### An introduction to Simplicial-map Neural Networks

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March 29, 2023



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# **REXASI** PRO

Reliable & Explainable Swarm Intelligence for People with Reduced Mobility



#### Consortium

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USE   ES	+
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SUPSI   CH	+
SCUOLA DI ROBOTICA   IT	+

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# The Project

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#### **Project Idea**

REliable eXplAinable Swarm Intelligence for People with Reduced mObility

To design a novel framework in which safety, security, ethics, and explainability are entangled to develop a Trustworthy Artificial Swarm Intelligence solution.

The framework will make a trustworthy collaboration among a swarm formed by autonomous wheelchairs and flying robots to allow a seamless doorto-door experience for people with reduced mobility.

This goal will result in benefits for these people, their families, caregivers, scientific community, industry, and environment, creating a scientific, economic, technological and social factors.



#### **Project Details**

**Duration** 01/10/2022 – 30/09/2025

Type of Action RIA

Grant Amount € 3.551.158.50

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3 main use cases



Navigation incrowded environment

Al for Autonomous Wheelchair in different scenarios: 1)Safety Assistant; 2) Driving Assistant; 3) Route Assistant; 4) Social Navigation. To adopt this technology in real-life scenario, new trustable social navigation approaches are required.



#### Flying robot mapping

#### HOVERING SOLUTIONS

Flying robots capable of flying autonomously in an indoor/underground environment and generating a map of the building that would be latter used by the wheelchair. The flying robot will collaborate with an orchestrator to optimize time and energy

consumption.



#### Collaborative Navigation

CN R

Mixed collaborative indoor environment where the swarm communicate with each other in emergency cases. The swarm would include the wheelchairs, the flying robots, the orchestrator, and intelligent camera for people detection and crowd monitoring.



#### USE role and team

CIMAGROUP



#### Dataset size reduction

#### USE

Dataset optimization by removing redundant data but ensuring shape and the model performance.



## Critical Configuration detection

#### US

Detection critical configuration in the dynamical system of the navigation process by the used of Persistent homology and partial matchings between the Persistent barcodes.







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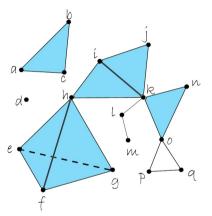


#### Universal approximation theorem

#### Theorem (Cybenko, 1989, Hornik, 1991)

Let A be any compact subset of  $\mathbb{R}^n$ . The space of real-valued continuous functions on A is denoted by C(A). Then, given any  $\varepsilon > 0$  and any continuous function  $g \in C(A)$ , there exists a one-hidden layer feedforward network  $\mathcal{N} : \mathbb{R}^n \to \mathbb{R}$  defined as  $\mathcal{N}(x) = f_2 \circ f_1(x)$  with  $f_1(y) = \phi_1(W^{(1)}; y; b_1)$  and  $f_2(y) = W^{(2)}y$ , such that  $\mathcal{N}$  is an approximation of the function g, that is,  $||g - \mathcal{N}|| < \varepsilon$ .

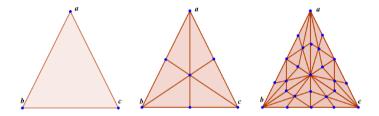
# Simplicial complexes and simplicial maps (1/4)



Things to recall: Face Maximal simplex Star Pure simplicial complex

A simplicial complex is a set of simplices such that each shared face is a simplex.

## Simplicial complexes and simplicial maps (2/4)



#### Definition

Let K be a simplicial complex with vertices in  $\mathbb{R}^d$ . The barycentric subdivision SdK can be written as an ordered set  $\{w_0, \ldots, w_k\}$  such that  $w_i = bar(\mu_i)$ , being  $\mu_i$  a face of  $\mu_j \in K$  for  $i, j \in \{0, \ldots, k\}$  and i < j.

#### An introduction to Simplicial-map Neural Networks

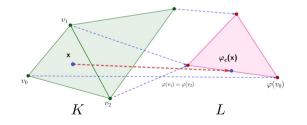
### Simplicial complexes and simplicial maps

#### Definition

Given two simplicial complexes K and L, a vertex map  $\varphi^{(0)} : K^{(0)} \to L^{(0)}$  is a function from the vertices of K to the vertices of L such that for any simplex  $\sigma \in K$ , the set

$$\varphi(\sigma) := \{ v \in L^{(0)} : \exists u \in \sigma, \varphi^{(0)}(u) = v \}$$

is a simplex of L.



