- We would like to thank the reviewers for their thorough evaluation and constructive feedback. They have been really
- helpful in improving our work. Below, we address the main comments. Our revisions will be incorporated in the
- camera-ready version along with the additional related work, corrections and comments brought forth by the reviewers.
- Implications of equivariance and independence to the initial choice of identifiers (R1) SMP's equivariance proper-
- ties ensure that a change in the one-hot encoding results in a permutation of the rows of each local context U_i . However,
- in order to produce a final output (for node or graph classification), the rows of each U_i are pooled into a vector (in an
- equivariant manner as well). As a result, the output of each node is independent of the initial one-hot encoding, and the
- latter need not be consistent across examples and/or layers. Equivariance has some other useful consequences:
- Local isomorphisms: if the subgraphs G_i^k and G_j^k induced by G on the k-hop neighborhoods of v_i and v_j are isomorphic, then on node classification, any k-layer SMP f will yield the same result for v_i and v_j . To prove it, we first observe
- 10
- that $f(G)_{v_i} = f(G_i^k)_{v_i}$ and $f(G)_{v_j} = f(G_j^k)_{v_j}$, and then write the definition of equivariance for an isomorphism π 11
- mapping G_i^k to G_i^k and i to j. 12
- Transductivity: since all equivariant functions can take a variable number of inputs, SMP can be used transductively. If 13
- a node is added to a graph, a new line is simply created in each local context and there is no need to retrain the model.
- Experimentally, we observed that SMP managed to generalize to larger graphs than those seen during training: e.g., 15
- when we trained SMP to detect 4-cycles on graphs with 20 nodes (where it reaches 100% test accuracy), we obtained
- 99.05% accuracy when evaluating the same task on graphs with 36 nodes.
- Isomorphism testing: To test isomorphism using SMP, one can pool after each layer the $n \times d$ local context of each node 18
- into a feature vector in \mathbb{R}^d . For this purpose, a universal approximator of functions on sets (such as Deep Sets) can be 19
- used. Similarly to MPNNs, isomorphism can then be tested by comparing the multisets of node features after each layer. 20
- Equivariance guarantees that these multisets do not depend on the initial choice of the one-hot encoding, so that there is 21
- no need to sum over permutations—a key difference between SMP and relational pooling methods from the literature. 22
- Discussion about the theoretical results (R2) We would like to elaborate on three of the reviewer's points:
- Universality with features: Theorem 2 can be extended to attributed undirected graphs, but $d_{\text{nodes}} + nd_{\text{edges}}$ more 24
- channels are required in this case. For the node features, d_{nodes} channels can be used to store the features of all nodes 25
- using a variation of max pooling. For edge features, the same sketch of proof as Theorem 2 can be used: if each node 26 can store tensors of size $n \times n \times d_{\text{edges}}$, they can all recover the edge features. However, another embedding is needed 27
- as Lemma 1 does not apply anymore. If the graph is undirected, the square root matrix of each feature (which may be 28 complex-valued) constitutes a valid embedding, as it permutes as desired. However, this embedding does not compress 29
- the representation, so that $n \times d_{\text{edges}}$ new channels are required. Corollary 1 follows in the same way as previously.
- Expressivity: We do not yet have any formal results stating whether SMP is strictly more expressive than Fast SMP. Still, 31
- we observe that the proof that PPGN is at least as expressive as Fast SMP does not apply to SMP. This stems from the 32
- fact that SMP computes messages of the form $m(U_i, U_i, e_{ij})$, while PPGN can only store messages of the form $m(U_i)$. 33
- Equality of the embeddings in the limit: This is an interesting question. As Lemma 1 is not constructive, it is indeed 34 unclear at this point whether all node embeddings will become equal at infinite depth. At this point we can only observe 35
- that it is a possible scenario.
- Scalability and lower bound on the complexity (R3, R4) Although SMP is more efficient than previous powerful 37
- equivariant methods, large graphs exhibiting the small-world property indeed constitute a challenge. In this case, the 38
- scalability of SMP can be improved by simply using fewer identifiers (and ignoring conflicts), at the cost of breaking 39
- the theoretical guarantees of the network. We plan to investigate this extension in our future work. 40
- We also agree that lower bounds on the complexity required for universality would be very valuable to the community.
- We are aware of two results towards this direction: (i) if the feature space is continuous, at least d_{max} width is required 42
- to make the aggregation function injective [20]. (ii) for all message-passing methods (including SMP), solving some 43
- simple combinatorial tasks necessitates depth \times width = $\Omega(n)$ [18].
- Additional experiments (R1, R2, R4) Following the reviewers' suggestion, we ran experiments on Ring-GNN and 45
- Relational Pooling (RP): (i) Ring-GNN could solve the cycle-detection problem up to k = 8, n = 50. However, in 46
- this configuration (k = 8, n = 50), it required 5× more epochs and $10\times$ more time than SMP to converge (ii) RP with 47
- π -SGD (summing over 8 permutations) obtained 100% accuracy on all training sets, but exhibited overfitting (which 48
- was not observed on equivariant methods): for k = 6, n = 56, test accuracy was 84.1% for RP against 99.8% for SMP.
- Finally, we acknowledge the importance of additional benchmarking on tasks where both features and structure
- play a role. We are currently working on the QM9 and ZINC datasets, and plan to make the method available in 51
- Pytorch-geometric.