

Knowledge Graph Structure as Prompt: Improving Small Language Models Capabilities for Knowledge-based Causal Discovery

No Author Given

No Institute Given

Abstract. Causal discovery aims to estimate causal structure among variables based on observational data. Large Language Models (LLMs) offer a fresh perspective to tackle the causal discovery problem by reasoning on the metadata associated with variables rather than their actual data values, an approach referred to as *knowledge-based causal discovery*. In this paper, we investigate the capabilities of Small Language Models (SLMs, defined as LLMs under 1 billion parameters) with prompt-based learning for knowledge-based causal discovery. Specifically, we present “KG Structure as Prompt”, a novel approach for integrating structural information from a knowledge graph, such as common neighbors nodes and metapaths, into prompt-based learning to enhance the capability of SLMs. Experimental results on three types of biomedical and an open-domain datasets under few-shot settings demonstrate the effectiveness of our approach, surpassing most baselines and even conventional fine-tuning approaches trained using full datasets. Our findings further highlight the strong capabilities of SLMs: in combination with knowledge graphs and prompt-based learning, SLMs demonstrate the potential to surpass LLMs with larger number of parameters. Our code and datasets are available as supplementary materials on GitHub.¹.

Keywords: causal discovery · language model · knowledge graph

1 Introduction

One of the fundamental tasks in various disciplines of science is to find the underlying causal relations and make use of them. Causal discovery is a branch of causality study which estimates causal structures from observational data and generates a causal graph as a result. A causal graph, as illustrated in Fig. 1, is a directed graph modeling the causal relationships between observed variables; a node represents a variable and an edge represents a causal relationship.

Conventionally, causal discovery involves learning causal relations from observational data by measuring how changes in one variable are associated with changes in the second variable, an approach referred to as *covariance-based causal discovery* [21]. Driven by the recent advancement of LLMs, recent work has explored the causal capabilities of LLMs using metadata such as variable names

¹ <https://anonymous.4open.science/r/kg-structure-as-prompt-7DCF/>



Fig. 1. Example of a causal graph.

rather than their actual data values, i.e., the causal relation is queried by natural language directly. This paper focuses on the latter, and to differentiate with *covariance-based causal discovery*, we refer to this approach as ***knowledge-based causal discovery***, following the definition of [21].

Typically, such metadata-based causal reasoning is performed by Subject Matter Experts (SMEs) as they construct a causal graph, drawing from their expertise in domain-specific subjects and common sense [21], or based on literature surveys on subjects related to the variables. The advancement in LLMs has simplified this formerly challenging process, as LLMs are now capable of providing the knowledge that previously can only be provided by SMEs. Recent works [18,37,40,43] also show promising results, notably, [21] explores causal capabilities of LLMs by experimenting on cause-effect pairs. Their findings suggest that LLM-based methods achieved state-of-the-art performance on several causal benchmarks. Similarly, [43] investigated the causal capability of LLMs by analyzing their behaviour given a certain causal question. However, in contrast to [21], their result suggests that LLMs currently lack the capability to offer satisfactory answers for discovering new knowledge. Meanwhile, a work by [18] focused on investigating the LLMs’ capability for causal association among events expressed in natural language. Thus, their study is more oriented towards extracting a causal diagram (e.g., a chain of events) from unstructured text instead of discovering new causal relations.

In this paper, we investigate the capabilities of language models for knowledge-based causal discovery between variable pairs given a textual context from text sources. Specifically, given a pair of variables e_1 and e_2 , the task is to predict if a causal relation can be inferred between the pair. Therefore, similar to [18], our focus also lies in inferring causal relations from text rather than discovering new causal relations. In particular, we present “**KG Structure as Prompt**”, a novel approach for integrating structural information from a Knowledge Graph (KG) into *prompt-based learning* with Small Language Models (SLMs). Prompt-based learning adapts LMs for specific tasks by incorporating prompts—text snippets combined with the input—to guide the models’ output for the downstream tasks. Our approach enhances this method by incorporating additional contextual information from KG structures, leveraging the strengths of KGs in providing context and background knowledge. We opted for SLMs because a smaller model that can outperform larger models is more cost-effective and therefore preferable. We conduct experiments on three types of biomedical and an open-domain datasets, and further evaluate the performance of the proposed approach under three different architectures of language models.

To summarize, our main contributions are:

1. We introduce “KG Structure as Prompt”, a new approach for injecting structural information from KG into prompt-based learning. Our proposed approach has also proven to be effective with different types of language model architectures and KGs, showcasing its flexibility and adaptability across various language models and KGs.
2. We demonstrate the robust capabilities of SLMs: fused with prompt-based learning and an access to a KG, SLMs are able to surpass LLMs with much larger parameter. Our experiments under *few-shot* settings further highlight the effectiveness of the proposed approach, as it outperformed the standard fine-tuning using a full dataset, even when utilizing limited samples.
3. We compiled datasets for detecting causality in natural language text sourced from publicly available datasets, and shared a new-annotated dataset.

