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Data-Driven Process Network Planning: A Distributionally Robust Optimization Approach

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Abstract: Process network planning is an important and challenging task in process systems engineering. Due to the penetration of uncertainties such as random demands and market prices, stochastic programming and robust optimization have been extensively used in process network planning for better protection against uncertainties. However, both methods fall short of addressing the ambiguity of probability distributions, which is quite common in practice. In this work, we apply distributionally robust optimization to handling the inexactness of probability distributions of uncertain demands in process network planning problems. By extracting useful information from historical data, ambiguity sets can be readily constructed, which seamlessly integrate statistical information into the optimization model. To account for the sequential decision-making structure in process network planning, we further develop multi-stage distributionally robust optimization models and adopt affine decision rules to address the computational issue. Finally, the optimization problem can be recast as a mixed-integer linear program. Applications in industrial-scale process network planning demonstrate that, the proposed distributionally robust optimization approach can better hedge against distributional ambiguity and yield rational long-term decisions by effectively utilizing demand data information.

Keywords: Data-based decision-making, distributionally robust optimization, multi-stage decision-making, process network planning.

1. INTRODUCTION

Nowadays, massive chemical complexes are erected and integrated by chemical manufacturers, which commonly leads to a large-scale process network. However, due to the increasingly fierce competitions in the global marketplace as well as stringent requirements in both economic and environmental aspects, making appropriate decisions for versatile activities involved in such a complicated network environment brings significant challenges in process industries (Wassick (2009)). On one hand, the synergies between dedicated and flexible processes provide multiple options to produce diversified products, and it is necessary to coordinate different decisions as a whole (Norton and Grossmann (1994)). On the other hand, some uncertain factors such as demand and price variations tend to exert significant influence on decision-making (Pistikopoulos (1995)). Since planning decisions are commonly made in a long horizon, it is impossible to obtain accurate predictions of long-term market variations. Therefore, uncertainties must be taken into account to yield rational planning decisions.

To address these challenges, optimization under uncertainties has been widely adopted as an effective tool in making planning decisions. The adopted methodologies can be generally classified into stochastic programming (SP) (Liu and Sahinidis (1996); You and Grossmann (2008)) and robust optimization (RO) (Gong et al. (2016); Shang et al. (2017)). In the context of SP, the expected performance is typically optimized with the random nature of uncertainties addressed by probability distribution functions (PDFs), which are assumed as known a priori (Birge and Louveaux (2011)). Nonetheless, an accurate distribution of uncertainties is commonly unavailable in practice, and the induced optimization problems are difficult to solve. RO optimizes the worst-case performance over the support of uncertainties, which is expressed as an uncertainty set of various shapes (Bertsimas et al. (2011)). However, RO bears no statistical interpretations, and the worst-case realization of uncertainties is typically excessively pessimistic, leading to over-conservative decisions.

As an intermediate approach, distributionally robust optimization (DRO) has gained increasing popularity in the operations research community in recent years (Delage and Ye (2010); Van Parys et al. (2016); Hanasusanto et al. (2017)). Different from RO and SP, DRO can be deemed as optimizing the worst-case expected performance on a set constituted by an infinite number of distributions, typically referred to as the *ambiguity set* and constructed based on uncertainty data, thereby seamlessly incorporating data information into optimization models. In this way, DRO could effectively hedge against the ambiguity of probability distributions of uncertainties in decision-making, which is a crucial issue unaddressed by both SP and RO.

Therefore, in this article, we propose a novel DRO model for process network planning under demand uncertainties. An ambiguity set is first constructed by extracting statistical information from historical demand data. In this way, partial data information can be organically integrated into the optimization model, leading to more reasonable planning decisions. In addition, to address the sequential nature of multi-period uncertain demands, a multi-stage DRO model is developed. To solve the resulting optimization problem, the affine decision rules (ADRs) have been adopted to yield a suboptimal yet tractable solution. The final optimization problem can be cast as a mixed-integer linear program (MILP) that can be conveniently solved using off-the-shelf solvers. Applications in an large-scale industrial process network planning task demonstrate that the proposed approach is advantageous to classic methods in utilizing data information and balancing between risks and profits.

The organization of this paper is given as follows: Section 2 develops the multi-stage DRO model for process network planning problem. Section 3 discusses a tractable solution approach based on ADRs. Section 4 reports the application results. Finally conclusions are drawn.

