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GNNs for generating molecules and PDE solutions

lundi 25 avril 2022 14:00 (1h 30m)

Graph Neural Networks (GNNs) have proven to be a versatile tool to predict properties of molecules, generative molecules and even predict solutions of a partial differential equation (PDE). Many physical application domains also exhibit symmetries which can be incorporated into the GNNs through equivariant convolutions or data augmentation. In this talk I will explain how this tool can be leveraged to generate molecules from their equilibrium distribution, possibly conditioned on some properties, and even predict solutions of a PDE.

Orateur: WELLING, Max (U. Amsterdam / MSR)

Classification de Session: Generative Models workshop