Universal Invariant and Equivariant Graph Neural Networks

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Graph Neural Networks (GNN) come in many flavors, but should always be either *invariant* (permutation of the nodes of the input graph does not affect the output) or *equivariant* (permutation of the input permutes the output). In this paper [1], we consider a specific class of invariant and equivariant networks, for which we prove new universality theorems.

More precisely, we consider networks with a single hidden layer, obtained by summing channels formed by applying an equivariant linear operator, a pointwise non-linearity, and either an invariant or equivariant linear output layer. Such linear invariant and equivariant operators between tensors have recently been completely characterized by Maron et al. [2]. Recently, the same authors [3] showed that by allowing higher-order tensorization inside the network, universal *invariant* GNNs can be obtained.

As a first contribution, we propose an alternative proof of this result, which relies on the Stone-Weierstrass theorem for algebra of real-valued functions. Our main contribution is then an extension of this result to the *equivariant* case, which appears in many practical applications but has been less studied from a theoretical point of view. The proof relies on a new generalized Stone-Weierstrass theorem for algebra of equivariant functions, which is of independent interest. Additionally, unlike many previous works that consider a fixed number of nodes, our results show that a GNN defined by a single set of parameters can approximate uniformly well a function defined on graphs of varying size.

References

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