2 Background and Related Work

Small Language Models. Small Language Models (SLMs) refer to language models with fewer parameters, resulting in limited capacity to process text compared to larger-parameter LLMs. However, SLMs typically require less computation resources, making them faster to train and to deploy, and maintaining them are generally more cost-effective. On the contrary, LLMs are trained on vast amounts of diverse data, thus have significantly more parameters and are capable of handling more complex language tasks than SLMs. Nevertheless, LLMs are expensive and difficult to train and deploy as they typically require more computational resource. For instance, GPT-3 [5], which consists of 175 billion parameters, is impractical to run on hardware with limited resources.

In this work, we define SLMs as LMs with less than 1 billion parameters. We explore the causal capability of SLMs with different architectures: (1) Masked Language Model (MLM) especially the encoder-only model, (2) Causal Language Model (CLM) or decoder-only language model, and (3) Sequence-to-Sequence Language Model (Seq2SeqLM) or encoder-decoder model. We provide an overview of each architecture below.

MLMs, especially the encoder-only model such as BERT [9], are a type of LMs that utilize encoder blocks within the transformer architecture and are trained to predict masked tokens based on the context provided by surrounding words. They excel in natural language understanding (NLU) tasks e.g., text classification, as they are able to capture relationships between words in a text sequence. CLMs, such as GPT-3 [5], use the decoder blocks within the transformer architecture and are trained to generate text one token at a time, by conditioning each token on the preceding tokens in the sequence. Meanwhile, Seq2SeqLMs, such as T5 [31], consist of both encoder and decoder blocks. The encoder transforms the input sequence into vector representation, while the decoder produces the output based on the encoded vector. CLMs and Seq2SeqLMs generally work well for natural language generation (NLG) and NLU tasks such as translation and summarization, as they can produce coherent and grammatically accurate sentences. We list our choice of language models in §5.

Prompt-based Learning & Knowledge Injection. Research on classifying causal relations from text have predominantly occurred within a supervised setting by *fine-tuning* a pre-trained language model, e.g., on biomedical-chemistry domains [19,6,28,11,32,18], and open-domain corpora [20,7,4,3]. Most of the works fine-tune a language model such as BERT [9], or propose a form of improvement for fine-tuning BERT [35]. Hence, we evaluate our proposed approach against those of conventional fine-tuning method as baselines.

Meanwhile, *prompt-based learning*, also known as *prompt-tuning*, has recently emerged as promising alternative to the conventional fine-tuning approach for a variety of Natural Language Processing (NLP) tasks [1,26,33,34]. Typically, a *prompt* is composed of discrete text (*hard prompt*); although, recent work has introduced *soft prompt*, a continuous vectors that can be optimized through backpropagation [23,25]. In the relation classification task, prompt-based learning often involves inserting a prompt template containing masked tokens into the input, essentially converting the task into *masked language modeling* or *text generation* problems [8,14,13]. This approach is particularly well-suited for few-shot or zero-shot scenarios, where only limited labeled data is available [34,10]. In such case, the prompt helps to *push* the model into the desired behavior, and the result has been impressive: it surpasses the models trained with conventional fine-tuning using a full dataset even when trained on limited samples. This motivates us to investigate such prompt-based learning under few-shot settings, given the scarcity of datasets for our causal relation classification task.

Other study has explored into **knowledge injection** for the prompt construction, for instance, KnowPrompt [8] injects latent knowledge contained in relation labels into prompt construction with learnable virtual words. KAPING [2] retrieves top-K similar triples of the target entities from WikiData and further augments them as prompt. KiPT [24] uses WordNet to calculate semantic correlation between the input and manually constructed core concepts to construct the prompts. Our work differs to them since we focus on leveraging *structural information* of a knowledge graph to construct the prompt, taking inspiration from Graph Neural Network (see §4).

3 Task Formulation

In this work, we focus on *pairwise* knowledge-based causal discovery: given a pair of entities e_1 and e_2 , i.e., variable or node pairs such as **FGF6** and **prostate cancer**, the task is to predict if a causal relation can be inferred between the pair. We formulate the task as *binary classification task*, classifying the relation as *causal* or *non-causal*. We evaluate our approach on dataset $\mathcal{D} = \{\mathcal{X}, \mathcal{Y}\}$, where \mathcal{X} is a set of training instance and $\mathcal{Y} = \{\text{causal}, \text{non-causal}\}$ is a set of relation labels. Each instance $x \in \mathcal{X}$ consists of a token sequence $x = \{w_1, w_2, \dots, w_{|n|}\}$ and the spans of a marked variable pair, and is annotated with a label $y_x \in \mathcal{Y}$.

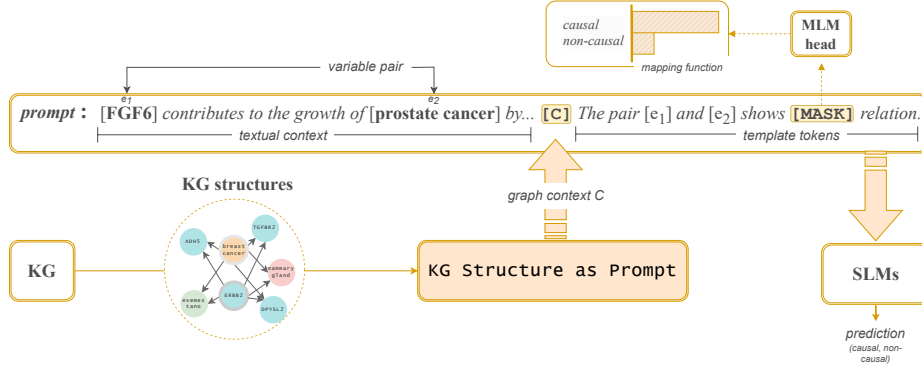


Fig. 2. Overall framework of our KG Structure as Prompt with prompt-based learning

4 Approach

We illustrate our proposed approach in Fig. 2. First, we generate a **graph context**, which is derived from the structural information of a knowledge graph with our KG Structure as Prompt method. Next, we feed the generated graph context and the inputs, i.e., the **variable pair** and its **textual context**, into the SLMs to train a prompt-based learning model.

