The use of group equivariant non-expansive operators in topological data analysis

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Building new GENEOSs
What does DATA COMPARISON mean?

The comparison of DATA is always a process depending on an observer. We could say that data comparison consists in the study of the relationship between an observer and the reality he/she can MEASURE. In this setting data coincide with measurements.

Observers receive and transform data. In some sense, they are defined by the way they perform this transformation.

In our approach observers are defined as a collection of suitable operators acting on measurements.
What does MEASUREMENT mean?

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. According to this definition, measurements (and hence data) can be seen as functions $\varphi$ 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). If we wish to develop a theory that can be applied in real situations, we need stability with respect to noise. This naturally leads us to use a topology on the set $\Phi$ of possible measurements on $X$. 
A topology on the space $X$ of characteristics

A natural topology on the set $\Phi$ of possible measurements is the one induced by the $L^\infty$ metric $D_\Phi(\phi_1, \phi_2) := \|\phi_1 - \phi_2\|_\infty$.

Since measurements are the central concept in our approach, the topology on $X$ is derived from $D_\Phi$.

We define this pseudometric $D_X$ on $X$ by setting

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

In plain words: Two points $x_1, x_2 \in X$ are close to each other if and only if every measurement in $\Phi$ takes similar values at those points.
Every function in $\Phi$ is continuous

In this talk we will assume that the topological space $\Phi$ is compact.

**EXAMPLE 1.** $X := S^1 = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 = 1\}$, $\Phi = \text{set of all } 1\text{-Lipschitzian functions from } S^1 \text{ to } [0,1]$.

**EXAMPLE 2.** $X := [-1,1] \times [-1,1]$, $\Phi = \text{set of all functions from } X \text{ to } [0,1] \text{ that are } 1\text{-Lipschitzian both in } X_1 := [-1,0] \times [-1,1] \text{ and in } X_2 := (0,1] \times [-1,1]$. Please observe that the functions in $\Phi$ can be discontinuous at the points $(x, y)$ with $x = 0$, with respect to the Euclidean topology on $X$. However, every function in $\Phi$ is continuous with respect to the topology induced by $D_X$.

**Theorem**

*If $\Phi$ is compact, then the topology induced by $D_X$ coincides with the initial topology on $X$, i.e. the coarsest topology on $X$ such that each function $\varphi \in \Phi$ is continuous.*
Homeomorphisms with respect to $D_X$

The next step consists in understanding what a $\Phi$-preserving homeomorphism with respect to $D_X$ is (a bijection $g : X \rightarrow X$ is called $\Phi$-preserving if $\varphi \circ g \in \Phi$ for every $\varphi \in \Phi$).

**Theorem**

*The $\Phi$-preserving homeomorphisms with respect to $D_X$ are exactly the $\Phi$-preserving bijections from $X$ to $X$.***

Let us now consider a group $G$ of homeomorphisms from $X$ to $X$, whose elements preserves $\Phi$ by right composition. We will say that $(\Phi, G)$ is a PERCEPTION PAIR.
A pseudo-metric on our $\Phi$-preserving group $G$

If a perception pair $(\Phi, G)$ is given, we can define the function

$$D_G(g_1, g_2) = \sup_{\varphi \in \Phi} D_\Phi(\varphi \circ g_1, \varphi \circ g_2) \quad (0.1)$$

from $G \times G$ to $\mathbb{R}$.

The function $D_G$ is a pseudo-metric on $G$.

Please note that also the definition of $D_G$ is inherited from the definition of $D_\Phi$.

**Theorem**

$G$ is a topological group with respect to the pseudo-metric topology and the action of $G$ on $\Phi$ through right composition is continuous.
Compactness of $X$ and $G$

We recall that we are assuming $\Phi$ compact.

**Theorem**

*If $X$ is complete then it is also compact with respect to $D_X$.***

**Theorem**

*If $G$ is complete then it is also compact with respect to $D_G$.***

In this talk we will assume that $X$ and $G$ are complete, and hence compact.
A mathematical framework for data comparison

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The link between the natural pseudo-distance and persistent homology via GENEOs

Building new GENEOs
Our ground truth: the natural pseudo-distance $d_G$

**Definition**

The pseudo-distance $d_G : \Phi \times \Phi \to \mathbb{R}$ is defined by setting

$$d_G(\varphi_1, \varphi_2) = \inf_{g \in G} D_\Phi(\varphi_1, \varphi_2 \circ g).$$

It is called the *natural pseudo-distance* associated with the group $G$.

If $G = \{Id : x \mapsto x\}$, then $d_G$ equals the sup-norm distance $D_\Phi$ on $\Phi$. If $G_1$ and $G_2$ are groups of $\Phi$-preserving self-homeomorphisms of $X$ and $G_1 \subseteq G_2$, then the definition of $d_G$ implies that

$$d_{G_2}(\varphi_1, \varphi_2) \leq d_{G_1}(\varphi_1, \varphi_2) \leq D_\Phi(\varphi_1, \varphi_2)$$

for every $\varphi_1, \varphi_2 \in \Phi$. 

