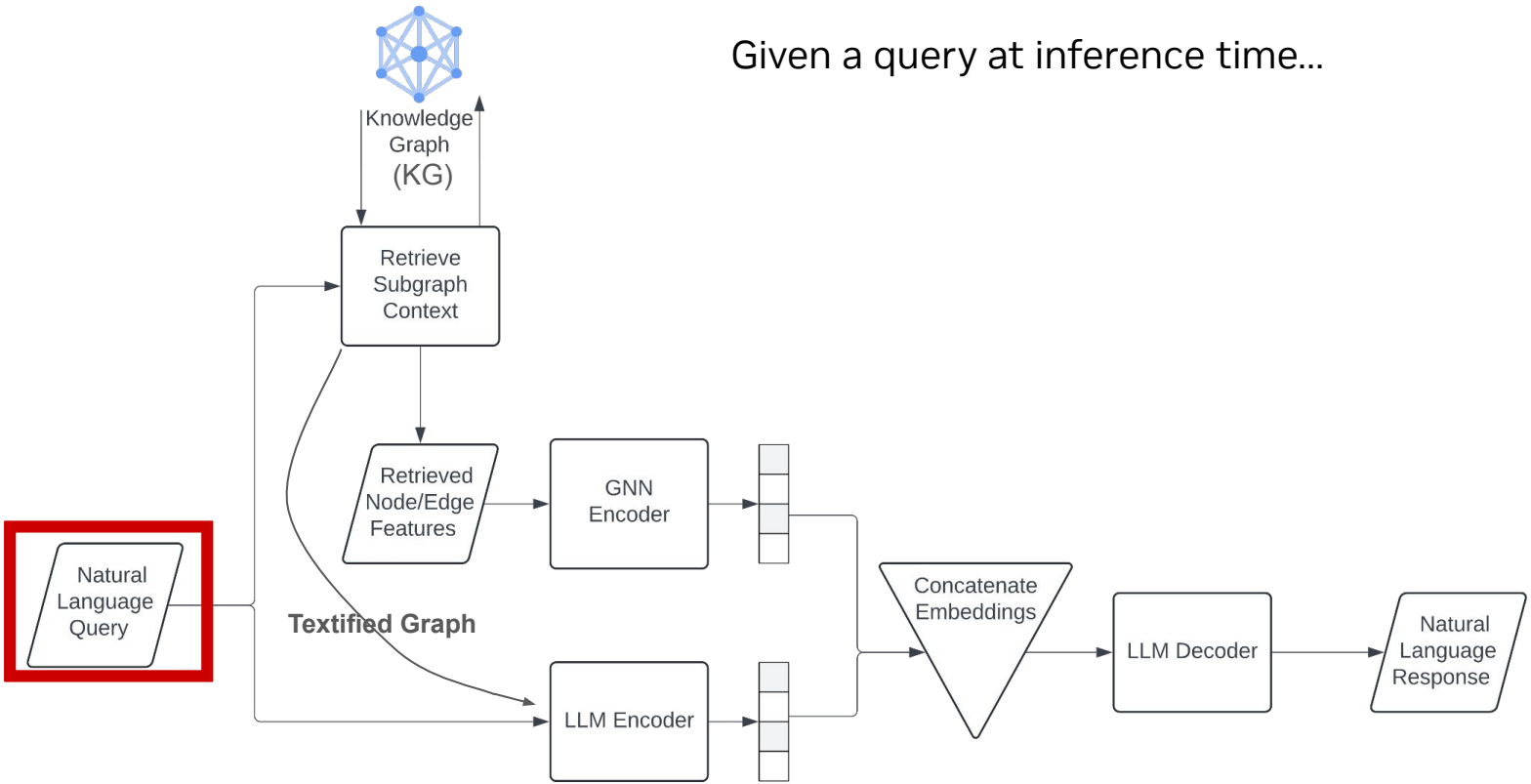
LLM: Wrong ❌
GNN+LLM: Correct ✅

GNNs Meet LLMs (History Lesson)

- “Attention is All You Need” (June 12, 2017 on Arxiv)
- GraphSAGE paper (June 7, 2017 on Arxiv)
- Since 2017, the industry has poured majority of effort into LLMs
- In parallel, small but strong PyG community grows in Academia
  - + Small Group of Companies Capitalizing on GNNs:
    - Pinterest, Kumo, Spotify …
- PyG GNN+LLM aims to combine the learnings of both work streams
  - Goal: Add GNNs to Advance AI systems past the limitations of LLMs

GNN+LLM Graph RAG (GNN Feeds LLM)

