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Geometric Deep Learning, Graph Neural Networks, and Neural Diffusion Equations

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Symmetry as an organising principle has played a pivotal role in Klein's Erlangen Programme unifying various types of geometry, in modern physics theory unifying different types of interactions. In machine learning, symmetry underlies Geometric Deep Learning, a group-theoretical framework for a principled design of geometric inductive biases by exploiting symmetries arising from the structure of the respective domains and data on these domains.

In this talk, I will first showcase the Geometric Deep Learning Blueprint and how it can be used to derive some of the most popular deep learning architectures. Focusing on Graph Neural Networks (GNNs), I will make make connections to non-Euclidean diffusion equations and show that drawing on methods from the domain of differential geometry, it is possible to provide a principled view on such GNN architectural choices as positional encoding and graph rewiring as well as explain and remedy the phenomena of over-squashing and bottlenecks.

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Classification de Session: Representation Learning workshop