2. DISTRIBUTIONALLY ROBUST PROCESS NETWORK PLANNING PROBLEM UNDER DEMAND UNCERTAINTY

2.1 Deterministic process network planning problem

In chemical complexes, a number of interconnected processes and versatile chemicals are involved. By synthesizing all factors and modeling the entire problem mathematically, a rational decision can be made from multiple manufacturing options for producing a certain chemical (Yue and You (2013)). Moreover, capacity expansions are allowed in each period to maximize the overall profit. We first introduce the deterministic process network planning problem, which is generally formulated as the following MILP (Liu and Sahinidis (1996)):

$$\begin{aligned}\max -&\sum_{i\in I}\sum_{t\in T}(\alpha_{it}\cdot QE_{it}+\beta_{it}\cdot Y_{it}+\delta_{it}\cdot W_{it})\\ +&\sum_{j\in J}\sum_{t\in T}(v_{jt}\cdot S_{jt}-\tau_{jt}\cdot P_{jt})\end{aligned} \tag{1}$$

$$\text{s.t. } qe_{it}^{L}\cdot Y_{it}\le QE_{it}\le qe_{it}^{U}\cdot Y_{it},\ \forall i,t \tag{2}$$

$$Q_{it}=Q_{i(t-1)}+QE_{it},\ \forall i,t \tag{3}$$

$$\sum_{t\in T}Y_{it}\le ce_i,\ \forall i \tag{4}$$

$$\sum_{i\in I}(\alpha_{it}\cdot QE_{it}+\beta_{it}\cdot Y_{it})\le ci_t,\ \forall t \tag{5}$$

$$W_{it}\le Q_{it},\ \forall i,t \tag{6}$$

$$P_{jt}-\sum_{i}\kappa_{ij}\cdot W_{it}-S_{jt}=0,\ \forall j,t \tag{7}$$

$$P_{jt}\le su_{jt},\ \forall j,t \tag{8}$$

$$S_{jt}\le du_{jt},\ \forall j,t \tag{9}$$

$$QE_{it},Q_{it},P_{jt},W_{it},S_{jt}\ge 0,\ \forall i,j,t \tag{10}$$

$$Y_{it}\in\{0,1\},\ \forall i,t \tag{11}$$

The objective (1) intends to maximize the net present value (NPV) of the process network over the entire planning horizon, which consists of investment costs, operating costs, material purchase costs, and sales profits. Constraint (2) enforces the upper and lower bounds of capacity expansions in each period, while (3) indicates the additive characteristic of expanded capacities. Inequalities (4) and (5) limit the budgets of capacity expansions in each time period. The equality (7) speaks about the mass balance. (8) and (9) enforce that the purchase amount and sales amount cannot exceed the limits of suppliers and markets. The non-negativity of continuous variables is ensured by (10). Binary variables $\{Y_{it}\}$ are used to indicate whether the capacity of process i will be expanded in time period t.

For clear expositions, we adopt the following compact description of the deterministic process network planning problem in the sequel:

$$\begin{aligned}\min_{\mathbf{x}}\ &\mathbf{c}^{\mathrm{T}}\mathbf{x}\\ \text{s.t. }&\mathbf{A}\mathbf{x}\le\mathbf{b}\\ &\mathbf{C}\mathbf{x}\le\boldsymbol{\xi}\\ &\mathbf{x}_{\text{int}}\in\{0,1\}\end{aligned} \tag{12}$$

where decision variables $\mathbf{x}$ include continuous decision variables $\{QE_{it},Q_{it},W_{it},S_{jt},P_{jt}\}$ and binary decision variables $\{Y_{it}\}$, and the latter ones are denoted by $\mathbf{x}_{\text{int}}$. The inequality $\mathbf{A}\mathbf{x}\le\mathbf{b}$ corresponds to constraints (2)-(8) and (10), and $\mathbf{C}\mathbf{x}\le\boldsymbol{\xi}$ stands for the demand constraints (9), which are further assumed to be affected by uncertain demands $\boldsymbol{\xi}$.

2.2 Modeling demand uncertainty with ambiguity set

We assume that uncertain demands are represented by an M-dimensional random vector $\boldsymbol{\xi}=[\xi_1\ \cdots\ \xi_M]^{\mathrm{T}}$. However, an exact knowledge about the distribution $\mathbb{P}$ of uncertainties $\boldsymbol{\xi}$ is commonly unavailable. In the context of DRO, we capture statistical properties of $\boldsymbol{\xi}$ by considering a set of probability distributions, termed as the *ambiguity set*. Here we employ the following formulation of ambiguity sets:

$$\mathcal{D}=\left\{\mathbb{P}_{\boldsymbol{\xi}}\in\mathcal{M}_{+}^{M}\ \middle|\ \begin{array}{l}\mathbb{P}\{\boldsymbol{\xi}\in\Xi\}=1\\ \mathbb{E}_{\mathbb{P}}\{g_i(\boldsymbol{\xi})\}\le\gamma_i,\ i=1,\cdots,I\end{array}\right\}. \tag{13}$$

