

# Empowering Language Models with Graph Learning

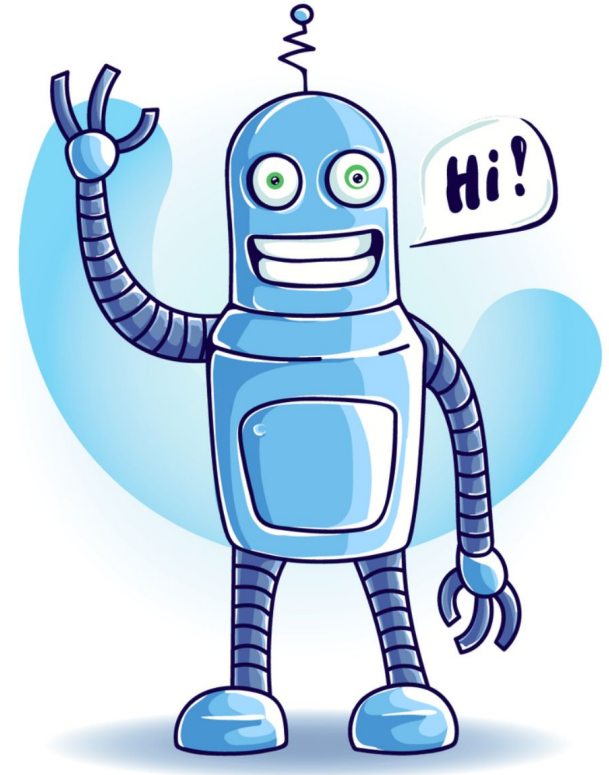
Michihiro Yasunaga

Joint work with Antoine Bosselut, Hongyu Ren, Xikun Zhang, Chris Manning, Percy Liang, Jure Leskovec



# What is Natural Language Processing (NLP)?

- Automated understanding of natural language input
- Coherent generation of natural language output



# NLP Applications

Machine Translation:



Question Answering:



Personal Assistants:



Specialized Applications:



Legal Documents

Health Records

Business Intelligence

Customer Research

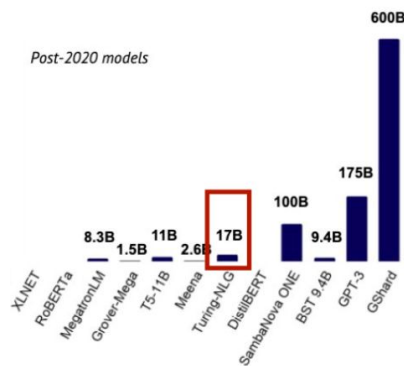
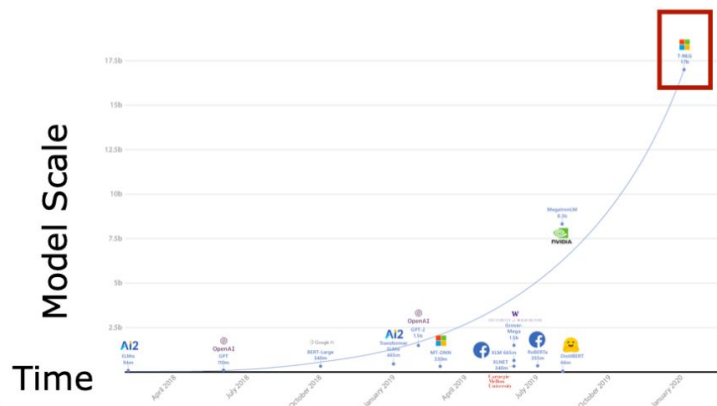
# Modern NLP – Powered by large language models



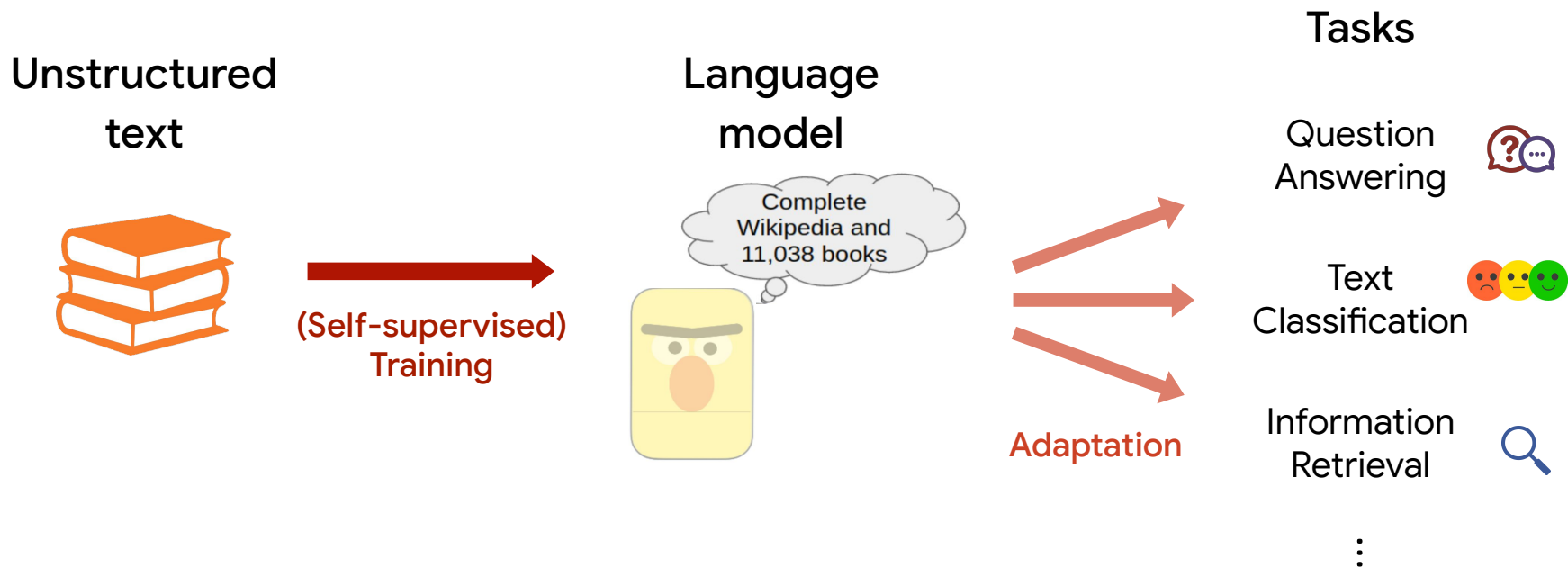
The New York Times  
A Breakthrough for A.I.  
Technology: Passing an  
8th-Grade Science Test

**Vox** How I'm using AI to  
write my next novel

The New York Times  
**Meet GPT-3. It Has Learned to  
Code (and Blog and Argue).**  
The latest natural-language system generates tweets, pens poetry,  
summarizes emails, answers trivia questions, translates  
languages and even writes its own computer programs.

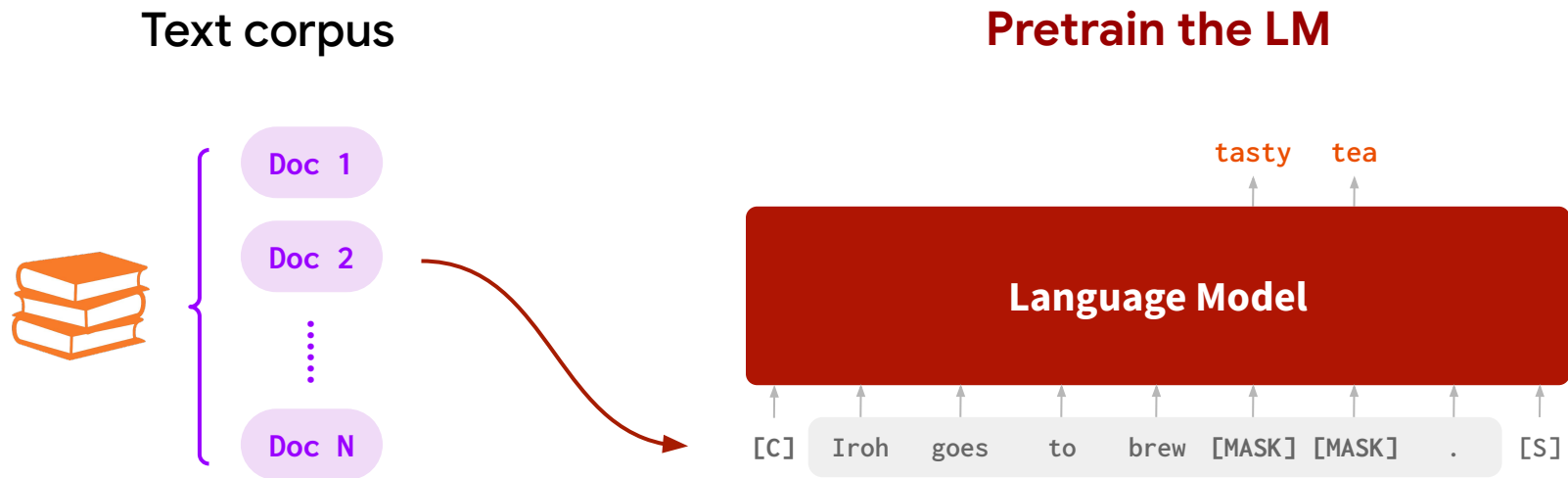


# Language Model (LM) Pretraining



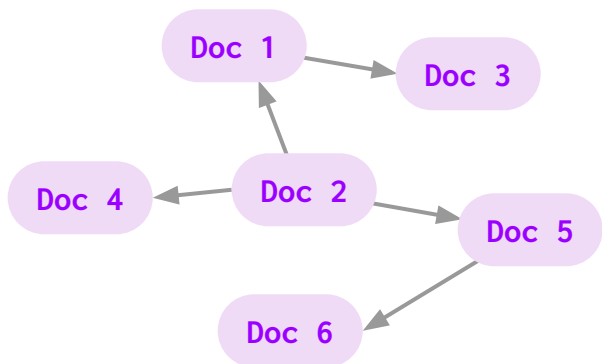
# Existing LM Pretraining

Take a document from text corpus, and perform language modeling over it

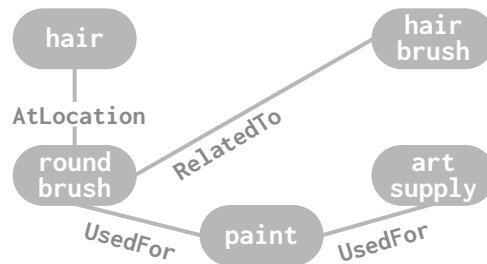


# How graphs are useful for LMs?

Hyperlink Graph



Knowledge Graph (KG)



**Graphs help make connections between concepts that may be far or latent in text**

# Graph can bring relevant concepts closer

[Tidal Basin, Washington D.C.]

**The Tidal Basin** is a man-made reservoir located between .... It is part of West Potomac Park, is near the National Mall and is a focal point of [the National Cherry Blossom Festival](#) held each spring. The Jefferson Memorial, ....

