Neural Bellman-Ford Networks: A General Graph Neural Network Framework for Link Prediction

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Abstract

Link prediction is a very fundamental task on graphs. Inspired by traditional path-based methods, in this paper we propose a general and flexible representation learning framework based on paths for link prediction. Specifically, we define the representation of a pair of nodes as the *generalized sum* of all path representations, with each path representation as the *generalized product* of the edge representations in the path. Motivated by the Bellman-Ford algorithm for solving the shortest path problem, we show that the proposed path formulation can be efficiently solved by the generalized Bellman-Ford algorithm. To further improve the capacity of the path formulation, we propose the Neural Bellman-Ford Network (NBFNet), a general graph neural network framework that solves the path formulation with learned operators in the generalized Bellman-Ford algorithm. The NBFNet parameterizes the generalized Bellman-Ford algorithm with 3 neural components, namely INDICATOR, MESSAGE and AGGREGATE functions, which corresponds to the boundary condition, *multiplication* operator, and *summation* operator respectively[1]. The NBFNet is very general, covers many traditional path-based methods, and can be applied to both homogeneous graphs and multi-relational graphs (e.g., knowledge graphs) in both transductive and inductive settings. Experiments on both homogeneous graphs and knowledge graphs show that the proposed NBFNet outperforms existing methods by a large margin in both transductive and inductive settings, achieving new state-of-the-art results.

1 Introduction

Predicting the interactions between nodes (a.k.a. link prediction) is a fundamental task in the field of graph machine learning. Given the ubiquitous existence of graphs, such a task has many applications, such as recommender system [28], knowledge graph completion [35] and drug repurposing [22].

Traditional methods of link prediction usually define different heuristic metrics over the paths between a pair of nodes. For example, Katz index [24] is defined as a weighted count of paths between two nodes. Personalized PageRank [36] measures the similarity of two nodes as the random walk probability from one to the other. Graph distance [31] uses the length of the shortest path between two nodes to predict their association. These methods have been shown effective on different types of graphs, scaling up to large graphs, and enjoying good interpretability. However, they are designed based on handcrafted metrics and may not be optimal for link prediction on real-world graphs.

To address these limitations, there are some recent advancements based on graph neural networks (GNNs) [66, 49], which automatically extract important features from local subgraphs for link

[1] Unless stated otherwise, we use *summation* and *multiplication* to refer the generalized operators in the path formulation, rather than the basic operations of arithmetic.

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prediction. Thanks to the high expressiveness of GNNs, these methods have shown state-of-the-art performance, and the learned models can generalize to new graphs, i.e., in the inductive setting. However, both scalability and intepretability of these methods is usually compromised. Therefore, we wonder if there exists an approach which has the advantages of both traditional path-based methods and recent approaches based on graph neural networks, i.e., **scalability**, **high model capacity**, **strong generalization in both transductive and inductive settings**, and **interpretability**.

In this paper, we propose such a solution. Inspired by traditional path-based methods, our goal is to develop a general and flexible representation learning framework for link prediction based on the paths between two nodes. Specifically, we define the representation of a pair of nodes as the *generalized sum* of all the path representations between them, where each path representation is defined as the *generalized product* of the edge representations in the path. Many link prediction methods, such as Katz index [24], personalized PageRank [36], graph distance [31], as well as graph theory algorithms like widest path [3] and most reliable path [3], are special instances of this path formulation with different *summation* and *multiplication* operators. Motivated by the polynomial-time algorithm for the shortest path problem [4], we show that such a formulation can be efficiently solved via the generalized Bellman-Ford algorithm [45] under mild conditions and scale up to large graphs.

The operators in the generalized Bellman-Ford algorithm—*summation* and *multiplication*—are handcrafted, which have limited flexibility. Therefore, we further propose the Neural Bellman-Ford Networks (NBFNet), a graph neural network framework that solves the above path formulation with learned operators in the generalized Bellman-Ford algorithm. Specifically, NBFNet parameterizes the generalized Bellman-Ford algorithm with three neural components, namely INDICATOR, MESSAGE and AGGREGATE functions. The INDICATOR function initializes a representation on each node, which is taken as the boundary condition of the generalized Bellman-Ford algorithm. The MESSAGE and the AGGREGATE functions learn the *multiplication* and *summation* operators respectively.

We show that the MESSAGE function can be defined according to the relational operators in knowledge graph embedding methods [5, 61, 52, 25, 46], e.g., as a translation in Euclidean space induced by the relational operators of TransE [5]. The AGGREGATE function can be defined as learnable set aggregation functions [64, 59, 7]. The whole framework can be efficiently optimized through back-propagation. With other instantiations of MESSAGE and AGGREGATE functions, our framework can also cover some existing works on learning logic rules [62, 40] for link prediction on knowledge graphs. A comparison of operators in our NBFNet and other existing works is listed in Table 1.

Our NBFNet framework is very general, which can be applied to not only single-relational graphs (e.g., homogeneous graphs) but also multi-relational graphs (e.g., knowledge graphs). We empirically evaluate the proposed NBFNet for link prediction on homogeneous graphs and knowledge graphs in both transductive and inductive settings. Experimental results show that the proposed NBFNet outperforms existing state-of-the-art methods by a large margin in all settings, with an average relative performance gain of 14% on knowledge graph completion (HITS@1) in transductive setting and 16% on inductive relation prediction (HITS@10). We also show that the proposed NBFNet is indeed interpretable by visualizing the top-k relevant paths for link prediction on knowledge graphs.

