Barycentric Coordinates in Neural Network-Based Function Approximation

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Joint work with Rocío González Díaz and Miguel A. Gutiérrez Naranjo

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Seville, Spain

Jornadas de Topología de Datos, Logroño, January 2025

Introduction

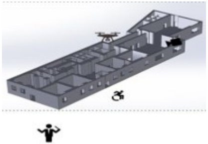
About me

- Graduate in Statistics.
- Specialised in Artificial Intelligence, with a master's degree.
- 2 years of experience working as a data scientist, focusing on the development of AI models, as well as data analysis.
- Currently, researcher at the USE in the REXASI-PRO European Project and doing a PhD in mathematics, which is focused on the intersection between TDA and AI.

REXASI-PRO

Wheelchair

Drone



Orchestrator

REXASI-PRO

Our aim is to use TDA for analyse the discrete model of the fleet behavior, contributing to safety navigation.

Outline

- Topogical Data Analysis and Barycentric Coordinates
- Neural Networks
- Barycentric Neural Network
- Continuous Piecewise Linear Function Representation using BNN
- Continuous Function Approximation using BNN
- Conclusion

TDA

What is Topology?

Topology[1], is a branch of Mathematics, which explores the properties of space that remain unchanged under continuous transformations, like stretching or vending, without tearing.

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- Problem-Solving Across Disciplines
- Broader Perspective

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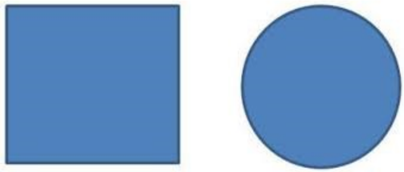

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What about algebraic topology?

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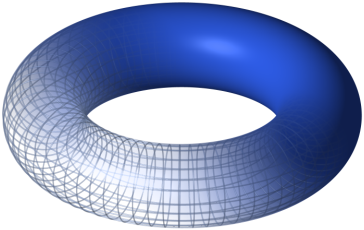

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Algebraic Topology Key concepts

- **Simplicial Complexes:** Discrete structures used to represent topological spaces for algebraic analysis.
- **Homology:** A tool to study the number and types of “holes” in a space.

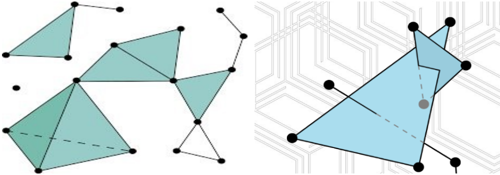
Simplicial Complexes

A **simplex** is a general geometric object that have dimension:

- 0-simplex: a point (called a vertex)
- 1-simplex: a line segment (called an edge)
- 2-simplex: a triangle (filled)
- 3-simplex: a tetrahedron
- ...

Simplicial Complexes

A **simplicial complex** is obtained by a nested family of simplices



(a) Simplicial complex example (b) This is not a simplicial complex!

Homology

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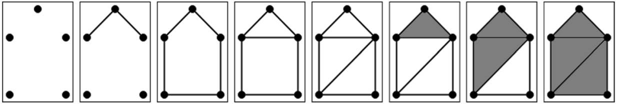
  - β_K: number of k-dimensional holes

Homology



A filtration for $t = 0,1,2,3,4,5,6,7$ (from left to right)

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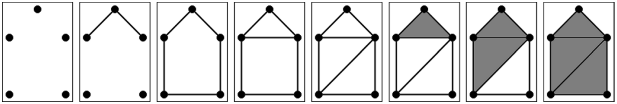

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- $t = 0 \rightarrow \beta_0 = 5, \beta_1 = 0, \beta_2 = 0$

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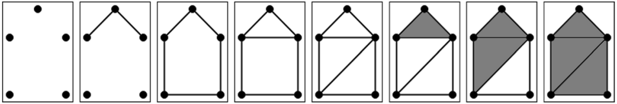

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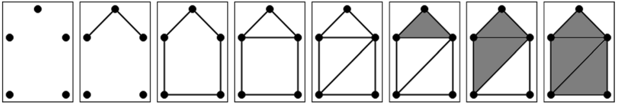

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- $t = 5 \rightarrow \beta_0 = 1, \beta_1 = 2, \beta_2 = 1$

What is TDA?

