Efficient Probabilistic Logic Reasoning with Graph Neural Networks

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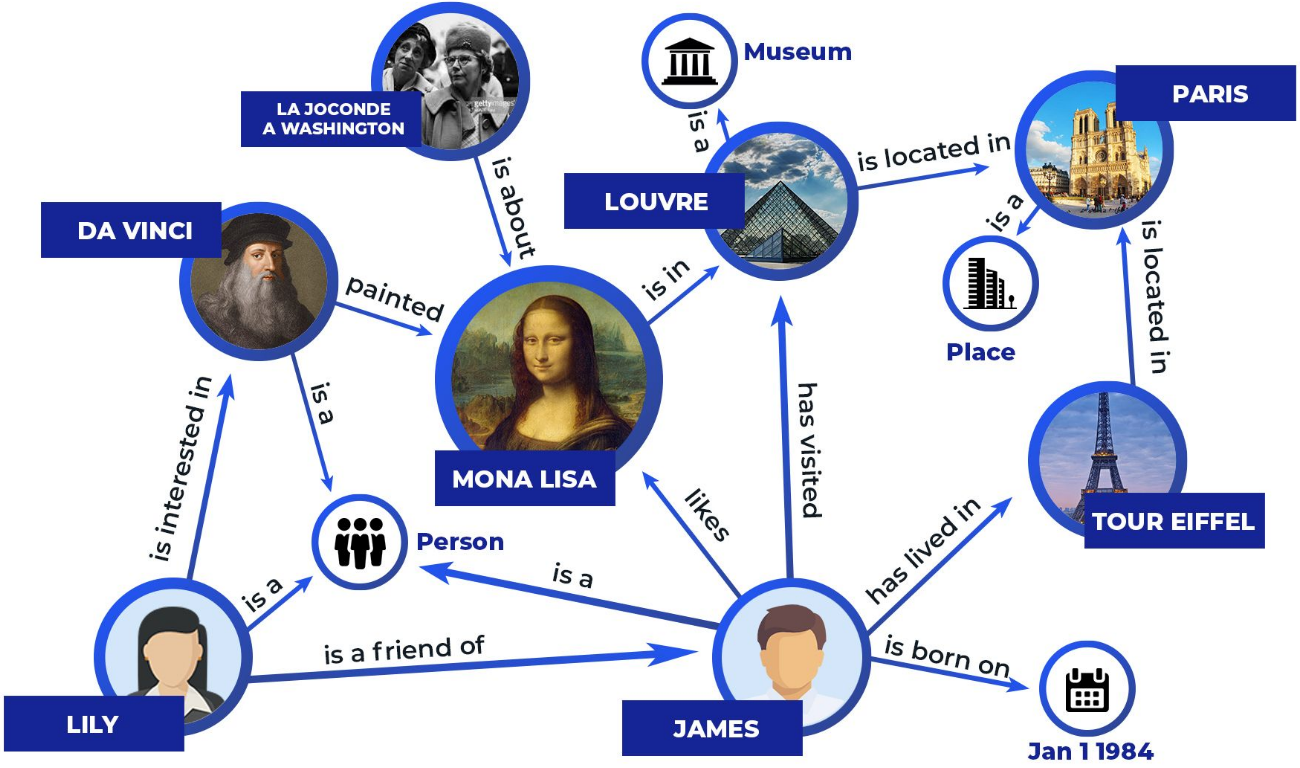
Knowledge Graph



Knowledge Graph

Knowledge Graph is a tuple $\mathcal{K} = (\mathcal{C}, \mathcal{R}, \mathcal{O})$

$\mathcal{C} = \{c_1, \ldots, c_M\}$ -- set of entities/constants

$\mathcal{R} = \{r_1, \ldots, r_N\}$ -- set of relations/predicates

$\mathcal{O} = \{o_1, \ldots, o_L\}$ -- set of observed facts

Knowledge Graph

Predicate is a logic function $\mathcal{C} \times \ldots \times \mathcal{C} \mapsto \{0, 1\}$

$r(c, c')$ -- c have relation with c' (asymmetric)

