D-HYPR: Harnessing Neighborhood Modeling and Asymmetry Preservation for Digraph Representation Learning

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DRL aims to learn representations for directed homogeneous graphs (digraphs).
Challenges of DRL

Challenge 1: Neighborhood Modeling

- The neighborhoods of a node may possess unique semantics.
The neighborhoods of a node in digraphs may possess unique semantics.

**Social Network**

- Sam
- Annie
- Mac
- Jack
- Doug
- Annie is following Sam, and followed by Jack.
- Harry
- Howard

**Citation Network**

Sources:
[1] An Example of A Social Network Graph. Friendship@seekpng.com.
[2] Daniel G. Fort, et al. “Mapping the Evolving Definitions of Translational Research”. Journal of Clinical and Translational Science 1, No. 1 (2017): 60-66.

**Challenge 1: Neighborhood Modeling**
Existing popular GNNs ignore the unique node neighborhood characteristics.

**Challenge 1: Neighborhood Modeling**

- Remove edge directions.

The information “Annie is following Sam, and followed by Jack” is lost!
Challenges of DRL

Challenge 1: Neighborhood Modeling

• The neighborhoods of a node may possess unique semantics.
• Existing popular GNN techniques (e.g., GCN\cite{1}, VGAE\cite{2}, GAT\cite{3}, HGCN\cite{4}, GIL\cite{5}) transform digraphs to undirected graphs to enable running experiments, or only consider the direct out-neighbors in graph convolution.

Challenge 2: Asymmetry Preservation

• Shall capture the asymmetric node connection probabilities for node pair \((i, j)\) and \((j, i)\).

\[1\] Thomas N Kipf and Max Welling. "Semi-Supervised Classification with Graph Convolutional Networks." ICLR 2017.
\[2\] Thomas N Kipf and Max Welling. “Variational Graph Auto-Encoders”. arXiv preprint arXiv:1611.07308 (2016).
\[3\] Petar Veličković, et al. “Graph Attention Networks”. ICLR 2018.
\[4\] Ines Chami, Zhitao Ying, Christopher Ré, and Jure Leskovec. “Hyperbolic Graph Convolutional Neural Networks”. NeurIPS 2019.
\[5\] Shichao Zhu et al. “Graph Geometry Interaction Learning”. NeurIPS 2020.
Node connection probabilities are unequal in digraphs.

Challenge 2: Asymmetry Preservation
What are the prior practices?

Challenge 1: Neighborhood Modeling

- Spectral-based DRL GNNs\(^1-4\) have been proposed.

Challenge 2: Asymmetry Preservation

- View directions of edges as a kind of edge feature\(^5\).
- Parametrize the node pair likelihood function by a neural network\(^6-7\).

Moreover, prior DRL techniques are often constrained to directed acyclic graphs (DAGs), are transductive, or have poor generalizability across tasks - some studies provide experimental evidence for a single task.

[1] Yi Ma, et al. “Spectral-based Graph Convolutional Network for Directed Graphs”. arXiv preprint arXiv:1907.08990 (2019).
[2] Zekun Tong, et al. "Digraph Inception Convolutional Networks". NeurIPS 2020.
[3] Zekun Tong, et al. "Directed Graph Convolutional Network". arXiv preprint arXiv:2004.13970 (2020).
[4] Xitong Zhang, et al. "MagNet: A Magnetic Neural Network for Directed Graphs". NeurIPS 2021.
[5] Liyu Gong and Qiang Cheng. "Exploiting Edge Features for Graph Neural Networks". CVPR 2019.
[6] Peter W Battaglia, et al. "Relational Inductive Biases, Deep Learning, and Graph Networks". arXiv preprint arXiv:1806.01261 (2018).
[7] Lei Shi, et al. "Skeleton-based Action Recognition with Directed Graph Neural Networks". CVPR 2019.
Our solution: D-HYPR

Challenge 1: Neighborhood Modeling

• D-HYPR utilizes hyperbolic collaborative learning from multi-ordered and partitioned neighborhoods.

