Region and Relations Based Multi Attention Network for Graph Classification

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Motivation: Region and Relations Based Multi Attention Network for Graph Classification

- Most of the existing pooling techniques cannot handle long-range dependencies between nodes.
- On the other hand, the node's co-relations with other nodes are also important for more expressive model.
- The existing pooling approaches are either global which cannot preserve the structure or hierarchical which can maintain the structure of the graph.
- Further, standard graph classification approaches use a classifier at the end of hierarchical structure which causes information loss.

Our Contributions

We propose a multi-attention network **R2MAN** which:

- includes our proposed pooling layer **R2POOL** that forms the new coarser version of the graph based on our proposed **region based attention** and **relation aware attention** layers.
- combines R2POOL layer with our **attention-aware multi-level prediction** mechanism to learn coarse to fine representations and restrict them to use only intermediate features weighted by the alignment scores for classification.
- leverages the proposed **branch training strategy** to learn importance of each level prediction.
- Experiments show that our model is able to achieve state-of-the-art performance on many real world datasets.

R2POOL Layer

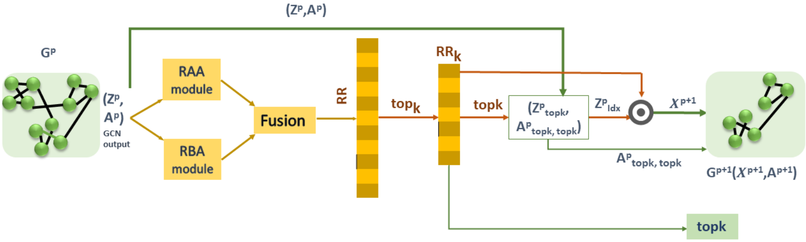

Figure: The R2POOL layer for graph pooling of the R2MAN network.

R2MAN

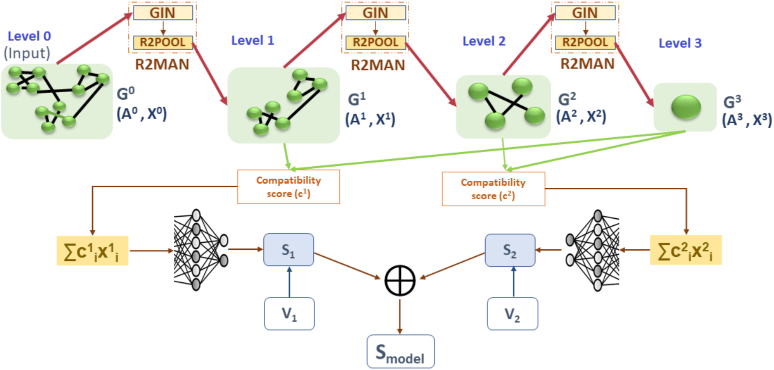

Figure: R2MAN architecture for graph classification

Hierarchical training strategy

Training part of R2MAN consists of majorly 3 steps:

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1. **Compatibility scores** (C^p) between each pth intermediate layer node representations (X^p) and vector of final level graph (O^P).

$$e_i^p = x_i^p O^P, \quad c_i^p = \frac{exp(e_i^p)}{\sum_{j=1}^{N_p} exp(e_j^p)}, \quad \forall i \in \{1, 2, \cdots, N_p\}$$

$$l^p = C^p X^p \;\; or \;\; l_p = \sum_{i=1}^{N_p} c_i^p x_i^p, \quad \forall p \in \{1, P-1\}$$

Hierarchical training strategy

Training part of R2MAN consists of majorly 3 steps:

2. **Branch nets** at each intermediate layer.

$$S_p = Branch\_net(I_p), \;\; \forall p \in \{1, P-1\} \tag{1}$$

Hierarchical training strategy

Training part of R2MAN consists of majorly 3 steps:

3. Finally, **branch training** is used to get the final predictions (S_{model}).

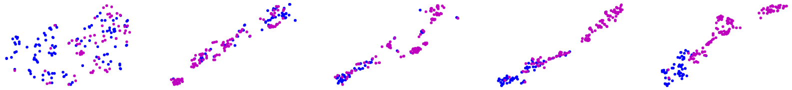
$$S_{model} = \sum_{p=1}^{P-1} V_p S_p \tag{2}$$

Here, v_p is the contribution of predictions at layer p.

