National Institute for Theory and Mathematics in Biology

Funded by the U.S. National Science Foundation and the Simons Foundation

Schur Nets: Higher Order GNN

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Higher order message passing neural networks (MPNNs), or Graph Neural Networks (GNN), assign (k+1)'th order tensors to subgraphs, for example, for k=2, a 6-cycle would output a 6x6xc tensor where the first two dimensions index the vertices of cycle while the third dimension corresponds to the channels. The general rules for permutation equivariant message passing between subgraphs carrying such tensors were derived in P-tensor framework [1].

While at the level of the graph as a whole such networks can capture structure in an expressive way, at the level of subgraphs, they enforce equivariance to the full symmetric group Sm of all permutations of vertices of the subgraph, which limits the space of equivariant maps. The true ambiguity of labeling of a graph is only up to the automorphism group, so one can consider the larger space of equivariant maps w.r.t. the automorphism group of the subgraph. A reason that this is not widely adopted might be the difficulty of determining those maps, which require finding the automorphism group and its linear representations. In our work, we present Schur Net, a novel Graph Neural Network architecture

Graph	Aut_S	**# of distinct λ_i (*Schur* Layer)**	$\sum_i(\kappa_i)^2$ Group theoretical approach
6-cycle	D_6	4	4
5-cycle	D_5	3	3
4-cycle	D_4	3	3
3-cycle	D_3	2	2
5-star	S_4	3	5
4-star	S_3	3	5
5-cycle with one branch	S_2	6	20
6-cycle with one branch	S_2	7	29

Table 2: Examples on EVD approach vs group theoretical approach towards # of equivariant maps w.r.t. Aut_S.

Corollary 1. *Consider a GNN on a graph that involves a neuron $\mathfrak{n}_S$ corresponding to a subgraph S with m vertices. Assume that the input of $\mathfrak{n}_S$ is a matrix $T \in \mathbb{R}^{m \times c_{in}}$, the rows of which transform covariantly with permutations of S and c_{in} is the number of channels. Let L be the combinatorial Laplacian of S, $U_1, \ldots, U_p$ be the eigenspaces of L, and M_i an orthognal basis for the i'th eigenspace stacked into an $\mathbb{R}^{n \times dim(U_i)}$ dimensional matrix. Then for any collection of learnable weight matrices $W_1, \ldots, W_p \in \mathbb{R}^{c_{in} \times c_{out}}$,*

$$\phi : T \longmapsto \sum_{i=1}^{p} M_i M_i^{\top} T W_i \tag{8}$$

is a permutation equivariant linear operation.

In the theory section of our paper, we derive sufficient condition for automorphism equivariant operations (Corollary 1) and the characterization of the learnable weights. Table 2 shows the extra possible equivariant maps.

We implemented Schur Net in P-tensor framework [1] to do higher-order message passing between subgraphs. We first do controlled ablation study to showcase the improvements Schur Net brings over Linmaps[2]. Table 3 demonstrates our absolute performance over existing MPNN as Schur Net achieves state-of-the-art result on ZINC-12k and OGB-HIV datasets.

Model	ZINC-12K MAE(↓)	OGB-HIV ROC-AUC(% ↑)
GCN	0.321 ± 0.009	76.07 ± 0.97
GIN	0.408 ± 0.008	75.58 ± 1.40
GINE	0.252 ± 0.014	75.58 ± 1.40
PNA	0.133 ± 0.011	79.05 ± 1.32
HIMP	0.151 ± 0.002	78.80 ± 0.82
N^2-GNN	$\mathbf{0.059 \pm 0.002}$	-
CIN	0.079 ± 0.006	80.94 ± 0.57
P-tensors	0.071 ± 0.004	80.76 ± 0.82
DS-GNN (EGO+)	0.105 ± 0.003	77.40 ± 2.19
DSS-GNN (EGO+)	0.097 ± 0.006	76.78 ± 1.66
GNN-AK+	0.091 ± 0.011	79.61 ± 1.19
SUN (EGO+)	0.084 ± 0.002	80.03 ± 0.55
Autobahn	0.106 ± 0.004	78.0 ± 0.30
Schur-Net	0.064 ± 0.002	$\mathbf{81.6 \pm 0.295}$

Table 3: Comparison of different models on the ZINC-12K and OGBG-MOLHIV datasets.

Reference: https://neurips.cc/virtual/2024/poster/95836 This research was supported in part by grants from NSF (MRI-1828629)

[1] A. Hands, T. Sun, R. Kondor: P-tensors: a General Formalism for Constructing Higher Order Message Passing Networks (AISTATS 2024).

[2]. Linmaps refer to only use equivariant maps w.r.t. S_n, which is the previously most general equivariant maps used by P-tensor.) code available at https://github.com/risi-kondor/ptens