# TRANSFORMER-XH: MULTI-HOP QUESTION AN-SWERING WITH EXTRA HOP ATTENTION

#### Anonymous authors

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#### Abstract

Transformers have obtained significant success modeling natural language as a sequence of text tokens. However, in many real world scenarios, textual data inherently exhibits structures beyond a linear sequence such as tree and graph; an important one being multi-hop question answering, where evidence required to answer questions are scattered across multiple related documents. This paper presents Transformer-XH, which uses eXtra Hop attention to enable the intrinsic modeling of structured texts in a fully data-driven way. Its new attention mechanism naturally "hops" across the connected text sequences in addition to attending over tokens within each sequence. Thus, Transformer-XH better answers multi-hop questions by propagating information between multiple documents, constructing global contextualized representations, and jointly reasoning over multiple pieces of evidence. This leads to a simpler multi-hop QA system which outperforms previous state-of-the-art on the HotpotQA FullWiki setting by large margins.

#### **1** INTRODUCTION

Transformers effectively model natural language in *sequential* form (Vaswani et al., 2017; Dai et al., 2019; Devlin et al., 2019; Yang et al., 2019). Nevertheless, in many NLP tasks, text does not simply appear as a linear sequence of tokens but rather carries meaningful structure in the form of paragraphs, headings, and hyperlinks. These structures can be abstracted into trees or graphs with nodes and edges. Multi-hop question answering (Yang et al., 2018) is one such task in which structure plays an important role, since the evidence required to formulate the answer is scattered across multiple documents, requiring systems to jointly reason across links between them.

Recent approaches leverage pre-trained Transformers (e.g., BERT) for multi-hop question answering (QA) by converting the structural reasoning task into sub-tasks that model flat sequences. For example, Min et al. (2019b) decompose a multi-hop question into a series of single-hop questions; Ding et al. (2019) conduct several steps of single-hop reading comprehension to simulate the multihop reasoning. The hope is that additional processing to fuse the outputs of the sub-models can recover all the necessary information from the original structure. While pre-trained Transformer language models have shown improvements on multi-hop QA, manipulating the inherent structure of the problem to fit the rigid requirements of out-of-the-box models can introduce problematic assumptions or information loss.

This paper presents Transformer-XH (meaning eXtra Hop), which upgrades Transformers with the ability to natively represent structured texts. Transformer-XH introduces extra hop attention in its layers that connects different text pieces following their inherent structure while also maintaining the powerful pre-trained Transformer abilities over each textual piece individually. Our extra hop attention enables 1) a more global representation of the evidence presented by each piece of text as it relates to the other evidence, and 2) a more natural way to jointly reason over an evidence graph by propagating information along edges necessary to complete the task at hand.

We apply Transformer-XH to HotpotQA, a challenging benchmark for the multi-hop question answering task (Yang et al., 2018). Rather than decomposing the task into a series of sub-tasks to fit the constraints of pre-trained Transformers, Transformer-XH is a solution that fits the problem as it naturally occurs. It is a single model that represents and combines evidence from multiple documents to construct the answer.



Figure 1: The eXtra Hop attention in Transformer-XH (a) and its application to multi-hop QA (b).

On HotpotQA's FullWiki setting, which is a more realistic setup and requires stronger multihop reasoning ability (Min et al., 2019b; Jiang & Bansal, 2019), Transformer-XH outperforms CogQA (Ding et al., 2019), the previous start-of-the-art, by 12 points on answer F1. It also beats the contemporary BERT based pipeline SR-MRS (Nie et al., 2019), by 3 points. The results follow from our simple yet effective design, with one unified model operating over the inherent structure of the task, rather than melding the outputs from disparate sub-tasks adapted to the sequential constraints of pre-trained Transformer. Our ablation analysis demonstrates Transformer-XH's efficacy on questions that are known to require multi-hop reasoning (Min et al., 2019b), and that the source of this success is due to the eXtra Hop attention mechanism's ability to combines information from multiple documents.

#### 2 Model

This section first discusses preliminaries on sequential Transformers, then we show how we incorporate eXtra hop attention to create Transformer-XH.

#### 2.1 PRELIMINARIES

Transformers represent a sequence of input text tokens  $X = \{x_1, ..., x_i, ..., x_n\}$  into contextualized distributed representations  $H = \{h_1, ..., h_i, ..., h_n\}$  (Vaswani et al., 2017). This process involves multiple stacked self-attention layers that converts the input X into  $\{H^0, H^1, ..., H^l, ..., H^l\}$ , starting from  $H^0$ , the embeddings, to the final layer of depth L.

