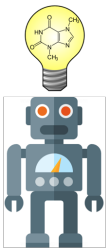

Novel Directions of Applying Machine Learning in Cheminformatics

Special session at 6th Symposium on Conformal and Probabilistic Prediction with Applications (COPA 2017) on 14-16 June, 2017, in Stockholm, Sweden

Session overview

There has been a renewed interest in novel machine learning techniques in drug discovery during the last years. This has been driven both by novel methods, access to larger and imbalanced datasets as well progress in high-performance computing. For example, methods like conformal prediction, deep learning and matrix factorization have already made significant impact and are part of making the drug discovery process more data driven and efficient. In this session we will mainly focus on the cheminformatics aspects. The speakers will describe the current state of the art, bottlenecks and future directions covering topics like de novo design of novel molecules, improve accuracy in activity prediction, and confidence estimation. The presentations will be followed by round table discussions focusing on current challenges and future opportunities.

Call for papers

Authors are invited to submit original, English-language contributions of all kinds related to machine learning in cheminformatics. Submitted papers will be refereed for quality, correctness, originality, and relevance. Notification and reviews will be communicated via email. All accepted papers must be presented at the conference and will be published by JMLR Workshop and Conference Proceedings (volume 60). The deadline for submissions is February 10th, 2017.

Accepted papers in the special session *Novel Directions of Applying Machine Learning in Cheminformatics* will be invited to submit an extended version of their manuscripts to a special issue in Journal of Cheminformatics.

For more information and submission guidelines - see COPA 2017 website:

http://clrc.rhul.ac.uk/copa2017/