

Recent advances in the theory of GENEOS and its application to Machine Learning

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CaLISTA kick-off meeting, Bologna, 5-9 June 2023

Outline

The key role of observers in data analysis

Topological and metric basics for the theory of GENEOS

Building linear and nonlinear GENEOS

How can we use GENEOS in applications?

The key role of observers in data analysis

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How can we use GENEOS in applications?

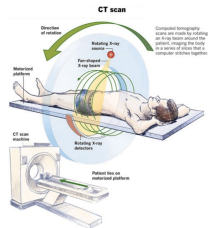
Some key principles in our model

LET US ILLUSTRATE
THE MAIN PRINCIPLES
IN OUR MODEL

Data can be often regarded as functions

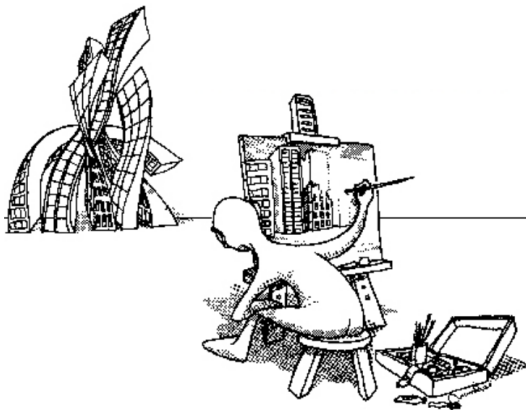
Some examples of data that can be seen as functions:

- An electrocardiogram (a function from \mathbb{R} to \mathbb{R});
- A gray-level image (a function from \mathbb{R}^2 to \mathbb{R});
- A computerized tomography scan (a function from a helix to \mathbb{R}).



Data are processed by observers

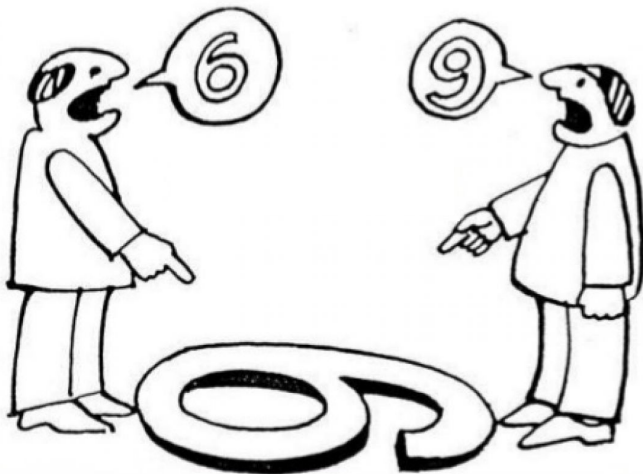
Data have no meaning if no observer elaborates them.



An observer is an agent that transforms data.

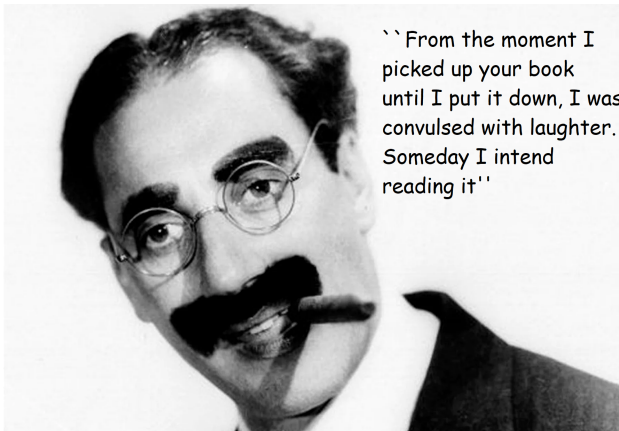
Observers are variables in data analysis

Data interpretation strongly depends on the chosen observer:



Our interest in data is greatly overrated

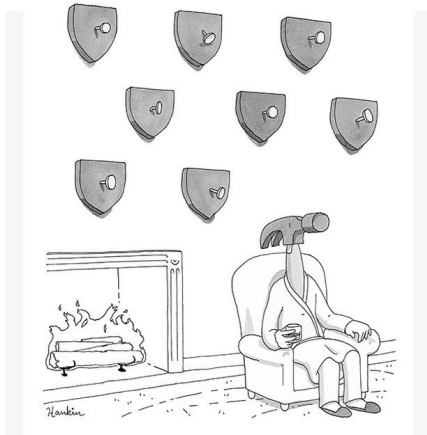
We are hardly ever interested directly in data but in the reaction of the observer to the presence of data.