Table 1: Comparison of operators in NBFNet and other methods from the view of path formulation.

Class	**Method**	**MESSAGE** $\boldsymbol{w}_q(e_i) \otimes \boldsymbol{w}_q(e_j)$	**AGGREGATE** $\boldsymbol{h}_q(P_i) \oplus \boldsymbol{h}_q(P_j)$	**INDICATOR** $⓪_q, ①_q$	**Edge Representation** $\boldsymbol{w}_q(e=(u,v))$
Traditional Link Prediction	Katz Index [24]	$\boldsymbol{w}_q(e_i) \times \boldsymbol{w}_q(e_j)$	$\boldsymbol{h}_q(P_i) + \boldsymbol{h}_q(P_j)$	$0, 1$	βw_e
	Personalized PageRank [36]	$\boldsymbol{w}_q(e_i) \times \boldsymbol{w}_q(e_j)$	$\boldsymbol{h}_q(P_i) + \boldsymbol{h}_q(P_j)$	$0, 1$	$\frac{\alpha w_{uv}}{\sum_{v' \in \mathcal{N}(u)} w_{uv'}}$
	Graph Distance [31]	$\boldsymbol{w}_q(e_i) + \boldsymbol{w}_q(e_j)$	$\min(\boldsymbol{h}_q(P_i), \boldsymbol{h}_q(P_j))$	$+\infty, 0$	w_e
Graph Theory Algorithms	Widest Path [3]	$\min(\boldsymbol{w}_q(e_i), \boldsymbol{w}_q(e_j))$	$\max(\boldsymbol{h}_q(P_i), \boldsymbol{h}_q(P_j))$	$-\infty, +\infty$	w_e
	Most Reliable Path [3]	$\boldsymbol{w}_q(e_i) \times \boldsymbol{w}_q(e_j)$	$\max(\boldsymbol{h}_q(P_i), \boldsymbol{h}_q(P_j))$	$0, 1$	w_e
Logic Rules	NeuralLP [62] / DRUM [40]	$\boldsymbol{w}_q(e_i) \times \boldsymbol{w}_q(e_j)$	$\boldsymbol{h}_q(P_i) + \boldsymbol{h}_q(P_j)$	$0, 1$	Weights learned by LSTM [21]
	NBFNet	Relational operators of knowledge graph embeddings [5, 61, 46]	Learned set aggregators [7]	Learned indicator functions	Learned relation embeddings

2 Related Work

Existing work on link prediction can be generally classified into 3 main paradigms: path-based methods, embedding methods, and graph neural networks.

Path-based Methods. Path-based methods have a long history in the literature of link prediction. Early methods on homogeneous graphs compute the similarity between two nodes based on the weighted count of paths (Katz index [24]), random walk probability (personalized PageRank [36]) or the length of the shortest path (graph distance [31]). SimRank [23] uses advanced metrics such as the expected meeting distance on homogeneous graphs, which is extended by PathSim [45] to heterogeneous graphs. On knowledge graphs, Path Ranking [29, 13] directly uses relational paths as symbolic features for prediction. Rule mining methods, such as NeuralLP [62] and DRUM [40], learn probabilistic logical rules to weight different paths. Path representation methods, such as Path-RNN [34] and its successors [9, 55], encode each path with recurrent neural networks (RNNs), and aggregate paths for prediction. However, these methods need to traverse an exponential number of paths and are limited to very short paths, e.g., ≤ 3 edges. Another stream of works [58, 8, 20] learns an agent to collect useful paths for link prediction. While these methods can produce explainable paths, they suffer from extremely sparse rewards and require careful engineering of the reward function [32] or the search strategy [44]. Some other works [6, 38] adopt variational inference to learn a path finder and a path reasoner for link prediction. The most relevant work to this paper is All-Paths [51], which computes all paths between two nodes with dynamic programming. However, All-Paths can only be applied with the bilinear model, while our NBFNet is general and enjoys a rich design space from existing knowledge graph embedding methods and set aggregation functions.

Embedding Methods. Embedding methods learn a distributed representation for each node and edge by preserving the edge structure of the graph. Representative methods include DeepWalk [37] and LINE [47] on homogeneous graphs, and TransE [5], DistMult [61] and RotatE [46] on knowledge graphs. Later works improve embedding methods with new score functions [52, 11, 25, 46, 48] that capture common semantic patterns of the relations, or search the score function in a general design space [68]. Embedding methods achieve promising results on link prediction, and can be scaled to very large graphs using multiple GPUs [70]. However, embedding methods do not explicitly encode local subgraphs between node pairs and cannot be applied to the inductive setting.