The first constraint in (13) ensures that $\mathcal{D}$ only contains valid distributions supported over the support set Ξ. Here, we use upper and lower bounds in each dimension to specify the support Ξ of uncertainties:

$$\Xi=\left\{\boldsymbol{\xi}\ \middle|\ \xi_m^{\min}\le\xi_m\le\xi_m^{\max},\ m=1,\cdots,M\right\}. \tag{14}$$

The second constraint in (13) characterizes generalized moment information of uncertainties via I functions $\{g_i(\cdot)\}$, and enforces the generalized moment $\mathbb{E}_{\mathbb{P}}\{g_i(\boldsymbol{\xi})\}$ cannot exceed a given threshold γ_i. For the sake of solvability and practicability of DRO approach, we adopt a piecewise linear formulation of moment functions $\{g_i(\cdot)\}$ in this study:

$$g_i(\boldsymbol{\xi})=\max\left\{\mathbf{f}_i^{\mathrm{T}}\boldsymbol{\xi}-q_i,0\right\},\ i=1,\cdots,I \tag{15}$$

which can be understood as the first-order deviation of uncertain parameters along a certain projection direction $\mathbf{f}_i$ truncated at q_i. Such a specification leads to equivalent robust counterparts of planning problems that can be efficiently solved, thereby benefiting decision-making in complicated process operations. In fact, the ambiguity set $\mathcal{D}$ can be reexpressed as the projection of a lifted ambiguity set $\bar{\mathcal{D}}$ by introducing an I-dimensional auxiliary random vector $\boldsymbol{\varphi}$:

$$\bar{\mathcal{D}} = \left\{ \mathbb{Q}_{\boldsymbol{\xi},\boldsymbol{\varphi}} \in \mathcal{M} \left| \begin{array}{l} \mathbb{P}\{(\boldsymbol{\xi},\boldsymbol{\varphi}) \in \bar{\Xi}\} = 1 \\ \mathbb{E}_{\mathbb{Q}}\{\boldsymbol{\varphi}\} \leq \boldsymbol{\gamma} \end{array} \right. \right\}, \tag{16}$$

where the domain of uncertainties is extended to a lifted support set $\bar{\Xi}$:

$$\bar{\Xi} = \left\{ (\boldsymbol{\xi},\boldsymbol{\varphi}) \left| \begin{array}{l} \boldsymbol{\xi} \in \Xi \\ g_i(\boldsymbol{\xi}) \leq \varphi_i, \ i = 1, \cdots, I \end{array} \right. \right\}. \tag{17}$$

It has been proved by Bertsimas et al. (2017) that the ambiguity set $\mathcal{D}$ is essentially tantamount to the set including all marginal distribution of $\boldsymbol{\xi}$ under $\mathbb{Q} \in \bar{\mathcal{D}}$. With the support set Ξ and functions $\{g_i(\cdot)\}$ determined by (14) and (15), we can easily rewrite the lifted support set $\bar{\Xi}$ as a set of linear inequalities:

$$\bar{\Xi} = \left\{ (\boldsymbol{\xi},\boldsymbol{\varphi}) \left| \begin{array}{l} \boldsymbol{\xi} \leq \boldsymbol{\xi}^{\max} \\ \boldsymbol{\xi}^{\min} \leq \boldsymbol{\xi} \\ 0 \leq \varphi_i, \ i = 1, \cdots, I \\ \mathbf{f}_i^{\mathrm{T}} \boldsymbol{\xi} - q_i \leq \varphi_i, \ i = 1, \cdots, I \end{array} \right. \right\}, \tag{18}$$

which can be further concisely expressed in a matrix form:

$$\bar{\Xi} = \{ (\boldsymbol{\xi},\boldsymbol{\varphi}) \,|\, \mathbf{G}\boldsymbol{\xi} + \mathbf{H}\boldsymbol{\varphi} \leq \mathbf{r} \}. \tag{19}$$

Here matrices $\mathbf{G}, \mathbf{H}$ and the vector $\mathbf{r}$ are given by:

$$\mathbf{G} = \begin{bmatrix} \mathbf{I} \\ -\mathbf{I} \\ \mathbf{0} \\ \mathbf{F}^{\mathrm{T}} \end{bmatrix}, \ \mathbf{H} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ -\mathbf{I} \\ -\mathbf{I} \end{bmatrix}, \ \mathbf{r} = \begin{bmatrix} \boldsymbol{\xi}^{\max} \\ -\boldsymbol{\xi}^{\min} \\ \mathbf{0} \\ \mathbf{q} \end{bmatrix}, \tag{20}$$

where $\mathbf{I}$ denotes unitary matrix with appropriate dimension, and $\mathbf{F}$ and $\mathbf{q}$ encompass parameters of piecewise linear functions $\{g_i(\cdot)\}$:

$$\mathbf{F} = [\mathbf{f}_1 \ \mathbf{f}_2 \ \cdots \mathbf{f}_I], \ \mathbf{q} = [q_1 \ q_2 \ \cdots \ q_I]^{\mathrm{T}}. \tag{21}$$