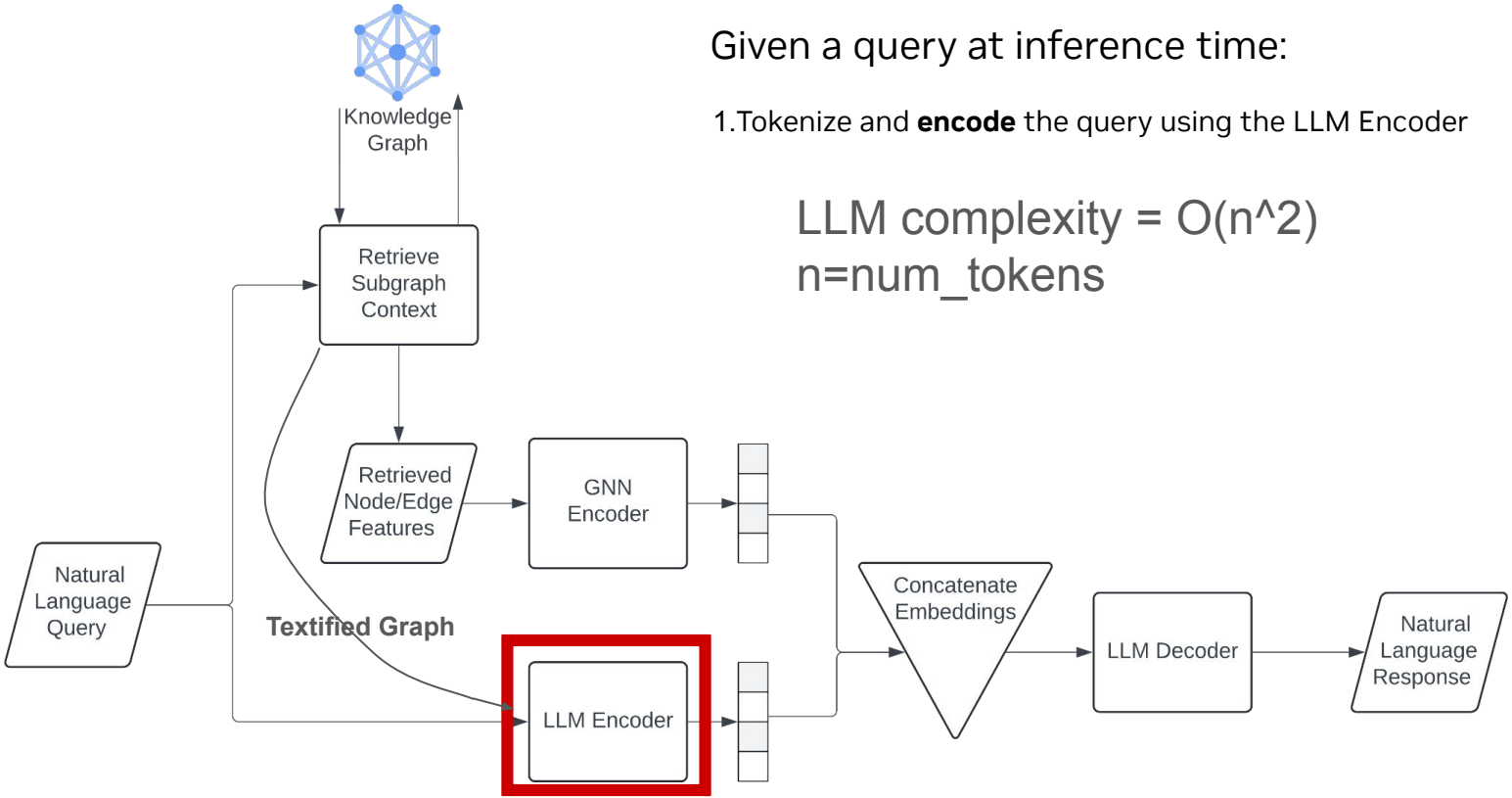
Given a query at inference time…



*RAG = Retrieval Augmented Generation

*G-retriever: https://arxiv.org/abs/2402.07630

GNN+LLM Graph RAG (GNN Feeds LLM)



Given a query at inference time:

1.Tokenize and **encode** the query using the LLM Encoder

LLM complexity = O(n^2)
n=num_tokens

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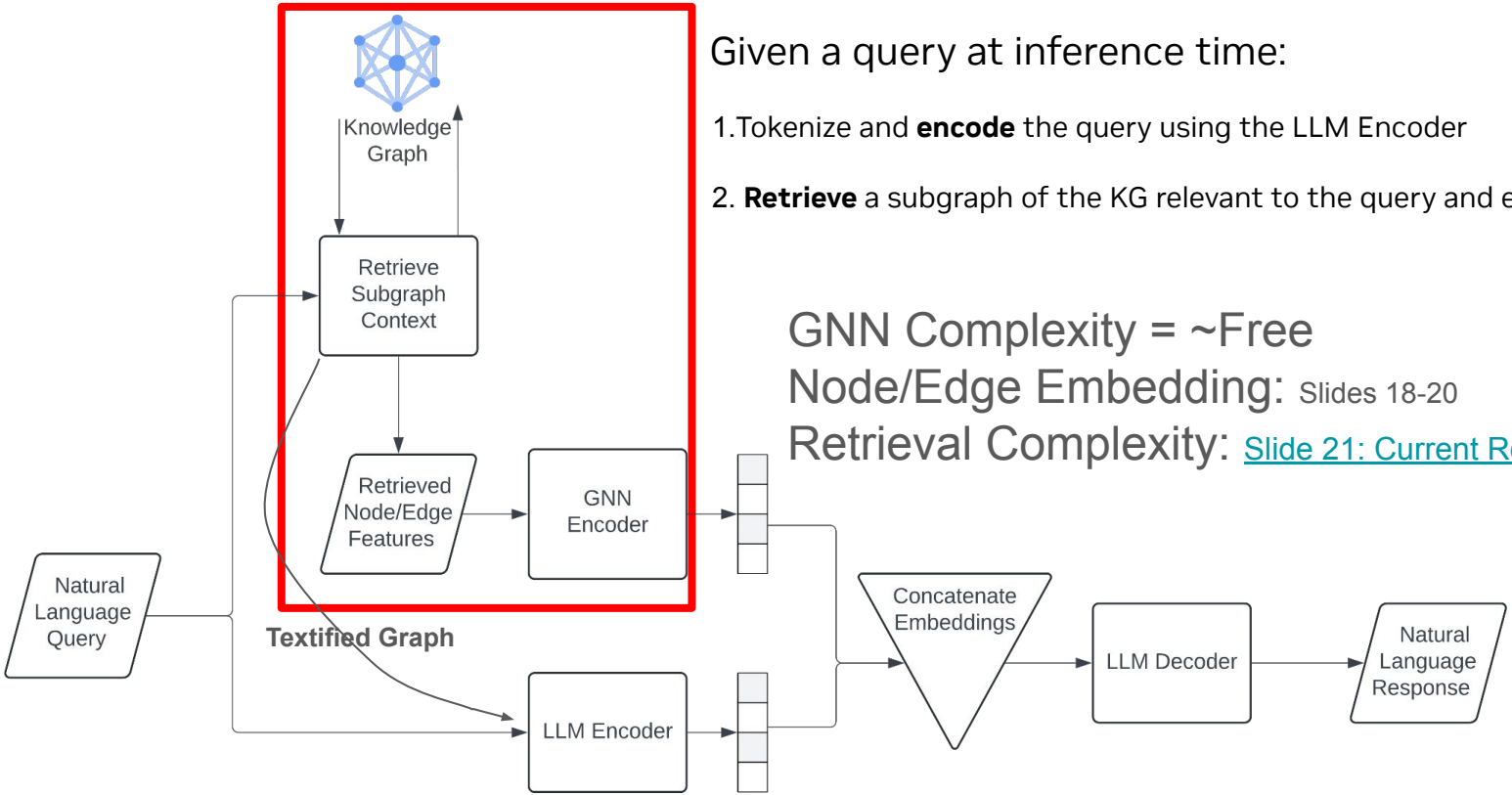
GNN+LLM Graph RAG (GNN Feeds LLM)



Given a query at inference time:

1.Tokenize and **encode** the query using the LLM Encoder

2. **Retrieve** a subgraph of the KG relevant to the query and encode it using a GNN

