QA-GNN: Reasoning with Language Models and Knowledge Graphs for Question Answering

Stanford University NAACL 2021

Introduction

"Question Answering" system

- 인간이 제시한 질문에 자동으로 응답하는 시스템
- 각각에 관련된 knowledge와 이에 대한 추론에 접근할 수 있어야 함.

Knowledge의 표시

- Unstructured text에 대해 Implicitly encode된 large language models(LMs)
- Structured한 knowledge graphs(KGs)로 Explicitly represented

Knowledge graph(KG)

- Node: Entities.
- Edge: Entity 간의 관계.
- 기존 Pre-trained LM은 광범위한 knowledge를 가졌지만, negation 처리와 같은 structured reasoning에는 부적합
- KG는 structured reasoning에 더 적합하지만, knowledge로 적용할 수 있는 범위가 적음
- → 두 가지 모두를 어떻게 효과적으로 추론하는지가 중요한 문제점.

Introduction

Question answering(QA)을 위한 end-to-end LM+KG 모델인 QA-GNN을 제안.

Key insight

- 1. Relevance Scoring:
- QA context에 대해서, 어떤 Entity node는 다른 node보다 관련성이 높다. 따라서 이를 표현하기 위해서 Relevance Scoring 도입.
- Entity를 QA context와 연결하고, pre-trained LM을 사용해 가능성을 계산하여 KG subgraph의 각각의 Entity에 점수를 매김.
- 2. Joint Reasoning:
- QA context와 KG를 joint한 graph 표현을 설계하는 것.
- QA context를 graph의 추가 node로 보고, KG subgraph의 topic entity에 연결

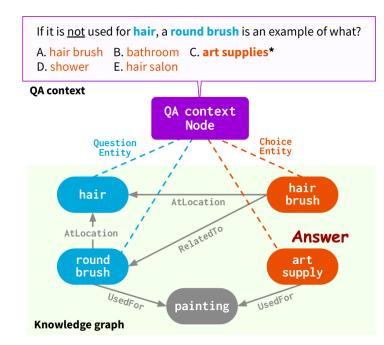


Figure 1: Given the QA context (question and answer choice; purple box), we aim to derive the answer by performing joint reasoning over the language and the knowledge graph (green box).

Introduction

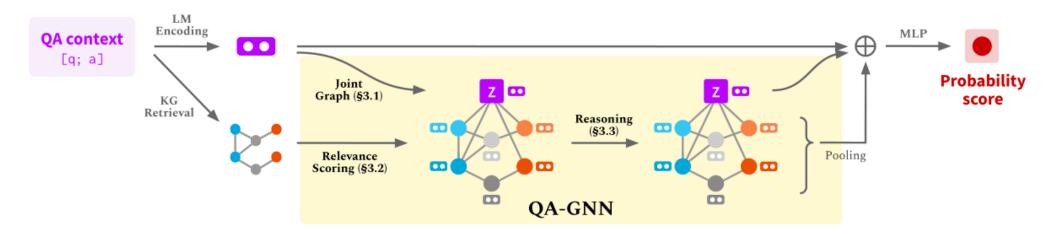


Figure 2: Overview of our approach. Given a QA context (z), we connect it with the retrieved KG to form a joint graph (working graph; §3.1), compute the relevance of each KG node conditioned on z (§3.2; node shading indicates the relevance score), and perform reasoning on the working graph (§3.3).

앞서서 결합한 graph를 working graph라고 하며, LM과 KG의 두 가지 양식을 1개의 Graph로 나타냄.

- Relevance score 이용해 각각의 node의 기능을 보강하고, reasoning을 위한 새로운 attention-based GNN 모듈 설계.
- Joint reasoning 알고리즘은, KG의 Entity와 QA context node의 표현을 동시에 업데이트
 - → 두 가지 정보 소스 간의 Gap을 해소할 수 있음.

Problem Statement

Language Model: 두 함수의 합성으로 생각. $f_{head}(f_{enc}(x))$

- $f_{enc}(x)$: Encoder로서 textual input x를 context화 된 vector \mathbf{h}^{LM} 에 매핑.
- f_{head} : f_{enc} 를 사용해서 원하는 작업을 수행.

 f_{enc} : masked language model (ex. RoBERTa)를 이용.

 \mathbf{h}^{LM} : 특별히 정해지지 않았으면, input sequence x 앞에 추가되는 [CLS] token의 output representation을 가리킴.

