Knowledge Graph Embeddings in Function Spaces

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Overview

Introduction to Knowledge Graphs

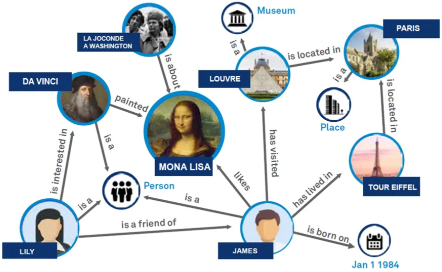


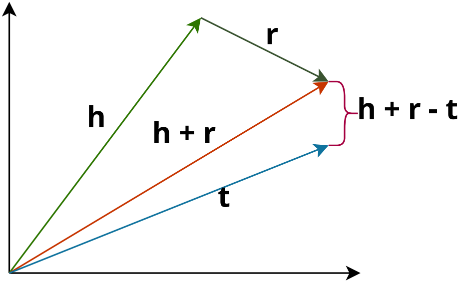
Figure: Knowledge Graph Example

- $\mathcal{G} := \{(h, r, t) \in \mathcal{E} \times \mathcal{R} \times \mathcal{E}\}$, where $\mathcal{E}$ and $\mathcal{R}$ represent a set of entities and relations respectively
- **Applications**: Enhance search engines, recommendation, and question-answering systems.

Knowledge Graph Embedding Models

- KGs are incomplete.
- KG Embedding models predict missing links, aiding in KG completion.
- Continuous vector representation for entities (h, t) and relations (r): $\mathbf{h} = [\theta_h]$, $\mathbf{r} = [\theta_r]$, $\mathbf{t} = [\theta_t]$.

Traditional Embedding Models



- TransE [1]: Models relationships as translations in the embedding space.
- Scoring function: $\psi_{TransE}(h, r, t) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|_{l_1/l_2}$

Model Scoring Functions

Model	**Scoring Function** ψ
TransE [1]	$\|\mathbf{h} + \mathbf{r} - \mathbf{t}\|_{l_1/l_2}$
DistMult [2]	$\mathbf{h}^\top \mathrm{diag}(\mathbf{r})\mathbf{t}$
ComplEx [4]	$\mathrm{Re}(\mathbf{h}^\top \mathrm{diag}(\mathbf{r})\bar{\mathbf{t}})$

Table: Scoring functions of various KG embedding models.

Moving Beyond Vector Embeddings

- Function-based embeddings: Representing $(\mathbf{h}, \mathbf{r}, \mathbf{t})$ as functions $f(\theta, x)$.
- θ: Parameters for each triple component.
- Domain X: The function operates over a domain X.
- Goal: Utilize expressiveness of function spaces for more effective learning and optimization.
- Examples:
  - $\mathbf{h} = f(\theta_h, x)$
  - $\mathbf{r} = f(\theta_r, x)$
  - $\mathbf{t} = f(\theta_t, x)$

Process Pipeline

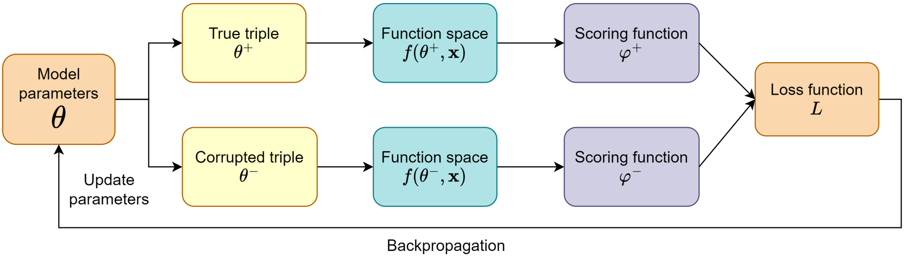


Figure: Schematic overview of the embedding as functions KG model.

Function Spaces Explored

- Polynomial Function Space.
- Complex Number Function Space.
- Neural Network Function Space.

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- Polynomial Function Space
- Complex Number Function Space
- Neural Network Function Space $\Leftarrow\Leftarrow$ Neural Architecture Search.

