

Brain Wiring Knowledge Graph Reasoning: A Region Embedding Approach for Logical Neuronal Relation Inference

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Abstract. Brain Wiring Knowledge Graph is a high-level abstraction from a physical neuronal wiring diagram with semantic information, helping us better understand brain functions. However, there is currently no approach that simultaneously learns both the physical connectivity and the conceptual semantic connectivity patterns within the connectome. In this paper, we propose using knowledge graphs to integrate physical connectivity and semantic connectivity. We construct knowledge graphs from the connectomes of *Drosophila* and a partial human cortex. Then, we further propose a brain wiring knowledge graph reasoning framework based on Lie Group Embedding for logical neuronal relation inference. By integrating multi-dimensional neuronal data, including synaptic connectivity, spatial localization, functional activity, cellular properties, and morphological characteristics, we construct a heterogeneous brain wiring knowledge graph to capture the intricate relationships between neurons. Link prediction and neuron classification tasks reveal the connection patterns of neurons in brain functions and the distribution patterns of functional regions. Experimental results demonstrate that the proposed method excels in logical reasoning tasks. The learned embeddings of neurons can reveal the taxonomy of complex neuronal functions. Our code is available at <https://github.com/zzy2018730/reasoning>.

Keywords: Brain Neural Networks · Neuronal Relation Inference · Neuronal link prediction.

1 Introduction

Understanding the brain’s neural circuits is fundamental to neuroscience research, as it provides insights into the brain’s complex functions and mechanisms

[1,2,3,4]. This knowledge is crucial for advancing our understanding of cognitive processes, brain disorders, and potential therapeutic strategies. The intricate networks formed by neurons enable various brain functions, and studying these connections is essential for decoding the brain’s structure and activities.

Traditional brain connectivity studies have largely relied on imaging technologies such as fMRI and DTI [5], as well as electrophysiological techniques like EEG and MEG [6], to map physical connections between neurons [7,8,9,10,11,12]. While these methods are effective at revealing physical contacts and signal propagation paths, they are limited in capturing the abstract, semantic relationships between neurons [13,14,15,16].

Knowledge graphs are powerful tools that can integrate multiple types of data and capture both structured and semantic information. Through knowledge graphs, the physical connections between neurons (such as synaptic links) can not only be modeled, but the abstract semantic relationships underlying neural logic and function can also be learned [17,18,19,20]. This enables a more comprehensive understanding of the brain’s connectivity structure. Therefore, by combining knowledge graph based reasoning methods, we can explore the functional characteristics and organizational structures of neurons at different levels and categories.

This study first constructed three brain connectivity knowledge graphs from the publicly available connectomes [21,23] that contain synaptic connectivity, spatial localization, functional activity, cellular properties, and morphological features. We then propose a novel knowledge graph reasoning framework based on Lie group embedding for logical neuronal relation inference, as shown in Fig.1. Through link prediction and neuron classification tasks, we reveal the connection patterns between neurons in brain functions and the distribution of functional regions. Experimental results demonstrate that our approach excels in both neuronal logical reasoning and functional classification tasks, significantly enhancing the understanding of brain wiring complexity. This study not only provides an innovative theoretical framework for interpreting brain wiring functions but also highlights the immense potential of Lie group embedding and knowledge graph reasoning in decoding the brain’s structure and function.

Our contributions:

- We construct heterogeneous knowledge graphs integrating multi-dimensional neuronal data.
- We propose a Lie group embedding-based brain wiring knowledge graph reasoning framework to model physical and semantic connectivity.
- Our framework can learn the hierarchical categories and functional characteristics of neurons, further enhancing the understanding of brain connectivity.

