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Interpretable Machine Learning for Astrochemistry

Friday 9 May 2025 09:40 (20 minutes)

Machine learning is revolutionizing astrochemistry by providing new ways to analyze complex datasets and accelerate computationally expensive models. However, interpretability remains a key challenge, especially when extracting physical insights from data-driven approaches. In this talk, I will present recent advancements in applying interpretable machine learning techniques to astrochemical problems, focusing on two case studies. First, I will discuss how neural networks and SHapley Additive exPlanations (SHAP) can be used to identify spectral features that retain key physical information in synthetic observations of prestellar cores. Second, I will showcase a novel approach that leverages autoencoders and optimization techniques to reduce the dimensionality of large chemical networks while maintaining accuracy and interpretability. These methods not only enhance our understanding of astrochemical processes but also provide practical tools for improving the efficiency of numerical simulations. I will conclude by discussing the broader implications of interpretable machine learning for astrophysical modeling and future directions for the field.

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