Challenge 2: Asymmetry Preservation

• D-HYPR takes advantage of self-supervised learning, using asymmetry-preserving regularizers supported by well-established socio-psychological theories.

We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
The real-world inductive bias: neighbors of a node can be partitioned into groups based on the semantics.

D-HYPR: Neighborhood Modeling with Partitioned and Larger Receptive Fields
The real-world inductive bias: neighbors of a node can be partitioned into groups based on the semantics.
The real-world inductive bias: neighbors of a node can be partitioned into groups based on the semantics.
Multi-Ordered 4 Canonical Types of Partitioned Neighborhoods

\[ k = 1 \]

\[ k = 2 \]

D-HYPR: Neighborhood Modeling with Partitioned and Larger Receptive Fields
We propose Digraph HYPERbolicolic Networks (D-HYPR) to address the problem.
Hyperbolic embeddings can incur smaller data distortion for real-world digraphs.

“Circle Limit 1” by M.C. Escher illustrates the Poincaré disc model of hyperbolic space. Each tile is of constant area in hyperbolic space, but vanishes in Euclidean space at the boundary [1].

[1] Benjamin Paul Chamberlain, James Clough, and Marc Peter Deisenroth. Neural Embeddings of Graphs in Hyperbolic Space. arXiv preprint arXiv:1705.10359 (2017).
We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
Homophily and preferential attachment are two driving forces of link formation.

**Homophily**
- Modeled by the Fermi-Dirac Decoder [1]

\[ p(i, j)_f = \frac{1}{e^{(d_{i,j}^H - r)/t} + 1} \]

**Preferential Attachment**
- Modeled by the Gravity Decoder [2]

\[ p(i, j)_g = \gamma \left( m_j - \lambda \log \left( d_{i,j}^H \right)^2 \right) \]

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[1] Dmitri Krioukov, et al. Hyperbolic Geometry of Complex Networks. Physical Review E 82, 3 (2010), 036106.
[2] Guillaume Salha, et al. Gravity-Inspired Graph Autoencoders for Directed Link Prediction. CIKM 2019.

D-HYPR: Self-Supervised Learning with Asymmetry-Preserving Regularizers
We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
**Results: Link Presence Prediction**

We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.

| Model (4/8-Dim) | 4-Dim | 8-Dim | 4-Dim | 8-Dim |
|-----------------|-------|-------|-------|-------|
|                 | AUC   | AP    | AUC   | AP    | AUC   | AP    | AUC   | AP    |
| GCN [22]        | 67.88 (61.73) | 67.88 (60.51) | 69.21 (64.05) | 69.68 (63.48) | 65.92 (61.00) | 65.92 (59.97) | 70.89 (65.67) | 71.26 (65.28) |
| Vgae [23]       | 69.77 (62.86) | 70.73 (62.55) | 73.49 (66.87) | 74.04 (66.95) | 63.86 (56.90) | 63.86 (55.39) | 66.60 (60.33) | 66.60 (58.75) |
| GAT [51]        | 69.02 (63.48) | 69.02 (62.86) | 71.31 (67.03) | 71.31 (67.01) | 68.18 (64.73) | 68.18 (64.31) | 72.70 (68.70) | 73.93 (69.08) |
| Gravity GCN † [40] | 65.20 (59.41) | 67.73 (60.98) | 74.00 (68.91) | 75.43 (69.14) | 70.37 (65.80) | 70.37 (64.65) | 75.29 (71.85) | 77.17 (72.50) |
| Gravity Vgae † [40] | 62.24 (55.48) | 62.24 (54.97) | 68.00 (60.23) | 68.00 (59.57) | 66.74 (61.79) | 66.74 (60.61) | 71.04 (65.45) | 71.04 (64.15) |
| DGCN † [49]     | 74.36 (65.75) | 71.42 (63.27) | 77.23 (70.60) | 75.86 (70.27) | 75.33 (71.88) | 71.95 (68.58) | 79.01 (75.30) | 79.01 (74.28) |
| DiGCN † [48]    | 72.59 (64.37) | 70.01 (61.66) | 74.65 (69.27) | 75.40 (68.29) | 70.61 (65.81) | 67.11 (61.57) | 74.63 (70.65) | 74.88 (69.86) |
| MagNet † [58]   | 72.26 (58.44) | 71.10 (57.92) | 76.64 (64.26) | 78.62 (64.69) | 77.45 (55.93) | 79.32 (56.84) | 77.46 (66.82) | 76.59 (63.96) |
| HAT § [59]      | 76.11 (71.24) | 73.72 (69.35) | 80.52 (75.13) | 79.73 (74.05) | 76.25 (72.84) | 74.38 (70.27) | 82.58 (77.82) | 82.05 (77.39) |
| HGCN § [8]      | 80.90 (66.63) | 80.90 (65.95) | 84.67 (77.65) | 85.97 (78.14) | 80.02 (67.37) | 82.16 (66.66) | 85.05 (83.07) | 88.04 (84.63) |
| D-HYPR (ours) †§ | **85.79** (*81.69) | **85.92** (*81.93) | **88.46** (*84.26) | **88.46** (*84.82) | **86.08** (*83.99) | **88.74** (*85.33) | **88.88** (*86.31) | **91.13** (*87.76) |