GNN Complexity = ~Free

Node/Edge Embedding: Slides 18-20

Retrieval Complexity: Slide 21: Current Retrieval Algorithm

*RAG = Retrieval Augmented Generation

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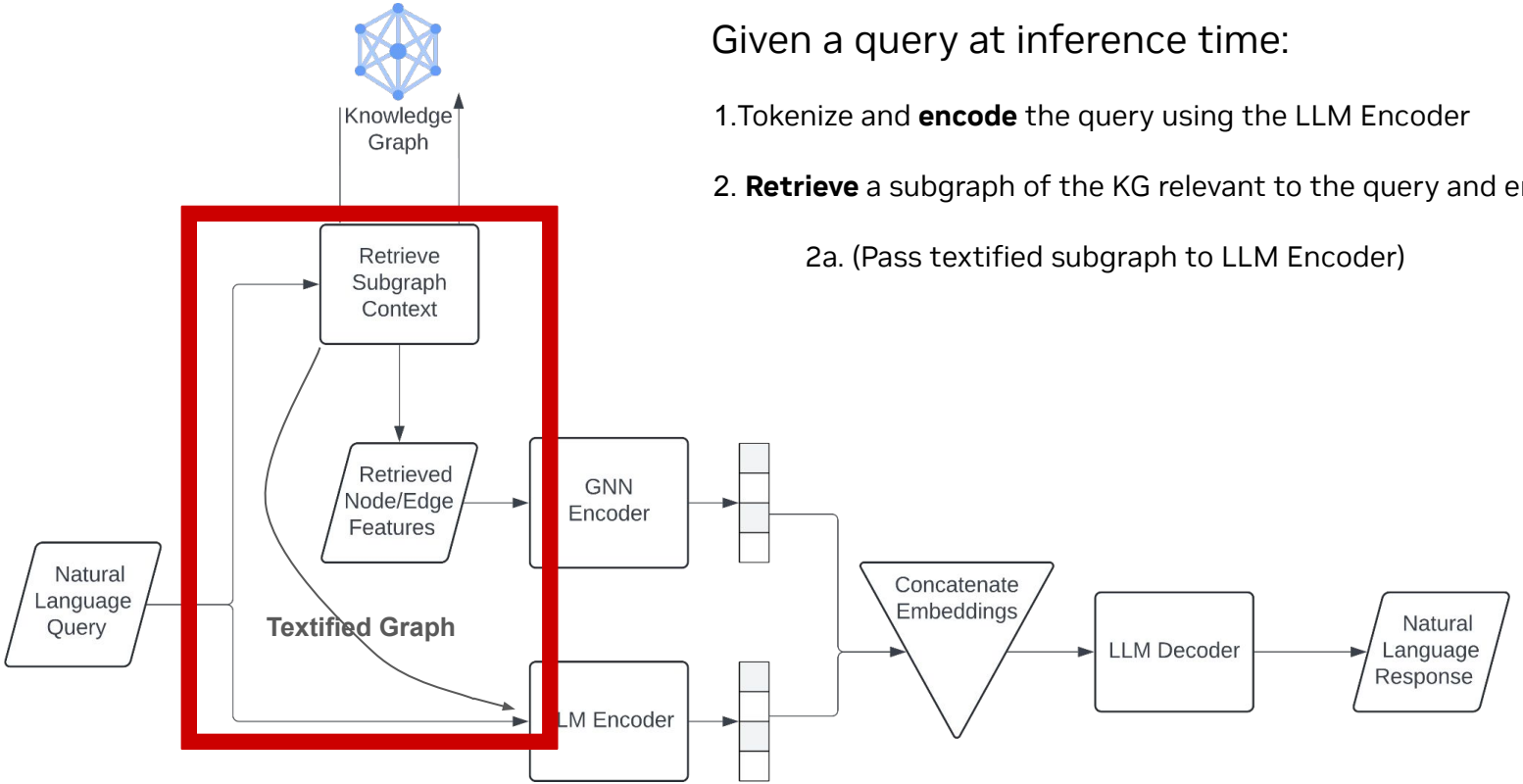
GNN+LLM Graph RAG (GNN Feeds LLM)



Given a query at inference time:

1.Tokenize and **encode** the query using the LLM Encoder

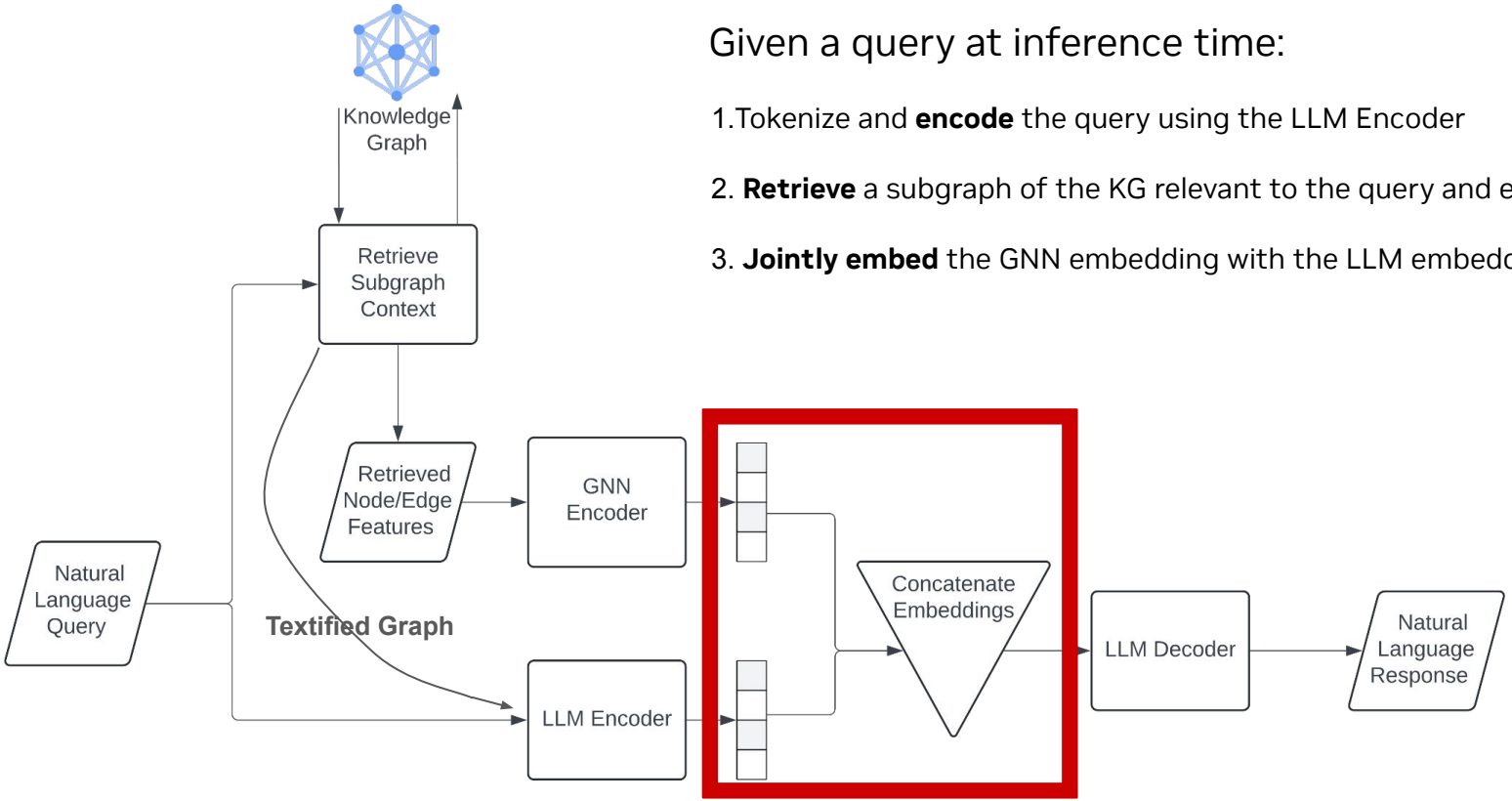
2. **Retrieve** a subgraph of the KG relevant to the query and encode it using a GNN

2a. (Pass textified subgraph to LLM Encoder)

*RAG = Retrieval Augmented Generation

*G-retriever: https://arxiv.org/abs/2402.07630

GNN+LLM Graph RAG (GNN Feeds LLM)



Given a query at inference time:

1.Tokenize and **encode** the query using the LLM Encoder

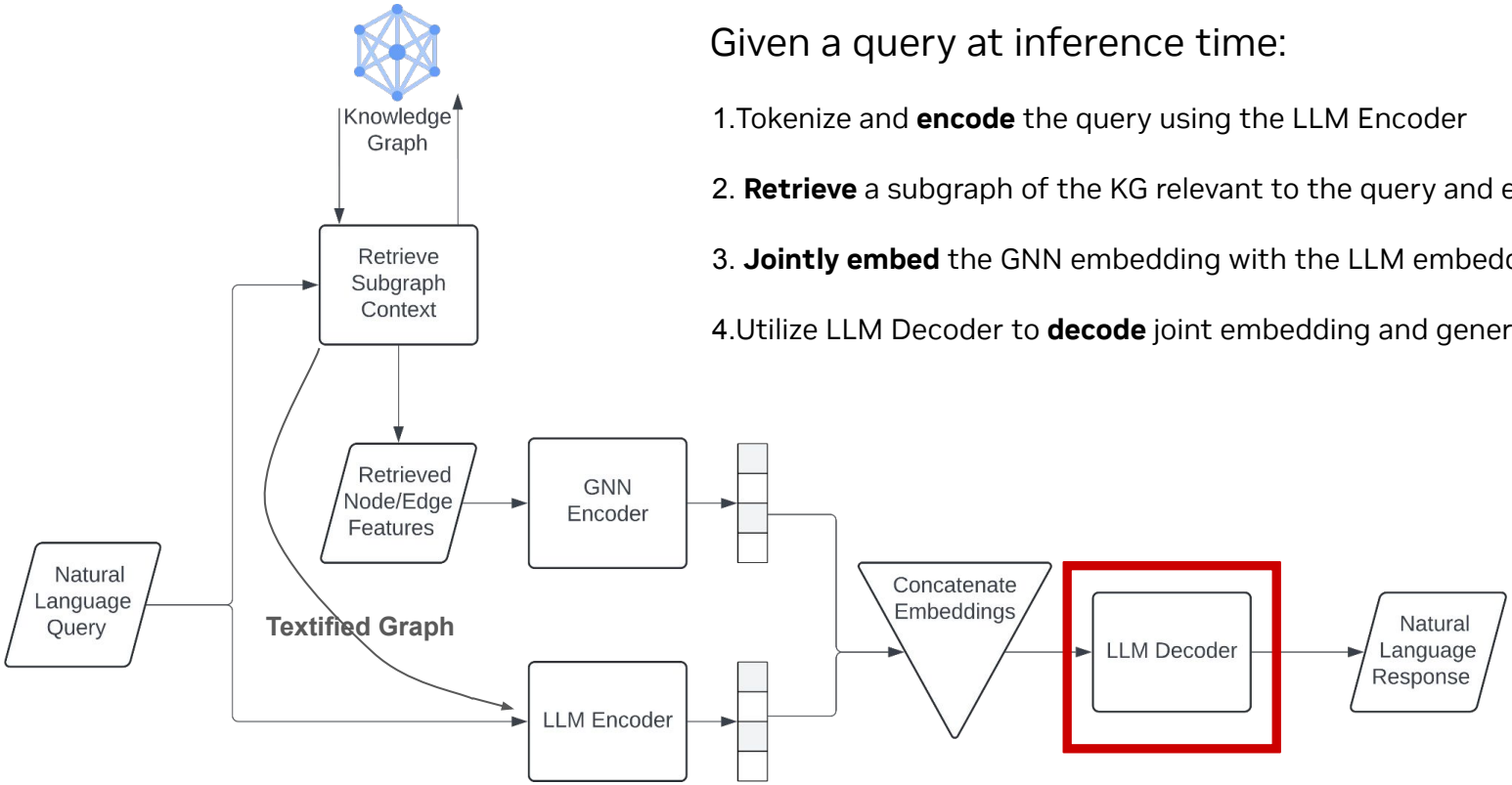
2. **Retrieve** a subgraph of the KG relevant to the query and encode it using a GNN

3. **Jointly embed** the GNN embedding with the LLM embedding

*RAG = Retrieval Augmented Generation

*G-retriever: https://arxiv.org/abs/2402.07630

GNN+LLM Graph RAG (GNN Feeds LLM)



Given a query at inference time:

1.Tokenize and **encode** the query using the LLM Encoder

2. **Retrieve** a subgraph of the KG relevant to the query and encode it using a GNN

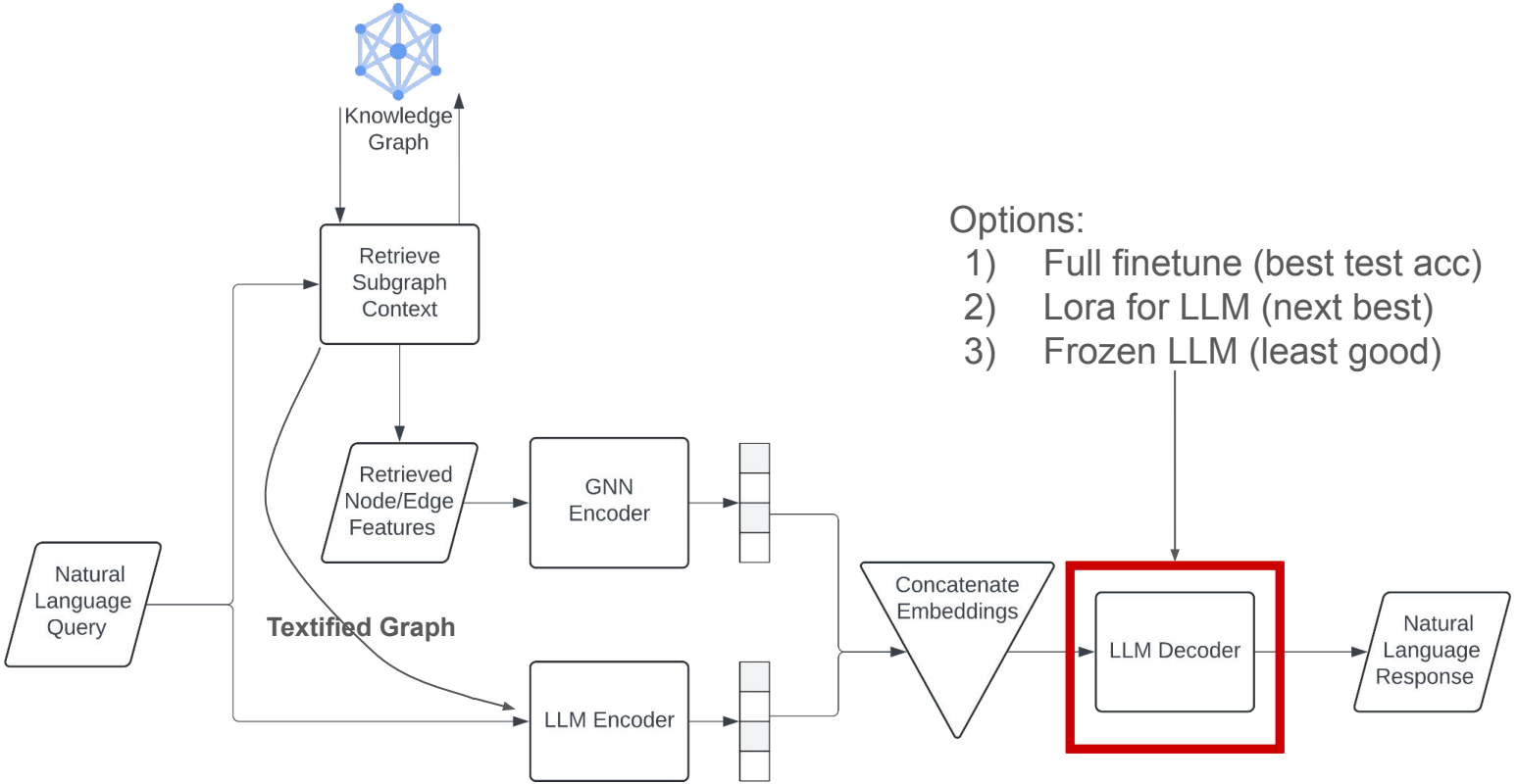
3. **Jointly embed** the GNN embedding with the LLM embedding