Knowledge Graph: G = (V, E)로 정의함.

- V: KG의 entity node set.
- $-E \subseteq V \times R \times V$: V의 node를 연결하는 edge들의 set. (이때, R은 relation type의 set)

Question q, Answer choice $a \in C$ 가 주어졌을 때, 각각에서 언급된 entity를 주어진 KG G에 연결함.

이때, V_q , V_a 는 각각 질문에서 언급된 KG entity와 answer choice로 나타냄.

 $V_{q,a} \coloneqq V_q \cup V_a$: 모든 question 또는 answer choice에서 나타나는 entity = "Topic Entity"

question-choice 쌍, $G_{sub}^{q,a} = (V_{sub}^{q,a}, E_{sub}^{q,a})$ 에 대해 G에서 subgraph를 추출.

 $G_{sub}^{q,a}$ 는 $V_{q,a}$ 의 node 사이 k-hop 경로에 있는 모든 node를 포함함.

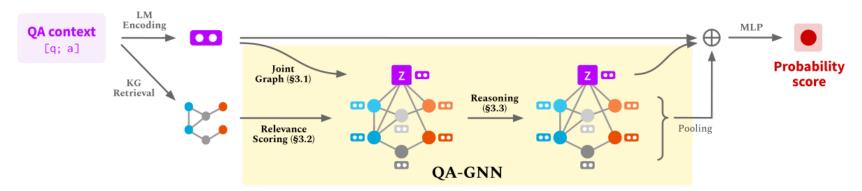


Figure 2: Overview of our approach. Given a QA context (z), we connect it with the retrieved KG to form a joint graph $(working\ graph; \S 3.1)$, compute the relevance of each KG node conditioned on z ($\S 3.2$; node shading indicates the relevance score), and perform reasoning on the working graph ($\S 3.3$).

Question q와 Answer choice a가 주어졌을 때, 이들을 concatenate 하여 QA context [q; a]를 얻음.

Overview:

LM, KG의 knowledge를 사용해서 주어진 QA context를 추론하기 위해서 QA-GNN은 다음과 같이 작동.

- 1. LM을 사용해 QA context에 대한 표현을 얻고, KG에서 subgraph G_{sub} 를 탐색.
- 2. QA context를 나타내는 context node z를 도입하고 topic entity $V_{q,a}$ 에 연결해 working graph G_W 제작
- 3. $\,$ QA context node와 G_W 의 다른 node 간 관계를 적용하기 위해 LM을 사용해서 relevance score를 계산.
- 4. 여러 round 동안 G_W 에서 message passing을 수행하는 attention-based GNN 모듈 제안.
- 5. LM 표현, QA context node 표현, Pooled working graph 표현을 사용해서 최종 예측을 수행.

Joint graph representation

- QA context를 나타내는 새로운 QA context node z 도입.
- 2개의 새로운 relation type $r_{z,q}$, $r_{z,a}$ 를 사용해 KG subgraph G_{sub} 에서 $V_{q,a}$ 의 각 topic entity에 z를 연결.
- 이러한 joint graph는 working graph $G_{W} = (V_{W}, E_{W})$ 라고 함.

$$(V_{W} = V_{sub} \cup \{z\}, E_{W} = E_{sub} \cup \{(z, r_{z,q}, v) | v \in V_{q}\} \cup \{(z, r_{z,a}, v) | v \in V_{a}\})$$

- G_W 의 각 node는 4가지 유형 중 하나. $T = \{Z, Q, A, O\}$
 - Z context node z
 - $-Q: V_q \supseteq \text{node}$
 - $-A: V_a \supseteq node$
 - 0: 기타 node
- QA context의 LM 표현을 사용해 z에 대한 node embedding 초기화.
- Entity embedding을 사용해서 G_{sub} 의 각 node 초기화.

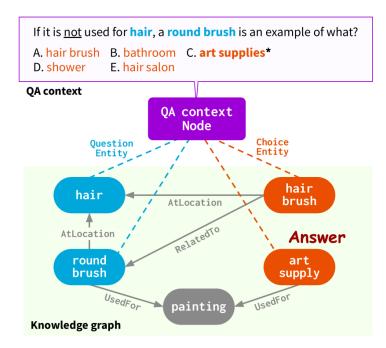


Figure 1: Given the QA context (question and answer choice; purple box), we aim to derive the answer by performing joint reasoning over the language and the knowledge graph (green box).

