A joint framework for path finding and path reasoning

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Abstract

In large knowledge graphs (KGs), many essential relations are missing. Therefore, inferring missing knowledge by synthesizing existing information has attracted a lot of interests from the research community. Here in this paper, we are particularly interested in solving a practical query answering task involving predicting the relation between given entities. In order to resolve the link prediction problem, many deep-learning based research has been done, they can be mainly classified into two categories, i.e. path-finding and path reasoning. The path finding model mainly focus on extracting more meaning links from the knowledge graph while the path reasoning model mainly focus on infer relation given an extracted KG path. None of the previous research has combined these two models into a unified framework and train them jointly. Our paper proposes a variational-inference based architecture to train these two models jointly so that they can complement each other and perform better on the reasoning task. Our empirical results have indicated very significant improvements over the other standalone algorithms.

Introduction

Automated reasoning, the ability of computing systems to make new inferences from observed evidence, has been a long standing goal of artificial intelligence, there is rising interests in applying deep learning and neural network in performing complex reasoning. Especially in large-KG scenarios, the multi-hop reasoning is even more challenging. In recent years, the Path-Ranking algorithm (PRA) (Lao, Mitchell, and Cohen 2011) have emerged and become the standard approach for KG reasoning, which uses a bounded depth-first search to pick more plausible paths using supervised learning. In order to vectorize the KG space and helps algorithm to generalize better, Deep-Path (Xiong, Hoang, and Wang 2017) has been proposed to view this process as a reinforcement learning problem (RL), which views the agent's every relation hop as an action and aims to encourage agent to find better paths. However, these two approaches not only fail to take the intermediate entity or entity type into consideration, but also needs different models for different reasoning tasks. In order to resolve these issues, Chains-of-Reasoning (Das et al. 2016) employs a single high-capacity RNN-based method to reason over all tasks. The existing deep neural models takes KG reasoning as two modules, i.e. ”Path-Finding” and ”Path-Reasoning” modules and train the two modules separately without interaction, which is known to cause error propagation problem. More specifically, ”Path-Finding” module only helps explore more paths while agnostic of the value of these newly explored paths, ”Path-Reasoning” module only learns to predict relation given the prefetched paths while agnostic of the procedure of path-finding. In order to train the two modules jointly and incorporate them closely to perform joint reasoning, we propose a novel perspective to this problem using graphic model. This graphic model views the path as the latent variables, the relation as the observed variables and the given entity pair as the conditional variables. Thus, the path-finding module can be viewed as a posterior distribution or prior distribution to infer the latent representation given the observed variable, while the path-reasoning can be viewed as the likelihood distribution selecting the correct relationship given the latetnt KG paths. With this assumption, we propose to use variational auto-encoder (Kingma and Welling 2013) to train these modules jointly. This variational framework closely incorporate the two components as a whole and alternatively use one to enhance the other. With this cooperation, the path-finding module can expose more possible links to the path-reasoning model to improve its generalizing ability, meanwhile, the path-reasoning module can alter the behavior of path-finding to search for more meaningful path links.

Model

Here we draw a schematic diagram of our model in Figure 1, formally, we write the following equation:

$$p(r|(e_s, e_d)) = \sum_L p_\beta(L|(e_s, e_d))p_\theta(r|L) \tag{1}$$

However, this probability is intractble since it needs to sum over the whole latent link space. Therefore, we propose to maximize its variational lower bound as follows: Formally, we achieve the following ELBO equation:

$$\begin{aligned} ELBO =& E_{L\sim q_\varphi} \log p_\theta(r|L) - \\ & KL(q_\varphi(L|r,(e_s,e_d))||p_\beta(L|(e_s,e_d))) \end{aligned} \tag{2}$$

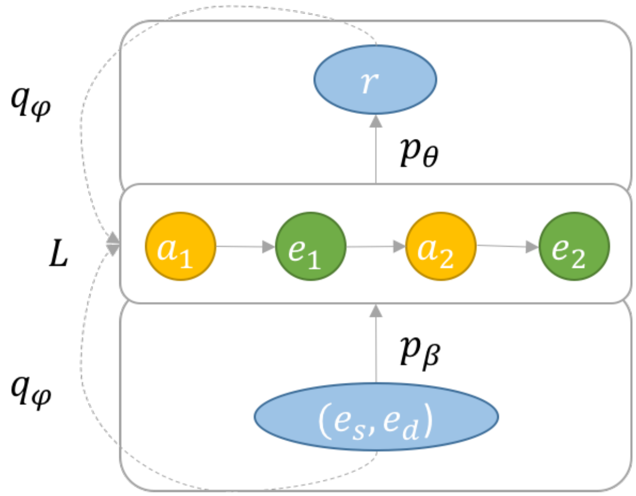

Figure 1: Dotted line represents the posterior distribution – Path-Finding module, which is modeled as a multinomial distribution over the whole link space, solid lines represents the prior probability of given path L and the likelihood probability of a relation represented by given path L.