The key idea of Transformer is its attention mechanism, which calculates the *l*-th layer output  $H^l$  using the input  $H^{l-1}$  from the previous layer:

$$H^{l} = \operatorname{softmax}\left(\frac{Q \cdot K^{T}}{\sqrt{d_{k}}}\right) \cdot V^{T},\tag{1}$$

$$Q^{T}; K^{T}; V^{T} = W^{q} \cdot H^{l-1}; W^{k} \cdot H^{l-1}; W^{v} \cdot H^{l-1}.$$
(2)

It includes three projections on the input  $H^{l-1}$ : Query (Q), Key (K), and Value (V).

Specifically, the slices of token  $h_i^l$  in Eqn.(2) is:

$$h_i^l = \sum_j \operatorname{softmax}_j(\frac{q_i^T \cdot k_j}{\sqrt{d_k}}) \cdot v_j, \tag{3}$$

which first calculates its attention to all other tokens j in the sequence and then combines the token values  $v_j$  into a new representation  $h_i^l$ , using the normalized attention weights. Multiple attentions can be used in one Transformer layer and concatenated as multi-head attention (Vaswani et al.,

2017). The architecture is stacked to form rather deep networks, which leads to significant success of large pre-trained Transformer models (Devlin et al., 2019; Liu et al., 2019).

A challenge of Transformer is that its attention is calculated over all token pairs (Eqn. 3), which is hard to scale to long text sequences. Transformer-XL (eXtra Long) addresses this challenge by breaking down longer texts, e.g., a multi-paragraph document, into a sequence of text segments:  $\{X_1, ..., X_{\tau}, ..., X_{\zeta}\}$ , and propagates the information between adjacent text segments using the following attention:

$$\tilde{H}_{\tau}^{l-1} = [\text{Freeze}(H_{\tau-1}^{l-1}) \circ H_{\tau}^{l-1}].$$
(4)

It concatenates ( $\circ$ ) the representation of the previous segment  $H_{\tau-1}^{l-1}$  to the current segment as segment level recurrences. The new representation  $\tilde{H}_{\tau}^{l-1}$  includes the information from previous segment and is integrated in the new attention mechanism:

$$\tilde{Q}^{T}; \tilde{K}^{T}; \tilde{V}^{T} = W^{q} \cdot H^{l-1}_{\tau}; W^{k} \cdot \tilde{H}^{l-1}_{\tau}; W^{v} \cdot \tilde{H}^{l-1}_{\tau}.$$
(5)

The attention over the previous segment allows Transformer-XL to effectively model long form text data recurrently as a sequence of text chunks (Dai et al., 2019).

Nevertheless, in many scenarios, the text segments are organized in nontrivial structures beyond a linear sequence. For example, documents are connected by hyperlinks in a graphical structure that does not readily simplify to form a linear sequence, prohibiting Transformer-XL's recurrent approach.

#### 2.2 TRANSFORMER-XH WITH EXTRA HOP ATTENTION

Transformer-XH models structured text sequence by linking them with eXtra Hop attention following their original structure. As illustrated in Figure 1a, to model three connected documents  $d_2 \rightarrow d_1 \rightarrow d_3$ , Transformer-XH uses eXtra Hop attention to propagate information along the graph edges, enabling information sharing between connected text sequence.

Formally, the structured text data includes a set of nodes,  $\mathcal{X} = \{X_1, ..., X_{\tau}, ..., X_{\zeta}\}$ , each corresponding to a text sequence, and an edge matrix E, which includes the connections (e.g., links) between them. The goal is to learn representations  $\mathcal{H} = \{\tilde{H}_1, ..., \tilde{H}_{\tau}, ..., \tilde{H}_{\zeta}\}$ , that incorporate not only the local information in each sequence X, but also the global contexts on the entire structured text  $\{\mathcal{X}, E\}$ .

Transformer-XH achieves this by two attention mechanisms: in-sequence attention and eXtra Hop attention. The *in-sequence attention* is the same as vanilla Transformer: in layer l, token i gathers information from other tokens inside the same text piece  $\tau$ :

$$h_{\tau,i}^{l} = \sum_{j} \operatorname{softmax}_{j} \left( \frac{q_{\tau,i}^{T} \cdot k_{\tau,j}}{\sqrt{d_{k}}} \right) \cdot v_{\tau,j}.$$

$$(6)$$

The *eXtra Hop attention* uses the first token in each sequence – the added special token "[CLS]" – as an "attention hub", which attends on all other connected nodes' hub token. In layer l, the  $\tau$ -th text sequence attends on other text sequence  $\eta$  if there is an edge between them  $(e_{\tau\eta} = 1)$ :

$$\hat{h}_{\tau,0}^{l} = \sum_{\eta; e_{\tau\eta} = 1} \operatorname{softmax}_{\eta} \left( \frac{\hat{q}_{\tau,0}^{T} \cdot \hat{k}_{\eta,0}}{\sqrt{d_k}} \right) \cdot \hat{v}_{\eta,0}.$$
(7)

Node  $\tau$  calculates the attention weight on its neighbor  $\eta$  using hop query  $\hat{q}_{\tau,0}$  and key  $\hat{k}_{\eta,0}$ . Then it uses the weights to combine its neighbors' value  $\hat{v}_{\eta,0}$  and forms a globalized representation  $\hat{h}_{\tau,0}^l$ .

