Stanford CS224W: Towards Foundation Models for Knowledge Graphs

CS224W: Machine Learning with Graphs

Charilaos Kanatsoulis and Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Announcements

- Homework 3 due **today**
  - Gradescope submissions close at 11:59 PM
- Exam opens in one week
  - Ed post soon about Exam Recitation
- Colab 5: **will be released today**
  - **Due Thurs 12/5**

Stanford CS224W: Foundation Models

CS224W: Machine Learning with Graphs

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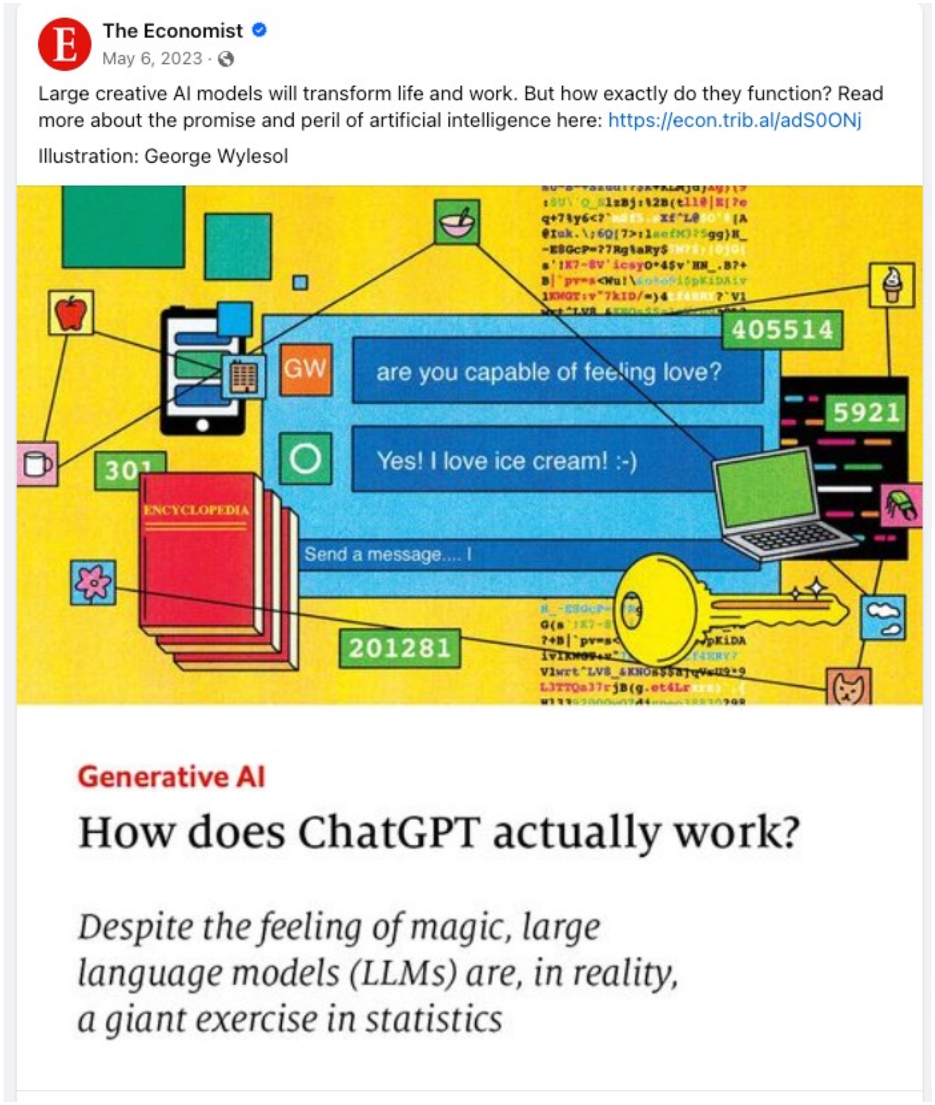
Large Language Models



The Economist
May 6, 2023

Large creative AI models will transform life and work. But how exactly do they function? Read more about the promise and peril of artificial intelligence here: https://econ.trib.al/adS0ONj

Illustration: George Wylesol

Generative AI

How does ChatGPT actually work?

Despite the feeling of magic, large language models (LLMs) are, in reality, a giant exercise in statistics

Language Models are Few-Shot Learners

Tom B. Brown* Benjamin Mann* Nick Ryder* Melanie Subbiah*
Jared Kaplan† Prafulla Dhariwal Arvind Neelakantan Pranav Shyam Girish Sastry
Amanda Askell Sandhini Agarwal Ariel Herbert-Voss Gretchen Krueger Tom Henighan
Rewon Child Aditya Ramesh Daniel M. Ziegler Jeffrey Wu Clemens Winter
Christopher Hesse Mark Chen Eric Sigler Mateusz Litwin Scott Gray
Benjamin Chess Jack Clark Christopher Berner
Sam McCandlish Alec Radford Ilya Sutskever Dario Amodei

OpenAI

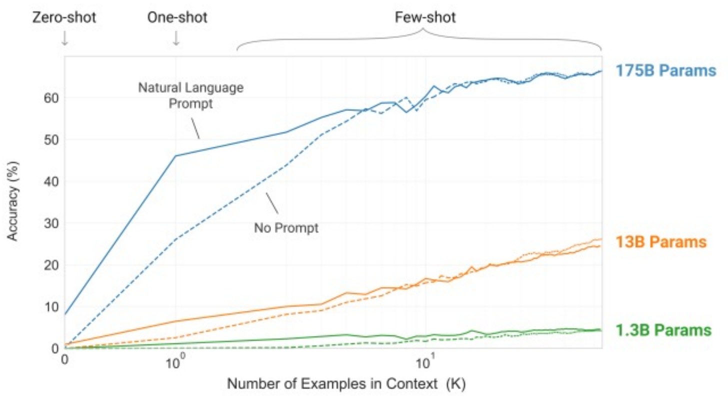


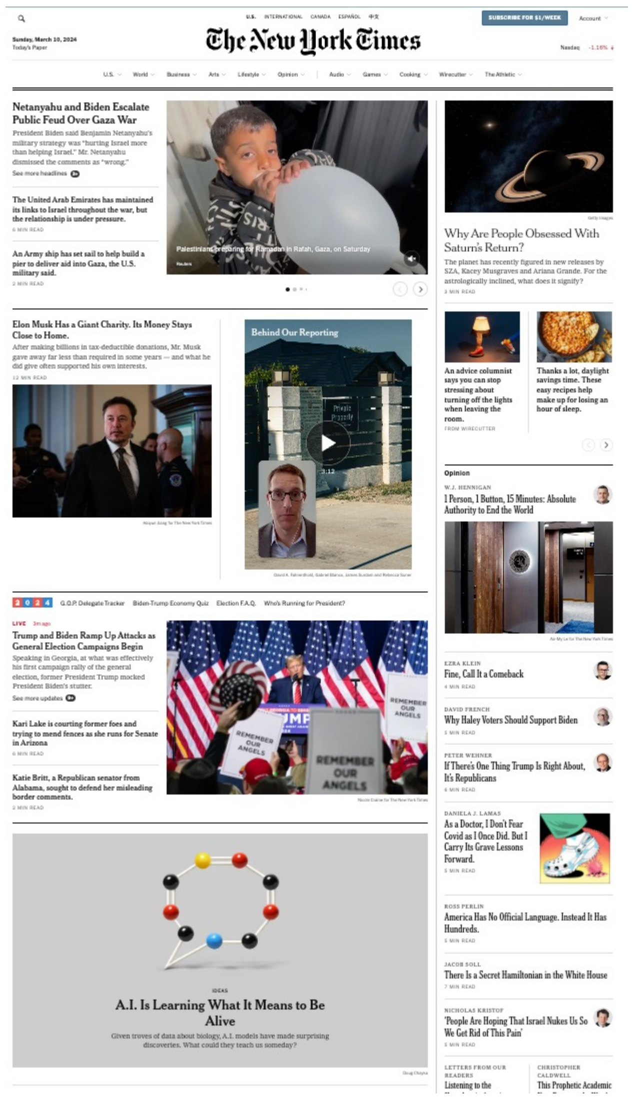
Figure 1.2: Larger models make increasingly efficient use of in-context information. We show in-context learning performance on a simple task requiring the model to remove random symbols from a word, both with and without a natural language task description (see Sec. 3.9.2). The steeper "in-context learning curves" for large models demonstrate improved ability to learn a task from contextual information. We see qualitatively similar behavior across a wide range of tasks.

Foundation Models for Comp. Vision

Figure 1. A building foundation — **Image: DALLE 2**

Source: https://medium.com/@tenyks_blogger/the-foundation-models-reshaping-computer-vision-b299a91527fb

Foundation Models for Biology



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Nasdaq -1.16%

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Netanyahu and Biden Escalate Public Feud Over Gaza War
President Biden said Benjamin Netanyahu's military strategy was "hurting Israel more than helping Israel." Mr. Netanyahu dismissed the comments as "wrong."
See more headlines

The United Arab Emirates has maintained its links to Israel throughout the war, but the relationship is under pressure.
6 MIN READ

An Army ship has set sail to help build a pier to deliver aid into Gaza, the U.S. military said.
2 MIN READ

Palestinians preparing for Ramadan in Rafah, Gaza, on Saturday
Reuters

Getty Images

Why Are People Obsessed With Saturn's Return?
The planet has recently figured in new releases by SZA, Kacey Musgraves and Ariana Grande. For the astrologically inclined, what does it signify?
3 MIN READ

Elon Musk Has a Giant Charity. Its Money Stays Close to Home.
After making billions in tax-deductible donations, Mr. Musk gave away far less than required in some years — and what he did give often supported his own interests.
12 MIN READ

Haiyun Jiang for The New York Times

Behind Our Reporting

3:12

David A. Fahrenthold, Gabriel Blanco, James Surdam and Rebecca Suner

An advice columnist says you can stop stressing about turning off the lights when leaving the room.
FROM WIRECUTTER

Thanks a lot, daylight savings time. These easy recipes help make up for losing an hour of sleep.

Opinion

W.J. HENNIGAN
1 Person, 1 Button, 15 Minutes: Absolute Authority to End the World

An-My Le for The New York Times

2024 G.O.P. Delegate Tracker Biden-Trump Economy Quiz Election F.A.Q. Who's Running for President?

LIVE 3m ago
Trump and Biden Ramp Up Attacks as General Election Campaigns Begin
Speaking in Georgia, at what was effectively his first campaign rally of the general election, former President Trump mocked President Biden's stutter.
See more updates

Kari Lake is courting former foes and trying to mend fences as she runs for Senate in Arizona
6 MIN READ

Katie Britt, a Republican senator from Alabama, sought to defend her misleading border comments.
2 MIN READ

Nicole Craine for The New York Times

EZRA KLEIN
Fine, Call It a Comeback
4 MIN READ

DAVID FRENCH
Why Haley Voters Should Support Biden
5 MIN READ

PETER WEHNER
If There's One Thing Trump Is Right About, It's Republicans
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DANIELA J. LAMAS
As a Doctor, I Don't Fear Covid as I Once Did. But I Carry Its Grave Lessons Forward.
5 MIN READ

ROSS PERLIN
America Has No Official Language. Instead It Has Hundreds.
5 MIN READ

JACOB SOLL
There Is a Secret Hamiltonian in the White House
7 MIN READ

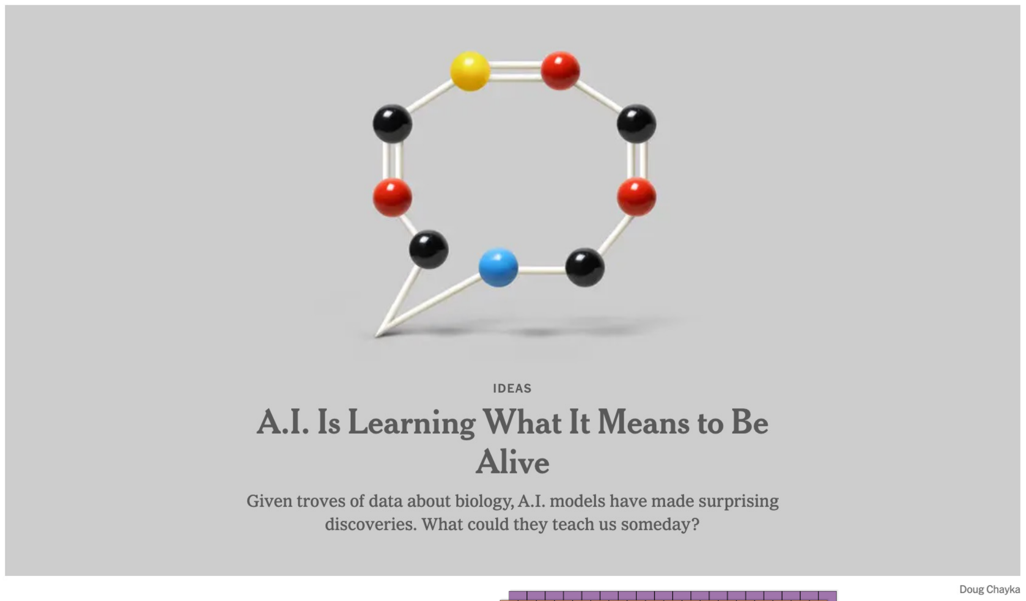
NICHOLAS KRISTOF
'People Are Hoping That Israel Nukes Us So We Get Rid of This Pain'
5 MIN READ

IDEAS
A.I. Is Learning What It Means to Be Alive
Given troves of data about biology, A.I. models have made surprising discoveries. What could they teach us someday?

Doug Chayka

LETTERS FROM OUR READERS
Listening to the

CHRISTOPHER CALDWELL
This Prophetic Academic

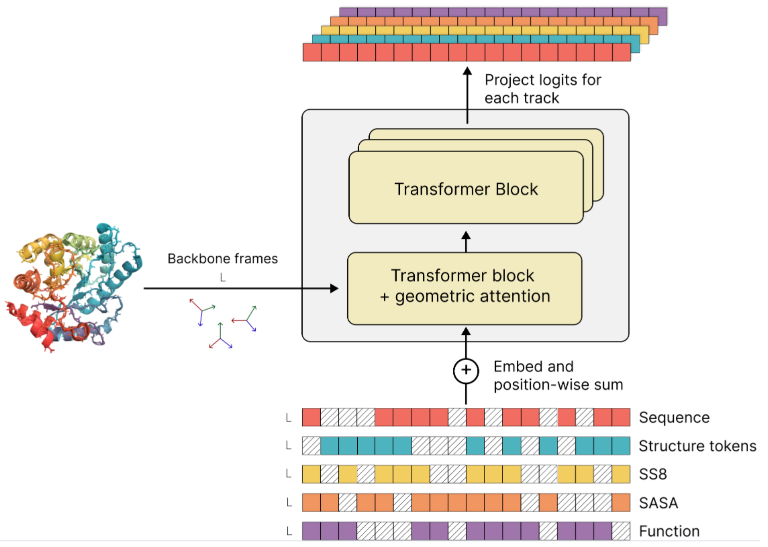


IDEAS

A.I. Is Learning What It Means to Be Alive

Given troves of data about biology, A.I. models have made surprising discoveries. What could they teach us someday?

