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TRA Colloquium: Symmetries in AI4Science

Tuesday, 22 October 2024 16:15 (45 minutes)

Symmetries are of fundamental importance in all of science and therefore critical for the success of deep learning systems used in this domain.

In this talk, I will give an overview of the different forms in which symmetries appear in physics and chemistry and explain the theoretical background behind equivariant neural networks.

Then, I will discuss common ways of constructing equivariant networks in different settings and contrast manifestly equivariant networks with other techniques for reaching equivariant models.

Finally, I will report on recent results about the symmetry properties of deep ensembles trained with data augmentation.

Presenter: Prof. GERKEN, Jan