We elaborate our proposed approach in the following subsections. We start with preliminary (§4.1), followed by the design of the KG structure as Prompt for generating the graph context (§4.2), and the incorporation of the generated graph context into the SLMs architecture with prompt-based learning (§4.3).

4.1 Preliminaries

Formally, we define a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where \mathcal{V} is a set of vertices or nodes, and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is a set of directed edges. A knowledge graph **KG** is a specific type of directed graph representing a network of entities and the relationship between them. Formally, we define a KG as a directed *labeled* graph $\mathcal{KG} = (N, E, R, \mathcal{F})$ where N is a set of nodes (entities), $E \subseteq N \times N$ is a set of edges (relations), R is a set of relation labels, and $\mathcal{F} : E \rightarrow R$, is a function assigning edges to relation labels. For instance, assignment label r to an edge $e = (x, y)$ can be viewed as triple (x, r, y) , e.g., (Tokyo, IsCapitalOf, Japan).

4.2 Knowledge Graph Structure as Prompt

In the field of Graph Neural Network (GNN), [42] explores whether LLMs can replace GNNs as the foundation model for graphs by using natural language to describe the geometric structure of the graph. They fine-tune LLMs to perform fundamental GNN tasks such as node classification, with a prompt template composed of a graph description. Their results on several graph datasets surpass

all traditional GNN-based methods, showing the potential of LLMs as a new foundational model for GNN. Inspired by their success, we similarly leverage the structural information of a specific type of graph, i.e., knowledge graph, to infer causal relationships between variable pairs. We select knowledge graphs due to their rich information combined from multiple sources, and we argue that their capability to express interconnected relationships is superior. We call our approach “**Knowledge Graph Structure as Prompt**”.

For instance, we may infer a causal relationship by looking at few hops relations between a node pair in a knowledge graph, as illustrated in Fig. 3.

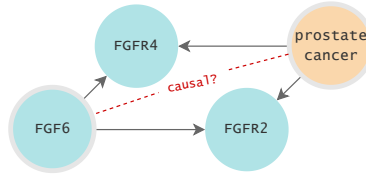


Fig. 3. Illustration of inferring a causal relationship in KG.

In Fig. 3, the node **FGF6** is *indirectly* connected to the node **prostate cancer** within one hop via the nodes **FGFR2** and **FGFR4**. As verified by a human-expert, there is indeed a causal relation between the nodes **FGF6** and **prostate cancer**. We argue that such graph structural information, in this example a *path*, adds background knowledge on top of internal knowledge of LMs, effectively assisting LMs in inferring causal relation between the variable pair. Specifically, we aim to use a natural language description of the structural information from the knowledge graph to be used as a prompt for prompt-based learning. We refer to such description of knowledge graph structure as **graph context**.

In this work, we specifically examine three kinds of vital structural information of a KG to be used as the graph context, namely **(1) neighbors nodes**, **(2) common neighbors nodes**, **(3) metapath**, described in detail as follows.

(1) Neighbors Nodes (\mathcal{NN}). The essence of a GNN lies in applying different aggregate functions to the graph structure, i.e., passing node features to *neighboring nodes*, where each node aggregates the feature vectors of its neighbors to further update its feature vector. Thus, it is evident that the neighbors nodes are the most crucial feature within a graph. Inspired by that, first we examine the neighboring nodes of the target node pairs to infer their causal relationship.

Formally, a node x is a **neighbor** of a node y in a knowledge graph $\mathcal{G} = (V, E)$ if there is an edge $\{x, y\} \in E$. We provide an example of neighbors nodes from Wikidata [38] in Fig. 4. According to the provided example, the node **prostate cancer** has **urology** as one of its neighbors nodes, while **FGF6** has **urinary bladder** as one of its neighbors. Thus, it becomes evident that a connection

exists between the node pair (**FGF6**, **prostate cancer**) due to their respective neighboring nodes: **urinary bladder** \leftrightarrow **urology**.

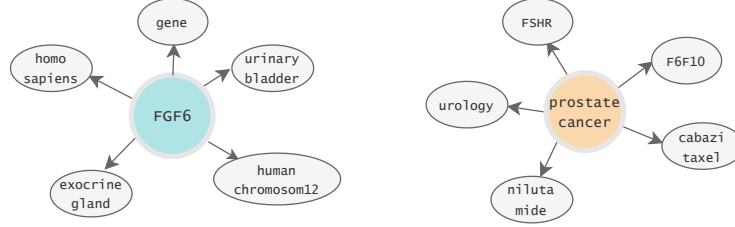


Fig. 4. Example of neighbors nodes for **FGF6** (left) and **prostate cancer** (right).

