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GENEOnet: a GENEIO based approach to Pocket Detection.

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Pocket detection is a key step inside the process of drug design and development. Its purpose is to prioritize specific areas of the protein surface with high chance of being binding sites. The primary byproduct of this is to avoid blind docking. During a blind docking, the software tries to fit the ligand into the target protein without prior knowledge, thus it scans the whole protein surface to choose the best possible location. This is a very computational intensive procedure and usually it doesn't give the best results. However, knowing in advance the putative binding sites allows to perform a targeted docking, reducing computational costs and possibly improving results.

GENEOnet is an algorithm for pocket detection based on Group Equivariant Non-Expansive Operators (GENEOs). It is also the first attempt to build a network of these operators to develop a machine learning pipeline. GENEOnet benefits of the theoretical properties of GENEOs such as: possibility of incorporating prior knowledge about the problem, exploitation of geometrical features of the data, reduction in the number of trainable parameters, need of fewer examples during training and higher interpretability of the final results. Combining all these advantages, GENEOnet provides a new solution to the problem of pocket detection that goes in the direction of explainable machine learning. Moreover, a comparison with other state-of-the-art methods for pocket detection, that usually lack some of the listed features, shows that GENEOnet has also competitive results.

Keywords

GENEOs, Pocket Detection, Explainable Machine Learning

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