Doug Chayka


Project logits for each track
Transformer Block
Transformer block + geometric attention
Backbone frames
L
Embed and position-wise sum
L
Sequence
L
Structure tokens
L
SS8
L
SASA
L
Function

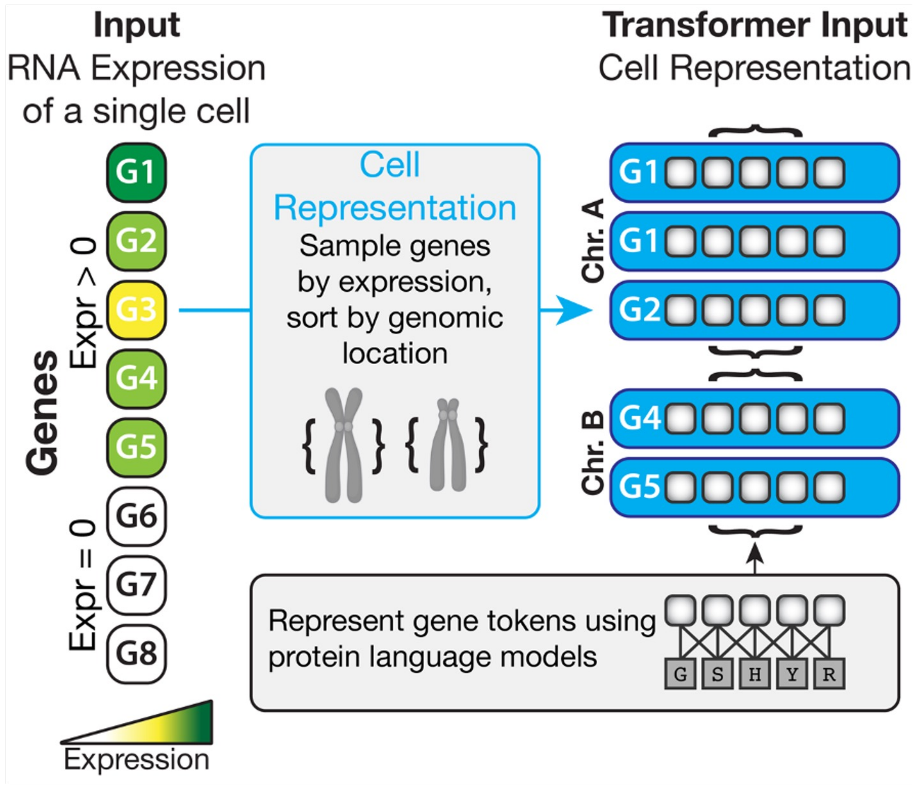
Source: https://github.com/evolutionaryscale/esm

Foundation Models for Cell Biology

- UCE creates universal representations of cells

Input:
RNA expression of a single cell/nucleus

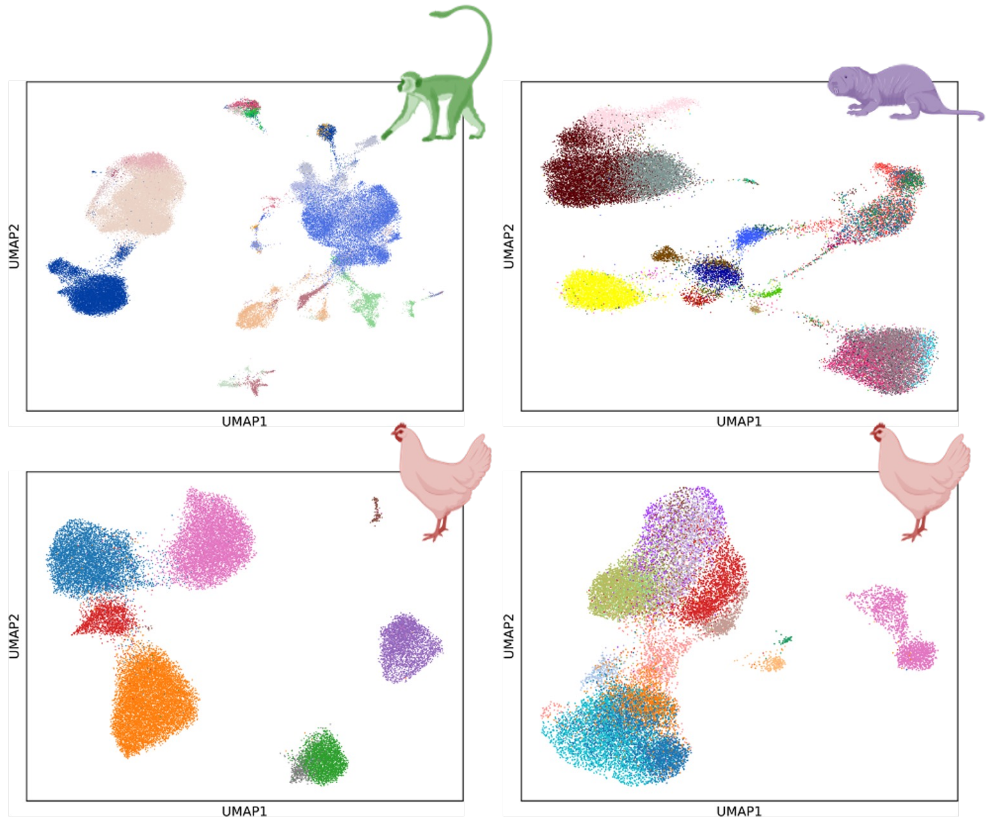
Output:
Cell Embedding



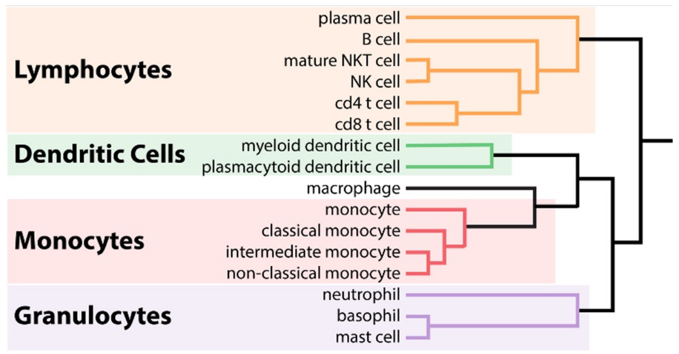
Input
RNA Expression of a single cell
Transformer Input
Cell Representation
Genes
Expr > 0
Expr = 0
G1
G2
G3
G4
G5
G6
G7
G8
Expression
Cell Representation
Sample genes by expression, sort by genomic location
Chr. A
Chr. B
G1
G1
G2
G4
G5
Represent gene tokens using protein language models
G
S
H
Y
R

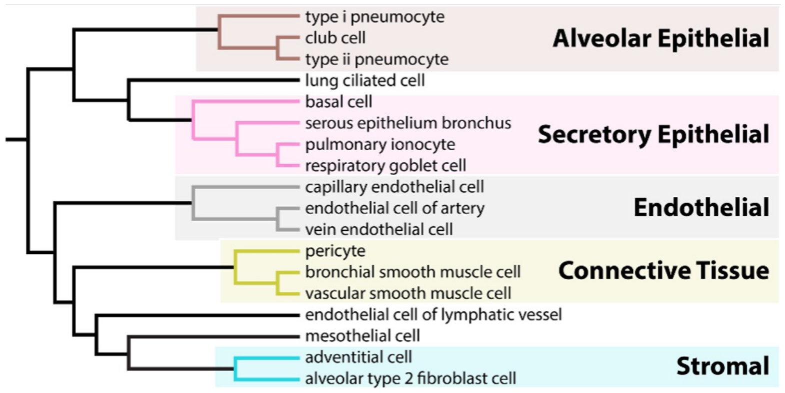
Foundation Models for Cell Biology

Visualize and transfer annotations



Infer Hierarchies





Foundation Models for Medicine

Perspective

Foundation models for generalist medical artificial intelligence

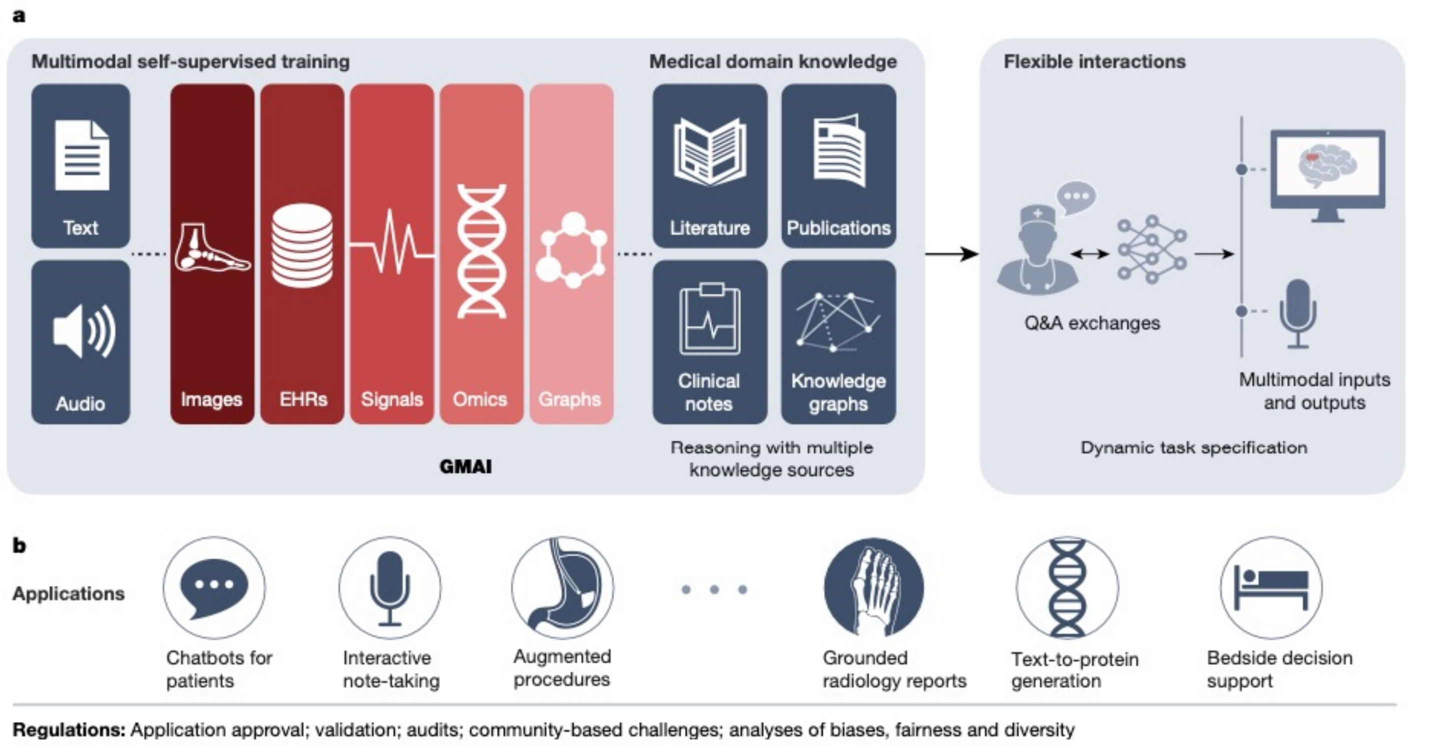
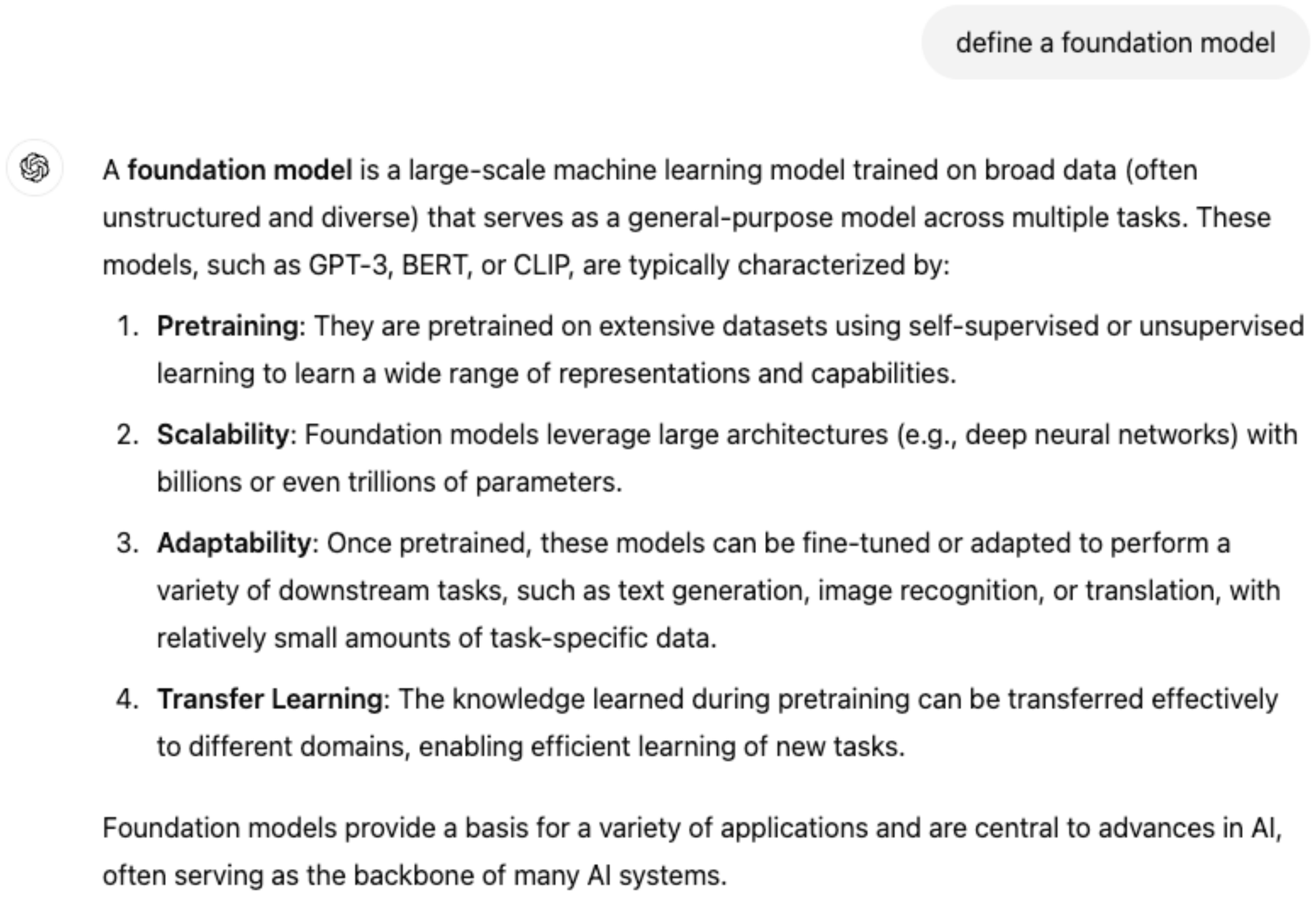

a
Multimodal self-supervised training
Text
Audio
Images
EHRs
Signals
Omics
Graphs
Medical domain knowledge
Literature
Publications
Clinical notes
Knowledge graphs
GMAI
Reasoning with multiple knowledge sources
Flexible interactions
Q&A exchanges
Multimodal inputs and outputs
Dynamic task specification
b
Applications
Chatbots for patients
Interactive note-taking
Augmented procedures
Grounded radiology reports
Text-to-protein generation
Bedside decision support
Regulations: Application approval; validation; audits; community-based challenges; analyses of biases, fairness and diversity

Fig. 1 | Overview of a GMAI model pipeline. a, A GMAI model is trained on multiple medical data modalities, through techniques such as self-supervised learning. To enable flexible interactions, data modalities such as images or data from EHRs can be paired with language, either in the form of text or speech data. Next, the GMAI model needs to access various sources of medical knowledge to carry out medical reasoning tasks, unlocking a wealth of capabilities that can be used in downstream applications. The resulting GMAI model then carries out tasks that the user can specify in real time. For this, the GMAI model can retrieve contextual information from sources such as knowledge graphs or databases, leveraging formal medical knowledge to reason about previously unseen tasks. **b**, The GMAI model builds the foundation for numerous applications across clinical disciplines, each requiring careful validation and regulatory assessment.

Foundation Models



define a foundation model

A **foundation model** is a large-scale machine learning model trained on broad data (often unstructured and diverse) that serves as a general-purpose model across multiple tasks. These models, such as GPT-3, BERT, or CLIP, are typically characterized by:

1. **Pretraining**: They are pretrained on extensive datasets using self-supervised or unsupervised learning to learn a wide range of representations and capabilities.
2. **Scalability**: Foundation models leverage large architectures (e.g., deep neural networks) with billions or even trillions of parameters.
3. **Adaptability**: Once pretrained, these models can be fine-tuned or adapted to perform a variety of downstream tasks, such as text generation, image recognition, or translation, with relatively small amounts of task-specific data.
4. **Transfer Learning**: The knowledge learned during pretraining can be transferred effectively to different domains, enabling efficient learning of new tasks.

Foundation models provide a basis for a variety of applications and are central to advances in AI, often serving as the backbone of many AI systems.