For utilizing the neighbors nodes structure as a prompt, we describe it in natural language to form a graph context \mathcal{C} , which we formally denote as:

$$\mathcal{C}(x, V, E) = \{x\} \text{ "is connected to" } \{[x_2]_{x_2 \in V_2^x}\} \quad (1)$$

We also create a variation of \mathcal{C} where we include the edge description on top of the neighbors nodes information, as follows:

$$\mathcal{C}(x, V, E) = \{x\} \text{ "is" } \{E_{x,x_2}\} \text{ "to" } \{[x_2]_{x_2 \in V_2^x}\} \quad (2)$$

where V_k^x represents the list of node x 's k -hop neighbors nodes and E_{x,x_2} represents the relation or edge description between the node x and its neighbors nodes. The additional template words "*is*", "*connected*", and "*to*" are optional, and can be replaced by any other fitting words in the experiment. Then, with Equation 1, the generated graph context \mathcal{C} for the node **prostate cancer** in Fig. 4 is shown in Example 1, as follows.

Example 1. **prostate cancer** is connected to *nilutamide*, *cabazitaxel*, *urology*, *FSHR*, *F6F10*

(2) Common Neighbors Nodes (\mathcal{CNN}). Different to neighbors nodes, **common neighbors nodes** capture the idea that the more common neighbors a pair of nodes (x, y) shares, the more likely for the pair to be connected i.e., there exists an edge $e = x, y$ between them. This can be best illustrated with: *someone who has mutual friends are more likely to be introduced than those who don't have any mutual friends*. We argue that common neighbors between two nodes help infer their relationship, so we examine the common neighbors information between the node pair as graph context, as well. Fig. 5 shows an example of common neighbors nodes for the pair (**breast cancer**, **ERBB2**), taken from Hetionet [17]. According to the provided example, the pair has in total 95 common neighbors, confirming a close relationship between them.

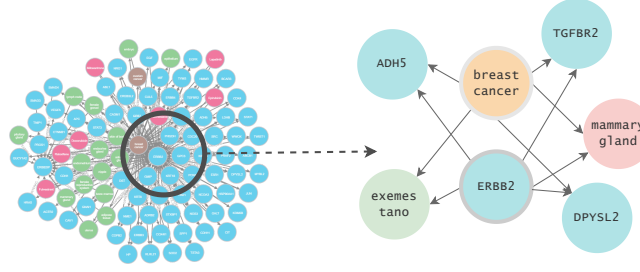


Fig. 5. Example of common neighbors nodes for the pair (**ERBB2**, **breast cancer**). Different colors of the nodes represents different node types.

Formally, common neighbors between node pairs x and y can be defined as:

$$\mathcal{CN}\{x, y\} = N(x) \cap N(y) \quad (3)$$

where $N(x)$ is the set of nodes adjacent to node x (the neighbors of x), and $N(y)$ is the set of nodes adjacent to node y (the neighbors of y). Subsequently, the graph context \mathcal{C} for describing the common neighbors between the pairs x and y can be formed as follows:

$$\mathcal{C}(x, \mathcal{CN}, y) = \text{"Common neighbors nodes of } \{x\} \text{ and } \{y\} \text{ are"} : \{[n]_{n \in \mathcal{CN}}\} \quad (4)$$

where \mathcal{CN} represents the list of common neighbors nodes of the pair x and y as defined in Equation 3. Again, the additional template words "*Common neighbors nodes of...*" are optional and can be replaced by other words. Then, we can generate the graph context \mathcal{C} including the common neighbors nodes information for the pair in Fig. 5, as follows:

Example 2. Common neighbors nodes of **breast cancer** and **ERBB2** are: *ADH5*, *mammary gland*, *exemes tano*, *TGFBR2*, *DPYSL2*

(3) Metapath (\mathcal{MP}). *Metapaths*, or *meta-paths* are sequences of node types which define a walk from an origin node to a destination node [36]. Metapaths are frequently used in biomedical network analysis, for instance, [39] developed a meta path-driven Transformer encoder to learn node representations for gene-disease association prediction, while [41] uses metapath-based GNN for drug-side effect association prediction. Due to its importance in biomedical network, we investigate the metapaths of two nodes for inferring their causal relationship. Moreover, causality is often observed in the biomedical domain and based on our observation, causal relations occasionally follow specific patterns. Fig. 6 shows examples of metapaths of **prostate cancer** and **FGF6**, from Hetionet [17].

Formally, a metapath \mathcal{MP} can be defined as a path $Z_1 \xrightarrow{R_1} Z_2 \xrightarrow{R_2} \dots \xrightarrow{R_n} Z_{n+1}$ describing a relation R between node types Z and Z_{n+1} . The followings show examples of metapaths with different path length n from Fig. 6:

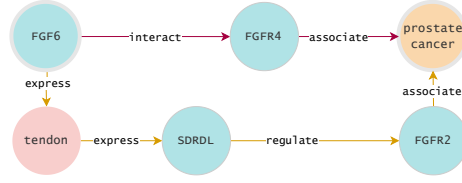


Fig. 6. Example of metapaths for the pair (FGF6, prostate cancer). Different colors of the nodes represents different node types.