- **Topological Data Analysis**[3] **(TDA)** consists in applying techniques from algebraic topology to the analysis of data, studying how the shape of the data is modified along the filtration.

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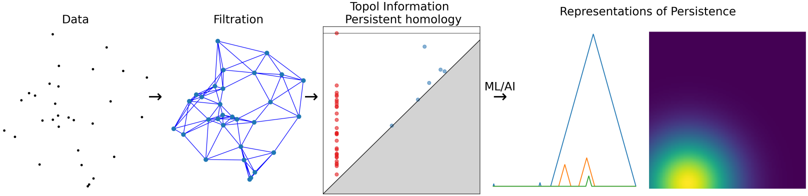

Typical TDA Pipeline

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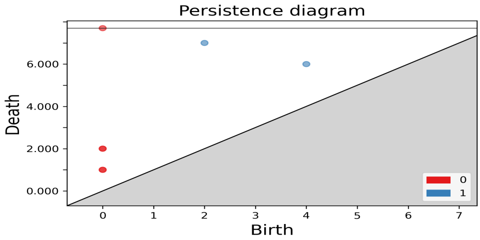

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Persistence entropy[4] is a measure of the complexity of a topological space based on its **persistence barcode**[5], measuring how different bars are in length.

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Maximum persistence entropy corresponds to the situation in which all the intervals in the barcode are of equal length, $\rightarrow H = \ln(n)$, being n the number of topological features (bars).

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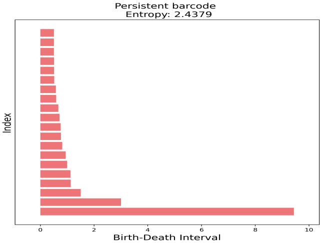

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For a point p in a $1D$ segment $[x_1, x_2]$, the barycentric coordinate t is defined as:

$$t = \frac{p - x_1}{x_2 - x_1}$$

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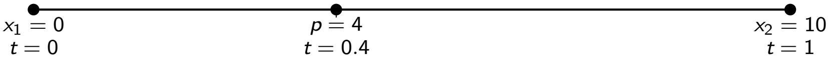
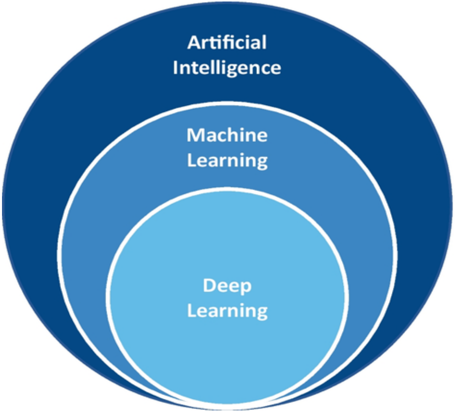


NNs

Artificial Intelligence



Artificial Intelligence (AI)

Computational programs perform intelligent tasks

Machine Learning (ML)

Automatically learns and improves from experience

Deep Learning (DL)

Multilayered artificial neural networks

Neural Networks

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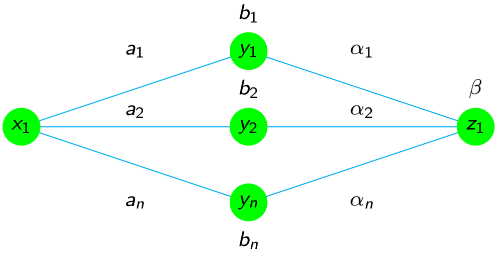

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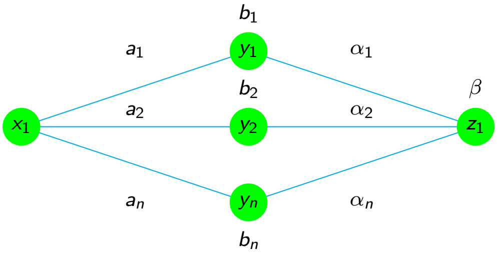
- Types:
  - MLP
  - CNNs
  - RNNs
  - ...