Foundation Models Characteristics

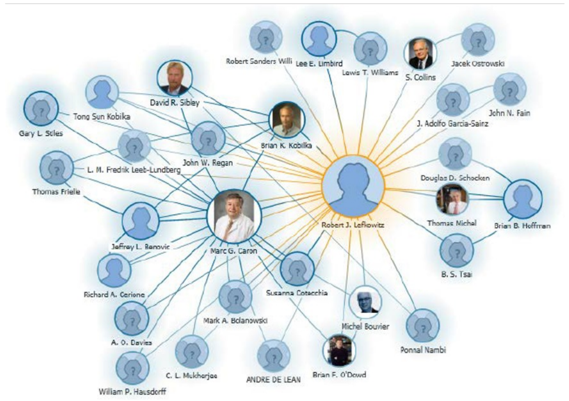
- Foundation models are pretrained architectures
- Modern AI trains very large models with a huge amount of data
- Foundation models can be used as zero-shot or few-shot learners
- They generalize to new entities that have not been observed during training

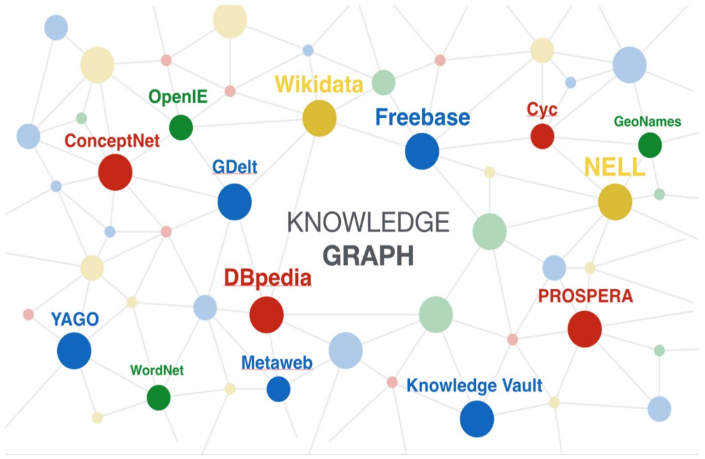
Graph Foundation Models

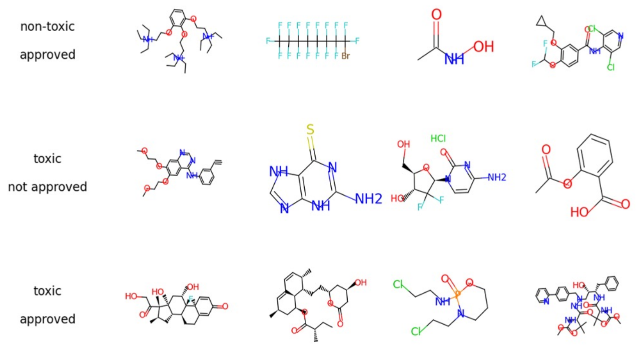
Challenges

- Multiple types of graphs

- Multiple types of tasks

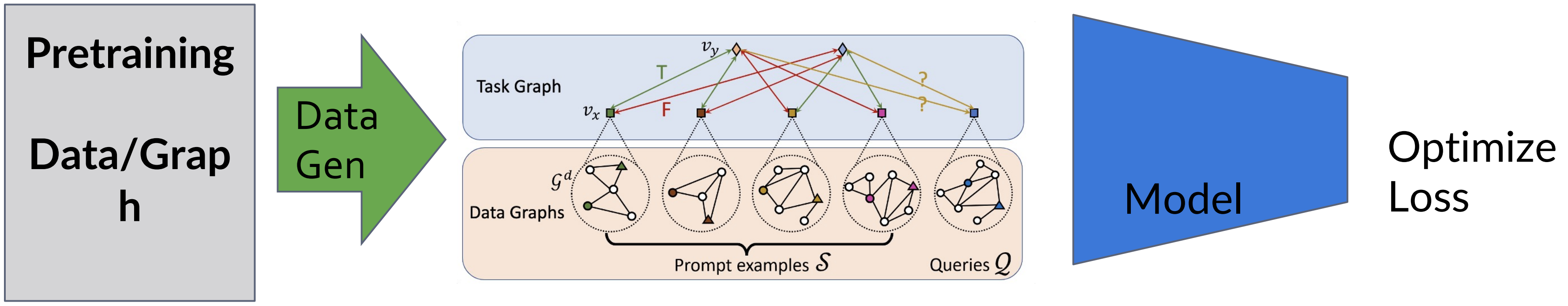






Recap: PRODIGY

- **Unified framework to learn graph tasks of multiple levels**
- **Agnostic of the graph type**



Towards Foundation Models for KGs

- Build a model that learns embeddings for entities and relations of any KG
- The model will be trained in an unsupervised fashion
- The model will transfer knowledge between different KGs
- We will not discuss scalability of the training data and the model

Stanford CS224W: Knowledge Graphs

CS224W: Machine Learning with Graphs
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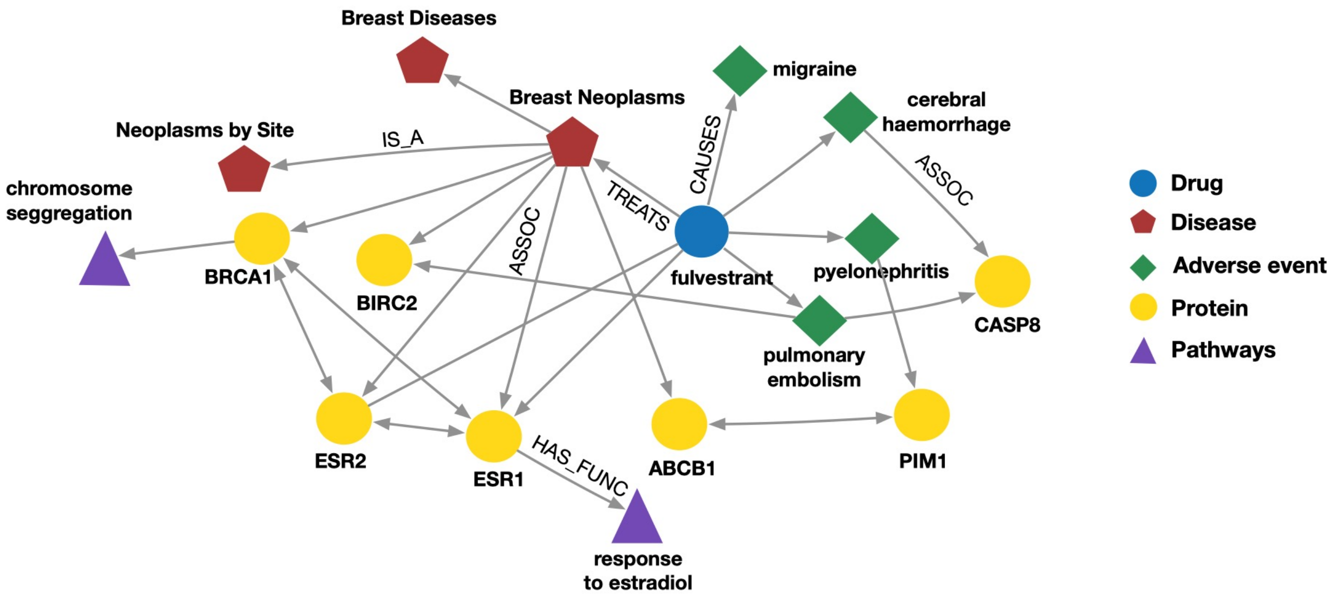
KG Representation

- Edges in KG are represented as **triples** (h, r, t)
  - head (h) has relation (r) with tail (t)
- **Key Idea:**
  - Model entities and relations in embedding space $\mathbb{R}^k$
    - Associate entities and relations with **shallow embeddings**
      - **Note we do not learn a GNN here!**
  - Given a triple (h, r, t), the goal is that the embedding of (h, r) **should be close** to the embedding of t.
    - How to embed (h, r)?
    - How to define score $f_r(h, t)$?
      - Score f_r is high if (h, r, t) exists, else f_r is low

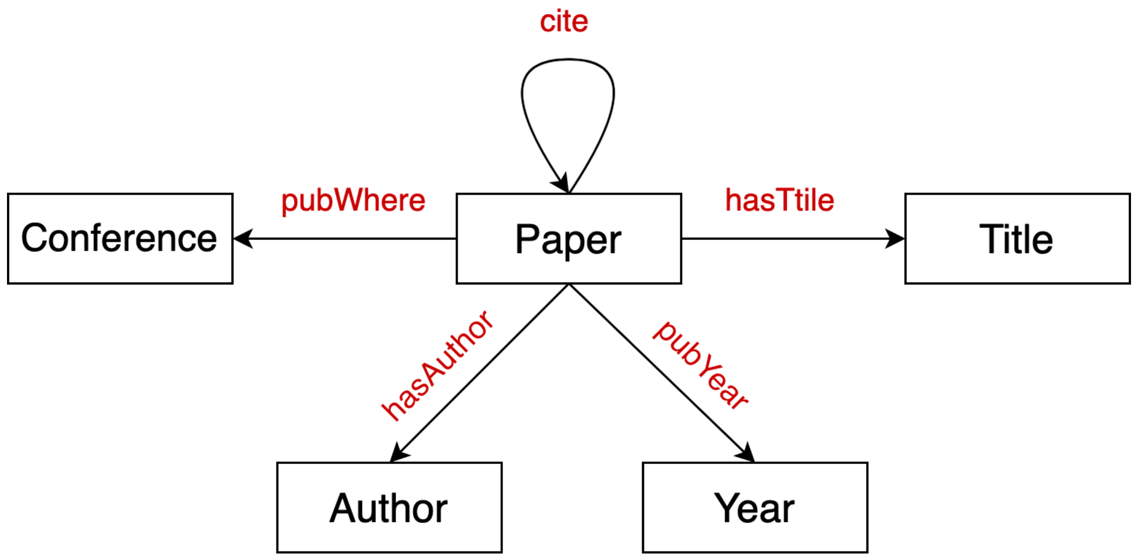
Example: Bio Knowledge Graphs

- **Node types**: drug, disease, adverse event, protein, pathways
- **Relation types**: has_func, causes, assoc, treats, is_a



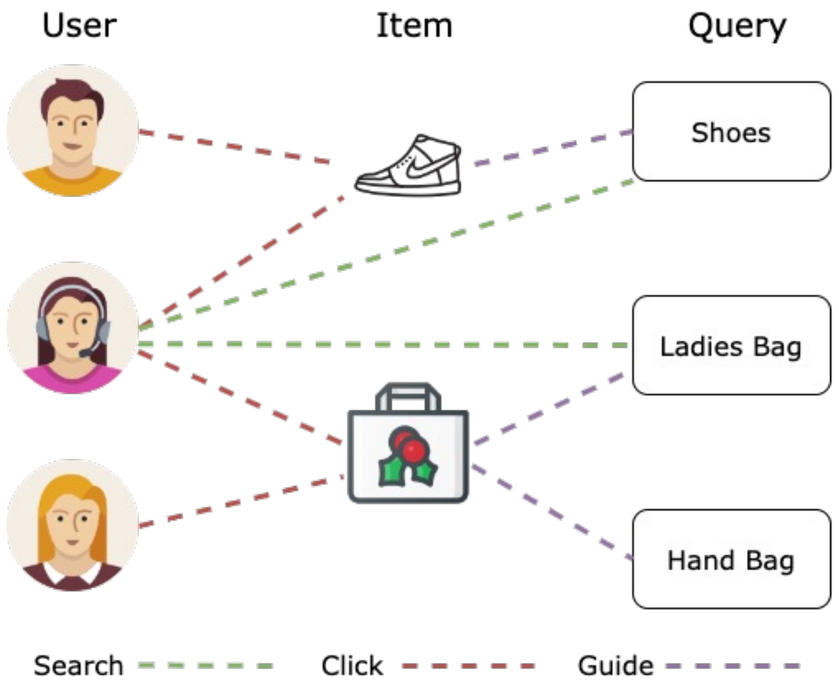
Example: Bibliographic Networks

- **Node types**: paper, title, author, conference, year
- **Relation types**: pubWhere, pubYear, hasTitle, hasAuthor, cite



Example: E-Commerce Networks

- Example: E-Commerce Graph
  - **Node types:** User, Item, Query, Location, ...
  - **Edge types:** Purchase, Visit, Guide, Search, ...
  - Different node type's features spaces can be different!



KG vs Natural Language

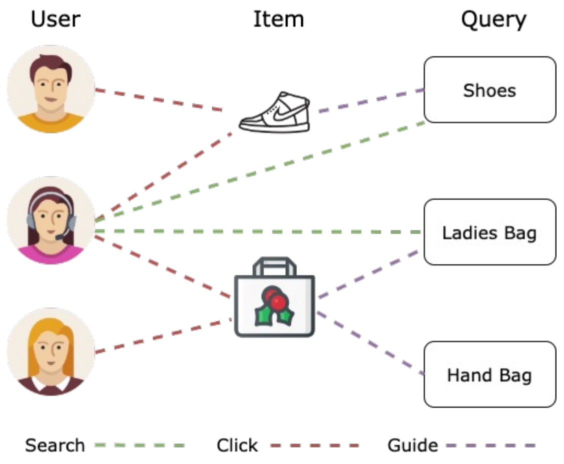
- Example: E-Commerce Graph
  - **Natural Language:**
  - User searches for shoes, User buys hand-bag

KG vs Natural Language

- Example: E-Commerce Graph
  - **Natural Language:**
  - User searches for shoes. User buys hand-bag
  - **All entities are words or tokens of the same type**
    - **Homogeneous vocabulary**
  - **Knowledge Graph:**
    - **User, shoes, hand-bag → entities**
    - **Searches, buys → relations**
    - **Two modalities, heterogeneous vocabulary**

KG vs Natural Language

- Example: E-Commerce Graph
  - **Natural Language:**
  - User searches for shoes. User buys hand-bag
  - **Tokens are connected sequentially**
  - **Knowledge Graph:**
    - **Entities have an underlying arbitrary graph structure**



Towards Foundation Models for KGs

- Build a model that learns embeddings for entities and relations of any KG
  - Double equivariant architectures
- Process the graph structure between entities
  - Use Graph Neural Networks
- Find a canonical task for unsupervised training
  - Knowledge Graph Completion

Stanford CS224W: Transductive Link prediction

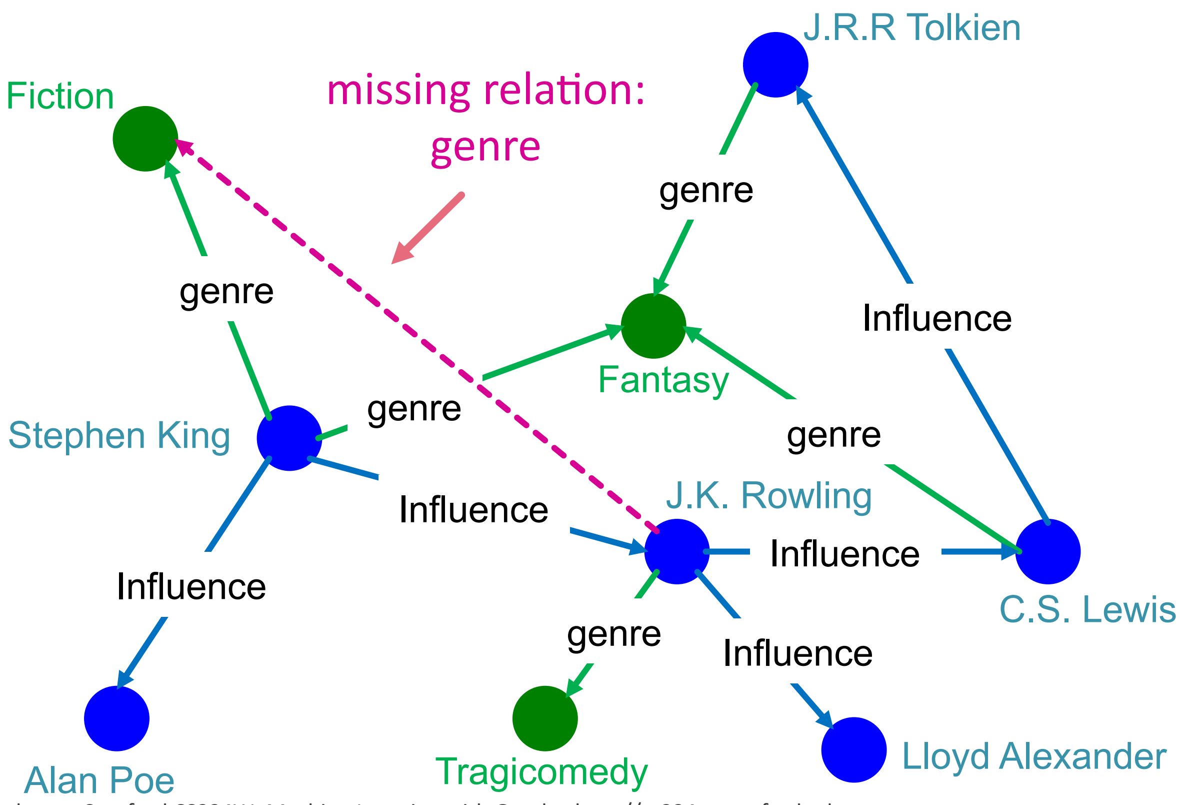
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Recap: KG Completion Task

Given an enormous KG, can we complete the KG?

