Palestra ACorner/IST

Ruth Misener

Professor in Computational Optimisation

Department of Computing

Imperial College London

https://www.imperial.ac.uk/people/r.misener

Autonomous research machines: Self-optimizing new chemistry

Our research seeks to boost R&D efficiency in the chemicals industry. As an example, consider "micro reactor flow systems", which are transforming chemical manufacturing by enabling flexible prototyping. Because these high-throughput microfluidic devices can control reaction conditions online, they are ideal for quantitatively characterizing diverse chemical synthesis techniques along new reaction pathways. The challenge is: How do we automate the design of experiments to "self-optimise" new chemistry? Together with the BASF Data Science for Materials & Chemistry teams, we're interested to solve Bayesian optimization challenges which may simultaneously exhibit: multiple objectives, mixed-feature spaces, asynchronous decisions, large batch sizes, input constraints, multi-fidelity observations, hierarchical choices, and costs associated with switching between experimental points. We review the machine learning contributions that we've found useful towards achieving these goals and discuss our own methodological and software contributions.

This work is a collaboration between Imperial (Jose Pablo Folch, Alexander Thebelt, Shiqiang Zhang, Jan Kronqvist, Calvin Tsay, Ruth Misener) and BASF (Robert Lee, Behrang Shafei, Nathan Sudermann-Merx, David Walz).

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