Ground predicate is predicate with a set of entities assigned

$a_r = (c, c')$ -- assignment ($r(c, c') \rightarrow r(a_r)$)

ground predicate ≡ binary random variable

unobserved facts ≡ latent variables

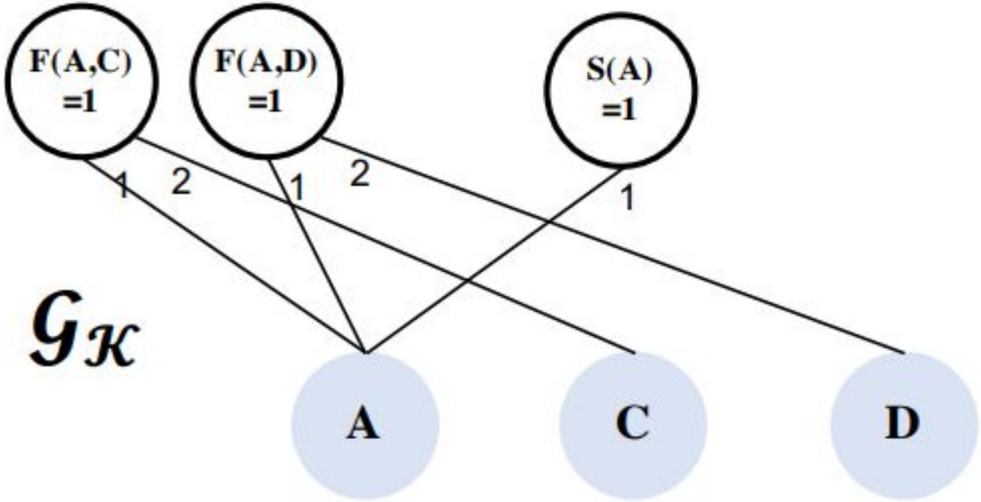
Observed fact is truth value {0, 1} assigned to a ground predicate

$\mathrm{L}(c, c') = 1$

Knowledge Graph

knowledge base $\mathcal{K}$ represented by a bipartite graph $\mathcal{G}_{\mathcal{K}} = (\mathcal{C}, \mathcal{O}, \mathcal{E})$

- $\mathcal{C}$ -- constant
- $\mathcal{O}$ -- observed facts (factor)
- $\mathcal{E}$ -- a set of edge



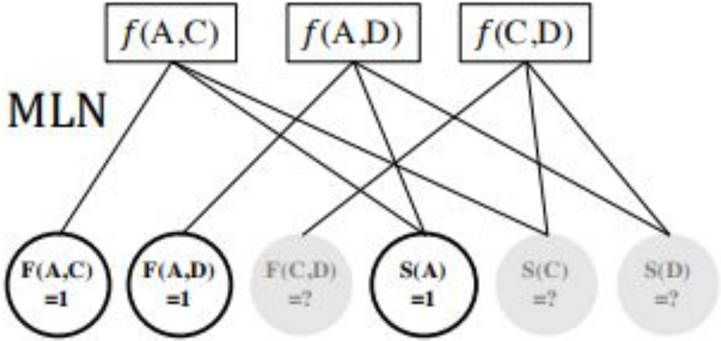
Markov Logic Networks

MLNs use logic formulae to define potential functions in undirected graphical models

logic formulae -- $f(\cdot) : \mathcal{C} \times \ldots \times \mathcal{C} \mapsto \{0, 1\}$ defined by composition of predicates

Example

$$f(c, c') := \mathtt{Smoke}(c) \wedge \mathtt{Friend}(c, c') \Rightarrow \mathtt{Smoke}(c')$$



Markov Logic Networks

MLN can be represented as a joint distribution over all observed facts O and unobserved facts H

$$P_w(\mathcal{O},\mathcal{H}) := \frac{1}{Z(w)} \exp\left(\sum_{f\in\mathcal{F}} w_f \sum_{a_f\in\mathcal{A}_f} \phi_f(a_f)\right)$$

$\mathcal{O}$ -- observed facts, $\mathcal{H}$ -- unobserved facts

$a_r = (c, c')$ -- assignment (similar to KG)