Graph Neural Networks. Graph neural networks (GNNs) [41] are a family of representation learning models that encode topological structures of graphs. Many works [26, 53, 59, 57] have been developed to learn better representations for nodes or graphs. For link prediction, the prevalent frameworks [27, 42, 10] adopt an auto-encoder formulation, which uses GNNs to encode node representations, and decodes edges as a function over node pairs. However, such frameworks do not capture the local subgraphs between nodes, and can be only applied to the transductive setting. Another stream of frameworks, such as SEAL [66] and GraIL [49], explicitly encodes the subgraph around each node pair for link prediction. While these frameworks are proved to be more powerful than the auto-encoder formulation [67] and can solve the inductive setting, they require to materialize a subgraph for each link, which is not scalable to large graphs. By contrast, our NBFNet explicitly captures the paths between two nodes for link prediction, meanwhile achieves a relatively low time complexity (Appendix C). There are also some works trying to scale GNNs for link prediction by dynamically pruning the set of nodes in message passing [60, 18]. These methods are complementary to our NBFNet, and may be incorporated into our method to get further acceleration.

3 Methodology

In this section, we first define a path formulation for link prediction. Our path formulation generalizes several traditional methods, and can be efficiently solved by the generalized Bellman-Ford algorithm. Then we propose Neural Bellman-Ford Networks to learn the path formulation with neural functions.

3.1 Path Formulation for Link Prediction

We consider the link prediction problem on both knowledge graphs and homogeneous graphs. A knowledge graph is denoted by $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{R})$, where $\mathcal{V}$ and $\mathcal{E}$ represent the set of entities (nodes) and relations (edges) respectively, and $\mathcal{R}$ is the set of relation types. We use the notation $\mathcal{N}(u)$ to denote the set of nodes connected to u, and $\mathcal{E}(u)$ to denote the set of edges ending with node u. A homogeneous graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ can be viewed as a special case of knowledge graphs, with only one relation type for all edges. Throughout this paper, we use **bold** terms, $\boldsymbol{w}_q(e)$ or $\boldsymbol{h}_q(u, v)$, to denote vector representations, and *italic* terms, w_e or w_{uv}, to denote scalars like the edge weight of

$e = (u, v)$. Without loss of generality, we derive our method based on knowledge graphs, while our method can also be applied to homogeneous graphs.

Path Formulation. Link prediction is aimed at predicting the existence of a query relation q between a head entity u and a tail entity v. From a representation learning perspective, this requires to learn a pairwise representation $\boldsymbol{h}_q(u, v)$, which captures the local subgraph structure between u and v w.r.t. the query relation q. In traditional methods [29], such a local structure is encoded by counting different types of random walks from u to v. Inspired by this construction, we formulate the pairwise representation as a *generalized sum* of path representations between u and v with a commutative *summation* operator $\oplus$. Each path representation $\boldsymbol{h}_q(P)$ is defined as a *generalized product* of the edge representations in the path with the *multiplication* operator $\otimes$.

$$\boldsymbol{h}_q(u, v) = \boldsymbol{h}_q(P_1) \oplus \boldsymbol{h}_q(P_2) \oplus ... \oplus \boldsymbol{h}_q(P_{|\mathcal{P}_{uv}|})|_{P_i \in \mathcal{P}_{uv}} \triangleq \bigoplus_{P \in \mathcal{P}_{uv}} \boldsymbol{h}_q(P) \tag{1}$$

$$\boldsymbol{h}_q(P = (e_1, e_2, ..., e_{|P|})) = \boldsymbol{w}_q(e_1) \otimes \boldsymbol{w}_q(e_2) \otimes ... \otimes \boldsymbol{w}_q(e_{|P|}) \triangleq \bigotimes_{i=1}^{|P|} \boldsymbol{w}_q(e_i) \tag{2}$$

where $\mathcal{P}_{uv}$ denotes the set of paths from u to v and $\boldsymbol{w}_q(e_i)$ is the representation of edge e_i. Note the *multiplication* operator $\otimes$ is not required to be commutative (e.g., matrix multiplication), therefore we define $\bigotimes$ to compute the product following the exact order. Intuitively, the path formulation can be interpreted as a depth-first-search (DFS) algorithm, where one searches all possible paths from u to v, computes their representations (Equation 2) and aggregates the results (Equation 1). Such a formulation is capable of modeling several traditional link prediction methods, as well as graph theory algorithms. Formally, Theorem 1-5 state the corresponding path formulations for 3 link prediction methods and 2 graph theory algorithms respectively. See Appendix A for proofs.

Theorem 1 *Katz index is a path formulation with* $\oplus = +$, $\otimes = \times$ *and* $\boldsymbol{w}_q(e) = \beta w_e$.

Theorem 2 *Personalized PageRank is a path formulation with* $\oplus = +$, $\otimes = \times$ *and* $\boldsymbol{w}_q(e) = \alpha w_{uv} / \sum_{v' \in \mathcal{N}(u)} w_{uv'}$.

Theorem 3 *Graph distance is a path formulation with* $\oplus = \min$, $\otimes = +$ *and* $\boldsymbol{w}_q(e) = w_e$.

Theorem 4 *Widest path is a path formulation with* $\oplus = \max$, $\otimes = \min$ *and* $\boldsymbol{w}_q(e) = w_e$.

Theorem 5 *Most reliable path is a path formulation with* $\oplus = \max$, $\otimes = \times$ *and* $\boldsymbol{w}_q(e) = w_e$.

