giotto-tda: A Topological Data Analysis Toolkit for Machine Learning and Data Exploration

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Abstract

We introduce giotto-tda, a Python library that integrates high-performance topological data analysis with machine learning via a scikit-learn–compatible API and state-of-the-art C++ implementations. The library’s ability to handle various types of data is rooted in a wide range of preprocessing techniques, and its strong focus on data exploration and interpretability is aided by an intuitive plotting API. Source code, binaries, examples, and documentation can be found at https://github.com/giotto-ai/giotto-tda.

Keywords: Topological Data Analysis, Persistent Homology, Mapper, Machine Learning, Data Exploration, Python

1. Introduction

Topological Data Analysis (TDA) uses tools from algebraic and combinatorial topology to extract features that capture the shape of data (Carlsson, 2009). In recent years, algorithms based on topology have proven very useful in the study of a wide range of problems. In particular, persistent homology has had significant impact on data intensive challenges including the classification of porous materials (Lee et al., 2018), the study of structures in the weight space of CNNs (Gabrielsson and Carlsson, 2018), and the discovery of links between structure and function in the brain (Reimann et al., 2017). The Mapper algorithm has also received considerable attention after its use in the identification of a highly treatable subgroup of breast cancers (Nicolau et al., 2011).

Despite its power, TDA has remained outside the toolbox of most Machine Learning (ML) practitioners, largely because current implementations are developed for research purposes and not in high-level languages. The aim of giotto-tda is to fill this gap by making TDA accessible to the Python data science community, while supporting research. To this end, giotto-tda inherits the flexibility of scikit-learn, the most popular all-purpose ML

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framework (Pedregosa et al., 2011), and extends it with TDA capabilities that include a wide range of persistent homology and Mapper-type algorithms. It enables TDA to be applied to univariate and multivariate time series, images, graphs, and their higher dimensional analogues, simplicial complexes. This makes giotto-tda the most comprehensive Python library for topological machine learning and data exploration to date.

2. Architecture

giotto-tda maintains compatibility with the scikit-learn API whenever possible. However, in order to apply certain TDA techniques one must first embed the input data into a higher-dimensional space. This causes the embedding Estimator to modify the number of samples in the input collection. To enable compatibility with scikit-learn a TransformerResamplerMixin base class was designed. It provides a resample method that modifies the number of samples in the target in accordance with how the input data is transformed. For users to be able to combine scikit-learn–based estimators and giotto-tda’s transformer-resamplers, an extended version of scikit-learn’s Pipeline is provided. It is adapted to the new mixin and allows the transformer-resamplers to resample the target. Compatibility with scikit-learn’s model selection algorithms is still ensured and highly relevant, as the hyperparameters of TDA algorithms are notoriously hard to select.

giotto-tda provides users with full flexibility in the design of TDA pipelines via modular estimators. This modularity enables the exploration of intermediate results, which are standard (possibly multi-dimensional) NumPy arrays. The highly visual nature of topological signatures is harnessed by giotto-tda via a plotting API. The latter is based on plotly and exposes a set of external functions and class methods to plot and interact with intermediate outputs.

3. Persistent Homology

Persistent homology is one of the main tools in TDA. It extracts and summarises, in so-called persistence diagrams, multi-scale relational information in a manner similar to hierarchical clustering that also considers higher-order connectivity. Few open-source Python libraries exist to calculate persistence diagrams. GUDHI (The GUDHI Project, 2020) provides the widest selection of efficient persistent homology algorithms in C++, together with Python bindings. It also contains scikit-learn–style transformers, but only to extract feature from persistence diagrams.

In giotto-tda, scikit-learn integration is extended to all steps involved in the creation of persistence diagrams, including persistent homology calculation and techniques to transform a wide variety of data inputs into forms suitable for it. The result is a framework for constructing end-to-end Pipeline objects to generate carefully crafted topological features from each sample in an input raw data collection.

Our library matches the code and documentation standards set by scikit-learn, and relies on state-of-the-art external C++ libraries (The GUDHI Project, 2020; Bauer, 2019; Kerber et al., 2017; Ltgehetmann et al., 2020) using new performance-oriented bindings based on pybind11 (Jakob et al., 2017). An example of a giotto-tda persistent homology Pipeline for images of handwritten digits is shown in Fig. 1.
4. Mapper

Mapper is a computational technique that applies “lenses” and partial clustering to high-dimensional data to obtain a simple, but topologically meaningful description in terms of a graph (or more generally, a simplicial complex). Mapper is primarily used as a data visualization tool to explore substructures of interest in data. In giotto-tda, the Mapper algorithm is realised as a well-defined sequence of steps in a scikit-learn Pipeline, where the clustering step can be parallelized. The resulting graph is visualized through an interactive plotting API. This design choice provides a great deal of interoperability and computational efficiency, allowing users to a) realize relevant steps of the Mapper algorithm through any scikit-learn estimator, b) integrate Mapper pipelines as part of a larger ML workflow, and c) make use of memory caching to avoid unnecessary re-computations. Memory caching is especially useful for interactive plotting, where giotto-tda allows users to tune Mapper’s hyperparameters and observe how the resulting graph changes in real time. An example is shown in Fig. 2.

