Make Knowledge Computable: Differentiable Neural Symbolic Reasoning

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1 Overview

The goal of making world knowledge computable has a long and distinguished history in artificial intelligence. Earlier symbolic AI systems attempt to hardly code expert-level knowledge into programs. Though powerful to solve very complex questions[1], these systems are mostly domain specific, require lots of human efforts to maintain the knowledge base and could not keep learning from data. Over the past years, deep learning have shown great capacity to memorize a surprising amount of world knowledge. By training from massive corpora in an end-to-end manner, recent large-scale neural models can even outperform humans in many languages and vision tasks, such as translation, open object recognition, and image captioning. Yet, as the knowledge is stored implicitly in the parameters of neural networks, existing neural models fail to handle many complex tasks that require reasoning over symbolic knowledge. For example, answering complex questions given a image/video requires inferring in-context and outside knowledge of objects and their relationships, based on which to conduct compositional and logical reasoning; synthesizing high-level hardware programs requires understanding structural and symbolic `C/C++` codes, predicting execution results and searching optimal programs in discrete space.

To address these issues, I attempt to propose a different direction: Instead of compiling the world knowledge statically into model weights, I aim to model these symbolic knowledge in a more modular design, such that both neural models and symbolic AI module could understand the knowledge, compute and conduct reasoning. This vision is close to the traditional **Neural-Symbolic learning systems** that integrate the two worlds. In these systems, the neural model focus on parsing input query x into symbolic programs z (such as SQL query or arithmetic circuit), on top of which a symbolic module, such as numerical and logical solver, focuses on planning, deduction, and reasoning, to generate output answer y. Despite the advantages of the Neural-Symbolic AI system, most previous works in this line face a crucial obstacle: as symbolic modules are not differentiable, we cannot train the whole Neural-Symbolic model in an end-to-end manner, i.e., only using (x, y) pairs to train the whole system. Instead, most prior efforts require annotating intermediate symbolic query z, to train the neural module. For most real-world applications, such high-quality intermediate labels are arduous or even impossible to obtain, limiting the usage of Neural-Symbolic AI systems.

My ultimate research goal is to enable neural model to interact with symbolic reasoning module in a differentiable manner, and train such Neural-Symbolic model end-to-end without intermediate labels. To bring this vision about, I have conducted works on:

- **Reasoning Module**: design differentiable neural modules that can conduct symbolic reasoning, including knowledge graph reasoning [1, 2] and complex Logical inference [3].
- **Self-Supervision**: train the neural model via self-supervision from structural symbolic knowledge [4, 5, 6].
- **Out-of-Distribution Generalization**: the modular design of neural-symbolic models by its nature help to generalize better for Out-of-Distribution [7], Out-of-Vocabulary [8], cross-lingual [9] and cross-type [10] tasks.

Putting these pieces together, I am pursuing the ultimate vision to build end-to-end Neural-Symbolic system that has the capacity of reasoning, advancing to true human intelligence.

2 Prior Research Achievements

My vision is supported by my prior research, which has led to more than 20 research papers published in top Machine Learning venues (NeurIPS, ICLR, AAAI), Data Mining venues (KDD, WWW, WSDM), and Nature Language Processing venues (ACL, EMNLP). Notably, I received the **Best Full Paper Award** at WWW 2019, **Best Student Paper Award** at DLG-KDD 2020, and **Best Paper Award** at SoCal-NLP 2022. Many models I design have been integrated into machine learning libraries such as Pytorch-Geometric and DGL[2], utilized in many industrial products, including Google Youtube Shorts recommendation, Microsoft Graph, Facebook hate speech detection, Tiktok & Toutial search engine [11] and stock trend prediction service by Microsoft [12]. Collectively, my papers have been cited more than 1500 times since 2018, according to Google Scholar. The software tools I developed have received over 1300 stars in total on Github, and also served as core building blocks for many NSF research grants.

[1] `https://www.ibm.com/ibm/history/ibm100/us/en/icons/watson/breakthroughs/`

[2] They have become basic building blocks for modern models for structured and geometric data and are widely used in academia and industry. My proposed HGT [1] model is used as official tutorial in PyG.