Polynomial Function Space

Embedding as a Polynomial Functions

$$f_{\text{poly}}(\theta, x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_{d-1} x^{d-1}. \quad (1)$$

Example

- Consider head entity parameters $\theta_h = \{1, -2, 3\}$ over the domain X.

$$f_{\text{poly}}(\theta_h, x) = 1 - 2x + 3x^2$$

Complex Number Function Space

Embedding as a Complex Number Function

$$f_{complex}(\theta, x) = \sum_{k=0}^{d-1} \theta_k \cdot \cos(x) + i \cdot \sum_{k=0}^{d-1} \theta_k \cdot \sin(x), \tag{2}$$

Example

- Consider head entity parameters $\theta_h = \{2, -1\}$ over the domain X.

$$f_{complex}(\theta_h, x) = (2-1) \cdot \cos(x) + i \cdot (2-1) \cdot \sin(x)$$

Neural Network Function Space Equation

- Parameter set:

$$\theta = [\theta_1, \theta_2, \ldots, \theta_d], \quad \text{where } d \text{ is the dimension.} \tag{3}$$

- Network function space :

$$f(\theta, X) = \sigma(\theta^{(n)}(\sigma(\theta^{(n-1)}(\ldots\sigma(\theta^{(2)}(\sigma(\theta^{(1)}X))))))). \tag{4}$$

- Layer-specific matrix size:

$$\theta^n = \sqrt{\frac{d}{n}} \times \sqrt{\frac{d}{n}}, \quad \text{for } n \text{ layers.} \tag{5}$$

Optimized Network Configuration

How to find Optimal Values:

- Dimension (d), number of layers (n), and Activation function (σ)?
- Network architecture type?
- Other network hyperparameters?

Neural Architecture Search

Overview of Neural Architecture Search (NAS)

Figure: The general framework of Neural Architecture Search.

- NAS aims to automate the design of neural network architectures, optimizing for performance on a given task.

Overview of Neural Architecture Search (NAS)

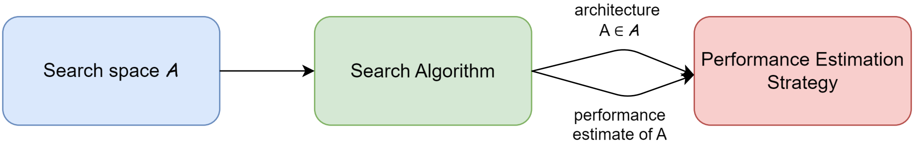

Figure: The general framework of Neural Architecture Search.

- NAS aims to automate the design of neural network architectures, optimizing for performance on a given task.
- **Search Space:** layer types, hyperparameters, and connectivity patterns.
- **Search Algorithm:** Uses techniques like reinforcement learning, Bayesian optimization, and evolutionary or gradient-based methods for efficient search.

NAS Frameworks

A variety of frameworks support NAS, each with unique features and methodologies:

- Microsoft's NNI (Neural Network Intelligence) [5].
- UniNAS [6].
- Auto-PyTorch [7].

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NNI Visualization

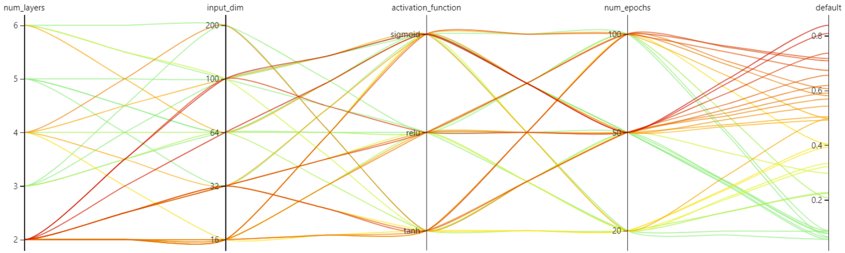
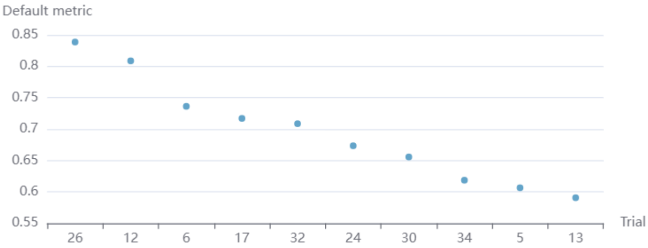


Figure: Parameters as the different axis in NNI

NNI Visualization

Top trials

Max | Min | Display top 10



	Trial No.	ID	Duration	Status	Default metric
>	26	klecB	1m 38s	SUCCEEDED	0.838603
>	12	C1axP	1m 21s	SUCCEEDED	0.808598
>	6	x4NIb	1m 58s	SUCCEEDED	0.736218
>	17	ex8X2	1m 41s	SUCCEEDED	0.717057

Optimal Network Configuration

$$f(\theta, X) = \sigma(\theta^{(n)}(\sigma(\theta^{(n-1)}(\ldots\sigma(\theta^{(2)}(\sigma(\theta^{(1)}X))))))). \tag{6}$$

The most effective configuration identified through NAS

- Two layers
- Layer normalization after each layer
- Residual connections
- Alternate relu activation function

Process Pipeline

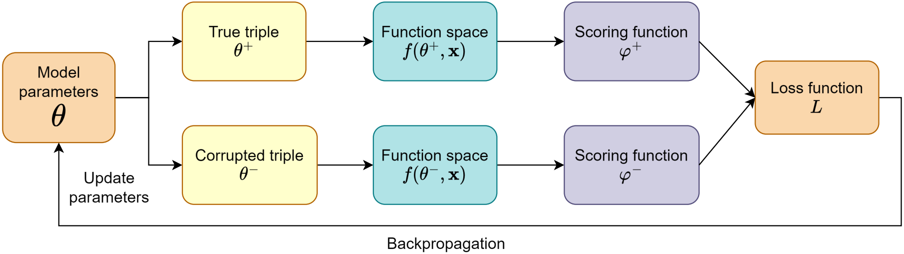


Figure: Schematic overview of the embedding as functions KG model.

