Special Issue

Novel Applications of Machine Learning and Bayesian Optimization, 2nd Edition

Message from the Guest Editors

Machine learning and Bayesian optimization are transforming applied sciences by enabling data-driven discovery, prediction, and decision-making. For example, in the chemical and molecular sciences, machine learning accelerates the discovery of novel materials and powers data-driven force fields. In biomedical and clinical sciences, it supports image analysis, disease diagnosis, and predictions of patient outcomes. In the environmental and Earth sciences, machine learning is used to forecast earthquake probabilities and automate the detection of environmental hazards such as litter. Large language models are opening further avenues, from automating hypothesis generation, to generating code for computational experiments. When data are scarce or expensive to obtain, Bayesian optimization plays a crucial role in experimental design, parameter tuning, and exploring trade-offs, and has a long history in engineering design. This Special Issue will publish high-quality, original research papers advancing the state of the art in the application of machine learning and/or Bayesian optimization

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As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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