KG node relevance scoring

- KG subgraph인 G_{sub} 의 많은 node는 QA context와 연관이 없을 수 있음.
 - → 이러한 irrelevant node는 overfitting 또는 추론에 어려움을 야기할 수 있음.
 - \rightarrow 이를 해결하기 위해 node relevance scoring을 사용해 QA context에 따라 KG node $v \in V_{sub}$ 의 관련성을 점수화.
- 각 node v에 대해, entity text(v)를 QA context text(z)와 concatenate하고 relevance score 계산.

$$\rho_v = f_{head}(f_{enc}([\text{text}(z), \text{text}(v)]))$$

- $f_{\text{head}} \circ f_{enc}$: LM에 의해 계산된 text(v)의 확률
- Relevance score ho_v : working graph $G_{
 m W}$ 를 추론, 정리하는데 사용되는 QA context에 관련된 KG node의 중요성을 파

악할 수 있음.

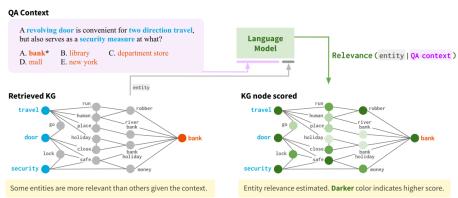


Figure 3: Relevance scoring of the retrieved KG: we use a pre-trained LM to calculate the relevance of each KG entity node conditioned on the QA context (§3.2).

GNN architecture

- L-layer QA-GNN에서 각 layer에 대해 각 node $t \in V_W$ 의 representation $h_t^{(l)} \in \mathbb{R}^D$ 를 다음과 같이 업데이트.

$$h_t^{(l+1)} = f_n \left(\sum_{s \in N_t \cup \{t\}} \alpha_{st} m_{st} \right) + h_t^{(l)}$$

- $-N_t$: node t의 neighborhood, $m_{st} \in \mathbb{R}^D$: s에서 t로의 각 인접 node의 message, α_{st} : attention weight
- 각 message의 합은 batch normalization을 통해 전달.
- GNN의 message passing은 working graph에서 작동 → QA context, KG의 표현을 같이 update.

$$m_{st} = f_m(h_s^{(l)}, u_s, r_{st})$$
 $u_t = f_u(u_t), r_{st} = f_r(e_{st}, u_s, u_t),$

$$\alpha_{st} = \frac{\exp(\gamma_{st})}{\sum_{t' \in N_s \cup \{s\}} \exp(\gamma_{st'})}, \qquad \gamma_{st} = \frac{q_s^T k_t}{\sqrt{D}}. \qquad \begin{aligned} \boldsymbol{\rho}_t &= f_{\rho}(\rho_t), \\ \boldsymbol{q}_s &= f_q(\boldsymbol{h}_s^{(\ell)}, \boldsymbol{u}_s, \boldsymbol{\rho}_s), \\ \boldsymbol{k}_t &= f_k(\boldsymbol{h}_t^{(\ell)}, \boldsymbol{u}_t, \boldsymbol{\rho}_t, \boldsymbol{r}_{st}), \end{aligned}$$

Inference & Learning

- Question q, Answer choice a가 주어졌을 때, 이것이 답일 확률을 계산.

$$p(a|q) \propto \exp\left(\text{MLP}(z^{\text{LM}}, z^{\text{GNN}}, g)\right)$$

- 이때, $z^{\text{GNN}}=h_z^{(L)}$ 이고, $g = \left\{h_v^{(L)} | v \in V_{sub}\right\}$ 의 pooling을 나타냄.
- Cross Entropy Loss를 사용해서 최적화.

Computation complexity

- Time: relation 수에 대해 일정. node 수에 대해서 선형
- Space: MHGRN과 동일.

MHGRN: relation에 대해 독립적인 graph network 가짐.

QA-GNN: embedding을 사용하는 방식.

