

Keynote: Knowledge Graphs for Explainable Scientific Discovery

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Abstract

Artificial intelligence is increasingly integrated into scientific discovery, but two key challenges remain: the integration of domain knowledge into models and the generation of explainable outputs that are scientifically relevant.

This talk explores the role of knowledge graphs in addressing these challenges through the lens of biomedical research with a particular focus on protein-protein interaction prediction and drug repurposing. It highlights the limitations of current knowledge graph embedding techniques, which, although able to integrate domain knowledge into models, often trade explainability for predictive performance, and examines recent advances in explainable approaches for semantic similarity, embeddings, and path-based reasoning.

It concludes with a vision of the future of scientific research, where artificial intelligence systems are able to generate scientifically meaningful outcomes grounded in domain knowledge, verifiable against existing evidence, and capable of advancing understanding.

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