TDA for TSP Solvers

Enhancing the performance of a Transformer-based NN solver with topological features

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Machine Learning Course, Skoltech, 2024

Motivation

- Traditional methods for solving the TSP may miss complex patterns in the data global structure.
- Persistent homology offers a lens to examine the solution space, uncovering structural insights that can improve solver performance.

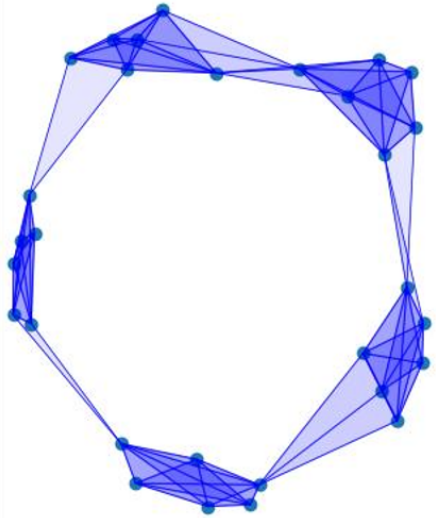


Figure: An example of the set of points with a global structure

Problem Statement

1. Can one augment the TSP dataset with topological features extracted from persistent homology to enhance neural network solvers?
2. Can one develop novel algorithms and heuristics informed by topological structures, potentially revolutionizing TSP solving methods?