The two attention mechanism are combined to form the new representation of layer *l*:

$$\hat{h}_{\tau,0}^{l} = \text{Linear}([h_{\tau,0}^{l} \circ \hat{h}_{\tau,0}^{l}]),$$
(8)

$$\tilde{h}_{\tau,i}^l = h_{\tau,i}^l; \forall i \neq 0.$$
(9)

Note that the non-hub tokens  $(i \neq 0)$  still have access to the hop attention in the previous layer through Eqn. (6).

One layer of eXtra Hop attention can be viewed as single-step of information propagation along edges E. For example, in Figure 1a, the document node  $d_3$  updates its representation by gathering information from its neighbor  $d_1$  using the hop attention  $d_1 \rightarrow d_3$ . When multiple Transformer-XH layers are stacked, this information in  $d_1$  includes both  $d_1$ 's local contexts from its in-sequence attention, and cross-sequence information from the hop attention  $d_2 \rightarrow d_1$  of the l-1 layer. Hence, an L-layer Transformer-XH can attend over information from up to L hops away.

Together, three main properties equip Transformer-XH to effectively model raw structured text data: the propagation of information (values) along edges, the importance of that information (hop attention weights), and the balance of in-sequence and cross-sequence information (attention combination). The representations learned in  $\mathcal{H}$  can innately express nuances in structured text that are required for complex chains of reasoning in tasks such as multi-hop QA.

# **3** APPLICATION TO MULTI-HOP QUESTION ANSWERING

This section describes how Transformer-XH applies to multi-hop QA. Given a question q, the task is to find an answer span a in a large open-domain document corpus, e.g. the first paragraph of all Wikipedia pages. By design, the questions are complex and often require information from multiple documents to answer. For example, in the case shown in Figure 1b, the correct answer "Cambridge" requires combining the information from both the Wikipedia pages "Facebook" and "Harvard University". To apply Transformer-XH in the open domain multi-hop QA task, we first construct an evidence graph and then apply Transformer-XH on the graph to find the answer.

**Evidence Graph Construction.** The first step is to find the relevant candidate documents D for the question q and connect them with edges E to form the graph G. Our set D consists of three sources. The first two sources are from canonical information retrieval and entity linking techniques:

- $D_{ir}$ : the top documents retrieved by TF-IDF matching on the question (e.g., "Facebook") (Chen et al., 2017),
- $D_{el}$ : the documents associated with the entities that appear in the question (e.g., "Mark Zuckerberg"), annotated by entity linking systems (Ferragina & Scaiella, 2010; Hasibi et al., 2017).

For better retrieval quality, we use a BERT ranker (Nogueira & Cho, 2019) on the set  $D_{ir} \cup D_{el}$  and keep top K ranked ones. Then the third source  $D_{exp}$  include all documents connected to or from any top ranked documents via Wikipedia hyperlinks (e.g., "Facebook"  $\rightarrow$  "Harvard University").

The final graph comprises all documents from the three sources as nodes  $\mathcal{X}$  and the Wikipedia links between them to form edge matrix E, i.e.  $e_{ij} = 1$  if there is a hyperlink from document i to j. Similar to previous work (Ding et al., 2019), the textual representation for each node in the graph is the [SEP]-delimited concatenation of the question, anchor text<sup>1</sup> and the paragraph itself. More details and analysis of the evidence graph construction are in Appendix Section A.1.

**Transformer-XH on Evidence Graph.** Transformer-XH takes the input nodes  $\mathcal{X}$  and edges E, and produces the global representation of all text sequences:

$$\mathcal{H}^{L} = \text{Transformer-XH}(\mathcal{X}, E).$$
(10)

Then we add two task-specific layers upon the last layer's representation  $\mathcal{H}^L$ : one auxiliary layer to predict the relevance score of the evidence node, and one layer to extract the answer span within it:

$$p(\text{relevance}|\tau) = \text{Linear}(h_0^L); \tag{11}$$

$$p(\text{start}|\tau, i), p(\text{end}|\tau, j) = \text{Linear}(\hat{h}_{\tau,i}^L), \text{Linear}(\hat{h}_{\tau,j}^L).$$
(12)

The final model is trained end-to-end with cross-entropy loss for both tasks in a multi-task setting. During inference, we first select the document with the highest relevance score, and then the start and end positions of the answer within that document.