$\mathcal{A}_f = \{a_f^1, a_f^2, \ldots\}$ -- entire collection of consistent assignments

$\phi_f(\cdot)$ potential function defined by a formula f

w_f -- confidence score of formula f

$Z(w)$ -- partition function summing over all ground predicates

KG vs MLN

Knowledge graphs	MLN
Sparse Number of edges linear to the number of entities	Denser number of edges high-order polynomials to the number of entities number of nodes can be quadratic or more tothe number of entities

Variational EM framework for MLN

Instead of optimizing the log-likelihood of all the observed facts

$$\log P_w(\mathcal{O})$$

Optimize the variational evidence lower bound (ELBO) of the data log-likelihood using variational EM algorithm

$$\mathcal{L}_{\text{ELBO}}(Q_\theta, P_w) := \mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}\Big[\log P_w(\mathcal{O}, \mathcal{H})\Big] - \mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}\Big[\log Q_\theta(\mathcal{H}|\mathcal{O})\Big]$$

$Q_\theta(\mathcal{H} \mid \mathcal{O})$ -- variational posterior distribution of the latent variables

$P_w(\mathcal{H}|\mathcal{O})$ -- true posterior

Variational EM framework for MLN

Derivation of lower bound:

- f(E[X]) >= E[f(X)] (Jensens)
- $$\begin{aligned} \log p(x) &= \log \int_z p(x, z) \\ &= \log \int_z p(x, z) \frac{q(z)}{q(z)} \\ &= \log \left(\mathrm{E}_q \left[\frac{p(x, Z)}{q(z)} \right] \right) \\ &\geq \mathrm{E}_q[\log p(x, Z)] - \mathrm{E}_q[\log q(Z)]. \end{aligned}$$

Variational EM algorithm E-step

Minimize the KL divergence between $Q_\theta(\mathcal{H}|\mathcal{O})$ and $P_w(\mathcal{H}|\mathcal{O})$

Exact inference of MLN is intractable and NP-complete

So use mean-field variational distribution to approximate, each unobserved ground predicate inferred as follows:

$$Q_\theta(\mathcal{H}|\mathcal{O}) := \prod_{r(a_r)\in\mathcal{H}} Q_\theta(r(a_r))$$

$Q_\theta(r(a_r))$ -- factorized distribution (follow bernoulli distribution)

Q_θ is parameterized using ExpressGNN

More about variational inference:
https://www.cs.cmu.edu/~epxing/Class/10708-17/notes-17/10708-scribe-lecture13.pdf

Variational EM algorithm E-step

After parameterization $\mathcal{L}_{\text{ELBO}}(Q_\theta, P_w)$ can be rewritten as:

$$\Big(\sum_{f\in\mathcal{F}} w_f \sum_{a_f\in\mathcal{A}_f} \mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}\Big[\phi_f(a_f)\Big] - \log Z(w)\Big) - \Big(\sum_{r(a_r)\in\mathcal{H}} \mathbb{E}_{Q_\theta(r(a_r))}\Big[\log Q_\theta(r(a_r))\Big]\Big)$$

Variational EM algorithm E-step

Both $\mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}[\log P_w(\mathcal{O}, \mathcal{H})]$ and $\mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}[\log Q_\theta(\mathcal{H}|\mathcal{O})]$ involves a large number of terms which can make it very computationally expensive

So the author uses mini-batches of ground formulae

- In each optimization iteration
- Sample a batch of ground formulae
- For each formulae sampled, compute $\left(\sum_{f \in \mathcal{F}} w_f \sum_{a_f \in \mathcal{A}_f} \mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}\left[\phi_f(a_f)\right] - \log Z(w)\right)$
    - By by taking the expectation of the corresponding potential function with respect to the posterior of the involved latent variables

Variational EM algorithm E step

If the task have sufficient label data, add supervised learning objective

$$\mathcal{L}_{\text{label}}(Q_\theta) = \sum_{r(a_r)\in\mathcal{O}} \log Q_\theta(r(a_r))$$

And the overall objective function is

$$\mathcal{L}_\theta = \mathcal{L}_{\text{ELBO}}(Q_\theta, P_w) + \lambda \mathcal{L}_{\text{label}}(Q_\theta)$$

