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

# HOI: A Python toolbox for high-performance estimation of Higher-Order Interactions from multivariate data

Matteo Neri <sup>1\*</sup>, Dishie Vinchi<sup>3\*</sup>, Christian Ferreyra<sup>1,5</sup>, Thomas Robiglio<sup>4</sup>, Onur Ates<sup>1</sup>, Marlis Ontivero-Ortega <sup>2</sup>, Andrea Brovelli <sup>1</sup>, Daniele Marinazzo <sup>2\*</sup>, and Etienne Combrisson <sup>1\*</sup>

1 Institut de Neurosciences de la Timone, Aix Marseille Université, UMR 7289 CNRS, 13005, Marseille, France 2 University of Ghent, Ghent, Belgium 3 Veermata Jijabai Technological Institute, Mumbai 4 Department of Network and Data Science, Central European University, Vienna, Austria 5 Laboratoire d'Informatique et des Systèmes, Aix Marseille Université, UMR 7020 CNRS, Marseille, France \* These authors contributed equally.

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## Summary

HOI (Higher-Order Interactions) is a Python toolbox to measure higher-order information theoretic metrics from multivariate data. Higher-order interactions refer to interactions that go beyond pairwise connections between nodes in a network (Battiston et al., 2021; Baudot et al., 2019; Gatica et al., 2021; Herzog et al., 2022; Luppi et al., 2024; Rosas et al., 2019). The HOI toolbox provides easy-to-use information theoretic metrics to estimate pairwise and higher-order information from multivariate data. The toolbox contains cutting-edge methods, along with core entropy and mutual information functions, which serve as building blocks for all metrics. In this way, HOI is accessible both to scientists with basic Python knowledge using pre-implemented functions and to experts who wish to develop new metrics on top of the core functions. Moreover, the toolbox supports computation on CPUs and GPUs. Finally, HOI provides tools for visualizing and presenting results to simplify the interpretation and analysis of the outputs.

## Statement of need

Recent research studying higher-order interactions with information theoretic measures provides new angles and valuable insights in different fields, such as neuroscience (Baudot et al., 2019; Combrisson et al., 2024; Gatica et al., 2021; Herzog et al., 2022; Luppi et al., 2022), music (Rosas et al., 2019), economics (Scagliarini et al., 2023), and psychology (Marinazzo et al., 2022). Information theory allows investigating higher-order interactions using a rich set of metrics that provide interpretable values of the statistical interdependency among multivariate data (Barrett, 2015; Mediano et al., 2021; Rosas et al., 2019; Scagliarini et al., 2023; Williams & Beer, 2010).

Despite the relevance of studying higher-order interactions across various fields, there is currently no toolkit that compiles the latest approaches and offers user-friendly functions for calculating higher-order information metrics. Computing higher-order information presents two main challenges. First, these metrics rely on entropy and mutual information, whose estimation must be adapted to different types of data (Czyż et al., 2024; Madukaife & Phuc, 2024). Second, the computational complexity increases exponentially as the number of variables and interaction orders grows. For example, a dataset with 100 variables, has approximately

$1.6 \times 10^5$  possible triplets,  $4 \times 10^6$  quadruplets, and  $7 \times 10^7$  quintuplets. Therefore, an efficient implementation, scalable on modern hardware is required.

## Related packages

Several toolboxes have implemented a few HOI metrics like `infotopo` (Baudot et al., 2019), `infotheory` (Candadai & Izquierdo, 2020) in C++, `DIT` (James et al., 2018), `IDTx1` (Wollstadt et al., 2019) and `pyphi` (Mayner et al., 2018), in Python. However, HOI is the only pure Python toolbox specialized in the study of higher-order interactions offering functions to estimate with an optimal computational cost a wide range of metrics as the O-information (Rosas et al., 2019), the topological information (Baudot et al., 2019) and the redundancy-synergy index (Timme & Lapish, 2018). Moreover, HOI allows to handle Gaussian, non-Gaussian, and discrete data using different state-of-the-art estimators (Czyż et al., 2024; Madukaife & Phuc, 2024). HOI also distinguishes itself from other toolboxes by leveraging `Jax`, a library optimized for fast and efficient linear algebra operations on both CPU, GPU and TPU. Taken together, HOI combines efficient implementations of current methods and is adaptable enough to host future metrics, facilitating comparisons between different approaches and promoting collaboration across various disciplines.

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