A New Framework to Primal Bounding Multistage Stochastic Programs under Endogenous and Exogenous Uncertainties

Zuo Zeng, Selen Cremaschi

Department of Chemical Engineering, Auburn University, Auburn, AL 36849, USA
selen-cremaschi@auburn.edu

Optimization problems with both decision-dependent (endogenous) and decision-independent (exogenous) uncertainties are typical in the chemical process industry, especially in planning and scheduling. Stochastic programming is a framework for modelling optimization problems that involve uncertainty. Multistage stochastic programming (MSSP) is one approach for modelling such problems that consider decisions and recourse actions and that involve realization of uncertainties in multiple stages. However, MSSP models grow exponentially with increasing number of scenarios and time periods, and they quickly become computationally intractable for real-world problems. In this paper, we propose a general primal-bounding framework for large-scale MSSP models with both endogenous and exogenous uncertainties based on extending the concepts of expected value solution from MSSP under exogenous uncertainties. The proposed framework utilizes already known information and assumes the expected results for unrealized information to determine current state decisions. We applied the framework to solve instances of process-network-synthesis problem, which involves both uncertain process yields (endogenous uncertainty) and uncertain demand (exogenous uncertainty) with up to 1024 scenarios. The computational results reveal that proposed approach yielded feasible solutions within 22.3%, 13.4%, and 6.5% of the true solutions for the first, second and third instances, and obtained these solutions up to three order of magnitude faster than solving the original MSSP models.

1. Introduction

Stochastic programming is a framework for modelling optimization problems, which involve uncertainties, and has been widely used by the process systems engineering (PSE) community. Many engineering applications have been considered under uncertainties such as gas and oil field developments (Goel and Grossmann, 2004), synthesis of process networks with uncertain yields (Goel and Grossmann, 2006; Tarhan and Grossmann, 2008), and artificial lift infrastructure planning with uncertain production rate (Zeng and Cremaschi, 2017). Multistage stochastic programming (MSSP) is one of the approaches for modeling optimization problems with sequential decisions that can be made at discrete stages under both exogenous (i.e., decision-independent) and/or endogenous (i.e., decision-dependent) uncertainties in multiple time periods. It is a scenario-based method that considers decisions and recourse actions in multiple stages. Scenarios represent possible future states of the system and are generated by enumerating combinations of possible outcomes of uncertain parameters. In MSSP, non-anticipativity constraints (NACs) prevent decision variable values from anticipating unrealized future outcomes. Unfortunately, MSSP models the uncertainty at all decision stages and take into account all possible scenarios and their impacts, which cause, typically, an exponential growth in the number of NACs making the MSSP model computationally intractable for real-world problems due to both space and time complexities. In other words, the model cannot be generated with the available RAM in a typical workstation, and the optimal solution cannot be obtained within a reasonable duration of time. The structure of MSSP models, more specifically its scenario-based structure, is generally exploited to develop algorithms that decompose the original model into smaller sub-problems. Most of these algorithms separate the scenario set into different scenario groups, remove NACs between scenario groups, and enforce NACs in each scenario group. The sub-problems then include subsets of scenarios and NACs, and they are easier to solve than the original MSSP model. The solutions of these sub-problems provide a...
dual bound for the original model. Then, heuristic and approximation approaches are generally employed to generate a feasible solution (and a primal bound), such as a rolling-horizon heuristic approach (Colvin and Maravelias, 2009), sample average approximation algorithm (Solak et al., 2010), and generalized knapsack-based decomposition algorithm (GKDA) (Zeng et al., 2018). Several approaches combine heuristics with scenario decomposition algorithms to solve the MSSPs. Recent examples include improved Lagrangean decomposition framework (Gupta and Grossmann, 2014), sequential scenario decomposition approach (Apap and Grossmann, 2017), and branch and bound algorithm (Christian and Cremaschi, 2018). However, the decomposition algorithms still enumerate all scenarios and the corresponding decision variables in sub-problems. Some of these scenarios may never be realized due to the decisions and recourse actions taken in the solution of MSSP problems with endogenous uncertainty.

