



A Comparative Theoretical and Computational Study on Robust Counterpart Optimization: III. Improving the Quality of Robust Solutions

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ABSTRACT: In this paper, we study the solution quality of robust optimization problems when they are used to approximate probabilistic constraints and propose a novel method to improve the quality. Two solution frameworks are first compared: (1) the traditional robust optimization framework which only uses the a priori probability bounds and (3) the approximation framework which uses the a posteriori probability bound. We illustrate that the traditional robust optimization method is computationally efficient but its solution is in general conservative. On the other hand, the a posteriori probability bound based method provides less conservative solution but it is computationally more difficult because a nonconvex optimization problem is solved. Based on the comparative study of the two methods, we propose a novel iterative solution framework which combines the advantage of the a priori bound and the a posteriori probability bound. The proposed method can improve the solution quality of traditional robust optimization framework without significantly increasing the computational effort. The effectiveness of the proposed method is illustrated through numerical examples and applications in planning and scheduling problems.

1. INTRODUCTION

Data uncertainty widely exists in realistic problems due to their random nature, measurement errors, or other reasons. As a result, decision making inherently involves consideration of such uncertainties since the solution of an optimization problem often exhibits high sensitivity to data perturbations, and ignoring the uncertainty could lead to suboptimal or even infeasible solutions. In past decades, developing optimization methods and tools to facilitate decision making under uncertainty has become one of the most important topics in both the operations research community and also the process systems engineering community.

Robust optimization belongs to an important methodology for dealing with optimization problems with data uncertainty. This type of method enforces the constraint satisfaction for all possible realizations of uncertain parameters inside a predefined uncertainty set. Comparing it to other methodologies that deal with uncertainty, one major motivation of robust optimization is that in many applications the data set is an appropriate notion of parameter uncertainty, especially for those cases that the parameter uncertainty is not stochastic, or for instances where no distributional information is available.

One of the earliest papers on robust counterpart optimization is the work of Soyster,¹ who considered simple perturbations in the data and aimed to find a reformulation of the original linear programming problem such that the resulting solution would be feasible under all possible perturbations. The approach admits the highest protection and is the most conservative one since it ensures feasibility against all potential realizations. Thus, it is highly desirable to provide a mechanism to allow for the trade-off between robustness and performance. The work by Ben-Tal and Nemirovski,^{2,3} El-Ghaoui et al.,^{4,5} and Bertsimas and Sim⁶ investigated the framework of robust counterpart optimization by introducing different types of uncertainty sets. Ben-Tal and

Nemirovski³ proposed the ellipsoidal set based robust counterpart formulation. El-Ghaoui and Lebret⁴ introduced a robust optimization approach for least-squares problems with uncertain data. Bertsimas and Sim⁶ studied robust linear programming with coefficient uncertainty using an uncertainty set with budgets. In this robust counterpart optimization formulation, a budget parameter (which takes a value between zero and the number of uncertain coefficient parameters in the constraints and is not necessarily integer) is introduced to control the degree of conservatism of the solution. Lin et al.⁷ and Janak et al.⁸ developed the theory of the robust optimization framework for general mixed-integer linear programming problems and considered both bounded uncertainty and several known probability distributions. The robust optimization framework was later extended by Verderame and Floudas⁹ and they studied both continuous (general, bounded, uniform, normal) and discrete (general, binomial, Poisson) uncertainty distributions and applied the framework to operational planning problems. The work was further compared with the conditional value-at-risk based method in Verderame and Floudas.¹⁰ In the first two parts of this paper series,^{11,12} we systematically studied the set induced robust counterpart optimization technique for linear and mixed integer linear optimization problems. Different uncertainty sets were extensively studied, including those studied in literature and novel ones were introduced in this work. The relationship between different representative uncertainty sets was discussed, and their corresponding robust counterpart formulations for both linear optimization (LP) and mixed integer linear optimization (MILP) problems were derived. Probabilistic guarantees

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on constraint satisfaction for the robust solution of those different uncertainty set induced robust counterpart optimization models were derived, for both bounded and unbounded uncertainty, with and without detail probability distribution information.

A key element in applying the robust optimization framework is the selection of the type and the size of the uncertainty set, which is strongly related to the desired reliability of the solution (i.e., the probability of constraint satisfaction). It is known that chance constraint/probabilistic constraint is the most direct way to enforce the reliability of the solution of an optimization problem,^{13,18} where the reliability is expressed as a minimum requirement on the probability of satisfying constraints. Chance constrained optimization problems face a lot of challenges for their solution. For example, even evaluating the distribution of a sum of uniformly distributed independent random variables is very difficult.¹⁹ When the program has structural properties that allow for an equivalent deterministic formulation, a chance constrained problem can be converted to a deterministic problem and can be solved directly.⁸ However, if the model does not admit sufficient structure that can be exploited, an approximation method has to be used. The various approximation methods can be divided into sampling based methods and analytical approximation based methods.

First, sampling based methods are designed based on the assumption that it is possible to draw observations from the distribution of the uncertainty. Sampling based methods fall broadly into two categories: scenario approximation and sample average approximation. For scenario approximation, it draws a finite number of samples from a given distribution, and enforces all sampled constraints to hold.¹⁴ Sample average approximation refers to replacing the distribution with another “easy-to-use” distribution, typically the empirical distribution determined from a sample drawn from the original distribution.¹⁵ While solving the approximation problem represents one aspect of complexity, the size of the sample required to guarantee the quality of the approximation is another important limitation.

Second, analytical approximation methods are based on either robust optimization¹⁶ or well-known probability inequalities.¹⁷ Since the type and the size of the uncertainty set is determined based on an initial assumption on the constraint satisfaction and the a priori probability bound formulation,¹² robust optimization provides a safe approximation of probabilistic constraint. In contrast to sampling based approximation, robust optimization based approximation is a promising deterministic alternative for certain classes of chance constrained problems. In addition, other forms of deterministic analytical approximation use probability inequalities, such as the Markov inequality, Chebyshev's inequality, Bernstein's inequality, Hoeffding's inequality, etc.

Although robust optimization has been used widely in different areas to achieve solution robustness/reliability, the quality of the solution is often ignored. In other words, while the desired solution feasibility (i.e., desired probability of constraint satisfaction) is met, how far is the solution from optimality? In this work, we will first illustrate the above issues and then propose an iterative strategy for improving the robust solution. In the proposed method, the tight a posteriori probability bounds are used to improve the robust solution within an iterative framework. Compared to the single-step classical robust optimization method, the quality of the robust solution can be improved. On the other hand, compared to the pure a posteriori probability bound based methods, the proposed method has the advantage

that it does not require the global optimization of nonconvex problem.

The rest of the paper is organized as follows. In section 2, we first present the problem of optimization with probabilistic guarantee on constraint satisfaction, that is, probabilistically constrained problem, and then introduce the traditional robust optimization based approximation framework. Next, the a posteriori probability bound based approximation framework is presented in section 3. Both methods are studied through a numerical example. In section 4, we present a novel iterative framework which combines the advantage of the previous two different methods. The proposed method and the traditional methods are studied through production planning and process scheduling problems in section 5, and the paper is concluded in section 6.

2. FRAMEWORK FOR ROBUST OPTIMIZATION

2.1. Problem Description. Consider the following linear optimization problem

$$\begin{aligned} &\max cx \\ &\text{s.t. } \sum_{j \notin J_i} a_{ij}x_j + \sum_{j \in J_i} \tilde{a}_{ij}x_j \leq b_i \quad \forall i \end{aligned} \quad (1)$$

where $x \in \mathbb{R}^n$ and x_j ($j = 1, \dots, n$) can be either continuous or integer variables, the left-hand-side (LHS) constraint coefficients \tilde{a}_{ij} are subject to uncertainty, and J_i represents the index subset that contains the variable indices whose corresponding coefficients are subject to uncertainty. The uncertainties in the constraint coefficients are normalized by $\tilde{a}_{ij} = a_{ij} + \xi_{ij}\hat{a}_{ij} \forall j \in J_i$ with a_{ij} being the nominal value and \hat{a}_{ij} being a constant perturbation amplitude ($\hat{a}_{ij} > 0$), $\{\xi_{ij}\}_{j \in J_i}$ are random variables which are subject to uncertainty. With the above definition, the i th constraint in problem 1 can be rewritten as the follows:

$$\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_{ij}\hat{a}_{ij}x_j \leq b_i \quad (2)$$

In many practical applications, enforcing constraint satisfaction for all possible values of the uncertain parameters (i.e., worst-case scenario) can be too costly or even impossible. Probabilistic constraint (also called chance constraint) provides a compromise to avoid this situation and ensures that the constraints are satisfied under certain given probability. A probabilistic version of the above constraint is written as follows so that a probabilistic guarantee on constraint satisfaction is applied:

$$\Pr\left\{\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_{ij}\hat{a}_{ij}x_j \leq b_i\right\} \geq 1 - \varepsilon \quad (3)$$

or an upper bound on the probability of constraint violation is applied

$$\Pr\left\{\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_{ij}\hat{a}_{ij}x_j > b_i\right\} \leq \varepsilon \quad (4)$$

where ε ($0 < \varepsilon < 1$) is the allowed degree of constraint violation. For instance, $\varepsilon = 0.05$ means that the constraint must be satisfied with a probability larger than 0.95 or the probability of constraint violation must be less than 0.05. While joint probabilistic constraints are alternative for modeling solution reliability, individual probabilistic constraints are investigated in this paper.