| Relative Gains (%) | 6.04 (14.67) | 6.21 (18.14) | 4.48 (8.51) | 2.90 (8.55) | 7.57 (15.31) | 8.01 (21.43) | 4.5 (3.9) | 3.51 (3.7) |

**Metrics:**
- AUC (Area under the ROC Curve)
- AP (Average Precision)

†: DRL method
§: hyperbolic space used
*: statistically superior

**Best score (Average score)**
## Results: Link Presence Prediction

We propose **Digraph HYPERbolic Networks (D-HYPR)** to address the problem.

| Model (32-Dim) | AUC (Air) | AP | AUC (Cora) | AP | AUC (Blog) | AP | AUC (Survey) | AP | AUC (DBLP) | AP |
|---------------|-----------|----|------------|----|------------|----|-------------|----|------------|----|
| MLP           | 81.29     | 76.52 | 83.53      | 78.18 | 84.47     | 81.67 | 87.70        | 83.69 | 93.31      | 92.48 | 91.21       | 89.98 | 92.46       | 90.75 | 51.22       | 49.98 | 51.22       |
| NERD † [19]   | 60.62     | 56.39 | 67.37      | 60.19 | 65.62     | 62.02 | 71.68        | 65.66 | 95.03      | 94.00 | 95.03      | 93.47 | 77.12       | 69.30 | 79.60       | 70.80 | 95.78       | 95.37 | 95.93       |
| ATP † [44]    | 68.99     | 66.40 | 68.99      | 64.99 | 88.47     | 86.44 | 88.47        | 86.04 | 85.05      | 83.46 | 85.05      | 79.30 | 73.53       | 71.47 | 73.53       | 70.64 | 60.43       | 59.21 | 60.43       |
| APP † [61]    | 85.08     | 82.72 | 86.35      | 84.58 | 86.65     | 85.50 | 89.80        | 87.22 | 92.33      | 91.65 | 92.33      | 90.55 | 91.16       | 90.34 | 92.77       | 91.14 | 95.58       | 95.33 | 95.73       |
| GCN [22]      | 76.71     | 72.27 | 80.95      | 75.13 | 80.77     | 78.73 | 85.67        | 81.21 | 91.87      | 90.18 | 92.16      | 90.54 | 89.29       | 87.98 | 91.78       | 89.42 | 92.98       | 92.34 | 94.37       |
| VGAE [23]     | 77.79     | 73.75 | 82.73      | 76.75 | 80.80     | 79.24 | 85.47        | 81.57 | 92.25      | 91.39 | 92.80      | 91.85 | 90.07       | 88.78 | 92.39       | 90.14 | 93.36       | 92.64 | 94.85       |
| GAT [51]      | 84.21     | 80.24 | 84.79      | 81.46 | 85.40     | 82.58 | 88.53        | 84.60 | 92.69      | 89.95 | 92.69      | 89.83 | 92.01       | 91.05 | 93.09       | 91.65 | 95.94       | 95.62 | 96.28       |
| Gravity GCN † [40] | 85.16     | 82.22 | 86.86      | 83.50 | 85.62     | 83.87 | 88.73        | 85.62 | 95.11      | 94.46 | 95.11      | 94.31 | 91.63       | 90.86 | 93.11       | 91.76 | 96.89       | 96.78 | 97.46       |
