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