Motivating Example. Consider the following linear optimization problem

$$\begin{aligned}
&\max \quad 8x_1 + 12x_2 \\
&\text{s.t.} \quad \tilde{a}_{11}x_1 + \tilde{a}_{12}x_2 \leq 140 \\
&\quad \quad \tilde{a}_{21}x_1 + \tilde{a}_{22}x_2 \leq 72 \\
&\quad \quad x_1, x_2 \geq 0
\end{aligned}$$

and assume that the LHS constraint coefficients of the constraints are uncertain and subject to uncertainty with $\tilde{a}_{11} = 10 + \xi_{11}$, $\tilde{a}_{12} = 20 + 2\xi_{12}$, $\tilde{a}_{21} = 6 + 0.6\xi_{21}$, and $\tilde{a}_{22} = 8 + 0.8\xi_{22}$ and ξ_{11} , ξ_{12} , ξ_{21} , ξ_{22} are independent uncertain parameters uniformly distributed in $[-1, 1]$. For the above problem, if we set the allowed violation probability for each of the constraint as 0.05, then the probabilistic constrained version of the problem is

$$\begin{aligned}
&\max \quad 8x_1 + 12x_2 \\
&\text{s.t.} \quad \Pr\{10x_1 + 20x_2 + (\xi_{11}x_1 + 2\xi_{12}x_2) > 140\} \leq 0.05 \\
&\quad \quad \Pr\{6x_1 + 8x_2 + (0.6\xi_{21}x_1 + 0.8\xi_{22}x_2) > 72\} \leq 0.05 \\
&\quad \quad x_1, x_2 \geq 0
\end{aligned}$$

2.2. Traditional Application Framework of Robust Optimization. In set induced robust optimization, the uncertain data is assumed to be varying in a given uncertainty set and the aim is to choose the best solution among those “immunized” against data uncertainty. For constraint 2, the set induced robust optimization method aims to find solutions that remain feasible for any ξ in the given uncertainty set U so as to immunize against infeasibility, that is

$$\sum_j a_{ij}x_j + \max_{\xi \in U} \sum_{j \in I_i} \xi_{ij}\hat{a}_{ij}x_j \leq b_i \quad \forall i \quad (5)$$

The corresponding robust optimization problem is

$$\begin{aligned}
&\max \quad cx \\
&\text{s.t.} \quad \sum_j a_{ij}x_j + \max_{\xi \in U} \sum_{j \in I_i} \xi_{ij}\hat{a}_{ij}x_j \leq b_i \quad \forall i
\end{aligned} \quad (6)$$

For different uncertainty sets, the robust counterpart formulation is distinct. Furthermore, under specific probability distribution assumption, the probabilistic guarantee on the constraint satisfaction can be quantified using the size of the uncertainty set. In our previous work, we have systematically derived the robust counterpart formulations under different uncertainty sets¹¹ and also derived their probability bounds on constraint violation.¹² For example, if the uncertainty set is given by a box

$$U_\infty = \{\xi \mid \|\xi\| \leq \Psi, \quad \forall j \in I_i\} \quad (7)$$

where Ψ is the size of the box, then the robust optimization counterpart constraint is

$$\sum_j a_{ij}x_j + \Psi \sum_{j \in I_i} \hat{a}_{ij}|x_j| \leq b_i \quad \forall i \quad (8)$$

If the uncertain parameters are subject to independent bounded symmetric distribution, then the following a priori probability bound is valid

$$\text{prob}_{\text{violation}}^{\text{prioriUB}}(\Psi) = \exp\left(-\frac{\Psi^2}{2}\right) \quad (9)$$

A priori probability bound means that if the size of the box set is Ψ , then the solution of the robust optimization problem will ensure that the probability of constraint violation is less than or equal to the following bound:

$$\Pr\left\{\sum_j a_{ij}x_j + \sum_{j \in I_i} \xi_{ij}\hat{a}_{ij}x_j > b_i\right\} \leq \text{prob}_{\text{violation}}^{\text{prioriUB}}(\Psi) \quad \forall i \quad (10)$$

In the literature, the traditional way of applying robust optimization^{7,24} to solve the probabilistically constrained problem is as follows. First, the reliability level ε in the probabilistic constraint is set, and the type of the robust optimization model (i.e., uncertainty set) is selected by the distribution of the uncertainty. Next, the size of the uncertainty set is evaluated based on the a priori probability bounds. For example, assuming that the box type uncertainty set is selected for applying robust optimization, the size of the uncertainty set can be determined by the following problem

$$\begin{aligned}
&\min \quad \Psi \\
&\text{s.t.} \quad \exp\left(-\frac{\Psi^2}{2}\right) \leq \varepsilon
\end{aligned} \quad (11)$$

Using the size parameter value determined from the above problem, the robust counterpart optimization problem can be solved and the solution ensures that the constraint is satisfied with the desired probability $1-\varepsilon$.

$$\begin{aligned}
&\max \quad cx \\
&\text{s.t.} \quad \sum_j a_{ij}x_j + \Psi \sum_{j \in I_i} \hat{a}_{ij}|x_j| \leq b_i \quad \forall i
\end{aligned} \quad (12)$$

As a summary, the traditional framework of applying robust optimization to address the probabilistic guarantee on constraint satisfaction is shown in Figure 1.

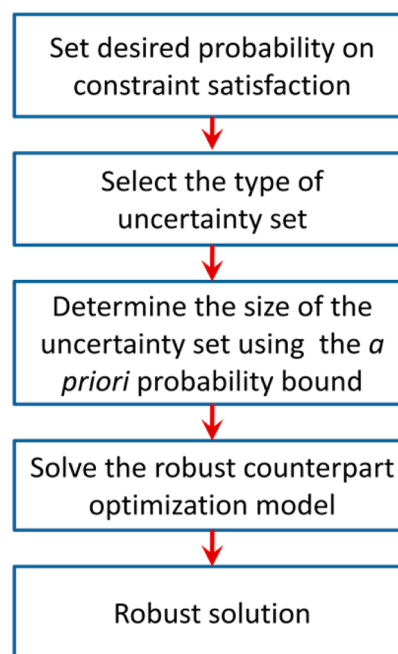


Figure 1. Traditional framework of applying robust optimization^{7,24} for probabilistically constrained optimization problem.

The robust optimization problem provides a safe and conservative approximation of the probabilistically constrained problem. Notice that the minimum possible value for Ψ is used to find the best possible solution within this framework. In the following, we illustrate the approximation of the probabilistic

constrained problem using the robust counterpart optimization through the motivating example.

Motivating Example (Continued). The “interval + ellipsoidal” uncertainty set induced robust counterpart optimization model is applied to solve the motivating example problem. The robust counterpart optimization problem under the interval + ellipsoidal uncertainty set is as follows

$$\begin{aligned} \max \quad & 8x_1 + 12x_2 \\ \text{s.t.} \quad & 10x_1 + 20x_2 + u_{11} + 2u_{12} + \Omega_1 \sqrt{z_{11}^2 + 4z_{12}^2} \\ & \leq 140 \\ & -u_{11} \leq x_1 - z_{11} \leq u_{11}, -u_{12} \leq x_2 - z_{12} \leq u_{12} \\ & 6x_1 + 8x_2 + 0.6u_{21} + 0.8u_{22} \\ & + \Omega_2 \sqrt{0.36z_{21}^2 + 0.64z_{22}^2} \leq 72 \\ & -u_{21} \leq x_1 - z_{21} \leq u_{21}, -u_{22} \leq x_2 - z_{22} \leq u_{22} \\ & x_1, x_2 \geq 0 \end{aligned}$$

where Ω_1 and Ω_2 are parameters determining the size of the interval + ellipsoidal uncertainty set. Using the probability bound on constraint violation for this type of robust counterpart optimization model (under the assumption that the uncertainty is bounded and symmetric which is satisfied in this example)

$$\exp\left(-\frac{\Omega^2}{2}\right) \leq 0.05, \exp\left(-\frac{\Omega^2}{2|J_i|}\right) \leq 0.05, B(|J_i|, \Omega) \leq 0.05$$

we obtained the smallest possible value: $\Omega_1 = \Omega_2 = 2.4477$. The above robust optimization problem is convex and can be efficiently solved using convex nonlinear optimization solvers. With this value, the robust counterpart optimization problem can be solved, the optimal objective value is $\text{Obj}^* = 90.9091$ and the robust solution is $\bar{x} = (7.2727, 2.7273)$. This solution ensures that the constraints are satisfied with the desired probability 0.95 on constraint satisfaction.

Once a robust solution is obtained, the probability of constraint violation can also be quantified by a posteriori probability bound. In our previous paper,¹² we studied those a posteriori probability bounds. If the probabilistic distribution information on the uncertain parameters is known, then the following relationship holds:¹²

$$\begin{aligned} \Pr\left\{\sum_j a_{ij}x_j + \sum_{j \in I_i} \xi_{ij}\hat{a}_{ij}x_j > b_i\right\} & \leq \exp(-\theta(b_i - \sum_j a_{ij}x_j) \\ & + \sum_{j \in I_i} \ln E[e^{\theta \xi_{ij}\hat{a}_{ij}x_j}]) \quad \forall i \end{aligned} \quad (13)$$

In the above derivation, θ is an arbitrary positive number. As studied in our previous work,¹² with the above probability inequality, we can evaluate the a posteriori probability bound on constraint violation as follows once we have a set of solution x , (i.e., we have \bar{x}_j as the solution):

$$\begin{aligned} \Pr\left\{\sum_j a_{ij}\bar{x}_j + \sum_{j \in I_i} \xi_{ij}\hat{a}_{ij}\bar{x}_j > b_i\right\} \\ \leq \min_{\theta} \exp(-\theta(b_i - \sum_j a_{ij}\bar{x}_j) + \sum_{j \in I_i} \ln E[e^{\theta \xi_{ij}\hat{a}_{ij}\bar{x}_j}]) \quad \forall i \end{aligned} \quad (14)$$

Notice that in the above equation, a minimization with respect to θ (i.e., only one variable) is performed to find the tightest probability bound.