**Document**

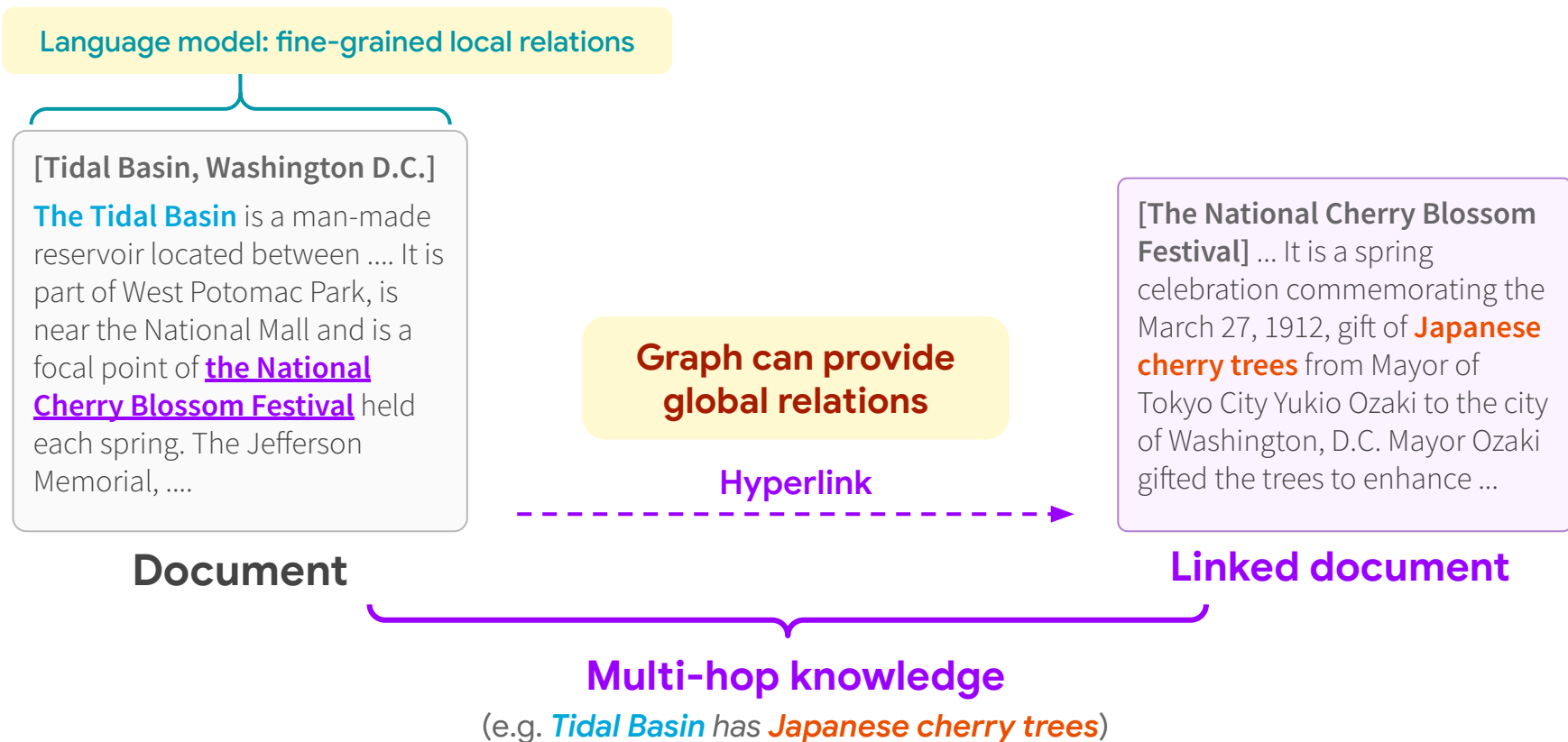
Hyperlink

[**The National Cherry Blossom Festival**] ... It is a spring celebration commemorating the March 27, 1912, gift of **Japanese cherry trees** from Mayor of Tokyo City Yukio Ozaki to the city of Washington, D.C. Mayor Ozaki gifted the trees to enhance ...

**Linked document**



# Graph can bring relevant concepts closer



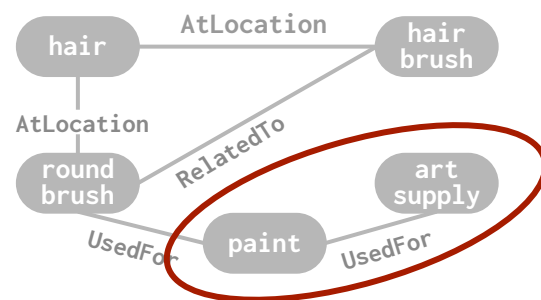
# Graph can bring relevant concepts closer

Graph can provide latent relations not mentioned in text

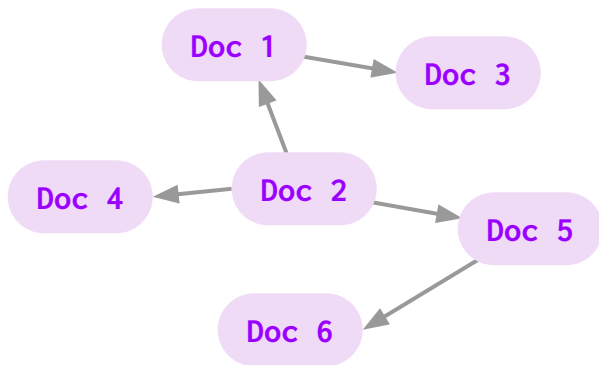
Text

If it is not used for hair,  
a round brush can be an  
example of what?

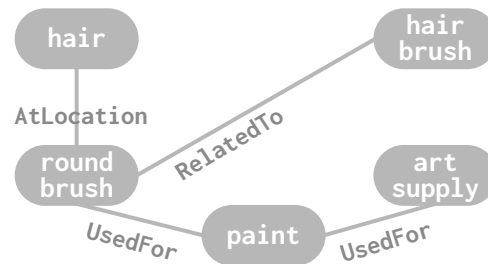
Knowledge Graph



# This talk



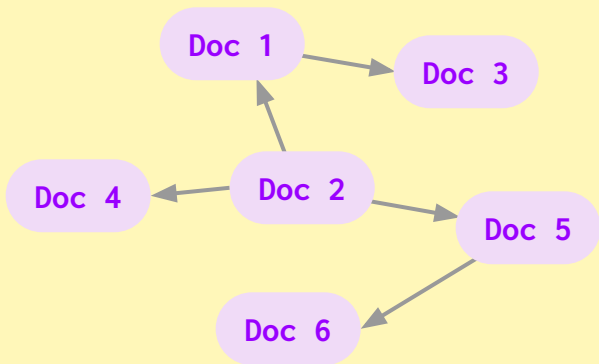
**LinkBERT**



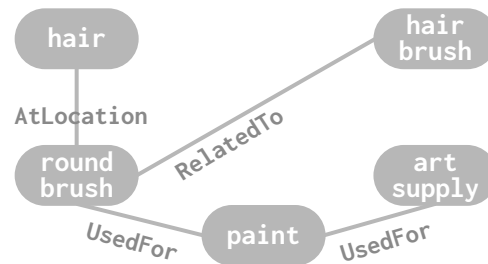
**DRAGON**

**General principle:** graphs bring relevant documents/concepts closer together

# This talk



**LinkBERT**



**DRAGON**

**General principle:** graphs bring relevant documents/concepts closer together

# LinkBERT: Pretraining Language Models with Document Links

 ACL 2022

Michihiro Yasunaga, Jure Leskovec\*, Percy Liang\*  
Stanford University



# But documents have rich dependencies

Corpus is not a list of documents, but a **graph** of documents!

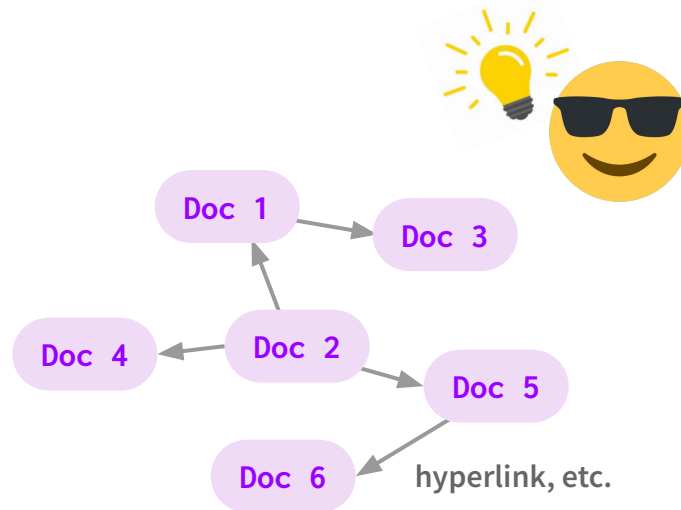
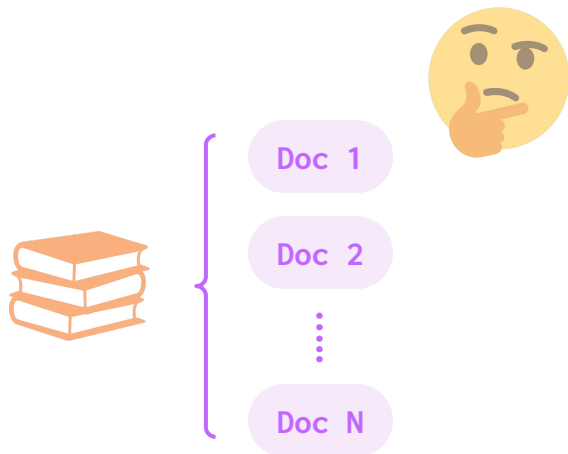
Web: **hyperlinks**