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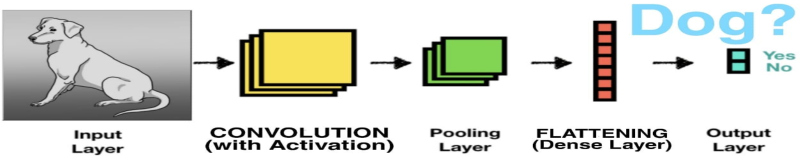

Barycentric Neural Network

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Using t, according to barycentric coordinates, we can perform linear interpolation to estimate a function value $f(x)$ at any x between two points, (x_1, y_1) and (x_2, y_2).

$$f(x) = mx + n = step(t) \cdot ReLU(1 - t) \cdot y_1 + step(1 - t) \cdot ReLU(t) \cdot y_2 = BNN(x)$$

where $step(t)$ activates the contribution of y_1 and y_2, and ReLU adjusts their weights based on t.

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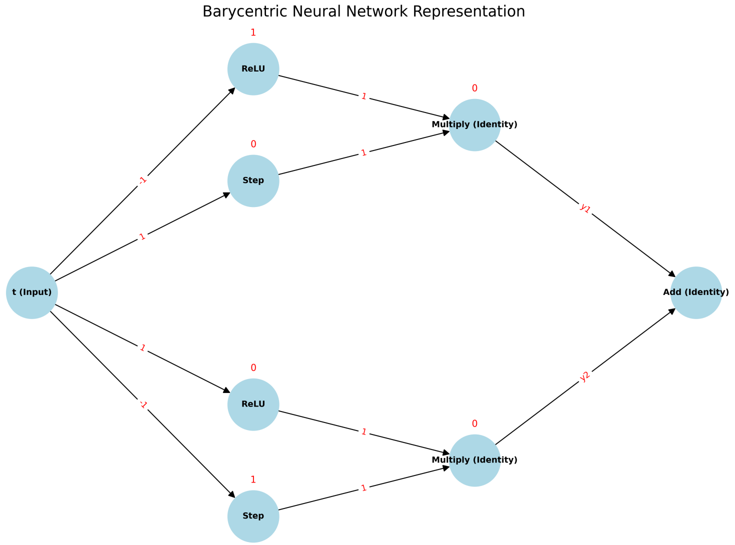
$$step(x) = \begin{cases} 1 & \textbf{si } x \geq 0 \\ 0 & \textbf{si } x < 0 \end{cases} \text{ and } ReLU(x) = max(0, x)$$

Barycentric Neural Network



Barycentric Neural Network

Barycentric coordinates simplify the neural network construction

↓

✖Training

CPLF representation

CPLF

A **Continuous Piecewise Linear Function** (CPLF) is a mathematical function defined by different linear expressions over different intervals of its domain, with the characteristic that it is continuous across its entire domain (no jumps or discontinuities).

$$CPLF(x) = \begin{cases} x + 2 & \text{if } x < 0, \\ -x + 2 & \text{if } x \in [0, 2), \\ x - 2 & \text{if } x \geq 2. \end{cases}$$

Remark 1

Remark

Let $f(x)$ be a continuous function linearly interpolated between points x_1 and x_2, with values $y_1 = f(x_1)$ and $y_2 = f(x_2)$. The proposed methodology, based on barycentric coordinates and a structure similar to a neural network, ensures the representation of $f(x)$ as a continuous linear function.

$$f(x) = BNN(t)$$

Extension to multiple points

This formulation can be extended to multiple points. Given a sequence of points $\{(x_i, y_i)\}$, the interpolation can represent a continuous piecewise linear function (CPLF). The function $f(x)$ is represented as:

$$CPLF(x) = BNN(t)$$

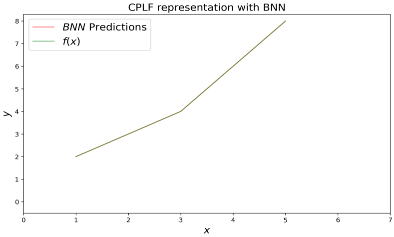
Remark 2

Remark

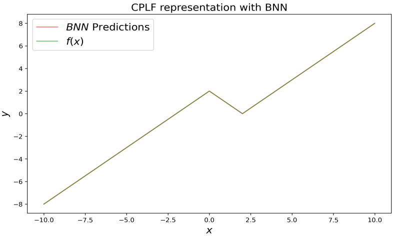
Let *CPLF* be a continuous function defined on $\mathbb{R} \to \mathbb{R}$, which can be divided into a finite number of intervals, each being linear. There exists a Barycentric Neural Network (BNN), such that for all $x \in \mathbb{R} \to \mathbb{R}$

$$CPLF(x) = BNN(t)$$

Examples



(a) $CPLF(x) = \begin{cases} x+1 & \text{if } x \in [1, 3) \\ x-2 & \text{if } x \in [3, 5) \end{cases}$

