SKM 2023 – SOE Thursday

SOE 14: Networks: From Topology to Dynamics II (joint session SOE/DY)

Time: Thursday 9:30–10:00 Location: ZEU 260

Invited Talk SOE 14.1 Thu 9:30 ZEU 260 Networks in space and time – Exploring the physics in graph learning — •Ingo Scholtes — Julius-Maximilians-Universität Würzburg, Chair of Machine Learning for Complex Networks, Center for Artificial Intelligence and Data Science, D-97074 Würzburg, Germany

Network Analysis and Graph Neural Networks have become cornerstones for the application of data science and machine learning to complex systems. Addressing geometric machine learning in non-Euclidean data, I will introduce key concepts that help to apply deep learning to graphs. We cover message passing algorithms, convolutional filters, discrete Laplacians and neural representation learning and highlight

relationships between graph learning and physics.

We finally explore how time-resolved data on dynamic networks helps us to better understand complex systems and how we can incorporate the time dimension into deep graph learning. We introduce De Bruijn Graph Neural Networks (DBGNNs), a novel time-aware graph neural network architecture. Our approach accounts for temporal-topological patterns that unfold via causal walks, i.e. temporally ordered sequences of links by which nodes can influence each other over time. We develop a graph neural network architecture that utilizes De Bruijn graphs of multiple higher orders to implement a message passing scheme that follows a non-Markovian dynamics, which enables us to learn patterns in the causal topology of complex networks.