Some recent results in the geometric-topological theory of group equivariant non-expansive operators

Patrizio Frosini

Department of Mathematics, ALMA-AI, AM^2 and ARCES, University of Bologna
patrizio.frosini@unibo.it

Methods and Applications of Artificial Intelligence and Machine Learning In Heterogeneous Brains, September 4-6, 2021

Outline

Data analysis is not just about data

Topological and metric basics for the theory of GENEOs

Compactness and convexity of the space of GENEOs

Methods to build GENEOs

GENEOs in the probabilistic setting

Data analysis is not just about data

Data interpretation depends on the observer:

Observers are often more important than data

We are usually not directly interested in data, but in data observers. For example, a patient is usually interested not in the data representing a computerized axial tomography of her body, but in the diagnosis that her doctor can make from these data.

Data analysis strongly depends on the chosen observer. If data analysis were not dependant on the chosen observer, then physicians' diagnoses would always be identical, scientists would always see the same causes for each phenomenon, and all people would agree in judging who the heroes and villains in a movie or a political event are.

It is indeed well known that different agents can have different reactions in the presence of the same data, and this suggests that **data analysis should study the pairs (data, observer) instead of data alone**.

What are data?

Data are usually produced by measurements (or actions) made by observers. Before proceeding, we have to determine what measurements are in our mathematical model.

Measurement is the assignment of a number to a characteristic of an object or event, which can be compared with other objects or events.

WIKIPEDIA

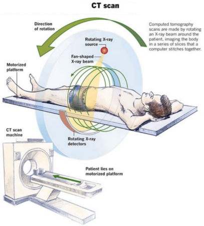
According to this definition, measurements (and hence data) can be often seen as functions φ associating a real number $\varphi(x)$ with each point x of a set X of characteristics. (This definition admits a natural extension to vector-valued functions but, for the sake of simplicity, we will treat here the case of scalar-valued functions).

Data are measurements made by observers

Some examples of data that can be seen as measurements (i.e., functions):

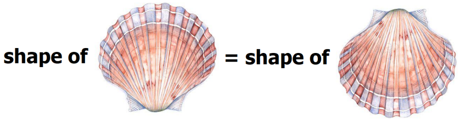
- An electrocardiogram (a function from $\mathbb{R}$ to $\mathbb{R}$);
- A gray-level image (a function from $\mathbb{R}^2$ to $\mathbb{R}$);
- A computerized tomography (CT) scan (a function from a helix to $\mathbb{R}$).



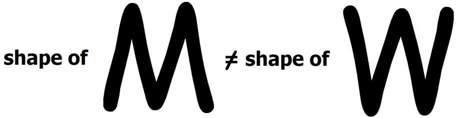


Observers are often associated with invariance groups

Observers often think that some data are equivalent to each other, according to an invariance group.



The group G is not established once and forever: when the observer changes, G changes too.



Data equivalence w.r.t. a group of permutations

Our data are represented by real-valued functions.

What do the expressions "data equivalence" and "data similarity" mean in our setting?

Two functions $\varphi_1, \varphi_2 : X \to \mathbb{R}$ *are* **equivalent** *with respect to a group* G *of permutations on* X *if a* $g \in G$ *exists, such that* $\varphi_1 = \varphi_2 \circ g$*.*

Two functions $\varphi_1, \varphi_2 : X \to \mathbb{R}$ *are* **similar** *with respect to a group* G *of permutations on* X *if a* $g \in G$ *exists, such that* $\|\varphi_1 - \varphi_2 \circ g\|_\infty$ *is small.*

Our general assumptions about data and observers

Our mathematical model is based on these assumptions:

- The space of observers is often more important than the space of data;
- The study of the space of observers requires the development of a new topological-geometric model.
- This new model could be of great use in data analysis, when the role of the observers is not negligible.

These assumptions suggest us to move from **Topological Data Analysis** to the new field of **Topological Observer Analysis**.

Observers can be seen as equivariant operators

Observers are structures able to change data into other data, and usually do that by respecting some data equivalences, i.e., by commuting with some transformations.

As a first approximation, observers can be represented as group equivariant operators (GEOs).

Many researchers are presently studying the use of group equivariant operators in deep learning (Yoshua Bengio, Tomaso Poggio, Max Welling, Stéphane Mallat...).

In this talk we will give some results on the theory of Group Equivariant Non-Expansive Operators (**GENEOs**).
(Why "non-expansive?" Because observers are often assumed to simplify the metric structure of data in order to produce meaningful interpretations.)

