# Group Equivariant Non-Expansive Operators (GENEOs) as geometric instruments to build transparent and robust AI models

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# Outline

Some epistemological assumptions

Some basics on the theory of GENEOs

**GENEOs** and XAI

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# Assumption 1: Data are often represented by functions

#### Many types of data can be represented as functions:

Images, electrocardiograms, computerized tomography scans, and more.

Additionally:

- A point cloud C in  $\mathbb{R}^n$  (where C is equivalent to the function  $d_C : \mathbb{R}^n \to \mathbb{R}$  that expresses the distance from C).
- A graph Γ (where Γ is equivalent to its adjacency matrix, which can be interpreted as a function).



# Assumption 2: Data are processed by observers

Data have no meaning without an observer to interpret them.



An observer is an agent that transforms data while preserving their symmetries.

### Assumption 3: Observers are variables

Data interpretation strongly depends on the chosen observer.



# Assumption 4: Observers are important

We are rarely directly interested in the data, but rather in how observers react to their presence.



Consequently, we should focus more on the properties of the observers than on the properties of the data.

# Assumption 5: There is no structure in the data

Generally speaking, data lack inherent structure. Instead, the structure of data reflects the observer's own structure.



The shape is not in the data but in the eyes of the observer.

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# Let's start by defining perception pairs

Let us consider

- 1. A collection  $\Phi$  of functions from a set X to  $\mathbb{R}$ ;
- A group G of bijections g : X → X such that φ ∈ Φ ⇒ φ ∘ g ∈ Φ for every φ ∈ Φ.

We say that  $(\Phi, G)$  is a perception pair.

The choice of a perception pair states which data can be considered as legitimate measurements (the functions in  $\Phi$ ) and which group represents the admissible symmetries between data (the group G).



# Admissible and not admissible data



ADMISSIBLE AS AN ELECTROCARDIOGRAM

NOT ADMISSIBLE AS AN ELECTROCARDIOGRAM





NOT ADMISSIBLE AS A NUMBER

### What metric can we consider on $\Phi$ , X and G?

We endow  $\Phi$  with the sup-norm metric:

$$D_{\Phi}(\varphi_1,\varphi_2) = \sup_{x \in X} |\varphi_1(x) - \varphi_2(x)|.$$

NB: What other metric could we put on  $\Phi$ , given that X is not endowed with any measure or structure?

Then, we endow X with the pseudo-metric

$$D_X(x_1,x_2) = \sup_{\varphi \in \Phi} |\varphi(x_1) - \varphi(x_2)|.$$

We recall that a pseudo-metric is just a metric *d* without the property  $d(x_1, x_2) = 0 \implies x_1 = x_2$ .

Finally, we put on G the pseudo-metric

$$D_G(g_1,g_2) := \sup_{\varphi \in \Phi} D_\Phi(\varphi \circ g_1, \varphi \circ g_2).$$

### Some mathematical properties

- Every function  $\varphi \in \Phi$  is non-expansive and hence continuous.
- 1. If  $\Phi$  is compact and X is complete, then X is compact.
  - 2. If  $\Phi$  is compact and G is complete, then G is compact.
  - 3. If  $\Phi$  is totally bounded, we can always assume that  $\Phi$ , X, and G are compact.
- G is a topological group for the topology induced by D<sub>G</sub>, and the action of G on Φ by composition on the right is continuous.
- Any Φ-preserving bijection is an isometry.

A mathematical theory has been developed on this topic.

# GEOs and GENEOs

Let us assume that two perception pairs  $(\Phi, G)$ ,  $(\Psi, K)$  are given.

Each pair  $(F : \Phi \to \Psi, T : G \to K)$  such that T is a homomorphism and  $F(\varphi \circ g) = F(\varphi) \circ T(g)$  for every  $\varphi \in \Phi, g \in G$  is called a *Group Equivariant Operator (GEO)*.

If *F* is also non-expansive (i.e.,  $D_{\Psi}(F(\varphi_1), F(\varphi_2)) \leq D_{\Phi}(\varphi_1, \varphi_2)$  for every  $\varphi_1, \varphi_2 \in \Phi$ ), then (F, T) is called a *Group Equivariant* Non-Expansive Operator (GENEO).

GENEOs represent observers in our setting.

# An example of GENEO

When we blur an image by applying a convolution with a rotationally symmetric kernel whose mass is less than 1 in  $L^1$ , we are applying a GENEO (here, we are considering the group of isometries).



# Another example of GENEO

When we compute the convex hull of a cloud of points, we are applying a GENEO (here, we are considering the group of isometries).



### Good news for applications

A metric can be naturally defined on the space of GENEOs between two fixed perception pairs  $(\Phi, G)$  and  $(\Psi, K)$ , given a fixed homomorphism T between the transformation groups G and K.

The following result holds.

#### Theorem

- If the input and output spaces of admissible data are compact, then the space of GENEOs is also compact.
- If the output space of admissible data is convex, then the space of GENEOs is also convex.

# Two key observations (1)

Our main goal is to develop a robust geometric and compositional theory for approximating an ideal observer through GENEOs.



# Two key observations (2)

GENEOs are functions and can be taken as inputs of higher-level GENEOs. Data obtained through measuring instruments can be seen as GENEOs of level 0. Therefore, hierarchies of GENEOs can be considered.



# Construction of GENEOs

How can we build GENEOs?

The space of GENEOs is closed under composition, computation of minimum and maximum, translation, direct product, and convex combination. (However there is much more than this...)



