Explainable Machine Learning with Group Equivariant Non-Expansive Operators (GENEOs). An industrial application to Protein Pocket Detection.

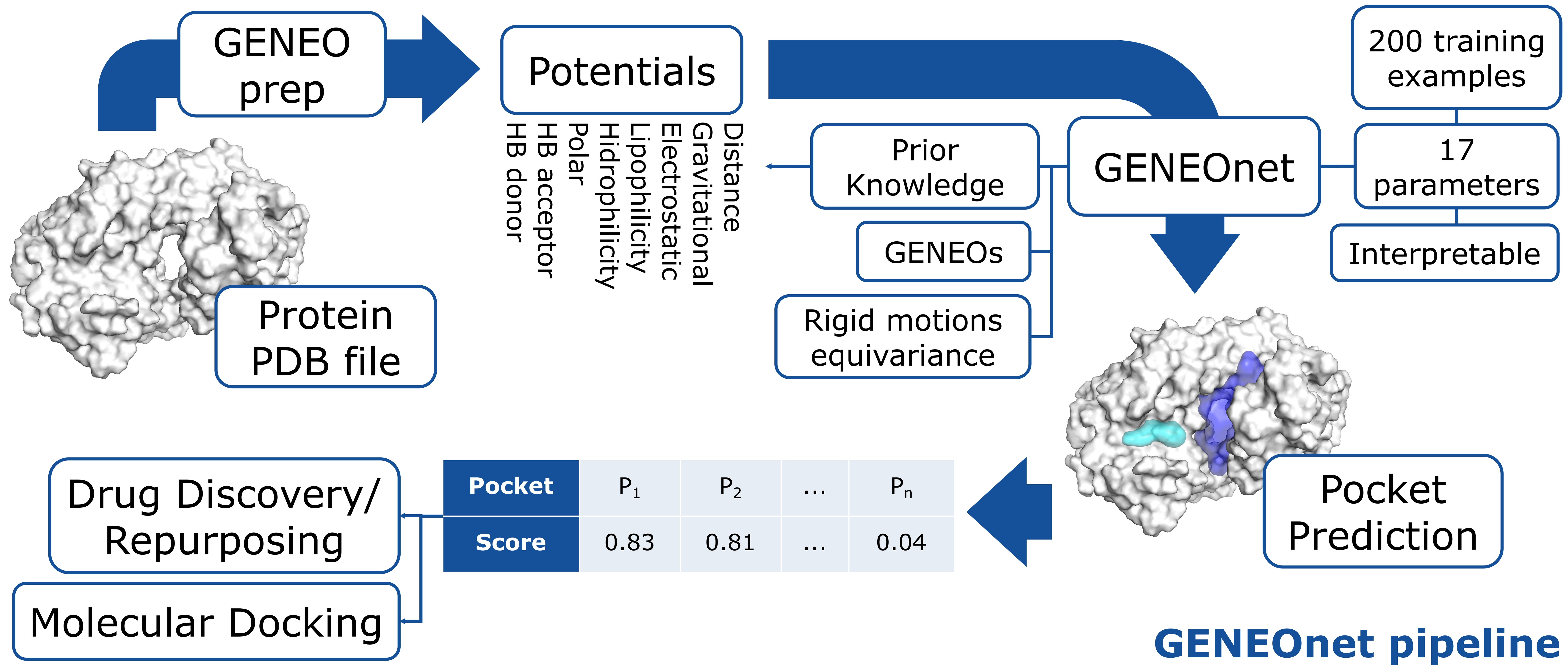
Giovanni Bocchi
Department of Environmental Science and Policy, University of Milan.