| Gravity VGAE † [40] | 83.98     | 80.06 | 85.67      | 81.61 | 87.17     | 84.46 | 89.51        | 86.22 | **96.15** | **95.59** | **96.15** | **95.42** | 91.64 | 90.96       | 93.23 | 91.82       | 95.98 | 95.57       | 96.24 | 95.81       |
| DGCN † [49]   | 77.83     | 73.68 | 80.79      | 75.64 | 83.57     | 81.34 | 85.48        | 83.00 | 87.74      | 86.74 | 88.13      | 86.75 | 90.47       | 89.49 | 91.27       | 89.94 | 92.26       | 91.83 | 90.16       | 89.52 |           |
| DiGCN † † [48] | 75.35     | 71.27 | 77.64      | 73.97 | 81.80     | 78.90 | 83.03        | 79.92 | 91.98      | 90.50 | 89.34      | 87.36 | 89.85       | 88.17 | 89.80       | 88.08 | 89.99       | 89.72 | 91.53       |
| MagNet † † [58] | 79.32     | 75.58 | 80.66      | 76.34 | 82.77     | 71.90 | 81.63        | 69.84 | 91.83      | 90.81 | 90.46      | 89.29 | 86.65       | 84.81 | 87.76       | 85.71 | 81.89       | 80.57 | 81.68       |
| HNN § [13]    | **88.42** | **85.79** | **88.95** | **86.40** | **88.75** | **86.33** | **90.81** | **87.81** | **95.80** | **95.39** | **95.80** | **95.16** | **92.07** | **91.39** | **93.40** | **92.04** | **97.43** | **97.14** | **97.43** |
| HGNC § [8]    | **88.26** | **86.12** | **88.88** | **86.64** | **89.24** | **87.68** | **91.54** | **88.97** | **95.64** | **95.23** | **95.64** | **95.00** | **92.15** | **91.50** | **93.38** | **92.08** | **97.54** | **97.33** | **97.26** |

**Best score (Average score)**

| Best, Second best, Third best |
|-------------------------------|

†: DRL method  
§: hyperbolic space used  
*: statistically superior

### Metrics:
- **AUC (Area under the ROC Curve)**
- **AP (Average Precision)**

We propose **Digraph HYPERbolic Networks (D-HYPR)** to address the problem.
# Results: Node Classification

We propose **Digraph HYPERbolic Networks (D-HYPR)** to address the problem.

| Model       | CiteSeer     | Cora-ML     |
|-------------|--------------|-------------|
| MLP         | 37.68 ± 3.0  | 51.19 ± 6.3 |
| GCN [22]    | 32.82 ± 7.9  | 60.56 ± 9.8 |
| GAT [51]    | 51.97 ± 4.2  | 68.38 ± 3.4 |
| DGCN [49]   | 38.67 ± 10.0 | 53.44 ± 11.1|
| DiGCN [48]  | 53.43 ± 10.3 | 71.35 ± 2.3 |
| HNN [13]    | 47.44 ± 2.9  | 52.76 ± 4.9 |
| HGCN [8]    | 42.24 ± 3.6  | 52.17 ± 5.9 |
| D-HYPR (ours) | 65.72 ± 2.9 | 74.63 ± 1.2 |
| Relative Gains (%) | 23.00 | 4.60 |