Variational EM algorithm M step

learn the weights of logic formulae in MLN with $Q_\theta(\mathcal{H}|\mathcal{O})$ fixed

$Z(w)$ is no longer a constant, and has exponential number of terms, so is intractable to directly optimize the ELBO

Use pseudo-log-likelihood:

$$P_w^*(\mathcal{O},\mathcal{H}) := \mathbb{E}_{Q_\theta(\mathcal{H}|\mathcal{O})}\left[\sum_{r(a_r)\in\mathcal{H}} \log P_w(r(a_r)\mid \mathrm{MB}_{r(a_r)})\right]$$

$\mathrm{MB}_{r(a_r)}$ -- Makarov blanket of $r(a_r)$

Variational EM algorithm M step

For each formula i that connects $r(a_r)$ to its Markov blanket, optimize weight w_i

Use gradient descent, with the derivative:

$$\nabla_{w_i} \mathbb{E}_{Q_\theta}[\log P_w(r(a_r) \mid \mathrm{MB}_{r(a_r)})] \simeq y_{r(a_r)} - P_w(r(a_r) \mid \mathrm{MB}_{r(a_r)})$$

$y_{r(a_r)}$ = 0 or 1, if $r(a_r)$ is observed fact

= $Q_\theta(r(a_r))$, otherwise

Variational EM algorithm M step

Computationally intractable to use all ground predicates to compute the gradients

So consider all the ground formulae with at most one latent predicate and pick up the ground predicate if its truth value determines the formula’s truth value

Only need to keep a small subset of ground predicates that can directly determine the true value of a ground formula

ExpressGNN

Need to have a expressive and efficient network to approximate true posterior distribution in step E

ExpressGNN involve three parts:

1. Vanilla graph neural network (GNN)
2. tunable embeddings
3. uses the embeddings to define the variational posterior

ExpressGNN

Build a GNN on the knowledge graph $\mathcal{G}_\mathcal{K}$

much smaller than MLN

$\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$ are shared across the entire graph and independent of the number of entities

GNN is a compact model with $O(d^2)$ parameters given d dimensional embeddings

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Algorithm 1: $\texttt{GNN}()$

Initialize entity node: $\mu_c^{(0)} = \mu_0, \ \forall c \in \mathcal{C}$

for $t = 0$ *to* $T - 1$ **do**

$\quad \triangleright$ Compute message $\forall r(c, c') \in \mathcal{O}$

$\quad m_{c' \to c}^{(t)} = \texttt{MLP}_1(\mu_{c'}^{(t)}, r; \boldsymbol{\theta}_1)$

$\quad \triangleright$ Aggregate message $\forall c \in \mathcal{C}$

$\quad m_c^{(t+1)} = \texttt{AGG}(\{m_{c' \to c}^{(t)}\}_{c' : r(c,c') \in \mathcal{O}})$

$\quad \triangleright$ Update embedding $\forall c \in \mathcal{C}$

$\quad \mu_c^{(t+1)} = \texttt{MLP}_2(\mu_c^{(t)}, m_c^{(t+1)}; \boldsymbol{\theta}_2)$

return embeddings $\{\mu_c^{(T)}\}$

ExpressGNN

For each entity in the KG, augment its GNN embedding with a tunable embedding $\boldsymbol{\omega}_c \in \mathbb{R}^k$ as $\hat{\mu}_c = [\mu_c, \boldsymbol{\omega}_c]$

The tunable embeddings increase the expressiveness of the model

Number of parameters in tunable embeddings is $O(kM)$

ExpressGNN

variational posterior defined as:

$$Q_\theta(r(c_1, c_2)) = \sigma(\mathrm{MLP}_3(\hat{\mu}_{c_1}, \hat{\mu}_{c_2}, r; \boldsymbol{\theta}_3))$$

$$\sigma(\cdot) = \frac{1}{1+\exp(-\cdot)}$$

number of parameters in $\boldsymbol{\theta}_3$ is $O(d+k)$

ExpressGNN

compact GNN assigns similar embeddings to similar entities in the KG

expressive tunable embeddings allows encoding of entity specific information beyond graph structures

overall number of trainable parameters is $O(d^2 + kM)$, and by controlling d and k, we can control the trade-off between compactness and expressiveness

