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A Comparative Theoretical and Computational Study on Robust Counterpart Optimization: II. Probabilistic Guarantees on Constraint Satisfaction

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S *Supporting Information*

ABSTRACT: Probabilistic guarantees on constraint satisfaction for robust counterpart optimization are studied in this paper. The robust counterpart optimization formulations studied are derived from box, ellipsoidal, polyhedral, "interval+ellipsoidal", and "interval+polyhedral" uncertainty sets (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). For those robust counterpart optimization formulations, their corresponding probability bounds on constraint satisfaction are derived for different types of uncertainty characteristic (i.e., bounded or unbounded uncertainty, with or without detailed probability distribution information). The findings of this work extend the results in the literature and provide greater flexibility for robust optimization practitioners in choosing tighter probability bounds so as to find less conservative robust solutions. Extensive numerical studies are performed to compare the tightness of the different probability bounds and the conservatism of different robust counterpart optimization formulations. Guiding rules for the selection of robust counterpart optimization models and for the determination of the size of the uncertainty set are discussed. Applications in production planning and process scheduling problems are presented.

1. INTRODUCTION

In the vast majority of optimization applications, problem data are often subject to uncertainty because of their random nature, measurement errors, or other reasons. The solution obtained without considering the data uncertainty may be suboptimal or even infeasible for practical applications. Thus, addressing uncertainty issues in optimization is of significant importance and has received a lot of attention in both academia and industry. Robust optimization belongs to an important methodology dealing with optimization problems with data uncertainty. With a predefined set within the uncertain parameter space, robust optimization techniques aim at finding the best solution which is feasible for any realization of the data uncertainty in the given set. The corresponding optimization problem is also called *robust counterpart optimization* problem.

While several other methods for optimization under uncertainty are available, one major motivation for studying robust optimization is that in many applications we do not have information on probability distributions, and in some applications infeasibility is not accepted at all. Compared to min−max optimization problem, robust optimization has the flexibility in controlling the solution quality, rather than only leading to worst-case scenario solutions. Compared to methods such as two/multiple stage stochastic programming and parametric optimization, the advantage of robust optimization is that it does not suffer from the exponential increase in the computational complexity when the number of uncertain parameters increases.

One of the earliest papers on robust counterpart optimization is the work of Soyster,[1] who considered simple perturbations in the data and aimed at reformulating the original linear programming problem such that the resulting solution would be feasible under all possible perturbations. Ben-Tal and Nemirovski,[2,3] El-Ghaoui et al.,[4,5] Bertsimas and Sim,[6] Lin et al.,[7] Janak et al.,[8] Verderame. and Floudas,[9,10] and Li et al.[11] extended the framework of robust counterpart optimization, and included sophisticated solution techniques with nontrivial uncertainty sets describing the data. El Ghaoui and Lebret[4] used a robust optimization approach for least-squares problems with uncertain data. Ben-Tal and Nemirovski[3] proposed the ellipsoidal set based robust counterpart formulation for linear programming problems with uncertain linear coefficients. Bertsimas and Sim[6] considered 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 0 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 and several known probability distributions (e.g., normal, uniform, binomial, poisson distribution). The robust optimization framework was later extended by Verderame and Floudas,[9] 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 Li et al.,[11] we studied different uncertainty sets, discussed their relationships and derived their

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corresponding robust counterpart optimization formulations for both linear optimization (LP) and mixed integer linear optimization (MILP) problems. Several recent publications (e.g., El Ghaoui et al.,[12] Chen et al.,[13] Chen and Sim,[14] Delage and Ye,[15] Ben-Tal et al.[16]) aim at bridging the gap between the conservatism of robust counterpart optimization models and the specificity of stochastic programming, where optimal decisions are sought for the worst-case probability distributions within a family of possible distributions, defined by certain properties such as their support and moments.

Although robust optimization does not require known probability distribution information of the uncertainty, one might ask for probabilistic guarantees for the robust counterpart solution's feasibility if there exists a particular probability distribution for the uncertainty. In other words, it is desirable to evaluate the lower bound on constraint satisfaction or upper bound on constraint violation, which depends on the characteristics of the uncertainty itself. Ben-Tal and Nemirovski[3] derived probability bounds for the "interval+ellipsoidal" uncertainty set (see eq 2.9d) based robust counterpart optimization model for bounded symmetric uncertainty. They showed that for ellipsoids with radius Ω, the corresponding robust feasible solutions must satisfy the original constraint with probability at least $(1 - e^{-\Omega^2/2})$. Bertsimas and Sim[6] derived probability bounds for the "interval+polyhedral" uncertainty set (see eq 2.9e) based robust counterpart optimization model for bounded symmetric uncertainty and showed that the robust feasible solution satisfies the constraint with probability at least $(1 - e^{-\Gamma^2/(2|J_i|)})$, where Γ is the parameter defining the size of the polyhedron and $|J_i|$ is the number of the uncertain parameters in the i-th constraint. Chen et al.[13] considered more general deviation measures which capture distributional asymmetry and lead to improved probability guarantees. Bertsimas et al.[17] presented probabilistic guarantees for the general norm based uncertainty model. Bertsimas and Sim[18] proposed a relaxed robust counterpart for general conic optimization problems and provided probability guarantees of the robust solution when the uncertain coefficients obey independent and identically distributed normal distributions. Paschalidis and Kang[19] studied probability bounds for the "interval+polyhedral" uncertainty set based robust counterpart optimization model when the entire probability distribution is available.

In this paper, probabilistic guarantees on constraint satisfaction are derived for different uncertainty set induced robust counterpart optimization models, for both bounded and unbounded uncertainty, with and without detailed probability distribution information. Extensive numerical studies are performed so as to compare the tightness of the different probability bounds and to assess the conservatism of several important robust counterpart optimization models.

The paper is organized as follows. In section 2, we review the set induced robust counterpart optimization for general linear optimization and mixed integer linear optimization problems. In section 3, we study the probabilistic guarantees of constraint violation of the robust counterpart optimization models (with detailed proofs given in the Appendix). These are derived from two directions: the uncertainty set and the solution of robust counterpart optimization model. In section 4, numerical examples are studied to compare the different probability bounds and a comparative study on the conservatism is performed. In section 5, applications in production planning and process scheduling are presented.

2. UNCERTAINTY SET INDUCED 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, that is, candidate solutions that remain feasible for all realizations of the data from the uncertainty set.

In general, consider the following linear optimization problem with uncertainty in the left-hand side (LHS) constraint coefficients, right-hand side (RHS) and objective function coefficients

$$\begin{aligned} \max_x \ & \sum_j \tilde{c}_j x_j \\ \text{s.t.} \ & \sum_j \tilde{a}_{ij} x_j \le \tilde{b}_i \ \forall \ i \end{aligned} \tag{2.1}$$

where $\tilde{a}_{ij}$, $\tilde{b}_i$, and $\tilde{c}_j$ represent the true value of the parameters which are subject to uncertainty. Problem 2.1 can be equivalently rewritten as

$$\begin{aligned} \max_{x,z} \ & z \\ \text{s.t.} \ & z - \sum_j \tilde{c}_j x_j \le 0 \\ & \tilde{b}_i x_0 + \sum_j \tilde{a}_{ij} x_j \le 0 \ \forall \ i \\ & x_0 = -1 \end{aligned} \tag{2.2}$$

In 2.2, the uncertain parameters are all moved to the LHS.

Similarly, consider a general mixed integer linear optimization problem with uncertainty in LHS, RHS, and objective function coefficients

$$\begin{aligned} \max_{x,y} \ & \sum_m \tilde{c}_m x_m + \sum_k \tilde{d}_k y_k \\ \text{s.t.} \ & \sum_m \tilde{a}_{im} x_m + \sum_k \tilde{b}_{ik} y_k \le \tilde{p}_i \ \ \forall \ i \end{aligned} \tag{2.3}$$

where x_m and y_k are continuous and integer variables, respectively, and $\tilde{a}_{im}$, $\tilde{b}_{ik}$, $\tilde{c}_m$, $\tilde{d}_k$, and $\tilde{p}_i$ represent the true value of the parameters which are subject to uncertainty.

We can rewrite problem 2.3 as

$$\begin{aligned} \max_{x,y,z} \ & z \\ \text{s.t.} \ & z - \sum_m \tilde{c}_m x_m - \sum_k \tilde{d}_k y_k \le 0 \\ & \tilde{p}_i x_0 + \sum_m \tilde{a}_{im} x_m + \sum_k \tilde{b}_{ik} y_k \le 0 \ \forall \ i \\ & x_0 = -1 \end{aligned} \tag{2.4}$$

thus, the uncertain parameters in 2.3 are all moved to the LHS of constraints in 2.4.

Based on the above analysis, without loss of generality, we focus on the following general i-th constraint of a (mixed integer) linear optimization problem considering only LHS uncertainty

$$\sum_j \tilde{a}_{ij} x_j \le b_i \tag{2.5}$$

where every x_j can be either a continuous or an integer variable and $\tilde{a}_{ij}$ are subject to uncertainty. Define the uncertainty as follows

$$\tilde{a}_{ij} = a_{ij} + \xi_{ij}\hat{a}_{ij} \ \forall\ j \in J_i \tag{2.6}$$

where a_{ij} represent the nominal value of the parameters, $\hat{a}_{ij}$ represent positive constant perturbations, ξ_{ij} represent independent random variables which are subject to uncertainty and J_i represents the index subset that contains the variables whose coefficients are subject to uncertainty.

Constraint 2.5 can be rewritten by grouping the deterministic part and the uncertain part for the LHS of 2.5 as follows

$$\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_{ij}\hat{a}_{ij}x_j \le b_i \tag{2.7}$$

In the set-induced robust optimization method, the aim is to find solutions that remain feasible for any ξ in the given uncertainty set U so as to immunize against infeasibility, that is,

$$\sum_j a_{ij}x_j + \max_{\xi\in U}\{\sum_{j\in J_i} \xi_{ij}\hat{a}_{ij}x_j\} \le b_i \tag{2.8}$$

The formulation of the robust counterpart optimization is connected with the selection of the uncertainty set U. On the basis of our previous work in Li et al.,[11] we summarize five important uncertainty sets and their corresponding robust counterpart formulations here. Notice that we eliminate the constraint index i for the random vector ξ for the sake of simplicity.

Box uncertainty set:

$$U_\infty = \{\xi \mid |\xi_j| \le \Psi,\ \forall\ j \in J_i\} \tag{2.9a}$$

Ellipsoidal uncertainty set:

$$U_2 = \{\xi \mid \sum_{j\in J_i} \xi_j^2 \le \Omega^2\} \tag{2.9b}$$

Polyhedral uncertainty set:

$$U_1 = \{\xi \mid \sum_{j\in J_i} |\xi_j| \le \Gamma\} \tag{2.9c}$$

Interval + Ellipsoidal uncertainty set:

$$U_{2\cap\infty} = \{\xi \mid \sum_{j\in J_i} \xi_j^2 \le \Omega^2,\ |\xi_j| \le 1,\ \forall\ j \in J_i\} \tag{2.9d}$$

Interval + Polyhedral uncertainty set:

$$U_{1\cap\infty} = \{\xi \mid \sum_{j\in J_i} |\xi_j| \le \Gamma,\ |\xi_j| \le 1,\ \forall\ j \in J_i\} \tag{2.9e}$$

Note that we use "interval" uncertainty set to denote the following special case of box uncertainty set: $U_\infty = \{\xi \mid |\xi_j| \le 1, \forall j \in J_i\}$, which is useful for the case of bounded uncertainty since the uncertainty set can be restricted inside the known bounds of the uncertainty. The corresponding robust counterpart optimization formulations induced from the above different uncertainty sets are presented as follows:

Box uncertainty set based robust counterpart optimization formulation

$$\sum_j a_{ij}x_j + \Psi[\sum_{j\in J_i} \hat{a}_{ij}|x_j|] \le b_i \tag{2.10a}$$

Ellipsoidal uncertainty set based robust counterpart optimization formulation

$$\sum_j a_{ij}x_j + [\Omega\sqrt{\sum_{j\in J_i} \hat{a}_{ij}^2 x_j^2}\,] \le b_i \tag{2.10b}$$

Polyhedral uncertainty set based robust counterpart optimization formulation

$$\begin{cases} \sum_j a_{ij}x_j + z_i\Gamma \le b_i \\ z_i \ge \hat{a}_{ij}|x_j| \ \forall\ j \in J_i \end{cases} \tag{2.10c}$$

Interval + ellipsoidal uncertainty set based robust counterpart optimization formulation

$$\sum_j a_{ij}x_j + \sum_{j\in J_i} \hat{a}_{ij}|x_j - z_{ij}| + \Omega\sqrt{\sum_{j\in J_i} \hat{a}_{ij}^2 z_{ij}^2} \le b_i \tag{2.10d}$$

Interval + polyhedral uncertainty set based robust counterpart optimization formulation

$$\begin{cases} \sum_j a_{ij}x_j + [z_i\Gamma + \sum_{j\in J_i} p_{ij}] \le b_i \\ z_i + p_{ij} \ge \hat{a}_{ij}|x_j| \ \forall\ j \in J_i \\ z_i \ge 0,\ p_{ij} \ge 0 \end{cases} \tag{2.10e}$$

The robust counterpart optimization model is obtained by replacing the original i-th constraint in 2.5 with its robust counterpart constraint. For example, the box uncertainty set induced robust counterpart optimization model for 2.2 is

$$\begin{aligned} \max\quad & z \\ \text{s.t.}\quad & z - \sum_j c_jx_j + \Psi\sum_{j\in J_0} \hat{c}_j|x_j| \le 0 \\ & b_ix_0 + \sum_j a_{ij}x_j + \Psi[\sum_{j\in J_i} \hat{a}_{ij}|x_j| + \hat{b}_i|x_0|] \le 0\ \forall\ i \\ & x_0 = -1 \end{aligned}$$

which can be further rewritten as

$$\begin{aligned} \max\quad & z \\ \text{s.t.}\quad & z - \sum_j c_jx_j + \Psi\sum_{j\in J_0} \hat{c}_j|x_j| \le 0 \\ & \sum_j a_{ij}x_j + \Psi[\sum_{j\in J_i} \hat{a}_{ij}|x_j| + \hat{b}_i] \le b_i\ \forall\ i \end{aligned} \tag{2.11}$$

Note that in eq 2.11 the same uncertainty set parameter Ψ is applied for all the constraints in the above problem. However, different parameters Ψ can be introduced for different constraints.

