Gaussian Processes for Hybridizing Analytical & Data-Driven Decision-Making

Surrogate models are widely appreciated in chemical engineering. The typical setting focuses on expensive-to-evaluate, possibly uncertain functions. Resources are typically limited, so effective decision-making requires data-efficient learning.

The data science and statistical machine learning communities typically focus on models learned solely from observed data. But chemical engineering applications may also require explicit, parametric models, e.g. modeling known process constraints, operations constraints, and cost objectives. So prior work has integrated semi-algebraic functions with those learned from data or developed semi-physical modeling techniques.

We consider new three probabilistic modeling applications and extend methodologies to meet these hybrid situations:

**Design of experiments for model discrimination.** We bridge the gap between classical, analytical methods and Monte Carlo-based approaches. Classical methods may have difficulty managing non-analytical model functions and data-driven Monte Carlo approaches come at a high computational cost. We replace the original, parametric models with probabilistic, non-parametric Gaussian process surrogates learned from model evaluations. The surrogates are flexible regression tools that extend classical analytical results to non-analytical models, while providing us with model prediction confidence bounds and avoiding the computational complexity of Monte-Carlo approaches.

**Multi-objective optimization.** We make novel extensions to Bayesian multi-objective optimization in the case of one analytical objective function and one black-box, i.e. simulation-based, objective function. The resulting method has been applied to a bone neotissue application and a more general test suite.

**Scheduling plant operations under uncertainty.** For processes with equipment degradation, we use historical data and Bayesian optimisation to approximate the uncertainty set for large-scale, mixed-integer optimization models.

We close by offering a broad outlook on applying probabilistic surrogate models to chemical engineering.

**Tuesday, Dec. 4, 2018**
Lecture at 4:00 p.m.
Room 1610, Engineering Hall
Refreshments will be served at 3:45 p.m.