$\mathcal{MP} = (\text{FGF6}, \text{FGFR4}, \text{prostate cancer})$, composed of node types $\{gene, gene, disease\}$, with $n = 3$

$\mathcal{MP} = (\text{FGF6}, \text{tendon}, \text{SDRDL}, \text{FGFR2}, \text{prostate cancer})$, composed of node types $\{gene, anatomy, gene, gene, disease\}$, with $n = 5$

As explained by the example provided in Fig. 3, we argue that an *indirect path* between two nodes can be useful for inferring a causal relation between two pairs, even when the edge itself does not describe a causal relation. Thus, an *indirect metapath*, or combination of meaningful node types could be a *latent* evidence of causality between pair of variables. We describe the metapath structure from KG in natural language to form a graph context \mathcal{C} , as follows:

$$\mathcal{C}(x, y, \mathcal{MP}\{V, E\}) = \{x\} \text{“is connected to” } \{y\} \text{“via the following path: ”} \{v\} \{E_{v,v_2}\} \{v_2\} \quad (5)$$

where $\mathcal{MP}\{V, E\}$ is a metapath \mathcal{MP} with length n containing a set of nodes $V(v_1, v_2, \dots, v_{|n|})$ and a set of edges $E(v_1, v_{1+n})$. Additional tokens “*is connected to...*” are optional and can be replaced by other tokens. Then, the graph context \mathcal{C} with metapath information for the example in Fig. 6 would be:

Example 3. FGF6 is connected to prostate cancer via the following paths: FGF6 expressed in tendon, tendon expresses SQRDL, FGFR2 regulates SQRDL, FGFR2 associates with prostate cancer

To prevent bias in prediction by the LMs, we avoid the *direct* path. For instance, for the pair (x, y) , we avoid the path $\mathcal{MP} = (x, y)$ and $\mathcal{MP} = (y, x)$, when such path exists in the KG.

4.3 Prompt-based learning with graph context

As illustrated in the model architecture in Fig. 2, we feed the the **textual context** into SLMs together with the **graph context** generated with KG Structure as Prompt. We further design a prompt-based learning approach utilizing both contexts elaborated in this section. To get a clear distinction between conventional fine-tuning and our proposed prompt-based learning approach, first we provide a short overview of the conventional fine-tuning approach, as follows.

Given a pre-trained LM \mathcal{L} to fine-tune on a dataset \mathcal{D} , the **conventional fine-tuning** method encodes the training sequence $x = \{w_1, w_2, \dots, w_{|n|}\}$ into the corresponding output hidden vectors of the LMs $h = \{h_1, h_2, \dots, h_{|n|}\}$. For MLMs such as BERT [9], the special token “[CLS]” is inserted at the beginning of the sequence, and this special token is used as final sequence representation h' , since it is supposed to contain information from the whole sequence. A fully-connected layer and a softmax layer are further applied on top of this representation to calculate the probability distribution over class set \mathcal{Y} , as follows.

$$p = \text{softmax}(W_f h' + b_f) \quad (6)$$

Prompt-based learning, on the other hand, adapts the pre-trained LMs for the downstream task via priming on natural language **prompt**—pieces of text that are combined with the input and fed to the LMs to produce an output for downstream tasks [1]. Concretely, we first convert each input sequence x with a template \mathcal{T} to form a prompt x' : $\mathcal{T} : x \mapsto x'$. In addition, a mapping function \mathcal{M} is used to map the downstream task class set \mathcal{Y} to a set of label words \mathcal{V} constituting all vocabularies of the LM \mathcal{L} , i.e., $\mathcal{M} : \mathcal{Y} \mapsto \mathcal{V}$. As in the pre-training of LMs, we further insert the special token “[MASK]” into x' for \mathcal{L} to fill with the label words \mathcal{V} . We provide an example of the prompt formulation below.

Given $x = \text{“APC prevents tumor in adult male”}$, we set a template \mathcal{T} such as,

$\mathcal{T} = [x]$ “There is a [MASK] relation.”

Then, the prompt x' would be:

$x' = \text{“APC prevents tumor in adult male. There is a [MASK] relation.”}$

We further feed the prompt x' into \mathcal{L} to obtain the hidden vector $h_{[\text{MASK}]}$ of [MASK]. Next, with the mapping function \mathcal{M} connecting the class set \mathcal{Y} and the label words, we formalize the probability distribution over \mathcal{Y} at the masked position, i.e., $p(y|x) = p([\text{MASK}] = \mathcal{M}(y)|x')$. Here, the mapping function can also be set manually e.g., $\mathcal{M}(\text{true}) = \text{“positive”}$ and $\mathcal{M}(\text{false}) = \text{“negative”}$. Note that depending on the task, dataset, and the prompt design, the class labels themselves can be used directly without any mapping function \mathcal{M} .

In this study, our prompt-based learning combines the input sequence x with the graph context \mathcal{C} into the prompt x' , as illustrated in Fig. 2. Specifically, we formulate the prompt x' to include the following elements:

- (1) textual context: input sequence x containing the pair,
- (2) graph context \mathcal{C} : context generated from KG structures as described in §4.2,
- (3) target pair: pair e_1 and e_2 as the target, e.g., (FGF6, prostate cancer),
- (4) [MASK] token,
- (5) (optional) template tokens.