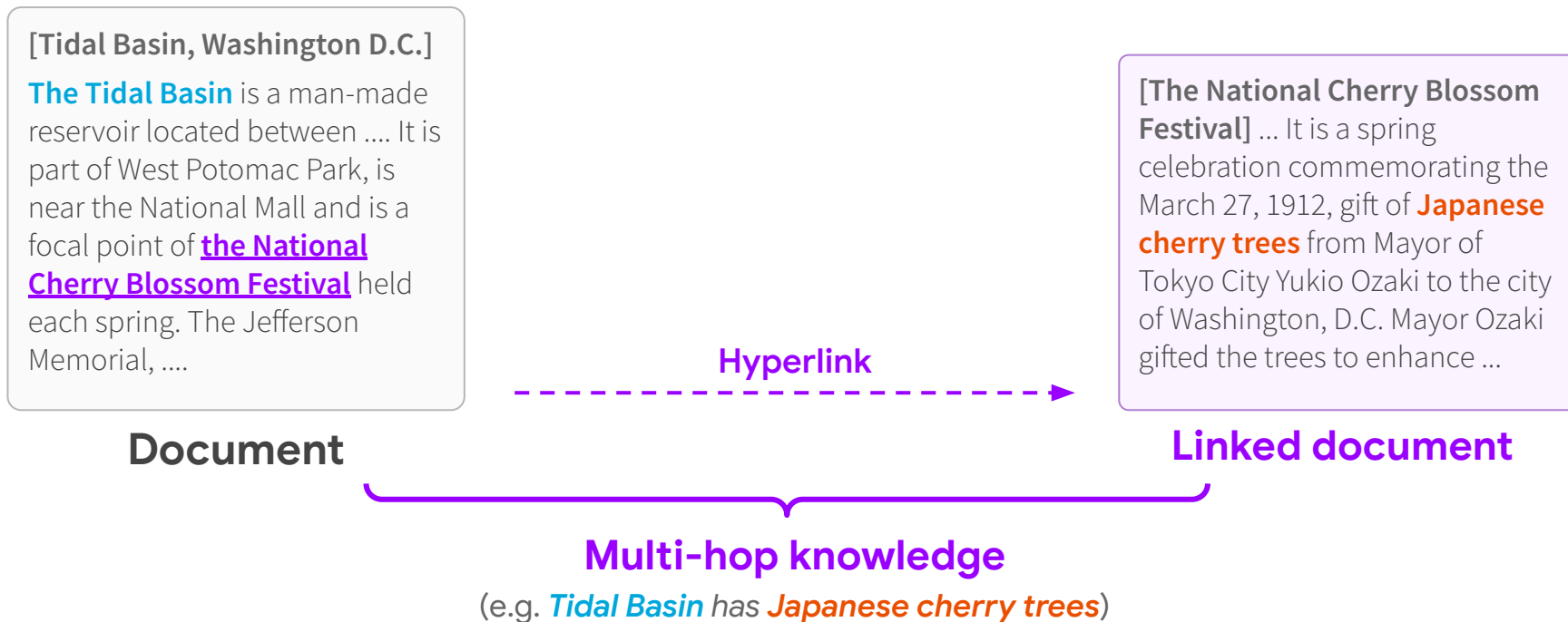
Literature: **citations**



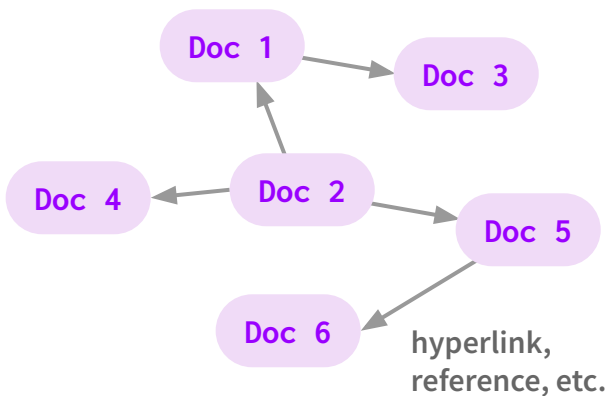
Code: **dependencies**



# Knowledge can span across documents



# Goal: Train LMs from a Graph of Docs



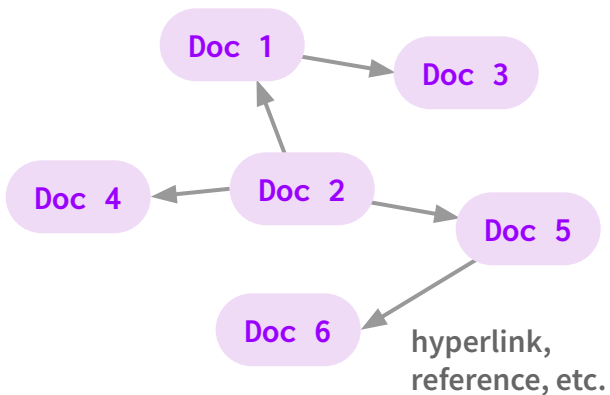
**Corpus of linked documents**



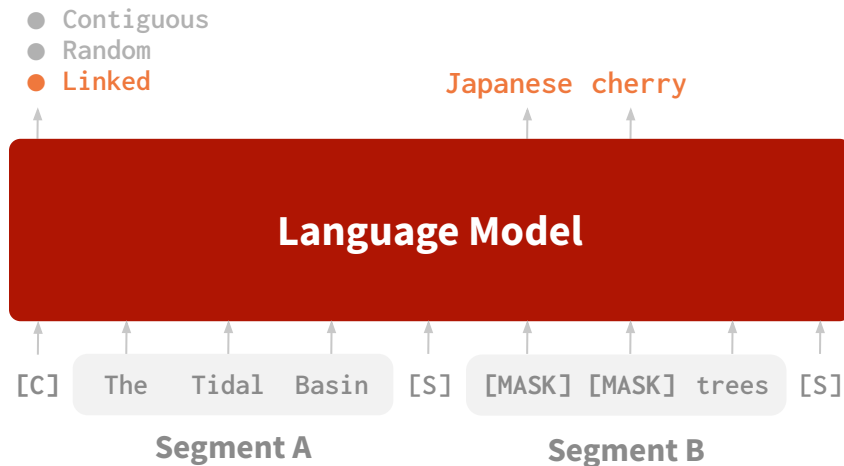
**Pretrain the LM**



# Proposed Idea: LinkBERT



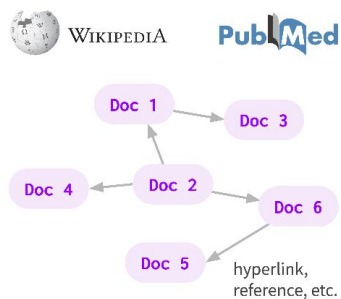
**Corpus of linked documents**



**Pretrain the LM**

# Proposed Idea: LinkBERT

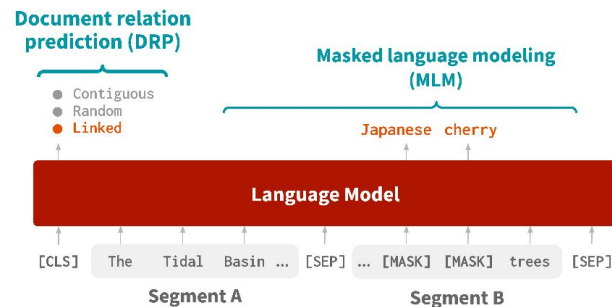
- (0) Document graph construction
- (1) Link-aware LM input creation
- (2) Link-aware LM pretraining
  - Masked language modeling (MLM)
  - Document relation prediction (DRP)



Corpus of linked documents



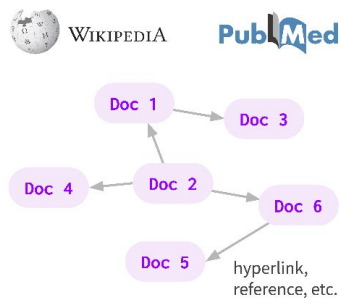
Create LM inputs



Pretrain the LM

# Proposed Idea: LinkBERT

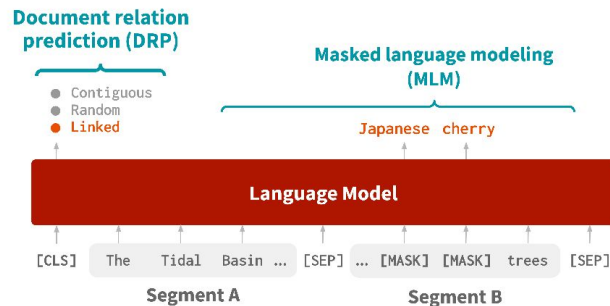
- (0) Document graph construction
- (1) Link-aware LM input creation
- (2) Link-aware LM pretraining
  - Masked language modeling (MLM)
  - Document relation prediction (DRP)



Corpus of linked documents



Create LM inputs



Pretrain the LM

# (0) Document Graph

## Idea

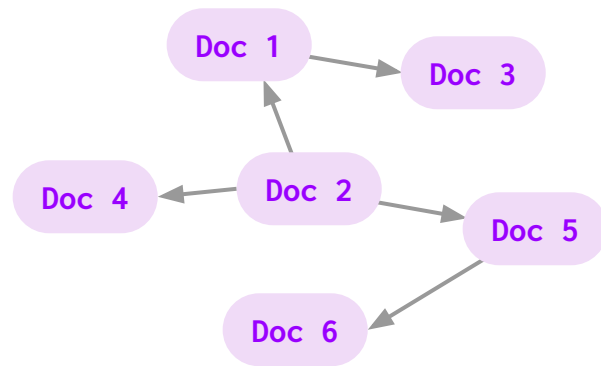
- Link related docs so that the links can bring together new knowledge

## How to link?

- Use **hyperlinks/citations**  
High quality of relevance. Easily gathered at scale.
- Could also use other linking methods  
e.g. lexical similarity

## Build document graph

- Node = document
- Edge  $(i, j)$  if there is a link from doc  $i$  to doc  $j$



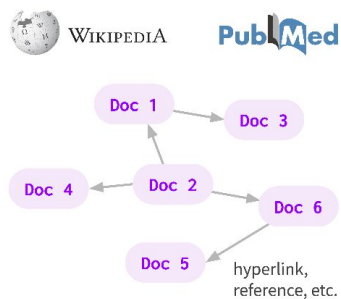
# Proposed Idea: LinkBERT

(0) Document graph construction

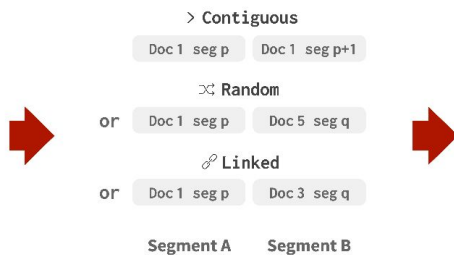
(1) Link-aware LM input creation

(2) Link-aware LM pretraining

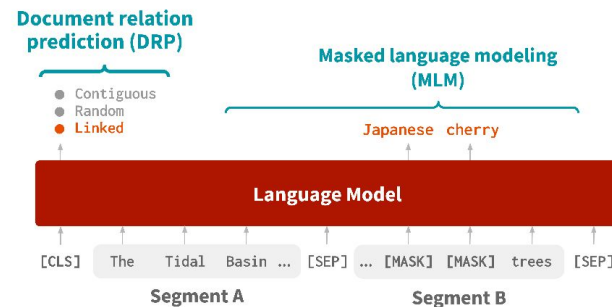
- Masked language modeling (MLM)
- Document relation prediction (DRP)



Corpus of linked documents



Create LM inputs

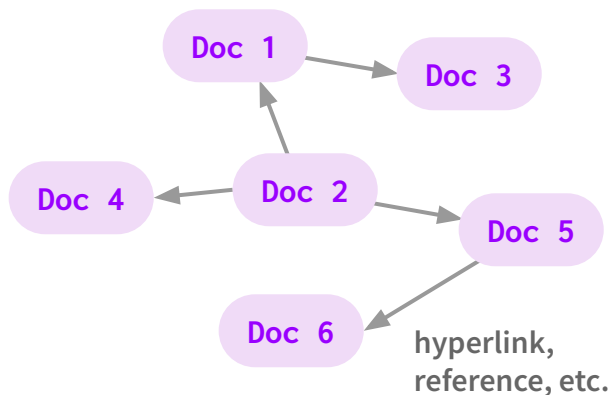


Pretrain the LM

# (1) Link-aware LM Input Creation

## Motivation

- LMs learn token dependency effectively if the tokens are shown in the same context ([Levine+2022](#)). Let's place linked docs together in the same context



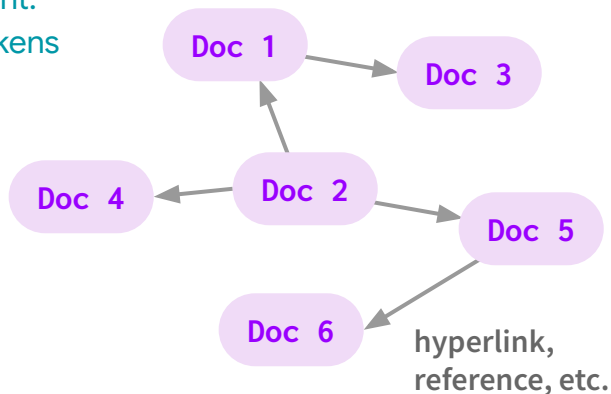
**Corpus of linked documents**

# (1) Link-aware LM Input Creation

## Idea

- Sample a pair of text segments (A, B) as input, using three options:  
(i) **contiguous**, (ii) **random**, (iii) **linked**

segment:  
~256 tokens



**Corpus of linked documents**



> Contiguous

Doc 1 seg p    Doc 1 seg p+1

↔ Random

or Doc 1 seg p    Doc 5 seg q

🔗 Linked

or Doc 1 seg p    Doc 3 seg q

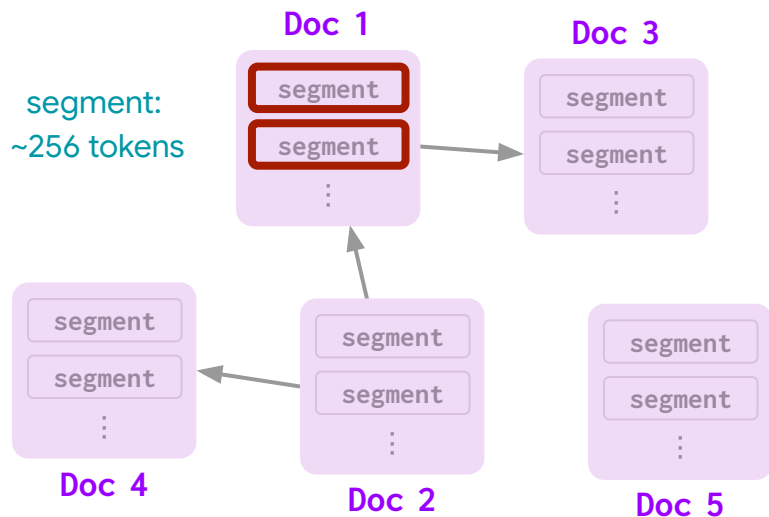
Segment A

Segment B

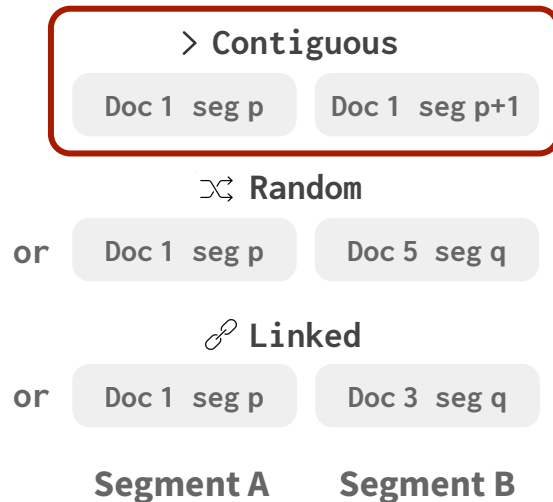
**Step 1. Create LM inputs**

# LM Input Option (i): “Contiguous”

After sampling segment **A**, take the contiguous segment from the same doc as **B** (same as BERT)



