Institute of Artificial Intelligence (Aii)

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Invited Speaker

Dr. Astrit Tola, Florida State University



"Topological Descriptors in Graph Representation Learning: From Persistent Homology to Scalable Embeddings"

Tuesday, March 3, 2026 • 1:00PM • SPRK 229 (Formerly Global) • Zoom

Abstract:
The intersection of algebraic topology and machine learning has opened new avenues for understanding the multi-scale structural properties of complex data. While Graph Neural Networks (GNNs) excel at capturing local neighborhood information, they often fail to account for higher-order topological features, such as cycles and voids, which are critical for structural robustness. In this talk, I will discuss how to mathematically formalize these features using Topological Data Analysis (TDA) and integrate them into modern learning architectures.

First, I will introduce TopoFormer (ICLR 2026), a scalable framework that integrates topological structure into attention-based architectures. TopoFormer uses a novel Topo-Scan module to convert graphs into ordered sequences of topological tokens, enabling the use of Transformers for graph-level representation learning. This approach preserves multi-scale structural information, provides theoretical stability guarantees, and achieves state-of-the-art results in graph classification and molecular property prediction, while remaining computationally efficient and parallelizable.

Next, I will present TopER - Topological Evolution Rate (NeurIPS 2025), which introduces a low-dimensional, interpretable graph embedding derived from a simplified persistent homology pipeline. By quantifying the evolution rate of graph substructures across filtrations, TopER produces intuitive representations that enable visualization and interpretability while achieving competitive or state-of-the-art performance on molecular, biological, and social network benchmarks. The method is also available as an open-source Python package on PyPI.

ogether, these works illustrate a broader research direction: embedding topological inductive biases into modern deep learning architectures to achieve interpretability, scalability, and strong predictive performance.

Bio:
Astrit Tola is a Postdoctoral Researcher in Mathematics at Florida State University. He received his Ph.D. in Mathematics from The University of Texas at Dallas, where his dissertation focused on integrating topological data analysis with graph representation learning.

His research lies at the intersection of topology and machine learning, where he develops mathematically grounded and computationally efficient methods for learning from graph-structured data. He studies how topological invariants and multi-scale structural information can be incorporated into modern deep learning architectures, including graph neural networks and attention-based models. His work has appeared in leading venues such as NeurIPS and ICLR and spans applications including graph classification, link prediction, molecular property prediction, and drug discovery.