<sup>&</sup>lt;sup>1</sup>i.e. the text in the hyperlink in parent nodes pointing to the child node

# 4 EXPERIMENTAL METHODOLOGIES

**Dataset.** We conduct our experiments on HotpotQA, the multi-hop question answering benchmark dataset (Yang et al., 2018). It includes 112k crowd-sourced questions designed to require multiple pieces of textual evidence, which are the first paragraphs of Wikipedia pages. It has two type of questions: bridge question require hopping via an outside entity, and comparison question compare a property of two entities. There are two settings in HotpotQA. The Distractor setting provides golden evidence paragraphs together with TF-IDF retrieved negatives. The FullWiki setting requires systems to retrieve evidence paragraphs from the full Wikipedia.

We focus on FullWiki setting since previous research found that the negative documents in Distractor may be too weak and mitigate the needs of multi-hop reasoning (Min et al., 2019b). There are 90k Train, 7k Dev and 7k Test questions. The ground truth answer and supporting evidence sentences in Train and Dev sets are provided. Test labels are hidden; only one submission is allowed to the leaderboard per 30 days<sup>2</sup>. We evaluate our best model on Test and conduct ablations on Dev.

**Metrics.** We use official evaluation metrics of HotpotQA. They include exact match (EM) and F1 on answer (Ans), supporting facts (Supp), and the combination (Joint). The supporting facts prediction is an auxiliary task that evaluates model's ability to find the evidence sentences. Joint EM is the product of the two EM result. Joint F1 first multiplies the precision and recall from Ans and Supp, then combines the Joint precision and recall to F1.

**Baseline.** We compare with previous approaches on the FullWiki setting, including Official Baseline (Yang et al., 2018), MUPPET (Feldman & El-Yaniv, 2019), QFE (Nishida et al., 2019), DecompRC (Min et al., 2019a), Cognitive QA (CogQA, Ding et al. (2019)), and Semantic Retrieval MRS (SR-MRS, Nie et al. (2019)). We also build our BERT Pipeline baseline, which decomposes the task into several sub components and uses BERT based models on every component.

CogQA is our major baseline and was the previous public SOTA. It uses several fine-tuned BERT machine reading comprehension (MRC) models to find hop entities and candidate spans, and then uses Graph Convolution Network to rank the candidate spans, which is on top of BERT.

SR-MRS is a contemporary work<sup>3</sup> and was the previous leaderboard rank one. It is a BERT based pipeline and uses fine-tuned BERT models to first rank the documents (twice), then to rank sentences to find supporting facts, and finally conduct BERT MRC on the concatenated evidence sentences.

**Implementation Details.** The in-sequence attention and other standard Transformer components in Transformer-XH are initialized by the pre-trained BERT base model (Devlin et al., 2019). The extra hop attention parameters are initialized randomly and trained from scratch. We set the max hops in the reasoning graph to three, following the nature of HotpotQA (Yang et al., 2018). More details of Transformer-XH and our BERT Pipeline can be found in the Appendix A.2 and A.4.

# 5 EVALUATION RESULTS

This section presents the evaluation results on Hotpot QA and analyzes the influence of different design choices of Transformer-XH, and evidence graph structure.

# 5.1 OVERALL RESULT

We present the overall results of HotpotQA FullWiki setting in Table 1. Transformer-XH outperforms all previous methods by significant margins. Compared with CogQA, our main baseline, the improvements are consistently more than 10 absolute points.

The only exception is Supp F1, where SR-MRS performs slightly better, though with much lower Supp EM. We think the reason is mainly from the search space variation. After predicting the answer, we select the supporting facts along the inference path (i.e., from all the parents node) which naturally fits the task purpose but would hurt the recall (more details in Appendix).

<sup>&</sup>lt;sup>2</sup>https://hotpotqa.github.io/

<sup>&</sup>lt;sup>3</sup>The ArXiv version is released one week before the submission of this work

	Dev				Test							
	Ans		Supp		Joint		Ans		Supp		Joint	
	EM	F1	EM	F1	EM	F1	EM	F1	EM	F1	EM	F1
Official Baseline	23.9	32.9	5.1	40.9	47.2	40.8	24.0	32.9	3.9	37.7	1.9	16.2
DecompRC	-	43.3	-	-	-	-	30.0	40.7	-	-	-	-
QFE	-	-	-	-	-	-	28.7	38.1	14.2	44.4	8.7	23.1
MUPPET	31.1	40.4	17.0	47.7	11.8	27.6	30.6	40.3	16.7	47.3	10.9	27.0
CogQA	37.6	49.4	23.1	58.5	12.2	35.3	37.1	48.9	22.8	57.7	12.4	34.9
SR-MRS*	46.5	58.8	39.9	71.5	26.6	49.2	45.3	57.3	38.7	70.8	25.1	47.6
Our Pipeline	44.8	57.7	29.2	62.8	18.5	43.4	-	-	-	-	-	-
Transformer-XH	49.8	62.3	42.2	71.6	27.4	51.0	49.0	60.8	41.7	70.0	27.1	49.6

Table 1: Results (%) on HotpotQA FullWiki Setting. Dev results of previous methods are reported in their papers. Test results are from the leaderboard. Contemporary method is marked by \*. Best result is marked **bold**.