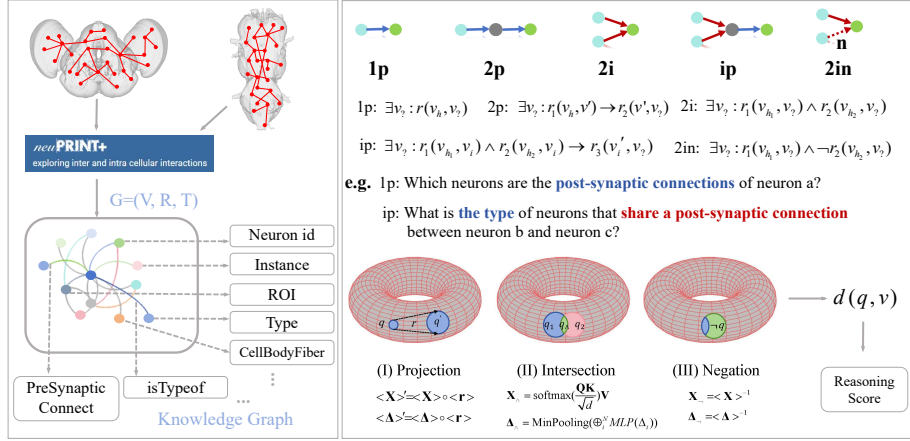


Fig. 1. The left frame illustrates the data source, representing the brain wiring knowledge graph constructed using the NeuPrint dataset. The graph includes various entities and edge types. The right frame presents our model architecture, where complex query types are constructed, and a Lie group-based reasoning method, including projection, conjunction, and disjunction operations, is applied. The reasoning results are derived by calculating the distance between the entity and the query.

2 Method

2.1 Constructing Brain Wiring Knowledge Graph

Brain Wiring Knowledge Graph. A knowledge graph is $G = (E, R, \mathcal{T})$, where E is the entity set, R is the relation set. $\mathcal{T} \subset E \times R \times E$ is a set of true facts, where each fact is represented as a triplet (h, r, t) corresponding to the assertion $r(h, t)$, where r is a 2-ary predicate, where h/t is the head/tail entity.

HemiBrain dataset [21] used in this study followed several key steps from the original *Drosophila* brain to model input. This involved microdissection, FIB-SEM imaging, FFNs-based segmentation and neuron reconstruction, synapse prediction, manual correction of segmentation errors, and cell-type identification using genetic and optical methods. The processed data were released on the neuPrint platform [22]. A similar process was applied by Shapson-Coe [23] for H01 sample to extract detailed neuron connection data from a partial human cortex.

This process yielded detailed neuron connection information, including presynaptic and postsynaptic connections, neuron region of interest (ROI), type, instance, and cell body fiber. Based on this, we constructed three heterogeneous knowledge graphs to explore brain wiring structure and function. The key entities in the graph include Neuron ID, ROI, Type, Instance, and Cell Body Fiber, with relationships such as CellBodyFiber, InputROI, isInstanceOf, isTypeOf, PreSynapticConnect, and PostSynapticConnect, which represent neuron con-

nectivity and interactions across brain regions. The dynamic illustration of the constructed knowledge graph can be found in the Supplementary Material.

Logical Neuronal Relation. Using this knowledge graph, we conducted logical inference on several motifs: 1p, 2p, 2i, ip, and 2in. Each motif corresponds to a specific query about neuronal connections, allowing for the extraction of relational information that deepens our understanding of brain structure and function. These motifs include:

- **1p:** $\exists v_? : r(v_h, v_?)$. Queries the postsynaptic connections of neuron a .
- **2p:** $\exists v_? : r_1(v_h, v') \rightarrow r_2(v', v_?)$. Queries the postsynaptic connections of the postsynaptic connections of neuron a .
- **2i:** $\exists v_? : r_1(v_{h_1}, v_?) \wedge r_2(v_{h_2}, v_?)$. Queries neurons that share postsynaptic connections with both neuron a and neuron b .
- **ip:** $\exists v_? : r_1(v_{h_1}, v_i) \wedge r_2(v_{h_2}, v_i) \rightarrow r_3(v_i', v_?)$. Queries the types of neurons that share postsynaptic connections with both neuron a and neuron b .
- **2in:** $\exists v_? : r_1(v_{h_1}, v_?) \wedge \neg r_2(v_{h_2}, v_?)$. Queries neurons that are postsynaptically connected to neuron a , but not to neuron b .

These logical motifs enable us to query and infer various relationships within the brain wiring knowledge graph, providing insights into the brain's complex neuronal network.

2.2 Modeling Logical Operators Using Region Embeddings

Lie Group. Since Neuronal Relation Inference relies on the logical relationships between neurons. Since logical reasoning requires closure under operations, it is important to choose an appropriate embedding space. Lie groups as compact manifolds constrain logical operators within the manifold, whereas Euclidean space is an open manifold and may lead to embedding divergence.

Region Embedding. Atomic queries, which retrieve basic facts or relationships between entities, serve as the fundamental units in knowledge graph reasoning. Each entity in a knowledge graph is represented as a point $\mathbf{X} = \langle x \rangle \in \mathbb{T}^n$, located on an n -dimensional torus. First-order logic queries [24] typically cover a closed region within \mathbb{T}^n [25]. This region is defined by a center point and a neighborhood, i.e., $q = (\mathbf{X}_c, \Delta)$, where $\mathbf{X}_c \in \mathbb{T}^n$ represents the center of the query region, and Δ denotes the extent of the region.