Scoring Functions

- Compositional Scoring Function.
- Trilinear Scoring Function.
- Vector Triple Product Scoring Function.

Scoring Function

$$\psi_{compositional} = \int_X f(\theta_r, f(\theta_h, x)) \circ f(\theta_t, x)\, dx. \tag{7}$$

$$\psi_{trilinear} = \int_X f(\theta_h, x) \circ f(\theta_r, x) \circ f(\theta_t, x)\, dx. \tag{8}$$

$$\begin{aligned} \psi_{vtp} = &- \int_X f(\theta_h, x)\, dx \times \int_X f(\theta_t, x) \circ f(\theta_r, x)\, dx \\ &+ \int_X f(\theta_r, x)\, dx \times \int_X f(\theta_t, x) \circ f(\theta_h, x)\, dx. \end{aligned} \tag{9}$$

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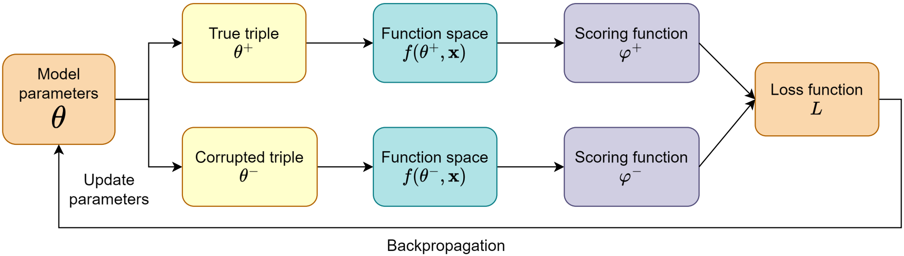

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Loss Functions Overview

- L2 Norm Loss.
- Margin Ranking Loss.
- Binary Cross-Entropy Logits Loss.

Loss Functions Overview

$$\mathcal{L}_{\text{l2}} = \sqrt{(1 - \psi(h, r, t) + \psi(h, r, \hat{t}))^2} \tag{10}$$

$$\mathcal{L}_{\text{margin}} = \max(0, \gamma - (\psi(h, r, t) - \psi(h, r, \hat{t}))) \tag{11}$$

$$\mathcal{L}_{\text{BCE}} = -y \cdot \log(\sigma(p)) - (1 - y) \cdot \log(1 - \sigma(p)) \tag{12}$$

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Result and Analysis

Evaluation Overview

Dataset	E	R	G^{Train}	$G^{\text{Val.}}$	G^{Test}
KINSHIP	104	25	8,544	1,068	1,074
UMLS	135	46	5,216	652	661
FB15K	14,951	1,345	483,142	50,000	59,071
WN18	40,943	18	141,442	5,000	5,000
NELL-995-h100	22,411	43	50,314	3,763	3,746
NELL-995-h50	34,667	86	72,767	5,440	5,393
NELL-995-h25	70,145	172	122,618	9,194	9,187

Dataset statistics.

Metrics Used:

- Mean Reciprocal Rank (MRR)
- Hits @n where $n = \{1, 3, 10\}$

UMLS Dataset Result

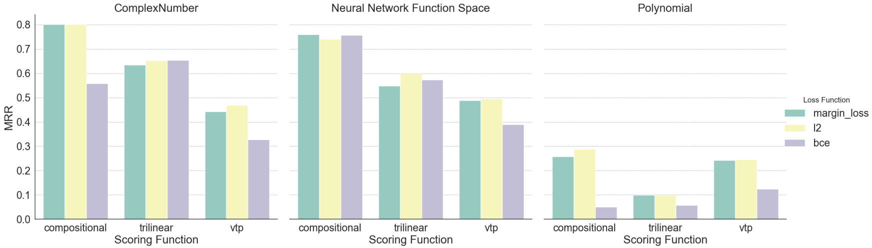

Figure: MRR performance of different function spaces with different loss and scoring functions for 64-dim vector on UMLS test dataset