Measurements as 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

$$D_\Phi(\varphi_1, \varphi_2) := \|\varphi_1 - \varphi_2\|_\infty . \qquad (0.1)$$

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**. For example, a gray-level image can be represented as a function from the real plane to the interval $[0,1]$ (in this case $X = \mathbb{R}^2$).

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

$$D_X(x_1, x_2) = \sup_{\varphi \in \Phi} |\varphi(x_1) - \varphi(x_2)|. \quad (0.2)$$

D_X induces a topology τ_{D_X} on X.

Theorem

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}.

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

Theorem

If Φ is compact and X is complete, then X is compact w.r.t. D_X.

Each bijection is an isometry

Let $\mathrm{Bij}(X)$ be the set of all bijections from X to X, and denote by $\mathrm{Bij}_{\Phi}(X)$ the set of all $g \in \mathrm{Bij}(X)$ such that $\varphi \circ g \in \Phi$ and $\varphi \circ g^{-1} \in \Phi$ for every $\varphi \in \Phi$. Let $\mathrm{Homeo}(X)$ be the set of all homeomorphisms from X a X with respect to D_X, and denote by $\mathrm{Homeo}_{\Phi}(X)$ the set of all $g \in \mathrm{Homeo}(X)$ such that $\varphi \circ g \in \Phi$ and $\varphi \circ g^{-1} \in \Phi$ for every $\varphi \in \Phi$. Let $\mathrm{Iso}(X)$ be the set of all isometries from X a X, and denote by $\mathrm{Iso}_{\Phi}(X)$ the set of all $g \in \mathrm{Iso}(X)$ such that $\varphi \circ g \in \Phi$ and $\varphi \circ g^{-1} \in \Phi$ for every $\varphi \in \Phi$.

Proposition

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

Remark

The condition of preserving Φ is quite restrictive for permutations.

A pseudo-metric on G

Let us now focus our attention on a subgroup G of $\mathrm{Homeo}_\Phi(X)$.
We can define a pseudo-metric D_G on G by setting

$$D_G(g_1, g_2) := \sup_{\varphi \in \Phi} D_\Phi(\varphi \circ g_1, \varphi \circ g_2). \tag{0.3}$$

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 it is also compact with respect to D_G.

GEOs and GENEOs

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

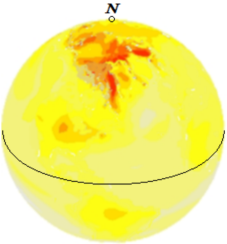
Let us now assume that two perception pairs (Φ, G), (Ψ, H) are given, and fix a group homomorphism $T : G \to H$.

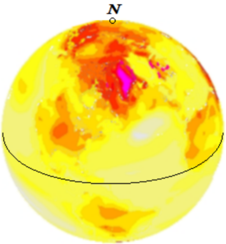
Each function $F : \Phi \to \Psi$ such that $\boxed{F(\varphi \circ g) = F(\varphi) \circ T(g)}$ for every $\varphi \in \Phi, g \in G$ is called a *Group Equivariant Operator (GEO)* associated with the homomorphism T.

If F is also non-expansive (i.e., $\boxed{D_{\Psi}(F(\varphi_1), F(\varphi_2)) \leq D_{\Phi}(\varphi_1, \varphi_2)}$ 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 GENEO

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 GENEO

In this case we can set

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

We can also consider the "equator" of our sphere, represented as the space S^1, and set

- $Y =$ 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

In this way we have defined two perception pairs (Φ, G) to (Ψ, H).

An example of GENEO

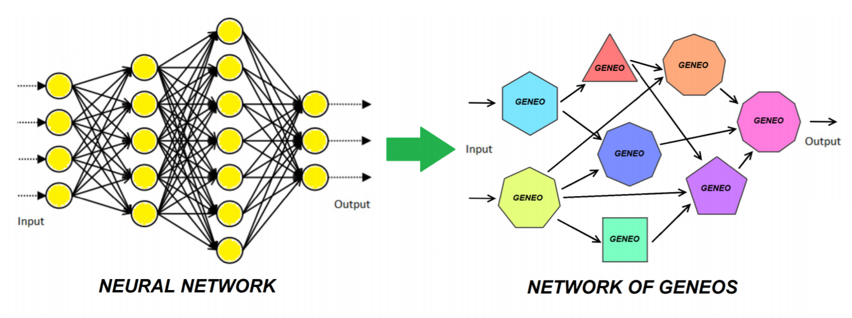
This is a simple example of GENEO from (Φ, G) to (Ψ, H):

- $T(g)$ 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 $T : G \to H$.