Subsequently, our final prompt x' as the input to the LM for the pair e_1 and e_2 can be formally defined as:

$$x' = [x] [\mathcal{C}] \text{ The pair } [e_1] \text{ and } [e_2] \text{ shows a [MASK] relation.} \quad (7)$$

In this study, we select three SLMs, one for each of the three architectures: MLM, CLM, Seq2SeqLM. Since each type of SLMs is trained differently, we design the prompt x' differently across each type of SLMs. For instance, the prompt x' in Equation 7, which is a *cloze-style task* prompt, suits the MLM architecture, since this model is trained to be able to see the preceding and succeeding words in texts. As for CLM and Seq2SeqLM, we cast the task as *generation-type*, with prompt x' such as:

$$x' = [x] [C] \text{ The pair } [e_1] \text{ and } [e_2] \text{ shows a causal relation: [MASK]}. \quad (8)$$

As mentioned earlier, the design of the mapping function \mathcal{M} to map the output into the downstream task labels varies depending on the task, dataset, and the prompt design. For instance, with the prompt x' as in Equation 7, we can directly use the class labels set $\mathcal{Y} = \{causal, non-causal\}$ without any mapping function. Meanwhile, for prompt x' in Equation 8, we manually define a mapping function, e.g., $\mathcal{M}(causal) = \text{"true"}$ and $\mathcal{M}(non-causal) = \text{"false"}$. Note that the template "*The pair shows...*" is optional and can be replaced with other text.

5 Evaluation

Experiment Settings. We evaluate the proposed approach under few-shot settings, using $k = 16$ training samples across all experiments. Precision (P), Recall (R), and F1-score (F1) metrics are employed to evaluate the performance.

Since fine-tuning on low-resource often suffers from instability and results may change given a different split of data [34], we apply 5-fold cross-validation and the metric scores are averaged. We restrict the number of contents from the KG structures to be included in the prompt since the length of the prompt for SLMs is limited, and we restrict the number of hops when querying the KG, as well. We experimented with different settings and reported the best performing models. Additional technical details are provided as supplementary materials.

Datasets. The evaluation datasets are summarized in Table 1. Causality is often observed in the biomedical domain, thus we primarily evaluate our approach within this field, supplemented by open-domain dataset. Each instance in the dataset comprises textual context where a variable pair co-occurs in text (see Example 4), and is annotated by human experts to determine if there is a causal relation between the pair.

Example 4. FGF6 contributes to the growth of prostate cancer by activating.

Choice of SLMs. In this work, we define SLMs as LMs with **less than 1 billion** of total parameters. We experimented with SLMs with three different architectures, as follows.

Table 1. Dataset sizes and types.

dataset	domain	total instances	description
GENEC (ours)	biomedical	5,834	gene-gene causality
DDI [16]	biomedical	33,508	drug-drug causality
COMAGC [22]	biomedical	821	gene-disease causality
SEMEVAL-2010 Task 8 [15]	open-domain	10,717	general domain causality

- (a) MLM: **roberta** [27] model adapted to the biomedical domain, with 125 million parameters (**biomed-roberta-base-125m** [12]),
- (b) CLM: **bloomz-560m** [29] with 560 million parameters,
- (c) Seq2SeqLM: **T5-base-220m** [31] model with 220 million parameters

Choice of KGs. We selected the following two KGs for the experiments:

- (a) Wikidata [38], as a representation of the general-domain KG,
- (b) Hetionet [17], a domain-specific KG assembled from 29 different databases, covering genes, compounds, and diseases.

We selected Wikidata for its broad coverage of numerous subjects and topics. As a comparison, we selected biomedical-KG Hetionet since we primarily evaluate our approach on the datasets from this particular domain.

Model Comparison. In the evaluation, we compare the following models:

- (1) ICL: In-Context Learning refers to a prompting method where few demonstrations of the task are provided to the LLMs as part of the prompt [5]. For this method, we selected **GPT-3.5-turbo-instruct** model by OpenAI.
- (2) FT_{full}: Conventional Fine-Tuning models trained using the full datasets.
- (3) FT_{few-shot}: Conventional Fine-Tuning models under few-shot $k = 16$ setting.
- (4) PT_{few-shot}: Original Prompt Tuning [23] implementation as baseline.
- (5) PBL _{\mathcal{NN} -Wiki-few-shot}: Our proposed Prompt-based Learning + **KG Structure as Prompt** using the neighbor nodes \mathcal{NN} structure from Wikidata.
- (6) PBL _{\mathcal{CN} -Wiki-few-shot}: Our proposed Prompt-based Learning + **KG Structure as Prompt** using the common neighbor nodes \mathcal{CN} structure from Hetionet.
- (7) PBL _{\mathcal{MP} -Wiki-few-shot}: Our proposed Prompt-based Learning + **KG Structure as Prompt** using the metapaths \mathcal{MP} structure from Hetionet.

6 Results and Discussion

Table 2 & 3 summarize the results. We report the averaged Precision (P), Recall (R), and F1 scores, including the standard deviation values of the F1 scores over the 5-folds cross-validation. We provide a summary of the primary findings (§6.1), followed by analysis and discussion of the results (§6.2).