GENEOs are like LEGO bricks that can be combined together to form more complex GENEOs.

### The main point in the approach based on GENEOs

In perspective, we are looking for a good compositional theory for building efficient and transparent networks of GENEOs. Some preliminary experiments suggest that replacing neurons with GENEOs could make deep learning more transparent and interpretable and speed up the learning process.



# What happens when we apply GENEOs to our data?

An example of use: comparison between real dice and fake dice.



(Experiment and computations by Giovanni Bocchi)

#### What happens to data when we apply GENEOs?

We produced 10000 dice (a training set of size 7000 and a test set of size 3000), then we applied PCA to the test set and to the test set transformed by a suitable GENEO, optimized on the training set:



For each die the first two principal components are plotted. Blue points are associated with **real dice**, while orange ones with **fake dice**. The GENEO we use was built by a convex combination of 3 GENEOs defined by permutant measures.

# **GENEOs and Machine Learning**

More details about the theory of GENEOs are available in this paper:

machine intelligence

ARTICLES https://doi.org/10.1038/s42256-019-0087-3

# Towards a topological-geometrical theory of group equivariant non-expansive operators for data analysis and machine learning

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https://rdcu.be/bP6HV

# **GENEOs and Machine Learning**

For more details about the use of GENEOs in Machine Learning, you can have a look at this paper:



#### https://ems.press/journals/mag/articles/10389352

# Current research projects (I)

CNIT / WiLab - Huawei Joint Innovation Center (JIC)

# Project on GENEOs for 6G





# Current research projects (II)

# PANDORA

#### Horizon Europe (HORIZON) Call: HORIZON-CL4-2023-HUMAN-01-CNECT Project: 101135775 — PANDORA Funding: approximately 9 million euros.

**Task 3.3 - Leveraging domain knowledge for explainable learning:** This task aims to investigate the use of domain knowledge in the development of explainable AI models. Tools like GENEOs for applications in TDA and ML and new theoretical methods of GENEOs for explainable AI will be used.



The project has received funding form the European Union's Horizon Europe Framework Programme (Horizon) under grant agreement No 101135775

# Current research projects (III)



The GENEOnet webservice represents the outcome of our partnership with Italian Pharmaceutical Company Dompé Farmaceutici S.p.A.: https://geneonet.exscalate.eu/

# Finding pockets in proteins by applying GENEOs

GENEOs can be used for the detection of druggable protein pockets.



**Model predictions for protein 2QWE**. In Figure a) the global view of the prediction is shown, where different pockets are depicted in different colors and are labelled with their scores. In Figure b) the zoomed of the pocket containing the ligand is shown.

#### Results



Percentage of correct answers when allowing n=1,2,3,4 attempts.

Please note that GENEOnet uses 17 parameters, while a CNN such as DeepPocket requires 665122 parameters.

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#### Basic idea

How can we mathematically and generally formalize the concept of an explanation provided by an agent, viewed as a functional operator?

**Informal idea:** We could say that the action of an agent A is explained by another agent B from the perspective of an agent C if:

- 1. C perceives A and B as similar to each other;
- 2. C perceives B as less complex than A.

Note that if A and B are represented as GENEOs, they are functions and can therefore be treated as inputs to a higher-level GENEO C.

### An extended pseudo-metric for ALL GENEOs

The first step in formalizing this idea is to introduce a metric between GENEOs that remains well-defined even when the GENEOs operate on different domains and produce outputs in distinct codomains. This is a non-trivial challenge.

$$(\Psi_{\alpha}, K_{\alpha}) \\ (F_{\alpha}, T_{\alpha}) \\ (\Phi_{\alpha}, G_{\alpha})$$

What's the distance between these two GENEOs?

 $(\Psi_{\beta}, K_{\beta})$   $(F_{\beta}, T_{\beta})$   $(\Phi_{\alpha}, G_{\alpha})$ 

In other words, what does it mean for two GENEOs to behave approximately the same way?

### An extended pseudo-metric for ALL GENEOs

Informally speaking, two GENEOs are considered similar if we can find two horizontal GENEOs that make this diagram nearly commutative:



# An extended pseudo-metric for ALL GENEOs

Therefore, we can define a distance *d* between GENEOs that measures how closely we can make the considered diagram commutative by choosing appropriate horizontal GENEOs (called *simplification GENEOs*). Naturally, this metric depends on which simplification GENEOs we consider admissible.

The non-expansiveness of GENEOs is a key component in proving that the function d is indeed a metric.

When the previous distance d is small, the GENEOs considered act approximately in the same way on the data they process.

# An example



# A mathematical concept of explanation

In summary, the pseudo-metric *d* enables us to introduce a precise mathematical concept of *explanation*. Specifically, we can define it as follows: the action of an agent represented by a GENEO  $(F_{\alpha}, T_{\alpha})$  is *explained at a level*  $\varepsilon$  by the action of another agent represented by a GENEO  $(F_{\beta}, T_{\beta})$  when  $d((F_{\alpha}, T_{\alpha}), (F_{\beta}, T_{\beta})) \leq \varepsilon$ .



A general mathematical model of explainability grounded in a precise operator theory could be beneficial for XAI.

# Summary

To sum up, GENEOs are

- novel mathematical tools designed to approximate observers
- particularly useful when some knowledge about the behavior of observers is available
- generally interpretable
- potentially useful for explainable artificial intelligence (XAI).