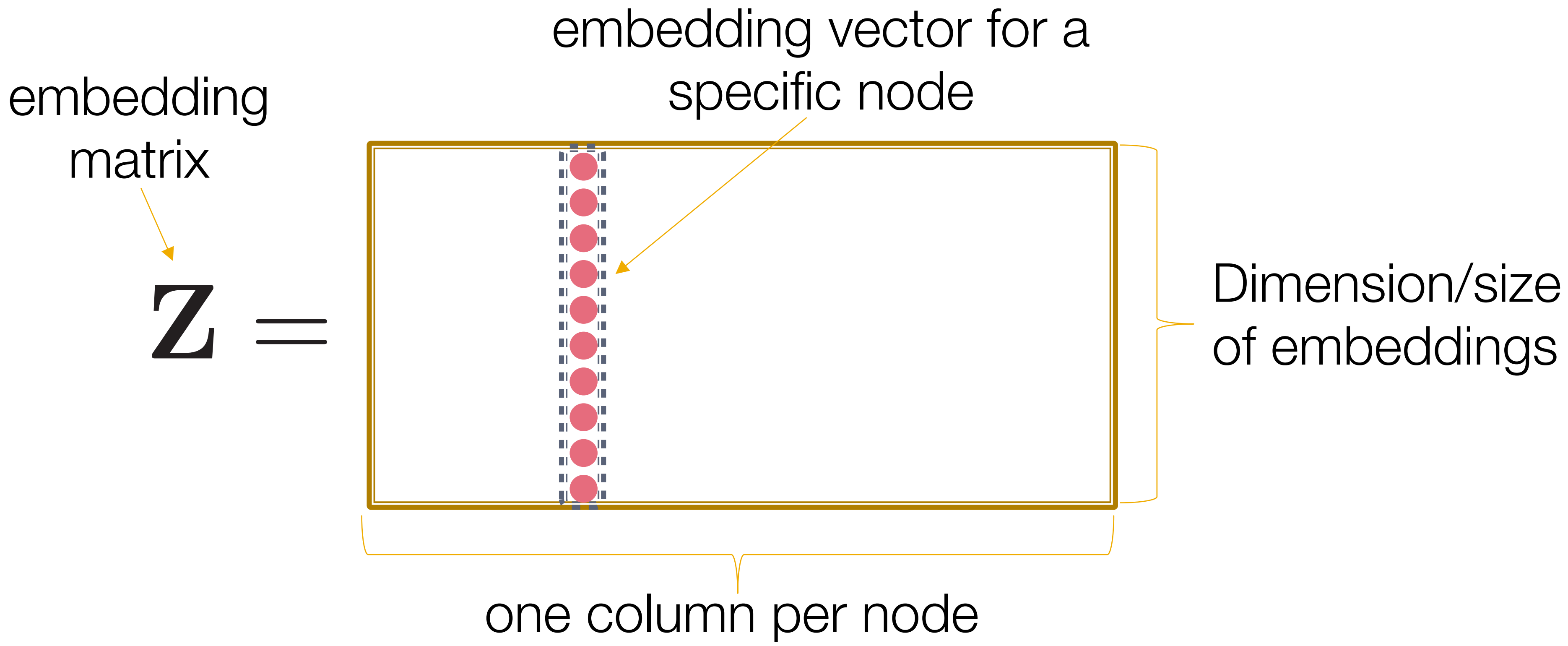
- For a given (**head**, **relation**), we predict missing **tails**.

Example task: predict the tail "Science Fiction" for ("J.K. Rowling", "genre")



Recap: "Shallow" Encoding

- Simplest encoding approach: **encoder is just an embedding-lookup**


embedding matrix
$\mathbf{Z} =$
embedding vector for a specific node
Dimension/size of embeddings
one column per node

Recap: KG Completion Models

KG embedding Models:

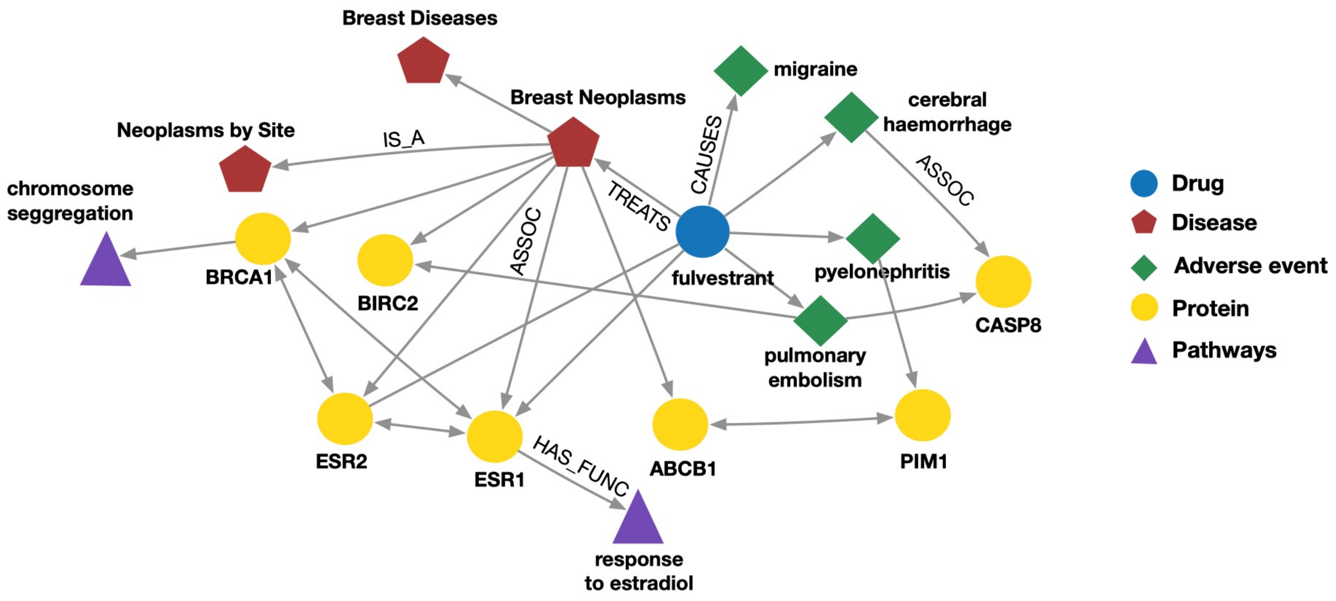
Model	Score	Embedding	Sym.	Antisym.	Inv.	Compos.	1-to-N
TransE	$-\lVert \mathbf{h}+\mathbf{r}-\mathbf{t}\rVert$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{R}^k$	✗	✓	✓	✓	✗
TransR	$-\lVert \boldsymbol{M}_r\mathbf{h}+\mathbf{r} - \boldsymbol{M}_r\mathbf{t}\rVert$	$\mathbf{h},\mathbf{t}\in\mathbb{R}^k$, $\mathbf{r}\in\mathbb{R}^d$, $\boldsymbol{M}_r\in\mathbb{R}^{d\times k}$	✓	✓	✓	✓	✓
DistMult	$<\mathbf{h},\mathbf{r},\mathbf{t}>$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{R}^k$	✓	✗	✗	✗	✓
ComplEx	$\mathrm{Re}(<\mathbf{h},\mathbf{r},\bar{\mathbf{t}}>)$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{C}^k$	✓	✓	✓	✗	✓
RotateE	$-\lVert \mathbf{h}\circ\mathbf{r}-t\rVert$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{C}^k$	✓	✓	✓	✓	✗

KG embedding methods

- Structure agnostic shallow encoders learn embeddings for entities and relations
  - The entity and relation embeddings are the trainable weights
- The structure of the KG is utilized in the loss function
- KG embedding methods can only be used on a single KG
  - They cannot transfer knowledge between KGs

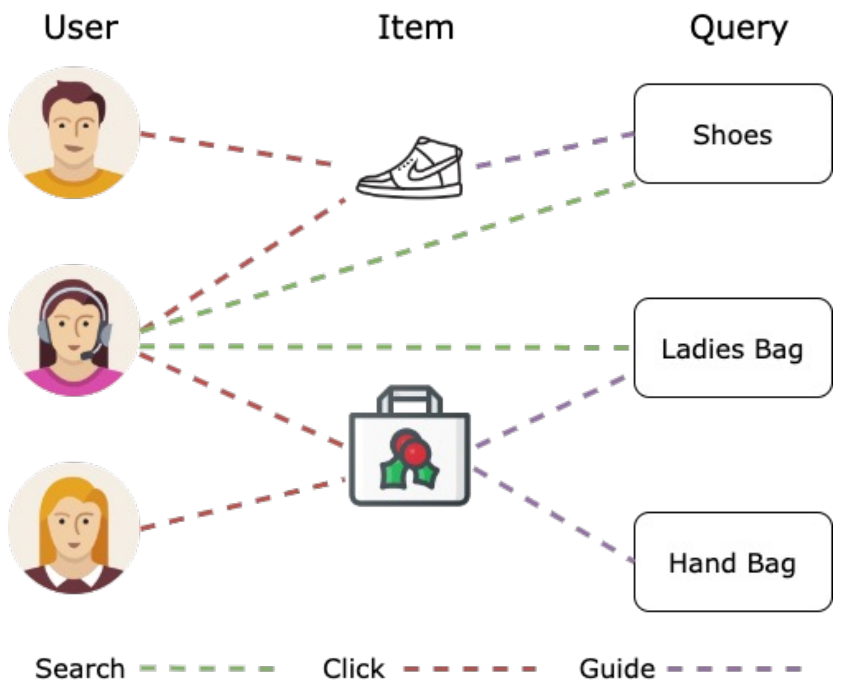
New entities in Bio KGs

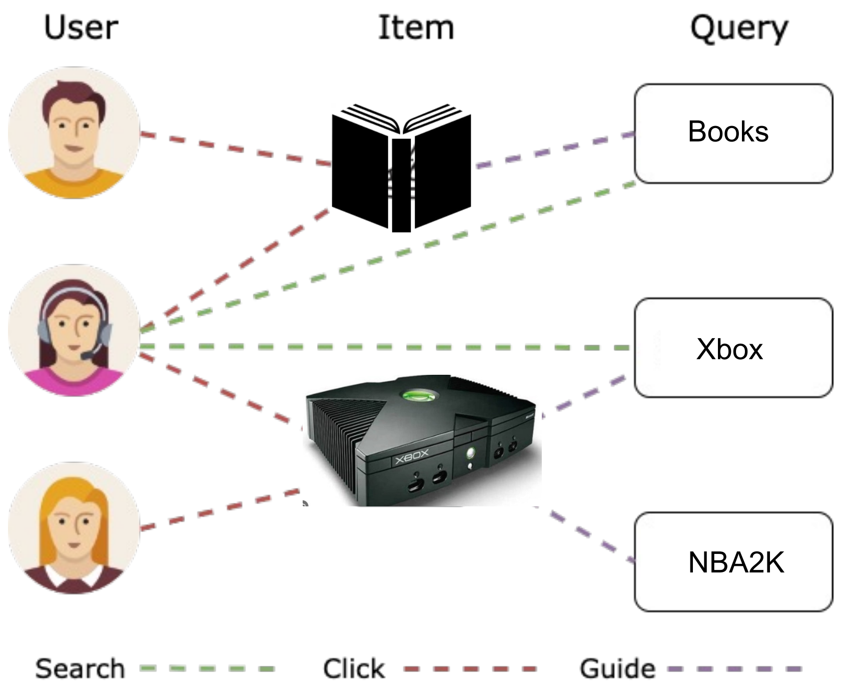
- **What if a new drug comes in?**
- **Need to retrain the shallow encoder**



Generalize across similar KGs

- What if I want to transfer knowledge from one KG to another?
- The KGs have the same relations





Stanford CS224W: Inductive Link prediction

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Generalize across similar KGs

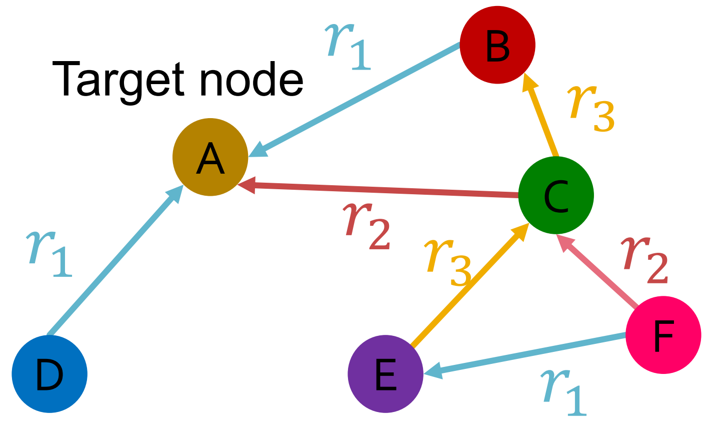
- **What if I want to transfer knowledge from one KG to another?**
- **The KGs have the same relations**

Solution:

- **Observe that a KG is a heterogeneous graph**
- **Use a heterogenous GNN**
  - **E.g., RGCN, Heterogenous Graph Transformer**

Relational GCN

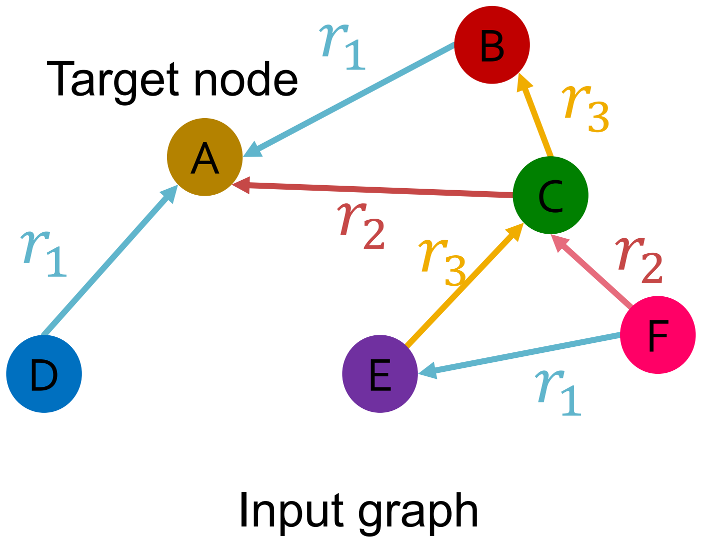
- **What if the graph has multiple relation types?**

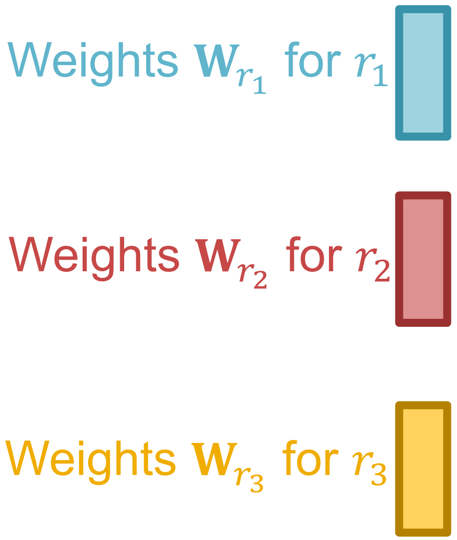


Input graph

Relational GCN (2)

- **What if the graph has multiple relation types?**
- Use different neural network weights for different relation types.

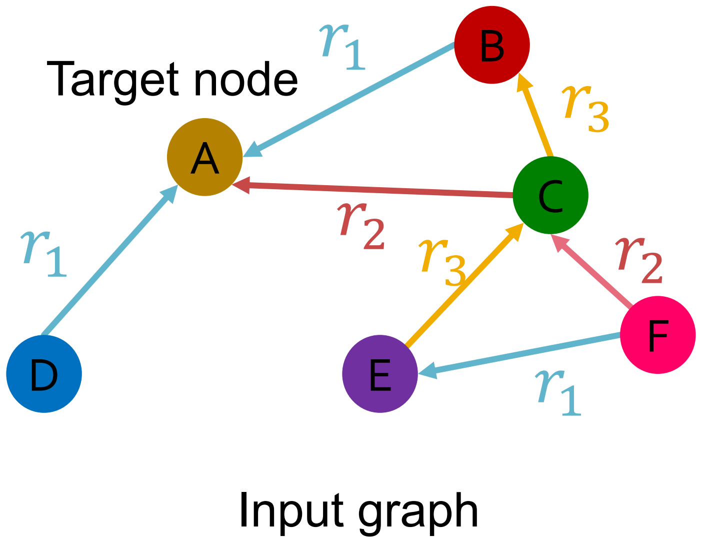


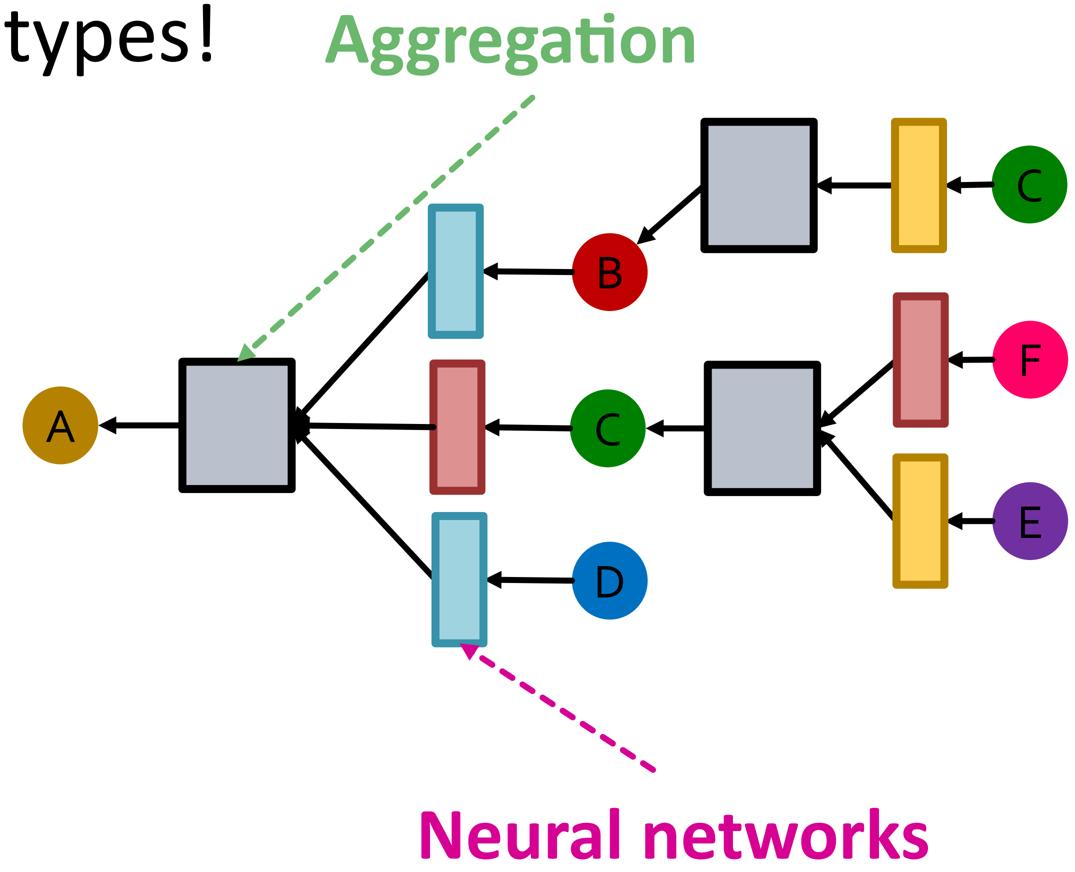


Weights $\mathbf{W}_{r_1}$ for r_1
Weights $\mathbf{W}_{r_2}$ for r_2
Weights $\mathbf{W}_{r_3}$ for r_3

Relational GCN (3)

- **What if the graph has multiple relation types?**
- Use different neural network weights for different relation types!





