Graph Representation Learning (GRL)

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Networks/Graphs

Social Networks

Facebook

Twitter

…

Biological Networks

Brain

Protein-Protein

Drug-Target

…

Product Networks

User-Item

Product-Product

..

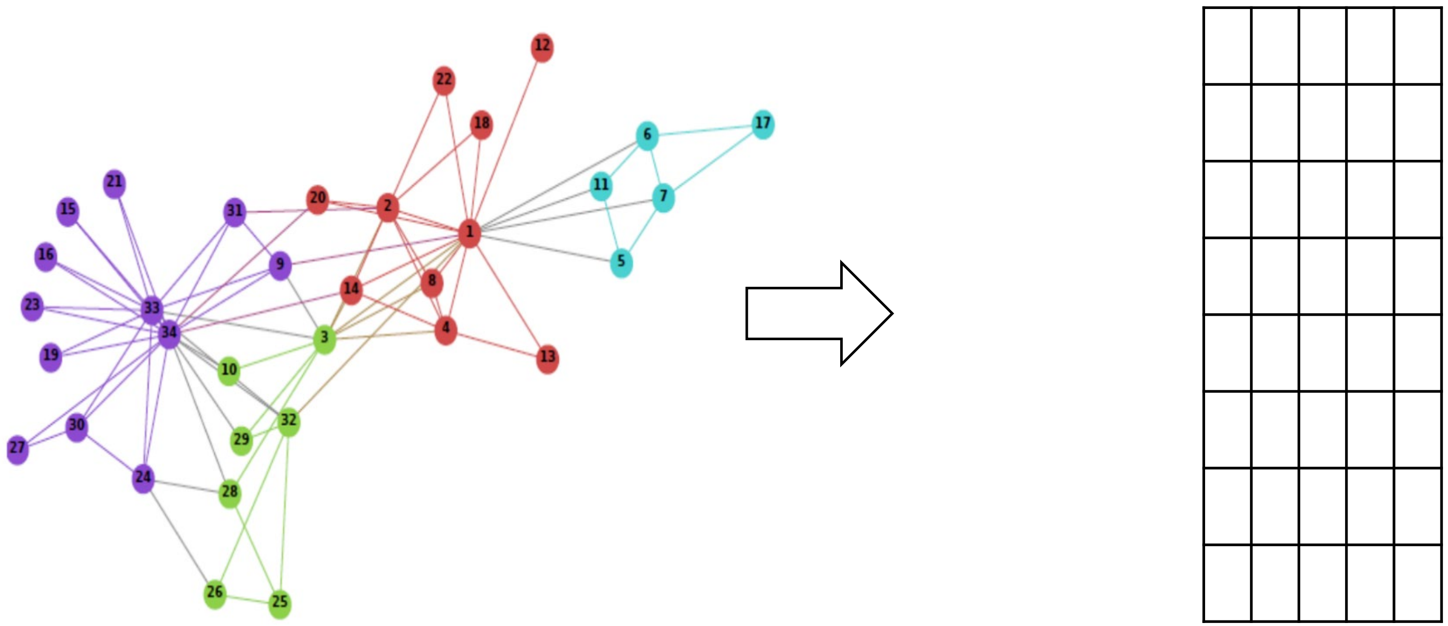
Basic Notations

- $G = (V, E)$
  - $N = |V|, M = |E|$
- $\boldsymbol{A} \in \{0, 1\}^{N \times N}$ – Adjacency matrix notation
  - $\boldsymbol{A}[i, j] = \begin{cases} 1, & (i, j) \in E \\ 0, & (i, j) \notin E \end{cases}$
- $\boldsymbol{X} \in \mathbb{R}^{N \times D}$ – Node feature matrix
  - $\boldsymbol{X}[i] = \boldsymbol{x}_i$- Node i's feature vector

What is GRL?

$N \times N$

$N \times d, d \ll N$



Input Space

Representation Space

What is GRL?

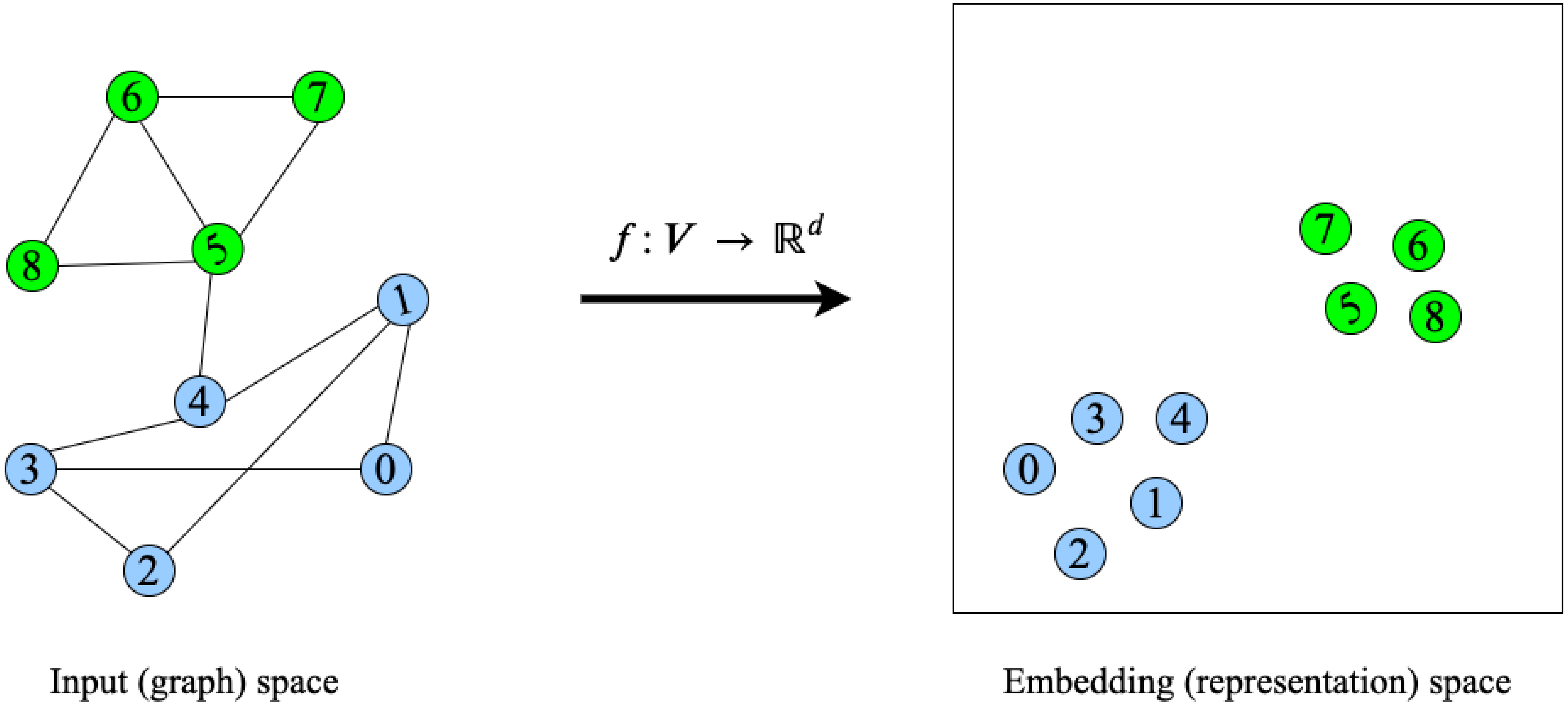
What makes a representation a good representation?