Model	Time	Space
	G is a dense graph	
L-hop KagNet L -hop MHGRN L -layer QA-GNN	$\mathcal{O}ig(\mathcal{R} ^L \mathcal{V} ^{L+1}Lig) \ \mathcal{O}ig(\mathcal{R} ^2 \mathcal{V} ^2Lig) \ \mathcal{O}ig(\mathcal{V} ^2Lig)$	$ \frac{\mathcal{O}(\mathcal{R} ^L \mathcal{V} ^{L+1} L)}{\mathcal{O}(\mathcal{R} \mathcal{V} L)} $ $ \mathcal{O}(\mathcal{R} \mathcal{V} L) $
G is a sparse graph	n with maximum noo	de degree $\Delta \ll \mathcal{V} $
L-hop KagNet L -hop MHGRN L -layer QA-GNN	$ \begin{array}{c} \mathcal{O} \big(\mathcal{R} ^L \mathcal{V} L \Delta^L \big) \\ \mathcal{O} \big(\mathcal{R} ^2 \mathcal{V} L \Delta \big) \\ \mathcal{O} \big(\mathcal{V} L \Delta \big) \end{array} $	$ \begin{array}{c} \mathcal{O} \big(\mathcal{R} ^L \mathcal{V} L \Delta^L \big) \\ \mathcal{O} (\mathcal{R} \mathcal{V} L) \\ \mathcal{O} (\mathcal{R} \mathcal{V} L) \end{array} $

Table 1: Computation complexity of different L-hop reasoning models on a dense/sparse graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with the relation set \mathcal{R} .

Experiment

Dataset

CommonsenseQA: 5지선다형 QA로 구성, 상식을 기반으로 추론해야 하는 질문.

OpenBookQA: 4지선다형 QA로 구성, 기초 과학 지식을 기반으로 추론해야 하는 질문.

Knowledge Graph

ConceptNet: hop-size k = 2로 structured knowledge source G에서 G_{sub} 를 탐색.

Baselines

- Fine-tuned LM: RoBERTa-large, AristoBoBERTa
- Existing LM+KG models: Relation Network(RN), RGCN, GconAttn, KagNet, MHGRN

Experiment

Methods	IHdev-Acc. (%)	IHtest-Acc. (%)
RoBERTa-large (w/o KG)	$73.07 (\pm 0.45)$	$68.69 (\pm 0.56)$
+ RGCN (Schlichtkrull et al., 2018)	$72.69 (\pm 0.19)$	68.41 (±0.66)
+ GconAttn (Wang et al., 2019a)	$72.61(\pm 0.39)$	$68.59 (\pm 0.96)$
+ KagNet (Lin et al., 2019)	$73.47 (\pm 0.22)$	$69.01 (\pm 0.76)$
+ RN (Santoro et al., 2017)	$74.57 (\pm 0.91)$	$69.08 (\pm 0.21)$
+ MHGRN (Feng et al., 2020)	74.45 (± 0.10)	$71.11 (\pm 0.81)$
+ QA-GNN (Ours)	76.54 (±0.21)	73.41 (±0.92)

Table 2: **Performance comparison on** *Commonsense QA* **in-house split** (controlled experiments). As the official test is hidden, here we report the in-house Dev (IHdev) and Test (IHtest) accuracy, following the data split of Lin et al. (2019).

Methods	RoBERTa-large	AristoRoBERTa
Fine-tuned LMs (w/o KG)	$64.80 (\pm 2.37)$	$78.40 (\pm 1.64)$
+ RGCN	62.45 (±1.57)	$74.60 (\pm 2.53)$
+ GconAtten	$64.75 (\pm 1.48)$	$71.80 (\pm 1.21)$
+RN	$65.20 (\pm 1.18)$	$75.35 (\pm 1.39)$
+ MHGRN	$66.85 (\pm 1.19)$	80.6
+ QA-GNN (Ours)	70.58 (±1.42)	82.77 (±1.56)

Table 4: **Test accuracy comparison on** *OpenBook QA* (controlled experiments). Methods with AristoRoBERTa use the textual evidence by Clark et al. (2019) as an additional input to the QA context.

Experiment

Methods	Test
RoBERTa (Liu et al., 2019)	72.1
RoBERTa+FreeLB (Zhu et al., 2020) (ensemble)	73.1
RoBERTa+HyKAS (Ma et al., 2019)	73.2
RoBERTa+KE (ensemble)	73.3
RoBERTa+KEDGN (ensemble)	74.4
XLNet+GraphReason (Lv et al., 2020)	
RoBERTa+MHGRN (Feng et al., 2020)	75.4
Albert+PG (Wang et al., 2020b)	75.6
Albert (Lan et al., 2020) (ensemble)	76.5
UnifiedQA* (Khashabi et al., 2020)	79.1
RoBERTa + QA-GNN (Ours)	

Table 3: **Test accuracy on** *CommonsenseQA***'s official leaderboard**. The top system, UnifiedQA (11B parameters) is 30x larger than our model.