Preliminaries: Persistent Homology

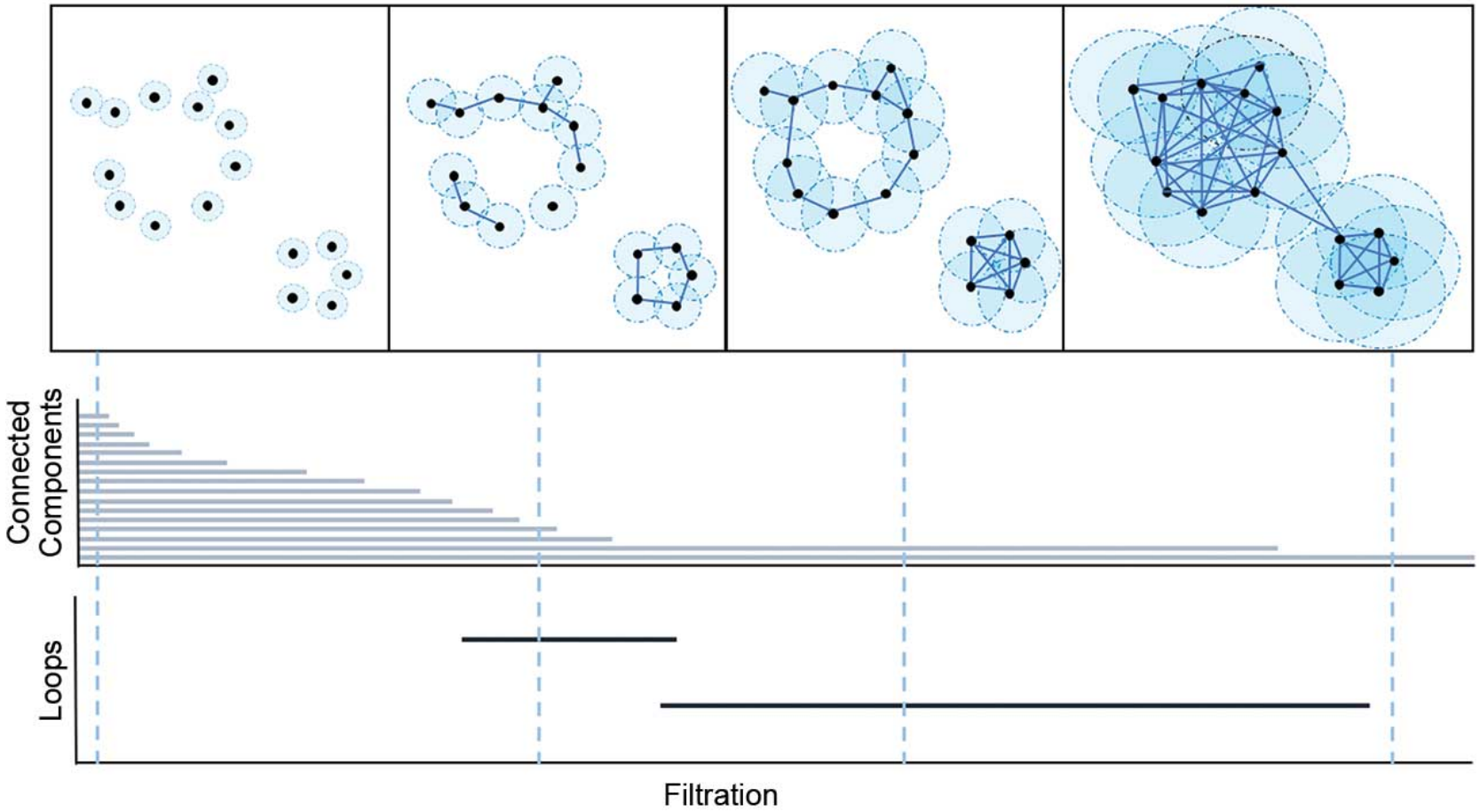


Figure: A set of points and its persistent barcode

Related Work: present TSP solvers

- **Exact Solvers:**
  - Branch and Bound,
  - Cutting Planes[5],
  - Dynamic Programming[1].
- **Heuristic Solvers:**
  - Greedy Algorithms (including the Christofides algorithm[3]),
  - Local Search[4],
  - Simulated Annealing[7],
  - Ant Colony Optimization[6].
- **Neural Network Solvers:**
  - Pointer Networks[9],
  - Graph Neural Networks assisted Monte Carlo Tree Search[10],
  - Transformer Networks (Kool et al.[8] and Bresson & Laurent[2]).

Baseline

1. The Transformer-based net [2] that takes the set of point coordinates as input.
2. The dynamics of its training on 10 and 20 points respectively will then be compared to the topologically-informed models.

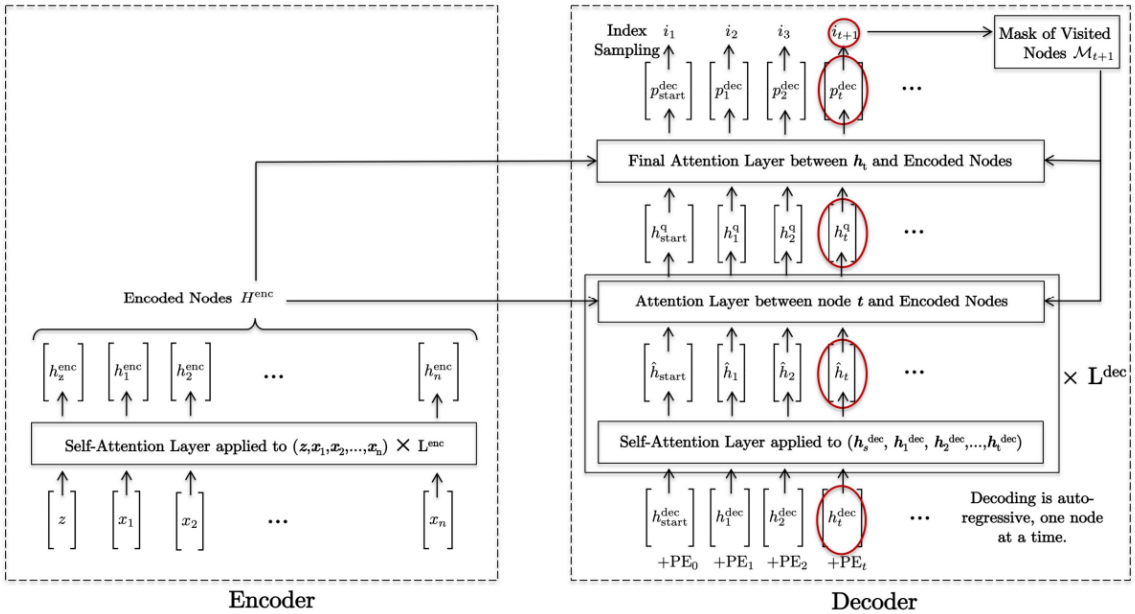


Figure 1: Proposed TSP Transformer architecture.