Similarly, the ellipsoidal set induced robust counterpart optimization model for MILP problem 2.4 is

$$
\begin{aligned}
&\max \quad z\\
&\text{s.t.} \quad z - \sum_m c_m x_m - \sum_k d_k y_k + \Omega\sqrt{\sum_m \hat{c}_m{}^2 x_m{}^2 + \sum_k \hat{d}_k{}^2 y_k{}^2} \le 0\\
&p_i x_0 + \sum_m a_{im} x_m + \sum_k b_{ik} y_k + \Omega\sqrt{\hat{p}_i^2 x_0{}^2 + \sum_m \hat{a}_{im}{}^2 x_m{}^2 + \sum_k \hat{b}_{ik}{}^2 y_k{}^2} \le 0 \ \forall i\\
&x_0 = -1
\end{aligned}
$$

which is further reduced to

$$
\begin{aligned}
&\max \quad z\\
&\text{s.t.} \quad z - \sum_m c_m x_m - \sum_k d_k y_k + \Omega\sqrt{\sum_m \hat{c}_m{}^2 x_m{}^2 + \sum_k \hat{d}_k{}^2 y_k{}^2} \le 0\\
&\sum_m a_{im} x_m + \sum_k b_{ik} y_k + \Omega\sqrt{\hat{p}_i^2 + \sum_m \hat{a}_{im}{}^2 x_m{}^2 + \sum_k \hat{b}_{ik}{}^2 y_k{}^2} \le p_i \ \forall i
\end{aligned} \tag{2.12}
$$

An equivalent presentation based on a unification approach of the uncertainty descriptions may be possible, but it is not selected so as to maintain the clarity of presentation. In the next section, probability guarantees on constraint satisfaction will be studied based on the above uncertainty sets and their corresponding robust counterpart formulations.

3. PROBABILISTIC GUARANTEES OF ROBUST COUNTERPART OPTIMIZATION SOLUTIONS

In the uncertainty set induced robust optimization framework, the uncertainty set is defined by the decision maker. If the uncertainty set covers the whole uncertain space containing all the possible realizations of uncertain parameters, then it is certain that the robust solution (if it exists) is feasible for any realizations of uncertainty (i.e., the probabilistic guarantee on constraint satisfaction is 1). However, in reality, the uncertainty set is not necessarily defined to cover the whole uncertain space because the decision maker might allow for a certain degree of constraint violation. For instance, it is impossible to define a finite set to cover unbounded uncertain parameter space.

For a given constraint, if we have a feasible solution and know the uncertain parameters' probability distribution, then the degree of constraint violation is exactly the probability that the constraint is violated. In those cases where the uncertainty set does not cover the whole uncertain parameter space, the following question naturally arises: Before we solve a robust optimization problem, what size of the uncertainty set is necessary to ensure that the degree of constraint violation does not exceed a certain level? Upon solution of the robust optimization problem, what is the degree of constraint violation? The answers to those questions are related to the probabilistic guarantees on the constraint satisfaction, or the upper bound on the probability of constraint violation.

In general, two different types of methodologies can be used in evaluating the probabilistic guarantees. The first type of methods derives the probability using the uncertainty set information before we solve the problem (i.e., from the robust counterpart constraint since the robust counterpart is derived from the uncertainty set) and the resulting bound is called a priori probability bound. The second method derives the probability directly from the solution of the robust counterpart optimization model, which can also be viewed as checking the probability of constraint violation, and the resulting bound is called a posteriori bound. For both methodologies, different probability bounds can be derived with different levels of uncertainty information.

3.1. A Priori Probabilistic Guarantees Based on Uncertainty Set Information. *Lemma 3.1.* For every robust counterpart constraint 2.10a–2.10e, if it is satisfied, then the following relationship, which represents an upper bound on the probability that the original constraint is violated, holds:

$$
\Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \Pr\{\sum_{j\in J_i} \xi_j \delta_j > \Delta\} \tag{3.1}
$$

where the parameters Δ and δ are defined as follows:

(1) For box uncertainty set based counterpart 2.10a

$$
\Delta = \Psi, -1 \le \delta_j \le 1, \forall j \in J_i, \sum_{j\in J_i} \delta_j \le 1 \tag{3.2a}
$$

(2) For ellipsoidal uncertainty set based robust counterpart 2.10b

$$
\Delta = \Omega, -1 \le \delta_j \le 1, \forall j \in J_i, \sum_{j\in J_i} \delta_j^2 = 1 \tag{3.2b}
$$

(3) For polyhedral uncertainty set based robust counterpart 2.10c

$$
\Delta = \Gamma, -1 \le \delta_j \le 1, \forall j \in J_i \tag{3.2c}
$$

(4) For interval + ellipsoidal uncertainty set based robust counterpart 2.10d

$$
\Delta = \Omega, -1 \le \delta_j \le 1, \forall j \in J_i, \sum_{j\in J_i} \delta_j^2 = 1 \tag{3.2d}
$$

(5) For interval + polyhedral uncertainty set based robust counterpart 2.10e

$$
\Delta = \Gamma, 0 \le \delta_j \le 1, \forall j \in J_i \tag{3.2e}
$$

Proof. See Appendix A for the proof.

From the above Lemma, it is observed that for the different types of robust counterparts 2.10a–2.10e, bounding the probability of constraint violation corresponds to the evaluation of the expression $\Pr\{\sum_{j\in J_i}\xi_j\delta_j > \Delta\}$.

Lemma 3.2. If $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to a ***symmetric*** probability distribution, then the following probability of constraint violation holds for any $\theta > 0$:

$$
\Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \mathrm{e}^{-\theta\Delta} \prod_{j\in J_i} \left\{ \int_{-\infty}^{\infty} \sum_{k=0}^{\infty} \frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!} \, \mathrm{d}F_{\xi_j}(\xi) \right\} \tag{3.3}
$$

where Δ and δ_j are detailed in Lemma 3.1.

Proof. See Appendix A for the proof.

Lemma 3.3. If $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to a ***bounded*** and ***symmetric*** probability distribution supported on

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$[-1, 1]$, then the following bound on the probability of constraint violation holds for any $\theta > 0$

$$\Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \exp\left(\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i} \frac{\theta^2\delta_j^2}{2}\right\}\right) \tag{3.4}$$

where Δ and δ_j are detailed in Lemma 3.1.

Proof. See Appendix A for the proof.

On the basis of the above analysis, explicit probability bounds on constraint violation can be derived as shown in Theorem 3.1.

Theorem 3.1. Let $\{\xi_j\}_{j\in J_i}$ be ***independent*** and subject to a ***bounded*** and ***symmetric*** probability distribution supported on [-1,1], then

(1) for all the five robust counterparts 2.10a−2.10e, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \exp\left(-\frac{\Delta^2}{2|J_i|}\right) \tag{3.5}$$

(2) for the box, ellipsoidal, and interval + ellipsoidal uncertainty sets induced robust counterparts 2.10a, 2.10b, and 2.10d, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \exp\left(-\frac{\Delta^2}{2}\right) \tag{3.6}$$

where Δ represents the adjustable parameter for the different uncertainty sets as detailed in Lemma 3.1.

Proof. See Appendix A for the proof.

Remark 3.1. Note that Ben-Tal and Nemirovski[3] derived the probability bound $e^{-\Omega^2/2}$ for the interval+ellipsoidal uncertainty set induced robust counterpart 2.10d and Bertsimas and Sim[6] derived the probability bound $e^{-\Gamma^2/(2|J_i|)}$ for the interval+ polyhedral uncertainty set induced robust counterpart 2.10e. Theorem 3.1 enhances them to more general robust counterpart optimization formulations.

Remark 3.2. Another bound $B(|J_i|,\Delta)$ proposed by Bertsimas and Sim[6] for the interval+polyhedral based robust counterpart is also valid for all the five robust counterparts in (2.10) since it is valid for $Pr\{\sum_{j\in J_i}\xi_j\delta_j \ge \Delta\}$, thus we have the following bounds for the robust counterparts 2.10a−2.10e:

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le B(|J_i|, \Delta) \tag{3.7}$$

where

$$B(|J_i|, \Delta) = \frac{1}{2^{|J_i|}}\left\{(1-\mu)\sum_{l=\lfloor\nu\rfloor}^{|J_i|}\binom{|J_i|}{l} + \mu\sum_{l=\lfloor\nu\rfloor+1}^{|J_i|}\binom{|J_i|}{l}\right\},$$
$$\nu = ((\Delta + |J_i|)/2),\ \mu = \nu - \lfloor\nu\rfloor$$

Considering the complexity in evaluating the combination terms in $B(|J_i|,\Delta)$, Bertsimas and Sim[6] also proposed the following simpler bound:

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le B'(|J_i|, \Delta) \tag{3.8}$$

where $B'(|J_i|,\Delta) = (1-\mu)C(n, \lfloor\nu\rfloor) + \sum_{k=\lfloor\nu\rfloor+1}^{n} C(n,k)$, $n = |J_i|$, $\nu = ((\Delta + |J_i|)/2)$, $\mu = \nu - \lfloor\nu\rfloor$

$$C(n,k) = \begin{cases} \dfrac{1}{2^n} & \text{if } k = 0 \text{ or } k = n \\ \dfrac{1}{\sqrt{2\pi}}\sqrt{\dfrac{n}{(n-k)k}}\exp\left[n\log\left(\dfrac{n}{2(n-k)}\right) + k\log\left(\dfrac{n-k}{k}\right)\right] & \text{otherwise} \end{cases}$$

The above bound 3.8 is still valid for robust counterparts 2.10a−2.10e.

The above probability bounds 3.5−3.8 are based on simple information on the uncertainty, that is, bounded, symmetric and independent. Once the full probability distribution information of the uncertainty is known, different bounds can be derived. Paschalidis and Kang[19] studied the probability bound for the interval+polyhedral uncertainty set induced robust counterpart optimization model. Here, we extend their conclusion to other robust counterpart formulations.

Theorem 3.2. If $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to ***symmetric*** probability distribution, then we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \exp(\min_{\theta>0}\{-\theta\Delta + \sum_{j\in J_i} \ln E[e^{\theta\xi_j}]\}) \tag{3.9}$$

where Δ represents the adjustable parameter for the different uncertainty sets as detailed in Lemma 3.1.

Proof. See Appendix A for the proof.

Note that evaluating the probability bound in 3.9 needs the moment generating function $E[e^{\theta\xi_j}]$ and the solution of an additional optimization problem.

3.2. A Posteriori Probabilistic Guarantees Based on Solutions of Robust Counterpart Optimization Model.

All the a priori probabilistic bounds are derived from the definition of the uncertainty set and the uncertainty characteristics. Once the solution of the robust counterpart optimization model is available, we can check the probability of constraint violation based on the robust solution x^*(which can be any feasible solution of the robust optimization problem) and the distribution characteristics of the uncertain parameters.

