







## Lothar-Collatz-Seminar

Mon, 10. February  $\cdot$  11:00  $\cdot$  Geom 142

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## On Symmetry-Informed Machine Learning: Theory and Applications

Abstract: One of the main challenges in machine learning is undoubtedly pattern recognition. Interestingly, the term 'pattern' does not have a single, universally accepted rigorous mathematical definition in this context. Instead, it is often hidden behind even less accessible terms, such as 'regularities' or 'structures' within data. Emmy Noether showed that symmetry is the only constant in change. Therefore, this talk will introduce 'patterns' as symmetries in algebras of some classes of functions (with codomain a fixed field). Doing so will show that groups are essential for 'pattern' recognition. Unfortunately, groups are unhandy for computers for real-world applications due to their combinatoric nature. The complexity of the symbolic manipulations increases very quickly, making meaningful work almost impossible. Therefore, in this talk, we will introduce an approach where groups play the role of inductive bias. With computational invariant theory, we can write down a symmetry-loss without listing all group elements. As an application, we explore symmetries in molecular graphs with differentiable programming to predict compounds' in-vitro activity.

For further information please contact

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