Kipf and Welling. Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017

Recap: Classical GNN Layers: GCN

- **(1) Graph Convolutional Networks (GCN)**

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}\right)$$

- **We add a self-loop**

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|} + \mathbf{W}^{(l)} \mathbf{h}_v^{(l-1)}\right)$$

Relational GCN (4)

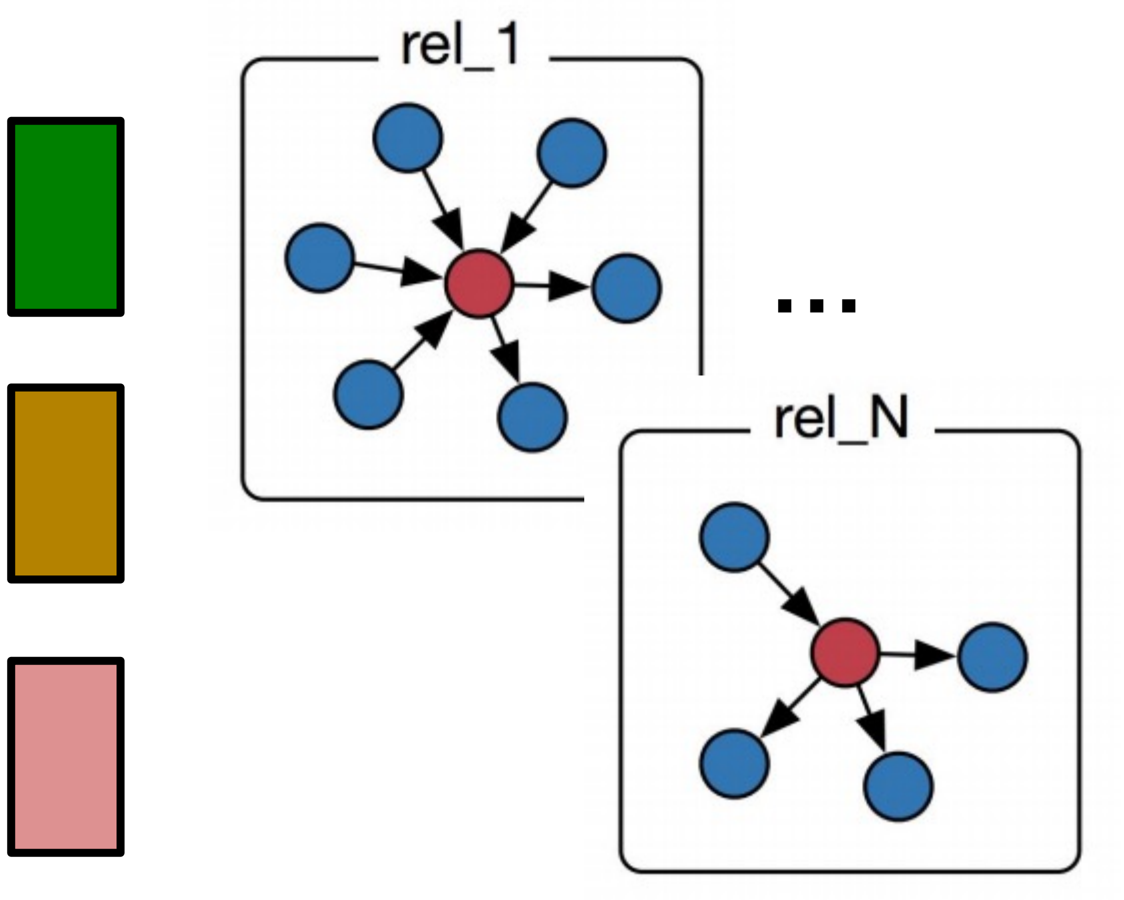
- Introduce a set of neural networks for each relation type!

Weight for rel_1

...

Weight for rel_N

Weight for self-loop



Relational GCN: Definition

- **Relational GCN (RGCN):**

$$\mathbf{h}_v^{(l+1)} = \sigma\left(\sum_{r\in R}\sum_{u\in N_v^r}\frac{1}{c_{v,r}}\mathbf{W}_r^{(l)}\mathbf{h}_u^{(l)} + \mathbf{W}_0^{(l)}\mathbf{h}_v^{(l)}\right)$$

- **How to write this as Message + Aggregation?**
- **Message:**
  - Each neighbor of a given relation:

$$\mathbf{m}_{u,r}^{(l)} = \frac{1}{c_{v,r}}\mathbf{W}_r^{(l)}\mathbf{h}_u^{(l)}$$

Normalized by node degree of the relation $c_{v,r} = |N_v^r|$

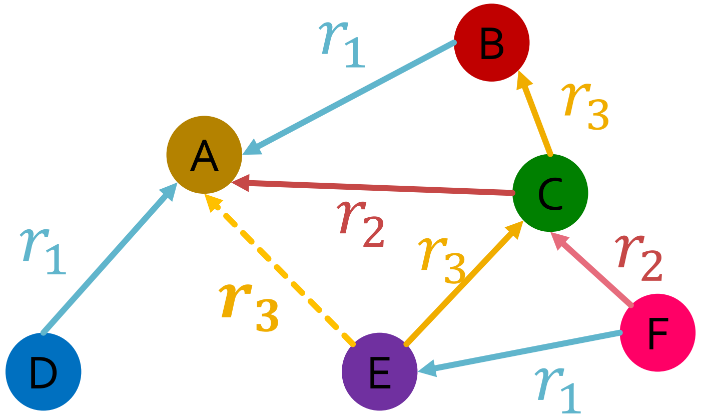
  - Self-loop:

$$\mathbf{m}_v^{(l)} = \mathbf{W}_0^{(l)}\mathbf{h}_v^{(l)}$$

- **Aggregation:**
  - Sum over messages from neighbors and self-loop, then apply activation
  - $\mathbf{h}_v^{(l+1)} = \sigma\left(\mathrm{Sum}\left(\left\{\mathbf{m}_{u,r}^{(l)}, u \in N(v)\right\} \cup \left\{\mathbf{m}_v^{(l)}\right\}\right)\right)$

RGCN for Link Prediction (1)

- **Assume (E, r_3, A) is training supervision edge, all the other edges are training message edges**
- **Use RGCN to score (E, r_3, A)!**
  - Take the final layer of E and A: $\mathbf{h}_E^{(L)}$ and $\mathbf{h}_A^{(L)} \in \mathbb{R}^d$
  - Relation-specific score function $f_r: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$
    - One example $f_{r_3}(\mathbf{h}_E, \mathbf{h}_A) = \mathbf{h}_E^T \mathbf{W}_{r_3} \mathbf{h}_A,\ \mathbf{W}_{r_3} \in \mathbb{R}^{d \times d}$



Input Graph

Heterogeneous GNNs

- Structure aware GNN encoders learn embeddings for entities
- Structure agnostic shallow encoders learn embeddings for relations
  - The relation embeddings are trainable weights
- The structure of the KG is also utilized in the loss function
- RGCN can be used for inductive link prediction across new entities
  - It cannot transfer knowledge between KGs with different relation types

Stanford CS224W: Inductive Link prediction for new entity and relation types

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Generalize across different KGs

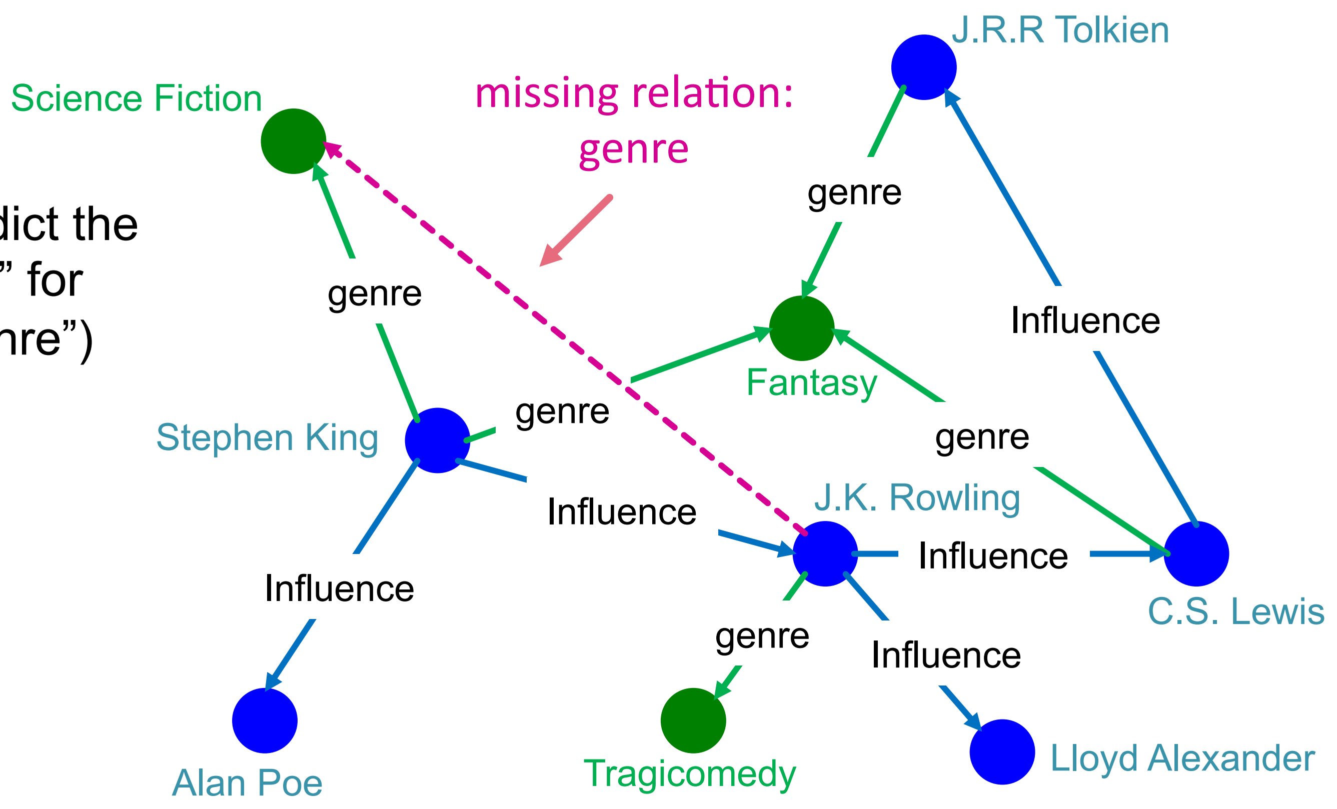
- **What if I want to transfer knowledge from one KG to another?**
- **The KGs have different entities and relations**

Recap: KG Completion Task

Given a KG, we train a model such that:

- For a given (**head**, **relation**), we predict missing **tails**.

Example task: predict the tail "Science Fiction" for ("J.K. Rowling", "genre")

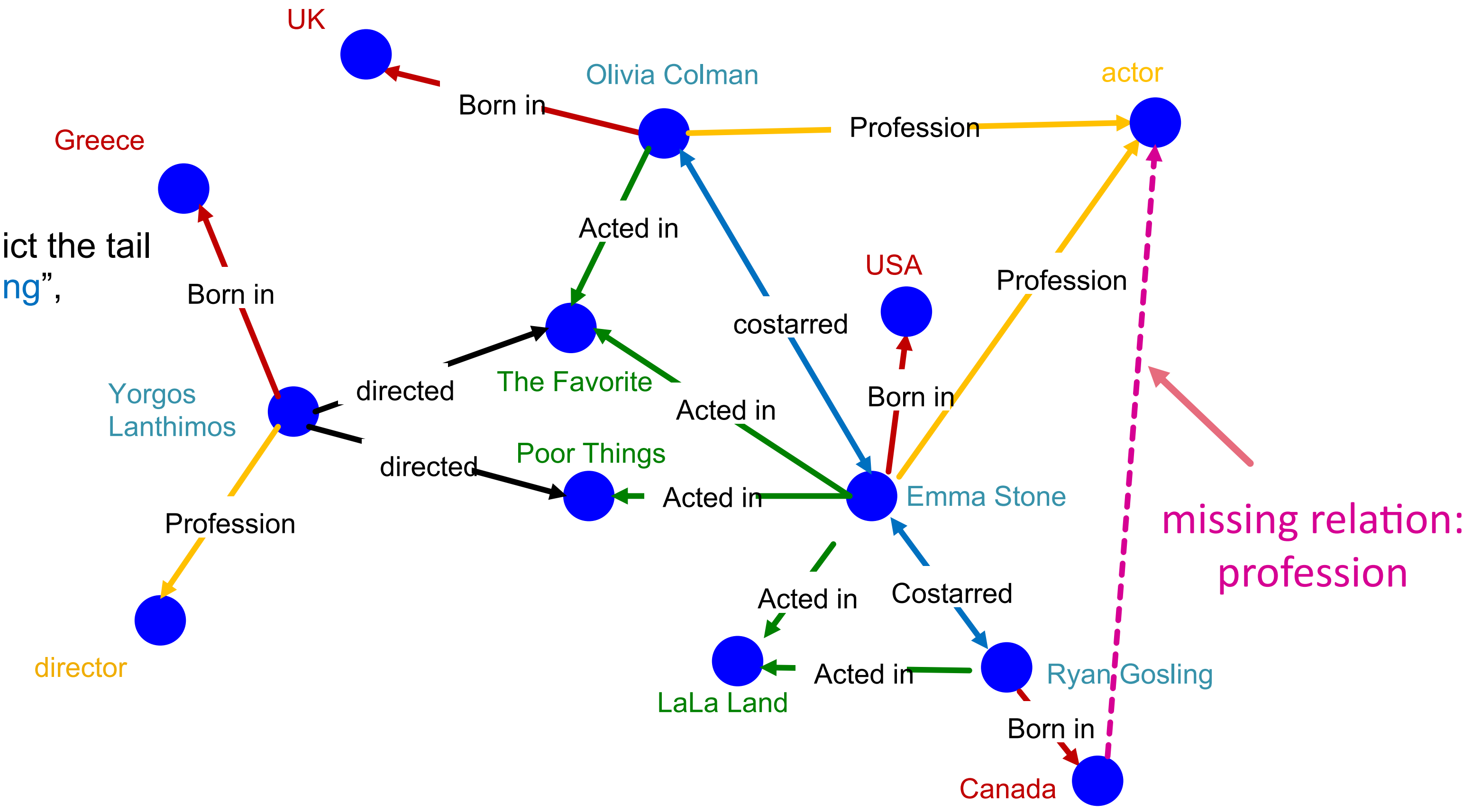


Recap: KG Completion Task

Given a trained model we want:

- For a given (**head**, **relation**), we predict missing **tails**.