Theorem 3.3. If the uncertain parameters $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to a ***bounded*** probability distribution supported on $[-1,1]$, and the robust counterpart solution is x^* with $d_i(x^*) > 0$, where $d_i(x) \triangleq b_i - \sum_j a_{ij}x_j - E[\sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j]$,

Table 3.1. Summary on Probabilistic Guarantees of Constraint Satisfaction[a]

	upper bound on the probability of constraint violation	robust counterpart applicable	assumption on uncertainty distribution
B1[b]	$\exp(-(\Delta^2)/2)$	IE[3], B, E	independent, symmetric, bounded
B2[b]	$\exp(-(\Delta^2)/2\|J_i\|)$	IP[6], B, E, IE, P	independent, symmetric, bounded
B3[bc]	$B'(\|J_i\|,\Delta)\ (1 \le \Delta \le \|J_i\|)$	IP[6], B, E, IE, P	independent, symmetric, bounded
B4[b]	$\exp(\min_{\theta>0}\{-\theta\Delta + \sum_{j\in J_i} \ln E[e^{\theta\xi_j}]\})$	IP[19], B, E, IE, P	independent, symmetric, known probability distribution function
B5[bd]	$\exp(-(d_i(x^*)^2)/(\sum_{i\in J_i} 2\hat{a}_{ij}^2 x^{*2}_j))$	B, E, IE, P, IP	independent, bounded
B6[be]	$\exp(\min_{\theta>0}\{-\theta h_i(x^*) + \sum_{j\in J_i} \ln E[e^{\theta\xi_j\hat{a}_{ij}x^*_j}]\})$	IP[19], B, E, IE, P	independent, known probability distribution function

[a]B, box set based robust counterpart; E, ellipsoidal set based robust counterpart; P, polyhedral set based robust counterpart; IE, interval + ellipsoidal set based robust counterpart; IP, interval + polyhedral set based robust counterpart. [b]Bounds B1, B2, B3, and B4 are a priori derived from uncertainty set definitions, bounds B5 and B6 are posteriori bound derived from robust counterpart solutions. [c]Detailed description on B3 can be found in eq 3.8. [d]For B5, $d_i(x) \triangleq b_i - \sum_j a_{ij}x_j - E[\sum_{j\in J_i}\xi_j\hat{a}_{ij}x^*_j]$. [e]For B6, $h_i(x) \triangleq b_i - \sum_j a_{ij}x^*_j$.

then we have

$$Pr\{\sum_j a_{ij}x^*_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x^*_j > b_i\} \le \exp\left(-\frac{d_i(x^*)^2}{\sum_{i\in J_i} 2\hat{a}_{ij}^2 x^{*2}_j}\right) \tag{3.10}$$

Proof. See Appendix A for the proof.

For those uncertainties with full probability distribution information, we can also derive the following probability bound.

Theorem 3.4. If the uncertain parameters $\{\xi_j\}_{j\in J_i}$ are ***independent*** and the robust counterpart solution is x^*, then for any $\theta > 0$, we have

$$\begin{aligned} &Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j > b_i\} \\ &\le \exp(\min_{\theta>0}\{-\theta(b_i - \sum_j a_{ij}x^*_j) + \sum_{j\in J_i} \ln E[e^{\theta\xi_j\hat{a}_{ij}x^*_j}]\}) \end{aligned} \tag{3.11}$$

Proof. See Appendix A for the proof.

Finally, we summarize the probabilistic bounds for the different robust counterpart optimization models in Table 3.1.

4. ILLUSTRATIVE COMPUTATIONAL STUDIES

To this point, we have systematically studied different uncertainty sets, their corresponding robust counterpart formulations, and presented several different a priori and a posteriori probability bounds on constraint violation for the resulting robust counterpart optimization formulations.

Based on the above theoretical results, we address the following two questions through a set of computational studies:

> Question 1: While we have several alternative types of uncertainty sets and robust counterpart optimization formulations, which one could be a better choice in constructing the robust counterpart model?
>
> Question 2: Once we have selected a particular type of uncertainty set and its resulting robust counterpart optimization formulation, what is an appropriate size for the uncertainty set such that a desired probability bound on constraint satisfaction is met?

4.1. Comparison of Different Probability Bounds.

To compare the different probability bounds for the uncertainty set induced robust counterpart optimization formulations, the following numerical examples with different numbers of uncertain parameters are studied.

Example 1. Consider the following linear optimization problem

$$\begin{aligned} \max\ & 8x_1 + 12x_2 \\ \text{s.t.}\ & \tilde{a}_1x_1 + \tilde{a}_2x_2 \le 140 \\ & 6x_1 + 8x_2 \le 72 \\ & x_1, x_2 \ge 0 \end{aligned}$$

In the above problem, $\tilde{a}_1$ and $\tilde{a}_2$ are uncertain coefficients and they are defined by

$$\tilde{a}_j = a_j + \hat{a}_j\xi_j,\ j = 1, 2$$

where $[a_1\ a_2] = [10\ 20]$, $\tilde{a}_j = 0.1a_j$, and ξ_1,ξ_2 are independent uncertain parameters.

Example 2. Consider the following linear optimization problem

$$\begin{aligned} \max\ & 2x_1 + 4x_2 + 3x_3 + x_4 \\ \text{s.t.}\ & \tilde{a}_1x_1 + \tilde{a}_2x_2 + \tilde{a}_3x_3 + \tilde{a}_4x_4 \le 12 \\ & x_1 - 3x_2 + 2x_3 + 3x_4 \le 7 \\ & 2x_1 + x_2 + 3x_3 - x_4 \le 10 \\ & x_1, x_2, x_3, x_4 \ge 0 \end{aligned}$$

In this problem, $\tilde{a}_1$, $\tilde{a}_2$, $\tilde{a}_3$, and $\tilde{a}_4$ are uncertain coefficients, and they are defined by

$$\tilde{a}_j = a_j + \hat{a}_j\xi_j,\ j = 1, 2, 3, 4$$

where $[a_1\ a_2\ a_3\ a_4] = [3\ 1\ 1\ 4]$, $\tilde{a}_j = 0.1a_j$, and ξ_1,ξ_2,ξ_3,ξ_4 are independent uncertain parameters.

Example 3 . Consider the following linear optimization problem

$$\begin{aligned} \max \quad & -0.18x_1 - 0.22x_2 - 0.1x_3 - 0.12x_4 - 0.1x_5 \\ & - 0.09x_6 - 0.4x_7 - 0.16x_8 - 0.5x_9 - 0.07x_{10} \\ \text{s.t.} \quad & \tilde{a}_1x_1 + \tilde{a}_2x_2 + \tilde{a}_3x_3 + \tilde{a}_4x_4 + \tilde{a}_5x_5 + \tilde{a}_6x_6 + \tilde{a}_7x_7 \\ & + \tilde{a}_8x_8 + \tilde{a}_9x_9 + \tilde{a}_{10}x_{10} \geq 4.2 \\ & 2x_2 + 2x_3 + 2x_4 + 5x_5 + 3x_6 + 4x_8 + x_{10} \leq 20 \\ & 2.7x_5 + 0.08x_6 + 0.12x_8 \leq 0.3 \\ & 6x_1 + 4x_2 + 2x_3 + 3x_4 + x_5 + x_7 + x_{10} \geq 5 \\ & 2x_1 + 4.8x_2 + 1.2x_3 + 0.8x_4 + 3x_5 + 5.2x_7 + 25x_8 \\ & + 0.3x_9 + 2.6x_{10} \geq 40 \\ & 3x_1 + 4x_2 + 5x_3 + 6x_4 + 7x_5 + 2x_6 + x_7 + 9x_8 \\ & + x_9 + 3x_{10} \geq 20 \\ & 5x_1 + 2x_2 + 3x_3 + 4x_4 + x_7 + 3x_{10} \geq 12 \\ & x_j \geq 0, \ j = 1, ..., 10 \end{aligned}$$

In the above problem, $\tilde{a}_j$, $j = 1, ..., 10$ are uncertain coefficients and they are defined by

$$\tilde{a}_j = a_j + \hat{a}_j\xi_j, \ j = 1, ..., 10$$

where $[a_1\ a_2\ a_3\ a_4\ a_5\ a_6\ a_7\ a_8\ a_9\ a_{10}] = [0.91\ 1.1\ 0.9\ 0.75\ 0.35\ 0.65\ 1\ 1.2\ 0.65]$, $\hat{a}_j = 0.1a_j$, and ξ_j, $j = 1, ..., 10$, are independent uncertain parameters.

For all the above three example problems, the LHS constraint coefficients of the first constraint are subject to bounded uncertainty with a maximum of 10% perturbation. For those uncertain constraints in those examples, the corresponding a priori bounds B1, B2, B3, and B4 are computed using only the value of Δ (i.e., the value of Ψ, Ω, Γ). Bounds B5 and B6 are computed after the solution of the different robust counterpart optimization problems based on formulations in (2.10) and the resulting robust solutions are used to evaluate the probability bounds.

For those numerical examples, the following different probability distributions are considered to study the probability bounds: (1) bounded uniform distribution, (2) bounded triangular distribution, and (3) bounded reverse triangular distribution. A detailed description of the distributions is in Table 4.1. Note that to compute the bounds B4 and B6, the moment-generating function (mgf) $E[e^{\theta\xi_j}]$ is needed and it is listed in Table 4.1.

Table 4.1. Probability Distribution Summary

	p.d.f. $f(x)$	m.g.f. $E[e^{\theta\xi_j}]$
uniform	$0.5, -1 \leq x \leq 1$	$(e^{\theta} - e^{-\theta})/(2\theta)$
triangular	$\begin{cases} x + 1, & -1 \leq x \leq 0 \\ 1 - x, & 0 \leq x \leq 1 \end{cases}$	$(e^{\theta} + e^{-\theta} - 2)/\theta^2$
reverse triangular	$\begin{cases} -x, & -1 \leq x \leq 0 \\ x, & 0 \leq x \leq 1 \end{cases}$	$(e^{\theta}(\theta - 1) - e^{-\theta}(\theta + 1) + 2)/\theta^2$

With the above settings, each example is studied under three different uncertainty distributions and the upper bounds on the probability of constraint violation are computed from different types of robust counterpart formulations. Representative results are shown in Figure 4.1−4.3. Note that in Figure 4.2, bound B1 is not plotted since it is not applicable to the polyhedral uncertainty set induced robust counterpart model. For complete results on those examples, the reader is directed to Supporting Information B.

On the basis those results, the following observations can be made.

Comparing the A Priori Probability Bounds B1, B2, B3, and B4. (1) Comparing the first three bounds B1, B2, and B3, which do not use the probability distribution function or the robust solution, it is seen that for the ellipsoidal and interval+ellipsoidal model, bound B1 is the tightest bound. For polyhedral and interval+polyhedral model, bound B3 is the tightest bound.

(2) Comparing the four bounds B1−B4 without using the robust solution information, it is observed that for ellipsoidal and interval+ellipsoidal model, bound B1 and bound B4 are in general tighter than the other two, but there is not a definite conclusion on which one is tighter between bound B1 and bound B4. For the polyhedral and interval+polyhedral model, bound B4 is tighter than bound B1 and bound B3, and bound B1 is the worst bound.

Comparing the A Posteriori Probability Bounds B5 and B6. Comparing bound B5 and B6, B6 is tighter than B5, since it takes into consideration the detailed probability distribution information of the uncertainty. Furthermore, bound B6 is applicable to not only bounded uncertainties but also unbounded general uncertainties. On the other hand, bound B5 is only valid for bounded uncertainty.

Comparing the Two Bounds B4 and B6 Using the Probability Distribution Information. It is also observed that bound B4 and bound B6 that have used detailed distribution function information are tighter than those a priori bounds B1, B2, and B3 that only use the symmetry information. Comparing bound B4 and bound B6, although both of them use the probability distribution information of the uncertainty, bound B6 is tighter than B4 since B6 further uses the specific robust counterpart solution to evaluate the probability of constraint violation. For example, for the case of bounded uncertainty, the entire support of the random variables is covered by the uncertainty set when $\Omega \geq (|J_i|)^{1/2}$ or $\Gamma \geq |J_i|$, so the real probability of constraint violation for the robust solution should be zero, it can be observed that the bound B6 is very close to this value, but bound B4 is not.

Guidelines for Selecting Δ. Finally, based on the above comparisons, we propose some guidelines in assigning a parameter value Δ for uncertainty sets:

(1) In the process of assigning a parameter value for a specific uncertainty set, the bounds B1, B2, B3, and B4 provide us the capability to select the tightest possible bound expression so as to define the size of the uncertainty better and to avoid overly conservative solutions. For example, if the probability distribution information of the uncertainty is known, we can use bound B4 to compute the parameter value defining the interval+polyhedral uncertainty set since that is the best one among the first four bounds.

(2) If the probability distribution information of the uncertainty is known, we have the capability to further improve the solution by using the tightest possible bound B6. A detailed algorithm that achieves the objective will be presented in our future work.

Remark 4.1. For a given desired probabilistic guarantee on constraint satisfaction (or an upper bound on constraint violation), no matter what type of uncertainty set is chosen for

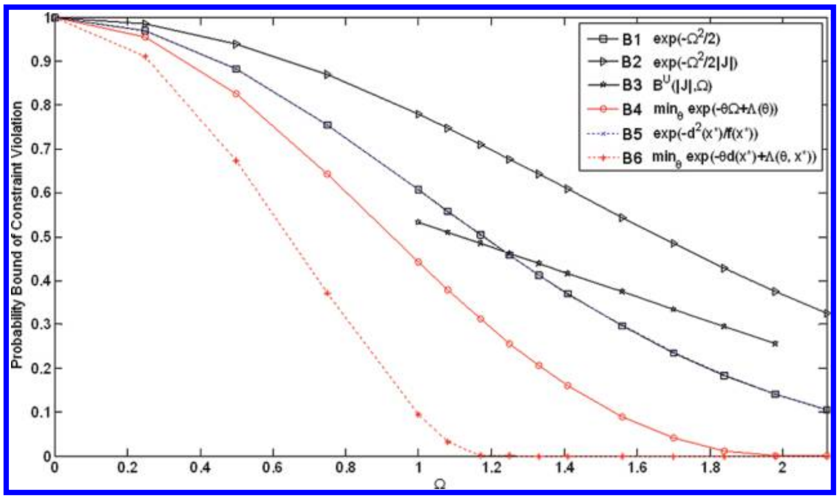

Figure 4.1. Example 1 ($|J| = 2$) under uniform probability distribution, ellipsoidal uncertainty set induced robust optimization model is used for evaluating B5 and B6.