	Question Type					Reasoning Type			
	Comparison (1487)		Bridge (5918)		Single-Hop (3426)		Multi-Hop (3979)		
	EM	F1	EM	F1	Node	EM	F1	EM	F1
CogQA	43.3	51.1	36.1	49.0	-	45.1	61.1	31.1	39.4
Our Pipeline	54.1	60.9	42.4	56.9	-	52.0	69.3	38.6	47.8
Transformer-XH	54.1	60.9	48.7	62.6	72.7	57.4	74.0	43.3	52.2

Table 2: Dev Answer Accuracy (%) on different scenarios. Reasoning Types are provided by Min et al. (2019b). We show the number of questions in each category in brackets.

Besides strong results, Transformer-XH's ability to natively represent structured data leads to much simpler QA system. Previously, in order to utilize pre-trained BERT, Hotpot QA approaches adapted the multi-hop reasoning task to comprise multiple sub-tasks. For example, given the re-trieved documents, our pipeline approach first leverages one BERT MRC model to find hop entities and then another BERT MRC model to find candidate answer spans. After that, it ranks the candidate answer spans using a BERT initialized GAT, which is the only structure modeling step. In comparison, Transformer-XH is a unified model which directly represents structured texts and incorporates pre-trained BERT weights.

Table 2 further inspects model performance on the Dev set by question type (Comparison or Bridge) and reasoning type (Single-Hop v.s. Multi-Hop). Compared with baselines, Transformer-XH consistently achieves stronger results on all categories. And on multi-hop questions, Transformer-XH has more relative gains (39% over CogQA on EM) than single-hop question (27%), which demonstrates its stronger multi-hop reasoning capability. We further study this property in Section 5.3.

#### 5.2 Ablation Studies

**Model Variations.** We show the results of different model variations on the top left of Table 3. *Single-Hop BERT* uses BERT MRC model on each document individually, which significantly decreases the accuracy, confirming the importance of multi-hop reasoning in FullWiki setting (Min et al., 2019a). *GAT* + *BERT* first uses Graph Attention Network (Veličković et al., 2017) on the evidence graph to predict the best node; then it uses BERT MRC on the best document. It is 10% worse than Transformer-XH since the MRC model has no access to the information from other documents. *No Node Prediction* eliminates the node prediction task and only trains on span prediction task; the accuracy difference shows node prediction task helps the model training.

**Graph Structures.** We show Transformer-XH's performance with different graph structures on the bottom left of Table 3. *Bidirectional Edges* adds reverse edges along the hyperlinks; *Fully Connected Graph* connects all document pairs; *Node Sequence* randomly permutes the documents and connects them into a sequence to simulate the Transformer-XL setting. Both *Bidirectional Links* and *Fully Connected Graph* have comparable performance with the original graph structure. Transformer-XH is able to learn meaningful connections using its hop attentions and is less dependent on the pre-existing graph structural. The fully connected graph can be used if there is no strong

Model Ablation		Ans	Hon Stone	Dev Ans	
		F1	The steps	EM	F1
Single-Hop BERT MRC on Individual Documents		42.2	One Hop	46.9	60.7
GAT (Node Prediction) + BERT (MRC on Best Node)		58.8	Two Hops	47.9	62.1
No Node Prediction Multi-Task		54.4	Four Hops	48.0	61.9
Bidirectional Edges on Hyperlinks		62.2	Five Hops	47.4	61.6
Fully Connected Graph		62.4	Six Hops	46.7	60.7
Node Sequence (Bidirectional Transformer-XL)		20.7	Transformer-XH	48.7	62.6

Table 3: Ablation studies on the bridge questions on Dev answer accuracy (%), including model components (top left), graph structures (bottom left), and hop steps (right). Transformer-XH's full model uses three hop steps and the original Wikipedia hyperlink graph.



Figure 2: Distributions of learned attention weights of three hops on three groups: From All (Node)  $\rightarrow$  (to) All, All  $\rightarrow$  (to) Ans (ground truth answer node), and Supp (nodes with the supporting facts)  $\rightarrow$  (to) Ans. X-axes are attention values scaled by number of nodes.

edge patterns available in the task. However, the performance drops significantly on *Node Sequence*, showing that structured texts cannot be treated as a linear sequence which cuts off many connections.

