Building Powerful and Equivariant Graph Neural Networks with Structural Message-Passing

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This paper [1] proposed a powerful and equivariant structural message-passing (SMP). Concretely, SMP maintains at each node a matrix $\mathbf{U}_i \in \mathbb{R}^{n \times c}$ called "local context" (instead of a feature vector), which are propagated and processed in a permutation equivariant way. The j-th row of $\mathbf{U}_i$ contains the c-dimensional representation that node v_i has of node v_j. The local context is initialized as a one-hot encoding $\mathbf{U}_i^{(0)} = \mathbf{1}_i \in \mathbb{R}^{n \times 1}$ for every $v_i \in \mathcal{V}$, which corresponds to having initially a unique identifier for each node. In addition, if there are features $\mathbf{x}_i$ associated with node v_i, they are appended to the same row of the local context as the identifiers: $\mathbf{U}_i^{(0)}[i,:] = [1, \mathbf{x}_i] \in \mathbb{R}^{1+c_{\mathbf{x}}}$. At layer $l+1$, the state of each node is updated as in standard MPNNs:

$$\boldsymbol{U}_i^{(l+1)} = u^{(l)}\left(\boldsymbol{U}_i^{(l)}, \tilde{\boldsymbol{U}}_i^{(l)}\right) \quad \text{with} \quad \tilde{\boldsymbol{U}}_i^{(l)} = \phi\left(\left\{m^{(l)}\left(\boldsymbol{U}_i^{(l)}, \boldsymbol{U}_j^{(l)}, \boldsymbol{y}_{ij}\right)\right\}_{v_j \in N_i}\right),$$

where $u^{(l)}$, $m^{(l)}$, ϕ are the update, message and aggregation functions of the $(l+1)$-th layer, respectively. SMP is powerful in that it can manipulate polynomials in the adjacency matrix and therefore learn spectral properties. For example, starting from a one-hot encoding and using the update rule $\boldsymbol{U}_i^{(l+1)} = \sum_{v_j \in \mathcal{N}_i} \mathbf{U}_j^{(l)}$ (no self-loop), SMP iteratively compute powers of $\mathbf{A}$. Specially, $\mathbf{A}_{ij}^l$ corresponds to the count of walks of length l between v_i and v_j. After all L message-passing layers have been applied, the aggregated contexts $\mathbf{U}^{(L)}$ can be pooled to a vector or to a matrix (e.g., for graph and node classification, respectively), which also should be permutation invariant (e.g., sum or average).

The equivariance properties and representation of SMP are given in the paper. Two implementations (i.e., how to design $u^{(l)}$, $m^{(l)}$, ϕ) are also provided.

References

[1] Clement Vignac, Andreas Loukas, and Pascal Frossard. Building powerful and equivariant graph neural networks with structural message-passing. *Advances in Neural Information Processing Systems*, 33:14143–14155, 2020.