Figure: The architecture proposed in [2]

Features and ideas

- We wanted to augment the set of coordinates with the features that encode the information about the generators of H_1
- We found a way to extract, for each segment of the barcode, a pair of simplices:
  1. one that is responsible for the birth of a nontrivial element in homology
  2. one that kills this element

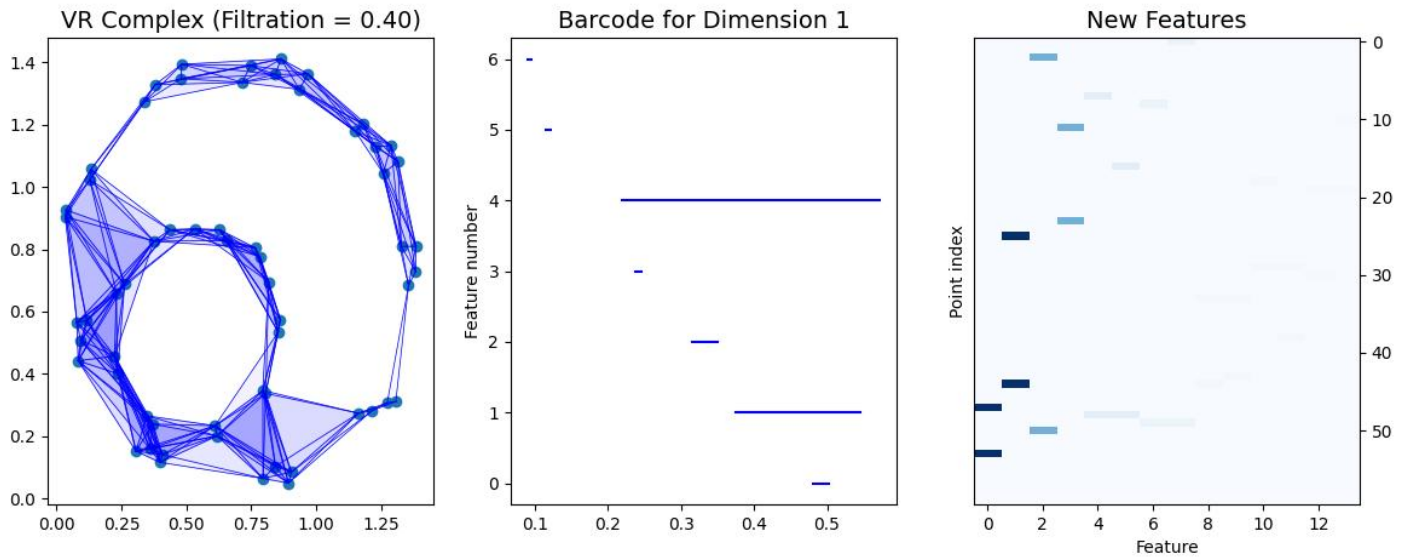
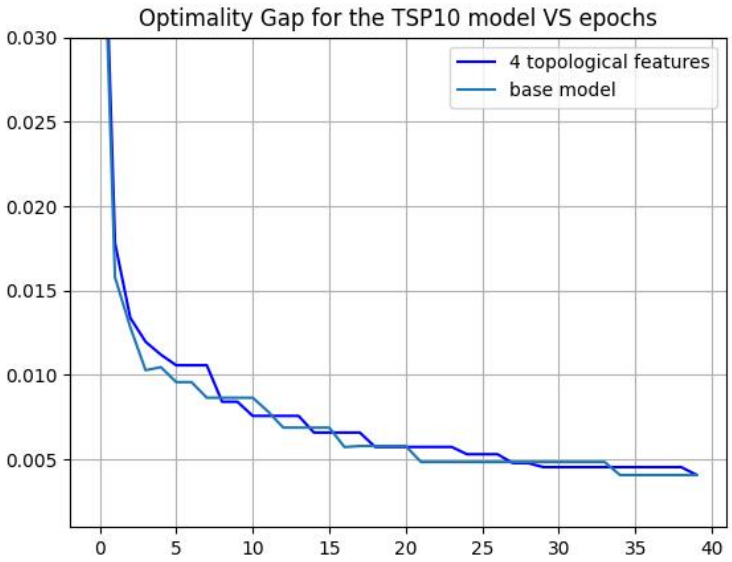
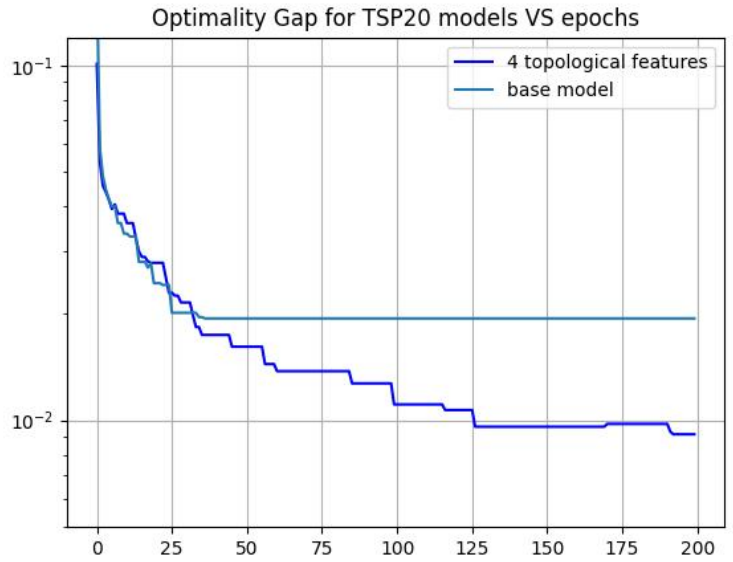