| Model       | CiteSeer     | Cora-ML     |
|-------------|--------------|-------------|
| MLP         | 51.70 ± 2.6  | 60.48 ± 1.8 |
| GCN [22]    | 36.26 ± 6.5  | 67.62 ± 10.8|    
| GAT [51]    | 50.81 ± 3.9  | 74.87 ± 1.8 |
| DGCN [49]   | 57.27 ± 2.4  | 77.16 ± 4.4 |
| DiGCN [48]  | 60.37 ± 2.6  | 78.38 ± 1.2 |
| HNN [13]    | 50.73 ± 3.1  | 61.54 ± 2.1 |
| HGCN [8]    | 52.57 ± 2.3  | 73.44 ± 2.3 |
| D-HYPR (ours) | 67.96 ± 1.6 | 81.55 ± 1.6 |
| Relative Gains (%) | 12.37 | 4.04 |

* : statistically superior

**Average score ± Standard Deviation**

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![Graph showing accuracy over label rate for CiteSeer and Cora-ML datasets]
We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.

| Model       | Node Classification | Link Sign Prediction |
|-------------|---------------------|----------------------|
| 4-Dim       |                     |                      |
| GCN [22]    | 17.01 ± 0.1         | 78.96 ± 0.4          |
| GAT [51]    | 40.75 ± 10.7        | 79.38 ± 0.2          |
| HGCN [8]    | 36.07 ± 5.3         | 78.72 ± 0.0          |
| D-HYPR (ours) | *71.27 ± 0.79     | *79.83 ± 0.0         |
| Relative Gains (%) | 74.90            | 0.57                 |
| 8-Dim       |                     |                      |
| GCN [22]    | 39.26 ± 9.5         | 78.76 ± 0.1          |
| GAT [51]    | 46.78 ± 10.5        | 79.41 ± 0.2          |
| HGCN [8]    | 58.40 ± 10.9        | 79.23 ± 0.2          |
| D-HYPR (ours) | *70.53 ± 1.6     | *79.47 ± 0.3         |
| Relative Gains (%) | 20.77            | 0.08                 |
| 32-Dim      |                     |                      |
| GCN [22]    | 37.77 ± 6.7         | 79.39 ± 0.1          |
| GAT [51]    | 46.12 ± 8.5         | 79.66 ± 0.1          |
| HGCN [8]    | 52.63 ± 5.8         | 79.21 ± 0.2          |
| D-HYPR (ours) | *71.65 ± 1.0     | *79.73 ± 0.2         |
| Relative Gains (%) | 36.14            | 0.09                 |

* : statistically superior
Average score ± Standard Deviation
We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
Parameter Sensitivity

Hyper-parameters:
(1) $\lambda \rightarrow$ a smaller $\lambda$ emphasizes the asymmetric node connectivity, used by the Gravity decoder.
(2) $K \rightarrow$ the maximal order of the $k$-order proximity matrix, larger means a wider receptive field and more scale information.

Parameter sensitivity analysis in terms of $K$

|       | 1      | 2      | 3      |
|-------|--------|--------|--------|
| CiteSeer | 69.23 ± 1.5 | 70.66 ± 1.2 | 69.76 ± 1.5 |
| Cora-ML  | 82.16 ± 1.3  | 82.16 ± 1.3  | 82.19 ± 1.3  |

Parameter sensitivity analysis in terms of $\lambda$

|       | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 | 2.50 | 2.75 | 3.00 | 3.25 | 3.50 | 3.75 | 4.00 | 4.25 | 4.50 | 4.75 | 5.00 | 10.0 |
|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| CiteSeer | 69.74 ± 1.6 | 70.66 ± 1.2 | 70.46 | 70.44 | 70.30 | 70.34 | 69.99 | 69.79 | 69.24 | 69.61 | 68.13 | 68.05 | 68.12 | 67.64 | 67.85 | 67.67 | 67.69 | 67.34 | 67.18 | 67.12 | 68.85 |
| Cora-ML  | 81.29 ± 1.3  | 81.18 ± 1.2  | 81.59 | 81.68 | 81.83 | 81.97 | 82.16 | 81.65 | 81.10 | 81.17 | 81.59 | 81.66 | 81.32 | 81.93 | 80.19 | 80.31 | 79.13 | 79.51 | 80.18 | 79.78 | 77.73 |