For the traditional robust counterpart optimization based framework, the adjustable parameter defining the size of the uncertainty set is initially selected based on the a priori probability bound which is a function of the adjustable parameter. However, usually, the resulting solution could be too conservative, since the actual probability of constraint violation is much smaller than the bound. For example, with the robust solution $\bar{x} = (7.2727, 2.7273)$ obtained for the motivating example, the probability of constraint violation can be evaluated using the above a posteriori probability bound 14, and the following upper bounds on constraint violation for the two constraints can be calculated:

$$\begin{aligned} \Pr\{10\bar{x}_1 + 20\bar{x}_2 + (\xi_{11}\bar{x}_1 + 2\xi_{12}\bar{x}_2) > 140\} \\ \leq 2.507 \times 10^{-6} \\ \Pr\{6\bar{x}_1 + 8\bar{x}_2 + (0.6\xi_{21}\bar{x}_1 + 0.8\xi_{22}\bar{x}_2) > 72\} \\ \leq 3.455 \times 10^{-6} \end{aligned}$$

which are far less than the desired violation probability 0.05. This implies that the obtained robust solution is conservative and there is room for improvement.

3. A POSTERIORI PROBABILITY BOUND BASED SOLUTION METHOD

While the a posteriori probability bound can be used to check the probability of constraint satisfaction with a given solution, it can also be used in another way to formulate a safe approximation of the probabilistic constraint. Using inequality 13, the following safe approximation of 4 is obtained:

$$\exp(-\theta_i(b_i - \sum_j a_{ij}x_j) + \sum_{j \in I_i} \ln E[e^{\theta_i \xi_{ij}\hat{a}_{ij}x_j}]) \leq \varepsilon \quad \forall i \quad (15)$$

because for any feasible solution satisfying 15, it also satisfies the constraint 4. Constraint 15 can be further rewritten as

$$-\theta_i(b_i - \sum_j a_{ij}x_j) + \sum_{j \in I_i} \ln E[e^{\theta_i \xi_{ij}\hat{a}_{ij}x_j}] \leq \ln \varepsilon \quad \forall i \quad (16)$$

and finally the following safe approximation of the probabilistic constrained problem is obtained:

$$\begin{aligned} \min_{x, \theta} \quad & cx \\ \text{s.t.} \quad & -\theta_i(b_i - \sum_j a_{ij}x_j) + \sum_{j \in I_i} \ln E[e^{\theta_i \xi_{ij}\hat{a}_{ij}x_j}] \leq \ln \varepsilon \quad \forall i \end{aligned} \quad (17)$$

Note that while for any fixed value of $\theta_i > 0$, 15 is an approximation of the original probabilistic constrained problem, here θ_i is set as a decision variables in problem 17 so as to find the tightest possible approximation and to seek the best possible solution.

The a posteriori probability bound based framework addressing the probabilistic constraint can be represented using Figure 2. It is seen that the approximation optimization problem is constructed based on the selected a posteriori bound, in comparison to the selection of uncertainty set in the traditional robust optimization framework.

Defining $\xi = \xi_{ij}\hat{a}_{ij}x_j$, then the explicit formulation of above approximation problem depends on the moment generating

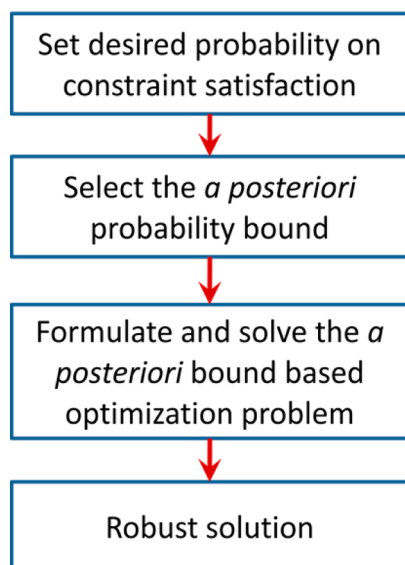


Figure 2. Solution framework of a posteriori bound based method.

Table 1. Summary on the pdf and mgf of Some Distributions

distribution of ξ	probability density function $f(\xi)$	moment generating function $E(e^{\theta\xi})$
uniform $U(a,b)$	$\begin{cases} 1/(b-a), & a \leq \xi \leq b \\ 0, & \text{otherwise} \end{cases}$	$\frac{e^{\theta b} - e^{\theta a}}{\theta(b-a)}$
triangular	$\begin{cases} \xi + 1, & -1 \leq \xi \leq 0 \\ -\xi + 1, & 0 \leq \xi \leq 1 \end{cases}$	$\frac{e^{\theta} + e^{-\theta} - 2}{\theta^2}$
exponential $\exp(\lambda)$	$\begin{cases} \lambda e^{-\lambda\xi} & \xi \geq 0 \\ 0 & \xi < 0 \end{cases}$	$(1 - \theta\lambda^{-1})^{-1}$ for $\lambda \geq \theta$
normal $N(\mu, \sigma)$	$\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\xi - \mu)^2}{2\sigma^2}\right)$	$e^{\theta\mu + 0.5\sigma^2\theta^2}$

function $E[e^{\theta\xi}]$. For several known distributions, their probability density functions and moment generating functions are listed in Table 1, which can be substituted into 17 and the resulting problem can be solved as a deterministic optimization problem. The above probability inequality based approximation framework is illustrated through the motivating example.

Motivating Example (Continued). Following the derivation in this section, the probability inequality based safe approximation of the probabilistic constrained problem of the motivating example is obtained:

$$\begin{aligned}
 \max_{x, \theta} \quad & 8x_1 + 12x_2 \\
 \text{s.t.} \quad & -\theta_1(140 - 10x_1 - 20x_2) + \ln E[e^{\theta_1\xi_{11}x_1}] \\
 & + \ln E[e^{2\theta_1\xi_{12}x_2}] \leq \ln 0.05 \\
 & -\theta_2(72 - 6x_1 - 8x_2) + \ln E[e^{0.6\theta_2\xi_{21}x_1}] \\
 & + \ln E[e^{0.8\theta_2\xi_{22}x_2}] \leq \ln 0.05 \\
 & x_1, x_2 \geq 0, \theta_1, \theta_2 > 0
 \end{aligned}$$

Since the random variable ξ_{11} is subject to uniform distribution in $[-1, 1]$, we have

$$E[e^{\theta_1\xi_{11}x_1}] = \frac{e^{\theta_1x_1} - e^{-\theta_1x_1}}{2\theta_1x_1}$$

Evaluate the expectation terms in the similar way and finally the following problem is obtained:

$$\begin{aligned}
 \max_{x, \theta} \quad & 8x_1 + 12x_2 \\
 \text{s.t.} \quad & -\theta_1(140 - 10x_1 - 20x_2) + \ln \left[\frac{e^{\theta_1x_1} - e^{-\theta_1x_1}}{2\theta_1x_1} \right] \\
 & + \ln \left[\frac{e^{2\theta_1x_2} - e^{-2\theta_1x_2}}{4\theta_1x_2} \right] \leq \ln \varepsilon \\
 & -\theta_2(72 - 6x_1 - 8x_2) + \ln \left[\frac{e^{0.6\theta_2x_1} - e^{-0.6\theta_2x_1}}{1.2\theta_2x_1} \right] \\
 & + \ln \left[\frac{e^{0.8\theta_2x_2} - e^{-0.8\theta_2x_2}}{1.6\theta_2x_2} \right] \leq \ln \varepsilon \\
 & x_1, x_2 \geq 0, \theta_1, \theta_2 > 0
 \end{aligned}$$

The above problem is a nonconvex optimization problem, which can be solved through a deterministic global optimization approach. We solve the above problem through global optimization solver ANTIGONE 1.1²³ in GAMS 24.2.2 (with relative optimality gap tolerance *optcr* = 0 and resource limit *reslim* = 10000) and obtain the following solution after 10 000 s (with a relative gap 0.11% to the upper bound 92.33):

$$\begin{aligned}
 \text{Obj}^* &= 92.2292, x^* = (7.3588, 2.7799), \\
 \theta &= (0.9501, 1.938)
 \end{aligned}$$

Comparing the above solution with the solution from the traditional robust optimization framework, it is observed that while both solutions ensure the desired probability on constraint satisfaction, the a posteriori probability bound based method generates a solution which is better than the classical method. Note though that the computational effort increases since global optimization is needed.