**Corpus of linked documents**

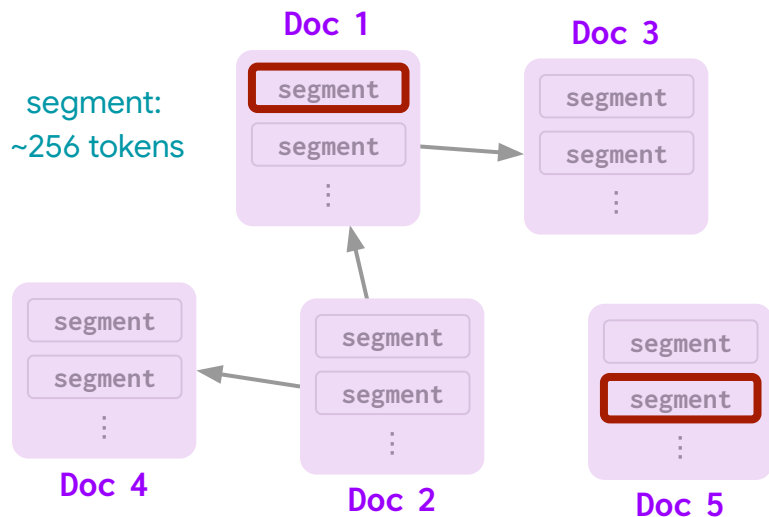


**Step 1. Create LM inputs**

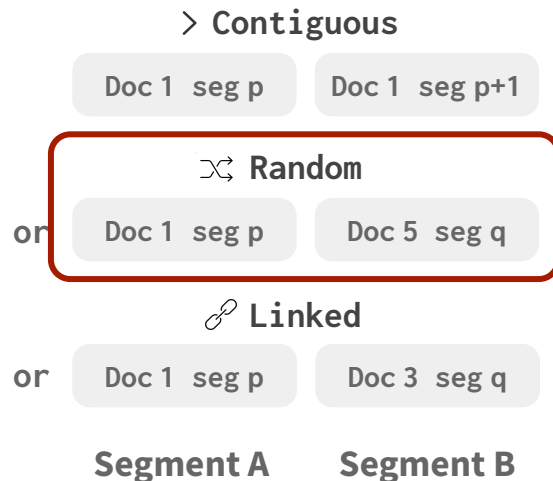


# LM Input Option (ii): “Random”

After sampling segment **A**, sample a segment from a random doc as **B** (same as BERT)



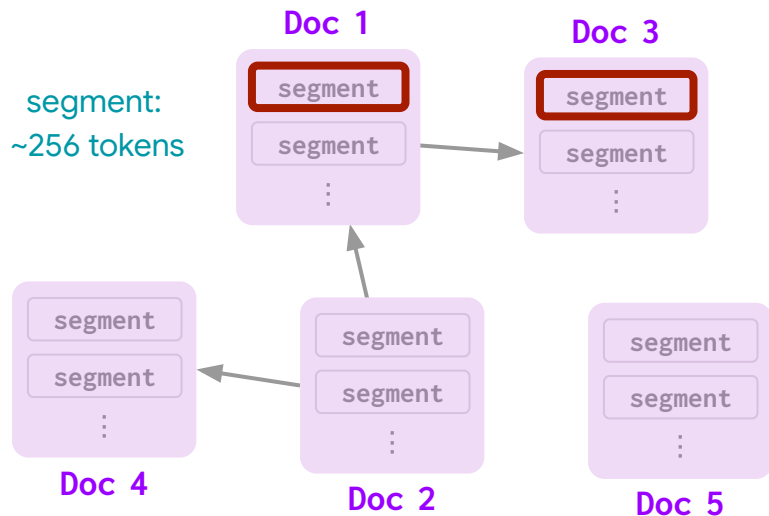
**Corpus of linked documents**



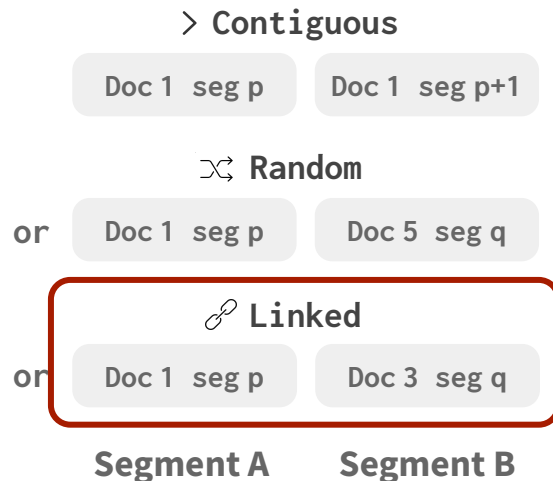
**Step 1. Create LM inputs**

# LM Input Option (iii): “Linked”

After sampling segment **A**, sample a segment from a linked doc as **B**  
(our new proposal)



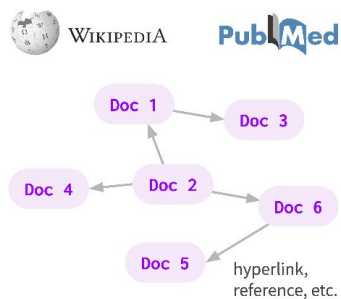
**Corpus of linked documents**



**Step 1. Create LM inputs**

# Proposed Idea: LinkBERT

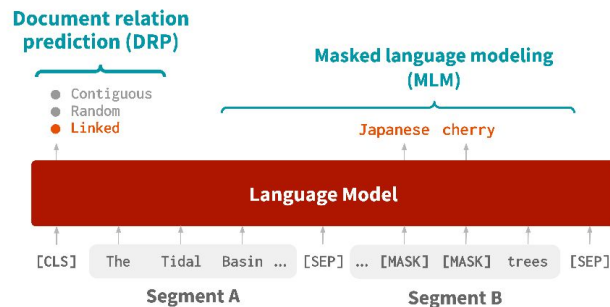
- (0) Document graph construction
- (1) Link-aware LM input creation
- (2) Link-aware LM pretraining
  - Masked language modeling (MLM)
  - Document relation prediction (DRP)



Corpus of linked documents



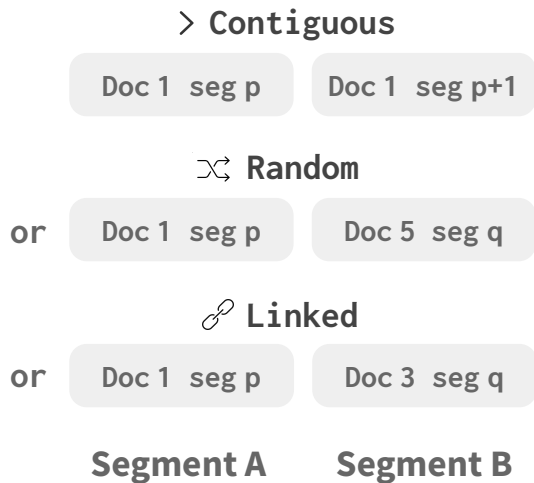
Create LM inputs



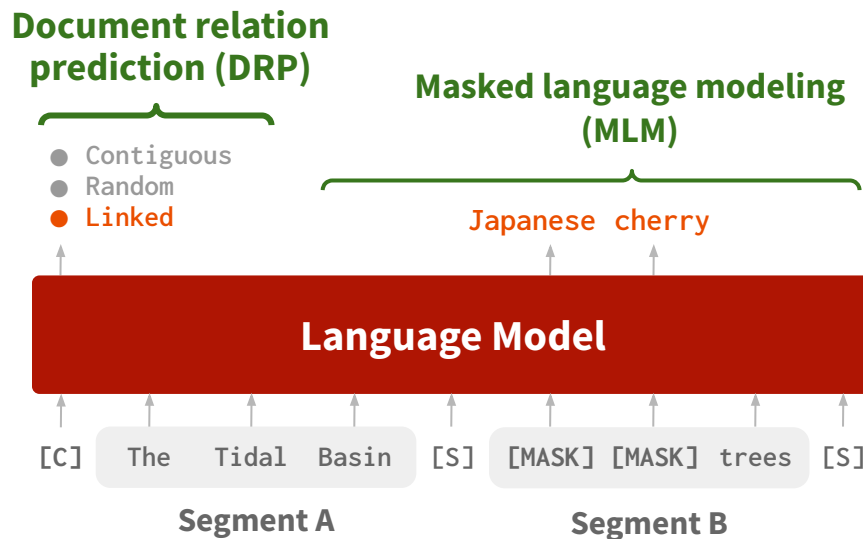
Pretrain the LM

## (2) Link-aware LM Pretraining

**Idea:** Pretrain LM with link-aware self-supervised tasks



**Step 1. Create LM inputs**



**Step 2. Pretrain the LM**

## (2) Link-aware LM Pretraining

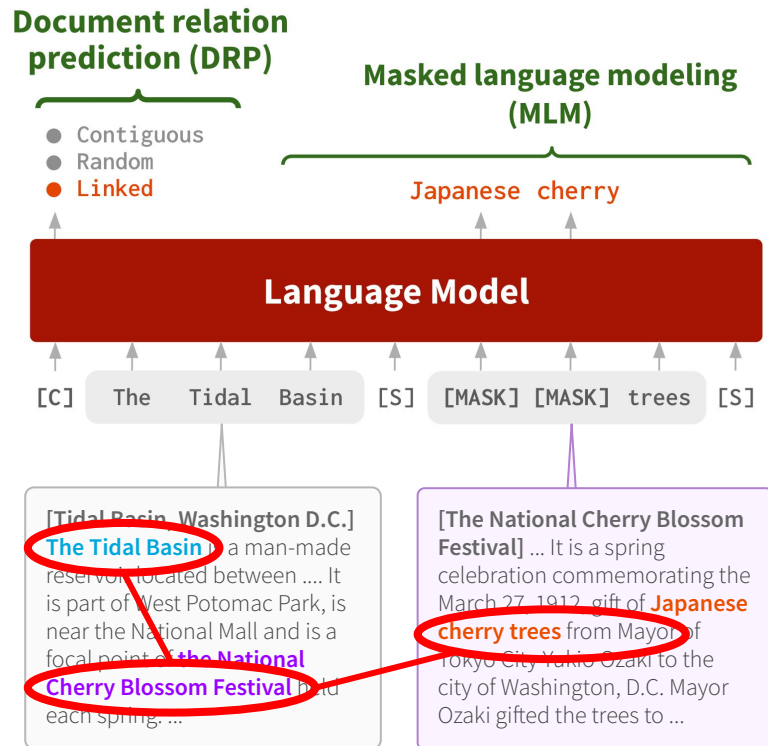
### Masked language modeling (MLM)

- Predict masked tokens
- Learn concepts brought into the same context by doc links, e.g. **multi-hop knowledge**

### Document relation prediction (DRP)

- Predict the relation between segment A and B
- Learn **relevance** between docs
- Learn the existence of **bridging concepts**

Jointly optimize MLM + DRP



# Graph Machine Learning Perspective

Interpretation as graph self-supervised learning on the doc graph

## MLM = Node Feature Prediction

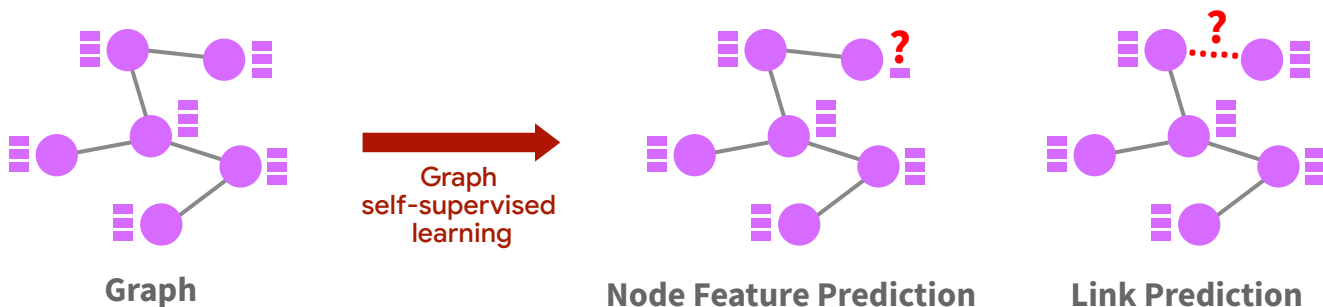
Predict masked features of a node using neighbor nodes