In practice, the values of these parameters can be estimated from historical demand data, thereby enabling a data-driven decision-making scheme. Based on the above choice of the ambiguity set $\mathcal{D}$, we deal with the tractability issue of the associated worst-case expectation problem

$$\sup_{\mathbb{Q} \in \bar{\mathcal{D}}} \mathbb{E}_{\mathbb{Q}} \{ L(\mathbf{x},\boldsymbol{\xi}) \}, \tag{22}$$

which will be useful in the sequel. Here $L(\mathbf{x},\boldsymbol{\xi})$ is a general objective function affected by uncertainties $\boldsymbol{\xi}$. In fact, we could translate (22) into a minimization problem by dualizations. An explicit expression of the inner problem is given by:

$$\begin{aligned} \sup_{\mathbb{Q}} \ & \int_{\bar{\Xi}} p(\boldsymbol{\xi},\boldsymbol{\varphi}) L(\mathbf{x},\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} \mathrm{d}\boldsymbol{\varphi} \\ \text{s.t.} \ & \int_{\bar{\Xi}} p(\boldsymbol{\xi},\boldsymbol{\varphi}) \mathrm{d}\boldsymbol{\xi} \mathrm{d}\boldsymbol{\varphi} = 1 \\ & \int_{\bar{\Xi}} p(\boldsymbol{\xi},\boldsymbol{\varphi}) \boldsymbol{\varphi} \mathrm{d}\boldsymbol{\xi} \mathrm{d}\boldsymbol{\varphi} \leq \boldsymbol{\gamma} \end{aligned} \tag{23}$$

Here the decision variable is the joint probability density function $p(\boldsymbol{\xi},\boldsymbol{\varphi})$ or the infinite-dimensional probability measure $\mathbb{Q}$. By associating Lagrangian multipliers η and $\boldsymbol{\beta}$ with constraints in (23), we can arrive at the dual form of (23) in the spirit of conic duality (Shapiro (2001)):

$$\begin{aligned} \min_{\eta,\boldsymbol{\beta}} \ & \eta + \boldsymbol{\gamma}^{\mathrm{T}} \boldsymbol{\beta} \\ \text{s.t.} \ & \boldsymbol{\beta} \geq 0 \\ & \eta + \boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{\beta} \geq L(\mathbf{x},\boldsymbol{\xi}), \ \forall (\boldsymbol{\xi},\boldsymbol{\varphi}) \in \bar{\Xi} \end{aligned} \tag{24}$$

where the last constraint is essentially a robust constraint on the uncertainty set $\bar{\Xi}$. In this sense (24) can be regarded as a classic RO problem.

2.3 Multi-stage DRO planning model

Process network planning typically involves a long planning horizon, in which the unknown demands in each period are revealed sequentially. This allows some decisions to be determined after uncertainties are known in each period, and hence leads to a sequential architecture of the decision-making process. To be more specific, variables $\{Y_{it}, QE_{it}, Q_{it}\}$ pertaining to capacity expansions should be specified at first as long-term planning decisions, while the operating levels $\{W_{it}\}$, purchase amounts $\{P_{jt}\}$ and sales amounts $\{S_{jt}\}$ can be determined in a more flexible manner after the uncertain demand $\mathbf{d}_t$ in period t becomes known. This can be mathematically expressed with the following multi-stage formulation:

$$\min_{\mathbf{x}} \left\{ \mathbf{c}_0^{\mathrm{T}} \mathbf{x}_0 + \sup_{\mathbb{P}_1 \in \mathcal{D}_1} \mathbb{E} \left\{ \min_{\mathbf{x}_1 \in \Omega_1} \mathbf{c}_1^{\mathrm{T}} \mathbf{x}_1 + \cdots + \min_{\mathbf{x}_T \in \Omega_T} \mathbf{c}_T^{\mathrm{T}} \mathbf{x}_T \right\} \right\}. \tag{25}$$