`` From the moment I
picked up your book
until I put it down, I was
convulsed with laughter.
Someday I intend
reading it''

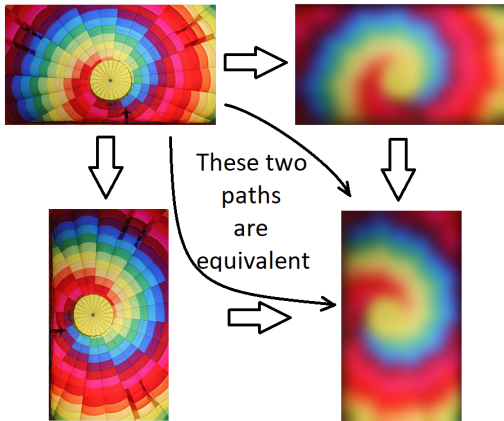
No data structure

Generally speaking, there is no structure in data. The structure of data is a projection of the structure of the observer.



Representing observers as equivariant operators

Observers are structures able to change data into other data, and usually do that by respecting some data symmetries, i.e., by commuting with some transformations (**equivariance**).



Representing observers as equivariant operators

As a first approximation, observers can be represented as **Group Equivariant Operators (GEOs)**.

In this talk we will illustrate some results on the theory of **Group Equivariant Non-Expansive Operators (GENEOs)**.

Why “non-expansive”?

Because

1. observers are often assumed to simplify the metric structure of data in order to produce meaningful interpretations;
2. non-expansiveness guarantees good topological properties.

The key role of observers in data analysis

Topological and metric basics for the theory of GENEOS

Building linear and nonlinear GENEOS

How can we use GENEOS in applications?

Some preliminary results

LET US NOW ILLUSTRATE
SOME PRELIMINARY
TOPOLOGICAL RESULTS

How could we represent observers?

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

Mattia G. Bergomi¹, Patrizio Frosini^{2,3*}, Daniela Giorgi⁴ and Nicola Quercioli^{2,3}

We provide a general mathematical framework for group and set equivariance in machine learning. We define group equivariant non-expansive operators (GENEOs) as maps between function spaces associated with groups of transformations. We study the topological and metric properties of the space of GENEOs to evaluate their approximating power and set the basis for general strategies to initialize and compose operators. We define suitable pseudo-metrics for the function spaces, the equivariance groups and the set of non-expansive operators. We prove that, under suitable assumptions, the space of GENEOs is compact and convex. These results provide fundamental guarantees in a machine learning perspective. By considering isometry-equivariant non-expansive operators, we describe a simple strategy to select and sample operators. Thereafter, we show how selected and sampled operators can be used both to perform classical metric learning and to inject knowledge in artificial neural networks.

<https://rdcu.be/bP6HV>

All begins with the space of admissible functions

Let X be a nonempty set. Let Φ be a topological subspace of the set \mathbb{R}_b^X of all bounded functions φ from X to \mathbb{R} , endowed with the topology induced by the metric

$$D_\Phi(\varphi_1, \varphi_2) := \|\varphi_1 - \varphi_2\|_\infty.$$

We can see X as the space where we can make our measurements, and Φ as the space of all possible measurements. We will say that Φ is the *set of admissible functions*. In other words, Φ **is the set of all functions from X to \mathbb{R} that can be produced by our measuring instruments (or by other observers)**. For example, a gray-level image can be represented as a function from the real plane to the interval $[0, 1]$ (in this case $X = \mathbb{R}^2$).

Perception pairs

Let us consider a group G of bijections $g : X \rightarrow X$ such that $\varphi \in \Phi \implies \varphi \circ g \in \Phi$ for every $\varphi \in \Phi$. We say that (Φ, G) is a **perception pair**.

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

To proceed, we need to introduce suitable topologies on X and G . Before doing that, we recall that the **initial topology** τ_{in} on X with respect to Φ is the coarsest topology on X such that every function φ in Φ is continuous.

A pseudo-metric on X

Let us define on X the pseudo-metric

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

D_X induces a topology τ_{D_X} on X .

The use of D_X implies that we can distinguish two points only if a measurement exists, taking those points to different values.

Proposition

The topology τ_{D_X} is finer than the initial topology τ_{in} on X with respect to Φ . If Φ is totally bounded, then τ_{D_X} coincides with τ_{in} .

A pseudo-metric on X

The following properties are of use in our model.

Proposition

Every function in Φ is non-expansive, and hence continuous.

Proposition

If Φ is compact and X is complete, then X is compact.

In the following, we will usually assume that Φ is compact and X is complete (and hence compact).