⇒ Predict masked tokens in Segment A using Segment B

## DRP = Link Prediction

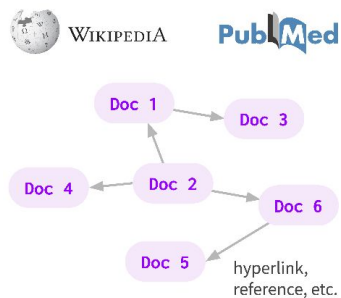
Predict the existence/type of an edge between two nodes

⇒ Predict if two segments are linked (edge), contiguous (self-loop), or random (no edge)

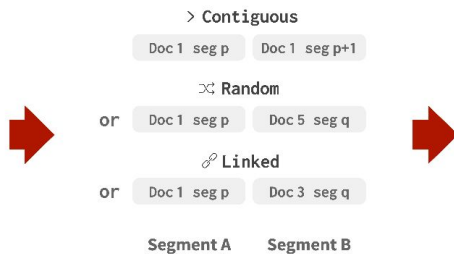


# Proposed Idea: LinkBERT

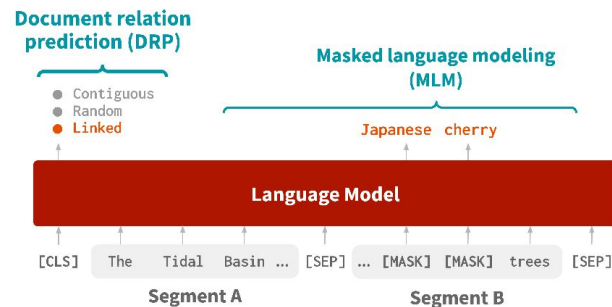
- (0) Document graph construction
- (1) Link-aware LM input creation
- (2) Link-aware LM pretraining
  - Masked language modeling (MLM)
  - Document relation prediction (DRP)



Corpus of linked documents



Create LM inputs



Pretrain the LM

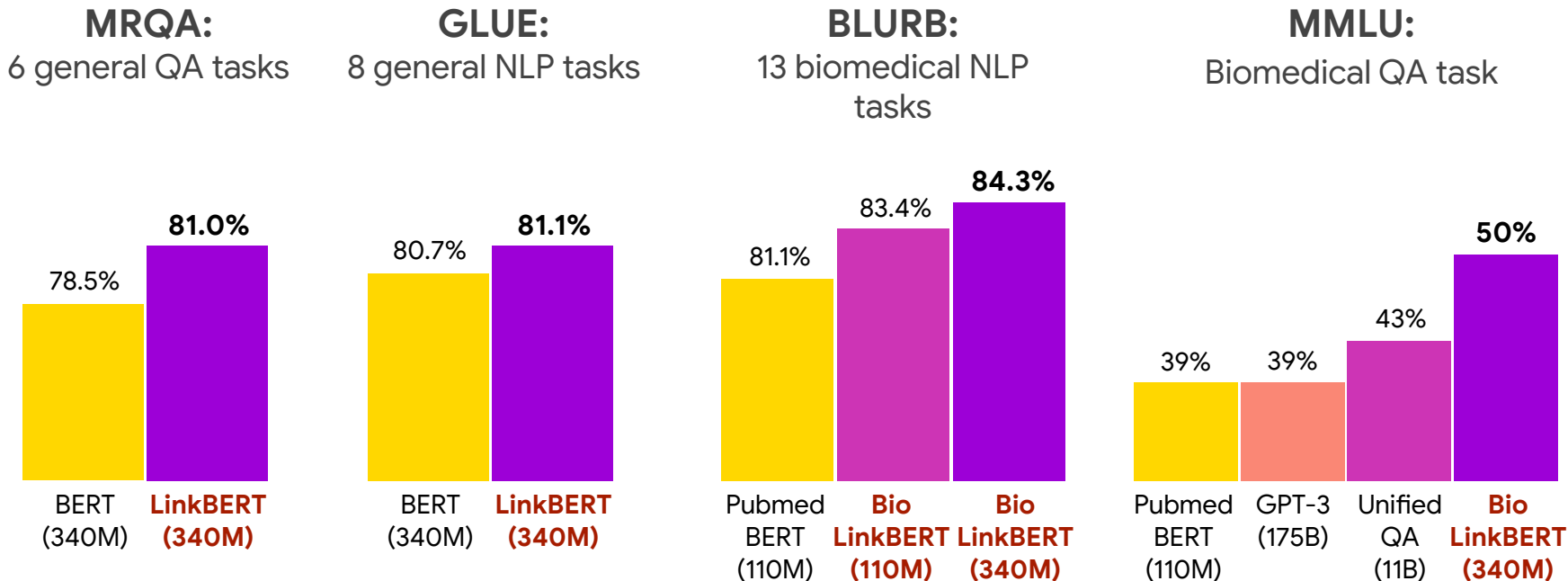
# Experiments

	General domain	Biomedical domain
<b>Pretraining corpus</b>	<b>Wikipedia (10GB) + Books (4GB)</b> <b>Links:</b> hyperlinks <b>Doc graph:</b> 3M nodes, 60M edges	<b>PubMed (20GB)</b> <b>Links:</b> citations <b>Doc graph:</b> 15M nodes, 120M edges
<b>Baseline</b> = Pretrained on same corpus, but no doc links	BERT ( <a href="#">Devlin+2019</a> )	PubmedBERT ( <a href="#">Gu+2020</a> )
<b>Downstream tasks</b>	<a href="#">GLUE</a> (NLP benchmark) <a href="#">MRQA</a> (QA benchmark)	<a href="#">BLURB</a> (NLP benchmark) <a href="#">MedQA-USMLE</a> (QA task) <a href="#">MMLU medicine</a> (QA task)



# Performance

LinkBERT makes consistent improvement across tasks and domains









# BioLinkBERT sets a new state of the art

BLURB

[Leaderboard](#) [Paper](#) [Models](#) [Tasks](#) [Submit](#) [News](#)

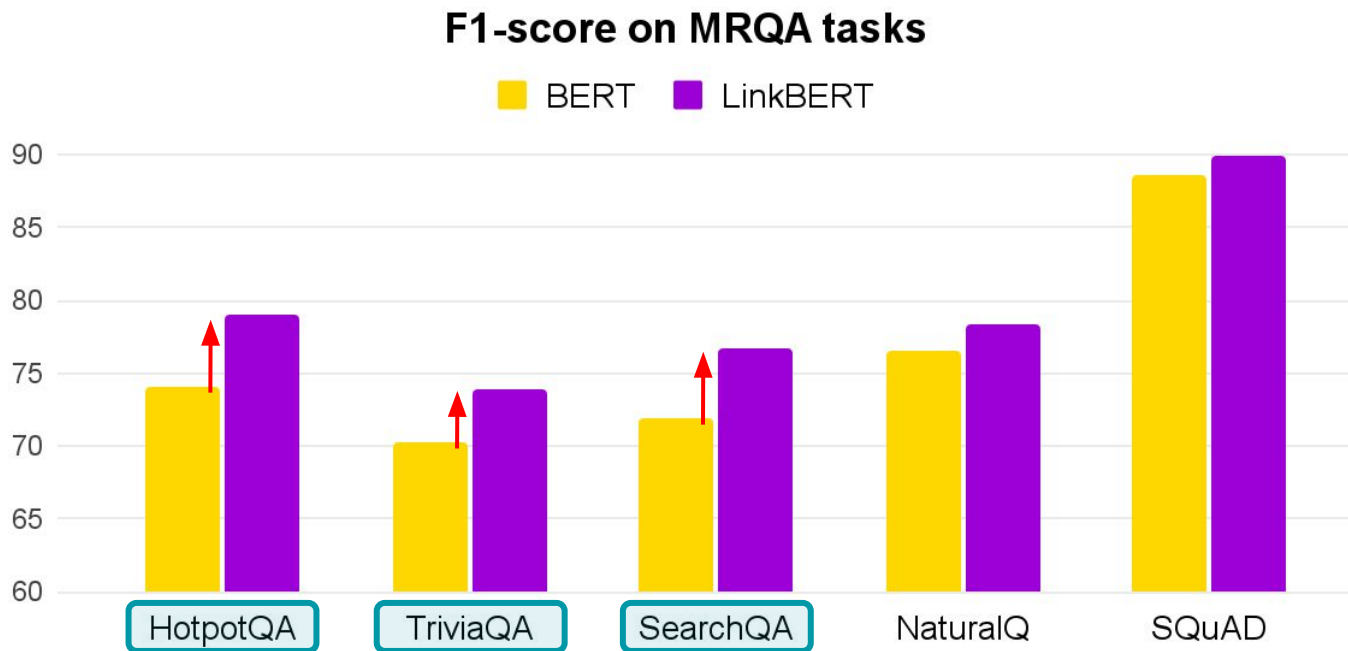
The Overall score is calculated as the macro-average performance over tasks. Details can be found within [our publication](#).

Show  entries

Rank	Model	BLURB Score (Macro Avg.)	Micro Avg.	NER	PICO	RE	SS	Class.	QA
1	<b>BioLinkBERT-Large</b> — Stanford  	84.30	84.80	86.89	74.19	82.74	93.63	84.88	83.50
2	<b>BioLinkBERT-Base</b> — Stanford  	83.39	83.84	86.39	73.97	81.56	93.27	84.35	80.81
3	<b>PubMedBERT-LARGE (fine-tuning stabilization; uncased; abstracts)</b> — Microsoft Research  	82.91	83.58	86.28	73.61	81.77	92.73	82.70	80.37

# Benefit 1: Multi-hop Reasoning

Large gains over BERT on tasks involving multi-hop reasoning



# Benefit 1: Multi-hop Reasoning

## HotpotQA example

**Question:** Roden Brothers were taken over in 1953 by a group headquartered in which Canadian city?

**Doc A:** Roden Brothers was founded June 1, 1891 in Toronto, Ontario, Canada by Thomas and Frank Roden. In the 1910s the firm became known as Roden Bros. Ltd. and were later taken over by Henry Birks and Sons in 1953. ...

**Doc B:** Birks Group (formerly Birks & Mayors) is a designer, manufacturer and retailer of jewellery, timepieces, silverware and gifts ... The company is headquartered in Montreal, Quebec, ...

LinkBERT predicts: “Montreal” (✓)

BERT predicts: “Toronto” (✗)

**Intuition:** seeing linked docs in the same context in pretraining helps reasoning with multiple docs in downstream

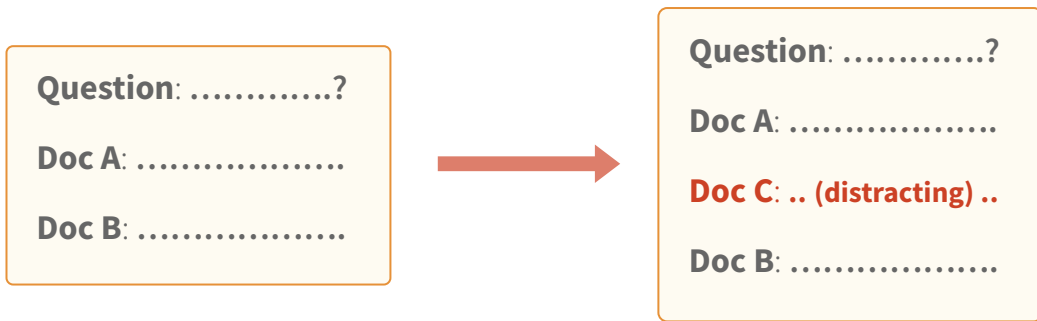
# Benefit 2: Document Relation Understanding

## Motivation

- In open-domain QA, QA model is given multiple retrieved (**noisy**) documents and needs to understand their relevance ([Chen+2017](#))