Here all uncertainties and recourse decisions decompose as

$$\mathbf{x} = [\mathbf{x}_1^{\mathrm{T}} \ \mathbf{x}_2^{\mathrm{T}} \ \cdots \mathbf{x}_T^{\mathrm{T}}]^{\mathrm{T}}, \ \boldsymbol{\xi} = [\boldsymbol{\xi}_1^{\mathrm{T}} \ \boldsymbol{\xi}_2^{\mathrm{T}} \ \cdots \boldsymbol{\xi}_T^{\mathrm{T}}]^{\mathrm{T}}, \tag{26}$$

where random demands $\boldsymbol{\xi}_t$ are revealed in Stages t, and afterwards $\mathbf{x}_t$ are are made. More precisely, decisions $\mathbf{x}_0 = \{Y_{it}, QE_{it}, Q_{it}\}$ shall be made in a *here-and-now* manner, and recourse variables $\mathbf{x}_t = \{W_{it}, P_{jt}, S_{jt}\}$ shall be made in a *wait-and-see* manner in response to demand uncertainties $\boldsymbol{\xi}_t$ observed at Stage t, which are described by the associated ambiguity set $\mathcal{D}_t$. Ω_t denotes the feasible region of recourse variables at Stage t, where we suppress the dependence of Ω_t on $\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_{t-1}$ and $\boldsymbol{\xi}_t$ for notational convenience.

3. TRACTABLE REFORMULATION BASED ON AFFINE DECISION RULES

In a multi-stage setting, deriving an explicit expression of optimal recourse policy and calculating the worst-case expectation are generally intractable, since they involve enumeration of all realizations of uncertainties within the lifted support set $\bar{\Xi}$ (Goh and Sim (2010)). A pragmatic strategy to circumvent the intractability issue is to employ the ADR with the nonanticipativity constraints (Ben-Tal et al. (2004)), which enforce the recourse variable $\mathbf{x}_t$ at Stage t to be affinely dependent on the uncertainty realizations $\boldsymbol{\xi}_{1:t} = [\boldsymbol{\xi}_1^{\mathrm{T}} \ \cdots \ \boldsymbol{\xi}_t^{\mathrm{T}}]^{\mathrm{T}}$ and the auxiliary random variables $\boldsymbol{\varphi}_{1:t} = [\boldsymbol{\varphi}_1^{\mathrm{T}} \ \cdots \ \boldsymbol{\varphi}_t^{\mathrm{T}}]^{\mathrm{T}}$ up to Stage t:

$$\mathbf{x}_t(\boldsymbol{\xi}_{1:t}, \boldsymbol{\varphi}_{1:t}) = \mathbf{x}_t^0 + \mathbf{X}_t^{\boldsymbol{\xi}} \boldsymbol{\xi}_{1:t} + \mathbf{X}_t^{\boldsymbol{\varphi}} \boldsymbol{\varphi}_{1:t}, \ \forall t. \tag{27}$$

where $\mathbf{x}_t^0$ denotes the constant, $\mathbf{X}_t^{\boldsymbol{\xi}}$ and $\mathbf{X}_t^{\boldsymbol{\varphi}}$ are coefficient matrices associated with the random variables $\boldsymbol{\xi}_{1:t}$ and the auxiliary random variables $\boldsymbol{\varphi}_{1:t}$, respectively. By stacking all affine equations in all periods, we can write (27) in a concise form:

$$\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi}) = \mathbf{x}^0 + \mathbf{X}^{\boldsymbol{\xi}} \boldsymbol{\xi} + \mathbf{X}^{\boldsymbol{\varphi}} \boldsymbol{\varphi}. \tag{28}$$

where some elements of $\mathbf{X}^{\boldsymbol{\xi}}$ and $\mathbf{X}^{\boldsymbol{\varphi}}$ are enforced to be zero to respect the spirit of nonanticipativity in (27). By substituting the ADR approximation (28) for the optimal decision policy, a conservative approximation to the multi-stage DRO problem (25) can be derived:

$$\begin{aligned}\min_{\mathbf{x}} \min_{\mathbf{x}(\boldsymbol{\xi},\boldsymbol{\varphi})} \ & \mathbf{c}_0^{\mathrm{T}}\mathbf{x}_0 + \sup_{\mathbb{P}\in\mathcal{D}} \mathbb{E}_{\mathbb{P}}\left\{\mathbf{c}_{1:T}^{\mathrm{T}}\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi})\right\} \\ \text{s.t. } & \mathbf{A}_0\mathbf{x}_0 + \mathbf{A}_{1:T}\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi}) \leq \mathbf{b},\ \forall(\boldsymbol{\xi},\boldsymbol{\varphi})\in\bar{\Xi} \\ & \mathbf{C}_0\mathbf{x}_0 + \mathbf{C}_{1:T}\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi}) \leq \boldsymbol{\xi},\ \forall(\boldsymbol{\xi},\boldsymbol{\varphi})\in\bar{\Xi} \\ & \text{Nonanticipativity constraints}\end{aligned} \tag{29}$$