**Hop Steps.** Recall that a Transformer-XH layer with extra hop attention corresponds to one information propagation (hop) step in the graph. Thus Transformer-XH with last K layers conducts K-step attention hops in the graph. We show results with different K on the right side of Table 3. Transformer-XH reaches its peak performance with three hops (our full-model). This is expected as most Hotpot QA questions can be answered by two documents (Yang et al., 2018).

#### 5.3 HOP ATTENTION ANALYSIS

This experiment analyzes the hop attentions using our full-model (three-hop) on the fully connected graph to study their behavior without pre-defined structure. Figure 2 plots the distributions of the learned hop attentions on the Dev set. It shows a strong shift away from the normal distribution with more hops. Transformer-XH learns to distinguish different nodes after multi-hop attention: the attention score becomes a bimodal distribution after three hops, ignoring some non-useful nodes. Transformer-XH also learns to focus on meaningful edges: the score is higher on the path Supp $\rightarrow$ Ans than All $\rightarrow$ Ans. And the margin is larger as the hop step increases from one to three.

# 5.4 CASE STUDY

Table 4 lists two examples from Transformer-XH and our BERT Pipeline. The first case has a clear evidence chain "2011/S/S"  $\rightarrow$  "Winner"  $\rightarrow$  "YG Entertainment"; both methods find the correct answer. However, the second case has too many distractors in the first document. Without additional clues from document 2, it is likely that the single-hop hop entity extraction component in our pipeline approach misses the correct answer document in its candidate sets; and the later structural reasoning component can not recover from this cascade error. In comparison, Transformer-XH finds the correct answer by combining the evidence with the hop attentions between the two evidence pieces. We leave more positive and negative cases in Appendix A.5.

Q: <u>2014 S/S</u> is the debut album of a South Ko-	Q: Which man who presented					
rean boy group that was formed by who?	2022 FIFA World Cup bid was born on					
<b>Document 1</b> : <u>2014 S/S</u> is the debut album of	October 22, 1930?					
South Korean group Winner.	<b>Document 1</b> : 2022 FIFA World Cup bid was					
<b>Document 2</b> : <u>Winner</u> is a South Korean boy	presented by Frank Lowy, Ben Buckley,					
group formed in 2013 by <b>YG Entertainment</b> .	Quentin Bryce and Elle Macpherson.					
Prediction:	Document 2: Frank Lowy (born 22 October					
Transformer-XH: YG Entertainment √	1930), is an Australian-Israeli businessman and					
<b>Pipeline</b> : YG Entertainment $\checkmark$	Chairman of Westfield Corporation.					
-	Prediction:					
	<b>Transformer-XH</b> : Frank Lowy √					
	<b>Pipeline</b> : Quentin Bryce X					

Table 4: Examples of Transformer-XH and BERT pipeline results in Hotpot QA.

# 6 RELATED WORK

Machine reading comprehension is an important task of natural language processing (Rajpurkar et al., 2016; Bajaj et al., 2016). The initial MRC questions are mostly single-hop, which only require single evidence sentence to answer (Min et al., 2018). One direction to make the task more realistic is open-domain question answering (QA), in which the evidence paragraph has to be retrieved from a large corpus (Chen et al., 2017). The other direction is multi-hop QA, where the questions require multiple pieces of evidence to answer (Welbl et al., 2018; Yang et al., 2018).

The FullWiki setting of HotpotQA is a combination of open-domain QA and multi-hop QA (Yang et al., 2018): the questions are designed to require multiple pieces of evidence and these evidence pieces are documents to retrieve from the entire Wikipedia. The combination makes this setting rather challenging. The retrieved documents are inevitably noisy and include much stronger distractors than the TF-IDF retrieved negative documents in the Distractor setting (Min et al., 2019a; Jiang & Bansal, 2019).

Various solutions have been proposed for Hotpot QA (Min et al., 2019b; Feldman & El-Yaniv, 2019; Nishida et al., 2019). These solutions often use complicated pipelines to adapt the multi-hop task into a combination of single-hop tasks, in order to leverage the advantage of pre-trained models. For example, CogQA (Ding et al., 2019) uses two BERT based MRC model to find candidate spans and then another BERT initialized Graph Neural Network (GNN) to rank spans; SR-MRS (Nie et al., 2019) uses three BERT based rankers to find supporting sentences, and then another BERT MRC model on the concatenated sentences to get the answer span. Transformer-XH is a simpler model that directly represents and reasons with multiple pieces of evidence using extra hop attentions.

