Optimization of Process Systems under Uncertainty

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Optimization under uncertainty has been an active and challenging area of research for many years. However, its application in Process Synthesis has faced a number of important barriers that have prevented its effective application. Barriers include availability of information on the uncertainty of the data (ad-hoc or historical), determination of the nature of the uncertainties (exogenous vs. endogenous), selection of an appropriate strategy for hedging against uncertainty (robust optimization vs. stochastic programming), handling of nonlinearities (most work addresses linear problems), large computational expense (orders of magnitude larger than deterministic models), and difficulty in the interpretation of the results by non-expert users.

In this course, we describe recent advances that address some of these barriers. We first describe the basic concepts of robust optimization, including the robust counterpart, showing its connections with semi-infinite programming. We also we explore the relationship between flexibility analysis and robust optimization for linear systems. A historical perspective is given, which shows that some of the fundamental concepts in robust optimization have already been developed in the area of flexibility analysis in the 1980s. We illustrate the application of robust optimization to a petrochemical complex with uncertain demands, as well as in the production scheduling of cryogenic energy storage systems under changes in the pricing of electric power and including management of reserve demand. We next consider two-stage and multi-stage stochastic programming in the case of exogenous parameter. We review Benders decomposition and Lagrangean decomposition to solve these problems for large number of scenarios. We describe acceleration techniques for Benders decomposition, hybrid sub-gradient/cutting plane methods for Lagrangean decomposition, and sampling techniques. We illustrate these techniques in the synthesis of integrated water networks under uncertainty, and in the design of supply chains under disruptions. We then address the the case of both exogenous and endogenous parameters, which gives rise to conditional scenario trees for which theoretical properties are described to reduce the problem size. We propose a heuristic solute method coupled with Lagrangean decomposition, and illustrate these techniques in the design of oil and gas fields. To avoid ad-hoc approaches for setting up the data for these problems, we describe approaches for handling of historical data for generating probabilities and outcomes for scenario trees. We apply these techniques to a process with uncertain yields and product demands, and for which historical data are available.