Projection Operator. The projection operation uses the relation embedding $\langle r \rangle$ to map the query region to a new region, as depicted in Fig 1(I). Let \circ represent the group operation. Projection operation is defined as $\circ \langle r \rangle$:

$$q' = \langle q \rangle \circ \langle r \rangle \iff \mathbf{X}' = \langle \mathbf{X} \rangle \circ \langle r \rangle, \quad \Delta' = \langle \Delta \rangle \circ \langle r \rangle, \quad (1)$$

where r denotes the relation embedding.

Conjunction Operator. The conjunction operation models the conjunction of the set $q_1 \wedge q_2 \wedge \dots \wedge q_n$, where q_1, q_2, \dots, q_n are the input queries, as shown in Figure 1(II). Due to the permutation invariance of the self-attention mechanism [26], it is applied to the input \mathbf{X} . Initially, each \mathbf{X}_i passes through an MLP to obtain \mathbf{Q} , \mathbf{K} , and \mathbf{V} . The new \mathbf{X} after the conjunction is: $\mathbf{X}_\wedge = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d}}\right)\mathbf{V}$. Subsequently, we apply min-pooling operation to Δ . The center and size after the conjunction operation are determined by \mathbf{X}_\wedge and Δ_\wedge :

$$\mathbf{X}_\wedge = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d}}\right)\mathbf{V}, \quad \Delta_\wedge = \text{MinPooling}\left(\bigoplus_{i=1}^n \text{MLP}(\Delta_i)\right), \quad (2)$$

where \oplus denotes the concatenation operation, $\mathbf{Q} = \bigoplus_{i=1}^n \text{MLP}_Q(\mathbf{X}_i)$, $\mathbf{K} = \bigoplus_{i=1}^n \text{MLP}_K(\mathbf{X}_i)$, $\mathbf{V} = \bigoplus_{i=1}^n (\mathbf{X}_i)$.

Negation Operator. Given a query q , the negation operation computes its inverse, as shown in Equation 3, yielding the negated result:

$$\neg q = \langle q \rangle^{-1}. \quad (3)$$

N-dimensional torus distance function. We use the p -norm of the minimum distance between corresponding points on each circle to calculate the distance:

$$d(x, y) = \|[g(x_1, y_1), \dots, g(x_n, y_n)]\|_p, \quad (4)$$

where $g(a, b)$ computes the shortest arc length between two points on the unit circle:

$$g(a, b) = \min(|\langle a \rangle -^* \langle b \rangle|, 1 - |\langle a \rangle -^* \langle b \rangle|), \quad (5)$$

where $-^*$ denotes group subtraction.

Entity-to-region distance. If there is a query $\langle q \rangle \in \mathbb{T}^n$ and an entity vector $\langle v \rangle \in \mathbb{T}^n$, the distance is defined as

$$d(q, v) = d_{out}(q, v) + \alpha \cdot d_{in}(q, v), \quad (6)$$

where $\langle q \rangle_{\max} = \mathbf{X} + \Delta$ and $\langle q \rangle_{\min} = \mathbf{X} - \Delta$, with $0 < \alpha < 1$. The external distance $d_{out}(q, v)$ is computed as:

$$d_{out}(q, v) = \|g(\max(v - q_{\max}, 0)) + g(\max(q_{\min} - v, 0))\|_2, \quad (7)$$

and the internal distance $d_{in}(q, v)$ is computed as:

$$d_{in}(q, v) = \|g(X(q)) - g(\min(q_{\max}, \min(q_{\max}, \max(q_{\min}, v))))\|_2. \quad (8)$$

The external distance refers to the distance from the entity to the nearest boundary, while the internal distance measures the distance from the side to the center of the query region.

Table 1. Statistical Information of Different Datasets

Dataset	Entities	Relations class	Train Triplets	Valid Triplets	Test Triplets
HemiBrain-KG	35,128	7	6,081,008	760,126	760,126
MANC-KG	32,059	6	608,009	76,001	76,001
H01-KG	15,562	3	57,624	7,203	7,203

Table 2. Performance of the proposed Logical Reasoning method on HemiBrain-KG, Manc-KG, and H01-KG datasets, evaluated using MRR and Hits@3/50 metrics.