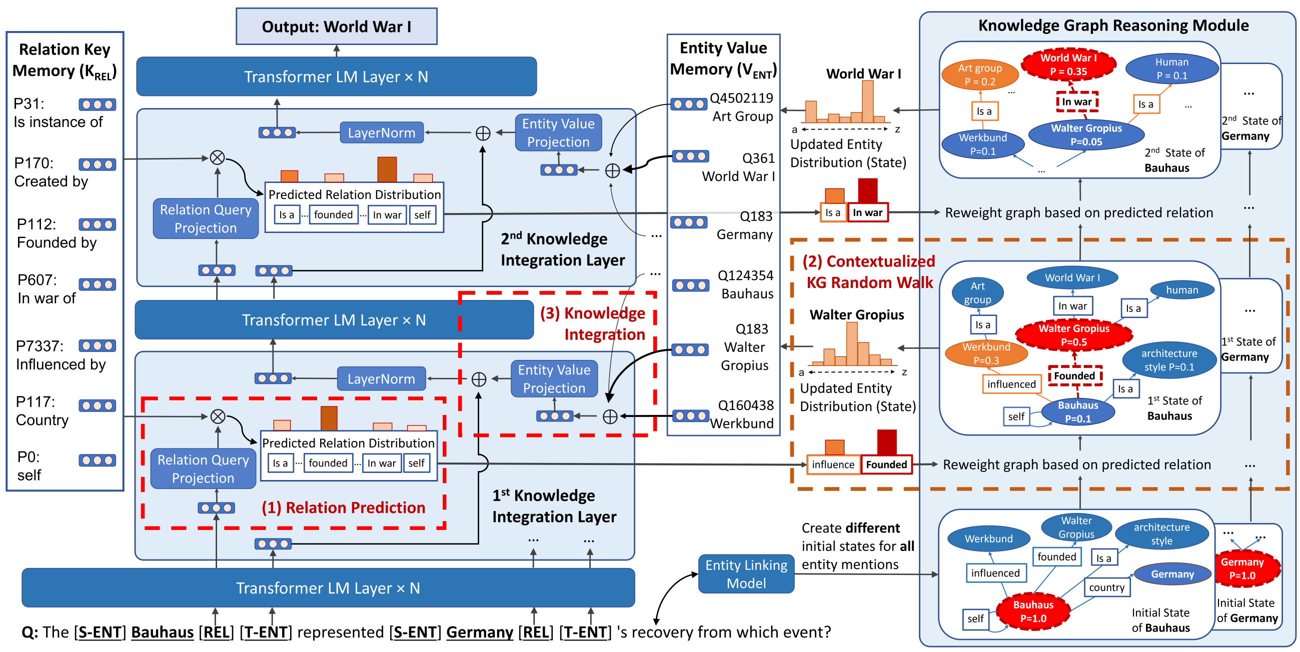

Figure 1: **OreoLM**: Integrating differentiable Knowledge Graph reasoning into neural Language Model. Three key procedures are highlighted in red dotted box: 1) *Relation Prediction*: predicts relation action for each entity mention. 2) *Contextualized KG Random Walk*: Based on the predicted relation, we re-weight each graph and conduct contextualized random walk to update entity distribution state. 3) *Knowledge Integration*: An weighted aggregated entity embedding is added into a placeholder token as retrieved knowledge.

2.1 Differentiable Symbolic Reasoning Module

The most important module to build an end-to-end Neural-Symbolic system is to make the symbolic reasoning step differentiable. My prior research focuses on **reasoning over Knowledge Graph** (KG), which consists of three central subtasks: 1) modeling heterogeneous KG via neural model; 2) reasoning over the knowledge graph to answer complex question; 3) answering first-order logical queries in embedding space.

HGT [1] addresses the first subtask to model complex multi-relational and large-scale knowledge graphs via Graph Neural Networks (GNNs). Before HGT, most existing GNNs are designed for homogeneous graphs, in which all nodes and edges belong to the same types, making them infeasible to represent more complex relational data, i.e., heterogeneous KG. To solve this problem, we propose Heterogeneous Graph Transformer (HGT) for modeling web-scale [13] heterogeneous graphs. As illustrated in Figure 2, we leverage the meta relation triplet to parameterize the weight matrices for calculating attention over each edge, empowering HGT to maintain dedicated representations for different nodes and edges. HGT can incorporate information from different types of high-order neighbors through messages passing across layers, so it can automatically learn "meta paths" which are essential for different downstream tasks. HGT significantly improve both benchmark performance and Microsoft Graph anomaly detection and Facebook hate speech detection service.

OreoLM [2] tackles the second subtask to conduct differentiable knowledge graph reasoning via graph walking, and is my first attempt to integrate such symbolic reasoning module with neural Language Model (LM). The proposed knOwledge REasOning empowered Language Model (OreoLM) consists of a fully differentiable Knowledge Interaction Layer that could be inserted amid arbitrary Transformer layers as the interface for LMs to interact with KG. As illustrated in Figure 1, KIL sends relational instructions for guiding knowledge graph reasoning and retrieves retrieved knowledge to solve the question. With the predicted relation, we conduct symbolic state transition for each reasoning path as walking over the graph. In this way, LM guides KG to walk towards the desired answer, while the retrieved knowledge improves LM. By adopting OreoLM to RoBERTa and T5, we show significant performance gain and state-of-art Closed-Book question answering performance and could summarize critical reasoning paths to interpret the model decision. OreoLM is being shifted to open-domain question-answering and summarizing system at Microsoft Azure Service.