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#### An introduction to Simplicial-map Neural Networks

# Simplicial complexes and simplicial maps (3/4)

#### Definition

Given two simplicial complexes K and L, a vertex map  $\varphi^{(0)} : K^{(0)} \to L^{(0)}$  is a function from the vertices of K to the vertices of L such that for any simplex  $\sigma \in K$ , the set

$$\varphi(\sigma) := \{ v \in L^{(0)} : \exists u \in \sigma, \varphi^{(0)}(u) = v \}$$

is a simplex of L.

The simplicial map  $\varphi_c : |K| \to |L|$  induced by the vertex map  $\varphi^{(0)}$  is a continuous function defined as:

$$\varphi^{c}(x) := \sum_{i=0}^{k} \lambda_{i} \varphi^{(0)}(u_{i})$$

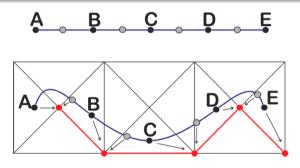
with  $\lambda_i \ge 0$  such that  $\sum_{i=0}^k \lambda_i = 1$  and  $x = \sum_{i=0}^k \lambda_i u_i$  where  $\sigma = \{u_0, \ldots, u_k\}$  is a simplex of K such that  $x \in |\sigma|$ .

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# Simplicial complexes and simplicial maps (4/4)

Theorem (Brower, 1910-1912)

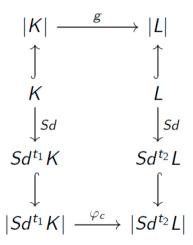
If  $g : |K| \to |L|$  is a continuous function, then there exists a sufficiently large t > 0 such that  $\varphi_c : |Sd^tK| \to |L|$  is a simplicial approximation of g.



 $g(|\operatorname{st} v|) \subset |\operatorname{st} \varphi(v)|$  (star condition)

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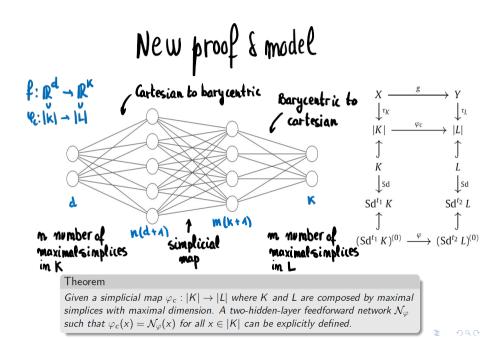
## The simplicial approximation extension



#### Proposition

Given  $\varepsilon > 0$  and a continuous function  $g : |K| \rightarrow |L|$  between the underlying spaces of two simplicial complexes K and L, there exists  $t_1, t_2 > 0$  such that  $\varphi_c : |Sd^{t_1}K| \rightarrow |Sd^{t_2}L|$  is a simplicial approximation of g and  $||g - \varphi_c|| \le \varepsilon$ .

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## For triangulations

We can follow what we did with the simplicial approximation theorem and extent it to get an approximation as close as desire:

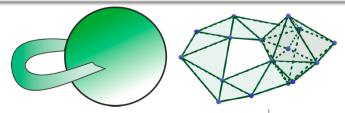
#### Theorem

Given a continuous function  $g : |K| \to |L|$  and  $\varepsilon > 0$ , a two-hidden-layer feedforward network  $\mathcal{N}$  such that  $||g - \mathcal{N}|| \le \varepsilon$  can be explicitly defined.

However, it works just for continuous functions between polyhedrons.

#### Definition

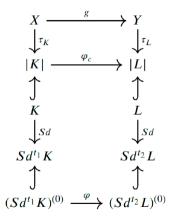
A triangulation of a topological space X consists of a simplicial complex K and a homeomorphism  $\tau : X \to |K|$ . We say that the triangulation is finite if K is finite.



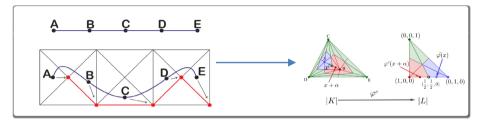
## For triangulations

#### Proposition

Let X and Y be two triangulable topological spaces,  $g: X \to Y$  a continuous map, and  $\varepsilon > 0$ . Then, there exists two triangulations  $(K, \tau_K)$ and  $(L, \tau_L)$  of X and Y, respectively, and a simplicial approximation  $\varphi_c: |Sd^{t_1}K| \to |Sd^{t_2}L|$  such that  $||g - \tau_L^{-1} \circ \varphi_c \circ \tau_K|| \leq \varepsilon$ .



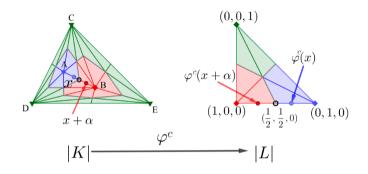
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- The classes are encoded in a maximal simplex |L|.
- Simplicial map is defined between a triangulation of the input dataset and |L|.