## Evaluation

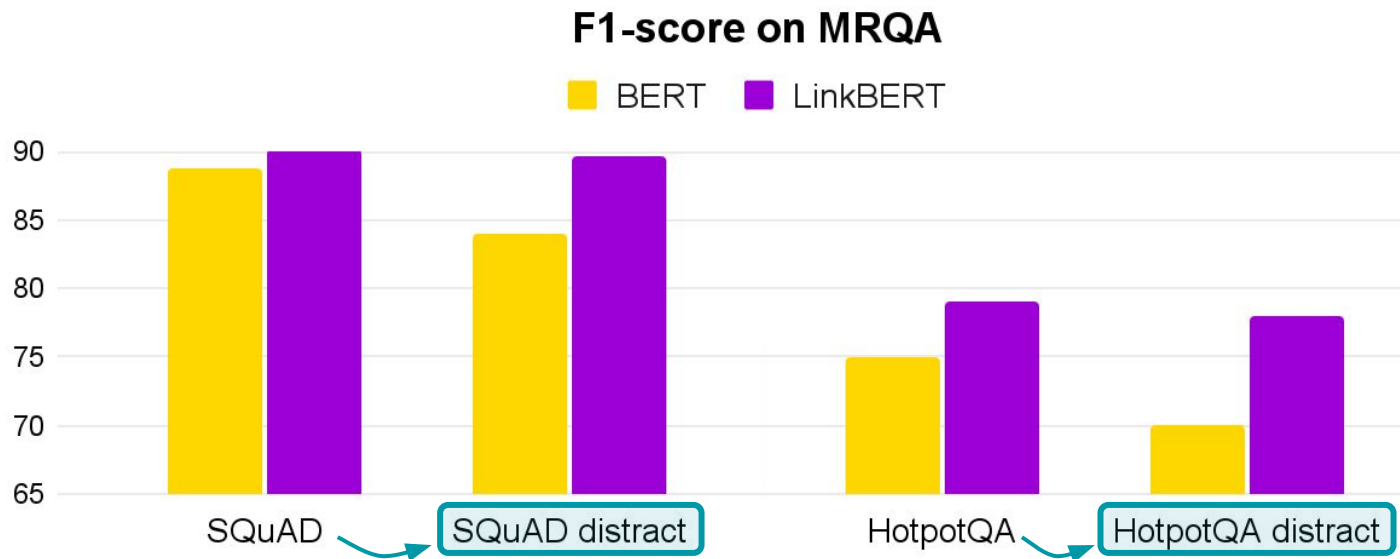
- Add distracting documents to the original MRQA datasets.  
Can LinkBERT still answer correctly?



# Benefit 2: Document Relation Understanding

## LinkBERT is robust to irrelevant documents

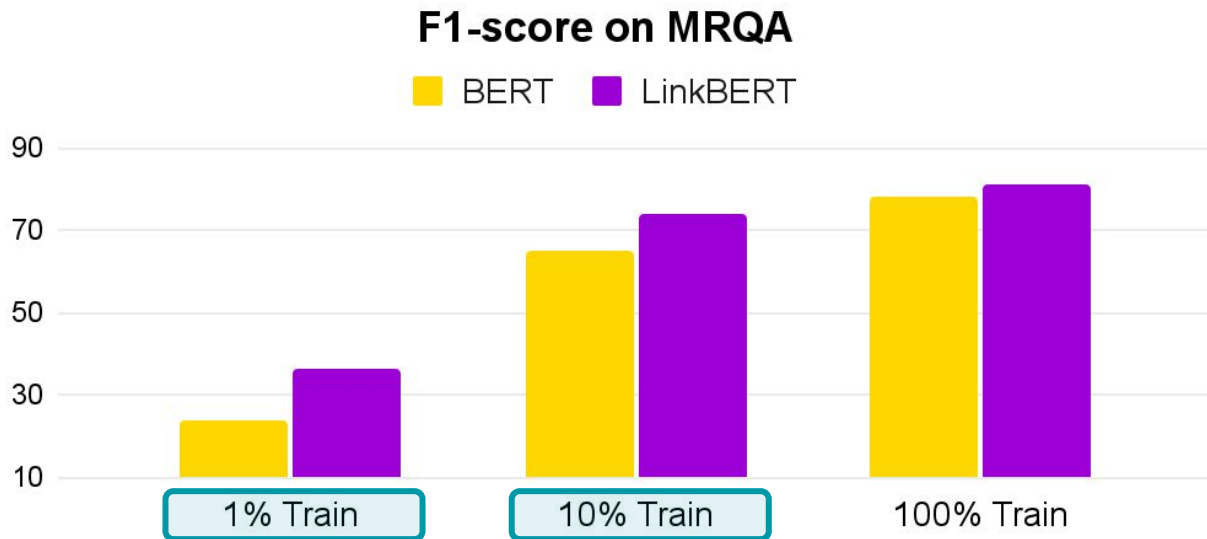
⇒ DRP task in pretraining helps recognizing doc relevance in downstream



# Benefit 3: Few-shot QA

Large gains over BERT on few-shot and data-efficient QA

⇒ LinkBERT internalized more knowledge during pretraining



# Try our models!

You can easily use LinkBERT on 🙌 HuggingFace!

## How to use

To use the model to get the features of a given text in PyTorch:

```
from transformers import AutoTokenizer, AutoModel
tokenizer = AutoTokenizer.from_pretrained('michiyasunaga/LinkBERT-large')
model = AutoModel.from_pretrained('michiyasunaga/LinkBERT-large')
inputs = tokenizer("Hello, my dog is cute", return_tensors="pt")
outputs = model(**inputs)
last_hidden_states = outputs.last_hidden_state
```



# Takeaways

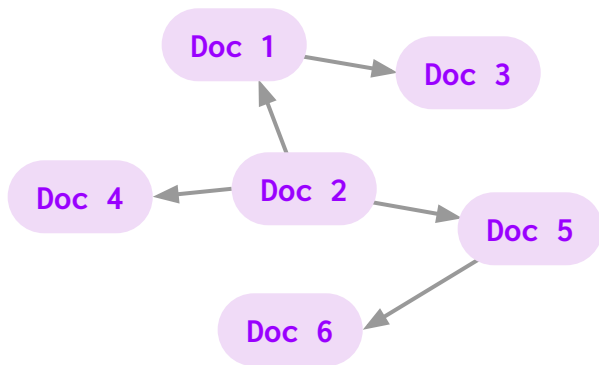
---

**LinkBERT**: train LMs using document links (hyperlinks, citations)

## Benefits

- Better captures document/concept relations  
⇒ Effective for **multi-hop** reasoning and **cross-document** understanding
- Internalizes more world knowledge  
⇒ Effective for **knowledge-intensive** tasks

# This talk



**LinkBERT**



**DRAGON**

**General principle:** graphs bring relevant documents/concepts closer together

# DRAGON: Deep Bidirectional Language-Knowledge Pretraining

Michihiro Yasunaga, Antoine Bosselut, Hongyu Ren, Xikun Zhang,  
Chris Manning, Percy Liang\*, Jure Leskovec\*  
Stanford University



# Text & KG offer complementary information

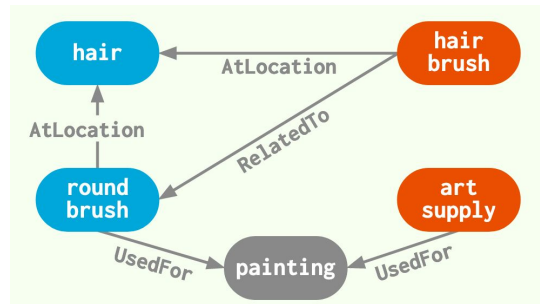
## Text & Pretrained Language Model (LM)

- Broad coverage (e.g. [Gao+2020](#))
- Captures rich context



## Knowledge Graph (KG)

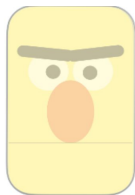
- Latent, structured relations
- Multihop reasoning (e.g. [Yasunaga+2021](#))



# Goal: Combine text & KG for pretraining

## Text

- Broad coverage (e.g. [Gao+2020](#))
- Captures rich context



Complete  
Wikipedia and  
11,038 books

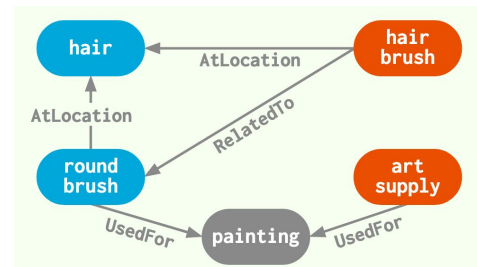
## Joint Pretraining



## Language-Knowledge Model

## Knowledge Graph (KG)

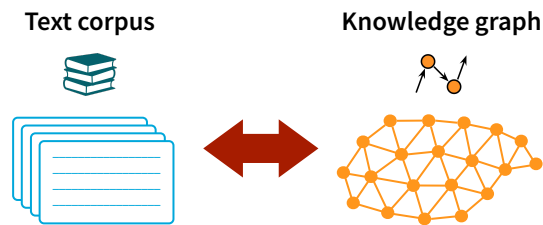
- Latent, structured relations
- Multihop reasoning  
(e.g. [Yasunaga+2021](#))



# Challenges

How to learn rich representations from text & KG?

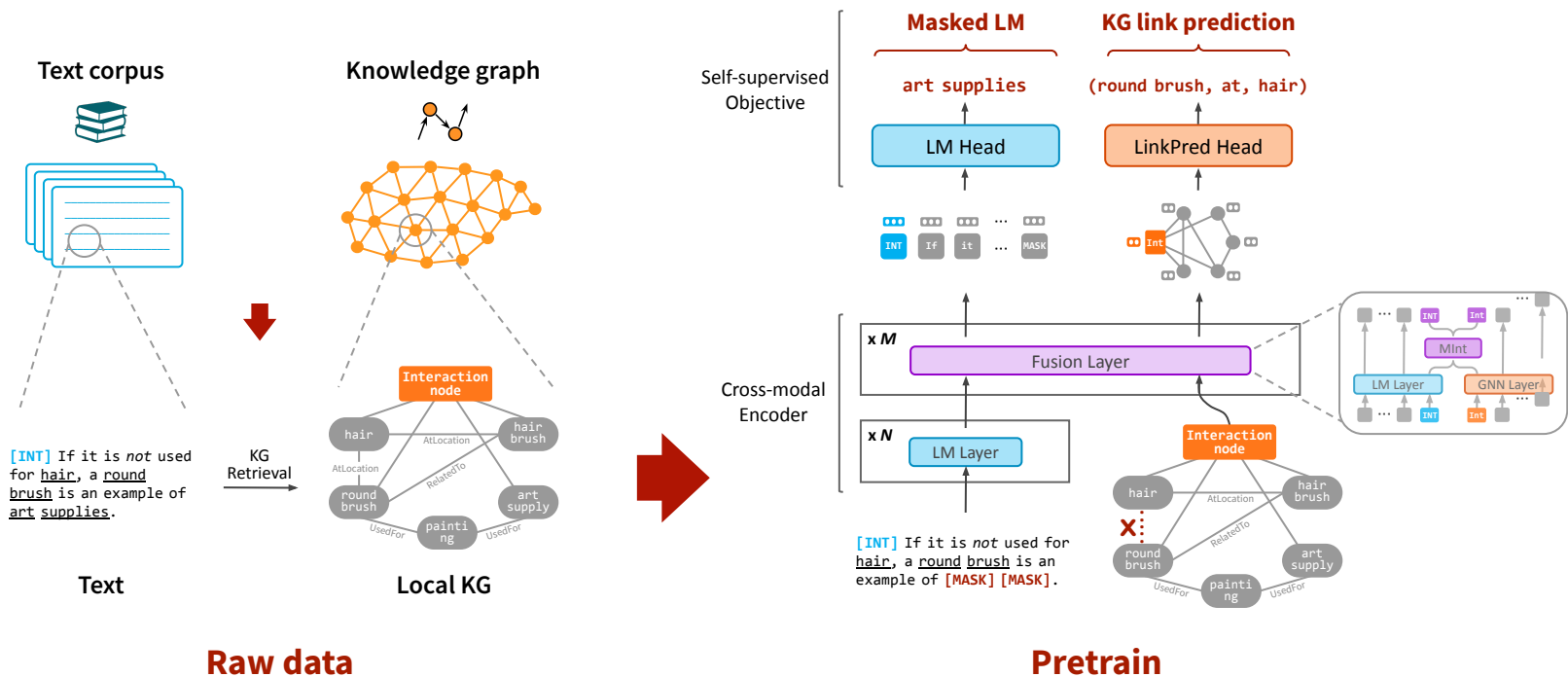
- (1) Deeply **bidirectional model** for the two modalities to interact
- (2) **Self-supervision** to learn joint reasoning over text and KG **at scale**