Some magic happens: each bijection is an isometry

- $\text{Bij}_\Phi(X) = \{\text{bijections } g: X \rightarrow X \text{ s.t. } \Phi \circ g, \Phi \circ g^{-1} \subseteq \Phi\};$
- $\text{Homeo}_\Phi(X) = \{\text{homeomorphisms } g: X \rightarrow X \text{ s.t. } \Phi \circ g, \Phi \circ g^{-1} \subseteq \Phi\};$
- $\text{Iso}_\Phi(X) = \{\text{isometries } g: X \rightarrow X \text{ s.t. } \Phi \circ g, \Phi \circ g^{-1} \subseteq \Phi\}.$

Proposition

$$\text{Bij}_\Phi(X) = \text{Homeo}_\Phi(X) = \text{Iso}_\Phi(X).$$

A pseudo-metric on G

Let us now focus our attention on a subgroup G of $\text{Homeo}_\Phi(X)$.

We can define a pseudo-metric D_G on G by setting

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

Theorem

G is a topological group with respect to D_G and the action of G on Φ by right composition is continuous.

Theorem

If Φ is compact and G is complete, then G is compact.

The concept of GENE0

WE ARE NOW READY
TO INTRODUCE
THE CONCEPT OF GENE0

GEOs and GENEOS

Each pair (Φ, G) with $G \subseteq \text{Homeo}_\Phi(X)$ is called a *perception pair*.

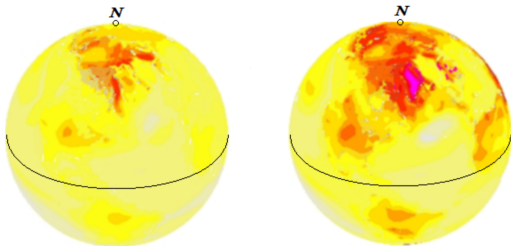
Let us assume that two perception pairs (Φ, G) , (Ψ, H) are given, and fix a group homomorphism $T : G \rightarrow H$.

Each function $F : \Phi \rightarrow \Psi$ such that $F(\varphi \circ g) = F(\varphi) \circ T(g)$ for every $\varphi \in \Phi, g \in G$ is called a *Group Equivariant Operator (GEO)* associated with the homomorphism T .

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 is called a *Group Equivariant Non-Expansive Operator (GENEO)* associated with the homomorphism T .

An example of GENE0

Let us assume to be interested in the comparison of the **distributions of temperatures** on a sphere, taken at two different times:



Let us also assume that only two opposite points N, S can be localized on the sphere.

An example of GENEIO

Let us introduce two perception pairs $(\Phi, G), (\Psi, H)$ by setting

- $X = S^2$
- $\Phi =$ set of 1-Lipschitz functions from S^2 to a fixed interval $[a, b]$
- $G =$ group of rotations of S^2 around the axis $N - S$

and

- $Y =$ the equator S^1 of S^2
- $\Psi =$ set of 1-Lipschitz functions from S^1 to $[a, b]$
- $H =$ group of rotations of S^1

An example of GENEIO

This is a simple example of GENEIO from (Φ, G) to (Ψ, H) :

- $T(g)$ is the rotation $h \in H$ of the equator S^1 that is induced by the rotation g of S^2 , for every $g \in G$.
- $F(\varphi)$ is the function ψ that takes each point y belonging to the equator S^1 to the average of the temperatures along the meridian containing y , for every $\varphi \in \Phi$;

We can easily check that F verifies the properties defining the concept of group equivariant non-expansive operator with respect to the isomorphism $T : G \rightarrow H$.

In plain words, our GENEIO simplifies the data by transforming “temperature distributions on the earth” into “temperature distributions on the equator”.

Two key results (and two good news for applications)

Let us assume that a homomorphism $T : G \rightarrow H$ has been fixed.
Let us define a metric D_{GENEO} on $\text{GENEO}((\Phi, G), (\Psi, H))$ by setting

$$D_{\text{GENEO}}(F_1, F_2) := \sup_{\varphi \in \Phi} D_{\Psi}(F_1(\varphi), F_2(\varphi)).$$

Theorem

If Φ and Ψ are **compact**, then $\text{GENEO}((\Phi, G), (\Psi, H))$ is **compact** with respect to D_{GENEO} .

Theorem

If Ψ is **convex**, then $\text{GENEO}((\Phi, G), (\Psi, H))$ is **convex**.

The key role of observers in data analysis

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How can we use GENEOS in applications?

Methods to build GENEOS

NOW THAT WE KNOW
THE ROLE OF GENEOS
WE NEED TO EXPLAIN
HOW WE CAN BUILD THEM

How can we build linear and nonlinear GENEOSs?



