# GENEOnet: a transparent AI method for drug design based on Group Equivariant Non Expansive Operators

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joint work with Giovanni Bocchi[1], Patrizio Frosini[2], Alessandro Pedretti[1], Carmine Talarico[3], Filippo Lunghini[3], Andrea R. Beccari[3], Carmen Gratteri[4]

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Equivariant operators are proving to be increasingly important in deep learning, in order to make neural networks more transparent and interpretable. The use of such operators corresponds to the rising interest in the so called "explainable artificial intelligence", which looks for methods and techniques whose functioning can be understood by humans. In accordance with this line of research, Group Equivariant Non-Expansive Operators (GENEOs) have been recently proposed as elementary components for building new kinds of networks [1, 2]. Their use is grounded in Topological Data Analysis (TDA) and guarantees good mathematical properties to the involved spaces, such as compactness, convexity, and finite approximability, under suitable assumptions on the space of data and by choosing appropriate topologies.

In this talk we will show promising results obtained by applying GENEOs to protein pocket detection [3, 4]. Protein pockets detection is a key problem in the context of drug design, since the ability to identify a small number of potential binding sites, allows to speed up drug discovery procedures. In this talk we will show how GENEOs can be used to build a robust geometrical machine learning method, able to detect protein pockets better than ML techniques already in use, but being based only on 17 unknown parameters.

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data analysis and machine learning. Nature Machine Intelligence (2019) doi: 10.1038/s42256-019-0087-3

[2] Bocchi, G., Botteghi, S., Brasini, M., Frosini, P., and Quercioli, N.: On the finite representation of group equivariant operators via permutant measures. Annals of Mathematics and Artificial Intelligence (2023) doi: 10.1007/s10472-022-09830-1

[3] Bocchi, G., Frosini, P., Micheletti, A., Pedretti, A. *et al.*: GENEOnet: A new machine learning paradigm based on Group Equivariant Non-Expansive Operators. An application to protein pocket detection. (2022) preprint at arXiv:2202.00451.

[4] Bocchi, G., Frosini, P., Micheletti, A., Pedretti, A., Gratteri, C., Lunghini, F.,Beccari, A.R.,Talarico, C. GENEOnet: statistical analysis supporting explainability and trustworthiness. Statistics, 1–26, (2025). doi: 10.1080/02331888.2025.2478203