4.Utilize LLM Decoder to **decode** joint embedding and generate a response

*RAG = Retrieval Augmented Generation

*G-retriever: https://arxiv.org/abs/2402.07630

GNN+LLM Graph RAG (GNN Feeds LLM)



*RAG = Retrieval Augmented Generation

*G-retriever: https://arxiv.org/abs/2402.07630

Text KG -> PyG Graph?

- PyG expects:
  - feature vector for each node
  - Optionally for each edge too
- Entities and relations are short phrases…
  - Example Triple: (cats, eat, dogs)
- Need Model(str) -> feature vector

Sentence Transformer Intro

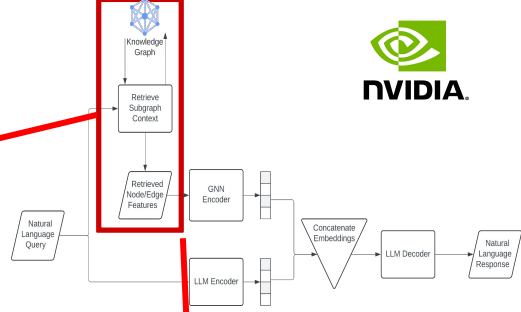
```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
model = SentenceTransformer(
    model_name='sentence-transformers/all-roberta-large-v1').to(device)
```

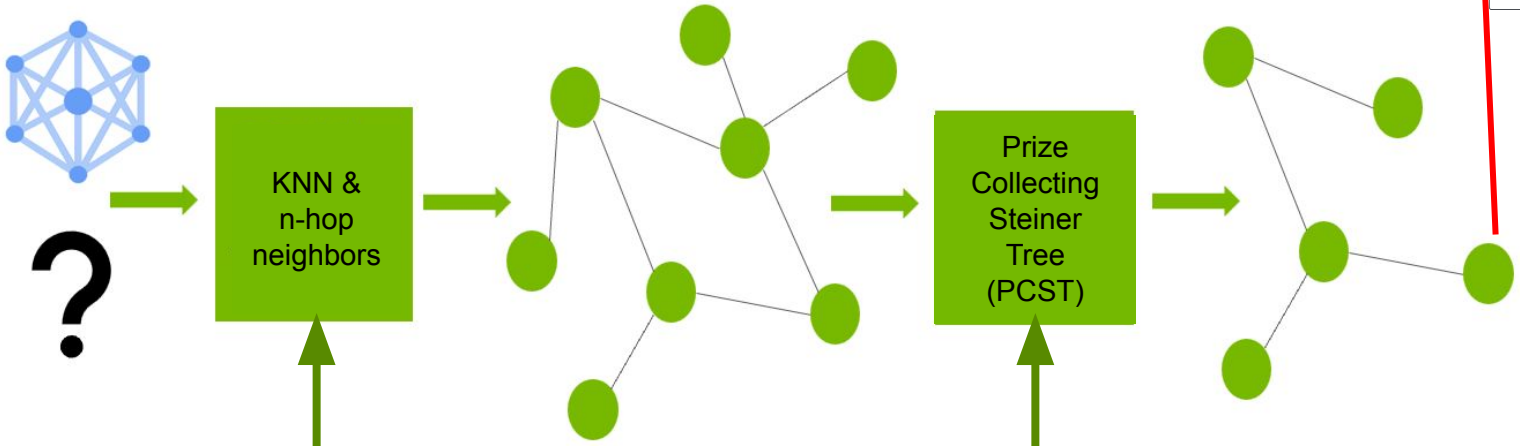
- Sentence Transformer: model(List[str]) -> Embedding Tensor
- Need to call model (3 * num_edges)
  - For each edge, call on both entities and the relation
  - -> Use small LM (SLM) like ModernBert for efficiency

Why Are Small LMs Okay as SentenceTransformers?

- Small LMs have sufficient understanding of short phrases
- Only need large LM for large/complex bodies of text
- Future work: Measure tradeoffs for SLM vs LLM
- Latest PyG supports VisionTransformer now!

Basic Retrieval Algorithm (GNN Feeds LLM)





Remote Knowledge Graph & Prompt (millions of nodes)

Untrimmed Subgraph (thousands of nodes)

Pruned Subgraph (dozens of nodes)

X nodes, n hops, fanout=f
-> O(X*K*f^n)

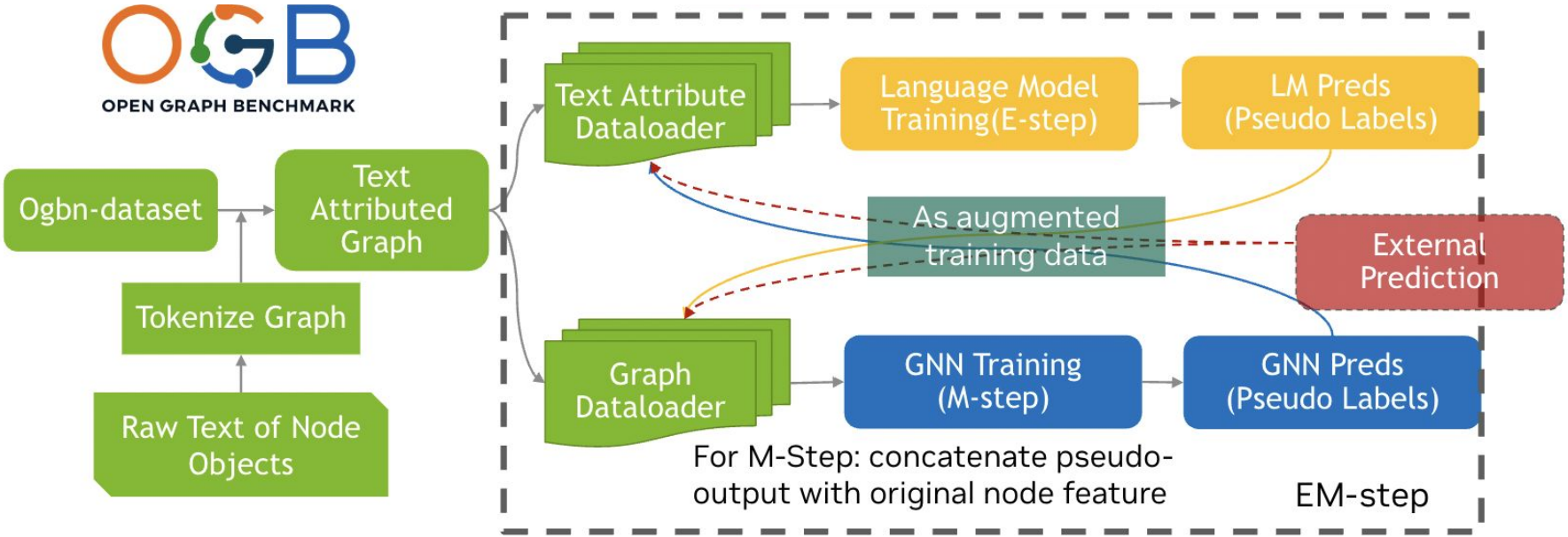
(similarity based graph traversal)
Linear on thousands -> Free