In addition to Transformer-XL (Dai et al., 2019), Transformer-XH is also inspired by GNN (Kipf & Welling, 2017; Schlichtkrull et al., 2017; Veličković et al., 2017), which leverages neural networks to model graph structured data. The key difference is that a "node" in Transformer-XH is a text sequence, and modeling of the structure is conducted jointly with the representation of the text. Transformer-XH combines the advantages Transformer has in understanding text with the power that GNN has in modeling structure.

# 7 CONCLUSION

Transformer-XH and its eXtra Hop attention mechanism is a simple yet powerful adaptation of Transformer to learn better representations of structured text data as it naturally occurs. It innately integrates with pre-trained language models to allow for complex reasoning across many hops of a textual evidence graph, where clues to the correct answer of a question are split across multiple documents. When applied to HotpotQA, Transformer-XH significantly shrinks the typical multi-hop QA pipeline, eliminating many cascading errors that arise from the linear sequence input constraints of pre-trained Transformers. Compared to previous SOTA baselines that use pipelines of BERT models to mimic multi-hop reasoning, one Transformer-XH model is all we need to obtain a much stronger answer accuracy. With its simplicity and efficacy, we envision Transformer-XH will benefit many applications in the near future.

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#### A APPENDIX

- A.1 HOTPOTQA EVIDENCE GRAPH CONSTRUCTION DETAILS
- A.1.1 GRAPH CONSTRUCTION DETAILS

To construct the evidence graph, we start with extracting documents directly from question. This step contains both documents from information retrieval  $D_{ir}$  and entity linking  $D_{el}$ . The goal of this step is to have a reasonable size set with high recall of necessary information, i.e., supporting pages.

	CogQA	Top2 IR/entities	Top5 IR/entities	Top10 IR/entities		
Supp Recall	70.8	72.3	76.5	78.9		
Graph Recall	-	88.1	89.6	91.1		

Table 5: Supporting facts recall (%) of first step extracted entities and answer recall of the evidence graph. CogQA includes Top-10 TFIDF ranked (IR) entities and linked question entities.

We use Top-100 ranked documents for  $D_{ir}$ . For  $D_{el}$ , to increase the recall of existing entity linking tool, we combine the output from two entity linking tools TagMe (Ferragina & Scaiella, 2010) and CMNS (Hasibi et al., 2017).

We use BERT ranker (Nogueira & Cho, 2019) to re-rank the initial set. The input to the BERT is the concatenation of question and first paragraph of document, and it outputs the relevance score of the document. To make sure the documents corresponding to question entities are extracted, we use SpaCy (Honnibal & Montani, 2017) to tag question named entities, and choose the top-1 ranked documents for each tagged entity from  $D_{el}$ . For  $D_{ir}$ , we choose the top-K documents. We experiment with different K in Sec A.1.2, and use K=2 as document set D for the next step.

Then we use Wikipedia hyperlinks over top-ranked documents D to get the expanded document set  $D_{exp}$ . We use the same BERT ranker to rank  $D_{exp}$  for the top-K documents. This step is for the memory efficiency purpose and we choose a relatively large K = 15. We report our final graph recall in Sec A.1.2.

## A.1.2 RETRIEVAL RESULT

Table 5 compares the coverage of supporting facts between CogQA and our approach. Our two-step ranking is helpful, which increases the coverage from 70.8% to 78.9%. Also the high answer recall of evidence graph provides a good basis for Transformer-XH modeling.

# A.2 OTHER HOTPOT QA COMPONENTS

This section describes the other components for HotpotQA dataset. The whole QA system starts with question classification. For bridge question, we use Transformer-XH over evidence graph to get the answer. For comparison question, we use BERT based model to predict the span or yes/no as answer. Besides answer prediction, we also adopt BERT based model for predicting supporting sentences.

#### A.2.1 QUESTION CLASSIFICATION

The first component of our system is to classify the question to bridge and comparison types. We adopt BERT classification fine-tuning setting on HotpotQA questions with 99.1% accuracy on the dev set.

#### A.2.2 SUPPORTING FACTS CLASSIFICATION

The supporting facts prediction task is to extract all sentences that help get the answer. For bridge question, these sentences usually cover different pieces of questions. And for comparison questions, the supporting facts are the properties of two question entities. We design one model architecture for this task, but we train two model on each type to reflect the inherent difference.

We use BERT as our base model and on top of BERT, we conduct multi-task learning scheme. The first task is document relevance prediction, similar as Transformer-XH, we add a linear layer on the [CLS] token of BERT to predict the relevance score. The other task is sentence binary classification, we concatenate the first and last token representation of each sentence in the document through a linear layer, the binary output decides whether this sentence is supporting sentence.