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A mathematical framework for data comparison

The natural pseudo-distance $d_G$

**Group equivariant non-expansive operators**

The link between the natural pseudo-distance and persistent homology via GENEOS

Building new GENEOS
The natural pseudo-distance $d_G$ represents our ground truth.

Unfortunately, $d_G$ is difficult to compute. This is also a consequence of the fact that we can easily find subgroups $G$ of $\text{Homeo}(X)$ that cannot be approximated with arbitrary precision by smaller finite subgroups of $G$ (i.e. $G = \text{group of rigid motions of } X = \mathbb{R}^3$).

Nevertheless, in this talk we will show that $d_G$ can be approximated with arbitrary precision by means of a DUAL approach based on persistent homology and group equivariant non-expansive operators (GENEOs).
The space of GENEOs

Definition

Assume that \((\Phi, G), (\Psi, H)\) are two perception pairs and that a homomorphism \(T : G \rightarrow H\) has been fixed. A Group Equivariant Non-Expansive Operator (GENEO) from \((\Phi, G)\) to \((\Psi, H)\) is a map \(F : \Phi \rightarrow \Psi\) such that the following properties hold for every \(\varphi_1, \varphi_2 \in \Phi\):

1. \(F(\varphi \circ g) = F(\varphi) \circ T(g)\) for every \(g \in G\);
2. \(D_{\Psi}(F(\varphi_1), F(\varphi_2)) \leq D_{\Phi}(\varphi_1, \varphi_2)\).

We will use the symbol \(\mathcal{F}^{\text{all}}\) to denote the set of all GENEOs from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\).
An example of GENEO

We give an example of the use of the definition of GENEO between two different perception pairs \((\Phi, G), (\Psi, H)\).

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 imagine that only two opposite points \(N, S\) can be localized on the sphere.
An example of GENEQO

In this case we can set

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

We can also consider the “equator” of our sphere, represented as the space $S^1$.

Therefore, we can also set

- $Y = \text{the equator } S^1 \text{ of } S^2$
- $\Psi = \text{set of } 1\text{-Lischitzian functions from } S^1 \text{ to } [a, b]$
- $H = \text{group of rotations of } S^1$
An example of GENEQ

In this case we can build a simple example of GENEQ from \((\Phi, G)\) to \((\Psi, H)\) by setting

- \(T(g)\) equal to the rotation \(h \in H\) of the equator \(S^1\) that is induced by the rotation \(g\) of \(S^2\), for every \(g \in G\).
- \(F(\varphi)\) equal to the function \(\psi\) 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 homomorphism \(T : G \to H\).
Another example of GENEO

Let us consider a set $\Phi$ of grey level images represented as 1-Lipschitzian compact supported functions from $X = \mathbb{R}^2$ to a suitable interval $[a, b]$. We set $G = \text{group of isometries of } \mathbb{R}^2$. We can build a simple example of GENEO from $(\Phi, G)$ to $(\Phi, G)$ with respect to $id: G \to G$ by taking a compact supported integrable function $f: \mathbb{R}^2 \to \mathbb{R}$ that is invariant with respect to every rotation around the point $(0, 0)$, and defining $F(\varphi)$ as the convolution of $\varphi$ with $f$. If we also assume that $\int_{\mathbb{R}^2} f(x, y) \, dx \, dy = 1$, we can easily check that $F$ verifies the properties defining the concept of group equivariant non-expansive operator with respect to the homomorphism $id: G \to G$. 
Another example of GENEO
Another example of GENEo
Another example of GENEO
Two pseudo-metrics for the space $\mathcal{F}^{\text{all}}$

The following two pseudo-metrics can be of use:

**Definition**

If $F_1, F_2 \in \mathcal{F}^{\text{all}}$, we set

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

$$D_{\text{GENEO},H}(F_1, F_2) := \sup_{\varphi \in \Phi} d_H(F_1(\varphi), F_2(\varphi)). \quad (0.2)$$

**Proposition**

$D_{\text{GENEO}}$ and $D_{\text{GENEO},H}$ are pseudo-metrics on $\mathcal{F}^{\text{all}}$. Moreover,

$D_{\text{GENEO},H} \leq D_{\text{GENEO}}$. 

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Some good news

Let \( \mathcal{F}^{\text{all}} \) be the set of all GENEOs from \((\Phi, G)\) to \((\Psi, H)\) with respect to a fixed homomorphism \( T : G \to H \).

**Theorem**

\( \mathcal{F}^{\text{all}} \) is **compact** with respect to both \( D_{\text{GENEO}} \) and \( D_{\text{GENEO,H}} \).