Generalized Bellman-Ford Algorithm. While the above formulation captures important heuristics for link prediction, it is computationally expensive since the number of paths grows exponentially with the path length. Previous works [34, 9, 55] that directly computes the exponential number of paths can only afford a maximal path length of 3. A more scalable solution is to use the generalized Bellman-Ford algorithm [3]. Specifically, assuming the operators $\langle \oplus, \otimes \rangle$ satisfy a semiring system [19] with *summation identity* $⓪_q$ and *multiplication identity* $①_q$, we have the following algorithm.

$$\boldsymbol{h}_q^{(0)}(u, v) \leftarrow \mathbb{1}_q(u = v) \tag{3}$$

$$\boldsymbol{h}_q^{(t)}(u, v) \leftarrow \left(\bigoplus_{(x,r,v) \in \mathcal{E}(v)} \boldsymbol{h}_q^{(t-1)}(u, x) \otimes \boldsymbol{w}_q(x, r, v) \right) \oplus \boldsymbol{h}_q^{(0)}(u, v) \tag{4}$$

where $\mathbb{1}_q(u = v)$ is the *indicator* function that outputs $①_q$ if $u = v$ and $⓪_q$ otherwise. $\boldsymbol{w}_q(x, r, v)$ is the representation for edge $e = (x, r, v)$ and r is the relation type of the edge. Equation 3 is known as the boundary condition, while Equation 4 is known as the Bellman-Ford iteration. The high-level idea of the generalized Bellman-Ford algorithm is to **compute the pairwise representation $\boldsymbol{h}_q(u, v)$ for all $v \in \mathcal{V}$ in parallel**, and reduce the total computation by the distributive property of *multiplication* over *summation*. When $\oplus = min$ and $\otimes = +$, it recovers the original Bellman-Ford algorithm for the shortest path problem [4]. See Appendix B for preliminaries and the proof of the above algorithm.

Theorem 6 *Katz index, personalized PageRank, graph distance, widest path and most reliable path can be solved via the generalized Bellman-Ford algorithm.*

3.2 Neural Bellman-Ford Networks

While the generalized Bellman-Ford algorithm can solve many classical methods (Theorem 6), these methods instantiate the path formulation with handcrafted operators (Table 1), and may not be optimal for link prediction. To improve the capacity of path formulation, we propose a general framework, Neural Bellman-Ford Networks (NBFNet), to learn the operators in the pairwise representations.

Neural Parameterization. We relax the semiring assumption and parameterize the generalized Bellman-Ford algorithm (Equation 3 and 4) with 3 neural functions, namely INDICATOR, MESSAGE and AGGREGATE functions. The INDICATOR function replaces the *indicator* function $\mathbb{1}_q(u = v)$. The MESSAGE function replaces the binary *multiplication* operator $\otimes$. The AGGREGATE function is a permutation invariant function over sets that replaces the n-ary *summation* operator $\bigoplus$. Note that one may alternatively define AGGREGATE as the commutative binary operator $\oplus$ and apply it to a sequence of messages. However, this will make the parameterization more complicated.

Now consider the generalized Bellman-Ford algorithm for a given entity u and relation q. In this context, we abbreviate $\boldsymbol{h}_q^{(t)}(u, v)$ as $\boldsymbol{h}_v^{(t)}$, i.e., a representation on entity v in the t-th iteration. It should be stressed that $\boldsymbol{h}_v^{(t)}$ is still a pairwise representation, rather than a node representation. By substituting the neural functions into Equation 3 and 4, we get our Neural Bellman-Ford Networks.

$$\boldsymbol{h}_v^{(0)} \leftarrow \text{INDICATOR}(u, v, q) \tag{5}$$

$$\boldsymbol{h}_v^{(t)} \leftarrow \text{AGGREGATE}\left(\left\{\text{MESSAGE}\left(\boldsymbol{h}_x^{(t-1)}, \boldsymbol{w}_q(x, r, v)\right) \middle| (x, r, v) \in \mathcal{E}(v)\right\} \cup \left\{\boldsymbol{h}_v^{(0)}\right\}\right) \tag{6}$$

NBFNet can be interpreted as a novel GNN framework for learning pairwise representations. Compared to common GNN frameworks [27, 42] that compute the pairwise representation as two independent node representations $\boldsymbol{h}_q(u)$ and $\boldsymbol{h}_q(v)$, NBFNet initializes a representation on the source node u, and readouts the pairwise representation on the target node v. Intuitively, our framework can be viewed as a source-specific message passing process, where every node learns a representation conditioned on the source node. The pseudo code of NBFNet is outlined in Algorithm 1.

Algorithm 1 Neural Bellman-Ford Networks

Input: source node u, query relation q, #layers T
Output: pair representations $\boldsymbol{h}_q(u, v)$ for all $v \in \mathcal{V}$

```
for v ∈ V do                                        ▷ Boundary condition
    h_v^(0) ← INDICATOR(u, v, q)
end for
for t ← 1 to T do                                   ▷ Bellman-Ford iteration
    for v ∈ V do
        M^(t) ← {h_v^(0)}                           ▷ Message augmentation
        for (x, r, v) ∈ E(v) do
            m_(x,r,v)^(t) ← MESSAGE^(t)(h_x^(t-1), w_q(x, r, v))
            M^(t) ← M^(t) ∪ {m_(x,r,v)^(t)}
        end for
        h_v^(t) ← AGGREGATE^(t)(M^(t))
    end for
end for
return h_v^(T) as h_q(u, v) for all v ∈ V
```

Design Space. Now we discuss some principled designs for MESSAGE, AGGREGATE and INDICATOR functions by drawing insights from traditional methods. Note the potential design space for NBFNet is way larger than what is presented here, as one can always borrow MESSAGE and AGGREGATE from the arsenal of message-passing GNNs [17, 14, 59].

