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PLENARY LECTURE

Leveraging combinatorial invariants and AI for classification of entangled structures in biopolymers

KEYNOTE SPEAKER

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PLENARY LECTURE ABSTRACT

Spontaneous physical entanglement, especially the formation of knots, occurs in polymers that are sufficiently long and densely packed. This phenomenon is not exclusive to synthetic polymers; biopolymers, including proteins and viral DNA, have been recognized for exhibiting knots as well. Recent advancements in AI-driven models have predicted that millions of proteins could potentially have a non-trivial topology. As biopolymers possess a highly complex geometric structure, recognizing, identifying, and classifying these entanglements presents a computational challenge. To speed up the computation of #P-hard knot invariants, which can detect the entanglement types, we implement topological methods that simplify the geometric representation and drastically decrease the computational complexity.

Additionally, we investigate the potential application of specific neural network architectures for predicting entanglement, further accelerating these computations. In the context of proteins, the AI approach also holds promise for unveiling amino-acid sequences that contribute to the formation of knots themselves.

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