Our goal

In perspective, we would like to obtain 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.



More details are available here

More details are available in this paper:

nature 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

Mattia G. Bergomi[1], Patrizio Frosini[2,3*], Daniela Giorgi[4] and Nicola Quercioli[2,3]

The paper is available at the link *https://rdcu.be/bP6HV*.

Two key results

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

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

Theorem

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

Theorem

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

Elementary methods to build GENEOs

Proposition (Composition)

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

Proposition (Image by a 1-Lipschitz function)

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

The next three statements follow from the last proposition.

Elementary methods to build GENEOs

Proposition (Maximization)

If $F_1, \ldots, F_n \in \mathrm{GENEO}((\Phi, G), (\Psi, H))$ *w.r.t.* $T : G \to H$ *e* $\max(F_1, \ldots, F_n)(\Phi) \subseteq \Phi$*, allora* $\max(F_1, \ldots, F_n) \in \mathrm{GENEO}((\Phi, G), (\Psi, H))$ *w.r.t.* T.

Proposition (Translation)

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

Proposition (Convex combination)

If $F_1, \ldots, F_n \in \mathrm{GENEO}((\Phi, G), (\Psi, H))$ *w.r.t.* $T : G \to H$, $(a_1, \ldots, a_n) \in \mathbb{R}^n$ *con* $\sum_{i=1}^n |a_i| \leq 1$ *and* $F_\Sigma(\Phi) \subseteq \Phi$ *for* $F_\Sigma(\varphi) := \sum_{i=1}^n a_i F_i(\varphi)$*, then* $F_\Sigma \in \mathrm{GENEO}((\Phi, G), (\Psi, H))$ *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 $X = \{x_1, \ldots, x_n\}$ to $\mathbb{R}$, and a subgroup G of the group $\mathrm{Bij}(X)$ of all permutations of X.

Definition

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

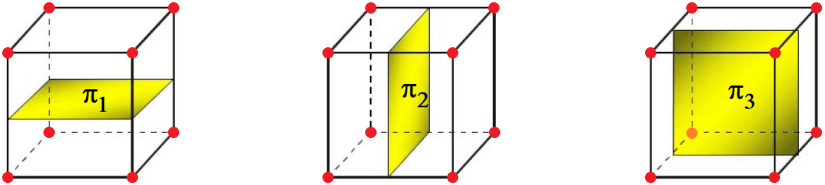
Proposition

If μ is a permutant measure with respect to G, then the map $F_\mu : \mathbb{R}^X \to \mathbb{R}^X$ defined by setting $F_\mu(\varphi) := \sum_{h \in \mathrm{Bij}(X)} \varphi \circ h^{-1}\ \mu(h)$ is a linear GEO.

An example of permutant measure

Let us consider the set X of the vertices of a cube in $\mathbb{R}^3$, and the group G of the orientation-preserving isometries of $\mathbb{R}^3$ that take X to X. Let π_1, π_2, π_3 be the three planes that contain the center of mass of X and are parallel to a face of the cube. Let $h_i : X \to X$ be the orthogonal symmetry with respect to π_i, for $i \in \{1,2,3\}$.

We can now define a permutant measure μ on the group $\mathrm{Bij}(X)$ by setting $\mu(h_1) = \mu(h_2) = \mu(h_3) = c$, where c is a positive real number, and $\mu(h) = 0$ for any $h \in \mathrm{Bij}(X)$ with $h \notin \{h_1, h_2, h_3\}$.



Building GENEOs by permutant measures

The following representation theorem holds.

Theorem

Let us assume that $G \subseteq \mathrm{Bij}(X)$ 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 GENEO from $(\mathbb{R}^X, G)$ to $(\mathbb{R}^X, G)$ (with respect to the identical homomorphism $\mathrm{id}_G : g \mapsto g$) if and only if a permutant measure μ with respect to G exists, such that $F(\varphi) = \sum_{h \in \mathrm{Bij}(X)} \varphi \circ h^{-1} \ \mu(h)$ for every $\varphi \in \mathbb{R}^X$, and $\sum_{h \in \mathrm{Bij}(X)} |\mu(h)| \leq 1$.