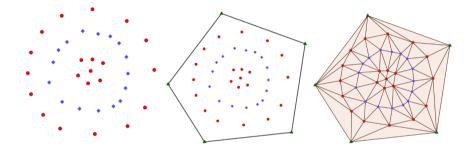
We need:

• To specify the "región of action" of the NN.



We need:

- A triangulation of the dataset.
- A maximal simplex to encode classes and predictions.
- A simplicial map.

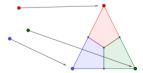


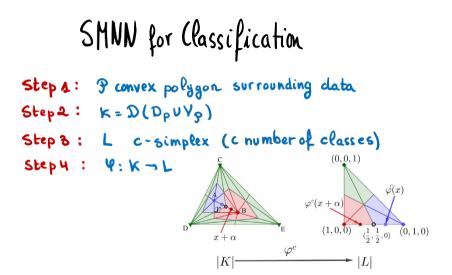
- Find a convex polytope surrounding the data points.
- Compute a Delaunay triangulation of the data points together with the vertices of the convex polytope.

#### Proposition

Let d, k > 0 be integers. Let L be the simplicial complex with only one maximal k-simplex  $\sigma = \{v_0, \ldots, v_k\}$  with  $v_i = e_i^k \times 0$  for  $i \in \{1, \ldots, k\}$  and  $v_0 = e_0^k \times 1$ . Let  $D \subset \mathbb{R}^d \times \mathbb{E}^k$  be a labelled dataset and let  $V_{\mathscr{P}}$  be the vertices of a convex polytope  $\mathscr{P}$  such that  $D_P \subset \mathscr{P}$ . Let us assume that  $D_P$  is in general position. Let  $K = \mathscr{D}(D_P \cup V_{\mathscr{P}})$ . Then, the map  $\varphi^{(0)} : K^{(0)} \to L^{(0)}$  defined as follows is a vertex map:

$$arphi^{(0)}(u) := \left\{ egin{array}{cc} \ell imes 0 & \mbox{if } (u,\ell) \in D \ v_0 & \mbox{if } u \in V_{\mathscr{P}} \end{array} 
ight.$$



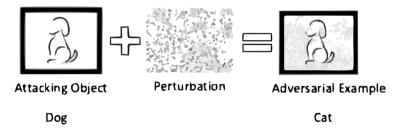


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## Adversarial examples

Definition

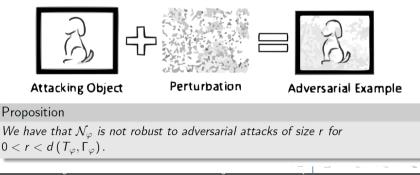
Let d, k > 0 be integers. Let  $D \subset \mathbb{R}^d \times \mathbb{E}^k$  be a labelled dataset and  $\mathcal{N}$  a neural network that characterizes D. Let  $B(r) = \{\alpha \in \mathbb{R}^d : ||\alpha|| \le r\}$  being  $||\cdot||$  a norm on  $\mathbb{R}^d$ . Let us suppose that  $x \in \mathbb{R}^d$  has label  $\ell$ . Then, an adversarial example of size r is defined as  $x' = x + \alpha$  with  $\alpha \in B(r)$  such that x' has label  $\ell'$  with  $\ell' \ne \ell$ . A neural network is called robust to adversarial attacks of size r if no labelled point  $x \in \mathbb{R}^d$  has an adversarial example of size r.



# Adversarial examples

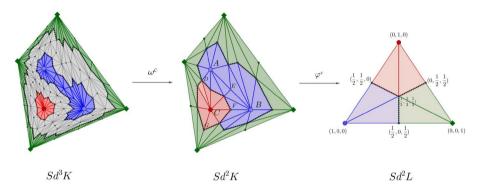
Definition

Let d, k > 0 be integers. Let  $D \subset \mathbb{R}^d \times \mathbb{E}^k$  be a labelled dataset and  $\mathcal{N}$  a neural network that characterizes D. Let  $B(r) = \{\alpha \in \mathbb{R}^d : ||\alpha|| \le r\}$  being  $||\cdot||$  a norm on  $\mathbb{R}^d$ . Let us suppose that  $x \in \mathbb{R}^d$  has label  $\ell$ . Then, an adversarial example of size r is defined as  $x' = x + \alpha$  with  $\alpha \in B(r)$  such that x' has label  $\ell'$  with  $\ell' \ne \ell$ . A neural network is called robust to adversarial attacks of size r if no labelled point  $x \in \mathbb{R}^d$  has an adversarial example of size r.