$\boldsymbol{z_i}$ is a d dimensional representation vector of node i

$\boldsymbol{Z}$ is the representation (embedding) matrix

Quality of Representation

- Preserve a certain property of the graph



Quality of Embedding

- We model the property we want to preserve using a similarity function in the input space

$$sim_g: V \times V \rightarrow \mathbb{R}$$

- Adjacency Matrix as a similarity function

$$sim_g(i,j) = \begin{cases} 1, & if\ \boldsymbol{A}[i,j] = 1 \\ 0, & if\ \boldsymbol{A}[i,j] = 0 \end{cases}$$

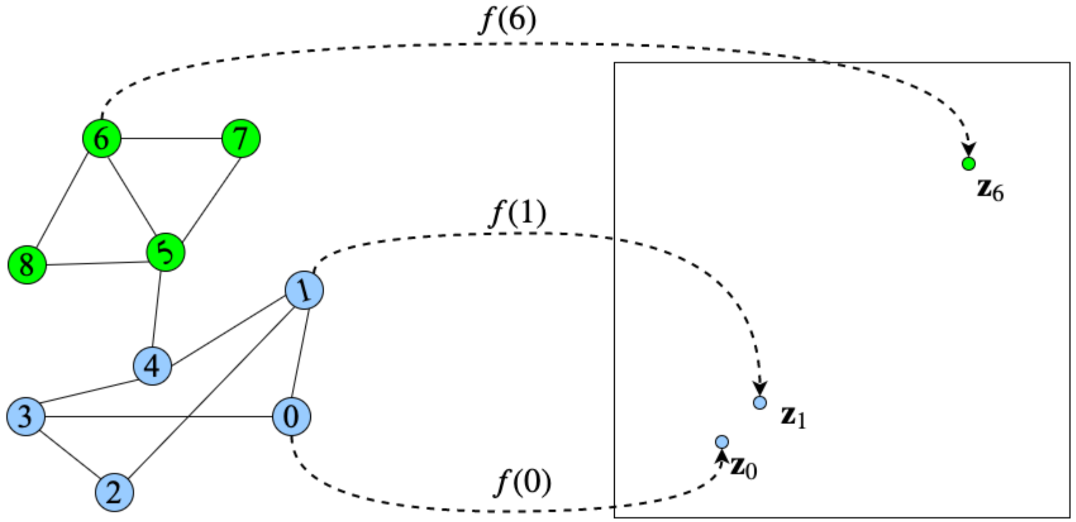
- Common Neighborhood
  - $sim_g(u,v) = |\mathcal{N}_u \cap \mathcal{N}_v|$
  - $\mathcal{N}_i = \{j: (i,j) \in E\}$
- Rooted Page Rank
  - $sim_g(u,v) = p$
  - p is the probability of reaching node v via a random walk starting from node u
- Generally, we use $\boldsymbol{W} \in [0,1]^{N \times N}$

