Graph Classification via Reference Distribution Learning: Theory and Practice

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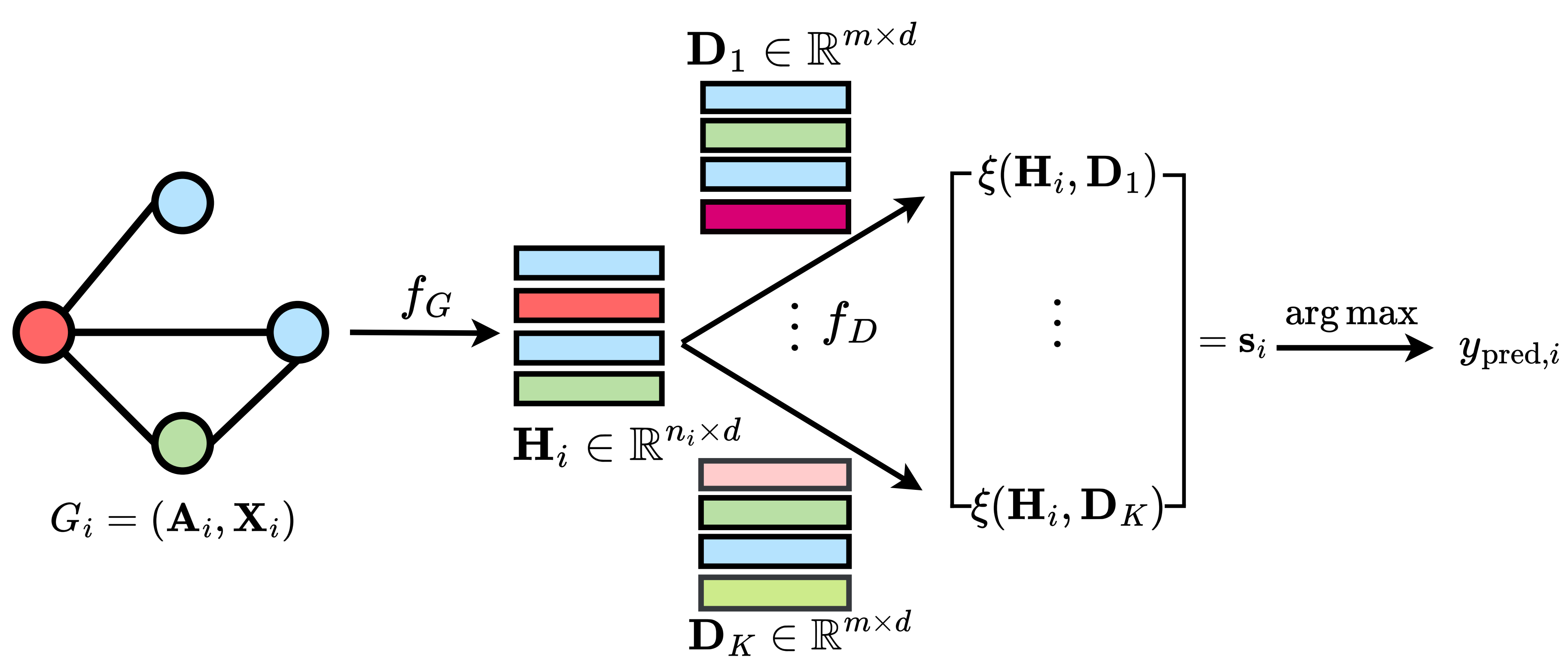
Motivation: Current global pooling methods suffer from information loss.

- Most of the global pooling methods are naive, often employing methods such as simple summation or averaging. These pooling methods collect only the first-order (statistics) information, leading to a loss of structural or semantic information.
- More sophisticated pooling operations retain more meaningful information, but still carry the inherent risk of information loss.