Table 2. Evaluation results. Values in parenthesis are the standard deviations of F1 scores over 5-cv test folds. \mathcal{NN} , \mathcal{CNN} , \mathcal{MP} indicate the KG structures: *neighbors nodes*, *common neighbors nodes*, and *metapath*, respectively. **bold**: highest F1 scores per LMs architecture and per dataset, underline: F1 scores where few-shot models surpassed the models with full dataset, *italic*: F1 scores of the highest-performed models per dataset.

	COMAGC			GENEC			DDI		
	P	R	F1	P	R	F1	P	R	F1
(baseline) ICL _(GPT-3.5-turbo)	64.1	67.7	65.5 _(.18)	55.4	77.2	62.6 _(.16)	53.2	99.0	68.9 _(.08)
MLM architecture (biomed-roberta-base-125m)									
FT _{full}	90.0	86.8	88.2 _(.02)	61.0	61.0	61.5 _(.03)	84.0	98.9	90.7 _(.04)
(baseline) FT _{few-shot}	87.0	71.0	76.8 _(.02)	52.0	52.0	52.0 _(.02)	64.9	87.0	73.9 _(.07)
(baseline) PT _{few-shot}	87.0	77.2	80.6 _(.03)	58.0	58.0	58.0 _(.02)	69.6	83.0	75.4 _(.03)
(ours) PBL _{\mathcal{NN}} -Wiki-few-shot	82.0	85.0	83.5 _(.02)	63.0	63.0	63.0 _(.03)	70.2	85.0	76.6 _(.03)
(ours) PBL _{\mathcal{CNN}} -Het-few-shot	77.4	89.5	82.7 _(.05)	54.5	54.4	54.4 _(.02)	65.1	89.9	74.6 _(.05)
(ours) PBL _{\mathcal{MP}} -Het-few-shot	80.0	89.3	83.9 _(.03)	60.5	60.5	60.5 _(.02)	67.0	87.6	75.4 _(.02)
CLM architecture (bloomz-560m)									
FT _{full}	58.0	91.8	71.3 _(.07)	53.8	73.0	60.7 _(.07)	83.0	91.4	86.7 _(.06)
(baseline) FT _{few-shot}	73.4	85.0	77.6 _(.04)	48.2	86.0	61.7 _(.01)	72.0	61.5	66.1 _(.04)
(baseline) PT _{few-shot}	64.1	95.0	76.3 _(.01)	51.3	97.0	67.6 _(.01)	60.2	92.0	72.7 _(.02)
(ours) PBL _{\mathcal{NN}} -Wiki-few-shot	71.7	90.9	79.0 _(.02)	54.1	90.0	67.4 _(.01)	63.3	88.0	72.6 _(.02)
(ours) PBL _{\mathcal{CNN}} -Het-few-shot	65.7	94.7	77.2 _(.05)	52.8	100	<u>69.1</u> _(.00)	60.4	93.9	72.8 _(.05)
(ours) PBL _{\mathcal{MP}} -Het-few-shot	76.9	89.0	81.8 _(.04)	52.8	91.0	68.5 _(.03)	65.5	90.8	74.8 _(.05)
Seq2SeqLM architecture (T5-base-220m)									
FT _{full}	88.5	78.0	82.6 _(.07)	60.6	43.0	50.0 _(.11)	96.3	83.0	88.8 _(.04)
(baseline) FT _{few-shot}	68.8	81.0	72.7 _(.06)	48.3	67.0	55.5 _(.01)	55.6	94.0	69.6 _(.04)
(baseline) PT _{few-shot}	64.5	91.0	75.0 _(.05)	63.0	83.0	69.3 _(.06)	63.3	82.0	70.3 _(.04)
(ours) PBL _{\mathcal{NN}} -Wiki-few-shot	65.3	90.0	74.7 _(.01)	66.5	76.0	70.3 _(.02)	57.5	95.0	70.9 _(.03)
(ours) PBL _{\mathcal{CNN}} -Het-few-shot	65.4	86.3	73.4 _(.02)	56.0	95.8	70.6 _(.01)	56.2	96.0	70.6 _(.02)
(ours) PBL _{\mathcal{MP}} -Het-few-shot	73.3	82.0	75.6 _(.03)	56.5	91.0	69.7 _(.02)	60.6	92.9	72.9 _(.03)

Table 3. Evaluation results for open-domain dataset: SEMEVAL-2010 Task 8

	P	R	F1	P	R	F1	P	R	F1
(baseline) ICL _{GPT-3.5-turbo}	52.2	97.2	67.5 _(.07)						
	MLM			CLM			Seq2SeqLM		
FT _{full}	94.8	88.7	91.6 _(.02)	73.0	74.0	71.3 _(.07)	82.8	77.0	79.4 _(.02)
(baseline) FT _{few-shot}	57.2	83.0	67.2 _(.04)	50.2	99.0	66.6 _(.01)	52.1	90.9	61.1 _(.04)
(baseline) PT _{few-shot}	51.9	94.0	66.9 _(.00)	51.7	98.0	67.6 _(.02)	52.5	93.0	66.7 _(.02)
(ours) PBL _{\mathcal{NN}} -Wiki-few-shot	55.7	93.0	69.7 _(.01)	53.4	91.2	67.4 _(.00)	53.7	93.0	67.9 _(.01)

6.1 Primary Findings

We listed the summary of the main results from Table 2 below.