Compare D-HYPR with SOTA

| Model     | CiteSeer | Cora-ML |
|-----------|----------|---------|
| MLP       | 53.18 ± 1.6 | 61.63 ± 1.8 |
| GCN [22]  | 53.20 ± 3.1  | 69.51 ± 8.5  |
| GAT [51]  | 63.03 ± 0.6  | 71.91 ± 0.9  |
| DGCN [49] | 64.17 ± 2.4  | 81.29 ± 1.6  |
| DiGCN [48] | 65.83 ± 1.8 | 78.08 ± 1.9 |
| HNN [13]  | 56.10 ± 2.2  | 62.49 ± 2.6  |
| HGCN [8]  | 59.02 ± 2.3  | 76.48 ± 1.5  |
| D-HYPR (ours) *70.66 ± 1.2* | *82.19 ± 1.3* |

Relative Gains (%) | 7.34 | 1.11 |

(32-Dim, the Node Classification task).

We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
We propose **Digraph HYPERbolic Networks (D-HYPR)** to address the problem.

| Method                                                        | CiteSeer     | Cora-ML     |
|---------------------------------------------------------------|--------------|-------------|
| D-HYPR (Our Full Design)                                      | 70.66 ± 1.2  | 82.19 ± 1.3 |
| No $A_{d_{in}}^k$                                             | 68.72 ± 1.2  | 82.11 ± 1.2 |
| No $A_{d_{out}}^k$                                            | 69.10 ± 0.9  | 81.33 ± 1.4 |
| No $A_{c_{in}}^k$                                             | 69.98 ± 1.0  | 81.86 ± 1.6 |
| No $A_{c_{out}}^k$                                            | 69.84 ± 1.3  | 81.74 ± 1.8 |
| No Hyperbolic Neighborhood Collaboration                      | 70.13 ± 1.5  | 82.03 ± 1.1 |
| No Gravity                                                    | 68.58 ± 1.3  | 79.21 ± 1.5 |
| No Fermi-Dirac                                                | 70.03 ± 1.2  | 82.05 ± 1.3 |
| No Self-Supervision                                           | 67.85 ± 1.9  | 78.15 ± 2.1 |
| Euclidean                                                     | 61.86 ± 5.4  | 73.38 ± 6.7 |
| Euclidean and No Neighborhood Collaboration                  | 51.01 ± 6.2  | 65.46 ± 12.1|
| $A$ + Three Learnable Matrices                               | 60.97 ± 12.7 | 78.92 ± 2.9 |
We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
Conclusion

- We propose **D-HYPR**: the Digraph HYPERbolic Network, as a novel GNN-based formalism for **Digraph Representation Learning** (DRL) by addressing **Neighborhood Modeling** and **Asymmetry Preservation**.

- Through extensive and rigorous evaluation involving **21** prior techniques, we empirically demonstrate the superiority of D-HYPR.

- D-HYPR retains effectiveness given a **low budget of embedding dimensionality or labeled training samples**, which is desirable for real-world applications.

**Limitations**: increased number of parameters, due to the use of multiple neighborhoods.

**Future work**:
- Automatic and dynamic neighborhood partitioning
- Parameter-sharing mechanism
- Theoretical analyses
- Novel large-scale applications

We propose Digraph HYPERbolic Networks (D-HYPR) to address the problem.
Thank you!

Code and data: [https://github.com/hongluzhou/dhypr](https://github.com/hongluzhou/dhypr)

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