**Corollary**

\( \mathcal{F}^{\text{all}} \) can be \( \epsilon \)-approximated by a finite subset for every \( \epsilon > 0 \).

**Theorem**

If \( \Psi \) is convex, then \( \mathcal{F}^{\text{all}} \) is convex.
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The link between the natural pseudo-distance and persistent homology via GENEOs

We recall that, with reference to the sublevel sets $X_t$ of a function $\varphi : X \to \mathbb{R}$, the persistence diagram in degree $k$ of $\varphi$ is the multiset of the pairs $(b_i, d_i)$ where $b_i$ and $d_i$ are the times of birth and death of the $i$-th hole of dimension $k$, and of the pairs $(u, u)$ endowed with infinite multiplicity.
The link between the natural pseudo-distance and persistent homology via GENEOSs

Persistent homology enters our theoretical framework by means of an equality allowing us to approximate the natural pseudo-distance:

**Theorem**

If \((\Phi, G) = (\Psi, H)\), then

\[ d_G(\varphi_1, \varphi_2) = \sup_{F \in \mathcal{F}} d_{\text{match}}(\text{Dgm}_0(F(\varphi_1)), \text{Dgm}_0(F(\varphi_2))) \]

where \(\text{Dgm}_0(F(\varphi))\) is the persistence diagram in degree 0 of the function \(F(\varphi)\) and \(d_{\text{match}}\) is the usual bottleneck distance.

The pseudo-metric $D_{\text{match}}$

Let us take a finite $\varepsilon$-approximation $\mathcal{F}$ of $\mathcal{F}^{\text{all}}$ and assume that the homology of $X$ is not trivial in degree $k$. We can then define the pseudo-metric

$$D_{\text{match}}(\varphi_1, \varphi_2) := \sup_{F \in \mathcal{F}} d_{\text{match}}(\text{Dgm}_k(F(\varphi_1)), \text{Dgm}_k(F(\varphi_2))).$$

The following properties hold for every $\varphi_1, \varphi_2 \in \Phi$ and every $g \in G$:

- $D_{\text{match}}(\varphi_1, \varphi_2 \circ g) = D_{\text{match}}(\varphi_1, \varphi_2)$;
- $D_{\text{match}}(\varphi_1, \varphi_2) \leq d_G(\varphi_1, \varphi_2) \leq \|\varphi_1 - \varphi_2\|_\infty$;
- $|d_G(\varphi_1, \varphi_2) - D_{\text{match}}(\varphi_1, \varphi_2)| \leq 2\varepsilon$. 
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Building new GENEOS
Building new GENEOS

Our approach to group equivariant Topological Data Analysis is based on the availability of GENEOS.

How could we build new GENEOS from other GENEOS?

A simple method consists in composing GENEOS:

**Proposition**

*If $F_1$ is a GENEO from $(\Phi_1, G_1)$ to $(\Phi_2, G_2)$ with respect to $T_1 : G_1 \to G_2$ and $F_2$ is a GENEO from $(\Phi_2, G_2)$ to $(\Phi_3, G_3)$, then $F_2 \circ F_1$ is a GENEO from $(\Phi_1, G_1)$ to $(\Phi_3, G_3)$ with respect to $T_2 \circ T_1 : G_1 \to G_3$.***
Building GENEOs via 1-Lipschitzian functions

We can also produce new GENEOs by means of a 1-Lipschitzian function applied to other GENEOs:

**Proposition**

Assume that two perception pairs \((\Phi, G), (\Psi, H)\) and a homomorphism \(T : G \rightarrow H\) are given. Let \(\mathcal{L}\) be a 1-Lipschitzian map from \(\mathbb{R}^n\) to \(\mathbb{R}\), where \(\mathbb{R}^n\) is endowed with the norm
\[
\|(x_1, \ldots, x_n)\|_\infty := \max_{1 \leq i \leq n} |x_i|.
\]
Assume also that \(F_1, \ldots, F_n\) are GENEOs from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\). Let us define \(\mathcal{L}^*(F_1, \ldots, F_n)\) by setting
\[
\mathcal{L}^*(F_1, \ldots, F_n)(\varphi)(x) := \mathcal{L}(F_1(\varphi)(x), \ldots, F_n(\varphi)(x)).
\]
If \(\mathcal{L}^*(F_1, \ldots, F_n)(\Phi) \subseteq \Psi\), then \(\mathcal{L}^*(F_1, \ldots, F_n)\) is a GENEO from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\).

From this proposition the following three results follow.
Building new GENEOSs via translations, the maximum operator and weighted averages

Assume that two perception pairs \((\Phi, G), (\Psi, H)\) and a homomorphism \(T : G \to H\) are given.