where L denotes the connecting links $L = l_1, l_2, l_3, \cdots, l_n$ between the entity pair, and $l_1 = (a_1, e_1), l_2 = (a_2, e_2), \cdots l_n = (a_n, e_n)$. More specifically, the ELBO is composed of three components, which we will talk in details as follows:

Approximate Posterior Distribution

Here we re-parameterize the approximate posterior distribution $q_\varphi(L|r, (e_s, e_d)$ as a multinomial distribution, which covers the whole path space $\mathbb{L}$. In order to model such a large and sparse space, we employ an RNN architecture (Hochreiter and Schmidhuber 1997) to break down the long sequence into consequent steps, which is modeled with Markov process, e.g. recursively picking outgoing edges based on the contexts and history. Formally, we write the probability distribution of t_{th} path node as follows:

$$s_t = RNN(s_{t-1}, l_t, r) \quad (3)$$
$$p(l_{t+1}) = softmax(g((e_s, e_d), r, s_t)) \quad (4)$$

where s_t denotes the hidden states of the RNN in t_{th} time step, we here also restrict the length limit to 4 to control the space.

Likelihood Distribution

Here we also re-parameterize the likelihood distribution $p_\theta(r|L)$ as multinomial distribution over the whole relation space $\mathbb{R}$. In order to model this probability, we propose another RNN architecture (Hochreiter and Schmidhuber 1997) to receive the sequential inputs $L = l_1, l_2, \cdots, l_n$ and apply classification based on the last hidden state h_n. Formally, we write the probability distribution $p(R)$ as follows:

$$h_t = RNN(h_{t-1}, l_t) \quad (5)$$
$$p(r) = softmax(f(h_n)) \quad (6)$$

where h_t is the state of the RNN in t_{th} step, after the RNN finishes n steps, we employ a function f with softmax to predict the probability over the relation space R. This model can be thought of as the path-reasoning module to understand the relation chains and tries to infer its relation type.

Prior Distribution

Here we formulate the path finder $p_\beta(L|(e_s, e_d))$ as an Markov decision process without knowing the actual relation R as input, which predicts actions l_t in every time step based on the history $l_1, \cdots, l_{t-1}$. We propose to adopt the same architecture as approximate posterior model and leave out the relation term r.

$$m_t = RNN(m_{t-1}, l_t) \quad (7)$$
$$p(l_{t+1}) = softmax(g((e_s, e_d), m_t)) \quad (8)$$

where m_t denotes the t_{th} hidden state of RNN model.

Training

In order to maximize our designed lower bound objective function $ELBO$, here we propose to use Monte-Carlo sampling algorithm for estimation as follows:

$$\frac{\partial ELBO}{\partial \varphi} = E_{L\sim q_\varphi(L))} - r(L)\frac{\partial \log q_\varphi(L|(e_s, e_d), r)}{\partial \varphi} \quad (9)$$

$$\frac{\partial ELBO}{\partial \theta} = E_{L\sim q_\varphi(L)}\frac{\partial \log p_\theta(r|L)}{\partial \theta} \quad (10)$$

$$\frac{\partial ELBO}{\partial \beta} = E_{L\sim q_\varphi(L)}\frac{\partial \log p_\beta(L|(e_s, e_d))}{\partial \beta} \quad (11)$$

here we can interpret these gradient terms as REINFORCE (Williams 1992) and RAML (Norouzi et al. 2016) frameworks and train them using gradient descent algorithm.

Implementation

In order to train this model on the current link prediction and fact prediction tasks like NELL-995 (Mitchell et al. 2015), we propose to use an alternative training algorithm to update three models. During test time, we can perform missing link prediction by firstly obtaining useful paths from the prior distribution and apply likelihood distribution to obtain its reasoning score for different relations.

Experimental Results

Here we compare our results with the state-of-art neural reasoning model (Xiong, Hoang, and Wang 2017) and demonstrate our results as follows: We can observe significant improvement on MAP evaluation metrics.

Model	12-rel MAP
RPA (Lao, Mitchell, and Cohen 2011)	67.5
DeepPath (Xiong, Hoang, and Wang 2017)	79.6
OUR MODEL	**88.6**

Table 1: MAP results on the NELL dataset.

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