$$\boldsymbol{W}[i,j] = sim_g(i,j)$$

Learning

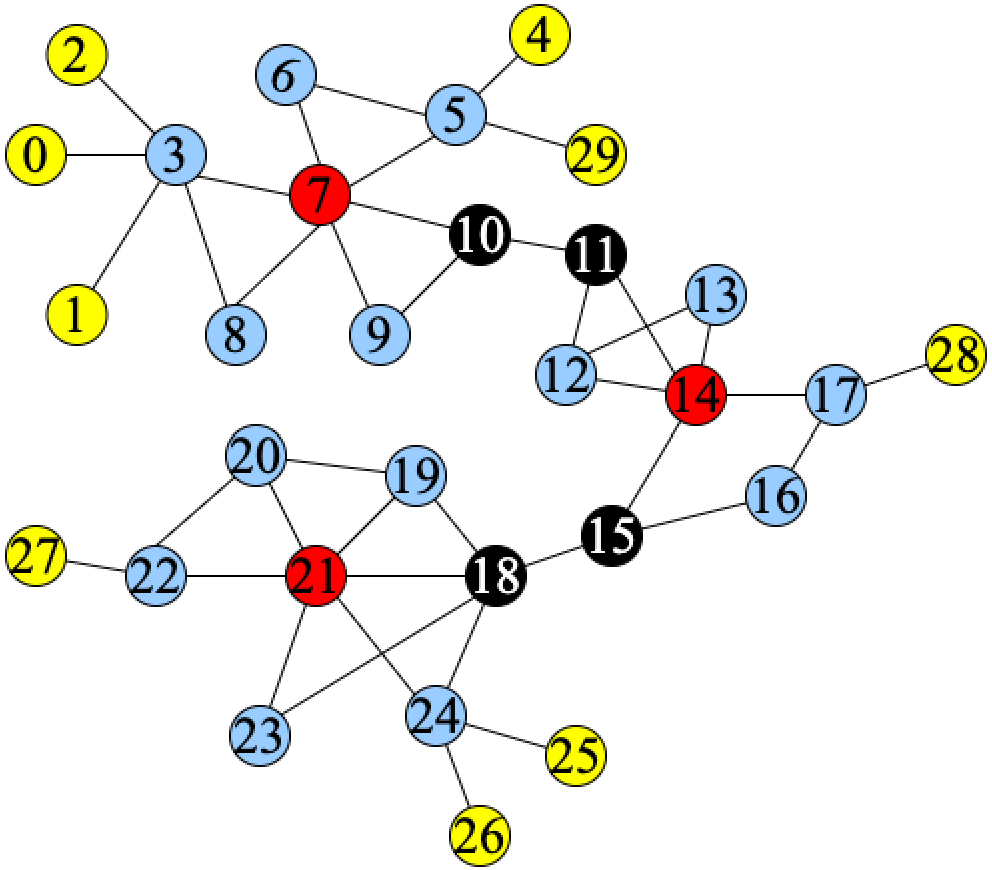
- Given a similarity function sim_g in the input space
- Learn a representation $\mathbf{z}_u = f(u) \in \mathbb{R}^d, u \in V$ that preserves sim_g
  - Similarity in the representation space, $sim_r: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$
  - sim_r Should approximate sim_g

$$sim_r(f(u), f(v)) \approx sim_g(u, v)$$



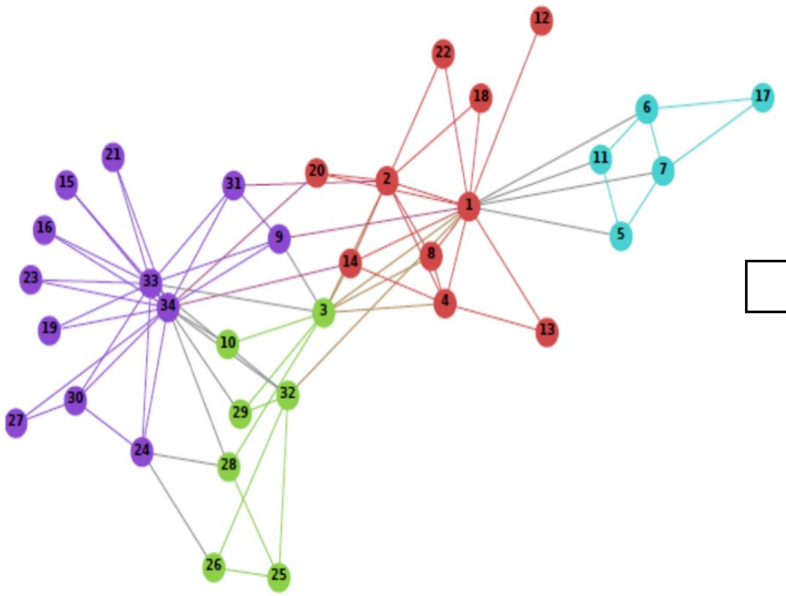
$$sim_r(f(0), f(1)) = sim_r(\mathbf{z}_0, \mathbf{z}_1) \approx sim_g(0,1)$$

Structural similarity



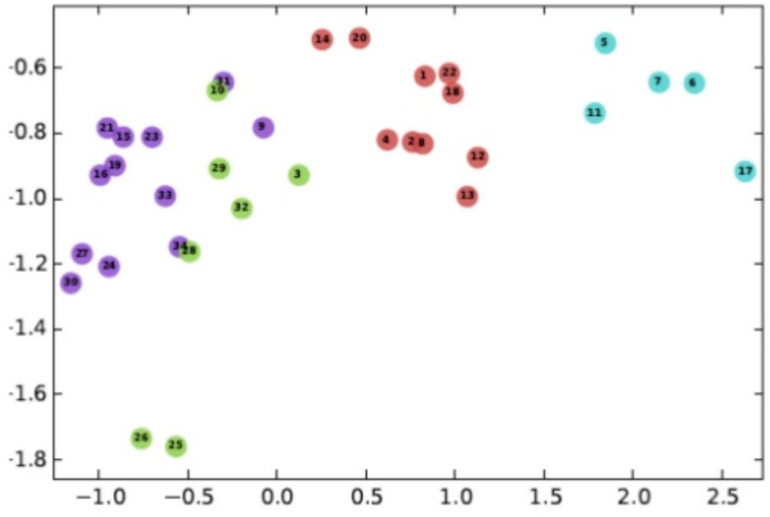
Why GRL?

$N \times N$



Input Space

$N \times d, d \ll N$



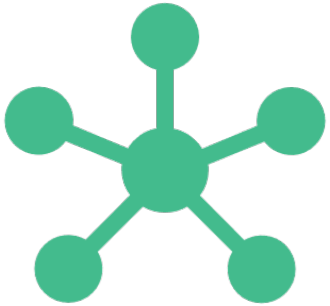
Representation Space

Network Analysis

- Link Prediction
- Node classification
- Clustering
- Recommendation
- ...