Figure: Features representing "critical" simplices of homology generators

Conducted experiments

1. Here we would compare optimality gaps for base model compared to that of augmented model – two pictures (10 and 20 nodes)





Results

1. Here is a demonstration of that out model predicts well

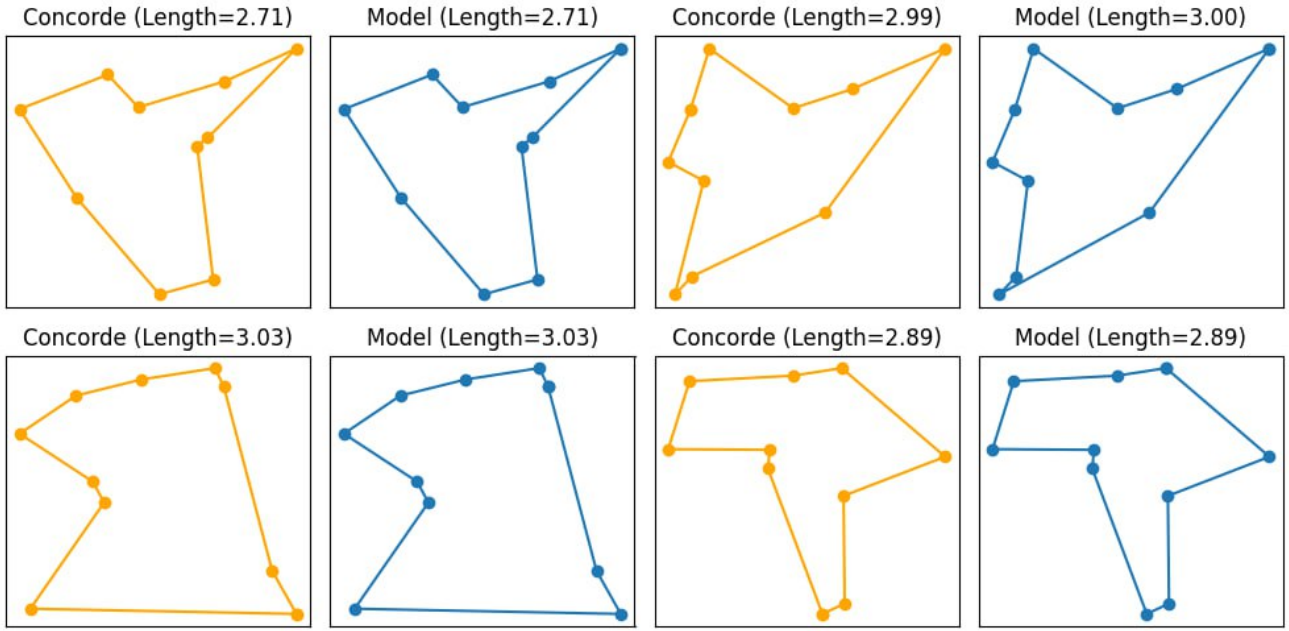


Figure: The performance of TSP10 net compared to optimal solutions

Further research

1. Optimize the use of topological features to accelerate the augmentation.
2. Investigate the impact of other homology dimensions.

Team Members' Contributions

- Elfat Sabitov: Training, technical support, inspiration.
- Ivan Gusev: Topological features development, massive research contribution.
- Alex Fokin: TDA research, visualization, training.

Acknowledgment

We are grateful to Anton Dmitriev, Eduard Tulchinskii and Serguei Barannikov for technical advice and research supervision.

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