GNN Feeds LLM vs LLM Feeds GNN

- GNN Feeds LLM:
  - Data: prompt conditioned on graph
  - Tasks: Token-level tasks (Ex. Question Answering)
  - Flow:
    - Graph -> GNN = GNN_out
    - (GNN_out + prompt) -> LLM = Answer Tokens
- LLM Feeds GNN:
  - Data: Graph where every node/edge has tokens attributed to it
  - Task: Graph learning (Ex. node classification or link prediction)
  - Flow:
    - feature vector for each node/edge (Sentence/VisionTransformer)
    - Feed this graph to GNN for Graph Learning Task

Node Classification: GLEM (LLM Feeds GNN)

- GLEM = SOTA Node Classification for Text Attributed Graphs (TAGs)
  - https://arxiv.org/abs/2210.14709
  - Ex: OGBN-Products (https://ogb.stanford.edu/docs/leader_nodeprop/#ogbn-products)



Node Classification in PyG (LLM Feeds GNN)

- Implementation in PyG 7x faster than original paper's code for OGBN-Products
- New Text Attributed Graph (TAG) Interface
- Also adds optional support for LLM finetuning w/ LoRA* (uses PEFT* library)
- See examples/llm/glem.py on PyG GitHub

PEFT = https://pyg.org/

LoRA = https://arxiv.org/abs/2106.09685

PEFT = https://huggingface.co/docs/peft/en/index

TAG Usage (LLM Feeds GNN)

```
dataset = PygNodePropPredDataset(f'ogbn-products', root=root)
split_idx = dataset.get_idx_split()
tag_dataset = TAGDataset("/root/path", dataset, "prajjwal1/bert-tiny",
                         token_on_disk=token_on_disk)
```

- Takes in path, dataset, and LM of choice
- Optional: save tokens on disk

GLEM Set Up (LLM Feeds GNN)

```
num_classes = dataset.num_classes
gnn = GAT(in_channels=1024,
          hidden_channels=1024,
          num_layers=4,
          out_channels=num_classes,
          heads=4,
         )
model = GLEM(lm_to_use="prajjwal1/bert-tiny", gnn_to_use=gnn, out_channels=num_classes,
             lm_use_lora=lm_use_lora, device=device)
```

- GLEM model: LM of choice, GNN of choice, num_classes
- Optional:
  - Use LoRa
  - Device (default cpu but cpu is **SUPER** slow)

G-retriever (GNN Feeds LLM) Set Up

```
gnn = GAT(
    in_channels=1024,
    hidden_channels=1024,
    out_channels=1024,
    num_layers=4,
    heads=4,
)

llm = LLM(model_name="meta-llama/Meta-Llama-3.1-8B-Instruct")
model = GRetriever(llm=llm, gnn=gnn)
```

- GRetriever: LLM + GNN
- Auto GPU Set Up!

G-retriever: Get Loss

```
model(
    batch.question, # ["list", "of", "questions", "here"]
    batch.x,  # [num_nodes, num_features]
    batch.edge_index,  # [2, num_edges]
    batch.batch,  # which nodes belong to which question
    batch.label,  # list answers (labels)
    batch.edge_attr,  # [num_edges, num_features]
    batch.desc  # list of text graph descriptions
)
```

G-retriever Inference

```
model.inference(["list", "of", "questions", "here"],
    batch.x # node features,
    batch.edge_index,
    batch.batch, # batch vector, assigns each element to a specific example.
    batch.edge_attr, # edge attributes, optional but recommended
    ["list", "of", "textified graphs", "here"]) # optional but recommended
```

Knowledge Graph Creation

- Most RAG Datasets only have unstructured text context
- Task: unstructured text -> KG
  - Format: (entity_1, relation, entity_2)
- LLMs specialized for unstructured text -> ideal model for task