On the Construction of Group Equivariant Non-Expansive Operators *via* Permutants and Symmetric Functions

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<https://www.frontiersin.org/articles/10.3389/frai.2022.786091/full>

How can we represent linear GENEOS?

Annals of Mathematics and Artificial Intelligence

<https://doi.org/10.1007/s10472-022-09830-1>

On the finite representation of linear group equivariant operators via permutant measures

Giovanni Bocchi¹ · Stefano Botteghi² · Martina Brasini² · Patrizio Frosini²  · Nicola Quercioli³

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<https://rdcu.be/c5Obw>

Elementary methods to build GNEOs

Proposition (Composition)

If $F_1 \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. $T_1 : G \rightarrow H$ and $F_2 \in \text{GENEO}((\Psi, H), (\chi, K))$ w.r.t. $T_2 : H \rightarrow K$ then $F_2 \circ F_1 \in \text{GENEO}((\Phi, G), (\chi, K))$ w.r.t. $T_2 \circ T_1 : G \rightarrow K$.

Proposition (Image by a 1-Lipschitz function)

If $F_1, \dots, F_n \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. $T : G \rightarrow H$, L is a 1-Lipschitz map from \mathbb{R}^n to \mathbb{R} , and $L^(F_1, \dots, F_n)(\Phi) \subseteq \Psi$ (where L^* is the map induced by L), then $L^*(F_1, \dots, F_n) \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. T .*

The next three statements follow from the last proposition.

Elementary methods to build GNEOs

Proposition (LATTICE OF GNEOS)

If $F_1, \dots, F_n \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. $T : G \rightarrow H$ and $\max(F_1, \dots, F_n)(\Phi), \min(F_1, \dots, F_n)(\Phi) \subseteq \Psi$, then $\max(F_1, \dots, F_n), \min(F_1, \dots, F_n) \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. T .

Proposition (Translation)

If $F \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. $T : G \rightarrow H$, and $F_b(\Phi) \subseteq \Psi$ for $F_b(\varphi) := F(\varphi) - b$, then $F_b \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. T .

Proposition (Convex combination)

If $F_1, \dots, F_n \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. $T : G \rightarrow H$, $(a_1, \dots, a_n) \in \mathbb{R}^n$ con $\sum_{i=1}^n |a_i| \leq 1$ and $F_\Sigma(\Phi) \subseteq \Psi$ for $F_\Sigma(\varphi) := \sum_{i=1}^n a_i F_i(\varphi)$, then $F_\Sigma \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. T .

Permutant measures

Let us consider the set $\Phi = \mathbb{R}^X \cong \mathbb{R}^n$ of all functions from a finite set $X = \{x_1, \dots, x_n\}$ to \mathbb{R} , and a subgroup G of the group $\text{Bij}(X)$ of all permutations of X .

Definition

A finite (signed) measure μ on $\text{Bij}(X)$ is called a *permutant measure* with respect to G if every subset H of $\text{Bij}(X)$ is measurable and μ is invariant under the conjugation action of G (i.e., $\mu(H) = \mu(gHg^{-1})$ for every $g \in G$).

Representation Theorem for linear GNEOs

Theorem (Representation Theorem for linear GNEOs)

Let us assume that $G \subseteq \text{Bij}(X)$ transitively acts on the finite set X and that F is a map from \mathbb{R}^X to \mathbb{R}^X . The map F is a linear GNEO from \mathbb{R}^X to \mathbb{R}^X with respect to the identical homomorphism $\text{id}_G: g \mapsto g$ **if and only if** a permutant measure μ with respect to G exists, such that $F(\varphi) = \sum_{h \in \text{Bij}(X)} \varphi h^{-1} \mu(h)$ for every $\varphi \in \mathbb{R}^X$, and $\sum_{h \in \text{Bij}(X)} |\mu(h)| \leq 1$.

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The use of GENEOS in applications

WE WILL NOW SHOW
HOW GENEOS CAN BE USED
IN APPLICATIONS

A real application: finding pockets in proteins

GENEOnet: A new machine learning paradigm based on Group Equivariant Non-Expansive Operators. An application to protein pocket detection.