For the MESSAGE function, traditional methods instantiate it as natural summation, natural multiplication or min over scalars. Therefore, we may use the vectorized version of summation or multiplication. Intuitively, summation of $\boldsymbol{h}_x^{(t-1)}$ and $\boldsymbol{w}_q(x, r, v)$ can be interpreted as a translation of $\boldsymbol{h}_x^{(t-1)}$ by $\boldsymbol{w}_q(x, r, v)$ in the pairwise representation space, while multiplication corresponds to scaling. Such transformations correspond to the relational operators [16, 39] in knowledge graph embeddings [5, 61, 52, 25, 46]. For example, translation and scaling are the relational operators used in TransE [5] and DistMult [61] respectively. We also consider the rotation operator in RotatE [46].

The AGGREGATE function is instantiated as natural summation, max or min in traditional methods, which are reminiscent of set aggregation functions [64, 59, 7] used in GNNs. Therefore, we specify the AGGREGATE function to be sum, mean, or max, followed by a linear transformation and a non-linear activation. We also consider the principal neighborhood aggregation (PNA) proposed in a recent work [7], which jointly learns the types and scales of the aggregation function.

The INDICATOR function is aimed at providing a non-trivial representation for the source node u as the boundary condition. Therefore, we learn a query embedding $\boldsymbol{q}$ for $①_q$ and define INDICATOR function as $\mathbb{1}(u = v) * \boldsymbol{q}$. Note it is also possible to additionally learn an embedding for $⓪_q$. However, we find a single query embedding works better in practice.

The edge representation $\boldsymbol{w}_q(x, r, v)$ is parameterized as a learnable relation embedding $\boldsymbol{r}^{(t)}$. Similar to NeuralLP [62] & DRUM [40], we use different embeddings for different iterations, but share the embeddings across different queries, i.e., $\boldsymbol{r}^{(t)}$ depends on t but not q. Note NBFNet only learns embeddings for relations but not entities, and therefore can solve the inductive setting.

Link Prediction. We now show how to apply the learned pair representations to the link prediction problem. We use the pair representations to predict the conditional likelihood of the tail entity $p(v|u, q) = \sigma(f(\boldsymbol{h}_q(u, v)))$, where $\sigma(\cdot)$ is the sigmoid function and $f(\cdot)$ is a feed-forward neural network. Following previous works [5, 46], we minimize the negative log-likelihood of positive and negative triplets (Equation 7). The negative samples are generated according to Partial Completeness Assumption (PCA) [12], which corrupts one of the entities in a positive triplet to create a negative sample. Since the edges in homogeneous graphs are undirected, we symmetrize the representations and define $p(u, v) = \sigma(f(\boldsymbol{h}(u, v) + \boldsymbol{h}(v, u)))$. Equation 8 shows the loss for homogeneous graphs.

$$\mathcal{L}_{KG} = \mathbb{E}_{(u,q,v)\in\mathcal{E}} \left[-\log p(u, q, v)\right] + \mathbb{E}_{(u',q',v')\in\text{PCA}(u,q,v)} \left[-\log(1 - p(u', q', v'))\right] \tag{7}$$

$$\mathcal{L}_{homo} = \mathbb{E}_{(u,v)\in\mathcal{E}} \left[-\log p(u, v)\right] + \mathbb{E}_{(u',v')\notin\mathcal{E}} \left[-\log(1 - p(u', v'))\right] \tag{8}$$

Time Complexity. One advantage of NBFNet is that it has a relatively low time complexity during inference[2]. Consider a scenario where a model is required to infer the conditional likelihood of all possible triplets $p(v|u, q)$. We group triplets with the same condition u, q together, where each group contains $|\mathcal{V}|$ triplets. For each group, we only need to execute Algorithm 1 once to get their predictions. Since a small constant number of iterations T is enough for NBFNet to converge (Table 5b), Algorithm 1 has a time complexity of $O(|\mathcal{E}|d + |\mathcal{V}|d^2)$, where d is the dimension of representations. Therefore, the amortized time complexity for a single triplet is $O\left(\frac{|\mathcal{E}|d}{|\mathcal{V}|} + d^2\right)$. For a detailed comparison on the time complexity of GNN frameworks, please refer to Appendix C.

4 Experiment

4.1 Experiment Setup

We evaluate NBFNet in three settings, knowledge graph completion, homogeneous graph link prediction and inductive relation prediction. The former two are transductive settings, while the last is an inductive setting. For knowledge graphs, we use FB15k-237 [50] and WN18RR [11]. We use the standard transductive splits [50, 11] and inductive splits [49] of these datasets. For homogeneous graphs, we use Cora, Citeseer and PubMed [43]. Following previous works [27, 10], we split the edges into train/valid/test with a ratio of 85:5:10. Statistics of datasets can be found in Appendix E.