Learning Algorithms

Random Walk Based



Message Passing Neural Networks

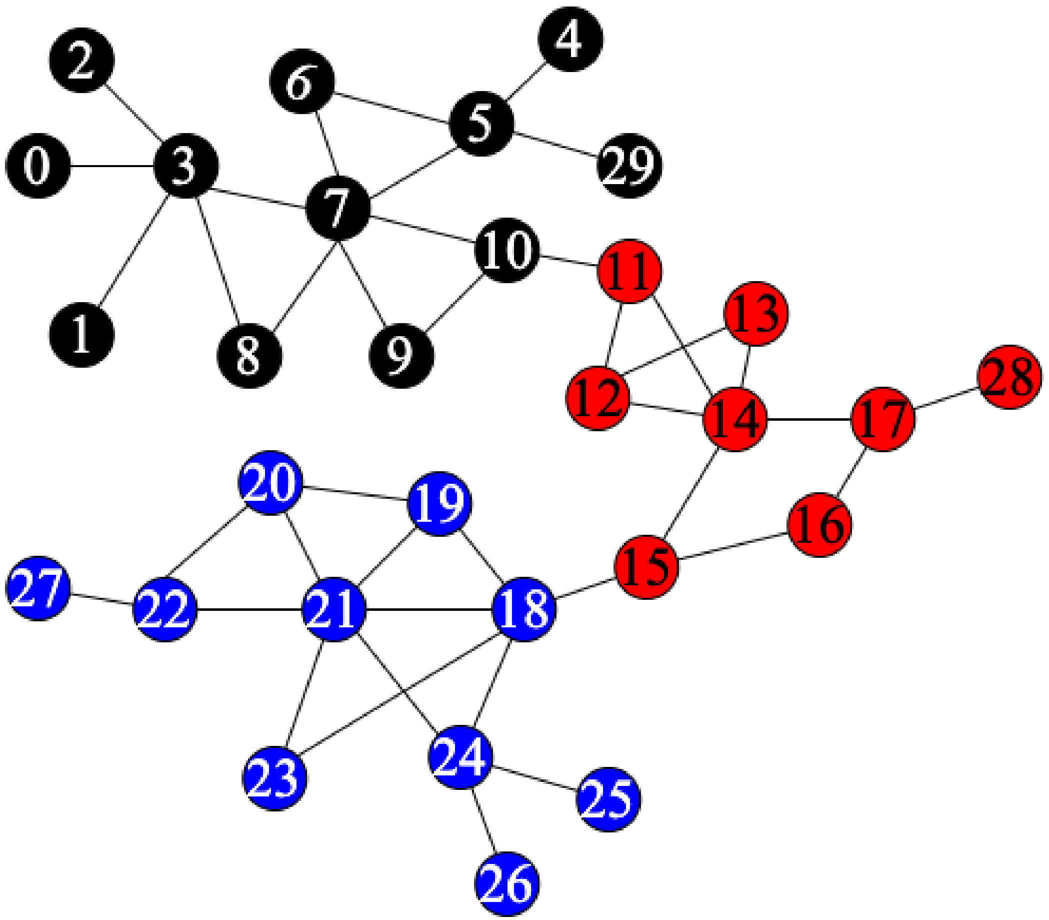
Random Walk (RW) Based

WALK SAMPLING

LEARNING

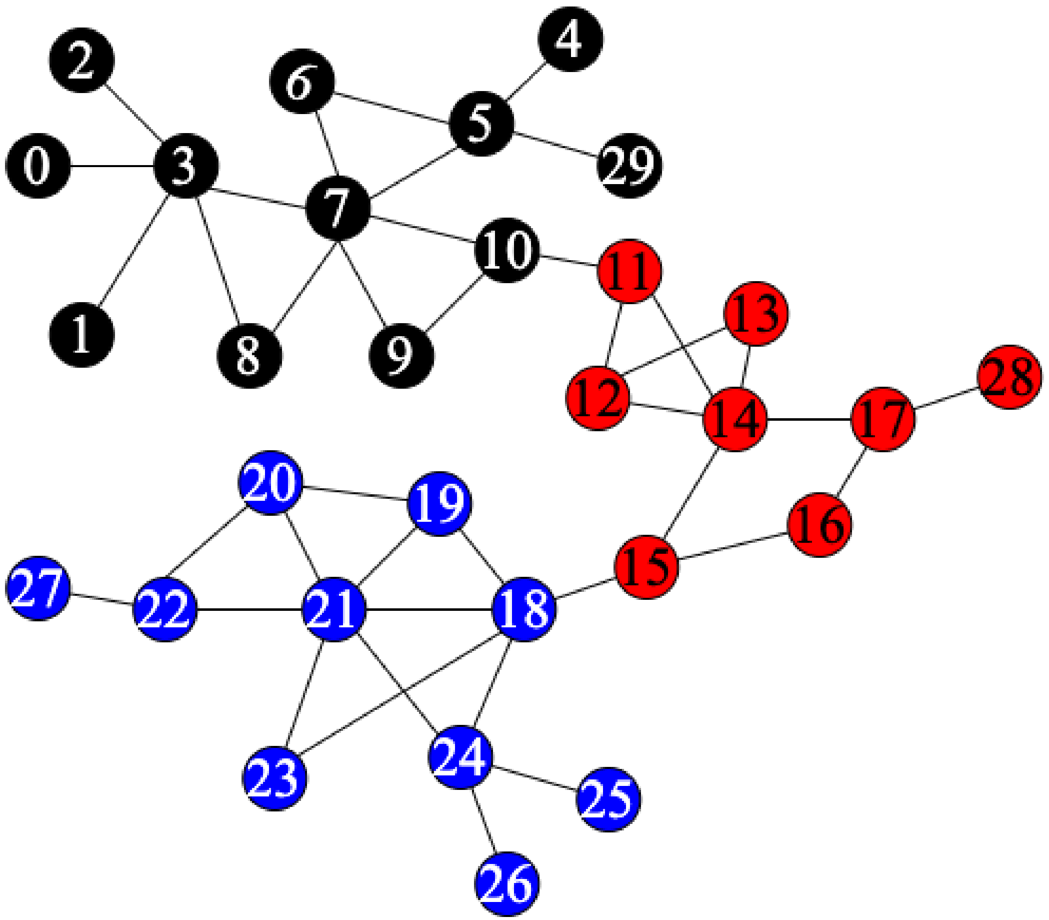
RW: Property

- Preserve Homophily: Similar nodes appear in the same neighborhood



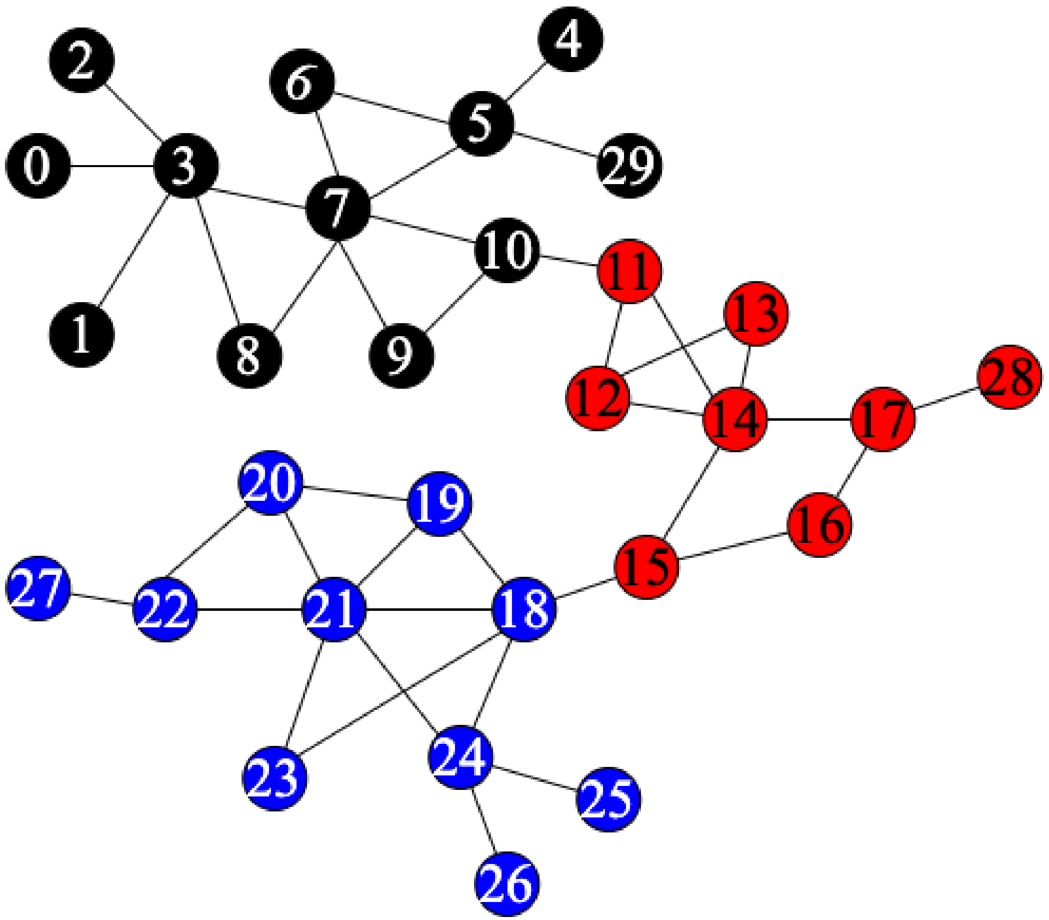
Challenge

- Graphs are arbitrary data structures
- GRL directly on top of graphs is difficult
- We need a different data structure that capture the homophily property (E.g., sequences)
    - Truncated random walks



RW Sampling

- Sample walks starting from node 21
  - 21, 24, 18, 23, 18
  - 21, 18, 19, 18, 15
  - 21, 19, 20, 22, 21
  - 21, 23, 18, 24, 21
- Sample walks starting from node 15
  - 15, 14, 12, 13, 12
  - 15, 14, 11, 14, 12
  - 15, 18, 15, 16, 17
  - 15, 14, 17, 28, 17
- …



Learning: Algorithm

- SkipGram: Used for word representation
- Key idea: Similar words frequently appear together in similar context
- E.g.:
  - Stockholm vs. Sweden
  - Vaccine vs. AstraZeneca
  - Darwin vs. Evolution
  - Arthur Conan Doyle vs. Sherlock Holmes
- Learning:
  - Given a target work, w_t
  - Learn its embedding, $\boldsymbol{z}_t$ by predicting its context words $w_c \in ctx(w_t)$

$$The, capital, of, Sweden, is, Stockholm$$

$$w_t = Sweden$$

$$ctx(w_t) = \{capital, stocholm\}$$

$$\max_{w_c \in ctx(w_t)} P(w_c | \boldsymbol{z}_t)$$

SkipGram for GRL

- Given a target node n_t from a random walk sequence
- Learn $\boldsymbol{z}_t$ by predicting its context nodes $n_c \in ctx(n_t)$

