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Recent advances in mathematical programming techniques for the optimization of process systems under uncertainty

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ABSTRACT

Optimization under uncertainty has been an active area of research for many years. However, its application in Process Systems Engineering 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/chance constrained optimization vs. stochastic programming), large computational expense (often orders of magnitude larger than deterministic models), and difficulty of interpretation of the results by non-expert users. In this paper, we describe recent advances that have addressed some of these barriers for mostly linear models.

1. Introduction

Optimization under uncertainty has been an active area of research in Process Systems Engineering, with applications ranging from synthesis and design, to planning, scheduling, control and supply chain optimization. General reviews on various aspects of uncertainty in Process Systems Engineering can be found in Sahinidis (2004), Li and Ierapetritou (2008a) and Grossmann et al. (2014).

It is interesting to note that there is a long history of optimization under uncertainty in Process Systems Engineering. The initial work was mostly focused on optimal design problems using stochastic programming as the major framework. Examples include the papers by Takamatsu et al. (1973), Dittmar and Hartmann (1976), Johns et al. (1978), and Grossmann and Sargent (1978). The next phase addressed planning problems under uncertainty, where examples of papers in this area include Liu and Sahinidis (1996), Acevedo and Pistikopoulos (1998), Gupta and Maranas (2000), and Applequist et al. (2000). The more recent trend has been to adopt robust optimization as a strategy for optimization under uncertainty, where it is interesting to point out that the work by Friedman and Reklaitis (1975a,b) was well ahead of its time with linear programming with uncertain coefficients; other examples include the papers by Swaney and Grossmann (1985) with the emphasis on flexibility, and Lin et al. (2004) with applications in the scheduling area. Finally, the other major approach has been based on chance constrained optimization which has been pioneered by Prof. Wozny (e.g., Li et al. (2008)).

Optimization under uncertainty has been motivated by the fact that parameters involved in optimization models for synthesis, design, planning, scheduling and supply chains are often uncertain. Typical parameters include product demands, prices of chemicals, product yields, oil reservoir sizes, and technical parameters like kinetic constants or transfer coefficients. Yet, despite the importance of accounting for uncertainties, the impact of techniques for optimization under uncertainty at the level of applications has been limited. This has been due to a number of modeling and computational barriers. In this paper, we first provide a brief overview of the area, and then describe some recent advances that are facilitating the wider deployment and application of optimization under uncertainty.

A major modeling decision in optimization under uncertainty is whether one should rely on robust optimization (Lin et al., 2004; Ben-Tal et al., 2009; Li and Ierapetritou, 2008b), or whether one should use stochastic programming (Ierapetritou and Pistikopoulos, 1994; Subrahmanyam et al., 1994; Iyer and Grossmann, 1998; Schultz, 2003; Ahmed and Garcia, 2003; Li and Ierapetritou, 2012). The basic idea in the robust optimization approach is to guarantee feasibility over a specified uncertainty set, while in stochastic programming a subset of decisions are made by anticipating that recourse actions can be taken once the uncertainties are revealed over a pre-specified scenario tree with discrete probabilities of the uncertainties. In general, this means that robust

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optimization will predict more conservative results compared to stochastic programming.

On the one hand, the robust optimization approach tends to be more appropriate for short-term scheduling problems in which feasibility over a specified set of uncertain parameters is a major concern, and when there is not much scope for recourse decisions. The stochastic programming approach, on the other hand, tends to be more appropriate for long-term production planning and strategic design decisions, since it does not fix all decisions at the initial point of the planning horizon as it allows recourse decisions to be made at future time points to adapt in response to how the uncertainties are revealed. It should also be noted that chance constrained optimization can be regarded as a generalization of robust optimization in which distribution functions are specified for the uncertainties with which a level of probability for meeting the feasibility of the constraints is specified (Li et al., 2008).

Computationally, stochastic programming problems tend to be very expensive to solve. This is particularly true if one has to deal with both exogenous and endogenous parameters, where the realization of the latter depends on the decisions taken (e.g., oilfield size), while the former are independent of decisions (e.g., demands) (Jonsbråten, 1998). Chance constrained programming is also computationally challenging, especially when the level of probability is specified for joint constraints. Robust optimization tends to be the least computationally expensive, especially for linear problems. In all cases, however, it is of great importance to have as a basis a computationally efficient deterministic model since adding uncertainty unavoidably adds complexity to the computations. Aside from the computational issues, there is also the question of how to specify the uncertainties (e.g., an intuitive guess or through statistical analysis of historical data) and how to interpret the results that are predicted from the various models.

