Advances in Robust Optimization and Opportunities for Process Operations

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Abstract

Robust optimization constitutes an approach for handling parameter uncertainty in the context of a mathematical optimization model. Despite having been around for a few decades and being a relatively well-known approach by now, it has arguably lagged behind other alternatives (e.g., stochastic or chance-constrained programming) in terms of applications in which it has been considered. This can be partly attributed to certain theoretical limitations in earlier robust optimization frameworks as well as to the misconception of "being too conservative" of an approach, steering many researchers and practitioners away from adopting it as a risk mitigation tool. However, recent advances in theory and methods have alleviated many of the previous concerns and have made robust optimization particularly attractive for practice, both from the viewpoint of conceptual fit as well as for the numerical tractability benefits it can offer. In this paper, we briefly review the current state-of-the-art in robust optimization and demonstrate its applicability in two example pieces of our work.

Keywords

Process operations, Robust optimization, Parameter uncertainty, Multi-stage decision-making

Introduction

A generic form of an optimization problem with uncertain parameters is presented in Formulation (1), where x represents a vector of decisions to be determined and ξ represents a vector of parameters whose exact value is unbeknownst to the decision-maker at the time of optimization.

$$\begin{aligned} \min_{x \in X} \quad & f(x, \xi) \\ \text{s.t.} \quad & g_i(x, \xi) \leq 0 \quad \forall i \end{aligned} \tag{1}$$

In order to cope with this uncertainty, Robust Optimization (RO) seeks to identify solutions that remain feasible under any realization of the parameters from within an *uncertainty set*, Ξ, which is chosen by the modeler a-priori. This set constitutes a comprehensive collection of all parameter realizations that the modeler wishes to insure against, and it can be linked to a confidence interval for probabilistic constraint satisfaction. In general, an uncertainty set may consist of a continuum of parameter realizations, collections of discrete scenarios, or their combinations. Out of all those solutions that retain their feasibility for all $\xi \in \Xi$, a.k.a., *robust feasible* solutions, RO selects the one that yields the best "worst-case" outcome given all possibilities.

Consequently, RO can be represented by the bi-level Formulation (2), which is referred to as the *robust counterpart* of the original problem, and which can be addressed via semi-infinite programming techniques. This typically involves the invocation of duality arguments to reformulate it into a monolithic formulation that can be solved directly.

$$\begin{aligned} \min_{x \in X} \quad & \max_{\xi \in \Xi} f(x, \xi) \\ \text{s.t} \quad & g_i(x, \xi) \leq 0 \quad \forall \xi \in \Xi, \forall i \end{aligned} \tag{2}$$

From a game-theory perspective, the above problem constitutes a Stackelberg game in which the leader controls the decision variables, x, and the adversarial follower controls the realization of uncertainty, ξ. The main principle governing this game is *Wald's maximin criterion*, which dates back to the 1940s and the development of statistical decision theory. Three decades later, Soyster (1973) studied this problem from a math-

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ematical optimization perspective and introduced a methodology that ensured feasibility of a linear problem under all possible perturbations around each uncertain parameter's nominal value. Since this may be too conservative in a practical setting, subsequent seminal works introduced more elaborate uncertainty sets that generally lead to less conservative solutions (we review such sets later). A concept similar to RO is that of Flexibility Analysis, which was developed independently in the context of studying feasibility of chemical process designs. Its relationship to RO was comprehensively articulated in Zhang et al. (2016).

Generally speaking, RO is particularly suitable in cases where loss of feasibility cannot be tolerated (e.g., due to system safety concerns), is not meaningful (e.g., equipment physical limitations), or cannot be reasonably penalized (e.g., no way to "monetize" infeasibility). However, RO can–and should–be considered also in contexts where the above do not hold. In fact, doing so may offer a number of advantages as compared to its alternatives. For one, RO often features good computational tractability, since in many cases the fully reformulated RO counterpart is in the same problem class as the deterministic problem itself. Furthermore, it can be applied in cases where detailed knowledge of probability distributions is not available. The more coarse description of uncertainty in the form of an uncertainty set, which is a collection of correlations among parameter values, can be readily extracted from any historical data. In general, these correlations may apply conditionally upon our own decisions, allowing us to capture also the endogenous stochastic behavior of a system.

