Special Issue

Machine Learning in Drug Discovery

Message from the Guest Editor

Time consumption, high cost, and great risk, significant attrition rates, among other factors, are hallmarks of drug discovery. Nevertheless, drug discovery has moved into a new paradigm with the introduction of machine learning technologies. Especially, the innovation and sophistication of machine learning algorithms as well as the development of high-throughput computing machines have further expedited the revolution. In fact, machine learning has been extensively applied to tasks including but not limited to homology modeling; hit identification; lead optimization; drug repurposing, de novo drug design; drug absorption, distribution, metabolism, excretion, and toxicity (ADME/Tox) assessments; and drug formulation development. The objective of this Special Issue is attempting to comprehensively cover all aspects associated with the applications and innovation of machine learning in drug discovery. In addition, it aims to explore the advantages and limitations of every machine learning algorithm and/or scheme. Finally, the future directions of machine learning and their applications will be addressed.

Guest Editor

Dr. Max Leong

Department of Chemistry and Department of Life Science and Institute of Biotechnology, National Dong Hwa University, Shoufeng, Hualien 97401, Taiwan

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Machine Learning and Knowledge Extraction
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
make@mdpi.com

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About the Journal

Message from the Editor-in-Chief

Machine learning deals with understanding intelligence to design algorithms that can learn from data, gain knowledge from experience and improve their learning behaviour over time. The challenge is to extract relevant structural and/or temporal patterns ("knowledge") from data, which is often hidden in high dimensional spaces, thus not accessible to humans. Many application domains, e.g., smart health, smart factory, etc. affect our daily life, e.g., recommender systems, speech recognition, autonomous driving, etc. The grand challenge is to understand the context in the real-world under uncertainty. Probabilistic inference can be of great help here as the inverse probability allows to learn from data, to infer unknowns, and to make predictions to support decision making.

Editor-in-Chief

Prof. Dr. Andreas Holzinger
1. Human-Centered AI Lab, Institute of Forest Engineering, Department of Ecosystem Management, Climate and Biodiversity, BOKU University, Vienna, Austria
2. Institute of Human-Centered Computing, Faculty of Computer Science and Biomedical Engineering, Graz University of Technology, Graz, Austria
3. xAI Lab, Alberta Machine Intelligence Institute, University of Alberta, Edmonton, AB, Canada

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