Dataset	1p		2p		2i		ip		2in	
	MRR	Hits@50	MRR	Hits@50	MRR	Hits@3	MRR	Hits@3	MRR	Hits@3
HemiBrain-KG	10.2	47.52	15.61	39.72	52.33	71.52	57.36	72.06	46.37	66.38
Manc-KG	35.67	89.25	45.32	50.06	87.63	99.05	91.66	99.89	76.53	89.33
H01-KG	32.01	86.53	41.67	77.69	84.79	98.82	89.54	99.51	72.32	80.63

Training objective. Using the query training set, the loss function is optimized through positive and negative sampling as follows:

$$\mathcal{L} = \sum_{(q,v) \in \Delta} \sum_{(q,v') \in \Delta'} [\gamma + f(q,v) - f(q,v')], \quad (9)$$

where γ is a fixed scalar margin, (q,v) denotes a positive query-answer pair, and (q,v') represents a negative pair sampled from disturbed triples.

3 Experiments

Dataset. We use HemiBrain-KG [21], MANC-KG [28], and H01-KG[23] to validate our proposed method. HemiBrain is a high-density reconstruction of the central brain of *Drosophila*, MANC is derived from the ventral nerve cord of a male *Drosophila*, and H01 comes from a partial human cortex. We processed the raw data, transforming the neuron and connection information into a knowledge graph. In H01-KG, 1p contains 60,953 triples, 2p contains 52,495 triples, 2i contains 42,130 triples, ip contains 4,042 triples, and 2in contains 2,061 triples. The dataset is split to train, valid, and test in an 8:1:1 ratio, as shown in Table 1.

Logical Reasoning Performance. We constructed five logical reasoning motifs (1p, 2p, 2i, ip, 2in) for HemiBrain-KG, Manc-KG, and H01-KG. Using MRR to measure ranking and Hits@3/50 to evaluate top predictions, our method performed well across all datasets. Since neurons have more postsynaptic connections, Hits@3 might not fully reflect reasoning performance for 1p and 2p, so we used Hits@50 instead. Our approach achieved high MRR and Hits@3/50 scores, particularly on the Manc-KG dataset, validating the quality of our datasets. We also compared our method with representative real-valued embedding methods on the H01 dataset. The Euclidean space-based method scored lower (31.67, 37.06, 80.12, 88.87 on 1p, 2p, 2i, and ip) compared to our Lie group-based approach, demonstrating the superior performance of our method.

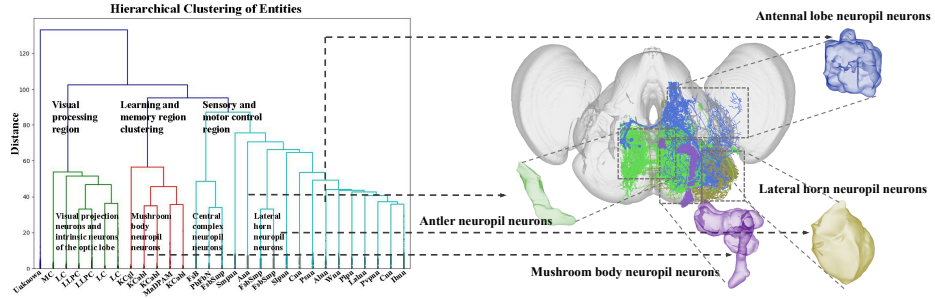


Fig. 2. The hierarchical clustering of neurons on HemiBrain successfully grouped neurons of the same type together. Our symbolic neural model can automatically learn the taxonomy of neuronal types.

Hierarchical Clustering Analysis. We input the learned entity embeddings into a density clustering algorithm, allowing our symbolic neural model to automatically learn the taxonomy of neuronal types. The hierarchical clustering results show that our model effectively captures neuronal features, revealing a hierarchical distribution that aligns with known brain regions such as the mushroom body, lateral horn, and antennal lobe, which are associated with memory formation, olfactory processing, and sensory integration, respectively. By combining neuronal morphological features and connectivity information, our method successfully assigns neurons to different functional regions, uncovering patterns related to visual processing, learning, memory, sensory, and motor control.

Entity Embedding Visualization. Fig.3 shows the t-SNE visualization of instance embeddings from three datasets. The plot clearly demonstrates the distinct clustering of neurons from different instances, where each color represents a different instance category. The results indicate that the embedding method successfully separates the instances, effectively capturing the differences between them.

Case Analysis. HemiBrain was used to predict the postsynaptic connections(task 1p) of specific neurons based on logical relation inference methods, as shown in Fig.4. The prediction results demonstrate that most neuron link predictions are accurate, with the model exhibiting high sensitivity and specificity in capturing the complex logical relationships between neurons. The prediction for neuron ID 5813080979 was accurate, indicating the model’s ability to handle complex link patterns. For neuron ID 602852509, the model successfully predicted the presence of its postsynaptic connections, confirming the model’s high precision and strong ability to capture neuron link characteristics.