Model and Optimization

- GRDL is composed of two parts.
  - f_G is a backbone GNN to transform each graph G_i with adjacency matrix $A_i \in \mathbb{R}^{n_i \times n_i}$ and node feature $X_i \in \mathbb{R}^{n_i \times d_0}$ to a node embedding matrix $H_i \in \mathbb{R}^{n_i \times d}$, which encodes the graph's information
$$H_i = f_G(G_i) = f_G(A_i, X_i),$$
  - A reference layer f_D computes the similarity between each graph embedding H_i and reference distributions $\{D_1, \ldots, D_K\}$
$$f_D(H_i) = [s_{i1}, s_{i2}, \ldots, s_{iK}] = [\xi(H_i, D_1), \xi(H_i, D_2), \ldots, \xi(H_i, D_K)]^\top \in \mathbb{R}^K$$
where $\xi(\cdot,\cdot)$ is a similarity measure between two distributions, and is chosen to be the negative squared maximum mean discrepancy (MMD) in our experiment:
$$\xi(H, D) = \frac{2}{mn}\sum_{i=1}^{n}\sum_{j=1}^{m} k(h_i, d_j) - \frac{1}{n^2}\sum_{i=1}^{n}\sum_{i'=1}^{n} k(h_i, h_{i'}) - \frac{1}{m^2}\sum_{j=1}^{m}\sum_{j'=1}^{m} k(d_j, d_{j'}),$$
$k(\cdot,\cdot)$ is chosen to be the Gaussian kernel $k(x, x') = \exp\left(-\theta\|x - x'\|_2^2\right)$.
  - The graph is assigned the label of the reference that exhibits the highest similarity
$$y_{\text{pred},i} = \arg\max_k s_{ik}$$

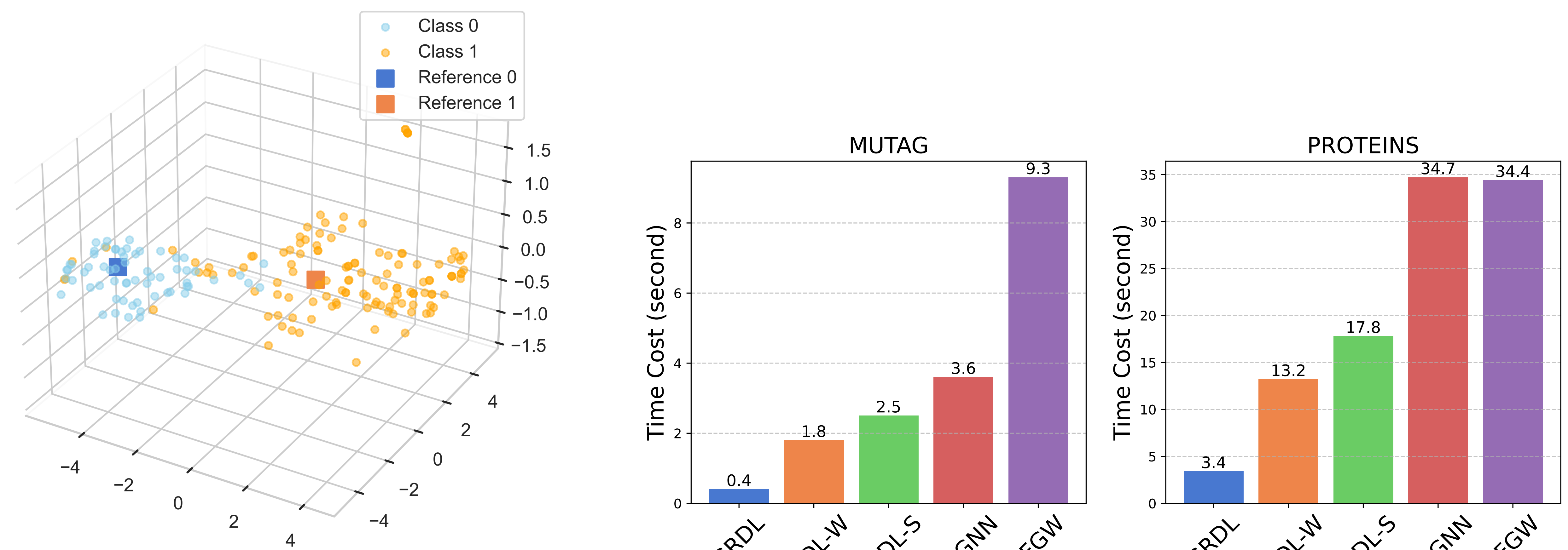


- Optimization problem of GRDL:
$$\min_{f_G, f_D} -\frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K} y_{ik}\log\frac{\exp(s_{ik})}{\sum_{j=1}^{K}\exp(s_{ij})} + \lambda\sum_{k}\sum_{k'\neq k}\xi(D_k, D_{k'})$$