Giovanni Bocchi¹, **Patrizio Frosini**², **Alessandra Micheletti**¹, **Alessandro Pedretti**³
Carmen Gratteri⁴, **Filippo Lunghini**⁵, **Andrea Rosario Beccari**⁵ and **Carmine Talarico**⁵

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² Department of Mathematics, Università degli Studi di Bologna

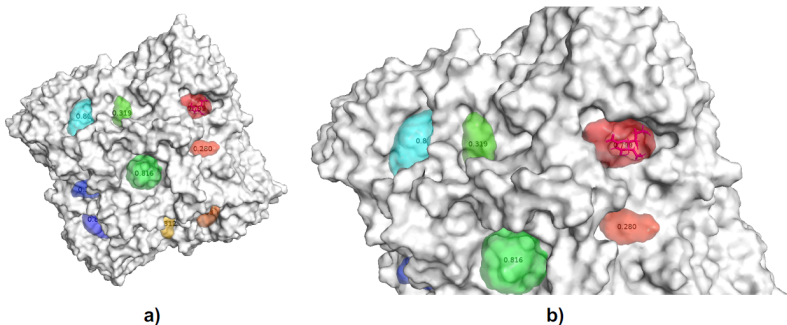
³ Department of Pharmaceutical Sciences, Università degli Studi di Milano

⁴ Dipartimento di Scienze della Salute, Università degli Studi "Magna Græcia di Catanzaro"

⁵ Dompé Farmaceutici SpA

<https://arxiv.org/ftp/arxiv/papers/2202/2202.00451.pdf>

A real application: finding pockets in proteins

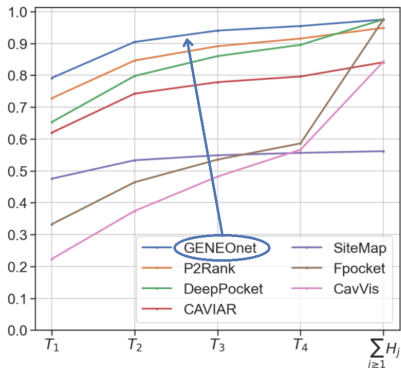


Model predictions for protein 2QWE. In Figure a) the global view of the prediction is shown, where different pockets are depicted in different colors and are labelled with their scores. In Figure b) the zoomed of the pocket containing the ligand is shown.

The search for the pockets was carried out by identifying an optimal GENE0 in the convex hull of 8 GENE0s (each focused on a particular property of the pockets).

A real application: finding pockets in proteins

Here are the results of our experiments:

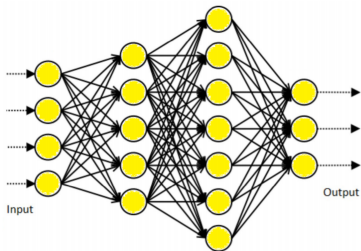


Please note that GENEOnet uses 17 parameters, while a CNN such as DeepPocket requires 665122 parameters.

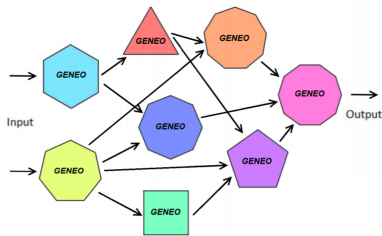
The main point in our approach

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.



NEURAL NETWORK



NETWORK OF GENEOS

GENEOs and Machine Learning

For more details about the use of GENEOS in Machine Learning:



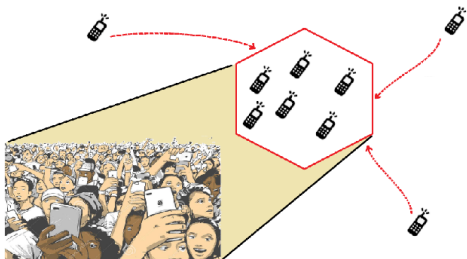
The screenshot shows the EMS Magazine website interface. At the top left is the logo for the European Mathematical Society (EMS). To the right of the logo is the text 'EUROPEAN MATHEMATICAL SOCIETY'. Further right is a 'Login' button. Below the logo and text is a navigation menu with items: News, Magazine, Membership, Services, Activities, and Society Overview. The main content area features a blue background with a white box on the left containing a thumbnail of the magazine cover. The cover has the title 'EMS Magazine' and a large blue abstract graphic. To the right of the thumbnail, the text reads: 'MAG > ONLINE FIRST > 24 APRIL 2023', followed by the article title 'A new paradigm for artificial intelligence based on group equivariant non-expansive operators' in large white font, and the author's name 'Alessandra Micheletti' and affiliation 'Università degli Studi di Milano, Italy' below it.

- A. Micheletti, *A new paradigm for artificial intelligence based on group equivariant non-expansive operators*, In: *EMS Magazine*, Online First, 24 April 2023.
- <https://ems.press/content/serial-article-files/27673>

A current research project

CNIT / WiLab - Huawei Joint Innovation Center (JIC)

Project on GENEOS for 6G



THANKS
FOR YOUR
ATTENTION