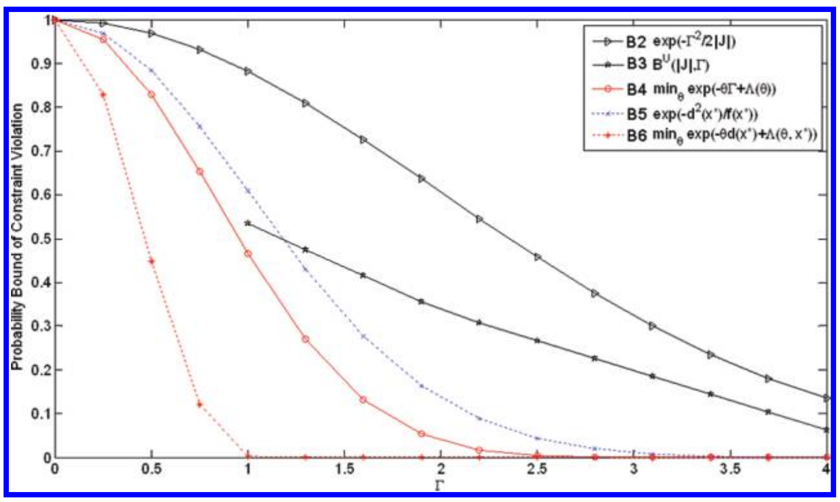

Figure 4.2. Example 2 ($|J| = 4$) under triangular probability distribution, polyhedral uncertainty set induced robust optimization model is used for evaluating B5 and B6.

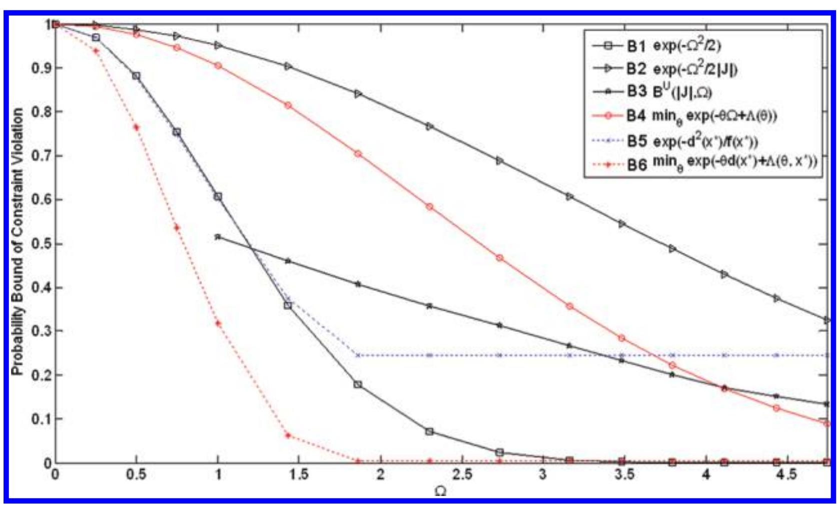

Figure 4.3. Example 3 ($|J| = 10$) under reverse triangular probability distribution, interval+ellipsoidal uncertainty set induced robust optimization model is used for evaluating B5 and B6.

the robust optimization application, we have to define the set with the right size (defined by Δ) such that the probability requirement is satisfied. One important guiding rule in defining the set is that the set should be as small as possible since a larger set leads to a worse solution (as illustrated in previous work[11]).

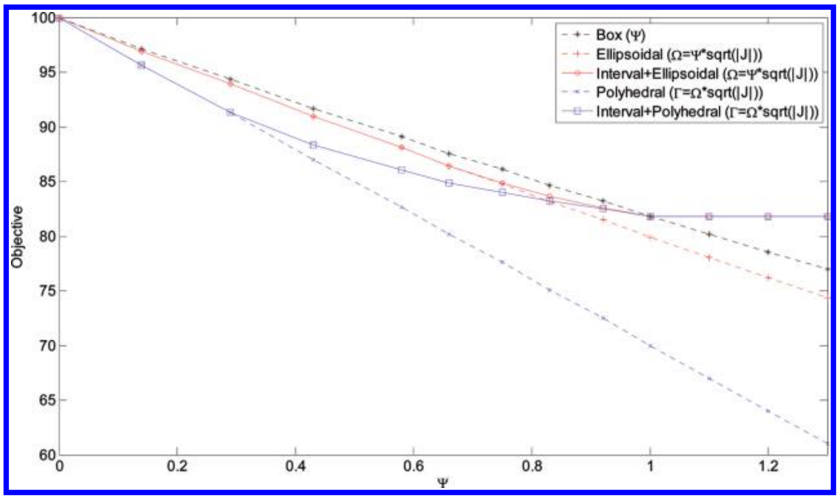

Figure 4.4. Example 4 with LHS+RHS uncertainty for both constraints ($|J| = 3$, $\Gamma = \Psi|J_i|$, $\Omega = \Psi(|J_i|)$).

Remark 4.2. Since the probability bounds are nonincreasing functions of the parameter Δ, the tightest probability bound expression is preferred to find the smallest uncertainty set so as to obtain the best solution.

4.2. Conservatism Comparison of the Different Robust Counterpart Optimization Models. As discussed in the previous subsection, while we are considering a single type of uncertainty set and its corresponding robust counterpart, the desired size for the uncertainty set is the smallest one among those satisfying the probability requirement on constraint satisfaction. However, since there are different uncertainty sets available for constructing robust counterpart optimization formulations, a natural question is: which type of uncertainty set (and robust formulation) should be used?

The above question is related to the issue of the different robust counterpart models' conservatism. Without considering other factors such as computational efforts, the decision-maker naturally wants to adopt the least conservative model. In other words, while the same probability of constraint violation is satisfied, the best possible solution is preferred.

4.2.1. Comparison from the Worst-Case Scenario Point of View. One of the most important distributions widely studied in practice is the bounded uncertainty. For this type of uncertainty, from the worst-case scenario point of view, to ensure that the solution is robust for any possible realization of uncertainties and that there is no constraint violation, the defined uncertainty set has to cover the whole uncertain space. While we compare the size of the different types of uncertainty sets, a conservatism recommendation could be made based on the following fact: the larger the uncertainty set is, the more conservatism the solution becomes.

First, comparing the box, ellipsoidal and polyhedral uncertainty sets, based on geometry it is observed that the minimum size of the uncertainty set necessary to cover the whole bounded support increases ($\Psi = 1$, $\Omega = (^{|J_i|})^{1/2}$, $\Gamma = |J_i|$), and correspondingly the model's conservatism increases in the following order: box, ellipsoidal, polyhedral.

Comparing the interval+ellipsoidal and the ellipsoidal set based model, the ellipsoidal model is more conservative since the interval+ellipsoidal set is always inside the ellipsoidal set with same parameter defining the set. Similarly, the interval +polyhedral set induced model is less conservative than the polyhedral set induced model.

To illustrate these points, the solution for the following example with both LHS and RHS uncertainty for two constraints is studied.

Example 4. Consider the following linear optimization problem

$$\begin{aligned} \max \quad & 8x_1 + 12x_2 \\ \text{s.t.} \quad & \tilde{a}_{11}x_1 + \tilde{a}_{12}x_2 \le \tilde{b}_1 \\ & \tilde{a}_{21}x_1 + \tilde{a}_{22}x_2 \le \tilde{b}_2 \\ & x_1, x_2 \ge 0 \end{aligned}$$

where the possible uncertainty is related to the left-hand side (LHS) constraint coefficients $\tilde{a}_{11}$, $\tilde{a}_{12}$, $\tilde{a}_{21}$, and $\tilde{a}_{22}$, and the right-hand side (RHS) parameters $\tilde{b}_1$ and $\tilde{b}_2$. Here, we define the uncertainty as follows:

$$\tilde{a}_{ij} = a_{ij} + \hat{a}_{ij}\xi_{ij},\ i = 1, 2,\ j = 1, 2$$

$$\tilde{b}_i = b_i + \hat{b}_i\xi_i,\ i = 1, 2$$

where $\hat{a}_{ij} = 0.1a_{ij}$, $\hat{b}_i = 0.1b_i$, represent constant perturbations around their nominal values, $\xi_{11},\xi_{12},\xi_{21},\xi_{22},\xi_1,\xi_2$ are independent uncertain parameters, and the nominal parameter values are given by

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} 10 & 20 \\ 6 & 8 \end{bmatrix}, \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 140 \\ 72 \end{bmatrix}$$

Five different robust counterpart formulations are solved for different Δ values which satisfy the relationship: $\Gamma=\Psi|J_i|$, $\Omega = \Psi(|J_i|)^{1/2}$, and the results are shown in Figure 4.4.

From the results, it can be observed that the solution of the different models is consistent with the above recommendation on robust counterpart optimization models' conservatism. For example, comparing the three dashed lines which represent the results of the box, ellipsoidal, and polyhedral set based solutions, for every Ψ value, the box set based solution is always better (larger for maximization problem in this case) than the ellipsoidal set based solution and the polyhedral set based solution is the worst. Comparing the red and blue solid line representing the interval+ellipsoidal and interval+polyhedral set based solutions, the red line is always above the blue line until the two lines overlap, and this shows that the interval +ellipsoidal set induced model is less conservative than the interval+polyhedral set induced model from the worst case scenario point of view.

4.2.2. Comparisons Based on Probability Distribution. As stated previously, it is important to address the following question: to satisfy the same probability of constraint violation, which model's solution is the best? There exist some comparisons in the literature, for example, the comparison between the "interval+ellipsoidal" set based model and the "interval+polyhedral" set based model.[20] However, the comparisons are generally based on assigning probability bounds $e^{-\Omega^2/2}$ and $e^{-\Gamma^2/(2|J_i|)}$ for the two models, respectively. Considering the bounds they selected, the conclusion they made is still worth to be further discussed.

On the basis of the analysis in section 4.1 and realizing that bound B4 and B6 are generally tighter than the other bounds since they use the probability distribution information, we quantify the probability of constraint violation using B4 and B6 in our comparison strategy. In the sequel, we plot the optimal objective of the robust counterpart optimization models and the probability bounds B4 or B6 on the same graph, so as to view and compare the results intuitively.

This numerical study is based on Example 4. First, we assume that only the first constraint's LHS coefficients in Example 4 are subject to uncertainty. With given probability distribution information of the uncertainty, we can check the probability of constraint violation. For example, if the uncertainty is subject to uniform distribution, the corresponding results are shown in Figure 4.5. We also studied the triangular and normal

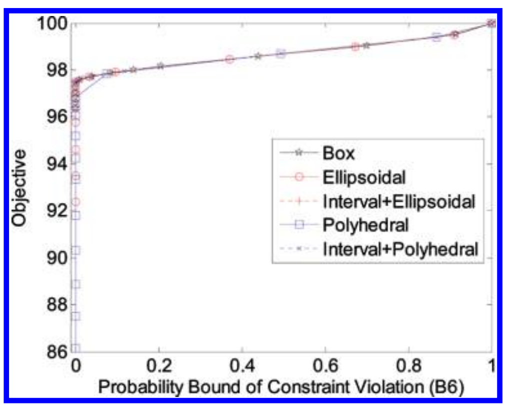

Figure 4.5. Probability bound B6 versus objective (uncertainty only in the first constraint, uniform probability distribution).

distribution, and the results are shown in Supporting Information C. It can be observed from those solutions that the different robust counterpart formulations have no difference in the conservatism since the objective-probability plots overlap.

Furthermore, treating both constraints' LHS coefficients of Example 4 subject to uniform probabilistic distribution for the uncertainty, we plot the results for the case of two uncertain constraints as shown in Figure 4.6. The corresponding results under the triangular and normal distribution can also be found in Supporting Information C. The results show that: for the first constraint, polyhedral and interval+polyhedral set based solutions are worse since for the same B6 value, the objective value is always smaller; but for the second constraint, the polyhedral and interval+polyhedral set based solutions are better. Thus, it is not possible to reach a conclusion based on the probability bound B6.

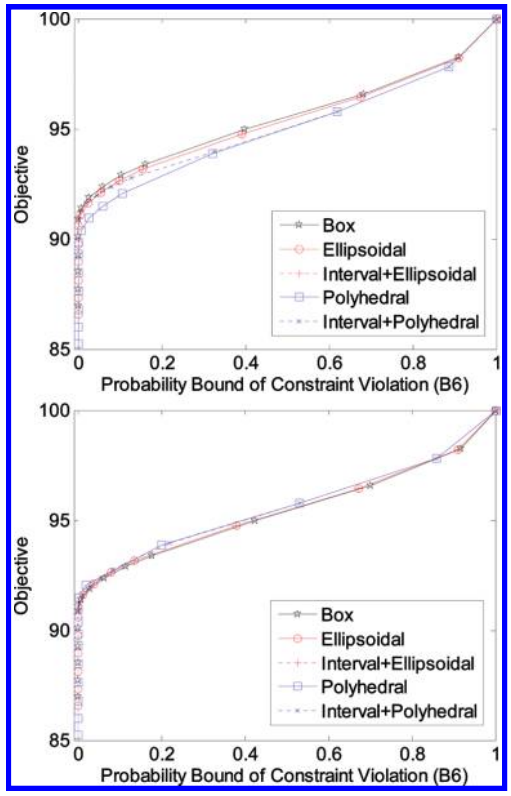

Figure 4.6. Probability bound B6 vs objective (uncertainty in both constraints, uniform probability distribution).