Further details can be found in this preprint:

S. Botteghi, M. Brasini, P. Frosini and N. Quercioli, On the finite representation of group equivariant operators via permutant measures **https://arxiv.org/pdf/2008.06340.pdf**

GENEOs in the probabilistic setting

When the space of data Φ is endowed with a probability measure, we can replace the pseudo-metrics D_X, D_G with the following two pseudo-metrics Δ_X, Δ_G, after choosing a G-invariant probability density f and a G-invariant probability measure λ on Φ:

$$\Delta_X(x_1,x_2) = \int_\Phi |\varphi(x_1) - \varphi(x_2)| f(\varphi)\, d\lambda, \quad \forall x_1,x_2 \in X;$$

$$\Delta_G(g_1,g_2) = \int_\Phi \|\varphi g_1 - \varphi g_2\| f(\varphi)\, d\lambda, \quad \forall g_1,g_2 \in G.$$

We will assume that Φ is compact.

GENEOs in the probabilistic setting

The following statements hold:

Proposition

Every function $\varphi \in \Phi$ is continuous with respect to Δ_X.

Proposition

X is totally bounded with respect to Δ_X.

Hence

Corollary

If X is complete, then X is compact with respect to Δ_X.

GENEOs in the probabilistic setting

Proposition

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

Proposition

G is totally bounded with respect to Δ_G.

Hence

Corollary

If G is complete, then it is also compact with respect to Δ_G.

GENEOs in the probabilistic setting

The concepts of GEO and GENEO can be adapted to the probabilistic setting and the following results can be proved:

Theorem

If the spaces of data are compact, then the space of all GENEOs is compact with respect to the norm $\|F\|_{L^2} := \left(\int_\Phi \|F(\varphi)\|^2 f(\varphi)\ d\lambda\right)^{\frac{1}{2}}$.

Proposition

If the spaces of data are convex, then also the set of all GENEOs is convex.

A Riemannian structure for manifolds of GENEOs

Important remark. $L^2(\Phi, V)$ is endowed with the inner product $\langle F_1, F_2 \rangle := \int_\Phi \langle F_1(\varphi), F_2(\varphi) \rangle f(\varphi)\, d\lambda$. Therefore, any C^k-submanifold of GENEOs in $L^2(\Phi, V)$ naturally inherits a Riemannian structure from $L^2(\Phi, V)$ (I am skipping some technical details here).

As a consequence, we can use the gradient flow of cost functions to look for optimal GENEOs in manifolds of GENEOs.

Further details can be found in this preprint:

P. Cascarano, P. Frosini, N. Quercioli and A. Saki, *On the geometric and Riemannian structure of the spaces of group equivariant non-expansive operators*, **https://arxiv.org/pdf/2103.02543.pdf**

Conclusions

The development of a compositional theory of GENEOs could make available a new kind of knowledge engineering for neural networks, based on using a relative small set of families of GENEOs.

Each family should be endowed with some kind of equivariance and focused on a particular activity on data. These GENEOs could replace the role of neurons and reduce the number of parameters we have to manage.

This approach would make available a method to decompose a network into elementary agents, endowed with an interpretable behaviour.

Open questions

- How can we approximate a real observer (let us say, e.g., a physician) by GENEOs, in order to emulate her behaviour with respect to data?
- Can we devise constructive procedures, allowing us to build any possible GENEO with respect to a given equivariance group?
- What is the right way of comparing GENEOs in a topological-statistical setting?
- How should we select representative sets in a probability space of GENEOs?
- How can we compute the basic statistics for GENEOs?
- How can we predict the behaviour of networks of GENEOs and control their actions?

Collaborators

Many results illustrated in this talk have been obtained in joint research conducted together with several collaborators and students: Faraz Ahmad, Mattia Bergomi, Silvia Biasotti, Stefano Botteghi, Martina Brasini, Francesco Camporesi, Pasquale Cascarano, Andrea Cerri, Barbara Di Fabio, Pietro Donatini, Bianca Falcidieno, Massimo Ferri, Leila De Floriani, Daniela Giorgi, Grzegorz Jabłoński, Claudia Landi, Laura Papaleo, Nicola Quercioli, Amir Saki, Michela Spagnuolo.

MAIN REFERENCES

- P. Frosini, G. Jabłoński, *Combining persistent homology and invariance groups for shape comparison*, **Discrete & Computational Geometry**, vol. 55 (2016), n. 2, 373-409.
- P. Frosini, *Towards an observer-oriented theory of shape comparison: Position paper*, **Proceedings of the Eurographics 2016 Workshop on 3D Object Retrieval**, Eurographics Association, 5–8 (2016).
- M. G. Bergomi, P. Frosini, D. Giorgi, N. Quercioli, *Towards a topological-geometrical theory of group equivariant non-expansive operators for data analysis and machine learning*, **Nature Machine Intelligence**, vol. 1, n. 9, 423–433 (2 September 2019).

THANKS FOR YOUR ATTENTION