Critics of RO have often dubbed it "too conservative," due to its focus on "worst-case" objective. It is important to highlight, however, that the choice of the uncertainty set rests with the modeler, who can judiciously choose the shape and size of the set so as to meet the tolerable risk profile. In fact, a hierarchy of optimal solutions across a range of uncertainty sets should be sought to better understand the *price of robustness* in each application of interest. In the author's view, a more substantial historical limitation of RO was the fact that it used to be restricted to single-stage decision-making settings, without the versatility to incorporate recourse decisions, or at least one had to make significant approximations in the form of applicable recourse. However, recent developments (briefly reviewed later) have opened many possibilities for multi-stage optimization via the RO approach.

In the context of Process Operations, in particular, where typically the mathematical models are of (mixed-integer) linear nature and feature too many parameters, using RO so as to mitigate the risk of our decisions makes good sense. In fact, in the usual paradigm of applying decision-making in a rolling horizon fashion, using a risk-averse framework like RO to obtain decisions at each iteration improves the likelihood of maintaining closed-loop feasibility over long periods of time, in contrast to using decisions based on deterministic or other stochastic models.

Uncertainty Sets

As discussed, a robust optimization model is associated with a specific uncertainty set that has been chosen by the modeler to this purpose. The most commonly utilized uncertainty sets are norm-based, as shown in Eq. (3). Here, ξ can be interpreted as the vector of normalized deviations of the uncertain parameters from their nominal values. For $p \to 0$, the set assumes that only a given number of uncertain parameters may deviate from their nominal values in any real-life scenario; for $p = 1$, the single budget set assumes that the cumulative absolute deviation from the nominal scenario shall be bounded; for $p = 2$, the ellipsoidal set assumes that the parameter realizations are jointly distributed normally; finally, for $p \to \infty$, the rectangular (a.k.a., "box") set assumes independent parameter realizations.

$$\Xi = \left\{ \xi \in \mathbb{R}^n \middle| \; \|\xi\|_p \leq \alpha \right\} \tag{3}$$

The prolific use of the above sets in RO literature is both due to their simplicity of representation as well as the fact that they often suffice to represent correlations among uncertain parameters that are observed in historical process data. Intersections among these sets are further suggested in Li et al. (2011). A straightforward extension is the general polyhedron uncertainty set of Eq. (4), which concurrently accommodates all affine correlations among subsets of parameters that can be postulated. Another polyhedral uncertainty set that one may use is the factor-model set (a.k.a., *net-alpha model*) of Eq. (5), which has been proposed to deal specifically with settings that feature a large number n of uncertain parameters. This set insures against all realizations whose weighted deviation from the nominal scenario is bounded. In effect, this reduces the dimensionality of the uncertainty down to a small number m ($m \ll n$) of random variables (i.e., the factors ϕ).

$$\Xi = \left\{ \xi \in \mathbb{R}^n \,\middle|\, \sum_{i=1}^{n} h_{ji}\xi_i \leq g_j,\ \forall\ j \right\} \tag{4}$$

$$\Xi = \left\{ (\xi, \phi) \in \mathbb{R}^n \times \mathbb{R}^m \,\middle|\, \begin{array}{c} \xi_i = \sum\limits_{f=1}^{m} \alpha_{if}\phi_f,\ \forall\ i \\ \left| \sum\limits_{f=1}^{m} \phi_f \right| \leq \beta m \\ \phi_f \in [-1, +1],\ \forall\ f \end{array} \right\} \tag{5}$$

The various coefficients and right-hand-sides referenced in a set are to be chosen by the modeler in a way that reflects the desirable level of risk tolerance. Efficient data-driven uncertainty set construction is currently an active field of research. As an example, we refer the interested reader to the work by Bertsimas et al. (2013), who proposed a scheme based on statistical hypothesis tests and machine learning techniques to determine the set. It should also be noted that, given distributional information about parameter realizations, bounds on the probability of constraint satisfaction as a function of the set's shape and size can be derived for many of the sets described above, while the sets themselves can be chosen so as to satisfy desirable confidence intervals (Guzman et al. (2016) and references therein).