GENEOs

A Group Equivariant Non-Expansive Operator F is a map between two functional spaces $\Phi = \{\varphi: \mathrm{X} \to \mathbb{R}\}$ and $\Psi = \{\psi: \mathrm{Y} \to \mathbb{R}\}$ that, given two subgroups $\mathrm{G} \trianglelefteq \mathrm{Homeo}(\mathrm{X})$ and $\mathrm{K} \trianglelefteq \mathrm{Homeo}(\mathrm{Y})$ and a fixed group homomorphism $\mathrm{T}: \mathrm{G} \to \mathrm{K}$, has two properties:

1. **Equivariance:** $\mathrm{F}(\varphi \circ g) = \mathrm{F}(\varphi) \circ \mathrm{T}(g)$ for all $\varphi \in \Phi$ and $g \in \mathrm{G}$.
2. **Non-Expansivity:** $\|\mathrm{F}(\varphi_1) - \mathrm{F}(\varphi_2)\|_\infty \leq \|\varphi_1 - \varphi_2\|_\infty$ for all $\varphi_1, \varphi_2 \in \Phi$

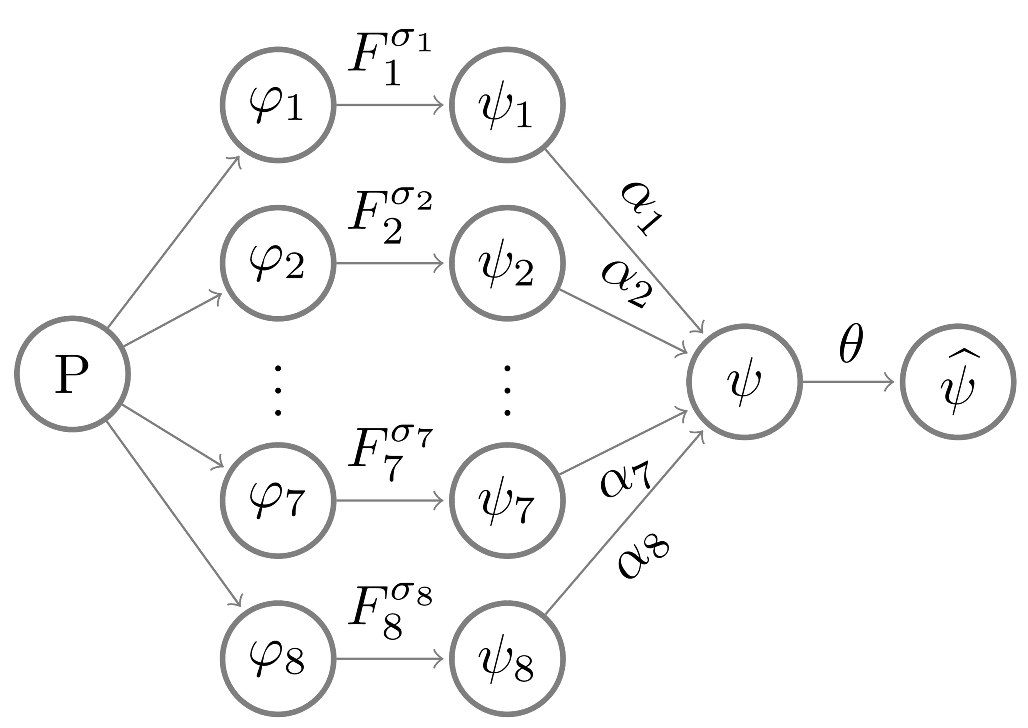
The problem



Pocket	P_1	P_2	...	P_n
Score	0.83	0.81	...	0.04

GENEOnet pipeline

GENEOnet



Results

Method	T_1	T_2	T_3	H_{1+}
GENEOnet	**0.792**	**0.905**	**0.941**	0.975
P2Rank	0.728	0.847	0.892	0.952
DeepPocket	0.652	0.798	0.860	**0.978**
CAVIAR	0.616	0.739	0.783	0.837
Fpocket	0.331	0.462	0.534	**0.978**
CavVis	0.224	0.376	0.483	0.842

Conclusions

GENEOs can be powerful mathematical tools for **eXplainable Machine Learning and AI.**

1. Few trainable parameters.
2. Intrepretability of the parameters.
3. Can incorporate Prior Knowledge.
4. Equivariance by design.
5. Necessity of fewer training data.
6. Lower computational complexity compared to similar deep networks.

Joint work with:
A. Micheletti, A. Pedretti (University of Milan) and P. Frosini (University of Pisa). C. Talarico, F. Lunghini, A. R. Beccari and C. Gratteri (Dompé Farmaceutici SpA).

Reach me at:
giovanni.bocchi1@unimi.it
www.linkedin.com/in/giovanni-bocchi-01998b197

Try it! **GENEOnet** **GENEOs**