4. ITERATIVE SOLUTION STRATEGY

Comparing the previous two methods, the following observations can be made:

- (1) In terms of the information needed, the a posteriori probability bound based approximation method needs the exact probability distribution function while the robust optimization method only needs partial information. For instance, in the studied robust optimization formulations, the assumptions on uncertainty are only bounded and symmetric so that a probabilistic guarantee is valid.
- (2) In terms of the solution complexity, the probability inequality based approximation problem can be nonconvex and global optimization is necessary (i.e., higher computation complexity). The robust optimization based approximation leads to convex problem which can be solved very efficiently.
- (3) In terms of the quality of the solution, the a posteriori probability bound based approximation method leads to less conservative solution because it is tighter than the a priori probability bound as illustrated in previous work.¹²

The aforementioned observations show that there is a trade-off between the two different types of approximations. To fully take advantage of both of them, an iterative solution framework, which is also the major contribution of this paper, is proposed

to combine the use of the traditional robust optimization approximation and the a posteriori probability bound. The objective is to improve the quality of robust solution while still ensure the probabilistic guarantee of the robust solution. At the same time, the computational complexity is decreased comparing to the a posteriori probability bound based approximation method.

The proposed solution framework is shown in Figure 3, which can be detailed as follows. Initially, the type of the uncertainty set

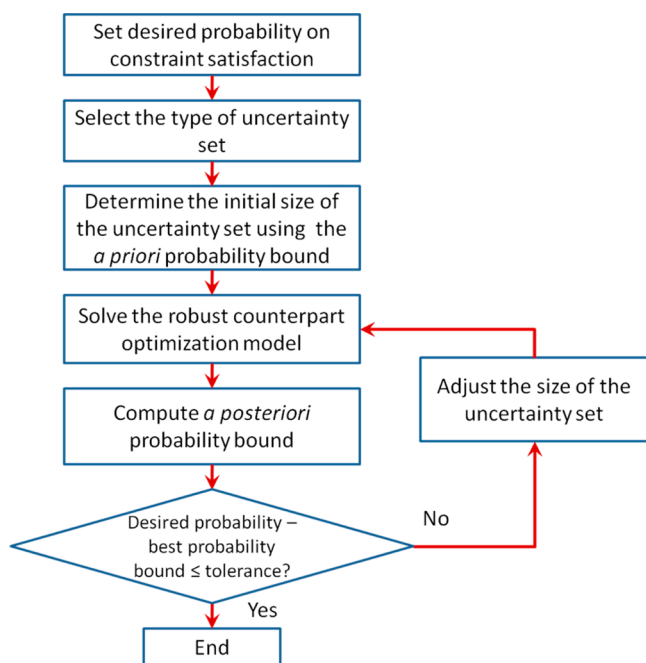


Figure 3. Proposed iterative solution framework to improve the quality of robust solution.

(i.e., the robust optimization formulation) is selected. Based on the desired degree of constraint satisfaction, the smallest possible size of the uncertainty set is determined using the specific a priori probability bounds (e.g., $\exp(-\Omega^2/2)$, $\exp(-\Omega^2/2|f|)$, etc.) of that type of robust formulation. With the determined size of the uncertainty set, the robust counterpart optimization problem is solved and the robust solution is obtained. Then, an upper bound on the constraint violation is evaluated using the derived solution and the a posteriori probability bound. This probability value is compared to the desired degree of constraint violation. If the gap between them is larger than a certain predefined tolerance, the size of the uncertainty set is adjusted and the robust optimization problem is solved again.

The size adjusting is the important step in the algorithm. Based on the fact that the a posteriori probability upper bound is monotonically decreasing function of the set size,¹² this adjustment can be made heuristically: if the probability upper bound exceeds the desired level, the set size should be decreased; if the bound is below the desired level, the set size should be increased. The above procedure is repeated until the gap between the desired degree of constraint violation and the computed upper bound on constraint violation is less than the tolerance. Finally, the solution from the last round robust optimization step is reported. A pseudo code of the iterative algorithm is given as follows:

Pseudo code for the Iterative algorithm

1. Initialize $\Delta_i^{\text{satisfy}} = M$, $\Delta_i^{\text{violate}} = 0$, where M is the set size computed using the a priori probability bound and the desired level of constraint satisfaction $1 - \varepsilon_i$. Set tolerance parameter δ (e.g., 0.01).
2. Set $\Delta_i = \Delta_i^{\text{satisfy}}$ for each constraint.
3. Solve the robust optimization problem.
4. Evaluate the a posteriori bounds $\text{prob}^{\text{posterioriUB}}_{\text{violation}}(i)$ on the probability of constraint violation for each constraint;
If $|\text{prob}^{\text{posterioriUB}}_{\text{violation}}(i) - \varepsilon_i| > \delta$ for any constraint, go to step 5; otherwise, go to step 6.
5. For each constraint
If $\text{prob}^{\text{posterioriUB}}_{\text{violation}}(i) \leq \varepsilon_i$ and $\Delta_i < \Delta_i^{\text{satisfy}}$
 $\Delta_i^{\text{satisfy}} = \Delta_i$
end
If $\text{prob}^{\text{posterioriUB}}_{\text{violation}}(i) > \varepsilon_i$ and $\Delta_i > \Delta_i^{\text{violate}}$
 $\Delta_i^{\text{violate}} = \Delta_i$
end
 $\Delta_i = 0.5(\Delta_i^{\text{violate}} + \Delta_i^{\text{satisfy}})$
End
Go to step 3.
6. Return the current robust solution.

Notice that in the proposed iterative framework, the problem of evaluating the a posteriori probability bound using the right-hand side (RHS) of 14 is an optimization problem. Since any feasible solution of the RHS of 14 will be a valid a posteriori upper bound on the probability of constraint violation, it is not necessary to obtain the global optimal solution here. Furthermore, since x is a known solution and taken fixed value, the RHS of 14 is a single variable optimization problem, which can be solved relatively efficiently.

Motivating Example (Continued). Applying the proposed framework and using the interval + ellipsoidal uncertainty set based robust counterpart optimization formulation, we obtain the following results for the motivating example as shown in Table 2 for different iterations (i.e., k stands for iteration):

Table 2. Solution Procedure

k	Ω_1, Ω_2	$\exp(-\Omega^2/2)$	Obj*	(x_1, x_2)	$\text{prob}^{\text{posterioriUB}}_{\text{violation}}$
1	(2.4477, 2.447)	(0.05, 0.05)	90.910	(7.2727, 2.7273)	$(2.51 \times 10^{-6}, 3.46 \times 10^{-6})$
2	(1.2238, 1.2238)	(0.4729, 0.4729)	91.807	(7.2745, 2.8009)	(0.0305, 0.0205)
3	(0.6119, 0.6119)	(0.8293, 0.8293)	95.695	(7.6045, 2.9049)	(0.5486, 0.5426)
4	(0.9179, 0.9179)	(0.6562, 0.6562)	93.685	(7.422, 2.859)	(0.222, 0.205)
5	(1.0709, 1.0709)	(0.5636, 0.5636)	92.712	(7.335, 2.836)	(0.105, 0.086)
6	(1.1474, 1.1474)	(0.5177, 0.5177)	92.236	(7.293, 2.824)	(0.062, 0.045)
7	(1.1856, 1.1474)	(0.4952, 0.5177)	92.153	(7.354, 2.777)	(0.045, 0.045)

The detailed solution procedure is explained as follows:

Step 1: Initialize $\Omega_1^{\text{satisfy}} = 2.4477$, $\Omega_1^{\text{violate}} = 0$, $\Omega_2^{\text{satisfy}} = 2.4477$, $\Omega_2^{\text{violate}} = 0$ using the a priori bound. Set tolerance parameter $\delta = 0.01$.

Step 2: Set $\Omega_1 = \Omega_1^{\text{satisfy}} = 2.477$, $\Omega_2 = \Omega_2^{\text{satisfy}} = 2.477$.

Iteration 1

Step 3: Solve the robust optimization problem and obtain solution $\text{Obj}^* = 90.91$, $x_1 = 7.2727$, $x_2 = 2.7273$.

Step 4: Compute the a posteriori probability bound from solution $P_1 = 2.51 \times 10^{-6}$, $P_2 = 3.46 \times 10^{-6}$.

Step 5: Since the probability violation upper bound is less than 0.05 for both constraints, there is room to contract the uncertainty set and improve the solution. So decrease the size of both uncertainty

sets based on the value in iteration 1: $\Omega_1 = \Omega_2 = (0 + 2.4477)/2 = 1.2238$.

Iteration 2

Step 3: Solve the robust model and obtain $\text{Obj}^* = 91.807$, $x_1 = 7.2745$, $x_2 = 2.8009$.

Step 4: Compute the a posteriori probability bound $P_1 = 0.0305$, $P_2 = 0.0205$.

Step 5: Since the probability violation upper bound is still less than 0.05 for both constraints, it is necessary to further decrease the size of both uncertainty sets based on the size value in iteration 1 $\Omega_1 = \Omega_2 = (0 + 1.2238)/2 = 0.6119$.

Iteration 3

Step 3: Solve the robust model and get $\text{Obj}^* = 95.6954$, $x_1 = 7.6045$, $x_2 = 2.9049$.

Step 4: Compute the a posteriori probability bound $P_1 = 0.5486$, $P_2 = 0.5426$.

Step 5: Since the probability violation upper bound becomes larger than 0.05 for both constraints, this means the uncertainty set should be enlarged to satisfy chance constraint. So we adjust the uncertainty sets based on smallest size leading to constraint satisfaction so far (1.2238 in iteration 2) and the size that leads to violation (0.6119 in iteration 3): $\Omega_1 = \Omega_2 = (0.6119 + 1.2238)/2 = 0.9179$.

Iteration 4

Step 3: Solve the robust model and obtain $\text{Obj}^* = 93.685$, $x_1 = 7.422$, $x_2 = 2.859$.