$ctx(18)$

$walk$

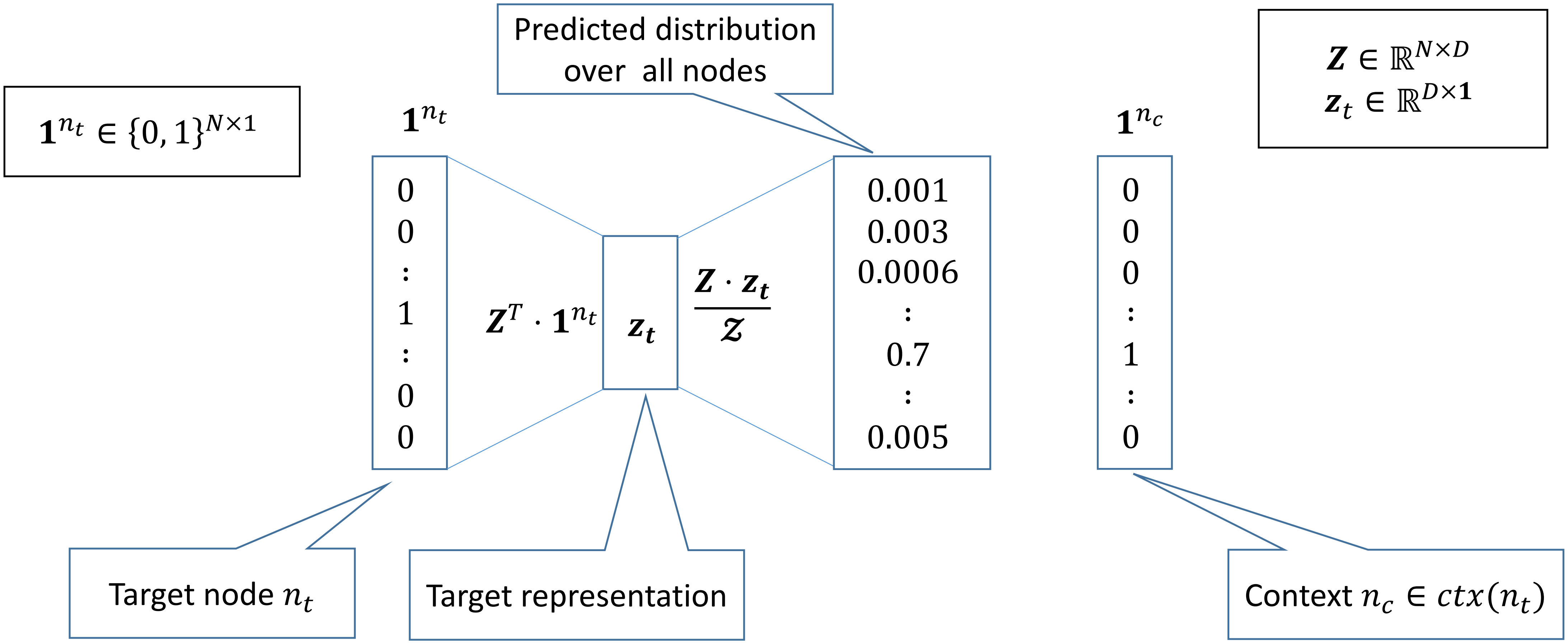
Finally update $\boldsymbol{z}_t$ using SGD according to the prediction errors

Current Context node

nt Target node=18

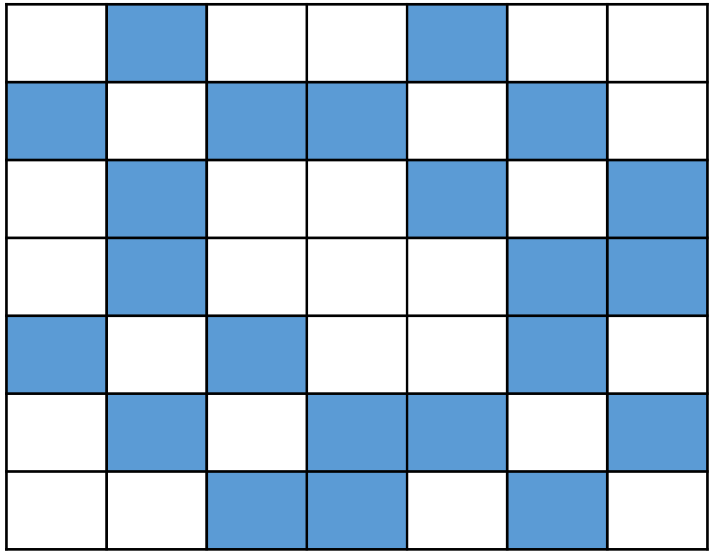
Pre	$Predict($	Pre	$Predict(24 \mid \boldsymbol{z}_{18})$

SkipGram Architecture

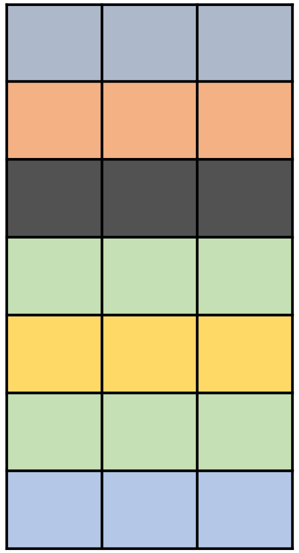


Message Passing Neural Networks (MPNN)