Methods	Test
Careful Selection (Banerjee et al., 2019)	72.0
AristoRoBERTa	77.8
KF + SIR (Banerjee and Baral, 2020)	80.0
AristoRoBERTa + PG (Wang et al., 2020b)	
AristoRoBERTa + MHGRN (Feng et al., 2020)	
Albert + KB	81.0
T5* (Raffel et al., 2020)	83.2
UnifiedQA* (Khashabi et al., 2020)	
AristoRoBERTa + QA-GNN (Ours)	82.8

Table 5: **Test accuracy on** *OpenBookQA* **leaderboard**. All listed methods use the provided science facts as an additional input to the language context. The top 2 systems, UnifiedQA (11B params) and T5 (3B params) are 30x and 8x larger than our model.

Ablation Study

Graph connection

- z node → KG의 QA entity node 연결: joint graph
- 없을 때: QA context, KG가 상호적 update 못함
 - → 성능 저하

KG node relevance scoring

- Context embedding과 비교했을 때, relevance scoring이 더 좋은 성능을 보임.

Graph Connection (§3.1)	Dev Acc.
No edge between Z and KG nodes	74.81
Connect Z to all KG nodes	76.38
Connect Z to QA entity nodes (final)	76.54

Relevance scoring (§3.2)	Dev Acc.
Nothing	75.56
w/ contextual embedding	76.31
w/ relevance score (final)	76.54
w/ both	76.52

GNN Attention & Message (§3.3)	Dev Acc.
Node type, relation, score-aware (final)	76.54
- type-aware	75.41
- relation-aware	75.61
- score-aware	75.56

GNN Layers (§3.3)	Dev Acc.
L=3	75.53
L = 4	76.34
L = 5 (final)	76.54
L=6	76.21
L = 7	75.96

Table 6: **Ablation study** of our model components, using the CommonsenseQA IHdev set.

GNN architecture

- GNN에서 각각에 해당하는 정보를 제거했을 때, 하나라도 빠지면 전체 모델의 성능이 저하됨.
- Layer수 = 5인 GNN에서 성능이 제일 좋았는데, QA context ↔ KG 사이 message passing이나 추론 패턴을 허용하는 5개의 layer가 존재한다는 것.

Model interpretability

(a)

QA context node → Question entity node → Other or Answer choice entity node

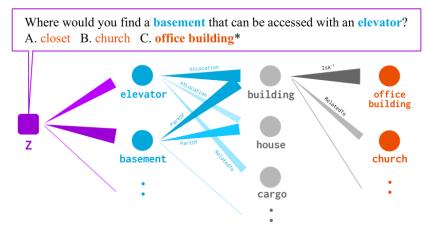
(b)

QA context node → Question entity node → Other or

QA context node → Answer choice entity node → Other

- 위의 두가지 방식으로 BFS를 사용하여 model을 해석할 수 있음.
- QA-GNN은 경로에 특정하지 않고 attention weight를 통해 추론을 진행.

(a) Attention visualization direction: BFS from Q



(b) Attention visualization direction: $Q \rightarrow Q$ and $A \rightarrow Q$

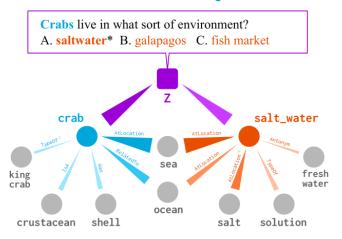


Figure 4: **Interpreting QA-GNN's reasoning process** by analyzing the node-to-node attention weights induced by the GNN. Darker and thicker edges indicate higher attention weights.

Structured reasoning

- 부정문 또는 단어의 대체를 정확하게 처리하는 것은 정확한 답 예측을 하는데 중요.
- 다른 model보다 QA-GNN은 이러한 상황에서의 예측 정확도가 높음.