Step 4: Compute the a posteriori probability bound $P_1 = 0.222$, $P_2 = 0.205$.

Step 5: Since the probability violation is still larger than 0.05 for both constraints by using size 0.9179, we need to further enlarge the uncertainty set to satisfy chance constraint. We adjust the parameter toward the smallest size leading to constraint satisfaction (1.2238 in iteration 2): $\Omega_1 = \Omega_2 = (0.9179 + 1.2238)/2 = 1.0709$.

Iteration 5

Step 3: Solve the robust model and obtain $\text{Obj}^* = 92.712$, $x_1 = 7.335$, $x_2 = 2.836$.

Step 4: Compute the a posteriori probability bound $P_1 = 0.105$, $P_2 = 0.086$.

Step 5: Since the probability violation is still larger than 0.05 for both constraints in the previous iteration, we need to further enlarge the uncertainty sets: $\Omega_1 = \Omega_2 = (1.0709 + 1.2238)/2 = 1.1474$.

Iteration 6

Step 3: Solve the robust model and obtain $\text{Obj}^* = 92.236$, $x_1 = 7.293$, $x_2 = 2.824$.

Step 4: Compute the a posteriori probability $P_1 = 0.062$, $P_2 = 0.045$.

Step 5: Since the probability violation is larger than 0.05 for the first constraints and the second constraint is satisfied, we keep Ω_2 unchanged and further increase Ω_1 as $\Omega_1 = (1.1474 + 1.2238)/2 = 1.1856$.

Iteration 7

Step 3: Solve the robust model and obtain $\text{Obj}^* = 92.153$, $x_1 = 7.354$, $x_2 = 2.777$.

Step 4: Compute the a posteriori probability $P_1 = 0.045$, $P_2 = 0.045$; both are less than 0.05 and the gap is smaller than $\delta = 0.01$, so the iteration stops.

Step 6: Return the final solution $\text{Obj}^* = 92.153$, $x_1 = 7.354$, $x_2 = 2.777$.

The solution procedure of the above iterative method is also illustrated in Figure 4, which shows how the constraint

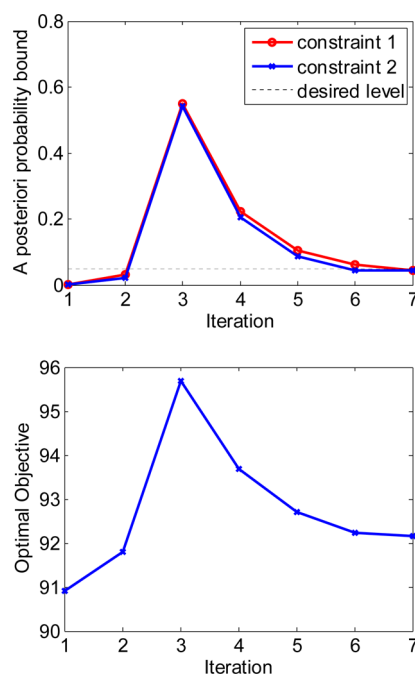


Figure 4. Iterative solution procedure for the motivating example: (upper) a posteriori probability bound; (lower) optimal objective value of robust solution.

satisfaction probability converges to the desired level and how the quality of the robust solution is eventually improved comparing to the traditional framework.

Finally, solutions from three different methods for the motivating example are summarized in Table 3. The columns

Table 3. Comparing the Different Solutions for the Motivating Example

	traditional	a posteriori	iterative
Obj^*	90.910 (1.43%)	92.2292	92.153 (0.08%)
$\text{prob}_{\text{violation}}^{\text{posterioriUB}}$	$(2.51 \times 10^{-6}, 3.46 \times 10^{-6})$	(0.05, 0.05)	(0.045, 0.045)
CPU time (s)	1.2	10000	8.4

“traditional”, “a posteriori”, and “iterative” represent the traditional robust optimization framework, the a posteriori probability bound based method, and the iterative method, respectively. The row “ Obj^* ” and “ $\text{prob}_{\text{violation}}^{\text{posterioriUB}}$ ” represent the optimal objective value of the robust optimization problem and the a posteriori probability bound based on the robust solution obtained. The percentage numbers represent the gaps between the traditional/iterative method’s solutions and the a posteriori method’s solution.

Comparing the traditional robust optimization based approximation framework and the proposed iterative method, we observed that it improves the quality of the solution while still ensures the degree of constraint satisfaction. Notice that the robust solution has been improved from 90.91 to 92.153. The percentage gap to the a posteriori solution 92.2292 has been decreased from 1.43% to 0.08% as shown Table 3. Comparing the pure a posteriori probability bound based approximation

method and the proposed iterative method, we observed that its computational complexity is decreased, since only a set of convex robust optimization problem is solved. The global optimization of the nonconvex optimization is avoided. In addition, when the gap tolerance is defined small enough, the solution of the proposed method will be close to the solution of the probability inequality based method. Finally, we summarize the characteristics of the three methods in Table 4.

Table 4. Summary of Different Methodologies

	traditional	a posteriori	iterative
uncertainty information needed	partial	full	full
solution complexity	low	high	low
solution quality	conservative	good	good

5. CASE STUDIES

In this section, we apply the different methods to solve a production planning problem and a process scheduling problem to compare their performances and illustrate the effectiveness of the proposed iterative method. All the optimization problems are solved on a UNIX workstation with 3.40 GHz Intel Core i7-2600 CPU and 8GB memory. The related global optimization problems are solved via ANTIGONE 1.1²³ and the (mixed integer) linear optimization problems are solved using CPLEX 12.0 in GAMS 24.2.2. Resource limit is set as 10 000 s for all cases.

5.1. Example 1. This example was introduced by Li et al.,¹² which addresses the problem of planning the production, storage and marketing of a product for a company. It is assumed that the company needs to make a production plan for the coming year, divided into six periods of 2 months each, to maximize the sales with a given cost budget. The production cost includes the cost of raw material, labor, machine time, etc., and the cost fluctuates from period to period. The product manufactured during a period can be sold in the same period, or stored and sold later on. Operations begin in period 1 with an initial stock of 500 tons of the product in storage, and the company would like to end up with the same amount of the product in storage at the end of period 6. This problem can be formulated as a linear optimization problem as follows:

$$\max \sum_j P_j z_j \quad (18a)$$

$$\text{s.t. } \sum_j \tilde{C}_j x_j + \sum_j V_j y_j \leq 400\,000 \quad (18b)$$

$$500 + x_1 - (y_1 + z_1) = 0 \quad (18c)$$

$$y_{j-1} + x_j - (y_j + z_j) = 0 \quad \forall j = 2, \dots, 6 \quad (18d)$$

$$y_6 = 500 \quad (18e)$$

$$x_j \leq U_j \quad \forall j = 1, \dots, 6 \quad (18f)$$

$$z_j \leq D_j \quad \forall j = 1, \dots, 6$$

$$x_j, y_j, z_j \geq 0 \quad \forall j = 1, \dots, 6 \quad (18g)$$

In this example, it is assumed that the production costs \tilde{C}_j are subject to independent uncertainty distributions. The uncertainty is normalized using 50% of the nominal value C_j as the base

perturbation amplitude. Then the original constraint 18b can be rewritten as

$$\sum_j (C_j + 0.5\xi_j C_j) x_j + \sum_j V_j y_j \leq 400\,000$$

where ξ_j are independent random variables. To ensure the reliability of the solution, the minimum probability for constraint 18b to be satisfied is set as 0.85 (i.e., the upper bound on the probability of constraint violation is set to 0.15), then the probabilistic constrained version for this constraint is

$$\Pr\left\{\sum_j \tilde{C}_j x_j + \sum_j V_j y_j > 400\,000\right\} \leq 0.15$$

In the sequel, this example is studied under different assumptions on the uncertainty distributions.

(a) Uniform Distribution. In this case, it is assumed that the production costs are subject to uniform uncertainty, that is, ξ_j are random variables that uniformly distributes in $[-1, 1]$. The traditional robust optimization method is applied first to solve the probabilistically constrained optimization problem. Using the interval + ellipsoidal type uncertainty set, the following robust counterpart optimization constraints can be formulated

$$\sum_j C_j x_j + \sum_j V_j y_j + \sum_j 0.5C_j u_j + \Omega \sqrt{\sum_j 0.25C_j^2 v_j^2} \leq 400\,000$$

$$-u_j \leq x_j - v_j \leq u_j$$

The robust optimization problem is obtained by replacing the original deterministic constraint 18b with the above constraints. Using the a priori probability bound for the interval + ellipsoidal set induced robust optimization model, the size of the uncertainty set is computed as $\Omega = 1.9479$. Then the robust optimization problem is solved and the corresponding objective is 2 356 977. The corresponding robust planning solution is shown in Figure 5.

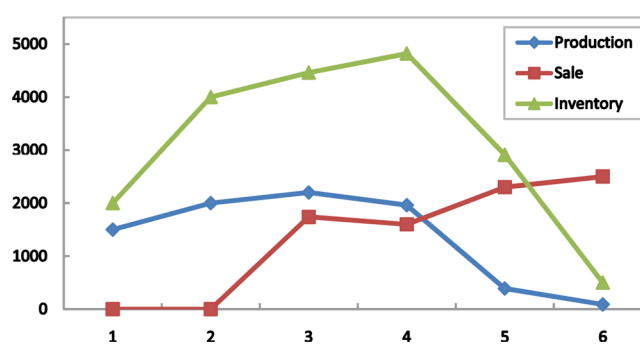


Figure 5. Solution of traditional robust optimization method.