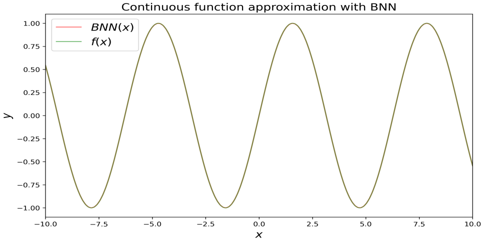


(b) $CPLF(x) = \begin{cases} x+2 & \text{if } x \in [-10, 3) \\ -x-2 & \text{if } x \in [0, 2) \\ x-2 & \text{if } x \in [2, 10) \end{cases}$

Continuous Function Approximation

Continuous Function

- Function $f(x)$, not neccesary to be linear, but continuous, as $sin(x)$.
- Divide it into m segments, obtaining a CPLF.
- Thanks to the *BNN*, we can represent the CPLF, serving as approximation of any continuous function.



Persistent entropy for optimal approximation

We use persistent entropy to find the smallest number of segments required to divide the function to satisfy a desired approximation precision ϵ.

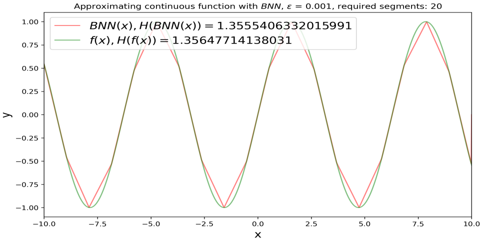
Given a continuous function $f : \mathbb{R} \to \mathbb{R}$, and a barycentric neural network *BNN* that approximates $f(x)$ by a CPLF with m equidistant segments, we want to find the minimum number of segments m_{min} such that:

$$|H(f(x)) - H(\hat{f}(x, m))| < \epsilon.$$

$\hat{f}(x, m)$ correspond to the *BNN* that represent the CPLF obtained dividing $f(x)$ in m equidistant segments.

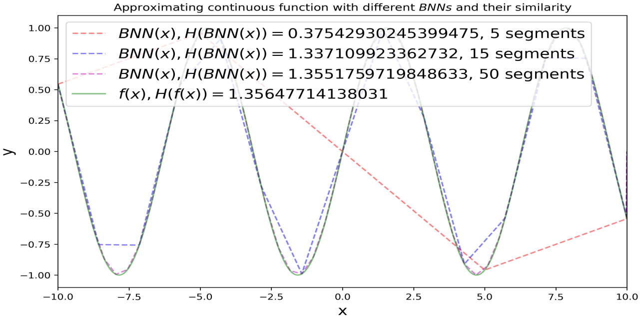
Persistent entropy for optimal approximation

1. Start with an initial number of segments m_0.
2. Evaluate the error $|H(f(x)) - H(\hat{f}(x, m_0))|$.
3. Increase m until the error $|H(f(x)) - H(\hat{f}(x, m))|)$ falls below the desired threshold ϵ.



$f(x) = sin(x)$ approximation using the BNN given a desired level of precision($\epsilon = 0.001$).

Persistent entropy as similarity metric



Barycentric Neural Network similarity according to persistent entropy approximating $sin(x)$ dividing it into different number of segments.

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- The use of geometrical-topological concepts provides a novel perspective for many machine-learning applications!
  - Effective neural network based on barycentric coordinates for represent CPLFs and approximate continuous functions without training.
  - Persistent entropy as a tool for optimal function approximation and similarity measure.
- Future work: Extend this approach to higher-dimensional function approximations, and explore its application in real-world scenarios.

Acknowledgement

- Rocío González Díaz and Miguel A. Gutierrez-Naranjo for the insightful discussions and ideas, as well as for their collaboration.
- European Union HORIZON-CL4-2021-HUMAN-01-01 under grant agreement 101070028 (REXASI-PRO).

HORIZON-CL4-HUMAN-01 grant agreement no.101070028

Funded by the European Union

Thanks for your time! ☺

If you have any question, please shoot!