- Now, we consider nodes with features



$\boldsymbol{A}$



$\boldsymbol{X}$

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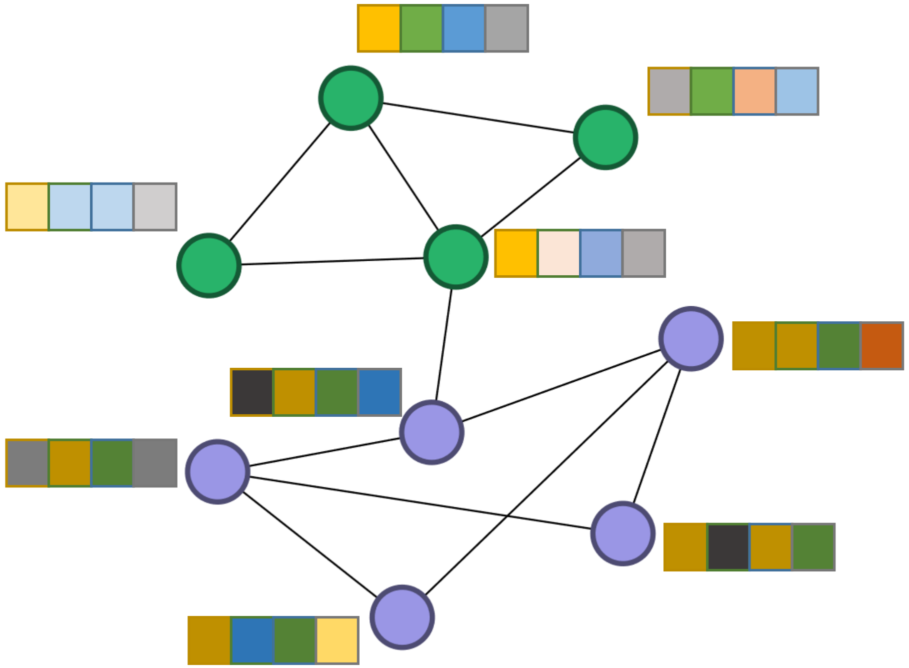
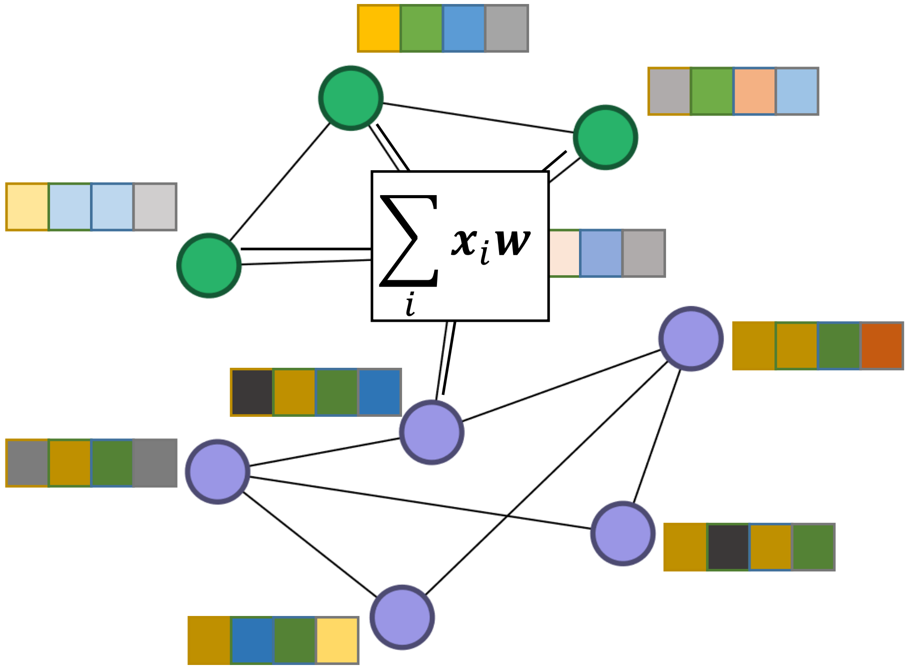