A typical RO approach utilizes uncertainty sets whose coefficients and right-hand-sides are predetermined constants. However, there are cases where the optimization decisions can have a direct impact upon the uncertainty itself. Such *endogenous* uncertainty arises when decisions lead a parameter to lose its physical meaning (e.g., the processing time of a task that never occurred), realize at a different point in time (e.g., we learn the true demand of a product only after the period we launch it into the market), or adhere to a different probability distribution (e.g., a decision to install a more established technology reduces the range of possible yields that will be achieved). In these contexts, one may use an uncertainty set where the various coefficients and right-hand-sides are functions of the decisions, x, appropriately modeling the underlying dependencies. For example, a decision-dependent counterpart of the generic polyhedron uncertainty set of Eq. (4) is shown in Eq. (6). More details about the use of decision-dependent sets in the context of RO can be found in Lappas and Gounaris (2017).

$$\Xi(x) = \left\{ \xi(x) \in \mathbb{R}^n \,\middle|\, \sum_{i=1}^{n} h_{ji}(x)\,\xi_i \leq g_j(x),\ \forall\ j \right\} \tag{6}$$

Solution Approaches

Although RO can be applied on non-linear problems (Ben-Tal et al., 2015) or even problems described via simulations (Bertsimas et al., 2010b), the majority of the literature focuses on problems whose deterministic instantiations can be represented as mixed-integer linear models.[1] With this in mind, two major solution avenues can be followed to obtain optimal solutions to the robust counterparts of those problems.

The standard approach is based on reformulating (2) by first converting the semi-infinite constraints into inner maximization subproblems, which can then be dualized towards a single-level optimization problem. When one utilizes polyhedral uncertainty sets, linear duality principles apply and the linear structure of the deterministic model persists in the robust counterpart. However, using ellipsoidal sets results to (convex) conic optimization problems. A second approach is the *robust cutting plane method* (Mutapcic and Boyd, 2009), which is based on the procedural enforcement of robust feasibility by adding select instantiations of constraints for some key parameter realizations from within the set. The process starts by optimizing a deterministic model for some nominal parameter realization, $\xi^0 \in \Xi$, after which the solution x^* is checked for robust feasibility across the whole set of interest. This entails solving a sequence of optimization problems (one per constraint)[2]–with the uncertain parameters being the variables–, in order to separate realizations $\xi^* \in \Xi$ under which the current solution x^* violates some constraint; the latter is then added in the master problem and the process repeats until full robust feasibility is satisfied.

It should be mentioned here that a well-known point of concern for the above RO solution approaches pertains to how to handle equality constraints that reference uncertain parameters. The challenge stems from the fact that satisfying an equality for any possible parameter realization reduces the feasible region dramatically. Gorissen et al. (2015) synopsize typical problem-specific workarounds, including relaxation to inequalities and state-variable elimination. In certain cases, it may possible to defer certain decisions for later, apply affine decision rules (discussed later) and reformulate the semi-infinite equalities via "coefficient-matching."

[1] This generally suffices for the vast majority of process operations applications.

[2] The separation problems can be merged into a single mixed-integer problem using disjunctive logic.

Multi-stage Robust Optimization

A multi-stage decision making setup is one where the set of parameters realizes gradually, with different subsets of parameters realizing at different points in time, and where decisions are to be taken at each time interval in-between. In general, decisions in stage t may depend on parameter realizations, but only those realizations that have occurred up and until stage $t-1$, since the decision maker has not yet had the opportunity to observe the rest. The T-stage setting is depicted below:

$$x^1 \to \xi^1 \to x^2(\xi^1) \to \ldots \to \xi^{T-1} \to x^T(\xi^1, \ldots, \xi^{T-1}).$$

A special case is that of two stages, where the decisions are split into two sets, the *here-and-now* decisions, which are taken before we had the opportunity to observe the realization of any parameters, and the *wait-and-see* decisions, which are taken after all parameter values have been revealed. The latter set of decisions often represent recourse actions to restore feasibility. The two-stage setting is generally adequate to address problems that fit into the classical "invest capacities–observe demands–operate network" or the "design control scheme–observe disturbances–tune controller" paradigms. In contrast, problems with more than two stages usually arise in multi-period planning problems, scheduling problems based on multiple event points, or moving-horizon estimation.

