Deep Thinking Hour @amsterdam

Talk by

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Topic

AI4Science at Microsoft Research

Abstract

In July 2022 Microsoft announced a new global team in Microsoft Research, spanning the UK, China and the Netherlands, to focus on AI for science. In September 2022 we announced that we have also opened a new lab in Berlin, Germany, and recently another team in Redmond (USA) joined our initiative. In this talk I will first discuss some of the research areas that we are currently exploring in AI4Science at Microsoft Research, covering topics such as drug discovery, material generation, neural PDE solvers, electronic structure theory. Then I will dive a little deeper into two recent works that were done at AI4Science. First, I will cover work on the use of score-based generative modeling for coarse-graining (CG) molecular dynamics simulations. By training a diffusion model on protein structures from molecular dynamics simulations we show that its score function approximates a force field that can directly be used to simulate CG molecular dynamics. While having a vastly simplified training that our approach leads to improved performance setup compared to previous work, we demonstrate that our approach leads to improved performance across several small- to medium-sized protein simulations, reproducing the CG equilibrium distribution, and preserving dynamics of all-atom simulations such as protein folding events. If time permits, I will discuss our recent work on Clifford Neural layers for PDE modeling. The PDEs of many physical processes describe the evolution of scalar and vector fields. In order to take into account the correlation between these different fields and their internal components, we represent these fields as multivectors, which consist of scalar, vector, as well as higher-order components. Their algebraic properties, such as multiplication, addition and other arithmetic operations can be described by Clifford algebras, which we use to design Clifford convolutions and Clifford Fourier transforms. We empirically evaluate the benefit of Clifford neural layers by replacing convolution and Fourier operations in common neural PDE surrogates by their Clifford counterparts on two-dimensional Navier-Stokes and weather modelling tasks, as well as three-dimensional Maxwell equations.

About

The Deep Thinking Hour @Amsterdam is a series of seminars and panel discussions on interesting questions in Deep Learning, Machine Learning, Computer Vision. The Deep Thinking Hour is organized by Efstratios Gavves and his students at the University of Amsterdam.

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