KINSHIP Dataset Result

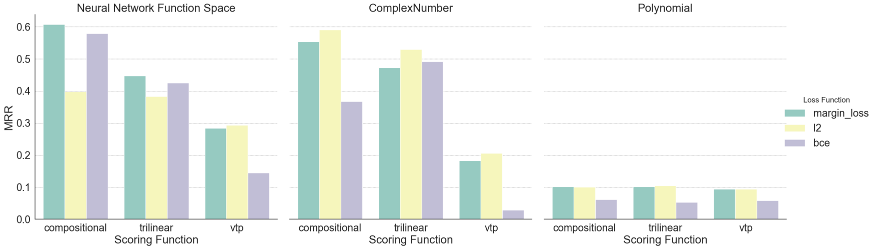

Figure: MRR performance of different function spaces with different loss and scoring functions for 64-dim vector on KINSHIP test dataset

Combined MRR Results for UMLS and KINSHIP Datasets

Model	MRR (Kinship)	MRR (UMLS)
TransE [1]	0.0545	0.6011
DistMult [2]	0.2299	0.1646
ComplEx [4]	0.1001	0.1142
QMult [3]	0.0670	0.1280
OMult [3]	0.0600	0.1043
Keci [8]	0.2193	0.1659
Complex Number FS	0.5236	0.6396
NNFS (NAS)	**0.7783**	**0.8798**

Table: MRR Comparison of Various KG Embedding Models Utilizing BCE Loss with a 1024-Dimensional Vector on the MLS and KINSHIP Test Dataset.

MRR for NELL-995 with h50 and h100

Model	MRR (h50)	MRR (h100)
TransE [1]	0.109	0.100
DistMult [2]	0.115	0.105
ComplEx [4]	0.066	0.044
QMult [3]	0.028	0.020
OMult [3]	0.035	0.019
Keci [8]	0.085	0.055
ComplexNumber FS	**0.172**	**0.158**
NNFS	0.099	0.130

Table: MRR Comparison of Various KG Embedding Models Utilizing BCE Loss with a 2048-Dimensional Vector on the NELL-995 Test Dataset

Combined MRR Results for WN18 and FB15K

Model	MRR (WN18)	MRR (FB15K)
TransE [1]	0.258	0.226
DistMult [2]	0.821	**0.479**
ComplEx [4]	**0.893**	0.466
QMult [3]	0.481	0.363
OMult [3]	0.637	0.380
Keci [8]	0.075	0.348
ComplexNumber FS	0.197	0.298
NNFS	0.826	0.360

Table: MRR Comparison of Various KG Embedding Models Utilizing BCE Loss with a 2048-Dimensional Vector on the WN18 and FB15K Test Dataset

Effect of embedding dimension

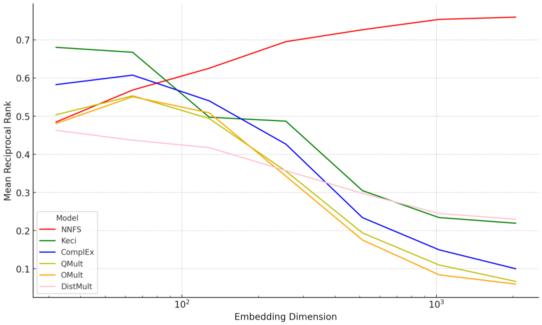

Figure: Comparison of Mean Reciprocal Rank for Various Models on the Kinship Test Dataset across Parameter Dimensions Ranging from 32 to 2048.

Effect of number of Negative Samples

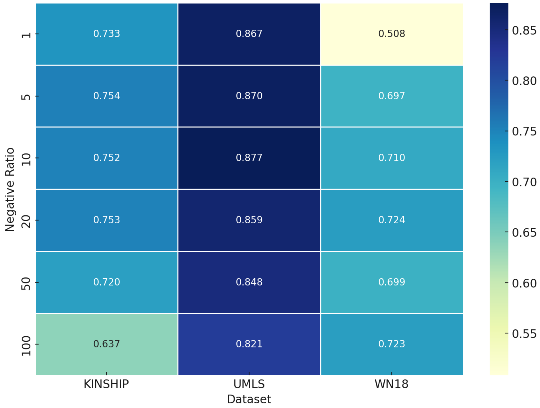

Figure: Heatmap reflecting the impact of varying negative ratios (k) on Mean Reciprocal Rank (MRR) scores across the KINSHIP, UMLS, and WN18 datasets.

Conclusions and Future Work

Conclusions:

- Compositional scoring function outperforms other.
- Different function spaces exhibit optimal performance with specific loss functions.
- NAS for automated discovery of optimal configurations.
- FS performs well at higher dimensions.
- Scalability issues on large datasets.

Future Directions:

- Enhance NNFS with NAS for scalability.
- Broaden scoring function research.
- Address large-scale dataset challenges.

The End

Questions? Comments?

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