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3D Equivariant Graph Neural Networks for Drug Discovery

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Abstract

In this talk I will first review a very useful machine learning tool for pharmaceutical applications: the Graph neural Network (GNN). A GNN analyses a signal on graph structured data, such as molecules or knowledge graphs. We then define the concept of equivariance, an organizing principle that embues the neural network with the right transformation properties under symmetry transformations. For instance, a molecule has the same properties whether we rotate it in space or not. We will finally apply the new 3D equivariant graph neural network to molecular data and show that it can successfully predict properties that are relevant for drug screening. If time permits we will briefly describe further relevant generalizations of this technnology.

Biography:

Prof. Dr. Max Welling is a research chair in Machine Learning at the University of Amsterdam and a VP Technologies at Qualcomm. He has a secondary appointment as a fellow at the Canadian Institute for Advanced Research (CIFAR). Max Welling has served as associate editor in chief of IEEE TPAMI from 2011-2015. He serves on the board of the Neurips foundation since 2015 and has been program chair and general chair of Neurips in 2013 and 2014 respectively. He was also program chair of AISTATS in 2009 and ECCV in 2016 and general chair of MIDL 2018. He is a founding board member of ELLIS. Max Welling is recipient of the ECCV Koenderink Prize in 2010. He directs the Amsterdam Machine Learning Lab (AMLAB), and co-directs the Qualcomm-UvA deep learning lab (QUVA) and the Bosch-UvA Deep Learning lab (DELTA). He has over 300 publications in machine learning and an h-index of 68.

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