Example task: predict the tail "Actor" for ("R. Gosling", "profession")



J. Lee, C. Chung, JJ. Whang, InGram: Inductive Knowledge Graph Embedding via Relation Graphs, ICML 2023

Stanford CS224W: InGram: Inductive KG Embedding via Relation Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Generalize across different KGs

- **What if I want to transfer knowledge from one KG to another?**
- **The KGs have different entities relations**

Solution:

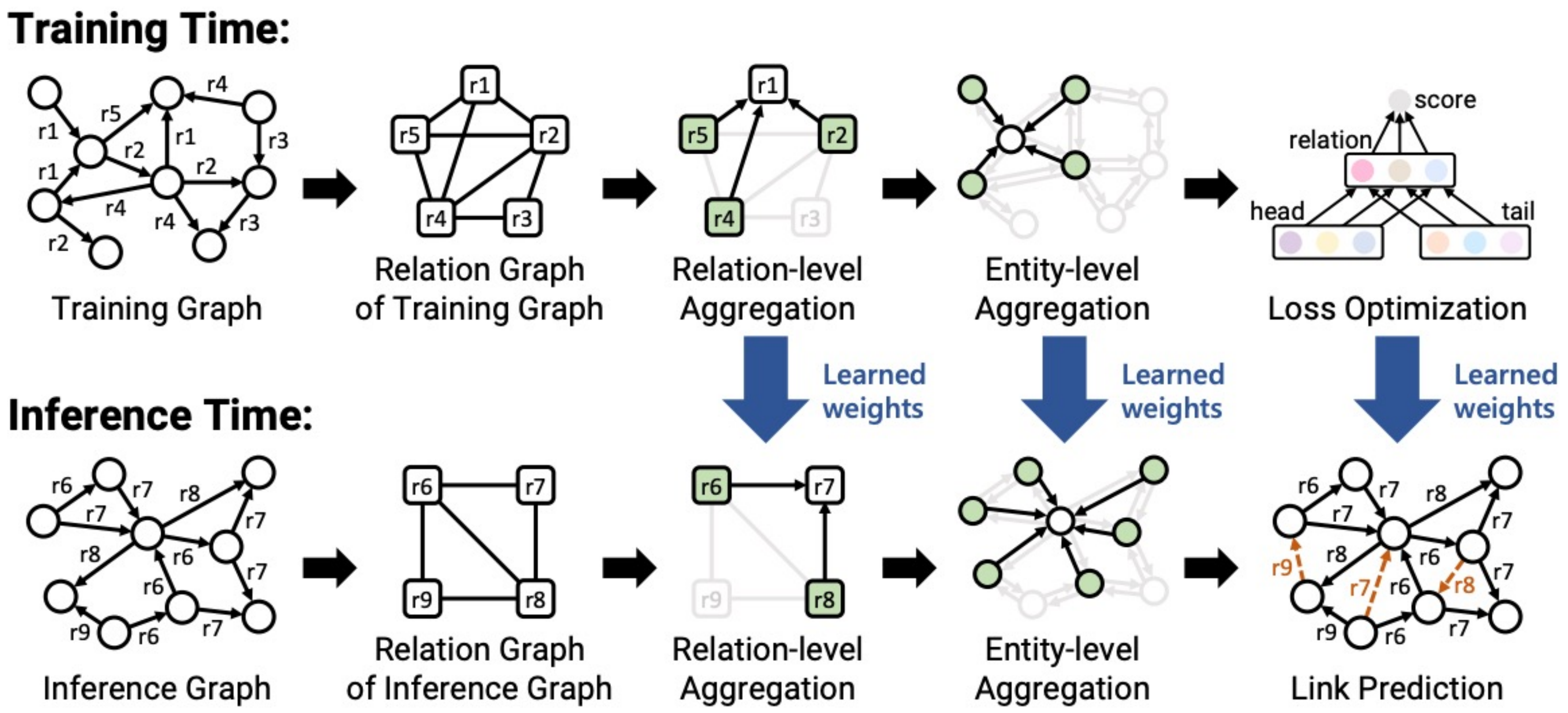
- **Build double equivariant models**
  - **E.g., InGram**

KG embedding methods

- **We achieve inductive link prediction on new entities by:**
  - **Structure agnostic shallow encoders to structure aware GNN encoders to learn embeddings for entities**
  - **The structure of the KG was moved from the loss function to the loss function and the model**
- **Let’s do the same for relations**
  - **Utilize the structure of relations to generate relation embeddings**

J. Lee, C. Chung, JJ. Whang, InGram: Inductive Knowledge Graph Embedding via Relation Graphs, ICML 2023

InGram Model



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- New component: **Relation Graph**

Relation graph

- We define tree **graph matrices**
- A_h: head **entities** **x** **relations** adjacency
  - $A_h[i,j] = 1$ if entity i is head in relation j
- A_t: tail **entities** **x** **relations** adjacency
  - $A_t[i,j] = 1$ if entity i is tail in relation j
- $D_{h,}$ $D_{t,}$: diagonal **entity** **x** **entity** matrices with entity degrees as heads and tails

Relation graph

- Then the **adjacency matrix of relations** is:

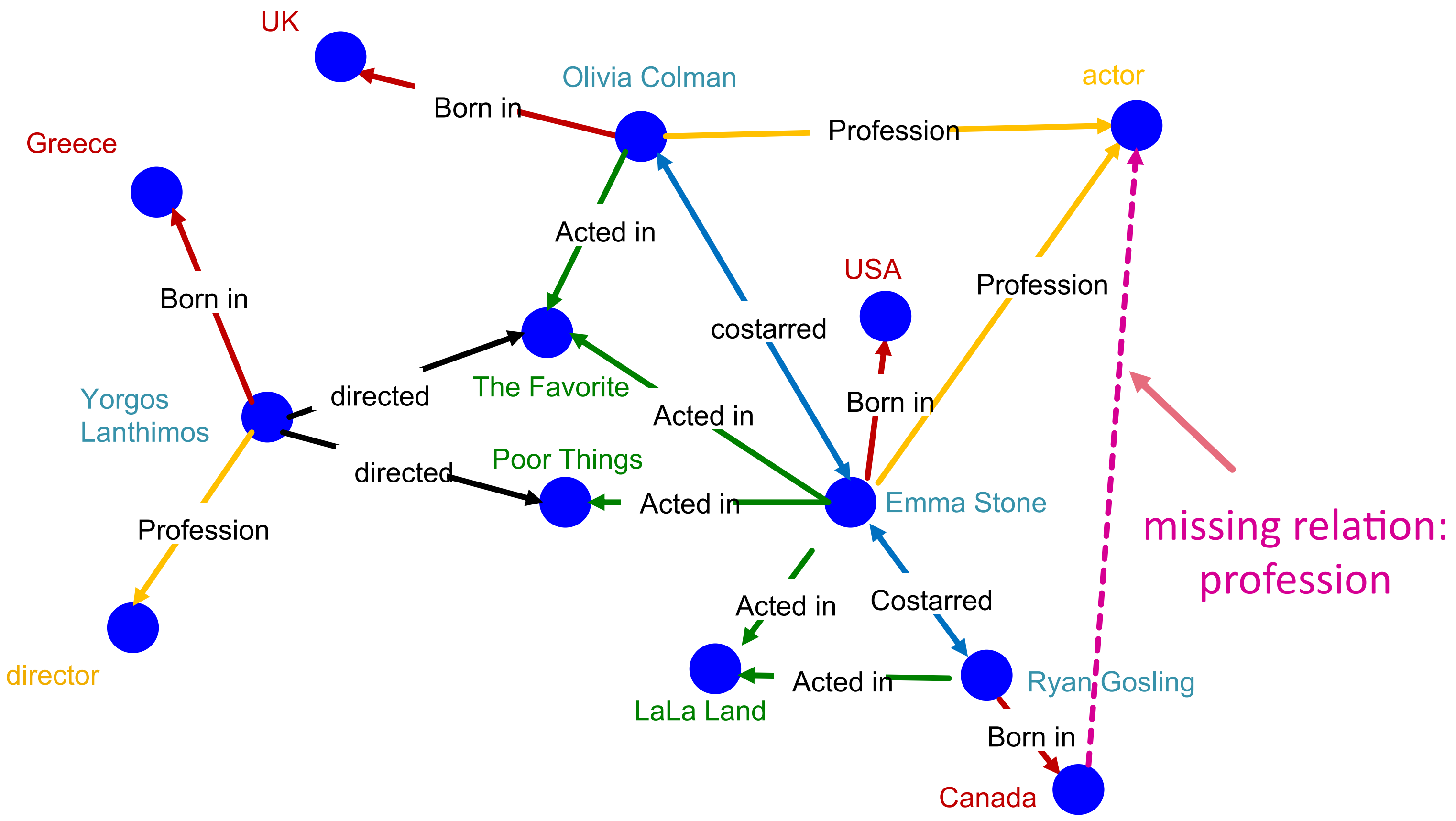
$$\boldsymbol{A} = \boldsymbol{E}_h^\top \boldsymbol{D}_h^{-2} \boldsymbol{E}_h + \boldsymbol{E}_t^\top \boldsymbol{D}_t^{-2} \boldsymbol{E}_t$$

- A is a **weighted adjacency matrix**
  - Every edge has a weight that determines the **importance of the edge**

- **In practice we are looking for entities that serve as heads and/or tails for relation pairs**

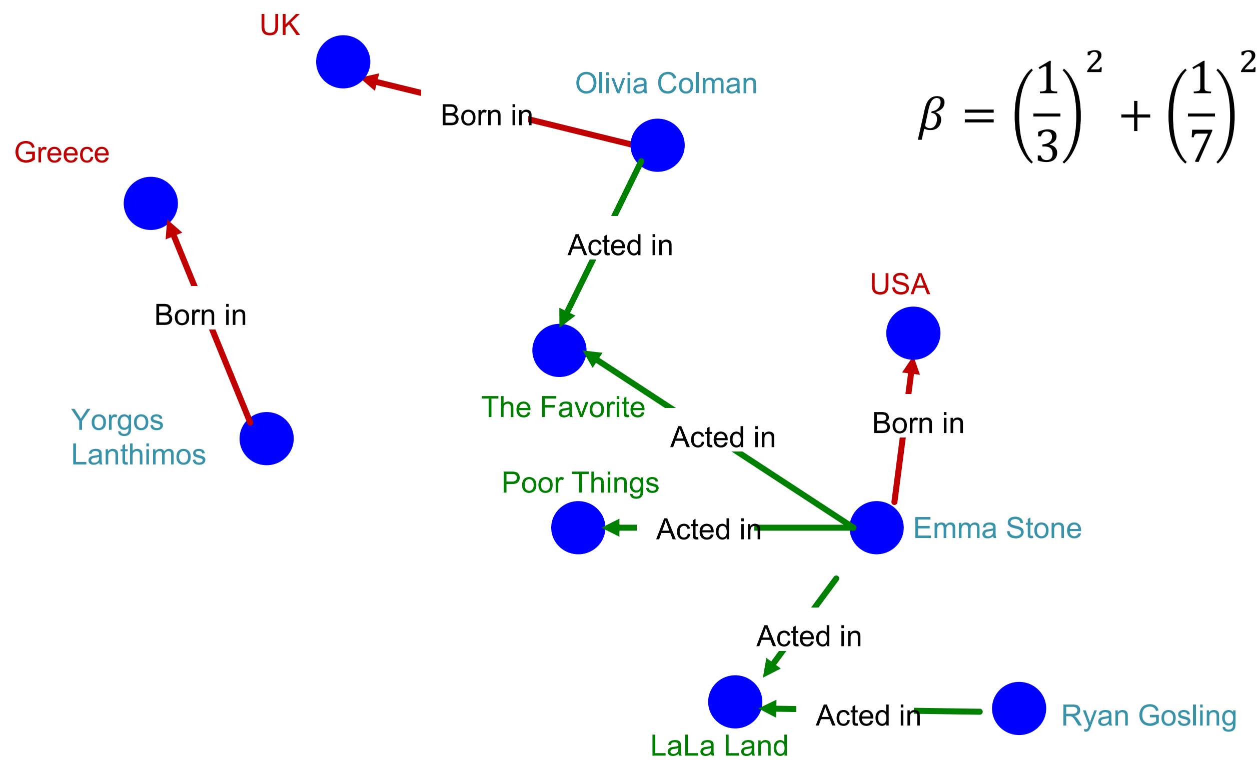
Relation Graph Construction

- **Consider relation pairs**
  - **Find entities that serve as heads and/or tails**



Recap: KG Completion Task

- **Consider relation pairs**
  - **Find entities that serve as heads and/or tails**

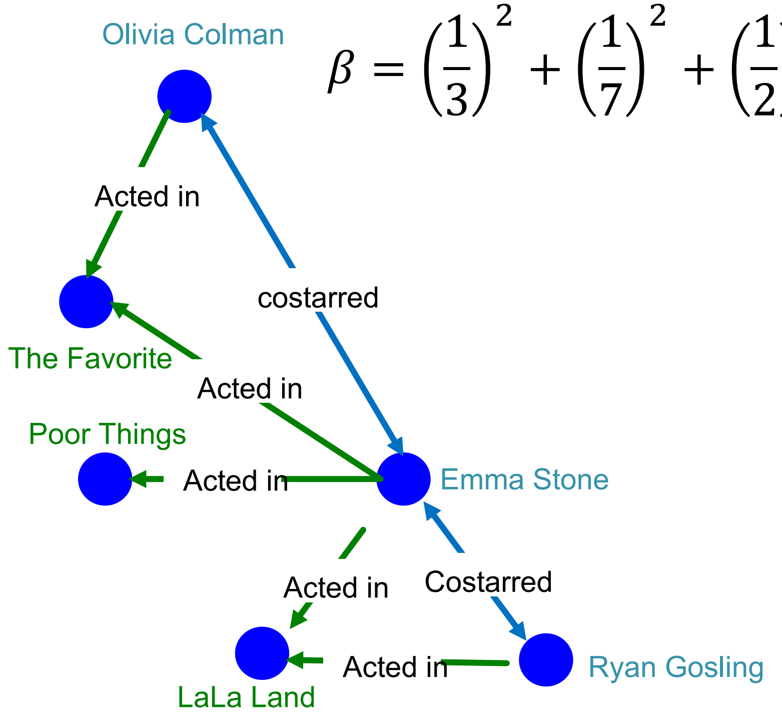


$$\beta = \left(\frac{1}{3}\right)^2 + \left(\frac{1}{7}\right)^2 = 0.13$$

Recap: KG Completion Task

- **Consider relation pairs**
  - **Find entities that serve as heads and/or tails**

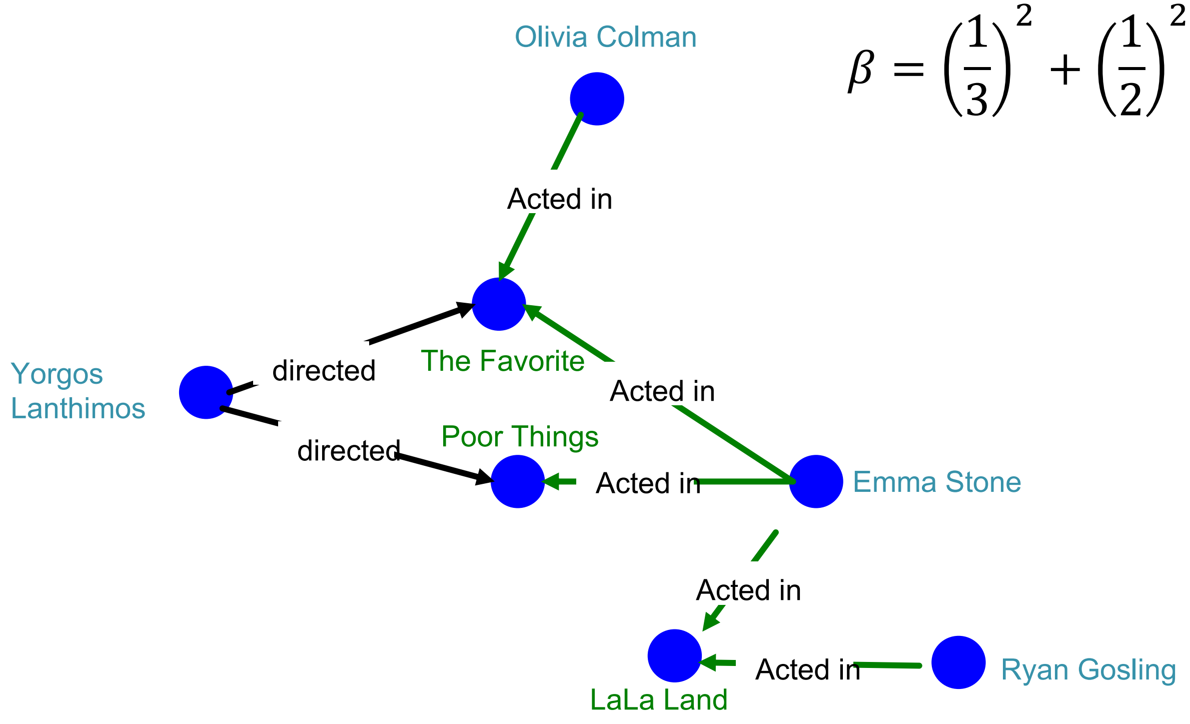
$$\beta = \left(\frac{1}{3}\right)^2 + \left(\frac{1}{7}\right)^2 + \left(\frac{1}{2}\right)^2 = 0.38$$