We also study Example 4 based on probability bound B4, which utilizes both the uncertainty set information and the probability distribution information of the uncertainty. On the basis of Example 4 and assuming uniform probability distributions for the LHS coefficients of the first constraint, the results are shown in Figure 4.7. By assuming uniform probability

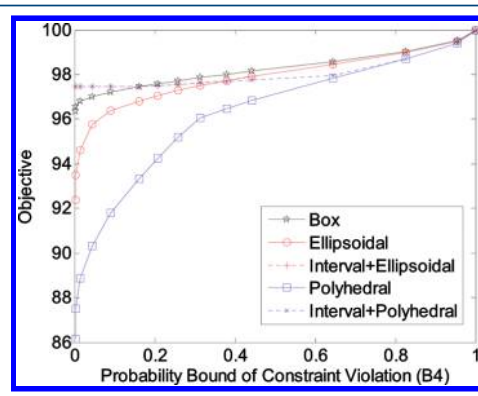

Figure 4.7. Probability bound B4 vs objective (uncertainty only in the first constraint's LHS, uniform probability distribution).

distributions for the LHS coefficients of both constraints, the results are shown in Figure 4.8. The results under triangular and normal distributions can be found in Supporting Information C. From the dashed lines in those plots, it can be observed that the interval+polyhedral set based model is more conservative than the interval +ellipsoidal set based model since under the same probability bound of constraint violation, the objective of the interval+polyhedral set based model is worse than the "interval+ellipsoidal" set based solution. Similarly, from the

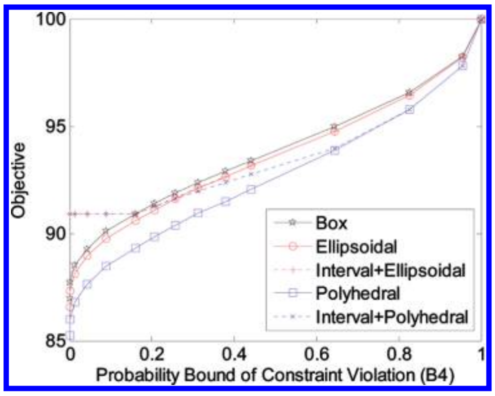

Figure 4.8. Probability bound B4 vs objective (uncertainty in both constraints' LHS, uniform probability distribution). Note: Same Δ is applied for both constraints, thus the bound B4 for the two constraints is the same.

solid lines in those plots, we can conclude that for the sets that are not combined with interval sets, their conservatism increases in the following order: box, ellipsoidal, polyhedral.

5. APPLICATION STUDIES ON PLANNING AND SCHEDULING

In this section, we study the application of the set induced robust counterpart formulations on a LP based production planning problem and a MILP based process scheduling problem. Specifically, we will focus on the utilization of the probabilistic guarantees derived in section 3 to find robust solutions for those problems.

5.1. Multiperiod Production Planning Problem: LP Model. This example is adapted from[21] and considers 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. A linear optimization formulation of this problem can be formulated as below:

$$\max \sum_j P_j z_j \tag{5.1a}$$

$$\text{s.t.} \sum_j C_j x_j + \sum_j V_j y_j \le 400000 \tag{5.1b}$$

$$500 + x_1 - (y_1 + z_1) = 0 \tag{5.1c}$$

$$y_{j-1} + x_j - (y_j + z_j) = 0 \ \forall\ j = 2, ..., 6 \tag{5.1d}$$

$$y_6 = 500 \tag{5.1e}$$

$$z_j \le D_j \ \forall\ j = 1, ..., 6 \tag{5.1f}$$

$$z_j \le D_j \ \forall\ j = 1, ..., 6 \tag{5.1g}$$

$$x_j, y_j, z_j \ge 0 \ \forall\ j = 1, ..., 6$$

In the above model, decision variables x_j represent the production amount during period j, y_j represent the amount of product left in storage (tons) at the end of period j and z_j represent the amount of product sold to market during period j. The objective function 5.1a maximizes the total sales. The first constraint 5.1b ensures that the total cost does not exceed a given budget. Constraints 5.1c and 5.1d represent the inventory material balances. Constraint 5.1e requires that the final inventory meet the desired level (i.e., 500 tons). Constraints 5.1f and 5.1g represent the production capacity limitations and demand upper bounds, respectively. Detailed data for the above LP problem are in Table 5.1.

Table 5.1. Problem Data for the Production Planning Problem

period j	selling price (\$/ton) P_j	production cost (\$/ton) C_j	storage cost (\$/ton) V_j	production capacity (tons) U_j	demand (tons) D_j
1	180	20	2	1500	1100
2	180	25	2	2000	1500
3	250	30	2	2200	1800
4	270	40	2	3000	1600
5	300	50	2	2700	2300
6	320	60	2	2500	2500

To study the robust counterpart optimization technique for the uncertain planning problem, we assume the production costs are subject to uncertainty and the cost budget constraint 5.1b is affected, where the parameters $\tilde{C}_j$ are the uncertain data in this constraint:

$$\sum_j \tilde{C}_j x_j + \sum_j V_j y_j \le 400000 \tag{5.2}$$

It is further assumed that the production costs are subject to a uniform probability distribution and that there is a maximum of 50% perturbation around their nominal values C_j as listed in Table 5.1. The desired probabilistic guarantee that constraint 5.1b is satisfied is set to 0.85 (i.e., the upper bound on the probability of constraint violation is set to 0.15).

Before we solve the robust production planning problem, the deterministic model and the worst-case scenario case (i.e., the uncertainty set is the interval set defined by the bounds on the uncertain parameters) are solved and the results are shown in Figure 5.1, which will be compared with the robust solution.

The general robust optimization methodology applied to the robust planning problem can be described as follows: first, with the desired probability bound on constraint violation, we calculate Δ using a priori bounds (B1, B2, B3 or B4); then with the Δ value, we solve the robust counterpart optimization problem and obtain the robust production plan. Finally, as an additional optional step, we can further check the a posteriori probability bound of constraint violation based on the robust solution using bounds B5 or B6.

For the uncertain constraint 5.2, we have $|J_i| = 6$. Then, from the a priori probability bound expressions B1−B4, we can obtain the following uncertainty set parameter values Δ

$$\Delta_{B1} = 1.9479,\ \Delta_{B2} = 4.7713,\ \Delta_{B3} = 3.7363,$$
$$\Delta_{B4} = 2.6704$$

Notice that for the box uncertainty set, the smallest Δ value derived above is 1.9479. Since it is larger than 1 (i.e., the

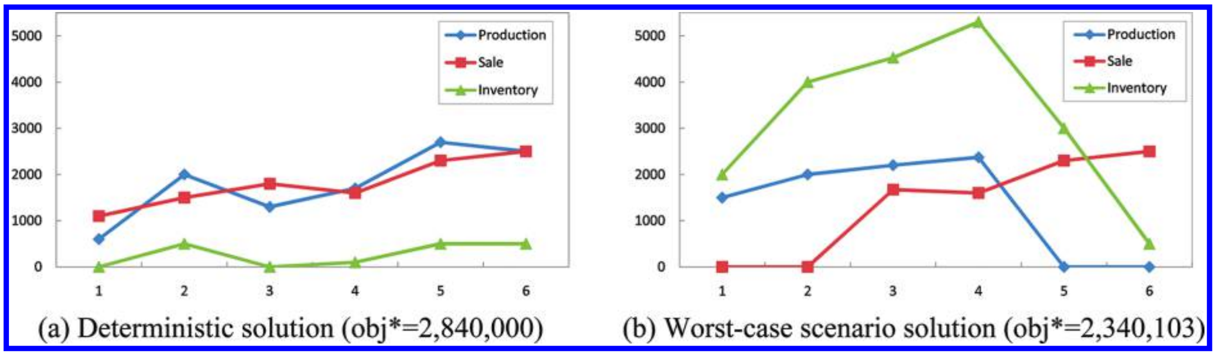

Figure 5.1. Deterministic and worst-case scenario solution.

corresponding uncertainty set has exceeded and totally covered the bounded support), it is not worth to apply the value Ψ = 1.9479 to solve the box set based robust counterpart optimization problem since the solution will be worse than the worst-case scenario (in this case, the optimal objective value is actually 1 969 209). While for the ellipsoidal and the interval + ellipsoidal uncertainty sets, the smallest Δ derived above is Δ_{B1} = 1.9479, and since 1.9479 < $(|J_i|)^{1/2}$ = 2.4495, the corresponding uncertainty set does not cover the whole uncertain space. Similarly, for the polyhedral and the interval+ polyhedral set, the smallest possible Δ value is Δ_{B4} = 2.6704, and since 2.6704 < $|J_i|$ = 6, the corresponding uncertainty set does not cover the whole uncertain space. The four different robust counterpart formulations are then applied to solve the robust planning problem by using their best possible uncertainty set parameter values and the results are listed in Table 5.2. With the robust solution, a posteriori probability

Table 5.2. Solution for Robust Planning Problem

	ellipsoidal	polyhedral	interval +ellipsoidal	interval +polyhedral
Δ	Ω = 1.9479	Γ = 2.6704	Ω = 1.9479	Γ = 2.6704
Obj*	2 350 433	2 459 972	2 356 977	2 475 824
B6	1.8429×10^{-4}	0.0014	1.6574×10^{-4}	0.0038

bound B6 on constraint violations is also evaluated and listed in Table 5.2. Detailed production plans for those different robust solutions are shown in Figure 5.2.

From the solutions, it is observed that although the polyhedral and the interval+polyhedral set based robust solution's objective is better than the ellipsoidal and interval+ellipsoidal set based solutions, their performances on probability of constraint violation (evaluated based on the tightest bound B6) are much higher, which illustrates the trade-off between optimality and feasibility.

Note that with the usage of a tighter probability bound, a smaller uncertainty set is derived while the probabilistic guarantee on constraint satisfaction is still met. For example, for the interval+polyhedral set based model, the robust solution with different Γ values derived from a priori probability bounds B2 and B3 are shown in Figure 5.3. Comparing Figure 5.3 with Figure 5.2d, it is seen that while using the bound B2, the solution is actually the same as the worst-case scenario solution, and the quality of the robust solution is greatly improved with tighter probability bounds (especially, B4).

5.2. Process Scheduling Problem: MILP Model. To further study the application of the different probabilistic bounds in addressing robust optimization problems for mixed integer linear optimization, MILP, models, here we consider a process scheduling problem studied in our previous work.[11,22−24] This example involves the scheduling of a batch chemical process related to the production of two chemical products using three raw materials. The state-task-network (STN) representation of this example is shown in Figure 5.4. The readers are directed to the paper[11] for the detailed mixed integer linear optimization formulation and problem data.

In this example, we specifically focus on the processing time uncertainty. Note that the demand uncertainty leads to only one uncertain parameter per constraint, and correspondingly, the different uncertainty sets are all reduced to the interval set case and the corresponding robust formulations are the same.

The constraints related to processing time uncertainty are listed as eq 5.3, where two uncertain parameters $\tilde{\alpha}_{i,j}$ and $\tilde{\beta}_{i,j}$ exist (i.e., $|J_i|$ = 2) for every such constraint:

$$Tf_{i,j,n} \geq Ts_{i,j,n} + \tilde{\alpha}_{i,j}wv_{i,j,n} + \tilde{\beta}_{i,j}b_{i,j,n} \ \forall\ i \in I,\ \forall\ j \in J_i,\quad \forall\ n \in N \tag{5.3}$$

In this study, we assume ***bounded triangular uncertainty*** on the processing time parameters $\tilde{\alpha}_{i,j}$ and $\tilde{\beta}_{i,j}$, and assign a maximum deviation of 5% of the nominal processing time data. We set the expected minimum probability level on constraint satisfaction to 0.9 (i.e., set the upper bound on constraint violation to 0.1).

First, we solve two extreme cases of the process scheduling problem: (1) the deterministic case, assuming no uncertainty on the parameters; (2) the "worst-case scenario" case, assuming that the schedule feasibility should be maintained for all the possible processing time perturbations, which can be performed by solving the box set based robust formulation with Ψ=1 (i.e., the uncertainty set is exactly the whole support defined by the bounds on the uncertainty). The results of the above two extreme cases are shown in Figure 5.5 and Figure 5.6, which will be further compared with the other robust solution cases.

