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Stochastic Optimization of Agrochemical Supply Chains with Risk Management

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Abstract

The global agrochemical market is highly consolidated, with large multinational companies accounting for a major share of the market. Thus, even for a single agrochemical product, its supply chain typically involves many possible paths connecting the raw material sources of active ingredients to final customers. In addition to structural complexity, agrochemical supply chains are also subject to seasonality and various unique uncertainties, thereby demanding high system resilience and implementation of risk management strategies in the face of these uncertainties and disruptions. In this study, we formulate and optimize the supply chain of an agrochemical active ingredient by formulating a stochastic mixed-integer nonlinear programming (MINLP) model. This MINLP formulation is scenario-based with demand uncertainty addressed by Value-at-Risk (VaR) and Conditional Value-at-Risk (CVaR). For the first time, we propose to reformulate these nonlinear CVaR constraints using perspective reformulation techniques. We show that these perspective cuts give a tight approximation of the original MINLP model. Through an illustrative case study, we compare the results and performance of the original MINLP and the reformulated MILP.

Keywords: Agrochemical supply chain, Value-at-Risk (VaR), Conditional Value-at-Risk (CVaR), perspective cuts, mixed-integer nonlinear programming.

1. Introduction

In 2050, the global population is expected to increase by 2 billion people to 9.7 billion, which puts unprecedented stress on food, energy, and water resources as the global food production must increase by at least 70% (Searchinger et al., 2018). Therefore, the manufacturing and supply chain of agrochemicals, including pesticides, herbicides, fungicides, and insecticides, are critical to ensuring food production and security. The global agrochemical market is highly consolidated, with 60-70% of the global market share dominated by four agrochemical companies alone (IEPS-Food, 2017). Each of these leading companies has a diversified product line, and its supply chains are multistage networks involving many possible paths connecting the raw material sources to active ingredients to final products. In addition, agrochemical supply chains are further complicated by seasonality and various uncertainties due to climate change, more frequent black swan events (e.g., COVID-19 pandemic), and increasingly complex geopolitical landscape (e.g., the Russia-Ukraine war). In particular, seasonal demand is a unique characteristic for agrochemical supply chains. To design cost-effective, resilient, and well-managed agrochemical supply chains, in this work, we develop an optimization framework to effectively model the risks associated with these seasonality and uncertainties and propose a reformulation strategy to solve the optimization problem.

Among numerous recent works on supply chain optimization (Garcia and You, 2015), Bassett and Gardner (2009) presented one of the first mixed-integer linear programming (MILP) formulations for global agrochemical supply chain optimization considering seasonality and uncertainties in customer demand. Liu and Papageorgiou (2012) extended the agrochemical supply chain optimization framework by modeling and comparing different plant expansion strategies. To further ensure continuous use and inactivity of warehouses for continuous periods of time, Brunaud et al. (2017) developed dynamic contract policy constraints for warehouses and incorporated them to the agrochemical supply chain model. In terms of quantifying uncertainties and risks, You et al. (2009) proposed a scenario-based two-stage stochastic linear programming framework and decomposition strategies for mid-term planning of multi-product supply chain under demand and freight rate uncertainties. Later, Carneiro et al. (2010) focused on the oil supply chain optimization problem, in which they incorporated Conditional Value-at-Risk (CVaR) as a risk assessment measure that quantifies the tail risk in their investment portfolio. In this work, we develop a scenario-based two-stage mixed-integer nonlinear programming (MINLP) model for global agrochemical supply chain optimization and adopt the concepts of Value-at-Risk (VaR) and CVaR to quantify and control the risks associated with demand unfulfillment. Note that these risk measures are highly nonlinear. Therefore, we introduce perspective cuts to linearize the CVaR constraint and reformulate the MINLP model. Perspective cuts were first introduced by Frangioni and Gentile (2006), who showed that the convex envelope of the objective function containing semicontinuous variables in a general mixed-integer program (MIP) is the perspective function of MIP's continuous part. More recently, Bestuzheva et al. (2021) extended perspective cuts to nonlinear constraints in MINLPs. Consider a MINLP with a linear objective function f: $\min f(x, y, z)$ subject to nonlinear constraints $g(x) \leq 0$, in which $y \in \Omega$, $z \in \{0,1\}^n$, and $x \in \mathbb{R}^n$ are semi-continuous variables (for every $i = 1, \cdots, n$, $x_i = 0$ when $z_i = 0$ and $x_i \in [l, u]$ when $z_i = 1$). The perspective cuts for linearizing nonlinear constraints $g(x) \leq 0$ are given by:

$$\langle \nabla g(\bar{x}), x \rangle + [g(\bar{x}) - \langle \nabla g(\bar{x}), \bar{x} \rangle] z \leq 0 \tag{1}$$

where $\bar{x} \in [l, u]$ is an arbitrary parameter. After replacing $g(x) \leq 0$ with these perspective cuts, the MINLP is reformulated to a MILP, which can be solved iteratively. Specifically, starting from the second iteration, $\bar{x}$ is chosen to be the solution of the MILP from the previous iteration. Bestuzheva et al. (2021) also conducted a detailed computational study of perspective reformulation for MINLPs with convex and nonconvex nonlinear constraints. They showed that the perspective reformulation of convex MINLPs provides much tighter approximation of the original problems compared to conventional branch-and-cut approaches, thereby leading to significant computational time reduction. Nevertheless, they also reported that adding perspective cuts for nonconvex MINLPs had less impact on computational time, although it reduces the size of branch-and-cut trees and strengthens the root node relaxation.

2. Problem Statement and Model Formulation

In this illustrative case study, we consider the three-echelon supply chain of one active ingredient (AI) produced in an agrochemical company involving five AI production plants, four warehouses/distribution centers, and three market regions. We are interested in midterm planning (1 year) divided into 52 periods (i.e., 1 week per period). AI production plants and warehouses are connected by one or more transportation links, and so are warehouses and market regions. We allow different types of transportation modes for each transportation link. AI production plants can either be active or inactive during each time period. The manufacturing capacity of an AI production plant can be expanded at most once in a year. During the expansion period, AI production must be inactive. The AI produced can either be transported to warehouses or stored as inventory. The inventory level must be larger than or equal to the safety stock. As shown in Figure 1, the yearly demand of an agrochemical product typically follows a bimodal distribution (Bassett, 2018). For this case study, we consider three scenarios in customer demand. Also, we consider the risk of demand loss or unsatisfaction due to uncertainties related to production planning and warehouse capacity limitations. We are given the safety stock of an inventory, initial inventory, as well as unit costs associated with inventory holding, AI manufacturing and expansion, material transportation, warehouse storage and expansion, and demand loss or unsatisfaction (see Table 1). The objective function is to minimize the total cost of the supply chain. Due to space limitations, we only highlight some of the key points in our MINLP model:

1. Following You et al. (2009), decision variables of the first time period (Week 1) are first-stage variables and are independent of scenarios. Second-stage variables and scenario-based stochasticity begins at the second time period (Week 2).

2. We adopt the dynamic contract policy formulation from Brunaud et al. (2018) and extend it to AI production plants – Each AI production plant must remain in production for at least U time periods, after which it might undergo cleanup for F time periods, during which no production activities would take place:

$$\begin{gathered}
-\alpha_i + \alpha_i^{start} \geq 0, \qquad \forall i \in I \\
\alpha_{i,t-1}^s - \alpha_{i,t}^s + \alpha_{i,t}^{s,start} \geq 0, \qquad \forall i \in I, s \in S, t \in T(t > 1) \\
\alpha_i + \sum_{\tau=2}^{R} \alpha_{i,\tau}^s \geq U\alpha_i^{start}, \qquad \forall i \in I,\ \ s \in S \\
\sum_{\tau=t}^{t+R-1} \alpha_{i,\tau}^s \geq U\alpha_{i,t}^{s,start}, \qquad \forall i \in I,\ \ s \in S,\ \ t \in T(t > 1, t + R - 1 \leq |T|) \\
\alpha_{i,t+1}^s - \alpha_{i,t}^s + \alpha_{i,t}^{s,final} \geq 0, \qquad \forall i \in I,\ \ s \in S,\ \ t \in T \\
\sum_{\tau=t+1}^{t+F} \alpha_{i,\tau}^s + F\alpha_{i,t}^{s,final} \leq F, \qquad \forall i \in I,\ \ s \in S,\ \ t \in T(t + F \leq |T|)
\end{gathered} \tag{2}$$