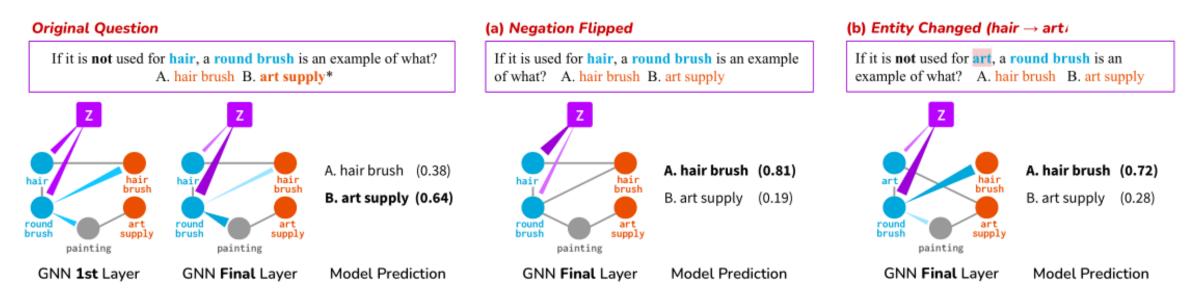


Figure 5: **Analysis of QA-GNN's behavior for structured reasoning**. Given an original question (left), we modify its negation (middle) or topic entity (right): we find that QA-GNN adapts attention weights and final predictions accordingly, suggesting its capability to handle structured reasoning.

Structured reasoning

Methods	IHtest-Acc. (Overall)	IHtest-Acc. (Question w/ negation)
RoBERTa-large (w/o KG)	68.7	54.2
+ KagNet + MHGRN	69.0 (+0.3) 71.1 (+2.4)	54.2 (+0.0) 54.8 (+0.6)
+ QA-GNN (Ours)	73.4 (+4.7)	58.8 (+4.6)
+ QA-GNN (no edge between Z and KG)	71.5 (+2.8)	55.1 (+0.9)

Table 7: Performance on **questions with negation** in *CommonsenseQA*. () shows the difference with RoBERTa. Existing LM+KG methods (KagNet, MH-GRN) provide limited improvements over RoBERTa (+0.6%); QA-GNN exhibits a bigger boost (+4.6%), suggesting its strength in structured reasoning.

Quantitative analysis

- QA context와 KG의 동시 update가 semantic한 부분을 통합 할 수 있음.

Qualitative analysis

- Entity간의 message 교환을 통해서, 부정 entity에는 약한 weight를, 관계가 큰 entity에는 큰 weight를 가지게 함.
- RoBERTa와는 다르게 부정문, entity 교체에도 좋은 결과를 보임.

Example (Original taken from CommonsenseQA Dev)	RoBERTa Prediction	Our Prediction
[Original] If it is not used for hair, a round brush is an example of what? A. hair brush B. art supply	A. hair brush (X)	B. art supply (✓)
[Negation flip] If it is used for hair, a round brush is an example of what?	A. hair brush (✓ just no change?)	A. hair brush (✓)
[Entity change] If it is not used for art a round brush is an example of what?	A. hair brush (✓ just no change?)	A. hair brush (✓)
[Original] If you have to read a book that is very dry you may become what? A. interested B. bored	B. bored (✓)	B. bored (✓)
[Negation ver 1] If you have to read a book that is very dry you may not become what?	B. bored (X)	A. interested (✓)
[Negation ver 2] If you have to read a book that is not dry you may become what?	B. bored (X)	A. interested (✓)
[Double negation] If you have to read a book that is not dry you may not become what?	B. bored (✓ just no change?)	A. interested (X)

Table 8: **Case study of structured reasoning**, comparing predictions by RoBERTa and our model (RoBERTa + QA-GNN). Our model correctly handles changes in negation and topic entities.

Effect of KG node relevance scoring

- G_{sub} 가 매우 클 때, KG node relevance score가 도움이 됨.
- 기존 LM+KG model은 G_{sub} 의 size, noize로 인해 더 많은 entity가 있는 질문에 대해 제한적인 성능.
- KG node relevance scoring이 이러한 병목현상을 완화
 - → 정확도 상승.

Methods	IHtest-Acc. (Question w/ ≤10 entities)	IHtest-Acc. (Question w/ >10 entities)
RoBERTa-large (w/o KG)	68.4	70.0
+ MHGRN	71.5	70.1
+ QA-GNN (w/o node relevance score)	72.8 (+1.3)	71.5 (+1.4)
+ QA-GNN (w/ node relevance score; final system)	73.4 (+1.9)	73.5 (+3.4)

Table 9: Performance on **questions with fewer/more entities** in *CommonsenseQA*. () shows the difference with MHGRN (LM+KG baseline). KG node relevance scoring (§3.2) boosts the performance on questions containing more entities (i.e. larger retrieved KG).