Here, coefficients $\{\mathbf{x}^0, \mathbf{X}^{\boldsymbol{\xi}}, \mathbf{X}^{\boldsymbol{\varphi}}\}$ of the decision rule (28) are absorbed into first-stage variables, thereby leading to a single-stage optimization problem that is easier to tackle. Based on the reformulation in Section 2.2, we could arrive at the following identical RO problem by dualizing the inner-most maximization problem:

$$\min \mathbf{c}_0^{\mathrm{T}}\mathbf{x}_0 + \eta + \boldsymbol{\gamma}^{\mathrm{T}}\boldsymbol{\beta} \tag{30}$$

$$\text{s.t. } \boldsymbol{\beta} \geq \mathbf{0} \tag{31}$$

$$\eta + \boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{\beta} \geq \mathbf{c}_{1:T}^{\mathrm{T}}\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi}),\ \forall(\boldsymbol{\xi},\boldsymbol{\varphi})\in\bar{\Xi} \tag{32}$$

$$\mathbf{A}_0\mathbf{x}_0 + \mathbf{A}_{1:T}\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi}) \leq \mathbf{b},\ \forall(\boldsymbol{\xi},\boldsymbol{\varphi})\in\bar{\Xi} \tag{33}$$

$$\mathbf{C}_0\mathbf{x}_0 + \mathbf{C}_{1:T}\mathbf{x}_{1:T}(\boldsymbol{\xi},\boldsymbol{\varphi}) \leq \boldsymbol{\xi},\ \forall(\boldsymbol{\xi},\boldsymbol{\varphi})\in\bar{\Xi} \tag{34}$$

$$\text{Nonanticipativity constraints} \tag{35}$$

Note that constraints (32)-(34) can be regarded as generic robust constraints on the polytopic uncertainty set $\bar{\Xi}$. We can then adopt existing results from RO literature to convert these infinite-dimensional constraints into their corresponding robust counterparts, leading to a tractable MILP reformulation of the multi-stage DRO process network planning problem. It is worth noting that an MILP reformulation owes to the piecewise linear formulations of $\{g_i(\cdot)\}$ (15) used in the ambiguity set $\mathcal{D}$ (13). Therefore it can be conveniently solved by using the state-of-the-art branch-and-cut methods implemented in solvers such as CPLEX.

4. APPLICATION CASE STUDY

In this section, the proposed DRO approach is applied to a large-scale process network involving 38 processes, 28 chemicals, 10 suppliers and 16 markets, whose structure is depicted in Fig. 1. The chemicals can be classified into raw materials (A-J), intermediates (AA,AB), and final products (K-Z). A ten-year planning horizon is considered here, which consists of five time periods in total, and each time period has two years. It is assumed that Processes 12, 13, 16, and 38 have initial capacities of 19.9, 12.5, 150 and 100 kton/year, respectively.

In this case, we consider random demands $\{du_{jt}\}$ over five time periods, which constitute a 80-dimensional random vector $\boldsymbol{\xi}$, and one thousand historical demand data samples are collected in total. We solve the planning case using the deterministic model, multi-stage DRO model and multi-stage adaptive robust optimization (ARO) model (Ben-Tal et al. (2004)). Parameters in the deterministic model are set as their nominal values. As with the multi-stage ARO model, the box uncertainty set is adopted with its size estimated with 1,000 available samples. Finally the multi-stage ARO problem is cast as an MILP by means of ADRs. In the multi-stage DRO model, we adopt principal component analysis (PCA) to estimate projection directions $\{\mathbf{f}_i\}$ in moment functions $\{g_i(\cdot)\}$ from data samples, and then set several truncation points $\{q_i\}$ evenly on each principal axis. In this way, partial statistical information within data can be incorporated into the ambiguity set $\mathcal{D}$, allowing for a systematic data-driven decision-making schema. All problems are modelled in GAMS 24.7.4, in which all induced MILPs are solved using CPLEX 12.7.0 with optimality gaps set as 0.1%.

Table 1 showcases the performance comparisons of solving various optimization problems under demand uncertainties. The multi-stage DRO problem has more variables and constraints than the other two problems, and is thus the most time-consuming. In spite of this, the computational burden is still affordable in practice. In terms of objectives, solving the multi-stage DRO problem returns 12.61% higher NPV than solving the multi-stage ARO problem, primarily due to different risk measures adopted. The optimal objective of the deterministic problem is much higher than those of two multi-stage problems. Such a gap in objectives is also due to the conservatism induced by ADRs for solving two multi-stage problems. Nonetheless, multi-stage problems are still preferred in an uncertain environment, since the deterministic problem organically falls short of addressing demand uncertainties and reducing potential risks.