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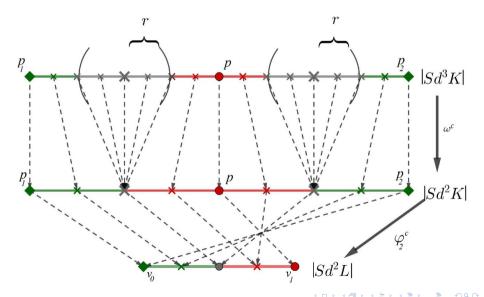
### Robustness against adversarial examples



#### Theorem

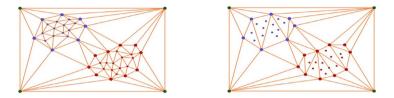
Let *D* be a labelled dataset. Then, there exists a two-hidden-layer neural network characterizing *D* and robust to adversarial attacks of size r > 0, for *r* being small enough.

### Robustness against adversarial examples



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## Optimizing its structure



Algorithm: Simplicial-map optimization

**Input:** A dataset *D*, a convex Polytope  $\mathcal{P}$  surrounding *D*, and  $\mathcal{N}_{\varphi} : |K| \to |L|$  that correctly classifies *D*.

**Output:**  $\tilde{\mathcal{N}}_{\tilde{\varphi}}$ 

**Step 1:** Create a set M with all  $\sigma = \{v_0, \ldots, v_n\} \subset D_P \cup V_P$  maximal simplex of K such that for some  $i \neq j \mathcal{N}_{\varphi}(v_i) \neq \mathcal{N}_{\varphi}(v_j)$ .

**Step 2:** Create the dataset  $\tilde{\mathcal{D}} = \{(v, \ell) : v \in M^{(0)} \text{ and } (v, \ell) \in D\}.$ 

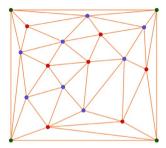
**Step 3:** Compute 
$$\hat{\mathcal{K}} = \mathcal{D}(\hat{D}_P \cup V_P)$$

**Step 4:** Define the simplicial-map neural network  $\tilde{\mathcal{N}}_{\tilde{\varphi}} : |\tilde{K}| \to |L|$  that correctly classifies  $\tilde{D}$ .

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### Optimizing its structure



 $\begin{array}{l} \mbox{Algorithm: Simplicial-map optimization} \\ \mbox{Input: A dataset $D$, a convex Polytope $\mathcal{P}$ surrounding $D$, and $\mathcal{N}_{\varphi}: |K| \rightarrow |L|$ that correctly classifies $D$. \\ \mbox{Output: $\vec{\mathcal{N}}_{\varphi}$} \\ \mbox{Step 1: Create a set $M$ with all $\sigma = \{v_0, \ldots, v_n\} \subset D_P \cup V_P$ maximal simplex of $K$ such that for some $i \neq ] $\mathcal{N}_{\varphi}(v_l) \neq \mathcal{N}_{\varphi}(v_l)$. \\ \mbox{Step 2: Create the dataset $\vec{D} = \{(v, \ell): v \in M^{(0)} \mbox{ and } (v, \ell) \in D\}$. \\ \mbox{Step 3: Compute $\vec{\mathcal{K}} = \mathcal{D}(\vec{D}_P \cup V_P)$. \\ \mbox{Step 4: Define the simplicial-map neural network $\vec{\mathcal{N}}_{\varphi}: |\vec{K}| \rightarrow |L|$ that correctly classifies $\vec{D}$. \\ \end{tabular}$ 

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Data Set Size	3-Simplices	3-Simplices (Reduced)	Data Set Size (Reduced)
14	34	29	13
104	551	391	75
1004	6331	1647	272
10,004	66,874	30,357	4556
100,004	672,097	147,029	21,955
1,000,004	6,762,603	1,858,204	274,635

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### Take-home message and future work

SMNNs are constructive by definition and universal
 approximation.

SMNNs can be refined to gain robustness against adversarial examples.

Its bottleneck is the computation of the triangulation and they are strongly data dependant.

Future work:

Can SMNNs be trained? Is it possible to optimize its architecture or avoid the Delaunay triangulation?

### Take-home message and future work

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 approximation.

SMNNs can be refined to gain robustness against adversarial examples.

Its bottleneck is the computation of the triangulation and they are strongly data dependant.

Future work:

Can SMNNs be trained? Is it possible to optimize its architecture or avoid the Delaunay triangulation? Thank you!

# Bibliography I

- 1 Eduardo Paluzo-Hidalgo, Rocio Gonzalez-Diaz, and Miguel A. Gutiérrez-Naranjo. "Two-hidden-layer feed-forward networks are universal approximators: A constructive approach". In: *Neural Networks* 131 (2020), pp. 29–36. doi: <u>10.1016/j.neunet.2020.07.021</u>. url: <u>https://doi.org/10.1016/j.neunet.2020.07.021</u>.
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