**Proposition (Translation)**

Let \(F\) be a GENEO from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\). The operator \(F_b(\phi) := \phi - b\) is a GENEO from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\), for every \(b \in \mathbb{R}\) such that \(F_b(\Phi) \subseteq \Psi\).

**Proposition (Maximum)**

If \(F_1, \ldots, F_n\) are GENEOSs from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\), then the operator \(F(\phi) := \max_i F_i(\phi)\) is a GENEO from \((\Phi, G)\) to \((\Psi, H)\) with respect to \(T\), provided that \(F(\Phi) \subseteq \Psi\).
Building new GENEOs via translations, weighted averages and the maximum operator

**Proposition (Weighted average)**

If \( F_1, \ldots, F_n \) are GENEOs from \((\Phi, G)\) to \((\Psi, H)\) with respect to \( T \) and \((a_1, \ldots, a_n) \in \mathbb{R}^n \) with \( \sum_{i=1}^{n} |a_i| \leq 1 \), then the operator \( F(\varphi) := \sum_{i=1}^{n} a_i F_i(\varphi) \) is a GENEO from \((\Phi, G)\) to \((\Psi, H)\) with respect to \( T \), provided that \( F(\Phi) \subseteq \Psi \).

Therefore, if we work with spaces \( \Phi, \Psi \) of measurements that are compact and convex, then the topological space of all GENEOs from \((\Phi, G)\) to \((\Psi, H)\) with respect to \( T \) is compact and convex.

For further information on building GENEOs: Nicola Quercioli, *Some new methods to build group equivariant non-expansive operators in TDA*, Session CPS01, 6 Dec, 17:20, Seminar Hall 2
An interesting GENEOS in kD persistent homology

Previous propositions imply the following statement.

**Proposition**

Assume $F_1, \ldots, F_n$ are GENEOS from $(\Phi, G)$ to $(\Psi, H)$ with respect to $T$, and that $(a_1, \ldots, a_n), (b_1, \ldots, b_n) \in \mathbb{R}^n$, with $a_1, \ldots, a_n > 0$, $\sum_{i=1}^n a_i = 1$ and $\sum_{i=1}^n b_i = 0$. Then the operator

$$F(\varphi) := \max \left\{ \frac{\min_j a_j}{a_1} \cdot (F_1(\varphi) - b_1), \ldots, \frac{\min_j a_j}{a_n} \cdot (F_n(\varphi) - b_n) \right\}$$

is a GENEO from $(\Phi, G)$ to $(\Psi, H)$ with respect to $T$, provided that $F(\Phi) \subseteq \Psi$.

This result can be easily generalized from the case $\Phi \subseteq C^0(X, \mathbb{R})$ to the case $\Phi \subseteq C^0(X, \mathbb{R}^m)$. 
An interesting GENE0 in kD persistent homology

Let us now take $G = H$, $T = id$ and $n = m$ in the extended version of the previous proposition. By considering the projection operators $F_i(\varphi) := \varphi_i$ for every $\varphi = (\varphi_1, \ldots, \varphi_n) \in \Phi \subseteq C^0(X, \mathbb{R}^n)$, we obtain the operator

$$F(\varphi) = \max \left\{ \frac{\min_j a_j}{a_1} \cdot (\varphi_1 - b_1), \ldots, \frac{\min_j a_j}{a_n} \cdot (\varphi_n - b_n) \right\}.$$

This operator is important in kD persistent homology, as a key tool to reduce kD persistent Betti number functions to families of 1D persistent Betti number functions. It is interesting to observe that such an operator is a group equivariant non-expansive operator.
Open questions

After defining an observer as a collection of GENEOS, our purpose consists in looking for methods to approximate the observer by a finite (and possible small) set of simple GENEOS. This leads us to the following open questions:

- How can we build a good library of GENEOS?
- How can we find a method to choose a finite set $\mathcal{F}^*$ of GENEOS that allows for both a good approximation of the natural pseudo-distance $d_G$ and a fast computation?
- How can we provide a suitable statistical theory for group equivariant non-expansive operators?

Further research is needed.
Our forward-looking goal: contributing to build a mathematical theory for GENEOS, in order to allow for their use in place of neurons in neural networks (extension of Hinton’s work on capsule networks).
Conclusions

- In our model, data comparison is based on measurements made by an observer. Each measurement can be represented as a function defined on a topological space $X$.
- The observer can be seen as a collection of GENEOs, applied to the measurements. The operators are allowed to change both the space of measurements and the invariance group.
- The functions describing the measurements can be compared by means of the natural pseudo-distance associated with a group $G$.
- Persistent homology can be used to approximate the natural pseudo-metric $d_G$. This can be done by means of a method that is based on GENEOs. This method is stable with respect to noise.
- The topological space of GENEOs deserves further research.
Thanks for your attention!