The a posteriori probability bound based method is applied next and the following constraint is applied to replace the original constraint 18b:

$$-\theta(400\,000 - \sum_j C_j x_j - \sum_j V_j y_j) + \sum_j \ln E[e^{0.5\theta\xi_j C_j x_j}] \leq \ln 0.15$$

For the a posteriori probability bound based method, the objective value is 2 550 538. It is seen that this solution is better (higher sales) than that of the classical robust optimization method. The robust planning solution is shown in Figure 6.

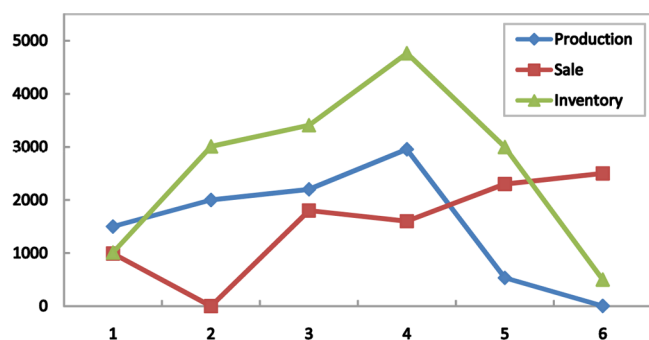


Figure 6. Solution of the a posteriori probability bound based approximation model.

Finally, the iterative framework is applied to solve the problem, the solution procedure is shown in Table 5 and the robust solution is shown in Figure 7.

Table 5. Solution Procedure of the Iterative Method for Example 1 under Uniform Distribution

k	Ω_k	$\exp(-\Omega^2/2)$	Obj*	$\text{prob}_{\text{violation}}^{\text{posterioriUB}}$
1	1.9479	0.15	2356977	1.66×10^{-4}
2	0.9739	0.6224	2569021	0.2003
3	1.4609	0.344	2451636	0.0170
4	1.2174	0.4766	2506754	0.0714
5	1.0957	0.5487	2536859	0.1249

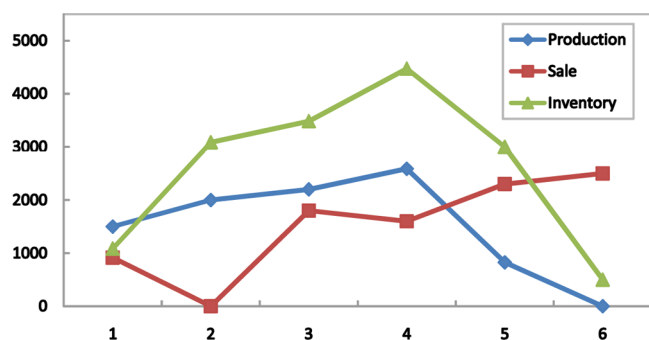


Figure 7. Solution of iterative framework.

In the above solution procedure, the parameter Ω is adjusted as follows: $\Omega_2 = 0.5\Omega_1$, $\Omega_3 = 0.5(\Omega_1 + \Omega_2)$, $\Omega_4 = 0.5(\Omega_2 + \Omega_3)$. Notice that although the parameter value is decreased in the fourth step, it is still a conservative solution ($0.0714 < 0.15$), so we do not adjust the parameter using $\Omega_5 = 0.5(\Omega_3 + \Omega_4)$, but rather $\Omega_5 = 0.5(\Omega_2 + \Omega_4)$.

The solutions of different methods are summarized in the following table. It is seen from Table 6 that while all the solutions

Table 6. Results Summary of Example 1 under Uniform Distribution

	traditional	a posteriori	iterative
Obj*	2356977 (7.6%)	2550538	2536859 (0.54%)
$\text{prob}_{\text{violation}}^{\text{posterioriUB}}$	1.66×10^{-4}	0.15	0.1249
CPU time (s)	0.04	26.6	0.2

satisfy the probabilistic requirement on constraint satisfaction, the solution of the a posteriori probability bound method (with relative optimality gap tolerance $\text{optcr} = 0$ and resource limit

$\text{reslim} = 10\,000$ s) is the best although global optimization is necessary. If we compare the classical robust optimization method and the iterative robust optimization method and consider the difference between their solution and the best solution (i.e., the a posteriori bound based solution), the gap has been decreased from 193 561 to 13 679 (a percentage of 92.93%), and the solution has been greatly improved through the iterative framework. Comparing the solution of the a posteriori probability bound based method (Figure 6) and the iterative method (Figure 7), it is seen that the difference between the solutions is very small. Note that global optimization is not needed in the iterative framework and only five convex robust counterpart optimization problems are solved.

(b) *Triangular Distribution*. In this case, it is assumed that the random variables ξ_j are subject to symmetric triangular distribution with support on $[-1, 1]$. Notice that this type of distribution is bounded and symmetric, so we can still apply the a priori probability bounds to determine the size of the uncertainty set and then apply the traditional robust optimization framework. Under the interval + ellipsoidal set induced robust optimization model, the solution will be the same as the previous uniform distribution since the a priori probability bound does not depend on the distribution. On the other hand, the solution of the other two methods will change since they depend on the distribution of the uncertainty. Specifically, while the a posteriori probability bound based method is applied, the solution is 2 626 457 after a 10 000 s resource limit reaches in GAMS (with a relative gap of 7.52% to the upper bound 2 840 000). When the iterative framework is applied, the final solution is 2 619 188 and the solution procedure is shown in Table 7.

Table 7. Solution Procedure of Iterative Method for Example 1 under Triangular Distribution

k	Ω_k	$\exp(-\Omega^2/2)$	Obj*	$\text{prob}_{\text{violation}}^{\text{posterioriUB}}$
1	1.9479	0.15	2356977	1.33×10^{-9}
2	0.9739	0.6223	2569021	0.0404
3	0.4870	0.8882	2707219	0.4829
4	0.7305	0.7658	2636392	0.181
5	0.8522	0.6955	2602086	0.0903
6	0.7913	0.7312	2619188	0.1304

Table 8. Results Summary of Example 1 under Triangular Distribution

	traditional	a posteriori	iterative
Obj*	2356977 (11.4%)	2626457	2619188 (0.28%)
$\text{prob}_{\text{violation}}^{\text{posterioriUB}}$	1.33×10^{-9}	0.15	0.1304
CPU time (s)	0.06	10000	0.4

The results of three different methods are compared in Table 8. While the traditional framework leads to an 11.4% difference to the a posteriori method solution, the iterative method's solution only has 0.28% difference. This shows that the iterative framework significantly improve the quality of the robust solution while the reliability of the solution is satisfied.

In the above studies, it is assumed that the uncertainty distribution is independent, bounded and symmetric, such that we can apply the traditional robust optimization framework based on only the a priori probability bounds. However, when the uncertainty distribution does not fall into this characteristic,

there is no basis for determining the size of the uncertainty set. Consequently, the traditional robust optimization framework cannot be directly applied (i.e., if we still use the a priori bound to determine the size, the solution will not ensure the probabilistic guarantee). On the other hand, with the proposed iterative framework, the robust optimization can still be applied to solve the problem. Next, we study two cases where the distribution does not satisfy the bounded or symmetric condition.

(c) *Exponential Distribution.* In this case, we assume the random variables are subject to exponential distribution with rate parameter $\lambda = 1$. Notice that this distribution is unbounded, so we apply the “ellipsoidal” type uncertainty set induced robust optimization model rather than interval + ellipsoidal type in this study. With the a posteriori probability bound based method, the final solution is 1 818 269. With the iterative solution framework, the solution is 1 803 310 and the corresponding a posteriori probability upper bound of constraint violation is 0.1474. The solution procedure is listed in Table 9. Notice that we do not list

Table 9. Solution Procedure of Iterative Method for Example 1 under Exponential Distribution

k	Ω_k	Obj*	prob ^{posterioriUB} _{violation}
1	1.9479	2350433	1.0
2	3.8958	1959758	0.3959
3	7.7916	1462763	0.0036
4	5.8437	1672734	0.05
5	4.8697	1806183	0.1505
6	4.8892	1803310	0.1474

the a priori bound value here, since it is not applicable for the asymmetric distribution in this case.

(d) *Normal Distribution.* It is assumed that each ξ_j is subject to normal distribution $N(0,0.5)$ in this case. Although for the case of the normal distribution, it is not necessary to apply an approximation scheme to solve the probabilistically constrained problem since analytical deterministic equivalent problem can be formulated and solved, we study the robust optimization approximation based method here to compare the solution quality. The “ellipsoidal” type uncertainty set is also used in this case to deal with the unbounded distribution. The a posteriori method lead to solution of 2 569 004, and the iterative method leads to 2 563 734, with the constraint violation probability less than 0.1394 as shown in Table 10.