In this paper, we address the following specific challenges in optimization under uncertainty: (a) how to account for recourse in robust optimization to make it less conservative, (b) how to effectively solve two- or multi-stage stochastic optimization problems to avoid excessive computational times, (c) how to effectively handle both exogenous and endogenous uncertainties in multi-stage stochastic programming, and (d) how to incorporate historical data in the generation of scenarios instead of relying on intuition. As will be shown, significant progress has been made to address these issues in MILP models with uncertainty.

2. Decision rule approach for modeling recourse in robust optimization

Robust optimization (Ben-Tal et al., 2009) is one approach for incorporating uncertainty in optimization models. The uncertainty is specified in terms of an uncertainty set in which any point is a possible realization of the uncertainty. The goal is to find a solution that is feasible for all possible realizations of the uncertainty while minimizing (or maximizing) the objective function. Since the worst-case scenario is one of the possible realizations, a robust optimization model returns a solution that is optimal for this particular scenario. However, considering the worst case is often overly conservative. One can reduce the level of conservatism by appropriately adjusting the size of the uncertainty set. Bertsimas and Sim (2004) propose such an approach in which a pre-specified "budget" parameter limits the number of uncertain parameters that can change at the same time.

The general robust formulation for a linear model is as follows:

$$\min_x \{c^T x : A(u)x \leq b \quad \forall u \in U\} \tag{1}$$

where the parameter u is uncertain and defined over the corresponding uncertainty set U in which we assume the uncertainty budget is included. Eq. (1) corresponds to a semi-infinite programming problem, but can be simplified by considering the dual of each row in the matrix A (robust counterpart), which yields a finite dimensional optimization problem. A drawback with this approach is that specifying the uncertainty set U is not trivial, not only because the uncertainty set might not be well known, but also because the user has to specify the uncertainty "budget" ranging from very conservative (all parameters vary independently) to less risk-averse (e.g., limiting the number of independent variations). Another reason for over-conservatism in traditional robust optimization is the disregard of recourse (i.e., reactive actions after the realization of the uncertainty), which is a very unrealistic assumption in many cases, such as in problems involving investment and long-term contract decisions. In this section, we present a recent development in robust optimization that allows recourse to a certain extent, and demonstrate the effectiveness of this method by applying it to an industrial scheduling problem.

2.1. The affine decision rule approach

Consider the following multi-stage (T stages) optimization problem under uncertainty:

$$\min_x \left\{ c^T x_1 : A_1(u)x_1 + \sum_{t=2}^{T} A_t x_t(u) \leq b \quad \forall u \in U \right\} \tag{2}$$

where x_t is the vector of the t-th-stage variables. We assume that the objective function only depends on x_1 and that only matrix A_1 is uncertain (fixed recourse). While x_1 does not depend on u, x_t for $t \geq 2$ are recourse variables and depend on the realization of the uncertainty. Note that x_t only depends on the u that are realized up to stage t.The problem given in Eq. (2) cannot be solved as such since the set of possible functions for $x_t(u)$ is infinitely large. The idea in the decision rule approach (Ben-Tal et al., 2004), also referred to as adjustable robust optimization, is to restrict oneself to a certain type of functions for $x_t(u)$, in particular to the set of affine functions. Hence, we set $x_t(u) = \alpha_t + B_t u$, and we obtain the following robust formulation by constraint-wise construction:

$$\min_{x_1,\alpha,B} \left\{ c^T x_1 : \max_{u \in U} \left\{ a_{1,i}^T(u)x_1 + \sum_{t=2}^{T} a_{ti}^T(\alpha_t + B_t u) \right\} \leq b_i \quad \forall i \right\} \tag{3}$$

which can be reformulated into a single-level problem for certain types of uncertainty sets by using techniques applying strong duality. This results in a robust counterpart formulation in which the decision variables are x_1 as well as the parameters for the affine decision rules, α and B. By applying the decision rule approach, the multi-stage problem is transformed into a single-stage problem to which the classic robust optimization reformulation is applied. Obviously, it is quite restrictive to only consider affine functions; however, this allows us to retain computational tractability and still account for recourse to a certain extent (for rigorous treatment of recourse see Grossmann et al. (2014), Zhang et al. (2016a)). The decision rule approach has been successfully applied to various operations research problems, such as inventory management (Ben-Tal et al., 2004), project management (Chen and Zhang, 2009), and logistics planning (Ben-Tal et al., 2011). In fact, it cannot only be applied to robust optimization, but also to stochastic programming (Kuhn et al., 2011). However, application of this approach in the process systems engineering literature is still very scarce.

2.2. Industrial case study: air separation plant providing interruptible load

To ensure the stability of the power grid, backup capacities are called upon when electricity supply does not meet demand due to unexpected changes in the grid. Traditionally, such operating reserve is provided by generating facilities with short ramp-up