To measure the importance of solving a stochastic model, Birge and Louveaux (2011) introduced the value of the stochastic solution \( VSS \) for two-stage stochastic models. The \( VSS \) is obtained as the difference between the solution of the two-stage stochastic model (SP) and the expected value of the solution of the deterministic model (EEV): \( VSS = SP - EEV \). The deterministic model is constructed by replacing all random variables with their expected values in the two-stage stochastic model, and the EEV is calculated by implementing the first-stage decisions obtained as the solution of the deterministic problem in two-stage stochastic model. Zeng and Cremaschi (2019) extended the concepts of expected value solution for MSSPs under only endogenous uncertainties and introduced a framework to obtain valid primal bounds, called Absolute Expected Value Solution (AEEV), for these problems under certain conditions. The AEEV framework yielded primal bounds within 1% of the optimal solutions in solution times up to four orders of magnitude faster than solving the original MSSP for the planning problems considered in the paper.

This paper extends the AEEV framework for large-scale MSSP problems under both endogenous and exogenous uncertainties with both continuous and discrete state variables and complete recourse. The proposed framework follows the nature of decision-making when planning in multiple decision stages under uncertainty as shown in Figure 1. Before any uncertainty is realized, the decision maker utilizes the expected results for future unrealized uncertainties to make state decisions. As new information becomes available with uncertainty observations, the recourse actions are taken, and the current state decisions are updated by using the current information along with expected results for future uncertainties at the current state. The process is repeated along the planning horizon (Figure 1). The remainder of the paper introduces a general MSSP formulation under endogenous and exogenous uncertainties that is addressed in this paper, explains the AEEV framework, defines the case study – process-network-synthesis problem from Apap and Grossmann (2017) – used to illustrate the framework, discusses the case study results, and summarizes conclusions.

\section*{2. A general MSSP model under endogenous and exogenous uncertainties}

Equations (1)-(10) define a general deterministic equivalent formulation of a MSSP problem with complete recourse under endogenous and exogenous uncertainties derived from Zeng and Cremaschi (2019).

\begin{align*}
RP &= \max \sum_{s} p_s \sum_{l} \sum_{t} G_{l,s}(v_{l,t}, \theta_{l,t}^{1}, \xi_{l,t}^{1}, b_{l,t}^{1}, y_{l,t}^{1}, r_{l,t}^{1}) \\
\forall i \in I, t \in T, s \in S & h(b_{l,t}^{1}, y_{l,t}^{1}, v_{l,t}^{1}, \theta_{l,t}^{1}, \xi_{l,t}^{1}) = 0 \\
\forall i \in I, t \in T, s \in S & g(b_{l,t}^{1}, y_{l,t}^{1}, v_{l,t}^{1}, \theta_{l,t}^{1}, \xi_{l,t}^{1}) \leq 0 \\
\forall i \in I, s \in S & b_{i}^{1} = b_{i}^{1} \\
\forall i \in I, \forall (s, s') \in S & y_{l,i}^{1} = y_{l,i}^{1} \end{align*}

Figure 1: Natural decision-making process when planning in multiple decision stages under uncertainty
\( b_{i,t} = b_{i,t}^e \quad \forall i, \forall t \in T, \forall (t,s,s') \in S_X \)  
(6)

\[ y_{i,t} = y_{i,t}^e \quad \forall i, \forall t \in T, \forall (t,s,s') \in S_X \]  
(7)

\[
\begin{align*}
Z_t^{s,s'} & = b_{i,t}^{s,s'} + K 
\left( -Z_t^{s,s'} \right) \\
& \quad \forall (s,s') \in S_E, \forall t \in T, t > 1
\end{align*}
\]  
(8)

\[
\begin{align*}
b_{i,t}^{s,s'}, Z_t^{s,s'} & \in \{0,1\}, y_{i,t}^{s,s'} \in \mathbb{R} \\
& \quad \forall (s,s') \in S_E, \forall t \in T, \forall i \in I
\end{align*}
\]  
(9)

In Eqs (1)-(10), decision variables are \((b_{i,t}^{s,s'}, y_{i,t}^{s,s'})\). We define the decision variables enforced by initial and conditional NACs as here-and-now decisions \((b_{i,t}^e, y_{i,t}^e)\). Other decision variables, which are determined by scenario specific constraints and are not enforced by any NACs, are defined as recourse actions \((y_{i,t}^r)\).