Recap: KG Completion Task

- **Consider relation pairs**
  - **Find entities that serve as heads and/or tails**

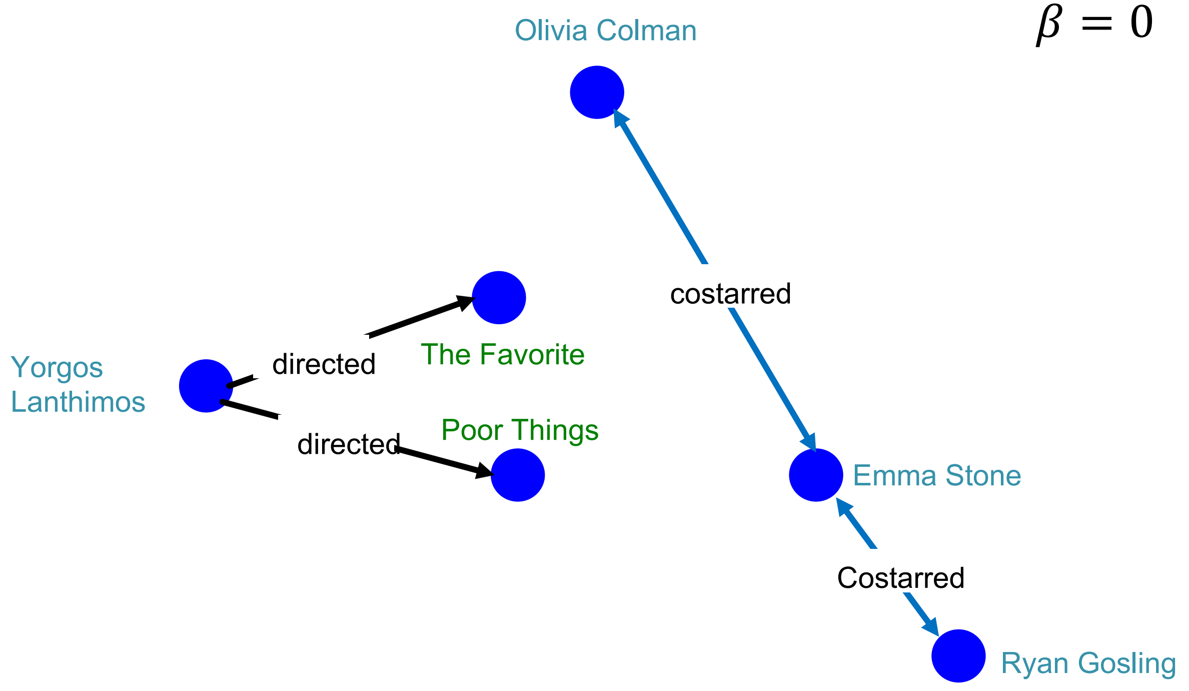
$$\beta = \left(\frac{1}{3}\right)^2 + \left(\frac{1}{2}\right)^2 = 0.36$$



Recap: KG Completion Task

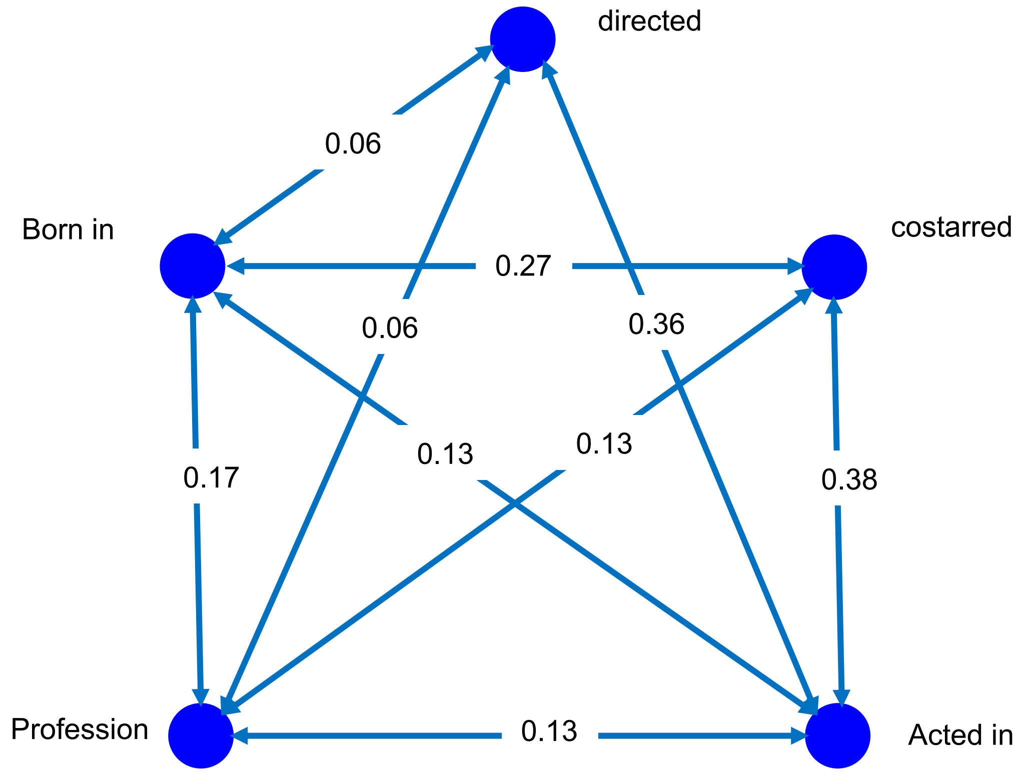
- **Consider relation pairs**
  - **Find entities that serve as heads and/or tails**

$\beta = 0$

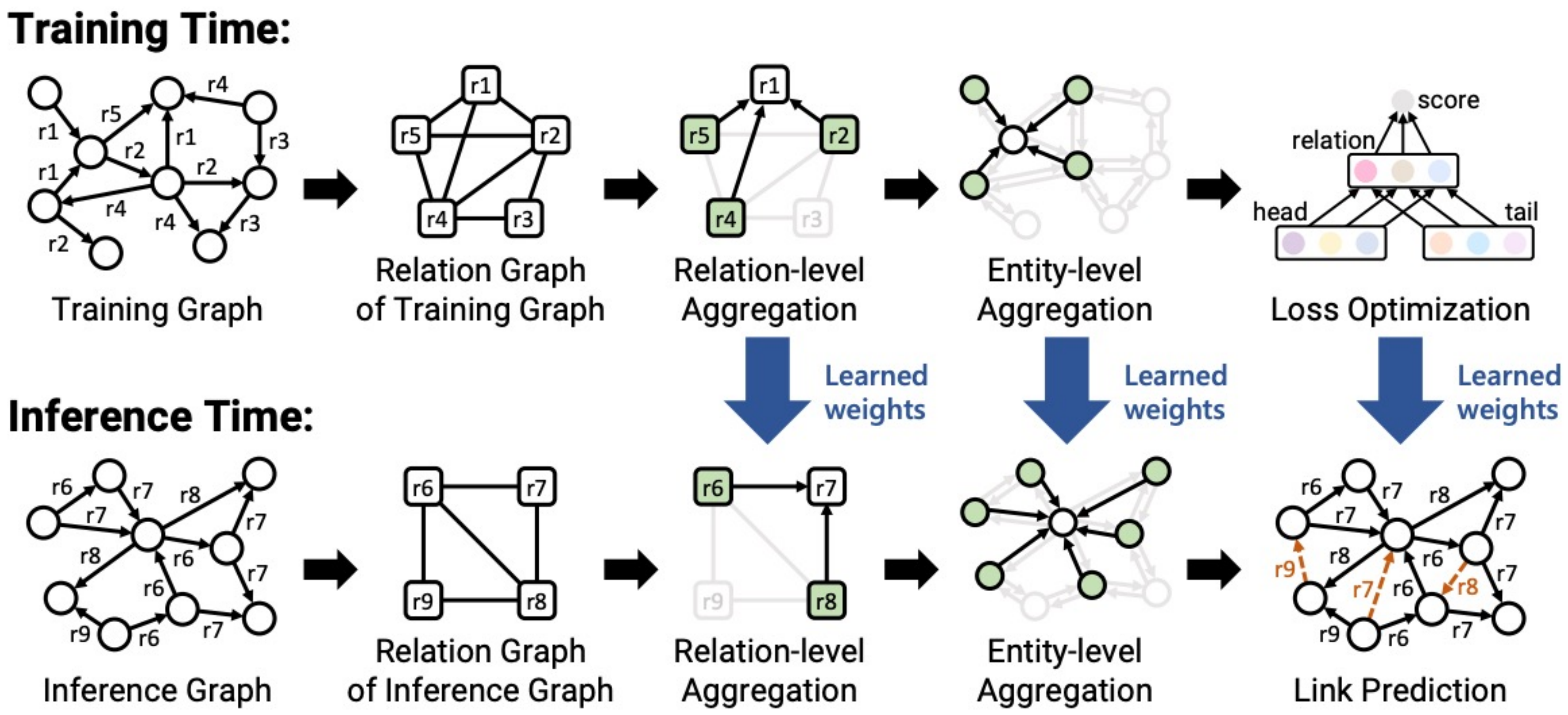


Relation Graph

- We can construct a graph **between relations**
  - **Encodes the proximity** between different relations



InGram Model



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- Next: **Relation-level message-passing**

Recap: Graph Attention Network

- **(3) Graph Attention Networks**

$$\mathbf{h}_v^{(l)} = \sigma\Big(\sum_{u\in N(v)} \underbrace{\boxed{\alpha_{vu}}}_{\text{Attention weights}} \mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}\Big)$$

Not all node's neighbors are equally important

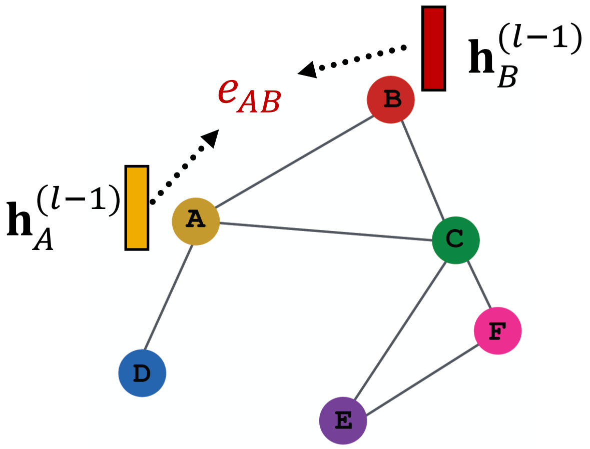
- **Attention** is inspired by cognitive attention.
- The **attention** $\boldsymbol{\alpha_{vu}}$ focuses on the important parts of the input data and fades out the rest.
  - **Idea:** the NN should devote more computing power on that small but important part of the data.
  - Which part of the data is more important depends on the context and is learned through training.

Recap: Attention Mechanism (1)

- Let α_{vu} be computed as a byproduct of an **attention mechanism a:**
  - (1) Let a compute **attention coefficients e_{vu}** across pairs of nodes u, v based on their messages:

$$e_{vu} = a(\mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}, \mathbf{W}^{(l)}\boldsymbol{h}_v^{(l-1)})$$

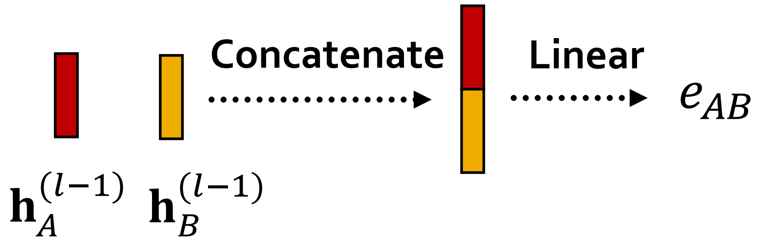
    - **e_{vu} indicates the importance of u's message to node v**



$$e_{AB} = a(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)})$$

Recap: Attention Mechanism (2)

- **What is the form of attention mechanism α?**
  - The approach is agnostic to the choice of α
    - E.g., use a simple single-layer neural network
      - α have trainable parameters (weights in the Linear layer)



$$e_{AB} = a\left(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)}\right)$$
$$= \text{Linear}\left(\text{Concat}\left(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)}\right)\right)$$

  - Parameters of α are trained jointly:
    - Learn the parameters together with weight matrices (i.e., other parameter of the neural net $\mathbf{W}^{(l)}$) in an end-to-end fashion

Recap: Attention Mechanism (3)

- **Normalize** e_{vu} into the **final attention weight** $\boldsymbol{\alpha_{vu}}$
  - Use the **softmax** function, so that $\sum_{u \in N(v)} \alpha_{vu} = 1$:

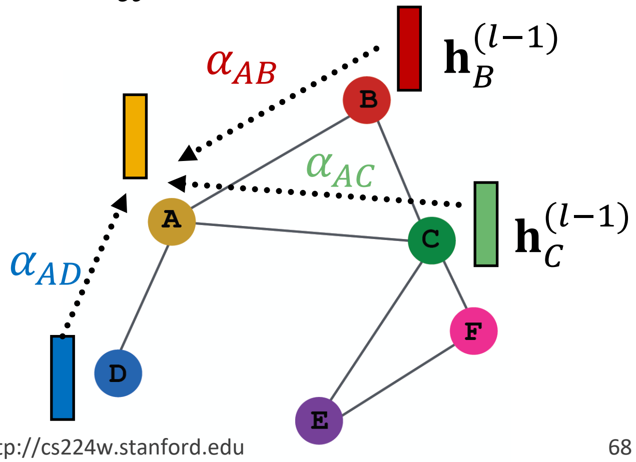
$$\alpha_{vu} = \frac{\exp(e_{vu})}{\sum_{k \in N(v)} \exp(e_{vk})}$$

- **Weighted sum** based on the **final attention weight** α_{vu}**:**

$$\mathbf{h}_v^{(l)} = \sigma(\textstyle\sum_{u \in N(v)} \alpha_{vu} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$

Weighted sum using α_{AB}, α_{AC}, α_{AD}**:**

$$\mathbf{h}_A^{(l)} = \sigma(\alpha_{AB}\mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)} + \alpha_{AC}\mathbf{W}^{(l)}\mathbf{h}_C^{(l-1)} + \alpha_{AD}\mathbf{W}^{(l)}\mathbf{h}_D^{(l-1)})$$



Relation Attention Mechanism

- **Normalize** e_{vu} into the **final attention weight** $\boldsymbol{\alpha_{vu}}$
  - Use the **softmax** function, so that $\sum_{u \in N(v)} \alpha_{vu} = 1$:

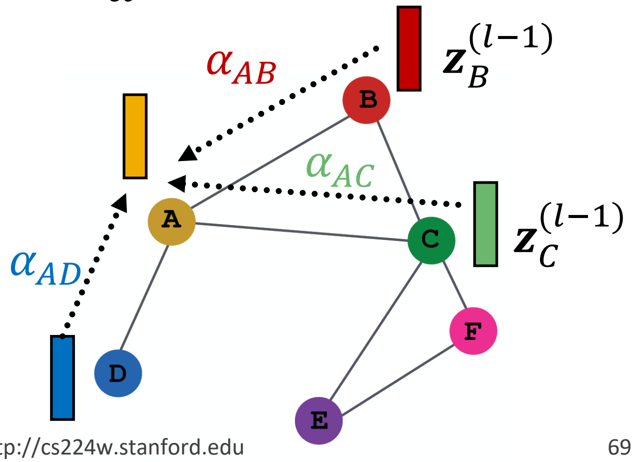
$$\alpha_{vu} = \frac{\exp(e_{vu} + \beta_{vu})}{\sum_{k \in N(v)} \exp(e_{vk} + \beta_{vk})}$$