Implementation Details. Our implementation generally follows the open source codebases of knowledge graph completion[3] and homogeneous graph link prediction[4]. For knowledge graphs, we follow [62, 40] and augment each triplet $\langle u, q, v\rangle$ with a flipped triplet $\langle v, q^{-1}, u\rangle$. For homogeneous graphs, we follow [26, 27] and augment each node u with a self loop $\langle u, u\rangle$. We instantiate NBFNet with 6 layers, each with 32 hidden units. The feed-forward network $f(\cdot)$ is set to a 2-layer MLP with 128 hidden units. ReLU is used as the activation function for all hidden layers. Our model is trained on 4 Tesla V100 GPUs for 20 epochs, with Adam optimizer. See Appendix F for more details.

Evaluation. We follow the filtered ranking protocol [5] for knowledge graph completion. For a test triplet $\langle u, q, v\rangle$, we rank it against all negative triplets $\langle u, q, v'\rangle$ or $\langle u', q, v\rangle$ that do not appear in the knowledge graph. We report mean rank (MR), mean reciprocal rank (MRR) and HITS at N (H@N) for knowledge graph completion. For inductive relation prediction, we follow [49] and draw 50 negative triplets for each positive triplet and use the above filtered ranking. We report HITS@10 for

[2] Although the same analysis can be applied to training on a fixed number of samples, we note it is less instructive since one can trade-off samples for performance, and the trade-off varies from method to method.

[3] `https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding`. MIT license.

[4] `https://github.com/tkipf/gae`. MIT license.

inductive relation prediction. For homogeneous graph link prediction, we follow [27] and compare the positive edges against the same number of negative edges. We report area under the receiver operating characteristic curve (AUROC) and average precision (AP) for homogeneous graphs.

Baselines. We compare NBFNet against path-based methods, embedding methods, and GNNs. These include 9 baselines for knowledge graph completion, 9 baselines for homogeneous graph link prediction and 4 baselines for inductive relation prediction. Note the inductive setting only includes path-based methods and GNNs, since existing embedding methods cannot handle this setting.

4.2 Main Results

Table 2: Knowledge graph completion results. Results of embedding methods are taken from [46]. Results of NeuraLP and DRUM are taken from [40]. Since GraIL has scalability issues in this setting, we evaluate it with 50 and 100 negative triplets for FB15k-237 and WN18RR respectively and report MR based on an unbiased estimation.

Class	Method	FB15k-237					WN18RR				
		MR	MRR	H@1	H@3	H@10	MR	MRR	H@1	H@3	H@10
Path-based	Path Ranking [29]	3521	0.174	0.119	0.186	0.285	22438	0.324	0.276	0.360	0.406
	NeuralLP [62]	-	0.240	-	-	0.362	-	0.435	0.371	0.434	0.566
	DRUM [40]	-	0.343	0.255	0.378	0.516	-	0.486	0.425	0.513	0.586
Embeddings	TransE [5]	357	0.294	-	-	0.465	3384	0.226	-	-	0.501
	DistMult [61]	254	0.241	0.155	0.263	0.419	5110	0.43	0.39	0.44	0.49
	ComplEx [52]	339	0.247	0.158	0.275	0.428	5261	0.44	0.41	0.46	0.51
	RotatE [46]	177	0.338	0.241	0.375	0.553	3340	0.476	0.428	0.492	0.571
GNNs	RGCN [42]	221	0.273	0.182	0.303	0.456	2719	0.402	0.345	0.437	0.494
	GraIL [49]	2053	-	-	-	-	2539	-	-	-	-
	NBFNet	**139**	**0.378**	**0.285**	**0.417**	**0.563**	**653**	**0.547**	**0.490**	**0.573**	**0.661**

Table 3: Homogeneous graphs link prediction results. Results of VGAE and S-VGAE are taken from their original papers [27, 10].

Class	Method	Cora		Citeseer		PubMed	
		AUROC	AP	AUROC	AP	AUROC	AP
Path-based	Katz Index [24]	0.834	0.889	0.768	0.810	0.757	0.856
	Personalized PageRank [36]	0.845	0.899	0.762	0.814	0.763	0.860
	SimRank [23]	0.838	0.888	0.755	0.805	0.743	0.829
Embeddings	DeepWalk [37]	0.831	0.850	0.805	0.836	0.844	0.841
	LINE [47]	0.844	0.876	0.791	0.826	0.849	0.888
	node2vec [15]	0.872	0.879	0.838	0.868	0.891	0.914
GNNs	VGAE [27]	0.914	0.926	0.908	0.920	0.944	0.947
	S-VGAE [10]	0.941	0.941	0.947	0.952	0.960	0.960
	SEAL [66]	0.933	0.942	0.905	0.924	0.978	0.979
	NBFNet	**0.963**	**0.970**	**0.956**	**0.967**	**0.988**	**0.988**

Table 4: Inductive relation prediction results (HITS@10). V1-v4 corresponds to the 4 standard versions of inductive splits. Results of compared methods are taken from [49].