Logical Relationship Modeling. Fig.5 focused on analyzing the embedding distribution of PostSynapticConnect, its inverse relationship PreSynapticConnect, and their product $\text{PostSynapticConnect} \circ \text{PreSynapticConnect}$ in the knowledge graph. The results show that the distributions of PostSynapticConnect and

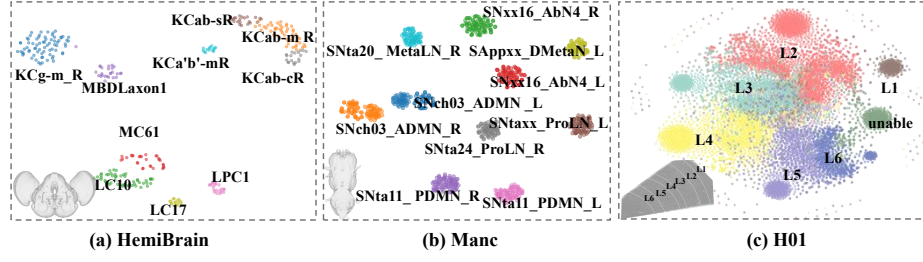


Fig. 3. t-SNE visualization of entity embeddings for instances in three datasets. The plot clearly demonstrates the distinct clustering of neurons from different instances, where each color represents a different instance category.

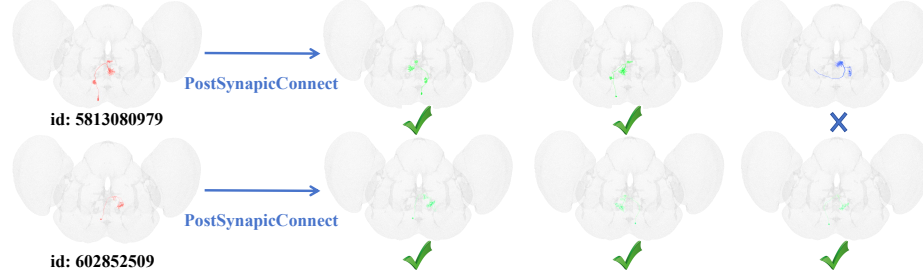


Fig. 4. Schematic diagram of reasoning task 1p, where the candidate set consists of all neurons. A check mark indicates correct reasoning, while a cross mark indicates incorrect reasoning.

PreSynapticConnect are relatively concentrated in the neural network, indicating that these two relationships occur frequently. The product of the inverse relationships tends to approach zero, which validates the effectiveness of our method for learning logical relationships. Additionally, the higher frequency of synaptic connection relationships within certain ranges suggests that there may be strong functional connections between some neurons.

4 Conclusion

We propose a brain wiring knowledge graph reasoning framework based on Lie group embedding to simultaneously learn both physical and semantic neuron connectivity patterns. By integrating multi-dimensional neuronal data, including synaptic connectivity, spatial localization, and functional activity, the framework captures the intricate relationships between neurons. Experimental results on datasets from *Drosophila* and a partial human cortex neurons show that this approach excels in neuronal logical reasoning and functional classification, providing new insights into the complexity of brain wiring and highlighting the

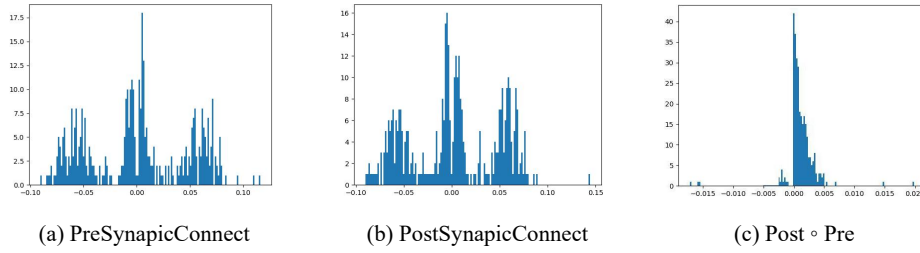


Fig. 5. Embedding frequency distribution of different relationship types in *Drosophila* HemiBrain-KG, the product of inverse relationship tends to approach zero, validating the effectiveness of our method in learning logical relationships.

potential of Lie group embedding and knowledge graph reasoning in advancing neuroscience research.

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