Existing works

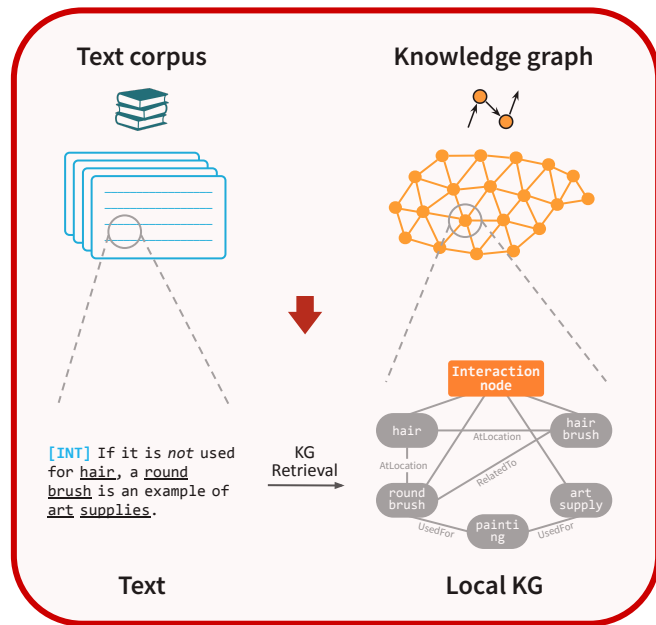
- Bidirectional model for text+KG, but only finetune on labeled data (e.g. [QAGNN](#), [GreaseLM](#))
- Self-supervised, but shallow or uni-directional interaction (e.g. [ERNIE](#), [WKLM](#), [KEPLER](#))

# Proposed Method: DRAGON

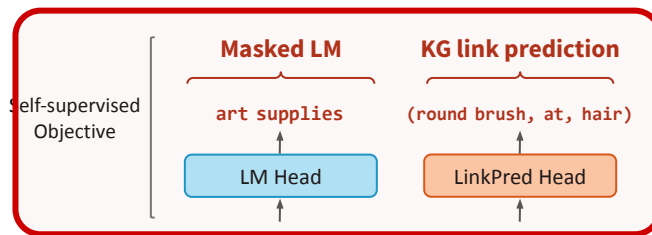


# Proposed Method: DRAGON

## Step (1)



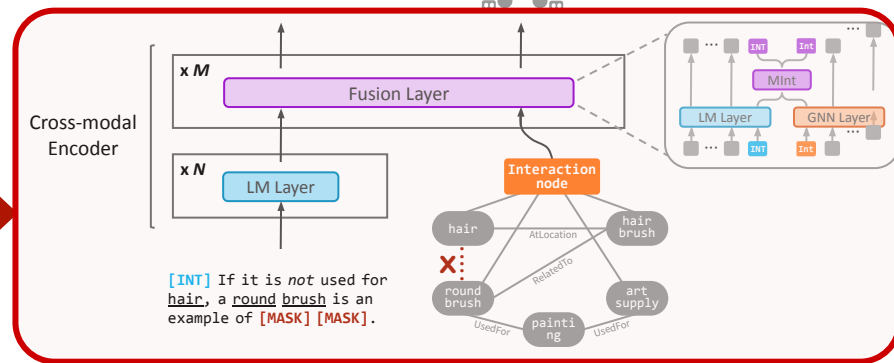
Raw data



Pretrain

## Step (3)

## Step (2)





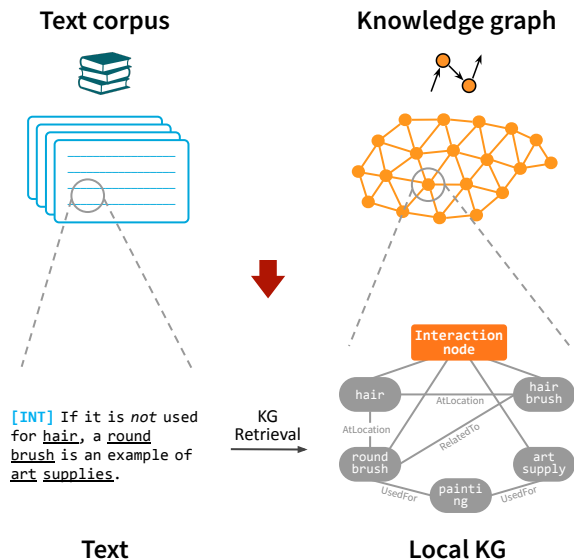
# (1) Text-KG Input

## Motivation

- Informative (text, local KG) pair:  
Text can contextualize the KG  
KG can ground the text

## Idea

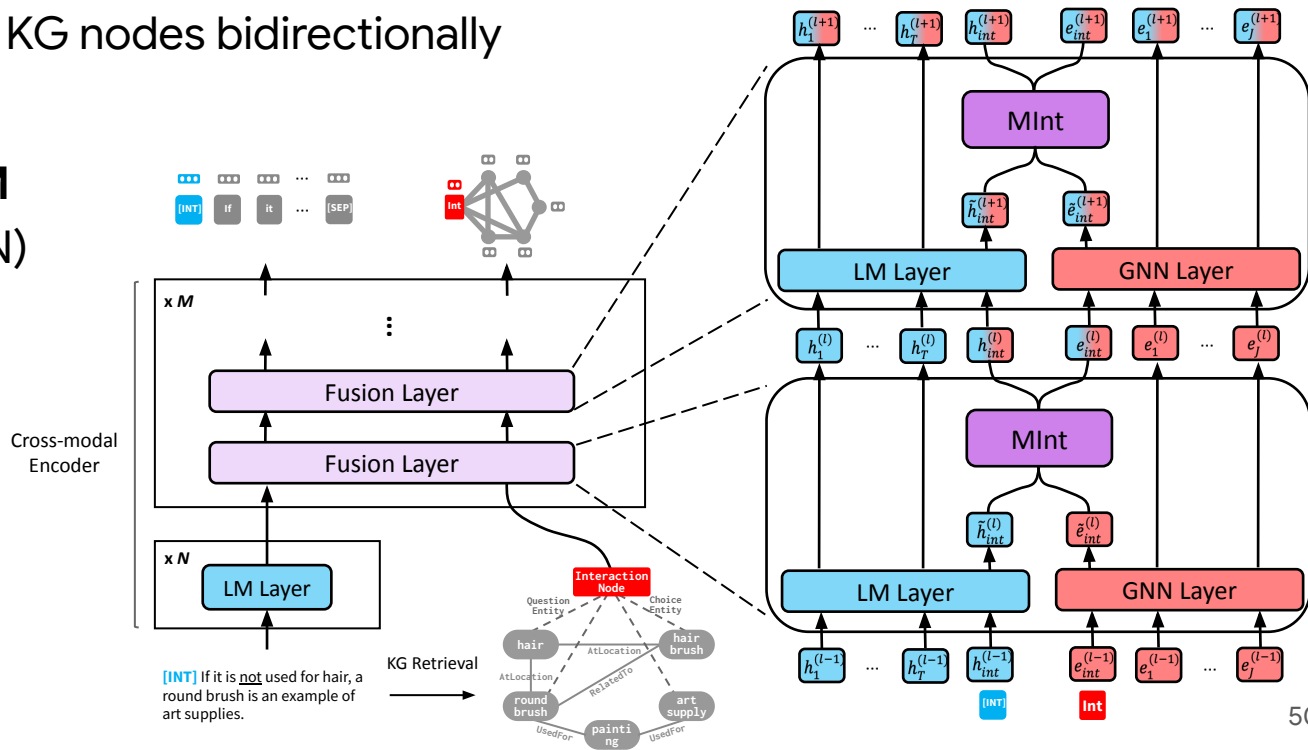
- Given text corpus and KG, create **aligned (text, local KG) pairs** by entity linking and getting neighbors in KG



## (2) Deep Bidirectional Cross-Modal Model

### Idea

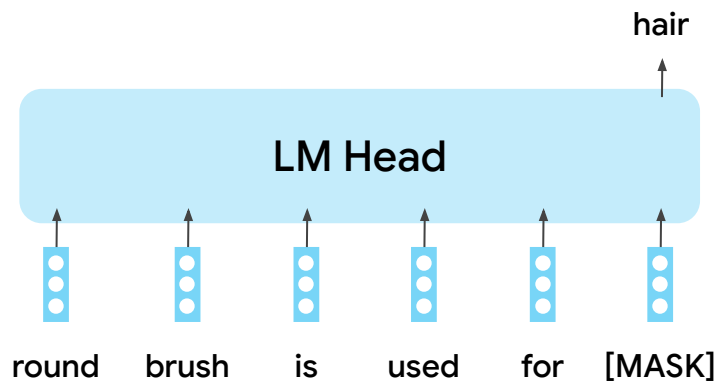
- Fuse text tokens & KG nodes bidirectionally for multiple layers
- Use the **GreaseLM** (Transformer+GNN) encoder