Class	Method	FB15k-237				WN18RR			
		v1	v2	v3	v4	v1	v2	v3	v4
Path-based	NeuralLP [14]	0.529	0.589	0.529	0.559	0.744	0.689	0.462	0.671
	DRUM [40]	0.529	0.587	0.529	0.559	0.744	0.689	0.462	0.671
	RuleN [33]	0.498	0.778	0.877	0.856	0.809	0.782	0.534	0.716
GNNs	GraIL [49]	0.642	0.818	0.828	0.893	0.825	0.787	0.584	0.734
	NBFNet	**0.692**	**0.858**	**0.898**	**0.923**	**0.942**	**0.895**	**0.900**	**0.881**

Table 2 summarizes the results on knowledge graph completion. NBFNet significantly outperforms existing methods on all metrics and both datasets. NBFNet achieves an average relative gain of 14% in HITS@1 compared to the best path-based method, DRUM [40], on two datasets. Since DRUM is a special instance of NBFNet with natural summation and multiplication operators, this indicates the importance of learning MESSAGE and AGGREGATE functions in NBFNet. NBFNet

also outperforms the best embedding method, RotatE [46], with an average relative performance gain of 16% in HITS@1 on two datasets. Meanwhile, NBFNet requires much less parameters than embedding methods. NBFNet only uses 381K parameters on FB15k-237, while RotatE needs 30M parameters. See Appendix D for details on the number of parameters.

Table 3 shows the results on homogeneous graph link prediction. NBFNet gets the best results on three datasets. One thing to note here is that unlike other GNN methods, NBFNet does not use the node features provided by the datasets but is still able to outperform other methods. We leave how to effectively combine node features and structural features for link prediction as our future work.

Table 4 summarizes the results on inductive relation prediction. On all inductive splits of two datasets, NBFNet achieves the best result. NBFNet outperforms the previous best method, GraIL [49], with an average relative performance gain of 16% in HITS@10. Note that GraIL explicitly encodes the local subgraph surrounding each node pair and has a high time complexity (Appendix C). Usually, GraIL can at most encode a 2-hop subgraph, while our NBFNet can efficiently explore longer paths.

4.3 Ablation Study

MESSAGE & AGGREGATE Functions. Table 5a shows the results of different MESSAGE and AGGREGATE functions. Generally, NBFNet benefits from advanced embedding methods (DistMult, RotatE > TransE) and aggregation functions (PNA > sum, mean, max). Among simple AGGREGATE functions (sum, mean, max), MESSAGE and AGGREGATE functions (TransE & max, DistMult & sum), which satisfy the semiring assumption[5] of the generalized Bellman-Ford algorithm, achieve locally optimal performance. PNA significantly improves over simple counterparts, which highlights the importance of learning more powerful AGGREGATE functions.

Number of GNN Layers. Table 5b compares the results of NBFNet with different number of layers. Although it has been reported that GNNs with deep layers often result in significant performance drop [30, 69], we observe NBFNet does not have this issue. The performance increases monotonically with more layers, hitting a saturation after 6 layers. We conjecture the reason is that longer paths have negligible contribution, and paths not longer than 6 are enough for link prediction.

Performance by Relation Category. We break down the performance of NBFNet by the categories of query relations: one-to-one, one-to-many, many-to-one and many-to-many[6]. Table 5c shows the prediction results for each category. It is observed that NBFNet not only improves on easy one-to-one cases, but also on hard cases where there are multiple true answers for the query.

Table 5: Ablation studies of NBFNet on FB15k-237. Due to space constraints, we only report MRR.

(a) Different MESSAGE and AGGREGATE functions.

MESSAGE	AGGREGATE			
	Sum	Mean	Max	PNA [7]
TransE [5]	0.249	0.236	0.294	0.300
DistMult [62]	0.324	0.305	0.302	**0.378**
RotatE [46]	0.313	0.264	0.292	0.372

(b) Different number of layers.

Method	#Layers (T)			
	2	4	6	8
NBFNet	0.304	0.368	**0.378**	**0.381**

(c) Performance w.r.t. relation category. The two scores are the rankings over heads and tails respectively.

Method	Relation Category			
	1-to-1	**1-to-N**	**N-to-1**	**N-to-N**
TransE [5]	0.498/0.488	0.455/0.071	0.079/0.744	0.224/0.330
RotatE [45]	0.487/0.484	**0.467**/0.070	0.081/0.747	0.234/0.338
NBFNet	**0.568/0.573**	0.459/**0.115**	**0.160/0.767**	**0.306/0.409**

4.4 Path Explanations of Predictions

One advantage of NBFNet is that we can explain its predictions through path groundings. Intuitively,

[5]Here semiring is discussed under the assumption of linear activation functions. Rigorously, no combination satisfies a semiring if we consider non-linearity in the model.

[6]The categories are defined same as [56]. We compute the average number of tails per head and the average number of heads per tail. The category is *one* if the average number is smaller than 1.5 and *many* otherwise.

the explanations should contain paths that contribute most to the prediction $p(u, q, v)$. Following local explanation methods [2, 65], we assume our NBFNet is locally linear w.r.t. the set of all paths, and define the importance of a path as its weight in the local linear model, i.e., the partial derivative of the prediction w.r.t. the path. Formally, the top-k path explanations for $p(u, q, v)$ are defined as

$$P_1, P_2, ..., P_k = \underset{P \in \mathcal{P}_{uv}}{\text{top-k}} \frac{\partial p(u, q, v)}{\partial P} \tag{9}$$

Note this formulation generalizes the definition of logical rules [62, 40] to non-linear models. While directly computing the importance of all paths is intractable, we approximate them with edge importance. Specifically, the importance of each path is approximated by the sum of the importance of edges in that path, where edge importance is obtained via auto differentiation. Then the top-k path explanations are equivalent to the top-k longest paths on the edge importance graph, which can be solved by a Bellman-Ford-style beam search. Better approximation is left as a future work.