Table 10. Solution Procedure of Iterative Method for Example 1 under Normal Distribution

k	Ω_k	Obj*	prob ^{posterioriUB} _{violation}
1	1.9479	2350433	0.0005
2	0.9739	2569021	0.1505
3	0.9934	2563734	0.1394

5.2. Example 2. In this example, a process scheduling problem^{11,20–22} is studied. This example involves the scheduling of a batch chemical process related to the production of two chemical products using three raw materials. The mixed integer linear optimization model for the scheduling problem is formulated as follows, and the readers are directed to the paper¹¹ for the detailed mixed integer linear optimization formulation and problem data

max profit

$$\text{s.t. profit} = \sum_{s \in S_p, n} \text{price}_s d_{s,n} + \sum_{s \in S_r} \text{price}_s (\text{STI}_s - \text{STF}_s) \quad (19a)$$

$$\sum_{i \in I_j} wv_{i,j,n} \leq 1 \quad \forall i \in I \quad (19b)$$

$$st_{s,n} = st_{s,n-1} - d_{s,n} - \sum_{i \in I_s} \rho_{s,i}^C \sum_{j \in J_i} b_{i,j,n} + \sum_{i \in I_s} \rho_{s,i}^P \sum_{j \in J_i} b_{i,j,n-1} \quad (19c)$$

$$\forall s \in S, \forall n \in N \quad (19d)$$

$$v_{i,j}^{\min} wv_{i,j,n} \leq b_{i,j,n} \leq v_{i,j}^{\max} wv_{i,j,n} \quad (19e)$$

$$\sum_n d_{s,n} \geq \tilde{r}_s \quad \forall s \in S_p \quad (19f)$$

$$Tf_{i,j,n} \geq Ts_{i,j,n} + \alpha_{i,j} wv_{i,j,n} + \beta_{i,j} b_{i,j,n} \quad (19g)$$

$$Ts_{i,j,n+1} \geq Tf_{i,j,n} - H(1 - wv_{i,j,n}) \quad (19h)$$

$$Ts_{i,j,n+1} \geq Tf_{i',j,n} - H(1 - wv_{i',j,n}) \quad (19i)$$

$$Ts_{i,j,n+1} \geq Tf_{i',j',n} - H(1 - wv_{i',j',n}) \quad (19j)$$

$$\forall i, i' \in I, i \neq i', \forall j, j' \in J, \forall n \in N \quad (19k)$$

$$Tf_{i,j,n+1} \geq Tf_{i,j,n} \quad \forall i \in I, \forall j \in J, \forall n \in N \quad (19l)$$

$$Ts_{i,j,n} \leq H \quad \forall i \in I, \forall j \in J, \forall n \in N \quad (19m)$$

$$Tf_{i,j,n} \leq H \quad \forall i \in I, \forall j \in J, \forall n \in N \quad (19n)$$

In this example, we consider the demand uncertainty only and the following constraints are affected:

$$\tilde{r}_s - \sum_n d_{s,n} \leq 0 \quad \forall s \in S_p$$

We assume independent uncertainty distributions on the product demand parameters \tilde{r}_s and assign a base perturbation of 20% of the nominal demand data ($r_{p1} = 50, r_{p2} = 75$): $\tilde{r}_s = r_s(1 + 0.2\xi_s)$. We set the expected minimum probability level on constraint satisfaction to 0.5 (i.e., set the upper bound on constraint violation to 0.5). Then the probabilistic constrained version is

$$\Pr\{\tilde{r}_s - \sum_n d_{s,n} > 0\} \leq 0.5 \quad \forall s \in S_p$$

Several different type of uncertainty distributions are considered to study the proposed method.

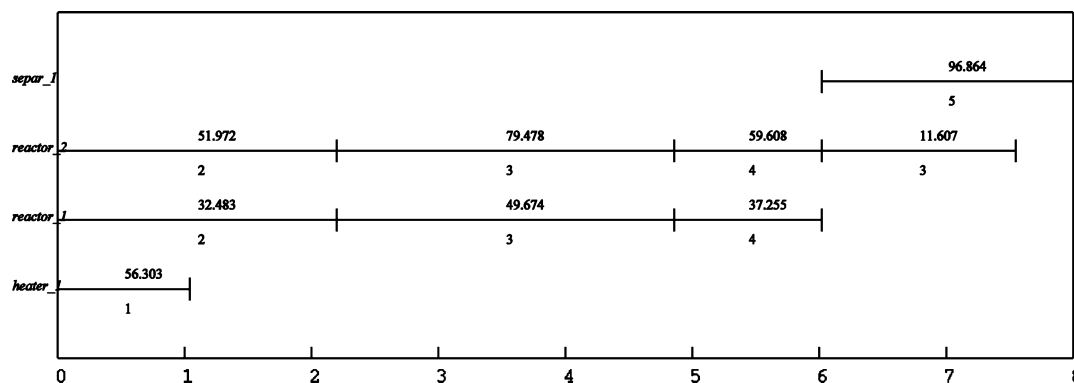


Figure 8. Schedule obtained from the a posteriori bound based method.

(a) *Bounded Distribution*. We consider a bounded symmetric distribution first. Specifically, we assume a uniform distribution on the product demand parameters \tilde{r}_s (i.e., ξ_s is uniformly distributed in $[-1, 1]$). Based on the traditional robust optimization method, the robust counterpart optimization constraint is formulated as follows:

$$r_s - \sum_n d_{s,n} + \Psi_s(0.2r_s) \leq 0 \quad \forall s \in S_p$$

which is equivalent for box, ellipsoidal, and polyhedral type of uncertainty sets since the number of uncertain parameter in each demand constraint is 1. From the desired bound on constraint violation 0.5, we get the uncertainty set size value 1.1774. Since the uncertainty is bounded, a set with size value 1 will cover the whole uncertainty space. However, size 1 still makes the robust optimization problem infeasible.

The a posteriori probability bound based method is applied next and the following constraint is applied:

$$\theta_s(r_s - \sum_n d_{s,n}) + \ln E[e^{0.2\theta_s \xi_s}] \leq \ln 0.5 \quad \forall s \in S_p$$

The resulting nonconvex mixed integer nonlinear optimization problem is solved using ANTIGONE 1.1²³ (with tolerance parameter $optcr = 0.01$ and $reslim = 10\,000$) and the objective is 1070.04 (with relative optimality gap 1.82% to the upper bound 1089.47 after 10 000 s). The corresponding schedule is shown in Figure 8. Finally, we apply the iterative solution framework to solve the problem. Since set size value 1 makes the robust optimization problem infeasible, in the iterative framework, we start from 0.5 for the parameter Ψ_s to make the problem feasible. The solution procedure is shown in Table 11. Notice that the

Table 11. Solution Procedure of Iterative Method for Example 2 under Uniform Distribution

k	Ψ_s	$\exp(-\Omega^2/2)$	Obj*	prob ^{posterioriUB} violation
1	(1.0, 1.0)	(0.6065, 0.6065)	infeasible	
2	(0.5, 0.5)	(0.8825, 0.8825)	1081.25	(0.6646, 0.2039)
3	(0.75, 0.25)	(0.7548, 0.9692)	1058.01	(0.3397, 0.3146)
4	(0.625, 0.375)	(0.8226, 0.9321)	1070.57	(0.5070, 0.2531)
5	(0.6875, 0.25)	(0.7895, 0.9692)	1064.29	(0.4240, 0.2839)
6	(0.6875, 0.125)	(0.7895, 0.9922)	1064.29	(0.4240, 0.2839)

adjustments of the parameter values are based on the change of the a posteriori bounds. For example, we realize that for the first demand constraint is 0.6646 in the 2nd iteration and 0.3397 in the third iteration. To move the bound close to less than 0.5, we

set the new parameter value Ψ_{p1} in the fourth iteration as $(0.5 + 0.75)/2 = 0.625$, and the resulting solution lead to a new probability bound 0.507. Notice in the sixth step, there is no change on the objective solution, so the solution procedure is stopped. The final optimal objective value is 1064.29, and the corresponding schedule is shown in Figure 9. This solution has only 0.54% difference to the a posteriori solution as shown in Table 12.

Comparing the solution from all the three different methods shown in Table 12, the following observations can be made. First, the traditional robust solution framework is conservative and even leads to an infeasible problem. However, the iterative framework successfully addresses the same problem and finds feasible solution. The reason is that the iterative framework utilizes not only the a priori probability bound but also the a posteriori probability bound, thus avoids the conservative solution. Second, comparing the a posteriori probability bound based method and the iterative method, it is seen that the optimal solutions are very close. However, with the iterative framework, we obtain a solution with almost same quality but far less computational efforts. This further validates the effectiveness of the proposed iterative method.

(b) *Unbounded Distribution (Exponential and Normal)*. For this scheduling example, two unbounded distributions are also studied. The traditional framework is not applicable in this situation because the a priori probability bound is based on the bounded distribution assumption. We first study the exponential distribution with parameter $\lambda = 5$. Box, ellipsoidal, and polyhedral type of uncertainty set lead to same robust optimization formulations here. The results of the different methods are summarized in Table 13, and the solution procedure of iterative method is given in Table 14. The iterative method's solution has only 0.6% difference to the a posteriori solution in this case.

Next, we study the case under normal distribution $N(0, 0.5)$. The results are given in Table 15, and the solution procedure of iterative method is summarized in Table 16. The a posteriori solution 1074.22 has a relative gap of 1.33% to the upper bound 1088.75 after 10 000 s. Iterative method's solution has only 0.1% difference when compared to the a posteriori solution.

From the above results, it is observed that while the traditional method is not applicable to the unbounded distribution cases, the iterative method applies the robust optimization approximation and uses the a posteriori bound to check the solution reliability. The solutions of iterative method are consistently very close to the a posteriori bound based method in terms of the optimal objective values while the computational complexity is greatly reduced since only convex robust optimization problem is solved in several iterations.