Results (acc. and std. dev.) of Graph Classification

Algorithms	MUTAG	PTC	PROTEINS	NCI1	NCI109	IMDB-B	IMDB-M
GK	81.39±1.7	55.65±0.5	71.39±0.3	62.49±0.3	62.35±0.3	NA	NA
RW	79.17±2.1	55.91±0.3	59.57±0.1	NA	NA	NA	NA
PK	76±2.7	59.5±2.4	73.68±0.7	82.54±0.5	NA	NA	NA
WL	84.11±1.9	57.97±2.5	74.68±0.5	**84.46±0.5**	**85.12±0.3**	NA	NA
AWE-DD	NA	NA	NA	NA	NA	74.45±5.8	51.54±3.6
AWE-FB	87.87±9.7	NA	NA	NA	NA	73.13±3.2	51.58±4.6
node2vec	72.63±10.20	58.85±8.00	57.49±3.57	54.89±1.61	52.68±1.56	NA	NA
sub2vec	61.05±15.79	59.99±6.38	53.03±5.55	52.84±1.47	50.67±1.50	55.26±1.54	36.67±0.83
graph2vec	83.15±9.25	60.17±6.86	73.30±2.05	73.22±1.81	74.26±1.47	71.1±0.54	50.44±0.87
InfoGraph	89.01±1.13	61.65±1.43	NA	NA	NA	73.03±0.87	49.69±0.53
SortPool	85.83±1.7	58.59±2.5	75.54±0.9	74.44±0.5	72.31	70.03±0.9	47.83±0.9
PSCN	88.95±4.4	62.29±5.7	75±2.5	76.34±1.7	NA	71±2.3	45.23±2.8
DCNN	NA	NA	61.29±1.6	56.61±1.0	NA	49.06±1.4	33.49±1.4
ECC	76.11	NA	NA	76.82	75.03	NA	NA
DGK	87.44±2.7	60.08±2.6	75.68±0.5	80.31±0.5	80.32±0.3	66.96±0.6	44.55±0.5
DIFFPOOL	85.56	62.8	76.25	NA	NA	74.3	50.3
SAGPool	81.9	61.6	72.1	74.2	74.1	72.2	50.4
gpool	80.3	NA	77.7	NA	NA	73.0	49.9
IGN	83.89±12.95	58.53±6.86	76.58±5.49	74.33±2.71	72.82±1.45	72.0±5.54	48.73±3.41
GIN	89.4±5.6	64.6±7.0	76.2±2.8	82.7±1.7	NA	75.1±5.1	**52.3±2.8**
1-2-3GNN	86.1±	60.9±	75.5±	76.2±	NA	74.2±	49.5±
R2MAN	**92.11±5.35**	**64.90±5.99**	**77.84±1.51**	79.01±2.53	77.80±1.73	**75.83±3.17**	51.80±3.35
Rank	1	1	1	5	3	1	2

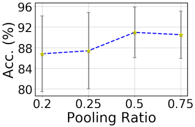
Model Ablation Study



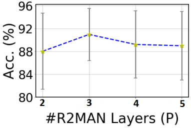
(a) DIFFPOOL (b) SAGPool (c) R2MAN-I (d) R2MAN-B (e) R2MAN

Figure: t-SNE visualization of the graphs from MUTAG dataset. The representations are generated by: (a) DIFFPOOL; (b) SAGPool; (c) R2MAN-I (Using Standard training procedure); (d) R2MAN-B (no branch training) and (e) R2MAN.

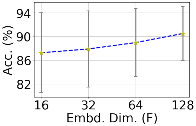
Sensitivity Analysis



(a)



(b)



(c)

Figure: Sensitivity analysis of R2MAN with respect to various hyper-parameters: (a) Pooling ratio, (b) Number of R2MAN layers and (c) Embedding dimension.

Thank you!!
Questions/Suggestions?