To the best of our knowledge, KeplerMapper (van Veen et al., 2019) is the only alternative open-source implementation of Mapper in Python that provides general-purpose functionality. Although KeplerMapper also provides the flexibility to use scikit-learn estimators to generate Mapper graphs, it implements all steps of the algorithm in a single class and is only partially compatible with scikit-learn pipelines. Moreover, it does not implement memory caching or provide real-time interactivity in the visualization.

5. Project management

Easy installation: Binary packages are available for all major operating systems on the PyPI package repository and can be installed easily by running pip install -U giotto-tda. Code quality: The code is unit-tested throughout using pytest and hypothesis and, as of v0.2.0, test coverage is 91%. The code follows the PEP8 standards and adheres to the Python coding guideline and numpy-style documentation. CI with Azure pipelines CI are used to ensure that new contributions can be easily integrated and maintain our quality standard. GNU AGPLv3 licensing: The library relies on a variety of GPL-licensed software. Community-based development: We base giotto-tdas development on collaborative tools such as Git, GitHub, and Slack. Contributions are encouraged, and we actively make use of GitHub’s issue tracker to provide support and discuss ideas.
Figure 2: Example of the Mapper graph (right) generated by giotto-tda on a 3D model of an alien (left). Nodes are colored according to the alien’s height. The alien example is adapted from Murugan and Robertson (2019).

Documentation: A detailed API reference \(^1\) is provided to the user using sphinx.

Learning resources: To lower the entry barrier for new users, we provide a theory glossary and a wide range of tutorials and examples that guide the users in understanding how TDA-based ML pipelines can be applied to datasets of various sorts.

Project relevance: At the time of writing, the repository has attracted over 220 stars on GitHub and is visited 1000 times per week. The PyPI package is downloaded 350 times per month.

6. Concluding remarks

The very active research field of TDA provides algorithms that can be used at any step of a ML pipeline. giotto-tda aims to make those algorithms available in a form that is useful to both the research and data science communities, allowing them to use TDA as a part of large-scale ML tasks. We have written giotto-tda under the code and documentation standards of scikit-learn and, alongside further performance optimization of the existing C++ code, future developments will include the first implementation of novel TDA algorithms such as persistence Steenrod diagrams (Medina-Mardones, 2018).

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\(^1\) Currently hosted at https://giotto-ai.github.io/gtda-docs/latest/modules/index.html
References

Ulrich Bauer. Ripser: efficient computation of Vietoris-Rips persistence barcodes, August 2019. Preprint.

Gunar Carlsson. Topology and data. Bull. Amer. Math. Soc. (N.S.), 46(2):255–308, 2009.

Rickard Brel Gabrielsson and Gunnar Carlsson. Exposition and interpretation of the topology of neural networks, 2018.

Adélie Garin and Guillaume Tauzin. A topological “reading” lesson: Classification of MNIST using TDA. In Proceedings of the 19th International Conference on Machine Learning and Applications (ICMLA 2020). IEEE, December 2019.

Wenzel Jakob, Jason Rhinelander, and Dean Moldovan. pybind11 – seamless operability between c++11 and python, 2017. URL https://github.com/pybind/pybind11.

Michael Kerber, Dmitriy Morozov, and Arnur Nigmetov. Geometry helps to compare persistence diagrams. Journal of Experimental Algorithmics, 22:1–20, 09 2017.

Yongjin Lee, Senja D Barthe, Pawe Dotko, et al. High-Throughput Screening Approach for Nanoporous Materials Genome Using Topological Data Analysis: Application to Zeolites. Journal of chemical theory and computation, 14(8):4427–4437, August 2018.

Daniel Ltehetmann, Dejan Govc, Jason P. Smith, et al. Computing persistent homology of directed flag complexes. Algorithms, 13(1), 2020.

A. M. Medina-Mardones. Persistence Steenrod modules, 2018. URL https://arxiv.org/abs/1812.05031.

Jeff Murugan and Duncan Robertson. An introduction to topological data analysis for physicists: From lgm to frbs, 2019.

Monica Nicolau, Arnold J. Levine, and Gunnar Carlsson. Topology based data analysis identifies a subgroup of breast cancers with a unique mutational profile and excellent survival. Proceedings of the National Academy of Sciences, 108(17):7265–7270, 2011.

F. Pedregosa, G. Varoquaux, A. Gramfort, et al. Scikit-learn: Machine learning in Python. Journal of Machine Learning Research, 12:2825–2830, 2011.

Michael W. Reimann, Max Nolte, Martina Scolamiero, et al. Cliques of neurons bound into cavities provide a missing link between structure and function. Frontiers in Computational Neuroscience, 11:48, 2017.

The GUDHI Project. GUDHI User and Reference Manual. GUDHI Editorial Board, 3.1.1 edition, 2020. URL https://gudhi.inria.fr/doc/3.1.1/.

Hendrik van Veen, Nathaniel Saul, David Eargle, et al. Kepler Mapper: A flexible Python implementation of the Mapper algorithm. Journal of Open Source Software, 4(42):1315, 2019. URL https://github.com/scikit-tda/kepler-mapper.