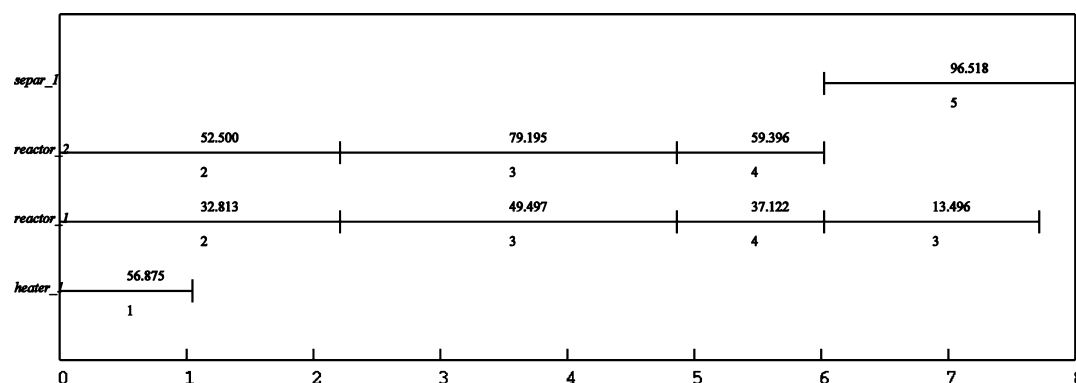


Figure 9. Schedule obtained from the iterative method.

Table 12. Results Summary of Example 2 under Uniform Distribution

	traditional	a posteriori	iterative
Obj*	infeasible	1070.04	1064.29 (0.54%)
prob ^{posterioriUB} _{violation}		(0.5, 0.2558)	(0.424, 0.2839)
CPU time (s)		10000	9.1

Table 13. Results Summary of Example 2 under Exponential Distribution

	traditional	a posteriori	iterative
Obj*	not applicable	1079.55	1073.09 (0.6%)
prob ^{posterioriUB} _{violation}		(0.5, 0.1672)	(0.406, 0.1827)
CPU time (s)		4.3	10.4

Table 14. Solution Procedure of Iterative Method for Example 2 under Exponential Distribution

k	Ψ_s	Obj*	prob ^{posterioriUB} _{violation}
1	(1.0, 1.0)	infeasible	
2	(0.5, 0.5)	1081.25	(0.5578, 0.1648)
3	(0.75, 0.25)	1058.01	(0.2397, 0.2240)
4	(0.8, 0.2)	1052.99	(0.1991, 0.2394)
5	(0.7, 0.3)	1063.04	(0.2873, 0.2094)
6	(0.6, 0.4)	1073.09	(0.406, 0.1827)

Table 15. Results Summary of Example 2 under Normal Distribution

	traditional	a posteriori	iterative
Obj*	not applicable	1074.22	1073.09 (0.1%)
prob ^{posterioriUB} _{violation}		(0.5, 0.2547)	(0.4868, 0.2582)
CPU time (s)		10000	4.8

Table 16. Solution Procedure of Iterative Method for Example 2 under Normal Distribution

k	Ψ_s	Obj*	prob ^{posterioriUB} _{violation}
1	(1.0, 1.0)	infeasible	
2	(0.5, 0.5)	1081.25	(0.6065, 0.2357)
3	(0.75, 0.25)	1058.01	(0.3247, 0.307)
4	(0.8, 0.2)	1052.99	(0.2780, 0.3243)
5	(0.7, 0.3)	1063.04	(0.3753, 0.2901)
6	(0.6, 0.4)	1073.09	(0.4868, 0.2582)

6. CONCLUSION

The traditional robust optimization framework can be used to approximate probabilistic constraints and provide safe solution. However, the solution can be conservative. When a detailed probability distribution on uncertainty is available, the a posteriori probability bound based method leads to less conservative approximation, but the trade-off is that the resulting nonconvex problem needs to be solved via a deterministic global optimization approach. A novel solution framework combining the robust optimization approximation and the a posteriori probability bound evaluation is proposed to improve the solution quality of traditional robust optimization framework without significant computation effort. The effectiveness of the proposed method has been illustrated through a motivating example, as well as planning and scheduling problems. Furthermore, while the traditional robust optimization method requires information on certain probability distribution on the uncertainty such that the a priori probability bound is valid, the proposed iterative framework extends the application to general distributions since we can always use the a posteriori probability bound to ensure the constraint is satisfied within desired probability. Finally, it is worth mentioning that the probability bounds used in this work are derived based on the assumption of independence on the uncertain parameters. One of the future research directions will be to investigate the correlation between uncertain parameters.

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Notes

The authors declare no competing financial interest.

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REFERENCES

- (1) Soyster, A. L. Convex programming with set-inclusive constraints and applications to inexact linear programming. *Operations Research* **1973**, *21*, 1154–1157.
- (2) Ben-Tal, A.; Nemirovski, A. Robust solutions of uncertain linear programs. *Operations Research Letters* **1999**, *25* (1), 1–13.

- (3) Ben-Tal, A.; Nemirovski, A. Robust solutions of Linear Programming problems contaminated with uncertain data. *Mathematical Programming* **2000**, *88*, 411–424.
- (4) El-Ghaoui, L.; Lebret, H. Robust solutions to least-squares problems with uncertain data. *Siam Journal on Matrix Analysis and Applications* **1997**, *18* (4), 1035–1064.
- (5) El-Ghaoui, L.; Oustry, F.; Lebret, H. Robust solutions to uncertain semidefinite programs. *SIAM J. Optim.* **1998**, *9*, 33–52.
- (6) Bertsimas, D.; Sim, M. The price of robustness. *Operations Research* **2004**, *52* (1), 35–53.
- (7) Lin, X.; Janak, S. L.; Floudas, C. A. A new robust optimization approach for scheduling under uncertainty: I. bounded uncertainty. *Comput. Chem. Eng.* **2004**, *28*, 1069–1085.
- (8) Janak, S. L.; Lin, X.; Floudas, C. A. A new robust optimization approach for scheduling under uncertainty: II. Uncertainty with known probability distribution. *Comput. Chem. Eng.* **2007**, *31*, 171–195.
- (9) Verderame, P. M.; Floudas, C. A. Operational Planning of Large-Scale Industrial Batch Plants under Demand Due Date and Amount Uncertainty. I. Robust Optimization Framework. *Ind. Eng. Chem. Res.* **2009**, *48* (15), 7214–7231.
- (10) Verderame, P. M.; Floudas, C. A. Operational Planning of Large-Scale Industrial Batch Plants under Demand Due Date and Amount Uncertainty: II. Conditional Value-at-Risk Framework. *Ind. Eng. Chem. Res.* **2010**, *49* (1), 260–275.
- (11) Li, Z.; Ding, R.; Floudas, C. A. A Comparative Theoretical and Computational Study on Robust Counterpart Optimization: I. Robust Linear and Robust Mixed Integer Linear Optimization. *Ind. Eng. Chem. Res.* **2011**, *50*, 10567–10603.
- (12) Li, Z.; Tang, Q.; Floudas, C. A. A Comparative Theoretical and Computational Study on Robust Counterpart Optimization: II. Probabilistic Guarantees on Constraint Satisfaction. *Ind. Eng. Chem. Res.* **2012**, *51*, 6769–6788.
- (13) Charnes, A.; Cooper, W. W.; Symonds, G. H. Cost Horizons and Certainty Equivalents - an Approach to Stochastic-Programming of Heating Oil. *Management Science* **1958**, *4* (3), 235–263.
- (14) Nemirovski, A.; Shapiro, A. Scenario approximations of chance constraints. In *Probabilistic and randomized methods for design under uncertainty*; Calafiore, G.; Dabbene, F., Eds.; Springer: London, 2005; pp 3–48.
- (15) Luedtke, J.; Ahmed, S. A Sample Approximation Approach for Optimization with Probabilistic Constraints. *SIAM Journal on Optimization* **2008**, *19* (2), 674–699.
- (16) Nemirovski, A.; Shapiro, A. Convex approximations of chance constrained programs. *SIAM Journal on Optimization* **2006**, *17* (4), 969–996.
- (17) Pinter, J. Deterministic approximations of probability inequalities. *ZOR - Method and Models of Operations Research* **1989**, *33*, 219–239.
- (18) Prekopa, A. *Stochastic Programming*; Kluwer: Dordrecht, 1995.
- (19) Mitra, S. K. Probability Distribution of Sum of Uniformly Distributed Random Variables. *Siam Journal on Applied Mathematics* **1971**, *20* (2), 195–198.
- (20) Ierapetritou, M. G.; Floudas, C. A. Effective continuous-time formulation for short-term scheduling. 2. Continuous and semi-continuous processes. *Ind. Eng. Chem. Res.* **1998**, *37* (11), 4360–4374.
- (21) Ierapetritou, M. G.; Floudas, C. A. Short-term scheduling: New mathematical models vs algorithmic improvements. *Comput. Chem. Eng.* **1998**, *22*, S419–S426.
- (22) Ierapetritou, M. G.; Hene, T. S.; Floudas, C. A. Effective continuous-time formulation for short-term scheduling. 3. Multiple intermediate due dates. *Ind. Eng. Chem. Res.* **1999**, *38* (9), 3446–3461.
- (23) Misener, R.; Floudas, C. A. ANTIGONE: Algorithms for coNTinuous/Integer Global Optimization of Nonlinear Equations. *Journal of Global Optimization* **2014**, *59*, 503–526, DOI: 10.1007/s10898-014-0166-2.
- (24) Li, Z.; Ierapetritou, M. G. Robust optimization for process scheduling under uncertainty. *Ind. Eng. Chem. Res.* **2008**, *47*, 4148–4157.