- (a) Our proposed approach outperformed other models in most of the experiments across different dataset domains: up to 15.1 points of improvement of F1 scores on biomedical datasets ($55.5 \rightarrow 70.6$, GENEC) and 6.8 points of improvement on open-domain dataset ($61.1 \rightarrow 67.9$, SEMEVAL).
- (b) Under few-shot settings with $k = 16$ training samples, our proposed approach achieved comparable scores to conventional fine-tuning models trained with full datasets, especially on GENEC and COMAGC datasets. Several even surpassed them (underlined values in Table 2).
- (c) Our models based on SLMs with less than 1 billion parameters surpassed a larger model across all experiments and datasets, underlining the importance of KG to support the constrained internal knowledge of smaller LMs.

6.2 Analysis and Discussion

\mathcal{NN} vs. \mathcal{CNN} vs. \mathcal{MP} : which performed best? To sum up, the KG structure *metapath* \mathcal{MP} contributed the most to the top-performed models, while the neighbors nodes \mathcal{NN} and common neighbors nodes \mathcal{CNN} roughly exhibited comparable performance across models and datasets. To train a robust model that is able to generalize well given any KG structure, we opted to not optimize the content selection of the KG structures in the current experiments. For instance, when there are more than m metapaths for a pair, we *randomly* select m of them, m being a *hyperparameter* of the number of metapaths to be included as prompt. In spite of that, our proposed approach achieved a relatively satisfactory performance, suggesting that rather than the content of the structure, the **type of the structural information**, i.e., \mathcal{NN} vs. \mathcal{CNN} vs. \mathcal{MP} , is arguably more important for our KG Structure as Prompt approach.

MLM vs. CLM vs. Seq2SeqLM: different LMs architecture. For classification tasks like ours, language models trained with MLM architecture are often preferred. This preference comes from the fact that MLMs are trained to consider both preceding and succeeding words, a crucial aspect for accurately predicting the correct class in a classification model. In line with that, our top-performed models are based on the MLM architecture, followed by the models based on Seq2SeqLM. Similar to MLM, Seq2SeqLM also includes encoder blocks and is trained to be able to see the surrounding words [31]. To conclude, selecting an appropriate architecture, specifically how the LMs are trained, is crucial when adapting LMs for downstream tasks. As demonstrated by the outcomes of our experiments, LMs trained with MLM and Seq2SeqLM architecture are more suitable for classification tasks than those with CLM architecture.

Wikidata vs. Hetionet. In biomedical datasets, the proposed approach injected with structural information from Hetionet demonstrates better performance in most experiments. This is expected considering the domain-specific nature of the dataset. Nevertheless, both Wikidata and Hetionet performed relatively well; the top-performed models for COMAGC and GENEC are attained

with Hetionet, while for DDI are achieved with Wikidata. We also achieved 6.8 points of improvement on SEMEVAL with Wikidata. This suggests that the proposed approach is rather flexible regarding the choice of KGs.

SLMs vs. LLMs, and the importance of KG. In this paper, we selected OpenAI’s `GPT-3.5-turbo-instruct` [30] as a representative of larger parameter-LLMs. However, they does not provide technical details such as the numbers of parameters; except the context windows which is 4,096 tokens in size for this model [30]. We chose this model since our choice of SLMs have a maximum token length ranging from 128 to 512, which is much smaller than this model. To summarize the result, all SLMs surpassed this model for all of the datasets in all experiments. This proved the potential of SLMs; fused with prompt-based learning and access to KG, our approach outperformed LLMs with considerably larger size and parameters. Note that we also provided $k = 16$ training samples as task demonstration to query the GPT model (ICL prompting), for a fair comparison with the few-shot settings.

Typically, SLMs are trained on significantly less data compared to LLMs, which leads to reduced capacity and inferior performance in downstream tasks. Therefore, the graph context derived from the structural information of KG by our **KG Structure as Prompt** effectively serves as an additional *evidence of causality*; in other words, it assists SLMs to rely not only on their constrained internal knowledge, but also by enhancing their capacity through denser information sourced from the KG.

7 Conclusion

In this paper, we presented “**KG Structure as Prompt**”, a novel approach for integrating structural information from KG into prompt-based learning, to further enhance the capability of Small Language Models (SLMs). We evaluated our approach on knowledge-based causal discovery tasks. Extensive experiments under few-shot settings on biomedical and open-domain datasets further highlight the effectiveness of the proposed approach, as it outperformed most of the baselines, including the conventional fine-tuning with a full dataset. Our proposed approach has also proven to be effective with three different types of LMs architectures, showing its flexibility and adaptability across various LMs and KGs. We also proved the robust capabilities of SLMs: in combination with prompt-based learning and a knowledge graph, SLMs are able to surpass LMs with considerably larger parameters.

Our work has been centered on discovering causal relationships between pairs of variables. In future work, we aim to tackle more complex scenarios by developing methods to analyze causal graphs with multiple interconnected variables, which will offer a deeper understanding of causalities.

Supplemental Material Statement: Datasets, source code, and other implementation details: <https://anonymous.4open.science/r/kg-structure-as-prompt-7DCF/>

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