While Δ can be evaluated from several a priori bounds, we first consider solving the robust scheduling problem without using the probability distribution information (i.e., bound B4). Thus, with a given probability bound on constraint violation 0.1, using the a priori probability bounds B1 and B2, we determine the value of Ψ, Ω, and Γ using $\exp(-(\Psi^2/2))$, $\exp(-(\Omega^2/2))$, and $\exp(-(\Gamma^2/2|J_i|))$, respectively, and the following parameter values are obtained: Ψ = 2.146, Ω = 2.146, Γ = 3.0349. Since Ψ = 2.146 > 1, Ω = 2.146 > $(|J_i|)^{1/2}$ = 1.414 and Γ = 3.0349 > $|J_i|$ = 2, the box, ellipsoidal and polyhedral uncertainty sets will all exceed the original bounds on uncertainty. Hence, the corresponding solution could be even worse than the worst-case scenario solution. Taking the box set based solution shown in Figure 5.7 and polyhedral set based

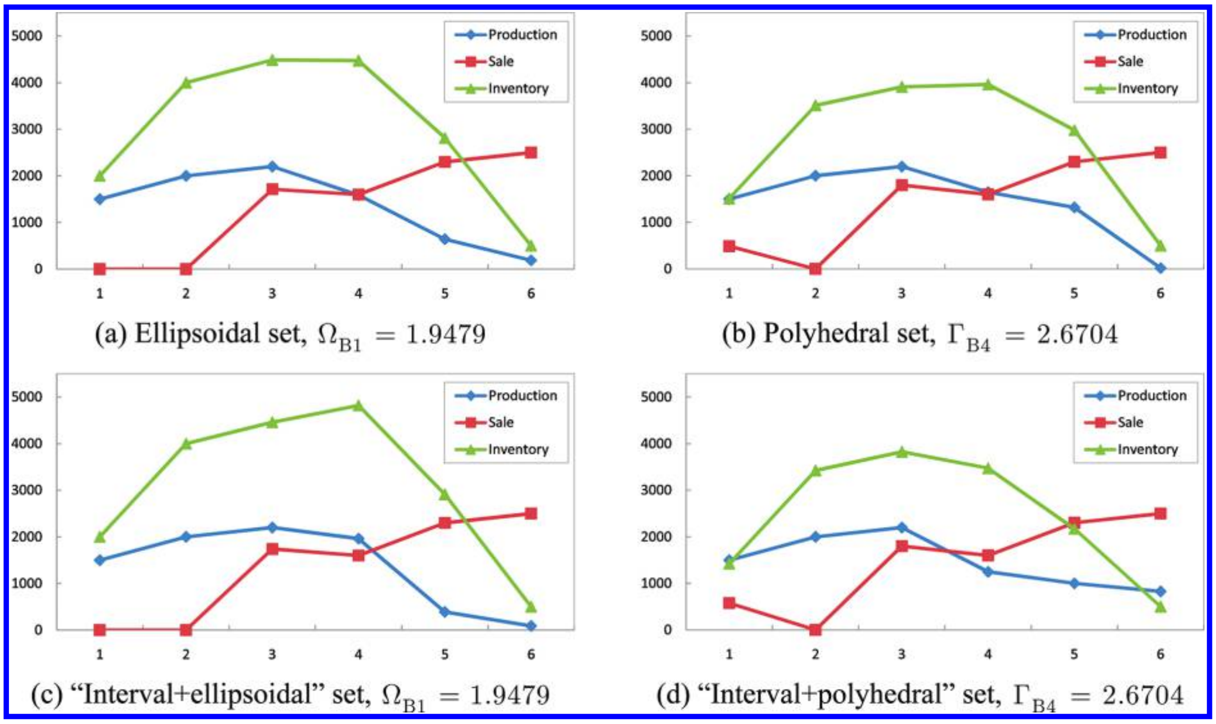

Figure 5.2. Different robust planning solutions.

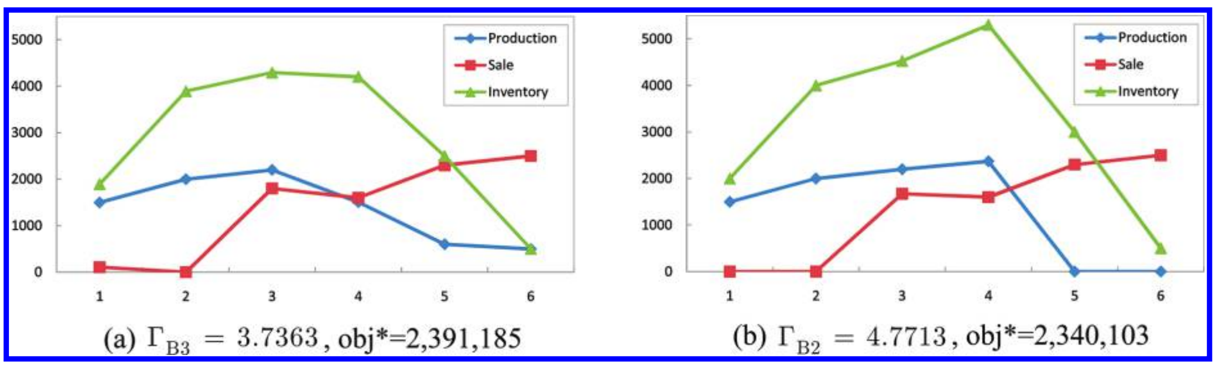

Figure 5.3. Interval+polyhedral set based robust solution with Γ derived from B2 and B3.

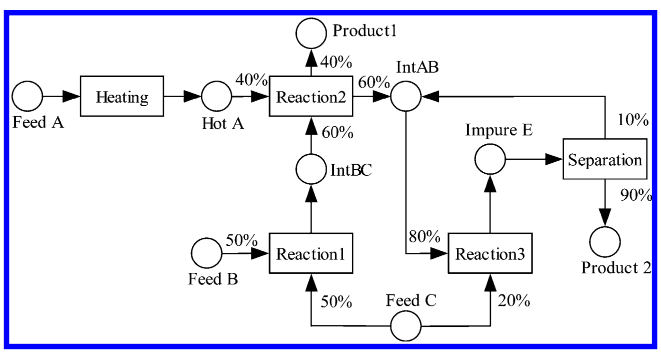

Figure 5.4. State task network (STN) representation of the batch chemical process.

robust solution in Figure 5.8 as examples, they are worse than the worst-case scenario solution in Figure 5.6. In this sense, although they are feasible solutions, they are not good robust solutions.

Based on the above Ω and Γ values, the corresponding "interval+ellipsoidal" and the "interval+ellipsoidal" uncertainty sets will be equal to the worst case scenario uncertainty set (i.e., the interval set described with the given bounds). Thus, the "Interval+ellipsoidal" set based solution with $\Omega = 2.146$ and the "Interval+polyhedral" set based solution with $\Gamma = 3.0349$ are the same as the worst-case scenario schedule, and they are shown in Figure 5.6.

From the above results, it is seen that using the probability bounds B1 and B2, the resulting robust solution is the same as the worst case scenario solution and hence conservative. The reason for this is that those two bounds are not tight for bounded triangular probability distribution when $|J_i| = 2$ (see Figure B.2 in Supporting Information B), thus leading to a relative large Δ and hence large uncertainty sets. To avoid those conservative solutions, we will further utilize the probability distribution information and the tighter probability bound B4 to evaluate the uncertainty set parameters, and then solve the resulting robust optimization problems.

For the given triangular distribution and $|J_i| = 2$, the relationship between the probability bound B4 and the uncertainty set parameter Δ (i.e., Ψ, Ω, and Γ) is plotted in Figure B.2 (see Supporting Information B). With the desired probabilistic guarantee on constraint satisfaction set to 0.9 (i.e., the probability of constraint violation does not exceed 0.1), we

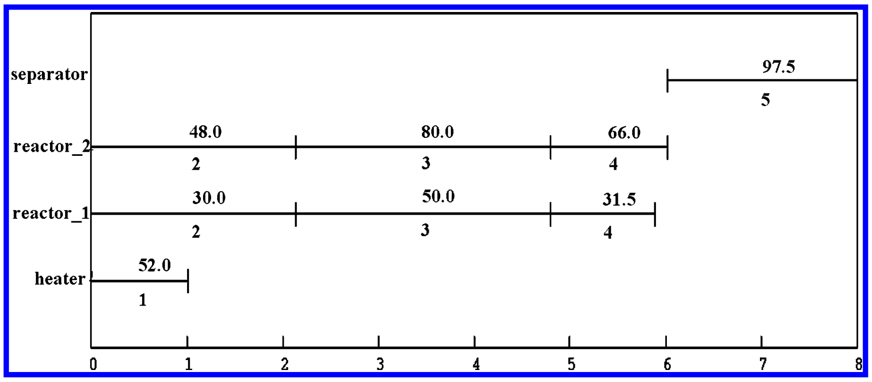

Figure 5.5. Deterministic schedule (obj* = 1088.75).

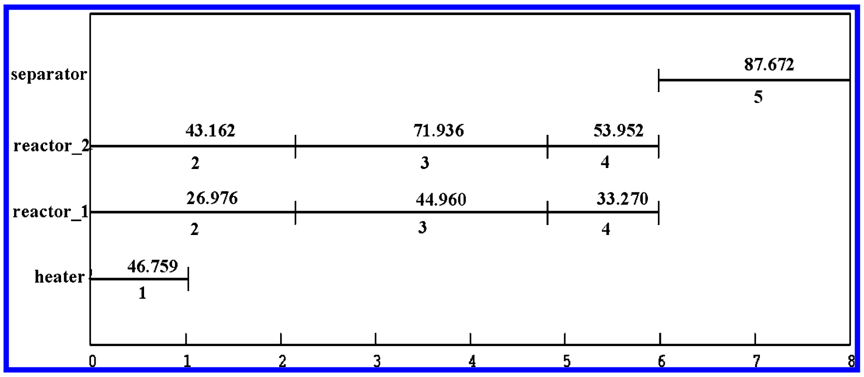

Figure 5.6. Worst-case scenario schedule (obj* = 979.01).

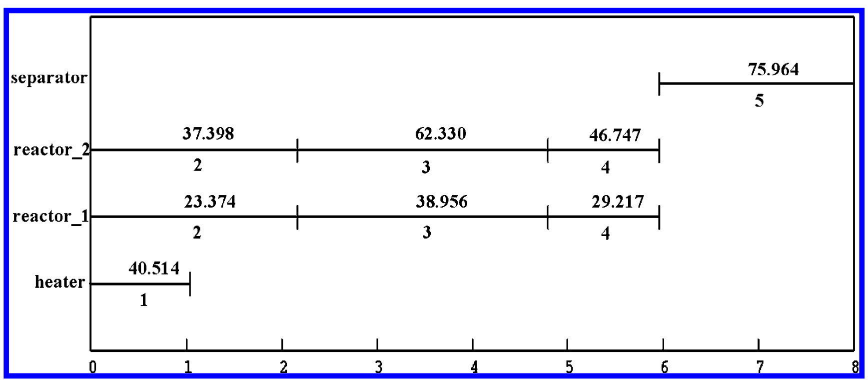

Figure 5.7. Box set based schedule, with $\Psi = 2.146$ derived from B1, obj* = 848.27.

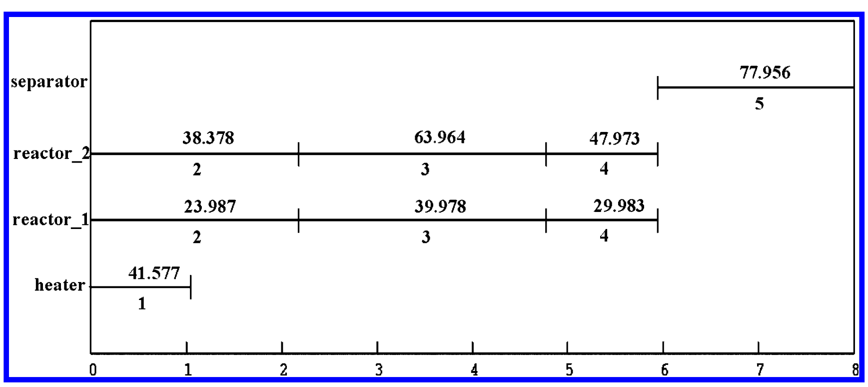

Figure 5.8. Polyhedral set based schedule, with $\Gamma = 3.0349$ derived from B2, obj* = 870.51.

can determine the parameters using the probability bound expression B4 and get $\Psi = \Omega = \Gamma = 1.1681$. Before we solve the robust counterpart optimization problems, we observe that the box set based robust counterpart will still lead to the worst case scenario solution because $\Psi = 1.1681 > 1$. On the other hand, the interval+ellipsoidal and interval+polyhedral set based

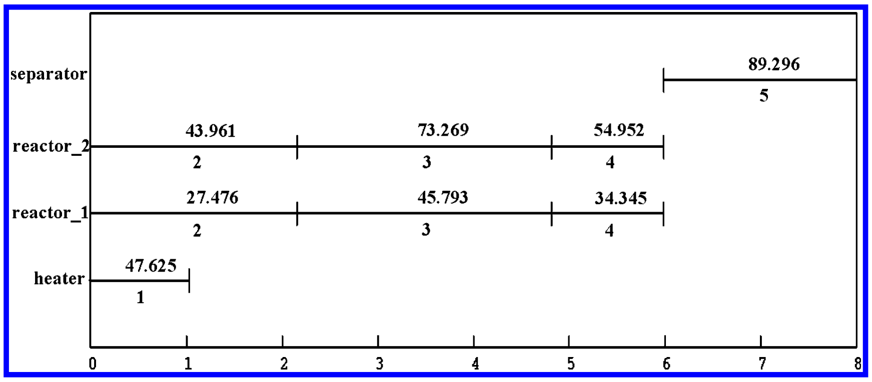

Figure 5.9. Interval+ellipsoidal uncertainty set based robust schedule, with $\Omega = 1.1681$ derived from B4 (obj* = 997.14).