FuzzQA [3] targets at the third and most challenging subtask of conducting first-order logical reasoning with existential quantification (∃), conjunction (∧), disjunction (∨), and negation (¬). Our proposed Fuzzy Query Embedding (FuzzQA) borrow the idea of fuzzy logic as differentiable logical operators, which fully satisfy the axioms of logical operations and can preserve logical operation properties in vector space. In addition, Our logical operations do not require learning any operator-specific parameters. We conduct experiments to show that even when our model is only trained with link prediction (without any complex query), it achieves better results than

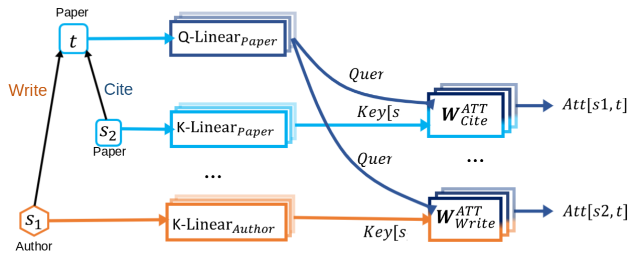

Figure 2: **HGT** (Heterogeneous Graph Transformer) models multi-relational knowledge graph by parametrize weights via meta relation triplets.

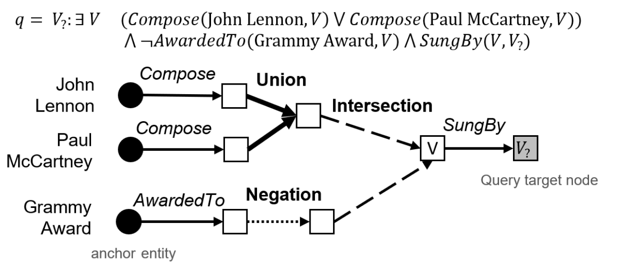

Figure 3: **FuzzQA** uses fuzzy logic as operators to build computational graph for answering First-Order Logic (FOL) Query over knowledge graph.

state-of-the-art logical query embedding models trained with extra complex query data.

2.2 Self-Supervised Learning from Structural Symbolic Knowledge

Recent deep learning is rapidly progressing from task-specific systems towards fundamental models that are trained from massive unlabelled datasets. To guide the proposed Neural-Symbolic models learning world knowledge without labeled data (especially intermediate annotations), I propose several attempts to utilize the structural symbolic knowledge (e.g., knowledge graph) as self-supervision to pre-train neural models.

GPT-GNN [5] aims to capture the intrinsic structural and semantic properties of the graph so that it can easily generalize to any downstream tasks on this graph with a few fine-tuning steps. To achieve this goal, we propose Generative Pre-Training of Graph Neural Networks (GPT-GNN), which models the graph distribution by directly learning to reconstruct the attributed graph. We factorize the likelihood of graph generation into two components: 1) attribute generation, and 2) edge generation. By modeling both components, GPT-GNN captures the inherent dependency between node attributes and graph structure during the generative process. GPT-GNN significantly outperforms state-of-the-art GNN models without pre-training by up to 9.1% over different datasets and downstream tasks. GPT-GNN is used by Facebook to pre-train HGT on billion-scale social media graph.

RGPT-QA [4] synthesizes a relational QA dataset covering a wide range of relations from both the Wikidata triplets and Wikipedia hyperlinks. We then pre-train a QA model to infer the latent relations from the question, and then conduct extractive QA to get the target answer entity. RGPT-QA enhances the performance of popular QA models, especially on questions with long-tail relations.

ReVeaL [6] (Retrieval-Augmented Visual Language Pre-Training) transforms multimodal world knowledge into a key-value memory using neural representation learning, and then retrieve from it to answer knowledge-intensive queries. By decoupling the knowledge memorization from reasoning, we enable our model to leverage various external sources of multimodal knowledge (Wikipedia passages and images, the WikiData knowledge graph, Web image-text pairs and visual question answering data). REVEAL achieves state-of-the-art performance on several knowledge-intensive Visual Question Answering and Image Captioning datasets.

Figure 4: **ReVeaL** augments a visual-language model with the ability to retrieve multiple knowledge from a diverse set of sources. Both retriever and generator are trained jointly in end-to-end manner.