**Bridge question supporting facts prediction** For bridge questions, we predict supporting facts after answer prediction from Transformer-XH to resume the inference chain. We start by predicting supporting facts in the answer document. The other document is chosen from the parents of the

answer document in the evidence graph.<sup>4</sup>. Compare with the contemporary model Nie et al. (2019), which does not limit the search space along the inference chain (i.e., the answer document may not be relevant to the other supporting page), our method more naturally fits the task purpose.

**Comparison question supporting facts prediction** For comparison questions, after extracting the first step documents D, we simply run this supporting facts prediction model to select the top-2 documents, and predict the corresponding supporting facts.

## A.2.3 ANSWER COMPARISON QUESTIONS

After predicting supporting facts, we concatenate the sentences and follow Min et al. (2019b) to run a BERT MRC model to predict either span or yes/no as the answer. As shown in Table 2, this straightforward approach achieves strong result.

## A.3 HOTPOT QA BERT PIPELINE APPROACH

This section discusses our implementation of pipeline approach for HotpotQA bridge question. We start with same methods for extracting the document set D.

## A.3.1 HOP ENTITY EXTRACTION

For each document from the previous step, we run BERT MRC model (Ding et al., 2019) and limit the span candidates as hyperlinked entities for hop entity extraction (e.g., in Figure 1, "Harvard University" is a hop entity). Follow Ding et al. (2019), we predict the top-3 entities that above the relative threshold that is the start span probability of [CLS] position.

## A.3.2 ANSWER SPAN EXTRACTION

For each document (add the hop entity document), follow Ding et al. (2019), we run BERT MRC model Ding et al. (2019) to extract spans (e.g., "Combridge" in Figure 1.). We predict the top-1 span that above the threshold that is the start span probability of [CLS] position.

We train both hop entity extraction and span extraction tasks with same BERT model but different prediction layers. For each training example, we extract the link between two given supporting pages. The page includes the link is the supporting page for hop entity extraction, while the other page is the answer page for answer span extraction.

# A.3.3 GAT MODELING

All the entities and answer spans form the final graph. The nodes are the entities and spans, and edges are the connections from the entities to the extracted hop entities or spans.

We use BERT for each node representation with question, anchor sentences and context, following Ding et al. (2019). We run standard GAT (Veličković et al., 2017) on top of BERT to predict the correct answer span node.

#### A.4 TRAINING DETAILS

We use DGL (Wang et al., 2019) for implementing Transformer-XH and pipeline GAT model with batch size 1 (i.e., one graph for each batch), and keep the other parameters same as default BERT setting. We train the model on bridge questions only for 2 epochs.

For all other BERT based models, we use the default BERT parameters and train the model for 1 epoch.

#### A.5 ADDITIONAL CASE STUDY

<sup>&</sup>lt;sup>4</sup>If the answer document does not have parent node, we choose from all documents

id	Example	Explanation
1(+)	<ul> <li>Q: In which year was the King who made the 1925 Birthday Honours born?</li> <li>P: 1865 √</li> <li>Document 1: The 1925 Birthday Honours were appointments by King George V to various orders and honours.</li> <li>Document 2: George V (3 June <u>1865</u> – 20 January 1936) was King of the United Kingdom.</li> </ul>	With necessary evidence available, Transformer-XH conducts multi-hop reasoning, and extracts the correct span.
2(-)	<ul> <li>Q: Where was the world cup hosted that Algeria qualified for the first time into the round of 16?</li> <li>A: Brazil P: Spain X</li> <li>Document 1 (Algeria at the FIFA World Cup): In 2014, Algeria qualified for the first time into the round of 16.</li> <li>Document 2 (2014 FIFA CUP): It took place in Brazil from 12 June to 13 July 2014, after the country was awarded the hosting rights in 2007.</li> </ul>	Transformer-XH does not predict the correct answer, since document 1 does not link to any other documents. Thus, the information does not propagate to the correct answer document 2014 FIFA CUP.
3(-)	Q: What government position was held by the woman who portrayed Corliss Archer in the film <u>Kiss and Tell</u> ? A: Chief of Protocol P: ambassador <del>X</del> <b>Document 1</b> : <u>Kiss and Tell</u> is a 1945 American comedy film starring then 17-year-old <u>Shirley Temple</u> as Corliss Archer. <b>Document 2</b> : As an adult, <u>Shirley Temple</u> was named United States ambassador to Ghana and to Czechoslo- vakia, and also served as <u>Chief of Protocol</u> of the United States.	Transformer-XH predicts the correct answer document Shirley Temple. However it could not distinguish from the wrong answer ambassador which she was named but not held that position.

Table 6: Additional examples for model prediction on HotpotQA dataset, the first example is the correct prediction (+), the other two examples are the wrong predictions (-).