- **Weighted sum** based on the **final attention weight** α_{vu}**:**

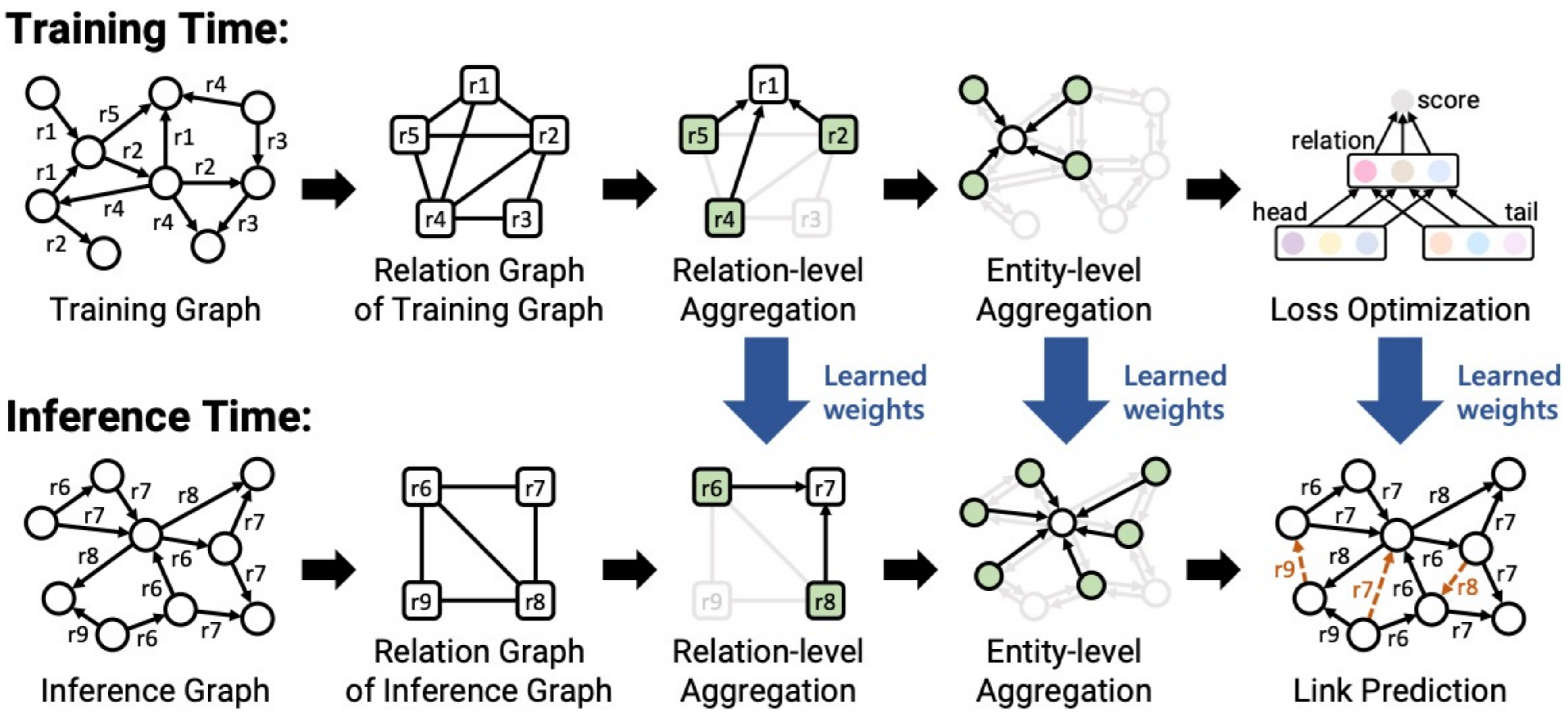
$$\mathbf{z}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \alpha_{vu} \mathbf{W}^{(l)} \mathbf{z}_u^{(l-1)}\right)$$

Weighted sum using $\alpha_{AB}, \alpha_{AC}, \alpha_{AD}$**:**

$\boldsymbol{z}_A^{(l)} = \sigma(\alpha_{AB} \mathbf{W}^{(l)} \boldsymbol{z}_B^{(l-1)} + \alpha_{AC} \mathbf{W}^{(l)} \boldsymbol{z}_C^{(l-1)} + \alpha_{AD} \mathbf{W}^{(l)} \boldsymbol{z}_D^{(l-1)})$



InGram Model



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- Next: **Entity-level message-passing**

Entity Attention Mechanism

- **Entity-level message-passing**

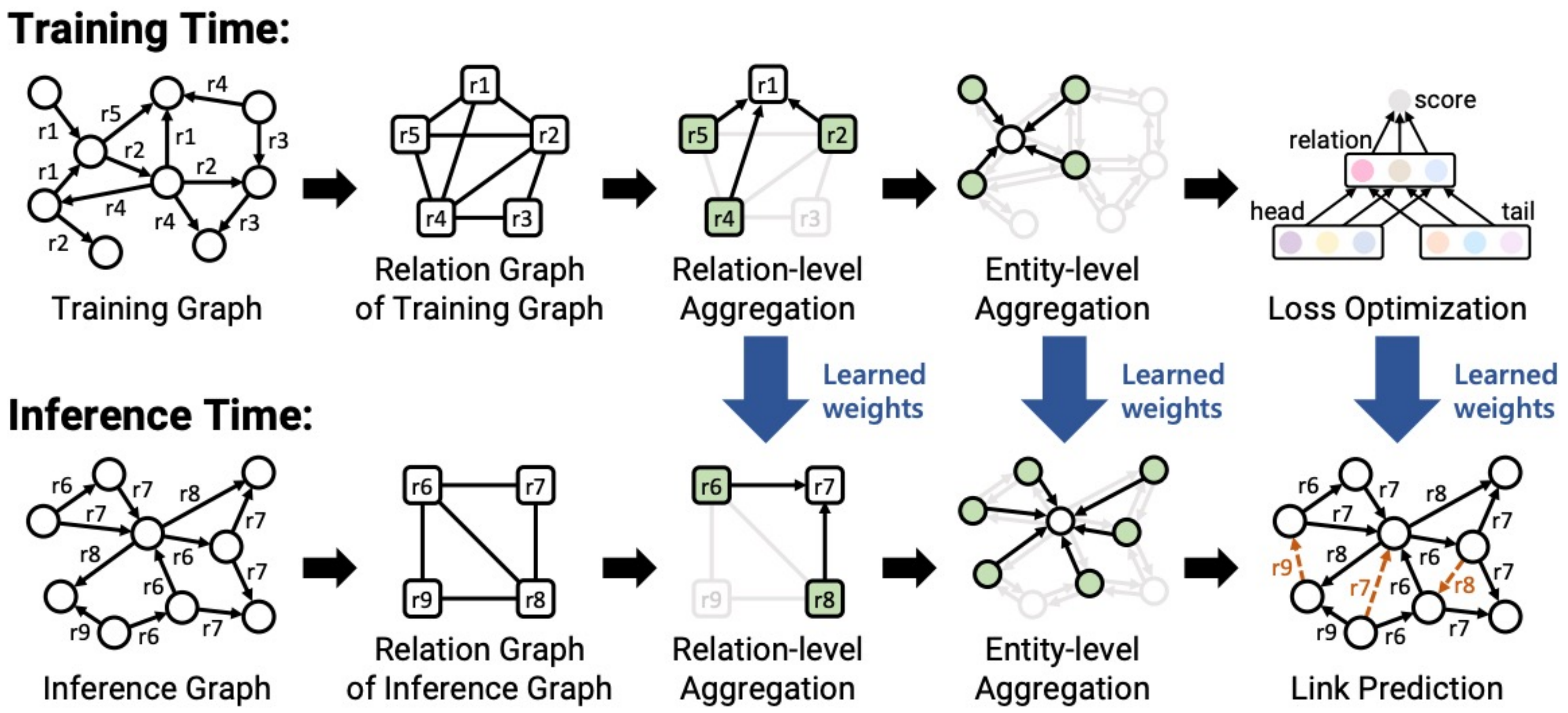
$$\boldsymbol{h}_v^{\dagger(l+1)} = \sigma\left(\sum_{r\in R}\sum_{u\in N_v^r} \mathbf{W}_1^{(l)}\mathbf{h}_u^{(l)} + \mathbf{W}_0^{(l)}\mathbf{h}_v^{(l)}\right)$$

$$\mathbf{h}_v^{*(l+1)} = \sigma\left(\sum_{r\in R}\sum_{u\in N_v^r} \alpha_{urv}\left(\mathbf{W}_1^{(l)}\mathbf{z}_r^{(l)} + \mathbf{W}_0^{(l)}\mathbf{h}_u^{(l)}\right)\right)$$

$$\boldsymbol{h}_v^{(l+1)} = \boldsymbol{h}_v^{\dagger(l+1)} + \boldsymbol{h}_v^{*(l+1)}$$

- The entity update depends on the relation update

InGram Model



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- Next: **Link-prediction head**

Link-Prediction Head

- Final embedding vectors computation

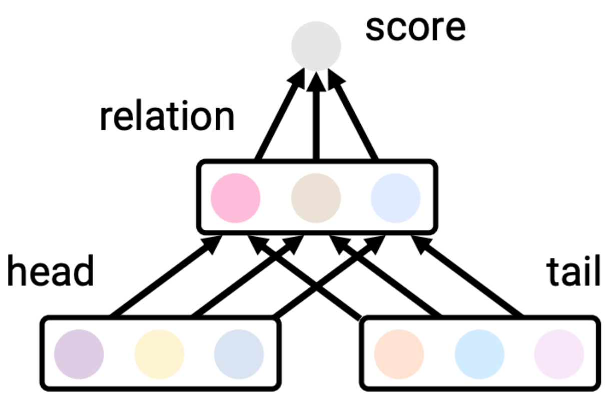
$$\boldsymbol{z}_k = \boldsymbol{M}\boldsymbol{z}_k^{(L)} \text{ and } \boldsymbol{h}_i = \widehat{\boldsymbol{M}}\boldsymbol{h}_i^{(\hat{L})}$$

- Scoring function

$$f(v_i, r_k, v_j) = \boldsymbol{h}_i^\top \operatorname{diag}(\overline{\boldsymbol{W}}\boldsymbol{z}_k)\boldsymbol{h}_j$$

- Loss

$$\sum_{(v_i,r_k,v_j)\in\mathcal{T}_{\text{tr}}} \sum_{(\mathring{v}_i,r_k,\mathring{v}_j)\in\mathring{\mathcal{T}}_{\text{tr}}} \max\left(0, \gamma - f(v_i, r_k, v_j) + f\left(\mathring{v}_i, r_k, \mathring{v}_j\right)\right)$$



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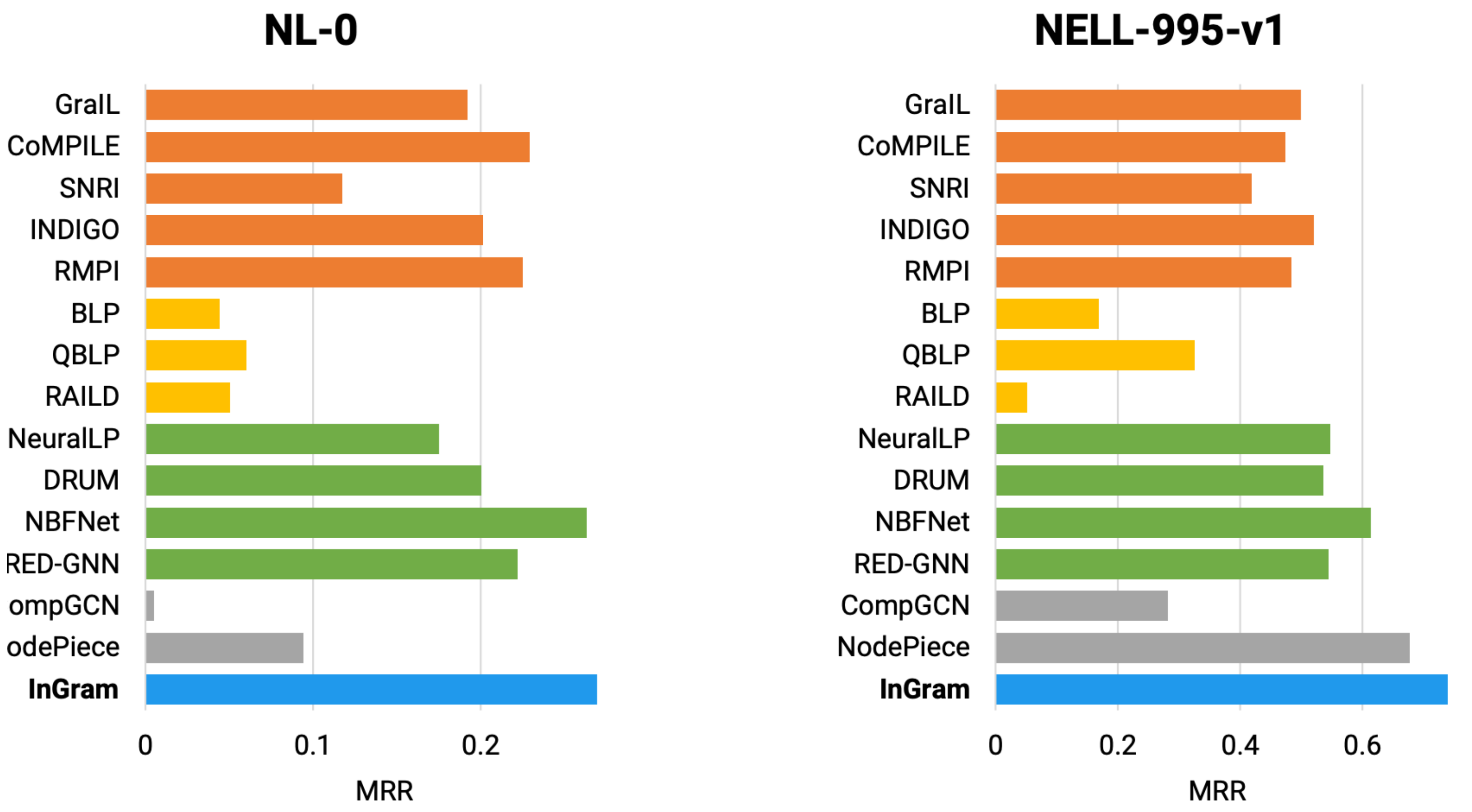
InGram

- Structure aware GNN encoders learn embeddings for entities
- Structure aware GNN encoders learn embeddings for relations
- The structure of the KG is also utilized in the loss function
- InGram can be used for inductive link prediction across new entities and new relation
  - It is a model we can use to train a foundation model

Experiments

- **Create different datasets from NELL, Wikidata, and Freebase**
- **Test the performance of InGram in Transductive and Inductive link prediction**

Transductive Link Prediction



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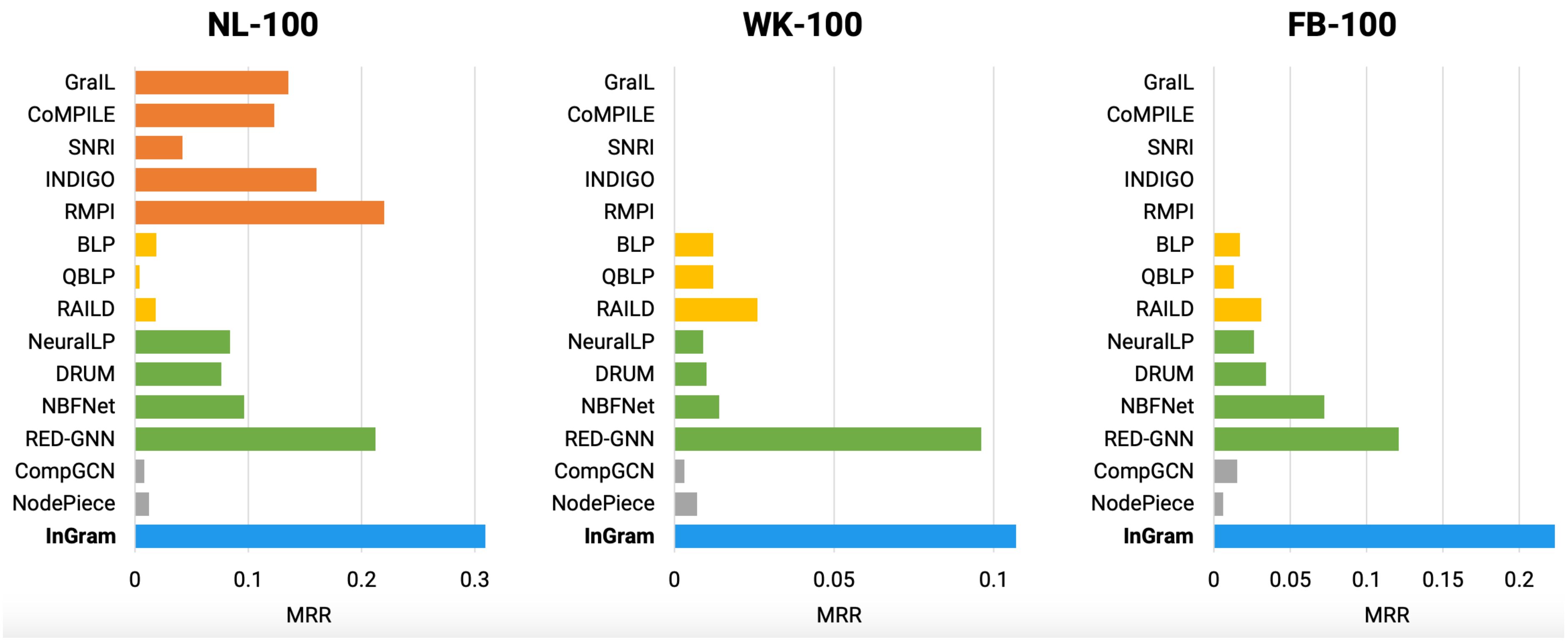
Inductive Link Prediction



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Summary of the Lecture

- Introduced a model that learns embeddings for entities and relations of any KG
- The model (InGram) is trained in an unsupervised fashion for KG completion
- The model can transfer knowledge between different KGs
- This is a step towards foundation models for KGs