The model contains deterministic parameters \((V_i,t)\), exogenous uncertain parameters \((\xi_t^s)\) and endogenous uncertain parameters \((\theta_t^d)\). Sets of exogenous and endogenous scenario pairs are defined as: \(S_X := \{ (t,s,s') : t \in T, \xi_t^s = \xi_t^{s}, \theta_t^d = \theta_t^{d} |_{\xi_t^{s}} \} \) and \(S_E := \{ (i,s,s') : i \in I, \theta_t^d = \theta_t^{d}, \xi_t^s = \xi_t^{s} |_{\theta_t^{d}} \} \).

Equations (2) and (3) are scenario specific inequality and equality constraints. Functions \(g_{i,s,t}(\cdot), h(\cdot), \) and \(g(\cdot)\) can either be linear or nonlinear. Initial NACs and NACs associated with exogenous uncertain parameters are given in Eqs (4)-(5) and Eqs (6)-(7).

Equation (8) is conditional NACs associated with endogenous uncertainty and uses Boolean variable, \(Z_t^{s,s'}\), which is equal to one if scenarios \(s\) and \(s'\) are indistinguishable at time period \(t\). The values of the Boolean variables \(Z_t^{s,s'}\) are determined by decisions made in previous time periods using function \(H(b_{i,t}^{s,s'}, b_{i,t}^{r}, \ldots, b_{i,t}^{s,s'}, y_{i,t}^{r}, y_{i,t}^{s,s'} , \ldots, y_{i,t}^{r})\).

The RP is the optimum objective function value.

3. The Absolute Expected Value Solution (AEEV) framework

In MSSP formulations (Eqs (1)-(10)), the numbers of both variables and constraints increases with number of scenarios, and NACs constitute a large portion of the constraints. The AEEV framework is a scenario-free approach that generates and solves a series of two deterministic sub-problems based on the observation of realized outcomes of uncertain parameters. These sub-problems are deterministic expected value sub-problems \((DEVSP_s)\) and recourse deterministic expected value sub-problems \((DEVSP_{s,recourse})\), whose formulations are introduced in Section 3.1. Here-and-now decisions are determined by solving \(DEVSP_s\) and recourse actions are determined by solving \(DEVSP_{s,recourse}\), using the solutions of \(DEVSP_s\).

3.1 The formulation of deterministic sub-problems

In \(DEVSP_s\) and \(DEVSP_{s,recourse}\), scenario indices and NACs are removed. Indicator variable \((Z_t^{s,s'})\) and Eq (7), are dropped from the models. The formulation of \(DEVSP_{s,2}\) for sub-problem \(n\) at time \(t\) is given in Eqs (11)-(16).

\[
\begin{align*}
\min & \sum_i \sum_{t'} G_{i,t'}^{n,t}(V_i,t', \theta_i, \xi_i^{n,t'} \in U_{n,\text{pro}}, b_{i,t'}, y_{i,t'}) \\
\text{s.t.} & h(b_{i,t'}, y_{i,t'}, \theta_i, \xi_i^{n,t'} \in U_{n,\text{pro}}) = 0, \quad \forall i \in I, t' \in T \\
g(b_{i,t'}, y_{i,t'}, \theta_i, \xi_i^{n,t'} \in U_{n,\text{pro}}) \leq 0, \quad \forall i \in I, t' \in T \\
b_{i,t'}^{n,t'} & \in F_{n,\text{pro}} |_{t', \in T}, b_{i,t'} \in [0,1] |_{t', \in I} \\
y_{i,t'}^{n,t'} & \in F_{n,\text{pro}} |_{t', \in T}, y_{i,t'} \in \mathbb{R} |_{t', \in I} \\
y_{i,t'}^{n,t'} & \in F_{n,\text{pro}} |_{t', \in T}, y_{i,t'} \in \mathbb{R} |_{t', \in I} \\
\end{align*}
\]  
(11)

(12)

(13)

(14)

(15)

(16)

In \(DEVSP_{s,2}\), \(n\) is the index for the sub-problem, and \(n,\text{pro}\) represents its parent subproblem. At time period \(t\), after solving \(DEVSP_{n,t}\), new child subproblems, \(DEVSP_{s,recourse}^{\text{child}}\), are generated if there are uncertainty
realizations. A set of DEVSP_{n,recourse} are generated based on the realized outcomes of uncertain parameters, the formulation for DEVSP_{n,recourse} are shown in Eqs (18)-(22).