Multi-stage RO problems are usually hard, and much of the methodological background necessary to tackle them tractably is still eluding researchers. Some sort of approximation is typically sought, which in turn results into models exhibiting a non-zero *adaptability gap*.[3] The most often used–and also most conservative–approximation is that of a static model, where all $x^t(\xi)$ are chosen as constant (in ξ). Static models are generalized with the concept of *adjustable* RO, where non-constant functional dependencies are postulated (Ben-Tal et al., 2004). Affine and piecewise-affine functions are the most commonly used, and a review of applications can be found in Bertsimas et al. (2011). Bertsimas et al. (2010a) discuss cases when such *decision rules* suffice for full adaptability (e.g., as shown in Gounaris et al. (2013) in the context of vehicle routing), but this is usually not the case. Another limitation of such decision rules is that they can only be used to adjust continuous decisions. For problems with integer recourse, piecewise-constant rules have been proposed (Bertsimas and Georghiou, 2014). Application of decision rules is generally possible in the case of fixed-recourse, with recent works extending them for random-recourse (Bertsimas and Georghiou, 2015). Note that the RO concept of decision-rule based approximation can also be applied to stochastic programming models (Kuhn et al., 2011).

Deriving optimal solutions to fully adaptable models is currently only possible for two-stage problems. One way to do this is to follow a Benders dual cutting-plane approach (Thiele et al., 2010), which can however only handle pure continuous recourse. Furthermore, this method does not provide an explicit solution for the second stage, rather only an implicit guarantee of robust feasibility. The main alternative is to work in the primal space via a constraint-and-column generation procedure (Zeng and Zhao, 2013), which identifies a violating scenario at each iteration and introduces a new scenario-specific policy to insure against it. Although this approach can accommodate mixed-integer recourse, one pays the price of having to solve increasingly larger subproblems. There is also no way to control the number of policies so derived, which may be undesirable in practice when the operators need to be trained on how to implement recourse actions. In these situations, the ability to derive only a limited number of "good" and collectively-robust contingency plans is of importance.

On a related note, Bertsimas and Caramanis (2010) proposed the concept of *finite adaptability*, whereby the fully adaptable solution is approximated by a finite set of a priori computed recourse policies. The goal is to identify which policy shall apply against each parameter realization. The authors derived conditions for when a finite adaptability approach may improve upon the static (i.e., "1-adaptable") robust solution, and they provided a heuristic algorithm to a-priori partition the uncertainty set into policy-specific regions. Alternative methods to partition the set were proposed in Bertsimas and Dunning (2016) and Postek and den Hertog (2016). Hanasusanto et al. (2015) were the first to propose a tractable method to address to guaranteed optimality two-stage finite adaptability problems for any a-priori chosen number of policies. They derived a mixed-integer linear model that yields the best set of K policies for the case of pure binary problems. Finally, it should be mentioned that the concepts of finite adaptability and decision rules can in principle be combined so as to enhance the approximation of the multi-stage problem.

[3] The adaptability gap of a model is defined as the ratio between its resulting solution and the best-possible–yet unknown–solution of any non-anticipative model.

Example Applications

In our first application, we apply affine decision rules in the multi-stage setting of process scheduling optimization (Lappas and Gounaris, 2016). Although various combinations of variables can be chosen for such adjustment, we found that adjusting only the timing variables provides for the best trade-off between solution quality and tractability (Figure 1). In this work we also introduced novel decision-dependent uncertainty sets to capture the endogenous nature of uncertain parameters, such as parameters associated with tasks that may or may not be chosen in the optimal solution. Other highlights included the fact that robust solutions were obtained for the first time in the open literature for instances with zero-wait states as well as instances with uncertainty in process yields. Our results illustrate that the multi-stage robust solutions significantly improve upon the static ones, both in terms of worst-case objective as well as objective in expectation.

