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ProteiNN: Intrinsic-Extrinsic Convolution and Pooling for Scalable Deep Protein Analysis

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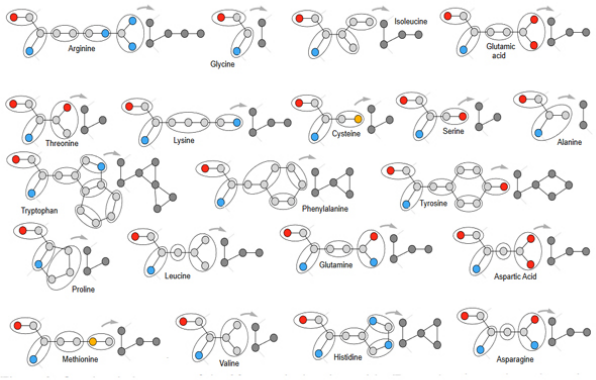

Proteins perform a large variety of functions in living organisms, thus playing a key role in biology. As of now, available learning algorithms to process protein data do not consider several particularities of such data and/or do not scale well for large protein conformations. To fill this gap, we propose two new learning operations enabling deep 3D analysis of large-scale protein data. First, we introduce a novel convolution operator which considers both, the intrinsic (invariant under protein folding) as well as extrinsic (invariant under bonding) structure, by using n-D convolutions defined on both the Euclidean distance, as well as multiple geodesic distances between atoms in a multi-graph. Second, we enable a multi-scale protein analysis by introducing hierarchical pooling operators, exploiting the fact that proteins are a recombination of a finite set of amino acids, which can be pooled using shared pooling matrices. Lastly, we evaluate the accuracy of our algorithms on several large-scale data sets for common protein analysis tasks, where we outperform state-of-the-art methods.

http://dx.doi.org/https://doi.org/10.1007/inventado

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