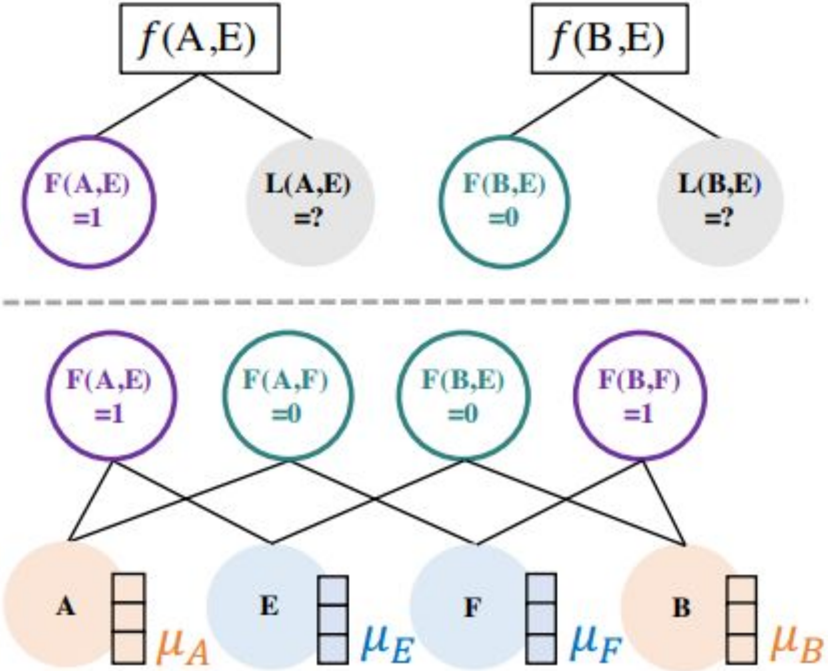
theoretical analysis on ExpressGNN

vanilla GNN produces the same embedding for some nodes that should be distinguished, for example

A and B have opposite relations with E, but GNN will produce same embedding

$\mathtt{L}(A, E)$ And $\mathtt{L}(B, E)$ have different posteriors, but they get same $Q_\theta(\mathtt{L}(A, E))$

ExpressGNN avoid this problem by allowing additional tunable embeddings



ExpressGNN

Efficient: works on the knowledge graph, instead of the huge MLN grounding graph, more efficient than the existing MLN inference methods

Compact: the GNN model with shared parameters can be very memory efficient

Expressive: the GNN model can capture structure knowledge in the knowledge graph, and the tunable embeddings can encode entity-specific information

Generalizable: with the GNN embeddings, ExpressGNN may generalize to new entities or even different but related knowledge graphs

Experimental Setup

Benchmark datasets

UW-CSE , Cora, synthetic Kinship datasets, and FB15K-237

General settings

Linux machine with RTX 2080 Ti, Intel Xeon Silver 4116 and 256GB RAM

Hyperparameters:

use 0.0005 as the initial learning rate, and decay it by half for every 10 epochs without improvement

two-layer MLP with ReLU activation function for each embedding update step

MLP parameters is different for steps, edge types and direction of embedding aggregation

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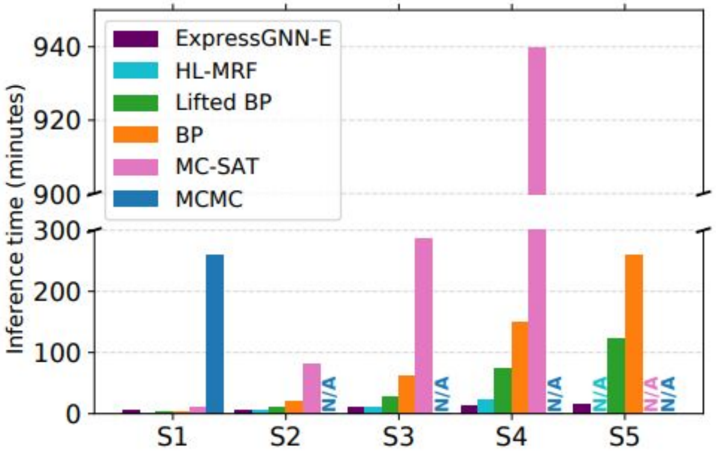
Experiment Result