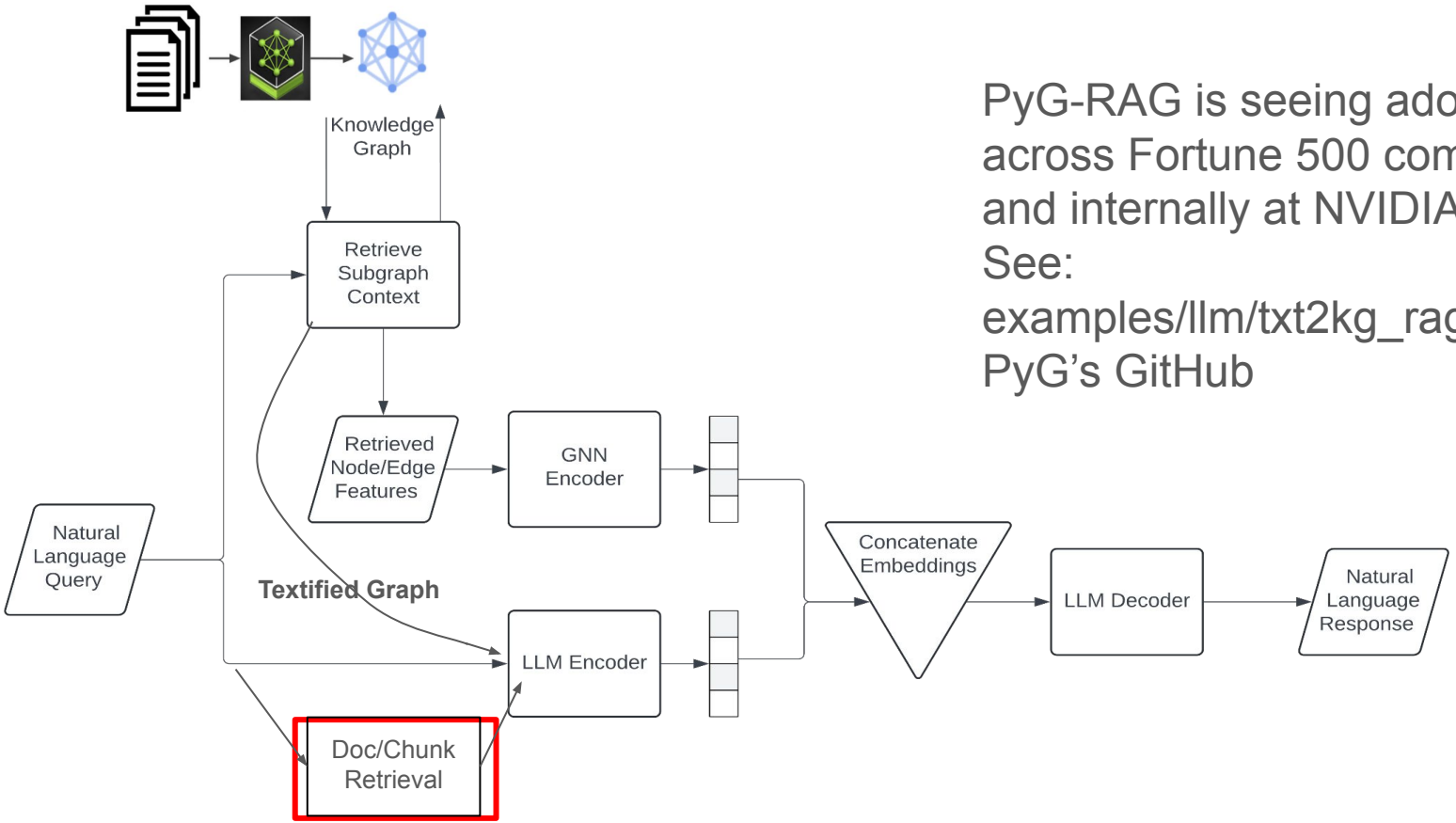
TXT2KG Class in PyG

- Released in PyG 2.7
- Prompt engineering + python filters

```
SYSTEM_PROMPT = "Please convert the above \
text into alist of knowledge triples with the form \
('entity', 'relation', 'entity'). \
Seperate each with a new line. \
Do not output anything else. \
Try to focus on key triples \
that form a connected graph. \
Try to focus on re-using the \
same entities whenever possible.""
```

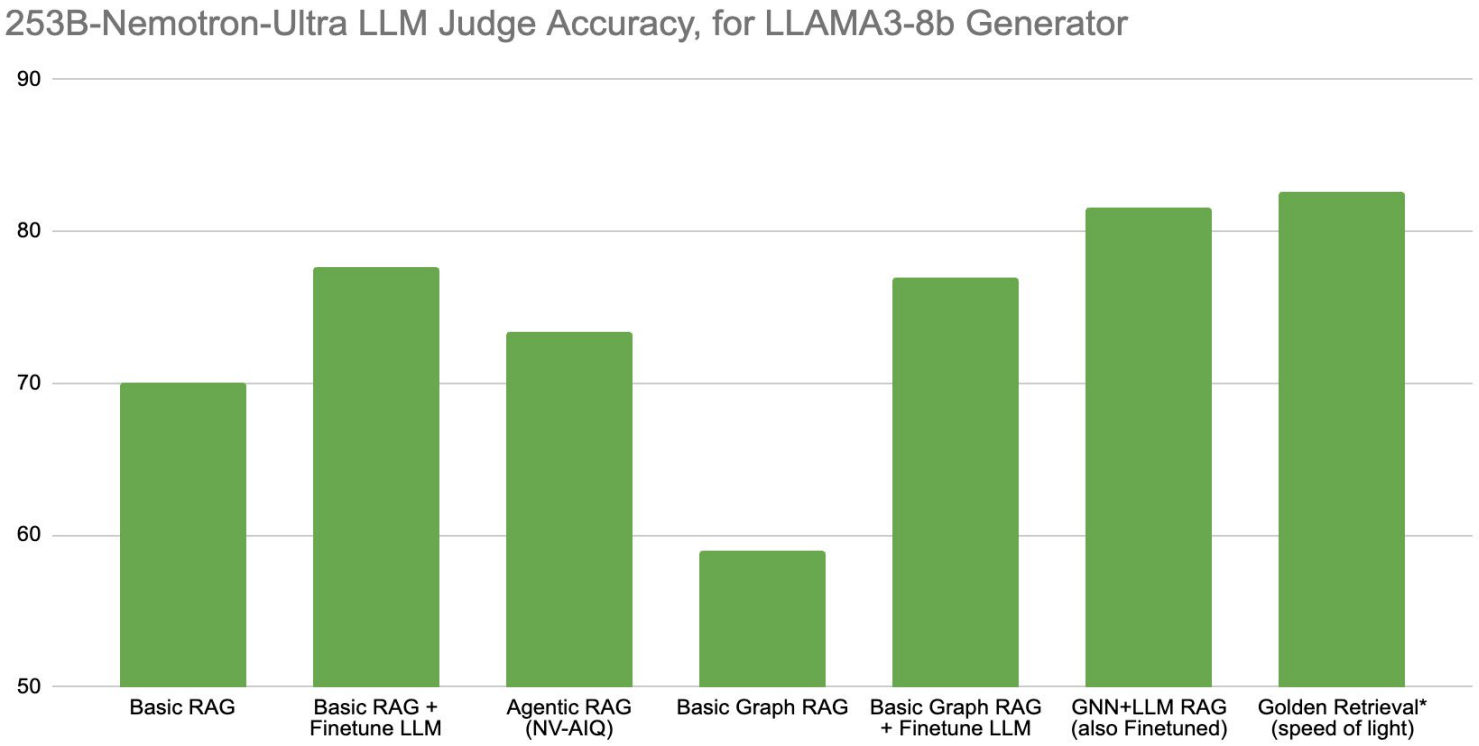
```
for context_doc in tqdm(context_docs, desc="Extracting KG triples"):
    kg_maker.add_doc_2_KG(txt=context_doc)
```

GraphRAG+VectorRAG (PyG-RAG)(torch_geometric.llm)



PyG-RAG is seeing adoption across Fortune 500 companies and internally at NVIDIA!!
See: examples/llm/txt2kg_rag.py on PyG's GitHub

Accuracy on Multi-Hop Synthetic Q & A for Lecture Corpus



*253b Nemotron for TXT2KG.