### (3) Bidirectional Self-Supervision

**Idea:** Joint self-supervised objectives

#### Masked LM

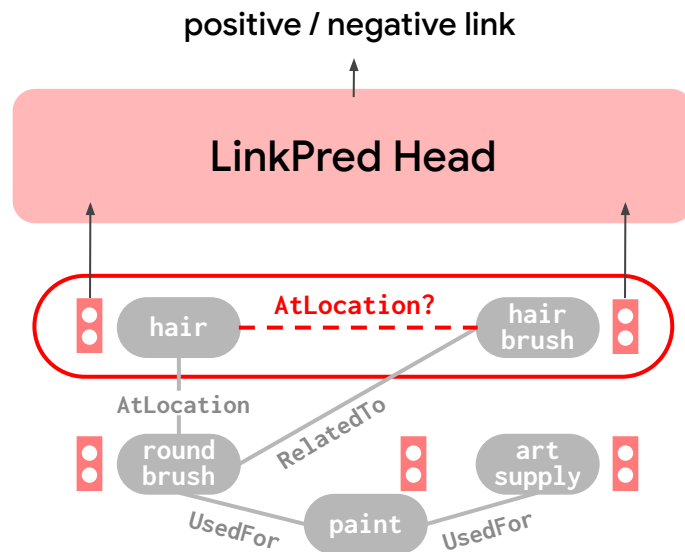


**Joint training**

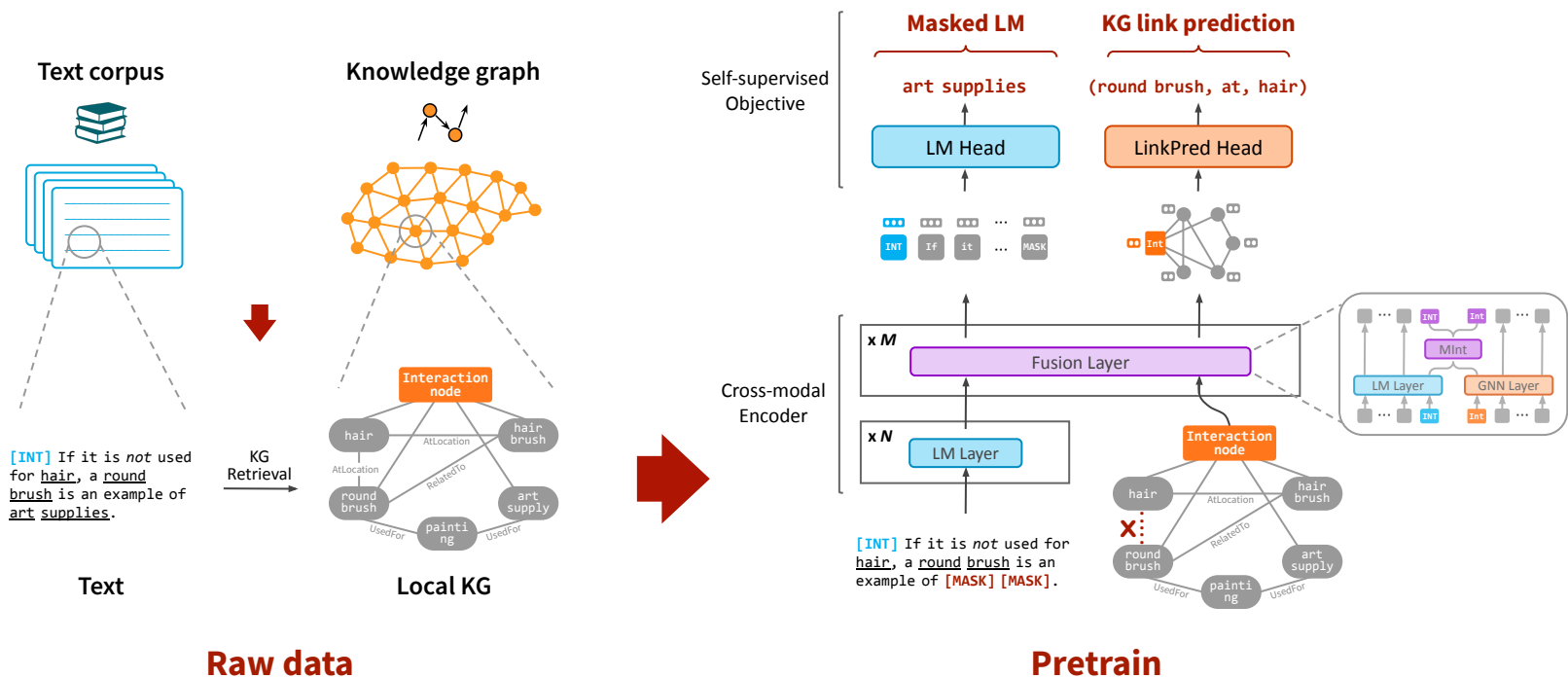


**Text & KG  
mutually inform  
each other**

#### KG Link Prediction



# Proposed Method: DRAGON



# Experiments

	General domain	Biomedical domain
Pretraining data	<b>Text:</b> <u>BookCorpus</u> (6GB) <b>KG:</b> <u>ConceptNet</u> (800K nodes, 2M edges)	<b>Text:</b> <u>PubMed</u> (20GB) <b>KG:</b> <u>UMLS</u> (300K nodes, 1M edges)
Downstream tasks	Commonsense reasoning ( <u>OBQA</u> , <u>RiddleSense</u> , <u>CommonsenseQA</u> , <u>CosmosQA</u> , <u>HellaSwag</u> , <u>PIQA</u> , <u>SIQA</u> , <u>aNLI</u> , <u>ARC</u> )	Biomedical reasoning ( <u>PubMedQA</u> , <u>BioASQ</u> , <u>MedQA-USMLE</u> )
Baseline: LM	RoBERTa ( <u>Liu+2019</u> )	BioLinkBERT ( <u>Yasunaga+2022</u> )
Baseline: LM finetuned with KG	RoBERTa + <u>GreaseLM</u>	BioLinkBERT + <u>GreaseLM</u>

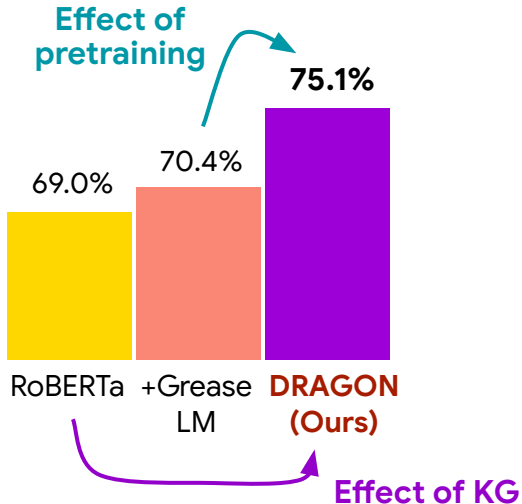
**Ours (DRAGON): LM *pretrained* with KG**

# Performance

## DRAGON makes consistent improvement across tasks and domains

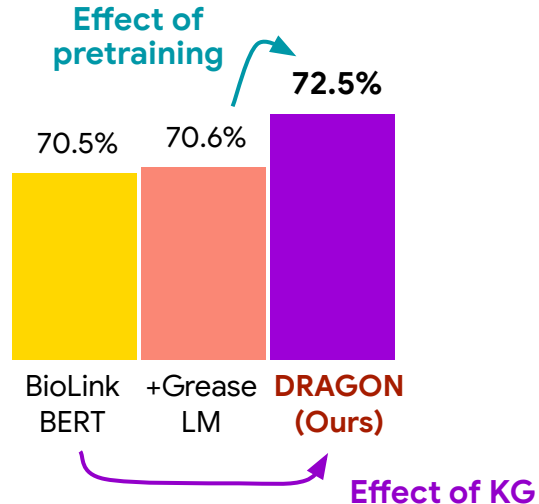
### Commonsense reasoning tasks

(e.g. OBQA, RiddleSense)



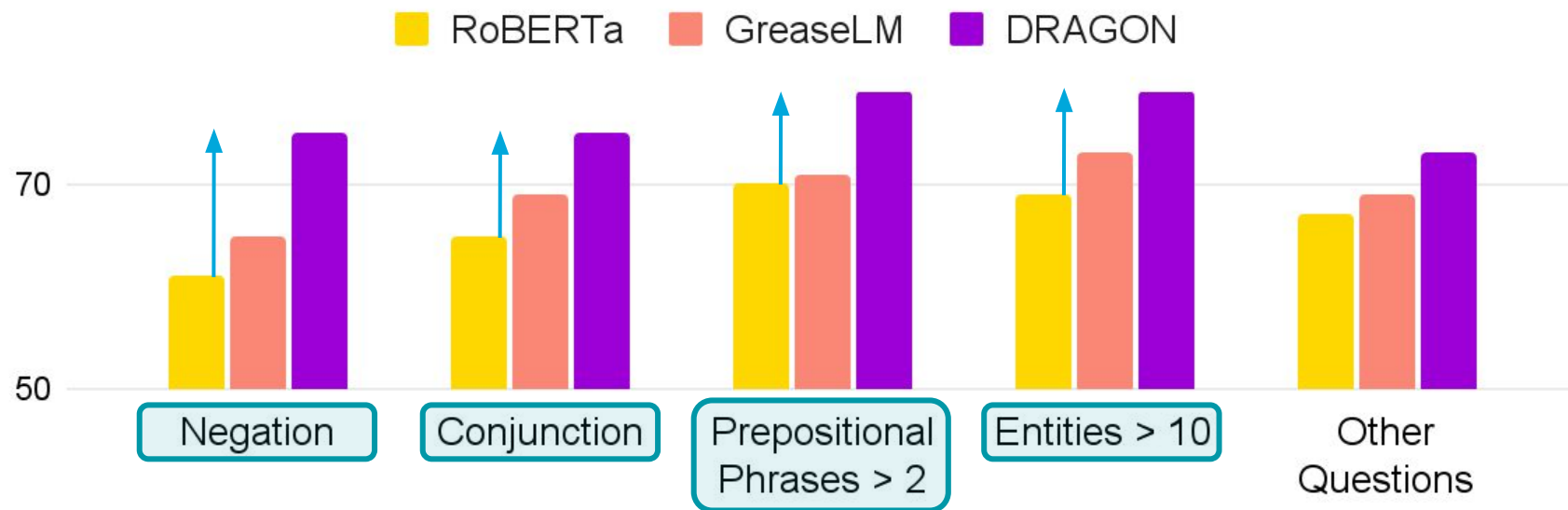
### Biomedical reasoning tasks

(e.g. PubMedQA, MedQA)



# Benefit: Complex Reasoning

Large gains on QA examples involving complex reasoning

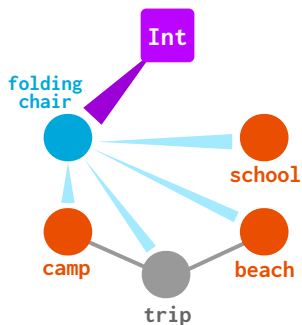


# Benefit: Complex Reasoning

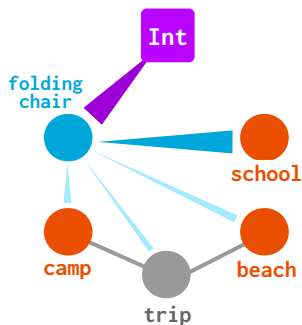
## Conjunction

Where would you use a **folding chair** and store one?

A. camp    **B. school**    C. beach



DRAGON  
GNN 1st Layer



DRAGON  
GNN Final Layer

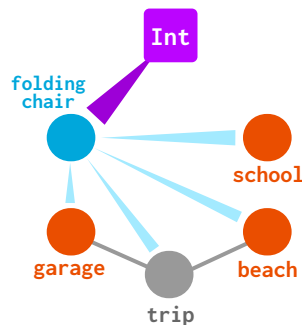
RoBERTa:  
A. camp (✗)  
  
GreaseLM:  
C. camp (✗)  
  
**DRAGON:**  
**B. school (✓)**

Model  
Prediction

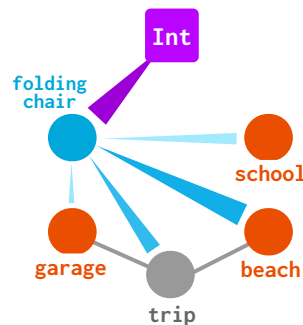
## Negation + Conjunction

Where would you use a **folding chair** but not store one?

A. garage    B. school    **C. beach**



DRAGON  
GNN 1st Layer



DRAGON  
GNN Final Layer

RoBERTa:  
B. school (✗)  
  
GreaseLM:  
B. school (✗)  
  
**DRAGON:**  
**C. beach (✓)**

Model  
Prediction

In DRAGON, KG serves as scaffold for performing structured/multi-step reasoning



# Summary

---

**DRAGON:** Pretrain a foundation model jointly on text & KGs

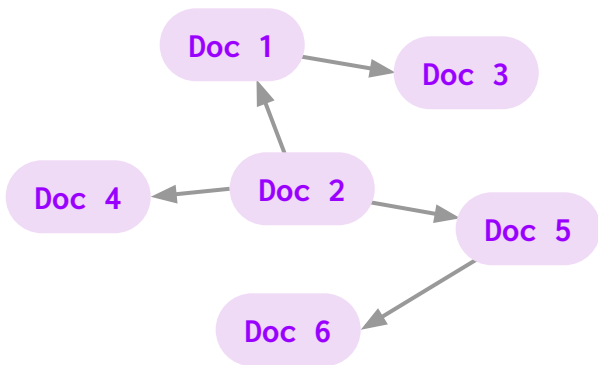
## Approach

- Deeply bidirectional model for the two modalities to interact
- Self-supervised objective to learn joint reasoning over text and KG at scale

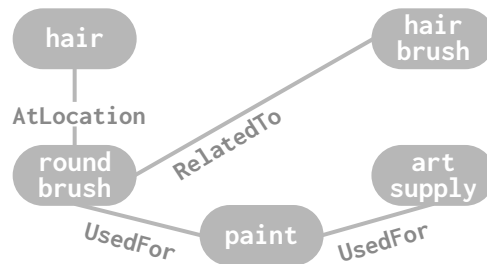
## Result

- Improved performance on knowledge- and reasoning-intensive applications (e.g. low-resource QA, multi-step reasoning)

# Final remarks



**LinkBERT**



**DRAGON**

**General principle:** graphs bring relevant documents/concepts closer together

**Open question:** how to better incorporate implicit relations (e.g., entity mentions w/o hyperlinks)

*...The campus occupies 8,180 acres (3,310 hectares), among the largest in the United States...*

**Open question:** how to perform more formal reasoning at scale?

# References

- Michihiro Yasunaga, Jure Leskovec, Percy Liang.  
[LinkBERT: Pretraining Language Models with Document Links](#). ACL 2022.
- Michihiro Yasunaga, Hongyu Ren, Antoine Bosselut, Percy Liang, Jure Leskovec.  
[QA-GNN: Reasoning with Language Models and Knowledge Graphs for Question Answering](#). NAACL 2021.
- Xikun Zhang, Antoine Bosselut, Michihiro Yasunaga, Hongyu Ren, Percy Liang, Chris Manning, Jure Leskovec.  
[GreaseLM: Graph REASoning Enhanced Language Models for Question Answering](#). ICLR 2022.
- Michihiro Yasunaga, Antoine Bosselut, Hongyu Ren, Xikun Zhang, Chris Manning, Percy Liang, Jure Leskovec.  
DRAGON: Deep Bidirectional Language-Knowledge Graph Pretraining. NeurIPS 2022.
- **Code/Models**
  - <https://github.com/michiyasunaga/LinkBERT>
  - <https://github.com/michiyasunaga/QAGNN>
  - <https://github.com/michiyasunaga/dragon>

# Collaborators