Experiments on Graph Dataset & Visualizations

Method	MUTAG	PROTEINS	NCI1	IMDB-B	IMDB-M	PTC-MR	BZR	COLLAB	Average
PATCHY-SAN	**92.6±4.2**	75.1±3.3	76.9±2.3	62.9±3.9	45.9±2.5	60.0±4.8	85.6±3.7	73.1±2.7	71.5
GIN	89.4±5.6	76.2±2.8	82.2±0.8	64.3±3.1	50.9±1.7	64.6±7.0	82.6±3.5	79.3±1.7	73.6
DropGIN	90.4±7.0	76.9±4.3	81.9±2.5	66.3±4.5	51.6±3.2	66.3±8.6	77.8±2.6	80.1±2.8	73.9
DIFFPOOL	89.4±4.6	76.2±1.4	80.9±0.7	61.1±3.0	45.8±1.4	60.0±5.2	79.8±3.6	80.8±1.6	71.8
SEP	89.4±6.1	76.4±0.4	78.4±0.6	**74.1±0.6**	51.5±0.7	68.5±5.2	86.9±0.8	**81.3±0.2**	75.8
GMT	89.9±4.2	75.1±0.6	79.9±0.4	**73.5±0.8**	50.7±0.8	**70.2±6.2**	85.6±0.8	80.7±0.5	75.7
MinCutPool	90.6±4.6	74.7±0.5	74.3±0.9	72.7±0.8	51.0±0.7	68.3±4.4	87.2±1.0	**80.9±0.3**	75.0
ASAP	87.4±5.7	73.9±0.6	71.5±0.4	72.8±0.5	50.8±0.8	64.6±6.8	85.3±1.3	78.6±0.5	73.1
WitTopoPool	89.4±5.4	80.0±3.2	79.9±1.3	72.6±1.8	**52.9±0.8**	64.6±6.8	87.8±2.4	80.1±1.6	75.9
OT-GNN	91.6±4.6	76.6±4.0	**82.9±2.1**	67.5±3.5	52.1±3.0	68.0±7.5	85.9±3.3	80.7±2.9	75.7
WEGL	91.0±3.4	73.7±1.9	75.5±1.4	66.4±2.1	50.3±1.0	66.2±6.9	84.4±4.6	79.6±0.5	73.4
FGW - ADJ	82.6±7.2	72.4±4.7	74.4±2.1	70.8±3.6	48.9±3.9	55.3±8.0	86.9±1.0	80.6±1.5	71.5
FGW - SP	84.4±7.3	74.3±3.3	72.8±1.5	65.0±4.7	47.8±3.8	55.5±7.0	86.9±1.0	77.8±2.4	70.6
WL	87.4±5.4	74.4±2.6	**85.6±1.2**	67.5±4.0	48.4±4.2	56.0±3.9	81.3±0.6	78.5±1.7	72.4
WWL	86.3±7.9	73.1±1.4	**85.7±0.8**	71.6±3.8	52.6±3.0	52.6±6.8	87.6±0.6	**81.4±2.1**	73.9
SAT	**92.6±4.3**	77.7±3.2	82.5±0.8	70.0±1.3	47.3±3.2	68.3±4.9	**91.7±2.1**	80.6±0.6	76.1
Graphormer	89.6±6.2	76.3±2.7	78.6±2.1	70.3±0.9	48.9±2.0	**71.4±5.2**	85.3±2.3	80.3±1.3	75.1
GRDL	**92.1±5.9**	**82.6±1.2**	80.4±0.8	**74.8±2.0**	**52.9±1.8**	68.3±5.4	**92.0±1.1**	79.8±0.9	**77.9**
GRDL-W	90.8±4.6	**82.1±0.9**	80.9±0.8	72.2±3.1	**53.1±0.9**	68.5±3.2	90.6±1.5	80.4±1.1	**77.3**
GRDL-S	90.6±5.7	**81.1±1.4**	81.2±1.5	72.4±3.3	52.5±1.1	64.2±3.2	**91.6±1.3**	78.6±1.3	76.5

Table: Classification accuracy (%). Bold text indicates the top 3 mean accuracy.



(a) MUTAG node embedding and reference distributions.

(b) Time cost comparison.

Theoretical Results

Generalization bound and its implications (see our paper).