On tactical and strategic decision making for chemical and energy systems under uncertainty

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Abstract

Most tactical and strategic decisions in process industries, such as research & development (R&D), capital, and infrastructure investments, are made in highly uncertain environments. The explosion of the alternatives with increasing uncertainty prohibits the generation of a comprehensive search space for such problems, and limits the applicability of existing tools and methods. This talk will give an overview of our research activities on surrogate model generation and derivative-free optimization for process synthesis and design of multi-scale processes, and on efficient solution algorithms for optimization under endogenous and exogenous uncertainty for strategic decision making. Superstructure optimization is, in theory, a very powerful approach to address tactical problems such as process synthesis for energy applications. However, the resulting mathematical program is difficult, and in some cases impossible, to solve. Surrogate models, simpler functional representations of the underlying complex system, can be used to simplify the problem. We developed sequential design algorithms to construct accurate surrogate models to be used in optimization problems. These algorithms scale well to problems in high dimensions, and investigate the trade-off between space-filling and adaptive nature of sampling methods. Our results reveal that an adaptive sampling approach is required in order to accurately model strong nonlinearities. Optimization problems with decision-dependent, i.e., endogenous, uncertainty are commonly observed in process industry, e.g., synthesis of process networks with uncertain process yields, R&D pipeline management, and biomass-to-commodity chemicals investment planning. Despite this, mostly due their challenging nature, the research community strayed away from these problems. We have recently developed a novel heuristic approach that decomposes the original multi-period multi-stage stochastic program into a series of Knapsack problems, which are then solved at appropriate decision points of the planning. Our computational results suggest that the solutions obtained provide tight lower bounds for the original problem (assuming maximization), and with several orders of magnitude reduction in solution times. The upper bounds are generated using progressive hedging and the lower bound solutions. The resulting algorithm is readily parallelizable with characteristics resembling embarrassingly parallel problems.

Short Bio

Dr. Cremaschi is an associate professor of chemical engineering at The University of Tulsa. Her research interests are risk management, optimization, and process synthesis under uncertainty. Her research group works at the intersection of operations research and chemical engineering, and develops systems analysis and decision support tools for complex systems, mainly focusing on energy area. She was the recipient of a Tulsa Tau Beta Pi Teaching Excellence award (2010), an NSF CAREER award (2011), and a Zelimir Schmidt Award for Outstanding Researcher (2013) among others. She earned her Ph.D. degree from Purdue University, and both her B.S. and M.S. degrees from Bogazici University (Turkey), all in chemical engineering.