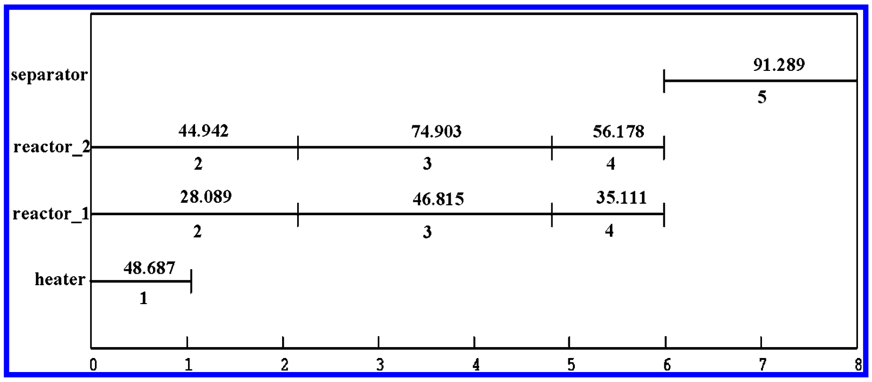

Figure 5.10. Interval+polyhedral uncertainty set based robust schedule, with $\Gamma = 1.1681$ derived from B4 (obj* = 1019.39).

robust counterparts will not lead to the worst case scenario solution because $\Omega = 1.1681 < (|J_i|)^{1/2} = 1.414$, $\Gamma = 1.1681 < |J_i| = 2$. Therefore, only the interval+ellipsoidal and interval +polyhedral set based robust counterpart optimization models are solved for the scheduling problem. The results are shown in Figure 5.9 and Figure 5.10, respectively.

Comparing the above two schedules, it can be observed that the task sequences are the same, and the differences lie on the batch sizes. For every task, the schedule shown in Figure 5.10 has a larger batch size than the schedule shown in Figure 5.9. This is explained by the fact that with $\Gamma = \Omega$, the ellipsoidal set is always larger than the polyhedral set since the polyhedron is circumscribed by the ellipsoid. Thus, the resulting ellipsoidal set based robust solution considers larger perturbations of the processing time, and as a result, the batch size that can be processed must be smaller so as to make feasible the positive perturbations which lead to large processing times for the tasks. Comparing the above two schedule solutions with the worst case scenario solution schedule in Figure 5.6, it can be seen that the solution has been improved since the batch processing size increased and the objective value increased.

One the basis of above analysis, it can be concluded that using the probability distribution information, we can improve the solution while still keeping the probabilistic guarantees on constraint satisfaction. This demonstrates the benefits of using the probability distribution information and tighter probability bounds.

6. CONCLUSIONS

Set induced robust counterpart optimization techniques are systematically studied in this paper based on their probabilistic guarantees on constraint satisfaction. We derive probability bounds for constraint violation of the robust solution for five different set induced robust counterpart formulations. Probabilistic guarantees are derived for both bounded and unbounded uncertainty, with and without detailed probability distribution information. The main findings on multiple probability bounds for several important robust optimization models extend the results in the literature and provide greater flexibility for robust optimization practitioners in choosing tighter probability bounds so as to find less conservative robust solutions. Illustrative numerical studies are performed to compare the tightness of different probability bounds and the conservatism of different robust formulations. The insights gained provide the basis for the application of the robust counterpart optimization in practical problems. We have also illustrated the usage of probability distribution information and tighter a priori probability bounds to find better robust solutions for a production planning and a process scheduling problem.

■ APPENDIX A

Lemma 3.1

For every robust counterpart constraint 2.10a-2.10e, if it is satisfied, then the following relationship, which represents an upper bound on the probability that the original constraint is violated, holds:

$$\Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij}x_j > b_i\} \le \Pr\{\sum_{j\in J_i} \xi_j\delta_j > \Delta\} \tag{3.1}$$

where the parameters Δ and δ are defined as follows:

(1) For box uncertainty set based counterpart 2.10a

$$\Delta = \Psi, \; -1 \le \delta_j \le 1, \; \forall\, j \in J_i, \; \sum_{j\in J_i} \delta_j \le 1 \tag{3.2a}$$

(2) For ellipsoidal uncertainty set based robust counterpart 2.10b

$$\Delta = \Omega, -1 \le \delta_j \le 1, \forall j \in J_i, \sum_{j \in J_i} \delta_j^2 = 1 \tag{3.2b}$$

(3) For polyhedral uncertainty set based robust counterpart 2.10c

$$\Delta = \Gamma, -1 \le \delta_j \le 1, \forall j \in J_i \tag{3.2c}$$

(4) For interval+ellipsoidal uncertainty set based robust counterpart 2.10d

$$\Delta = \Omega, -1 \le \delta_j \le 1, \forall j \in J_i, \sum_{j \in J_i} \delta_j = 1 \tag{3.2d}$$

(5) For interval+polyhedral uncertainty set based robust counterpart 2.10e

$$\Delta = \Gamma, 0 \le \delta_j \le 1, \forall j \in J_i \tag{3.2e}$$

Proof for Lemma 3.1

(1) For the box uncertainty set induced robust counterpart 2.10a, the following relationship holds:

$$\begin{aligned} & Pr\{\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \\ & \overset{(1)}{=} Pr\{(\sum_j a_{ij}x_j + \Psi \sum_{j \in J_i} \hat{a}_{ij}|x_j| - b_i) + \sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j \\ & > \Psi \sum_{j \in J_i} \hat{a}_{ij}|x_j|\} \overset{(2)}{\le} Pr\{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > \Psi \sum_{j \in J_i} \hat{a}_{ij}|x_j|\} \\ & = Pr\left\{\frac{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j}{\sum_{j \in J_i} \hat{a}_{ij}|x_j|} > \Psi\right\} = Pr\{\sum_{j \in J_i} \alpha_j \xi_j > \Psi\} \end{aligned}$$

where $\alpha_j = (\hat{a}_{ij}x_j)/(\sum_{j \in J_i}\hat{a}_{ij}|x_j|)$. Notice that while α_{ij} is a more accurate notation, for the simplicity in presentation, we omitted the index i here. Thus, we have $-1 \le \alpha_j \le 1\ \forall\ j \in J_i$, and $\sum_{j \in J_i}\alpha_j \le 1$.

In the above derivation, the equality (1) is obtained by adding $\Psi\sum_{j \in J_i}\hat{a}_{ij}|x_j|$ on both sides of the constraint and then moving b_i to the LHS; the inequality (2) is based on the box uncertainty set induced robust counterpart constraint 2.10a.

(2) For the ellipsoidal uncertainty set induced robust counterpart 2.10b

$$\begin{aligned} & Pr\{\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \\ & \overset{(1)}{=} Pr\{(\sum_j a_{ij}x_j + \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 x_j^2} - b_i) + \sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j \\ & > \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 x_j^2}\} \overset{(2)}{\le} Pr\{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 x_j^2}\} \\ & = Pr\left\{\frac{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j}{\sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 x_j^2}} > \Omega\right\} = Pr\{\sum_{j \in J_i} \xi_j \beta_j > \Omega\} \end{aligned}$$

where $\beta_j = (\hat{a}_{ij}x_j)/(\sum_{j \in J_i}\hat{a}_{ij}^2 x_j^2)$. Thus, we have $-1 \le \beta_j \le 1\ \forall\ j \in J_i$, and $\sum_{j \in J_i}\beta_j^2 = 1$.

In the above derivation, the equality (1) is based on adding term $\Omega(\sum_{j \in J_i}\hat{a}_{ij}^2 x_j^2)^{1/2}$ on both sides of the constraint; the inequality (2) is based on the ellipsoidal uncertainty set induced robust counterpart constraint 2.10b.

(3) For the polyhedral uncertainty set induced robust counterpart 2.10c

$$\begin{aligned} & Pr\{\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} = Pr\{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j \\ & > b_i - \sum_j a_{ij}x_j\} \overset{(1)}{\le} Pr\{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > z_i \Gamma\} \\ & \overset{(2)}{\le} Pr\{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > \Gamma \max_{j \in J_i} \hat{a}_{ij}|x_j|\} \\ & = Pr\left\{\frac{\sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j}{\max_{j \in J_i} \hat{a}_{ij}|x_j|} > \Gamma\right\} = Pr\{\sum_{j \in J_i} \xi_j \gamma_j > \Gamma\} \end{aligned}$$

where $\gamma_j = (\hat{a}_{ij}x_j)/(\max_{j \in J_i}\hat{a}_{ij}|x_j|)$. Thus, we have $-1 \le \gamma_j \le 1$ $\forall\ j \in J_i$.

The inequality (1) in the above derivation process is based on the first constraint of the robust counterpart constraints set 2.10c, the inequality (2) is based on the second constraint of 2.10c.

(4) For the interval+ellipsoidal uncertainty set induced robust counterpart 2.10d

$$\begin{aligned} & Pr\{\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \\ & = Pr\{(\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_j \hat{a}_{ij}(x_j - z_{ij}) - b_i + \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 z_{ij}^2}) \\ & + \sum_{j \in J_i} \xi_j \hat{a}_{ij} z_{ij} > \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 z_{ij}^2}\} \\ & \overset{(1)}{\le} Pr\{(\sum_j a_{ij}x_j + \sum_{j \in J_i} \xi_j \hat{a}_{ij}|x_j - z_{ij}| - b_i + \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 z_{ij}^2}) \\ & + \sum_{j \in J_i} \xi_j \hat{a}_{ij} z_{ij} > \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 z_{ij}^2}\} \\ & \overset{(2)}{\le} Pr\{\sum_{j \in J_i} \xi_j \hat{a}_{ij} z_{ij} > \Omega \sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 z_{ij}^2}\} \\ & = Pr\left\{\frac{\sum_{j \in J_i} \xi_j \hat{a}_{ij} z_{ij}}{\sqrt{\sum_{j \in J_i} \hat{a}_{ij}^2 z_{ij}^2}} > \Omega\right\} = Pr\{\sum_{j \in J_i} \xi_j \beta'_j > \Omega\} \end{aligned}$$

where β'_j is defined by $\beta'_j \equiv (\hat{a}_{ij}z_j)/((\sum_{j \in J_i}\hat{a}_{ij}^2 z_j^2)^{1/2})$. Thus, $-1 \le \beta'_j \le 1 \forall j \in J_i$, $\sum_{j \in J_i}\beta_j'^2 = 1$.

Note that in the above derivation procedure, the inequality (1) uses absolute value relaxation and the inequality (2) uses the robust counterpart constraint 2.10d.

(5) For the interval+polyhedral uncertainty set induced robust counterpart 2.10e:

It is proved by Bertsimas and Sim[6] that for the interval+polyhedral set based robust counterpart formulation 2.10e, the following inequality holds

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \hat{a}_{ij}x_j > b_i\} \le Pr\{\sum_{j\in J_i} \xi_j\gamma'_j > \Gamma\}$$

where $0 \le \gamma'_j \le 1\ \forall j \in J_i$.

Summarizing the above results, evaluating the probability of constraint violation under different uncertainty sets concludes to the evaluation of the expression $\Pr\{\sum_{j\in J_i}\xi_j\delta_j > \Delta\}$, where δ_j represents the coefficient α_j, β_j, β'_j, γ_j, γ'_j, and Δ represents the adjustable parameter Ψ, Ω, Ω, Γ, Γ for the different cases, respectively. This completes the proof.

Lemma 3.2

If $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to a ***symmetric*** probability distribution, then the following probability of constraint violation holds for any $\theta > 0$

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!}dF_{\xi_j}(\xi)\right\} \tag{3.3}$$

where Δ and δ_j are detailed in Lemma 3.1.

Proof for Lemma 3.2

Following the result in Lemma 3.1 (i.e., inequality 3.1), the following derivation holds for the robust counterpart formulations (2.10>):

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\} \le Pr\{\sum_{j\in J_i} \xi_j\delta_j > \Delta\}$$
$$\overset{(1)}{\le} Pr\{\sum_{j\in J_i}\xi_j\delta_j \ge \Delta\} \overset{(2)}{=} Pr\{\theta\sum_{j\in J_i}\xi_j\delta_j \ge \theta\Delta\}$$
$$\overset{(3)}{\le} e^{-\theta\Delta}E\{e^{\theta\sum_{j\in J_i}\xi_j\delta_j}\} \overset{(4)}{=} e^{-\theta\Delta}\prod_{j\in J_i}E\{e^{\theta\xi_j\delta_j}\}$$
$$\overset{(5)}{=} e^{-\theta\Delta}\prod_{j\in J_i}E\left\{\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^k}{k!}\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^k}{k!}\,dF_{\xi_j}(\xi)\right\}$$
$$\overset{(6)}{=} e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$
$$+ e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k+1}}{(2k+1)!}\,dF_{\xi_j}(\xi)\right\}$$
$$\overset{(7)}{=} e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$

Note that in the above derivation, inequality (1) uses direct relaxation of the strict inequality; equality (2) uses $\theta > 0$; inequality (3) uses the Markov inequality; equality (4) uses the independence condition; equality (5) uses the Maclaurin series; equality (6) separate the terms by odd and even value of k; equality (7) uses the symmetric distribution condition.