Method	Kinship					UW-CSE					Cora
	S1	S2	S3	S4	S5	AI	Graphics	Language	Systems	Theory	(avg)
MCMC	0.53	-	-	-	-	-	-	-	-	-	-
BP / Lifted BP	0.53	0.58	0.55	0.55	0.56	0.01	0.01	0.01	0.01	0.01	-
MC-SAT	0.54	0.60	0.55	0.55	-	0.03	0.05	0.06	0.02	0.02	-
HL-MRF	**1.00**	**1.00**	**1.00**	**1.00**	-	0.06	0.06	0.02	0.04	0.03	-
ExpressGNN-E	0.97	0.97	0.99	0.99	0.99	**0.09**	**0.19**	**0.14**	**0.06**	**0.09**	**0.64**

Experiment Result

Method	Inference Time (minutes)				
	AI	Graphics	Language	Systems	Theory
MCMC	>24h	>24h	>24h	>24h	>24h
BP	408	352	37	457	190
Lifted BP	321	270	32	525	243
MC-SAT	172	147	14	196	86
HL-MRF	135	132	18	178	72
ExpressGNN-E	**14**	**20**	**5**	**7**	**13**



Experiment Result

Configuration	Cora				
	S1	S2	S3	S4	S5
Tune64	0.57	0.74	0.34	0.55	0.70
GNN64	0.57	0.58	0.38	0.54	0.53
GNN64+Tune4	0.61	0.75	0.39	0.54	0.70
Tune128	**0.62**	0.76	0.42	**0.60**	0.73
GNN128	0.60	0.59	0.45	0.55	0.61
GNN64+Tune64	**0.62**	**0.79**	**0.46**	0.57	**0.75**

Experiment Result

Model	MRR					Hits@10				
	0%	5%	10%	20%	100%	0%	5%	10%	20%	100%
MLN	-	-	-	-	0.10	-	-	-	-	16.0
NTN	0.09	0.10	0.10	0.11	0.13	17.9	19.3	19.1	19.6	23.9
Neural LP	0.01	0.13	0.15	0.16	0.24	1.5	23.2	24.7	26.4	36.2
DistMult	0.23	0.24	0.24	0.24	0.31	40.0	40.4	40.7	41.4	48.5
ComplEx	0.24	0.24	0.24	0.25	0.32	41.1	41.3	41.9	42.5	51.1
TransE	0.24	0.25	0.25	0.25	0.33	42.7	43.1	43.4	43.9	52.7
RotatE	0.25	0.25	0.25	0.26	0.34	42.6	43.0	43.5	44.1	53.1
pLogicNet	-	-	-	-	0.33	-	-	-	-	52.8
ExpressGNN-E	**0.42**	**0.42**	0.42	0.44	0.45	53.1	53.1	53.3	55.2	57.3
ExpressGNN-EM	**0.42**	**0.42**	**0.43**	**0.45**	**0.49**	**53.8**	**54.6**	**55.3**	**55.6**	**60.8**

Demo

Quiz

1. What is a potential problem for applying GNN-based methods on knowledge graphs? (single choice)

a. There is no potential problem. GNN can perform well on all graph-related problems.
b. Long-tail nature of Knowledge Graph makes applying GNN hard since GNN requires sufficient labeled instances to achieve good performance.
c. Unobserved features in Knowledge Graph could never be learned by any neural network through any means.

2. Which of the following is true about Markov Logic Network(MLN)? (single choice)

a. Inference in MLN is computationally intense.
b. The MLN structure is normally sparser than knowledge graph
c. a and b

3. In regards to ExpressGNN, at which step is the GNN used in variational EM for Markov Logic Network(MLN)? (single choice)
a. E step
b. M step

Questions