Table 1. Optimization Results in the Process Network Planning Case

	Deterministic Planning	Multi-Stage DRO	Multi-Stage ARO
Cont. var.	851	753,732	189,012
Bin. var.	190	190	190
Constraints	1,224	407,775	103,215
CPU time (s)	0.11	1264.16	100.69
Objective (M$)	7,521	2,741	2,434

Next we investigate the conservatism of different approaches by taking a closer look at their decisions. The optimal process design and planning decisions in the entire planning horizon derived by solving the deterministic problem, the multi-stage DRO and ARO problems are listed in Table 2. We can see that compared with the deterministic planning model, less processes are operated by multi-stage DRO and ARO since capacities of Processes 34, 35, and 36 have not been expanded all along. It bears rationality because less capacity expansions are determined in a "here-and-now" manner by two multi-stage approaches and some unnecessary costs can be avoided in face of extremal realizations of random demands.

Table 2. Expansion Decisions Made in the Entire Planning Horizon by Different Models

Planning Model	Processes Selected for Expansions
Deterministic	8, 12, 13, 14, 16, 17, 28, 32, 34, 35, 36, 38
Multi-Stage DRO	8, 12, 13, 14, 16, 17, 28, 32, 38
Multi-Stage ARO	8, 12, 13, 14, 16, 17, 28, 32, 38

Although the same processes have been selected for capacity expansions by two multi-stage approaches, their exact amounts of expansions are different, especially for Processes 8, 14,17, 28, and 32. Fig. 2 further highlights the changes of capacities over the entire planning horizon determined by the two multi-stage approaches. Note that capacities of Processes 8, 14, 17, and 28 are expanded by all approaches at time period 2. As for Process 32, its capacity is expanded at time period 4 one more time by the multi-stage DRO approach. Therefore, it has a much larger

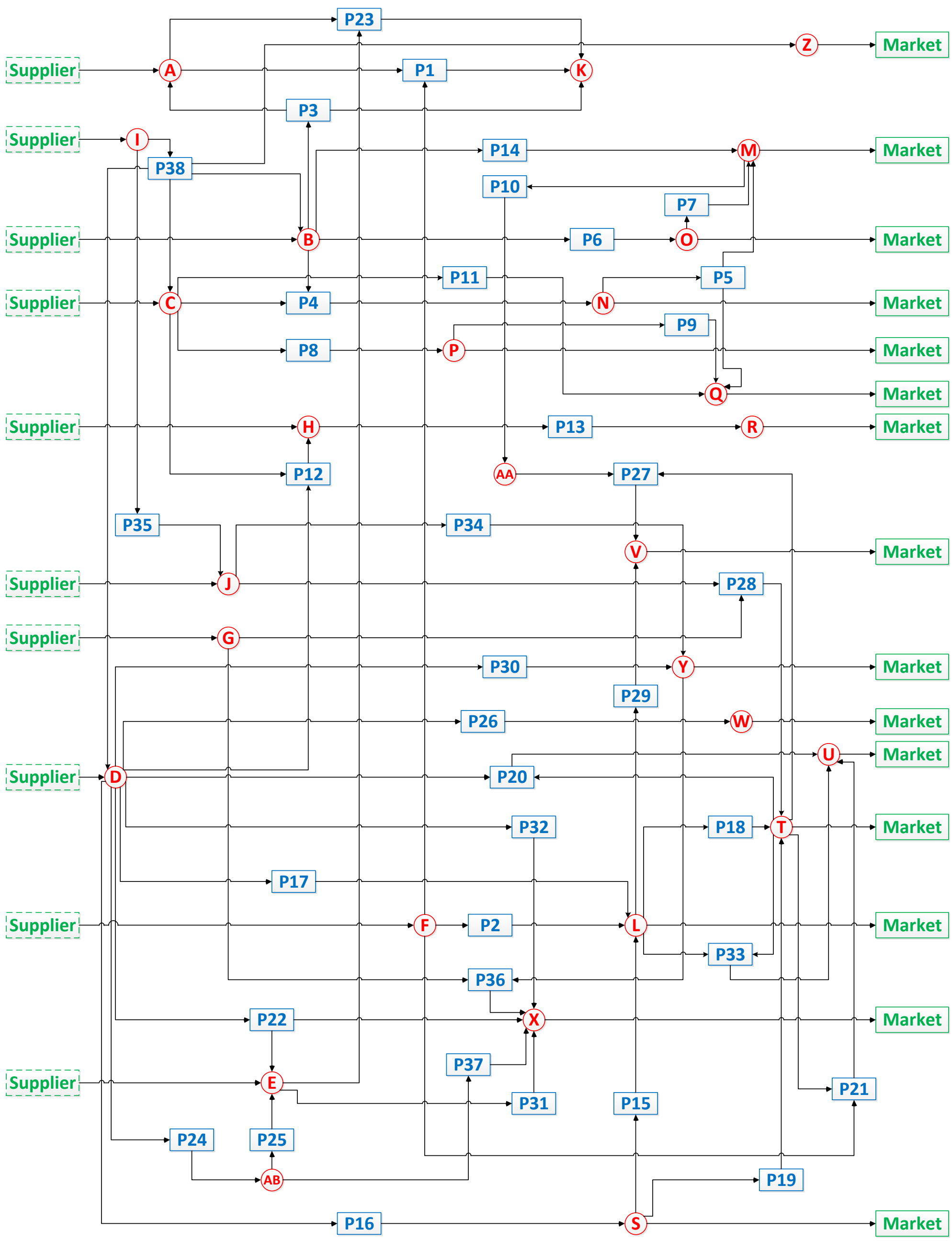
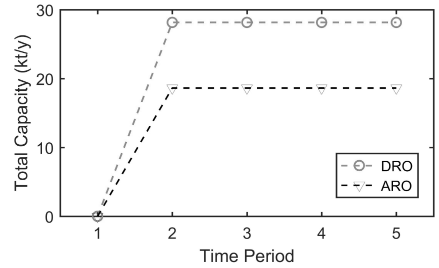