2.3 Generalize across Distributions via Modelling Symbolic Knowledge

One key advantage of symbolic reasoning over neural models is to better generalize to different distributions and domains [14]. By modelling data via a compositional and structural manner, we could regard each disentangled neural module to handle a specific functionality, and only change a particular module when we transfer to a new domain/distribution. More specifically, I conduct research to solve Out-of-Distribution, Out-of-Vocabulary, Cross-Lingual and Cross-Type tasks.

MT-CRL [7] (Multi-Task Causal Representation Learning) aims to improve Out-of-Distribution generalization of multi-task learning (MTL) via regularizing spurious correlation. We theoretically and empirically show that MTL is more prone to taking non-causal knowledge from other tasks than single-task learning, thus generalizing worse. To solve this problem, MT-CRL represents multi-task knowledge via disentangled neural modules, and learn which module is causally related to each task via MTL-specific invariant regularization. MT-CRL not only improves on official benchmarks, and also used in Google Youtube Shorts recommendation.

HiCE [8] (Hierarchical Context Encoder) aims to predict Out-Of-Vocabulary (OOV) word embedding based on corpus knowledge. We formulate the OOV embedding learning as a few-shot regression task by predicting oracle embedding vectors (trained with abundant observations) based on only K contexts. Specifically, we use Model-Agnostic Meta-Learning (MAML) for adapting model to the new corpus fast and robustly.

Emoji-LSA [9] improve cross-lingual sentiment classification performance. We utilize emojis, which are widely available in many languages, as a special symbolic knowledge to learn both the cross-language and language-specific sentiment patterns in different languages. The proposed method demonstrates the state-of-the-art performance on benchmark datasets, which are sustained even when sentiment labels are scarce.

KTN [10] (Knowledge Transfer Networks) studies transfering knowledge across different node types within a heterogeneous graph in zero-shot setup. We design a principled regularization to force embeddings of label-scarce node types close to their label-abundant neighborhood after aggregation.

3 Future Research Agenda

My research builds an end-to-end framework by combining neural models with symbolic reasoning, and utilizes it to solve different real-world tasks that require complex reasoning. In the past, I have been fortunate to collaborate with people from diverse backgrounds, covering machine learning, data mining, NLP, computer vision, and hardware infrastructure from both academia and industry. This experience gives me a broad vision for continuing this challenging but exciting research direction.

In the future, I am excited to further improve my proposed neural-symbolic reasoning framework, as well as using it to solve most fundamental and significant challenges in other areas in computer science, such as program synthesis, hardware design, mathematical auto-proving and scientific discovery:

1. Towards More Expressive Differentiable Symbolic Reasoning Systems. My past studies have been focused on symbolic reasoning over knowledge graphs. Outside this research domain, there exist many other interesting and powerful symbolic reasoning AI, including numerical reasoning, physics simulation, mathematical theorem prover, as well as many pre-defined APIs provided by industrial services. To enable integrating of these symbolic reasoning capacity into neural models, I plan to build a more general interface to bridge the two worlds, supporting free interaction and backpropagation. Many challenges remain to be addressed, including how to properly model this heterogeneous and structural knowledge in a principled manner (ideally in a unified graph view), choose appropriate abstractions for reasoning procedure, and make reasoning differentiable. I am also interested to improve the causal representation learning via modular design, and making the AI model capable to conduct causal inference and estimate uncertainty and risks.

2. Explore Program Synthesis via Neural-Symbolic Reasoning. Many fundamental tasks in computer science and artificial intelligence could be formalized as program synthesis. For example, dialogue chatbots require parsing human language into formal SQL programs; mathematical auto-proving requires transforming math equations; high-level synthesis of FPGA program requires compiling and latent execution of discrete C/C++ programs. My past research on graph representation learning and symbolic reasoning is a natural solution for conducting program synthesis. Therefore, I am excited to apply my proposed neural-symbolic models for solving these interesting and challenging tasks. Take hardware synthesis as an example, I aim to represent symbolic program as latent variables, which we could execute via neural module to infer results. Based on it, we could search best program via optimizing the latent program to maximize output, in a differentiable manner.

3. Empower Scientific Discovery via Neural-Symbolic Reasoning. My proposed Neural-Symbolic models have already shown improvement in a wide range of artificial intelligence tasks. Outside of AI domains, many general scientific problems could also be abstracted as symbolic reasoning. For example, the drug discovery and design could be represented molecule as geometric graph; physics simulation requires understanding complex physic environments (represented with graph with particles, fluids, plasma as nodes, and their mutual interactions as edges). I am particularly interested in whether my proposed neural-symbolic AI models could be applied and benefit these fundamental scientific problems, helping building better scientific simulation tools. In addition, I am interested in utilizing the neural-symbolic systems to automatically discover world knowledge, including constructing domain-specific knowledge graph, discovering new Physics or Chemical governing laws from experiments, and identifying causal structures from real-world social data.

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