For our second application, we study the tactical planning vehicle routing problem (VRP) with uncertain customer orders (Subramanyam et al., 2016), whereby a distributor plans a set of delivery routes for a number of upcoming periods. Uncertainty exists in the exact composition of the customer base, since customers are allowed to call in between deliveries and place additional orders. Consequently, it is important to derive routing plans that retain sufficient flexibility to be adapted once additional demand realizes (Figure 2). We derive a two-stage approximation of the full, multi-stage problem, and we prove that it always yields non-anticipative solutions. We also quantified their adaptability gap by computing anticipative lower bounds of the fully adaptable solutions. Results based on literature benchmarks indicate that a relatively small risk premium of the order of a few percent needs to be incurred so as to accommodate up to 50% additional customer orders placed later via calls. This work constitutes the first time in the open RO literature that addresses a multi-period VRP as well as the first time that the discrete uncertainty of customer presence is accounted for in an RO setting.

Conclusions

This article briefly highlighted some of the recent theoretical and methodological advances that have occurred in the field of RO. Our thesis is that these developments have positioned RO as a very meaningful and efficient approach for addressing uncertainty in process operations contexts, and we hope to have motivated more members of our community adopt it in their work.

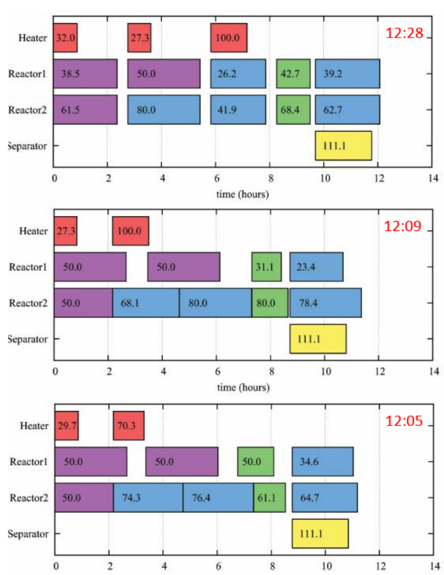

Figure 1. Three robust optimal minimum makespan schedules under the same level of uncertainty in task processing times, plotted here for the nominal realization. From top to bottom, adjusting more variables via affine decision rules leads to both better unit utilizations and worst-case objectives (reported in top-right corners).

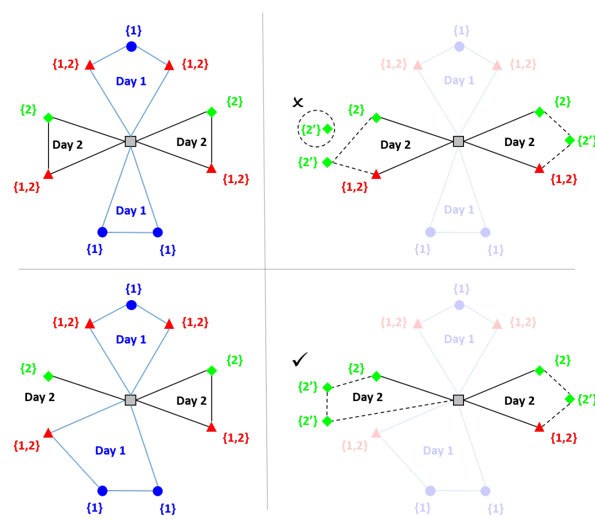

Figure 2. A non-robust (top left) and a robust (bottom left) plan for routing over the next two days. The non-robust plan myopically optimized the routes based on current information and did not have enough day 2 capacity left to serve the additional customers that called in after the day 1 routes were executed (top right). In contrast, the robust plan reserved more capacity and was able to cope with the additional demand (bottom right).

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