Lemma 3.3

If $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to a ***bounded*** and ***symmetric*** probability distribution supported on $[-1, 1]$, then the following bound on the probability of constraint violation holds for any $\theta > 0$

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le \exp\left(\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\}\right) \tag{3.4}$$

where Δ and δ_j are detailed in Lemma 3.1.

Proof for Lemma 3.3

Starting from the conclusion of Lemma 3.2 (i.e., inequality 3.3), we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\} \le e^{-\theta\Delta}$$
$$\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-1}^{1}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\left\{\sum_{k=0}^{\infty}\frac{(\theta\delta_j)^{2k}}{(2k)!}\int_{-1}^{1}\xi_j^{2k}\,dF_{\xi_j}(\xi)\right\}$$
$$\overset{(1)}{\le} e^{-\theta\Delta}\prod_{j\in J_i}\left\{\sum_{k=0}^{\infty}\frac{(\theta\delta_j)^{2k}}{(2k)!}\int_{-1}^{1}1\,dF_{\xi_j}(\xi)\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\left\{\sum_{k=0}^{\infty}\frac{(\theta\delta_j)^{2k}}{(2k)!}\right\} \overset{(2)}{\le} e^{-\theta\Delta}\prod_{j\in J_i}\left\{\sum_{k=0}^{\infty}\frac{(\theta\delta_j)^{2k}}{2^k k!}\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\left\{\sum_{k=0}^{\infty}\frac{(\theta^2\delta_j^2/2)^k}{k!}\right\} = e^{-\theta\Delta}\prod_{j\in J_i}\{e^{\theta^2\delta_j^2/2}\}$$
$$= \exp\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\}$$

In the above derivation, inequality (1) uses the $[-1, 1]$ bound condition; inequality (2) uses the fact $(2k)! > 2^k k!$. Finally, to obtain the best (smallest) upper bound by selecting the value of θ, we can solve the bound with respect to θ and the best upper bound is obtained, that is

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le \exp\left(\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\}\right)$$

Theorem 3.1

Let $\{\xi_j\}_{j\in J_i}$ be ***independent*** and subject to a ***bounded*** and ***symmetric*** probability distribution supported on $[-1,1]$, then (2) for all the five robust counterparts 2.10a–2.10e, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\} \le \exp\left(-\frac{\Delta^2}{2|J_i|}\right) \tag{3.5}$$

(4) for the box, ellipsoidal, and interval+ellipsoidal uncertainty sets induced robust counterparts 2.10a, 2.10b and 2.10d, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j \hat{a}_{ij} x_j > b_i\} \le \exp\left(-\frac{\Delta^2}{2}\right) \tag{3.6}$$

where Δ represents the adjustable parameter for the different uncertainty sets as detailed in Lemma 3.1.

Proof for Theorem 3.1

(1) On the basis of Lemma 3.1, for the box, ellipsoidal, polyhedral, interval+ellipsoidal, and interval+polyhedral uncertainty sets induced robust counterparts, we have $|\delta_j| \le 1$, $\forall j \in J_i$, so that $\sum_{j\in J_i}(1/\delta_j^2) \ge |J_i|$) and the following relationship holds:

$$\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\} = \min_{\theta>0}\left\{\frac{\delta_j^2}{2}\sum_{j\in J_i}\left(\theta^2 - \frac{2\Delta}{|J_i|\delta_j^2}\theta\right)\right\}$$
$$= -\frac{\Delta^2}{2|J_i|^2}\sum_{j\in J_i}\frac{1}{\delta_j^2} \le -\frac{\Delta^2}{2|J_i|}$$

Using the conclusion of Lemma 3.3, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le \exp\left(\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\}\right) \le \exp\left(-\frac{\Delta^2}{2|J_i|}\right)$$

(2) For the box, ellipsoidal, and interval+ellipsoidal uncertainty set induced robust counterparts, we have $|\delta_j| \le 1$, $\forall j \in J_i$, and $\sum_{j\in J_i}\delta_j^2 \le 1$), thus the following relationship holds:

$$\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\} \le \min_{\theta>0}\left\{-\theta\Delta + \frac{\theta^2}{2}\right\} = -\frac{\Delta^2}{2}$$

Similarly, using the conclusion of Lemma 3.3, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le \exp\left(\min_{\theta>0}\left\{-\theta\Delta + \sum_{j\in J_i}\frac{\theta^2\delta_j^2}{2}\right\}\right) \le \exp\left(-\frac{\Delta^2}{2}\right)$$

With the above analysis, we obtain the probability bounds presented in 3.5 and 3.6.

Theorem 3.2

If $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to ***symmetric*** probability distribution, then we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le \exp(\min_{\theta>0}\{-\theta\Delta + \sum_{j\in J_i}\ln E[e^{\theta\xi_j}]\}) \tag{3.9}$$

where Δ represents the adjustable parameter for the different uncertainty sets as detailed in Lemma 3.1.

Proof for Theorem 3.2

If the uncertainties are independent and subject to symmetric probability distribution assumption, then using the probability distribution information and starting from the conclusion in Lemma 3.2, we have

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j > b_i\}$$
$$\le e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j\delta_j)^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j)^{2k}\delta_j^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$
$$\overset{(1)}{\le} e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j)^{2k}}{(2k)!}\,dF_{\xi_j}(\xi)\right\}$$
$$\overset{(2)}{=} e^{-\theta\Delta}\prod_{j\in J_i}\left\{\int_{-\infty}^{\infty}\sum_{k=0}^{\infty}\frac{(\theta\xi_j)^{k}}{k!}\,dF_{\xi_j}(\xi)\right\}$$
$$= e^{-\theta\Delta}\prod_{j\in J_i}\{\int_{-\infty}^{\infty}e^{\theta\xi_j}\,dF_{\xi_j}(\xi)\} = e^{-\theta\Delta}\prod_{j\in J_i}E[e^{\theta\xi_j}]$$
$$= \exp(-\theta\Delta + \sum_{j\in J_i}\ln E[e^{\theta\xi_j}])$$

Note that in the above derivation, θ is a positive number, inequality (1) uses $|\delta_j| \le 1$; equality (2) uses the symmetric distribution condition. Finally, we obtain the best possible upper bound by selecting the optimal value of θ:

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j > b_i\} \le \exp(\min_{\theta>0}\{-\theta\Delta + \sum_{j\in J_i}\ln E[e^{\theta\xi_j}]\})$$

Theorem 3.3

If the uncertain parameters $\{\xi_j\}_{j\in J_i}$ are ***independent*** and subject to a ***bounded*** probability distribution supported on $[-1,1]$, and the robust counterpart solution is x^* with $d_i(x^*) > 0$, where $d_i(x) \triangleq b_i - \sum_j a_{ij} - E[\sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j]$, then we have

$$Pr\{\sum_j a_{ij}x_j^* + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j^* > b_i\} \le \exp\left(-\frac{d_i(x^*)^2}{\sum_{i\in J_i}2\hat{a}_{ij}^2x_j^{*2}}\right) \tag{3.10}$$

Proof for Theorem 3.3

$$Pr\{\sum_j a_{ij}x_j^* + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j^* > b_i\}$$
$$\overset{(1)}{\le} Pr\{\sum_j a_{ij}x_j^* + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j^* \ge b_i\}$$
$$\overset{(2)}{=} Pr((\sum_j a_{ij}x_j^* + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j^* - b_i) - (-d_i(x^*))$$
$$\ge d_i(x^*)) \overset{(3)}{=} Pr((\sum_j a_{ij}x_j^* + \sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j^* - b_i)$$
$$- (\sum_j a_{ij}x_j + E[\sum_{j\in J_i}\xi_j\hat{a}_{ij}x_j] - b_i) \ge d_i(x^*))$$
$$\overset{(4)}{\le} \exp\left(-\frac{2d_i(x^*)^2}{\sum_{i\in J_i}(2\hat{a}_{ij}x_j^*)^2}\right) = \exp\left(-\frac{d_i(x^*)^2}{\sum_{i\in J_i}2\hat{a}_{ij}^2x_j^{*2}}\right)$$

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In the above derivation, the inequality (1) is based on relaxation of strict inequality; the equality (2) is based on adding $d_i(x^*)$ on both sides of the constraint; the equality (3) is based on the definition of $d_i(x^*)$ and the inequality (4) is based on Hoeffding's inequality.[25]

Theorem 3.4

If the uncertain parameters $\{\xi_j\}_{j\in J_i}$ are ***independent*** and the robust counterpart solution is x^*, then for any $\theta > 0$, we have:

$$Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\} \leq \exp(\min_{\theta>0}\{-\theta(b_i - \sum_j a_{ij}x_j^*) + \sum_{j\in J_i} \ln E[e^{\theta\xi_j\hat{a}_{ij}x_j^*}]\}) \tag{3.11}$$

Proof for Theorem 3.4

$$\begin{aligned} & Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j > b_i\} \\ & \overset{(1)}{\leq} Pr\{\sum_j a_{ij}x_j + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j \geq b_i\} \\ & = Pr(\sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j \geq b_i - \sum_j a_{ij}x_j) \\ & = Pr(\theta\sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j \geq \theta(b_i - \sum_j a_{ij}x_j)) \\ & \overset{(2)}{\leq} \exp(-\theta(b_i - \sum_j a_{ij}x_j))E[\exp\{\theta\sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j\}] \\ & = \exp(-\theta(b_i - \sum_j a_{ij}x_j))\prod_{j\in J_i} E[e^{\theta\xi_j\hat{a}_{ij}x_j}] \\ & = \exp(-\theta(b_i - \sum_j a_{ij}x_j) + \sum_{j\in J_i} \ln E[e^{\theta\xi_j\hat{a}_{ij}x_j}]) \end{aligned}$$

In the above derivation, θ is a positive number, the inequality (1) is based on direct relaxation of strict inequality and the inequality (2) is based on the Markov inequality. Finally, the following probability bound is obtained through selecting optimal value of θ

$$Pr\{\sum_j a_{ij}x_j^* + \sum_{j\in J_i} \xi_j\hat{a}_{ij}x_j^* > b_i\} \leq \exp(\min_{\theta>0}\{-\theta(b_i - \sum_j a_{ij}x_j^*) + \sum_{j\in J_i} \ln E[e^{\theta\xi_j\hat{a}_{ij}x_j^*}]\})$$

ASSOCIATED CONTENT

Supporting Information

The Markov inequality, the Hoeffding's inequality, complete results on comparison of the tightness of probability bounds, and comparison of the conservatism of robust counterpart models for examples 1, 2, and 3. This material is available free of charge via the Internet at http://pubs.acs.org.

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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. *Oper. Res.* **1973**, *21*, 1154−1157.
(2) Ben-Tal, A.; Nemirovski, A. Robust solutions of uncertain linear programs. *Oper. Res. Lett.* **1999**, *25* (1), 1−13.
(3) Ben-Tal, A.; Nemirovski, A. Robust solutions of Linear Programming problems contaminated with uncertain data. *Math. Programming* **2000**, *88*, 411−424.
(4) ElGhaoui, L.; Lebret, H. Robust solutions to least-squares problems with uncertain data. *Siam J. Matrix Anal. Appl.* **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. *Oper. Res.* **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* (18), 10567−10603.
(12) El Ghaoui, L.; Oks, M.; Oustry, F. Worst-case value-at-risk and robust portfolio optimization: A conic programming approach. *Oper. Res.* **2003**, *51* (4), 543−556.
(13) Chen, X.; Sim, M.; Sun, P. A robust optimization perspective to stochastic programming. *Oper. Res.* **2007**, *55* (6), 1058−1071.
(14) Chen, W. Q.; Sim, M. Goal-driven optimization. *Oper. Res.* **2009**, *57* (2), 342−357.
(15) Delage, E.; Ye, Y. Distributionally robust optimization under moment uncertainty with application to data-driven problems. *Oper. Res.* **2010**, *58* (3), 595−612.
(16) Ben-Tal, A.; Bertsimas, D.; Brown, D. B. A soft robust model for optimization under ambiguity. *Oper. Res.* **2010**, *58* (4), 1220−1234.
(17) Bertsimas, D.; Pachamanova, D.; Sim, M. Robust linear optimization under general norms. *Oper. Res. Lett.* **2004**, *32* (6), 510−516.
(18) Bertsimas, D.; Sim, M. Tractable approximations to robust conic optimization problems. *Math. Programming* **2006**, *107* (1−2), 5−36.
(19) Paschalidis, I. C.; Kang, S.-C. In *Robust Linear Optimization: On the Benefits of Distributional Information and Applications in Inventory Control*, 44th IEEE Conference on Decision and Control, Seville, Spain, 2005; IEEE: Seville, Spain, 2005.
(20) Ben-Tal, A.; Ghaoui, L. E.; Nemirovski, A. *Robust Optimization*; Princeton University Press: Princeton, NJ, 2009.
(21) Ravindran, A. R. *Operations Research Methodologies*; CRC Press: New York, 2008.
(22) 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.

(23) Ierapetritou, M. G.; Floudas, C. A. Short-term scheduling: New mathematical models vs algorithmic improvements. *Comput. Chem. Eng.* **1998**, *22*, S419−S426.
(24) 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.
(25) Hoeffding, W. Probability-inequalities for sums of bounded random-variables. *J. Am. Stat. Assoc.* **1963**, *58* (301), 13−30.