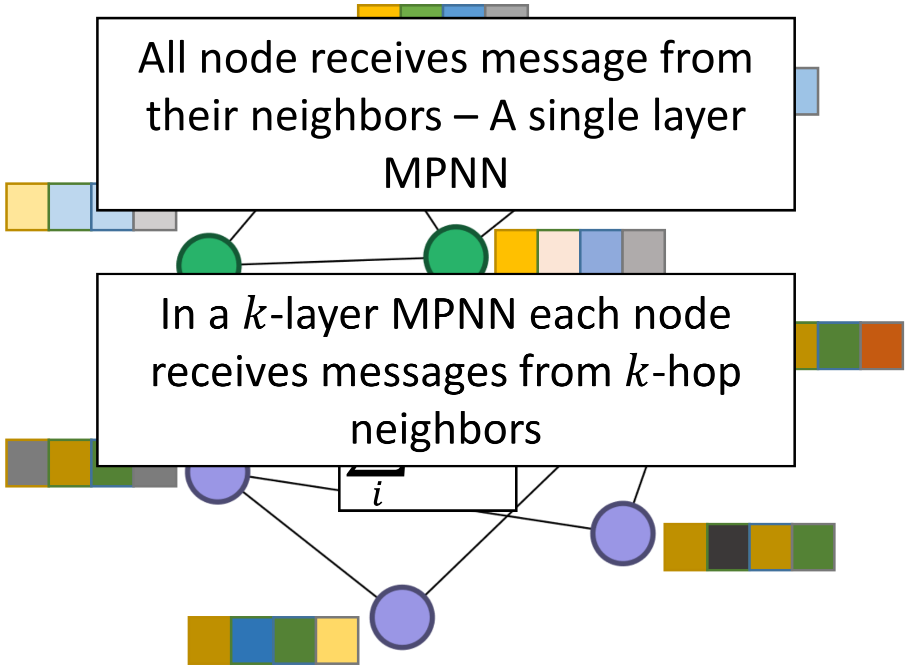
MPNN

- Key Idea: Each node sends and receives messages



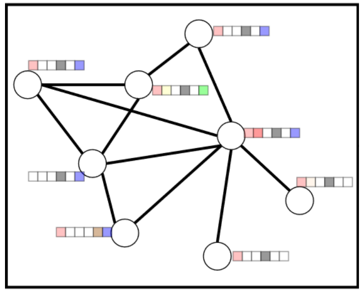
MPNN

- Key Idea: Each node sends and receives messages

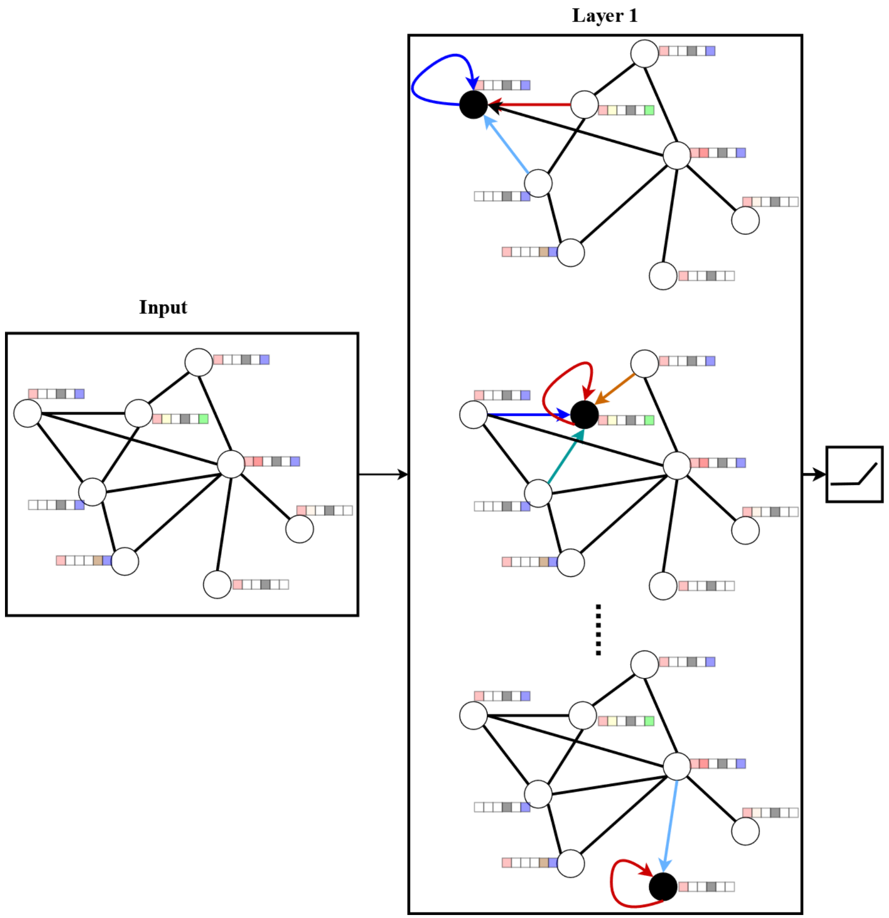


GCN

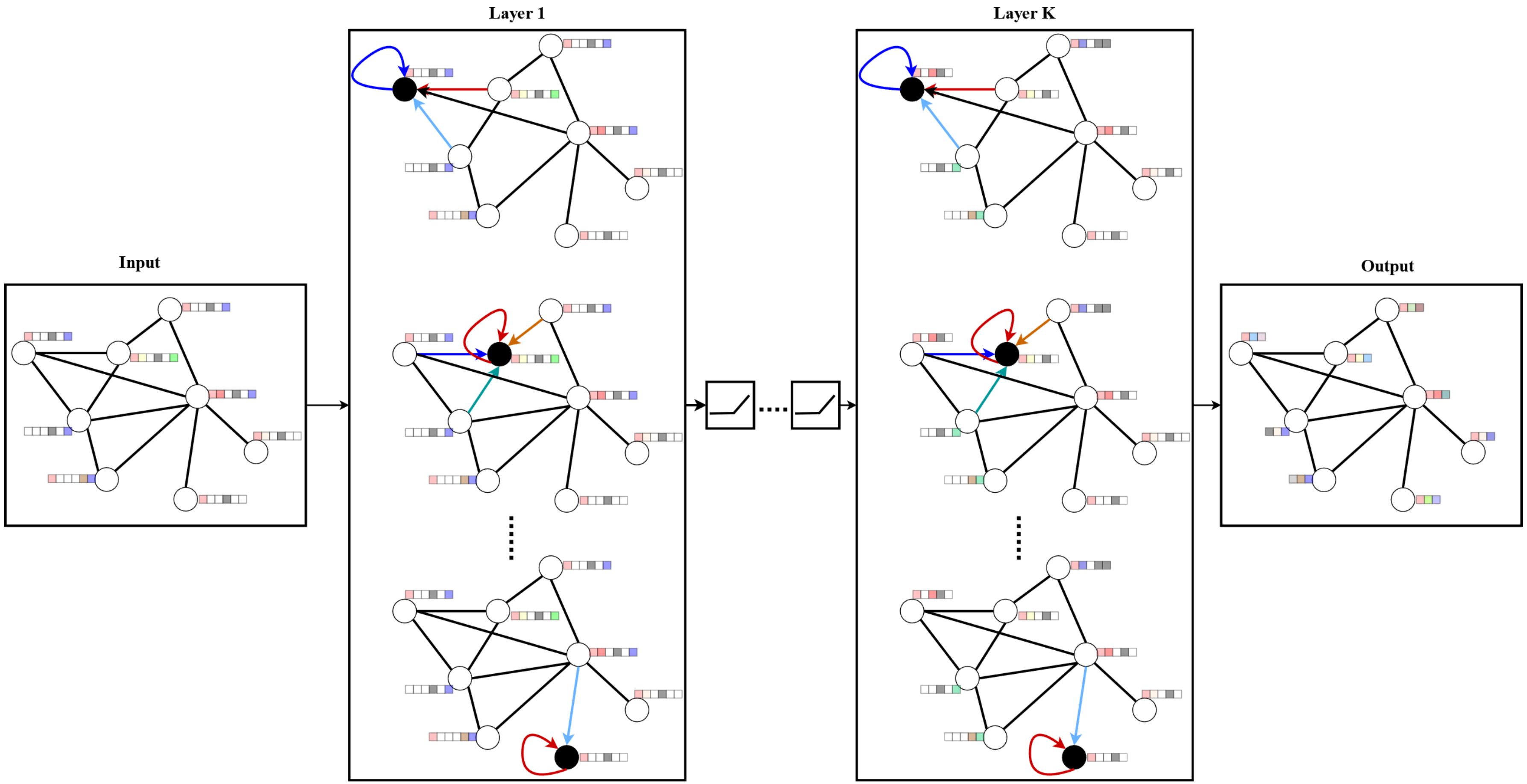
Input



GCN



GCN



Applications of GRL

- Social Networks
  - Friendship recommendation
- Recommendation Systems
  - Content (e.g., book, movie, …) recommendation
- Biomedical Systems
  - Drug discovery
  - Predicting functions of proteins
  - Predicting molecular properties
- …

Referrences

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