Table 6 visualizes some path explanations from FB15k-237 test set. 1) In the first example, NBFNet learns soft logical entailment, such as *impersonate*$^{-1} \wedge$*nationality* $\implies$ *nationality* and *ethnicity*$^{-1} \wedge$ *distribution* $\implies$ *nationality*. 2) In second example, NBFNet performs analogical reasoning by leveraging the facts from an analogous entity *Rome*. 3) In the last example, NBFNet extracts longer paths, as there is no obvious connection between *Pearl Harbor (film)* and *Japanese language*.

Table 6: Path explanations of predictions on FB15k-237 test set. For each query triplet, we visualize the top-2 path explanations and their weights. Inverse relations are denoted with a superscript $^{-1}$.

Query	$\langle$*O. Hardy, nationality, U.S.*$\rangle$
0.243	$\langle$*O. Hardy, impersonate*$^{-1}$*, R. Little*$\rangle \wedge \langle$*R. Little, nationality, U.S.*$\rangle$
0.224	$\langle$*O. Hardy, ethnicity*$^{-1}$*, Scottish American*$\rangle \wedge \langle$*Scottish American, distribution, U.S.*$\rangle$
Query	$\langle$*Florence, vacationer, D.C. Henrie*$\rangle$
0.251	$\langle$*Florence, contain*$^{-1}$*, Italy*$\rangle \wedge \langle$*Italy, capital, Rome*$\rangle \wedge \langle$*Rome, vacationer, D.C. Henrie*$\rangle$
0.183	$\langle$*Florence, place live*$^{-1}$*, G.F. Handel*$\rangle \wedge \langle$*G.F. Handel, place live, Rome*$\rangle \wedge \langle$*Rome, vacationer, D.C. Henrie*$\rangle$
Query	$\langle$*Pearl Harbor (film), language, Japanese*$\rangle$
0.211	$\langle$*Pearl Harbor (film), film actor, C.-H. Tagawa*$\rangle \wedge \langle$*C.-H. Tagawa, nationality, Japan*$\rangle$ $\wedge \langle$*Japan, country of origin, Yu-Gi-Oh!*$\rangle \wedge \langle$*Yu-Gi-Oh!, language, Japanese*$\rangle$
0.208	$\langle$*Pearl Harbor (film), film actor, C.-H. Tagawa*$\rangle \wedge \langle$*C.-H. Tagawa, nationality, Japan*$\rangle$ $\wedge \langle$*Japan, official language, Japanese*$\rangle$

5 Discussion and Conclusion

Limitations. We observe there are a few limitations for the proposed NBFNet. First, the assumption of the generalized Bellman-Ford algorithm requires the operators $\langle \oplus, \otimes \rangle$ to satisfy a semiring. Due to the non-linear activation functions in neural networks, this assumption does not hold for NBFNet, and we do not have a theoretical guarantee on the loss incurred by this relaxation. Second, NBFNet is only verified on simple edge prediction, while there are other link prediction variants. For instance, one may want to handle logical queries with conjunctions ($\wedge$) and disjunctions ($\vee$) [16, 39], or queries with question-answering contexts [63]. In the future, we would like to understand how NBFNet approximates the path formulation, as well as apply NBFNet to other link prediction settings.

Social Impacts. Link prediction has a wide range of beneficial applications, including recommender systems, knowledge graph completion and drug repurposing. However, there are also some potentially negative impacts. First, NBFNet may encode the bias present in the training data, which leads to stereotyped predictions when the prediction is applied to a user on a social or e-commerce platform. Second, some harmful network activities could be augmented by powerful link prediction models, e.g., spamming, phishing, and social engineering. We expect future studies will mitigate these issues.

Conclusion. We present a representation learning framework based on paths for link prediction. Our path formulation generalizes several traditional methods, and can be efficiently solved via the generalized Bellman-Ford algorithm. To improve the capacity of the path formulation, we propose NBFNet, which parameterizes the generalized Bellman-Ford algorithm with learned INDICATOR, MESSAGE, AGGREGATE functions. Experiments on knowledge graphs and homogeneous graphs show that NBFNet outperforms a wide range of methods in both transductive and inductive settings.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Section 5.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section 5.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 3.1 and Appendix B.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendix A, B and C.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] Our codebase is developed based on an internal graph representation learning library which has not been released yet, but we have included comprehensive implementation details in Appendix F. We will also release our code once the paper is published.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 4.1 and Appendix F.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Section 4.1 and Table 13 in Appendix F.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] See Section 4.1.
   (b) Did you mention the license of the assets? [Yes] See Footnote 3 and 4.
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A] This work only uses existing data.
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A] This work only uses standard public datasets.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A] The knowledge graphs only contain open knowledge like Wikipedia. The homogeneous graphs only contain anonymous publications and citations.
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]