Fig. 1. The chemical process network.

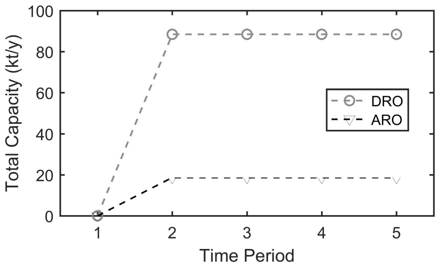
capacity at the final stage, which is much less conservative than that obtained by multi-stage ARO, and could enable higher profits under demand randomness. It indicates that ARO only accounts for the worst-case realization within the support set, thereby resulting in conservative solutions. By contrast, the proposed DRO-based planning approach is able to utilize more meaningful distributional information from data by using the ambiguity set, thereby better hedging against uncertainties.

5. CONCLUSION

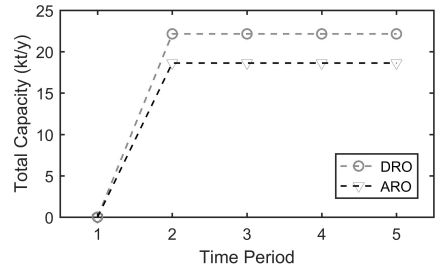
In this paper, we put forward a novel DRO approach to hedge against the ambiguity of probability distributions of uncertain demands in process network planning. An ambiguity set is constructed from data to capture partial statistical information, on which the worst-case expected objective value is optimized without knowing the exact distribution of uncertainties. To describe the sequential nature of uncertain demands revealed in multiple periods, a multi-stage DRO model is developed. To address the computational challenge, ADRs have been adopted to furnish a conservative yet tractable solution. An application case study on an industrial-scale process network planning problem demonstrate that, the proposed approach can of fully utilize statistical information underlying data, hedge against distributional ambiguity, and hence leads to less conservative solutions in comparison with classical ARO approach.



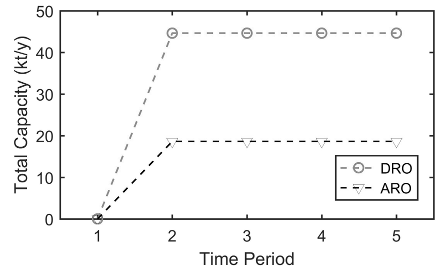
(a) Process 8



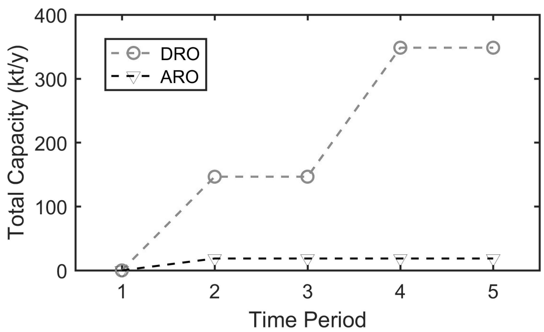
(b) Process 14



(c) Process 17



(d) Process 28



(e) Process 32

Fig. 2. Optimal capacity expansion decisions over the entire planning horizon determined by multi-stage DRO and ARO.

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