\[
\min \sum_{t'} \sum_{t_1} G_{1,t_1}^2(t', t''; \theta_n \in U_{n,child}, \xi_n \in U_{n,child}, b_{t', t''}, y_{t', t''})
\]

(17)

\[h(b_{t', t''}, y_{t', t''}, \theta_n \in U_{n,child}, \xi_n \in U_{n,child}) = 0 \quad \forall i \in I, t' \in T
\]

(18)

\[g(b_{t', t''}, y_{t', t''}, \theta_n \in U_{n,child}, \xi_n \in U_{n,child}) \leq 0 \quad \forall i \in I, t' \in T
\]

(19)

\[b_{t', t''} \in F_{n, t' \in T, t''} \in [0, 1] \quad \forall t' \in T, \forall i \in I
\]

(20)

\[y_{t', t''} \in F_{n, t' \in T, t''} \quad \forall t' \in T, \forall i \in I
\]

(21)

\[y_{t', t''} \in F_{n, t' \in T, t''} \quad \forall t' \in T, \forall i \in I
\]

(22)

In DEVSP_{n,recourse} the values of realized endogenous and exogenous uncertain parameters \(\theta_n, \xi_n\) are updated corresponding to \(U_{n,recourse}\). After obtaining here-and-now decisions and if there are uncertainty realizations, the values of realized uncertain parameters \(\theta_n, \xi_n\) in \(U_{n,child}\) are updated with corresponding outcomes. After solving DEVSP_{n,recourse} and DEVSP_{n,child}, here-and-now decisions \((b_{t', t''}, y_{t', t''})\) are obtained for \(t' \leq t\), and the recourse actions are obtained for \(t' < t\).

3.2 Implementation of the AEEV framework

At initialization, there is only one sub-problem, \(n = 0\). \(U_0\) is initialized to the expected values of all uncertain parameters, and DEVSP_{1,1} is generated at \(t = 1\). At \(t = 2\), the algorithm first determines if there have been any uncertainty realizations. If there are no uncertainty realizations, the sub-problem is inherited and solved at \(t = 2\). If there are uncertainty realizations, it generates a set of sub-problems based on the realized outcomes of uncertain parameters. For exogenous uncertainties, the values of uncertain parameters are realized based on time periods. For endogenous uncertainties, the realizations of uncertain parameters are based on here-and-now decisions. The generation of sub-problems in the framework are based on both time period (exogenous) and here-and-now decisions (endogenous) of previous stages. If an uncertain parameter is observed, the value of that uncertain parameter in \(U_n\) takes its realized value for sub-problem \(n\). For all other uncertain parameters, \(U_n\) contains their expected values. If there are realized uncertain parameters and recourse actions should be taken, DEVSP_{n,recourse} are generated and solved to determine the recourse actions. The generation and solution of sub-problems continue until all uncertain parameters are observed or until the end of planning horizon. At termination, the framework generates a feasible solution and its corresponding AEEV.


The problem involves uncertain process yields \(\theta_1, \theta_2\) (endogenous uncertainty) and uncertain product demands \(d_1\) (exogenous uncertainty). The goal is to determine optimal design decisions and recourse actions in production planning for maximizing the total expected profit from the sales of the final product. In the case study considered (Figure 2), the final product A is currently produced using Process 3, which has a known and fixed yield. There are two new processes, Process 1 and Process 2, which are available to be installed for producing the intermediate product used by Process 3. The yields of Process 1 and Process 2 are uncertain, and are assumed to have two possible outcomes, which are only realized once the processes are installed and operated. Demand uncertainty is realized at the end of every time period.