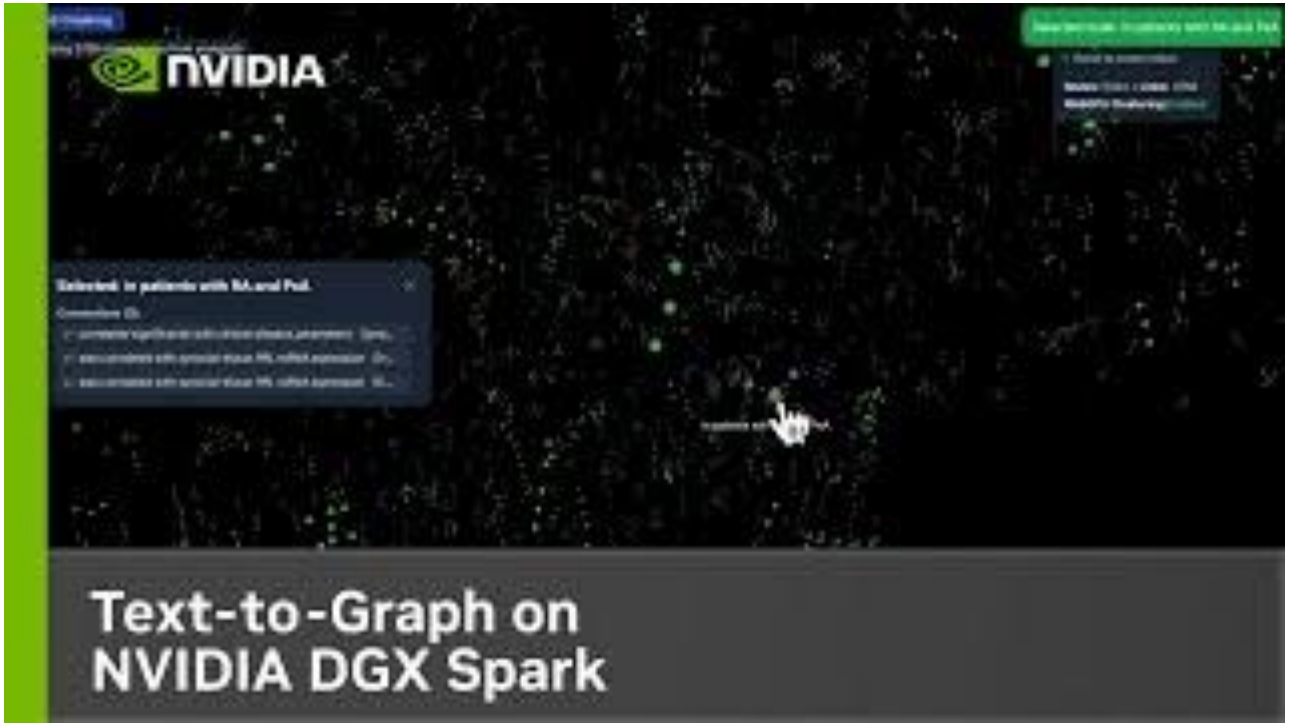
*ModernBert for vector embeddings.

*Feed generator same docs used to generate synthetic Q&A pairs.

Synthetic Q n A made with [NVIDIA TrueQuery]

Vibe Coded GUI

- PyG Codebase is easy to build with
  - Example: Our PM Santosh Bhavani Vibe Coded a GUI using Cursor
- https://build.nvidia.com/spark/txt2kg



Next Steps

- Continued improvements of codebase…
  - Speed, usability, accuracy, understandability, etc
- Accelerate retrieval w/ CuGraph+CuVs
  - Scale up to and beyond trillion edges
- Align TXT2KG w/ KGGen: https://github.com/stair-lab/kg-gen
- More modalities and interesting new problems to solve…
- New retrieval techniques

More Modalities…

- Idea of GNN embeddings to prefix Transformer/LLM is highly general…

Scientific GNN+LLM Community Sprint (Biology/Chemistry)

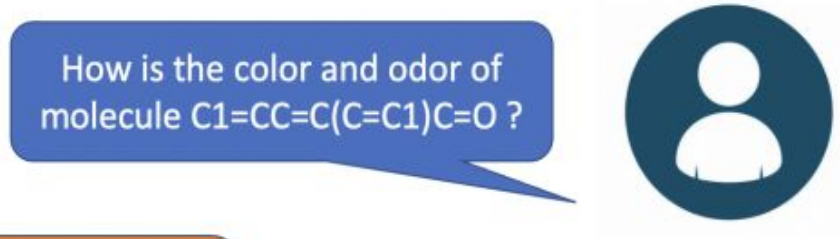
- Goal: Add GNN+LLM support for the sciences like biology and chemistry
- 3 Biology papers & 1 Chemistry paper
- General goal: advance medicine and science
- see examples/llm/README.md on PyG GitHub or NVIDIA Container

Example: MoleculeGPT

- “Talk to your Molecule” (GNN+LLM)

PyG Example link:

MoleculeGPT Paper link:



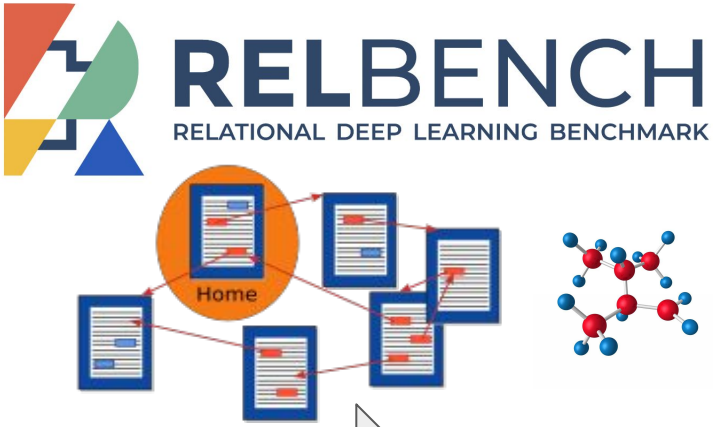
Qformer Paper:

More Modalities…

- Idea of GNN embeddings to prefix sequence prompt is highly general
  - Ex 1: Graphs = molecule/cell/etc, NLP task=Bio/Chem/Drug Discovery
  - Ex 2: Graphs = customer data, NLP task=talk to customer data
  - Ex 3: Graphs = docs w hyperlinks, NLP task=talk to docs
- Imagine graphs that include multiple modalities.
- Ex:
  - Amazon products, where each node has a text review and a photo
  - Relational Database heterographs as seen in RelBench*/Kumo.ai*
  - Node features could be:
    - Text: Natural Language or Code
    - Images
    - Audio
    - Video
    - Molecule/Cell/etc embeddings

* https://relbench.stanford.edu/
* https://kumo.ai/

Unstructured vs Structured Graph Data



- Less Accurate
- They Likely cover different knowledge
- Most enterprises have multiple
- Combine:
  - Separate GNN per Graph Type
- Highly Accurate

Graph Transformers vs Message Passing (Future)

- Today 2 Kinds of GNN:
  - Message Passing (traditional)
  - Graph Transformer (newer)
- More Graph Transformers Coming Soon to PyG
  - Future Goal: See how effects accuracy of previously discussed GNN+LLM systems

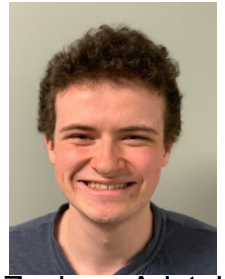
Webinar:

Conclusion

- General AI rule: Data is King!
- Ex: Even the best model can’t learn on randomly labeled data
- Key Takeaway:
  - Structured Data(GNN) + Unstructured Data(LLM) = Better GenAI
- Built & Optimized for NVIDIA PyG container
  - https://catalog.ngc.nvidia.com/orgs/nvidia/containers/pyg
- Stay tuned to LinkedIn for new updates

Acknowledgements


Serge Panev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And all the PyG contributors: https://github.com/pyg-team/pytorch_geometric/graphs/contributors

Thank You!