Here-and-now decisions are which processes (indexed by \(i\)) should be operated \((y_{t, i}^{oper})\) and expanded \((y_{t, i}^{exp})\). Capacity level of expansions \(w_{t, i}^{cap} \in R_{t, i}^{exp}\) and inflow rates of chemicals B, C, and D \(w_{t, i}^{inflow} \in R_{t, i}^{exp}\) are also here-and-now decisions. To satisfy the demand at time period \(t\) in scenario \(s\) \(d_1\), the recourse actions are inventory level \(w_{t, i}^{invent}\), purchases \(x_{t, i}^{purch}\), and sales \(x_{t, i}^{sales}\) of product A. The original nomenclature and MSSP formulation of the problem can be found in Goel and Grossmann (2006). The DEVSP_{n,recourse} generated and solved by the AEEV framework are obtained using the MSSP formulation and are given in Figure 3.
In Eq(19) of Figure 3, endogenous and exogenous uncertain parameters $\theta_1, \theta_2, d_t$ are updated using $U_n$. Here-and-now decisions $(y_{it}^{\text{exp}}, y_{it}^{\text{oper}}, r_{it}^{\text{rate}}, s_{it}^{\text{QF}}, s_{it}^{\text{QF}} \in \mathbb{R}^2, k = \{1, 2, 6\}, w_{it}^{\text{QF}} \in \mathbb{R}^2)$ are fixed for $t' < t$ (Figure 3, Eq(20)) using solutions of the parent problems. The $\text{DEVSP}_{n,t}^{\text{precourse}}$ has the same formulations as $\text{DEVSP}_{n,t}^{\text{synthesis}}$, where the values of here-and-now decisions are fixed to their corresponding values in the solution of $\text{DEVSP}_{n,t}^{\text{synthesis}}$. The algorithm starts by taking the expected values of the uncertain yields, 0.7 (for Processes 1 and 2) and uncertain demands for constructing the algorithm generates the corresponding recourse sub-problems for realized uncertain parameters and obtain recourse actions $(x_{it}^{\text{parc}}, x_{it}^{\text{sales}}, w_{it}^{\text{inv}}, w_{it}^{\text{rate}} \in \mathbb{R}^2, k = \{3, 4, 5, 7, 8\})$ for $t = 1$ for each realization. At the next time period, $t = 2$, all decision variables of the previous time periods and the realized uncertain parameters are fixed. The algorithm continues to generate and solve $\text{DEVSP}_{n,t}^{\text{synthesis}}$ and $\text{DEVSP}_{n,t}^{\text{precourse}}$.

We solved three instances of the process-network-synthesis problem using the AEEV framework. The first instance is a two time-period 3-stage problem and has 16 scenarios. The second problem has seven time periods and has 512 scenarios. The third problem has eight time periods with 1024 scenario due to increased demand uncertainty outcomes from a longer planning horizon. The optimum solutions for these instances are obtained by solving the deterministic equivalents of the MSSP models. All models and algorithms were
implemented in Pyomo and solved using CPLEX 12.6.3 on a standard node of Auburn University Hopper Cluster. Data for both instances are available upon request. In first instance, the optimum ENPV is $1.04285 \times 10^6$. The AEEV is $1.42125 \times 10^5$ with 22.3% relative gap. The solution generated by the AEEV framework has the same capacity expansion and operation decisions included in the optimum solution, but it recommends larger inflow rates than the optimum solution. In second instance, the optimum ENPV is $4.7908 \times 10^5$, while the AEEV is $4.1482 \times 10^5$ yielding a 13.4% relative gap. In the largest third instance, the optimum ENPV is $7.1548 \times 10^6$, while the AEEV is $6.6907 \times 10^6$ yielding a 6.5% relative gap. The solution times for first instance for MSSP and AEEV are both within a second. For second instance, the AEEV framework obtains the solution using 46 seconds, while CPLEX takes 4483 seconds to solve the MSSP. For the third instance, the AEEV framework obtains the solution using 140 seconds, while MSSP takes 901937 seconds.

5. Conclusions
This paper presents a new framework for solving a class of large-scale MSSP models under both endogenous and exogenous uncertainties. The class contains here-and-now decisions and complete recourse actions, which can be discrete or continuous. The proposed framework extends the expected value solution approach and obtains a feasible and implementable solution for this class of MSSP problems. By generating and solving a series of deterministic problems based on the observation of realized outcomes of uncertain parameters, the framework has a scenario-free structure and eliminates scenario indices and NACs. The proposed AEEV generates a feasible solution and a primal bound for this class of MSSP models relatively quickly. The proposed framework has been applied to two instances of process-network-synthesis problem under uncertain yields and demands with up to 1024 scenarios. The results reveal that the proposed framework can obtain feasible solutions up to three orders of magnitude faster and the quality of the solutions improves as the problem becomes larger.

Acknowledgments
This work was partially funded by RAPID Manufacturing Institute, the U.S.A.

References