where α_i, α_i^{start}, $\alpha_{i,t}^s$, $\alpha_{i,t}^{s,start}$, $\alpha_{i,t}^{s,final}$ are binary variables indicating whether the AI production plant $i \in I$ is in production (1) or not (0) at time period 1, starting at time period 1, at time period t under scenario s, starting at time t under scenario s, and ending at time t under scenario s respectively. $|T|$ is the total number of time periods.

3. The total demand loss χ_t^s for time period t under scenario s is the sum of demand loss from all market regions. To quantify the risks due to demand loss, we introduce the CVaR constraint in the model. We assume that the demand loss follows a normal distribution, which enables us to express VaR in terms of χ_t^s: $\mathrm{VaR}^s = \frac{\sigma^s z_\beta}{\sqrt{|T|}}$, where z_β

is z-score at confidence interval β, $|T|$ is the total number of time periods (i.e., 52), and $\sigma^s = \sqrt{\frac{1}{|T|-1}\left(\sum_{t\in T} {\chi_t^s}^2 - \frac{(\sum_{t\in T}\chi_t^s)^2}{|T|}\right)}$ is the standard deviation of the total demand loss as for scenario s. From VaR, we calculate CVaR as $\frac{1}{1-\beta}\sum_{s\in S} p_s \mathrm{VaR}^s$ following Carneiro et al. (2010), where p_s is the probability of scenario s. By specifying a lower bound P on CVaR (e.g., 30 mass units), we obtain the following CVaR constraint and add it into the formulation:

$$\mathrm{CVaR} = \frac{z_\beta}{(1-\beta)\sqrt{|T|(|T|-1)}}\sum_{s\in S} p_s \sqrt{\left(\sum_{t\in T} {\chi_t^s}^2 - \frac{(\sum_{t\in T}\chi_t^s)^2}{|T|}\right)} \geq P \qquad \forall s \in S, \tag{2}$$

4. Since Equation (2) is nonconvex and nonlinear, we introduce perspective cuts and reformulate the original MINLP into a MILP by substituting Equation (2) to Equation (1):

$$\left(P - R\sum_{s\in S} p_s Q_s - R\sum_{s\in S} p_s \frac{\bar{\chi}_t^s(\bar{\chi}_t^s - \frac{\sum_{t\in T}\bar{\chi}_t^s}{|T|})}{Q_s}\right) z_t - R\sum_{s\in S} p_s \frac{\chi_t^s\left(\bar{\chi}_t^s - \frac{\sum_{t\in T}\bar{\chi}_t^s}{|T|}\right)}{Q_s} \leq 0 \qquad \forall t \in T, \tag{3}$$

where $R := \frac{z_\beta}{(1-\beta)\sqrt{|T|(|T|-1)}}$, $Q_s := \sqrt{\left(\sum_{t\in T}(\bar{\chi}_t^s)^2 - \frac{(\sum_{t\in T}\bar{\chi}_t^s)^2}{|T|}\right)}$, $z_t \in \{0,1\}$, and $\bar{\chi}_t^s$ is the optimal demand loss from the previous iteration of introducing perspective cuts.

5. We point out that this is the first linearization of CVaR constraint reported in the literature. Both problems are solved using SCIP v8.0 in GAMS 40.2.0 in a Dell Precision 7920 workstation with Intel Xeon Gold 6226R CPU @ 2.90 GHz and 96 GB of RAM, and the results are compared.

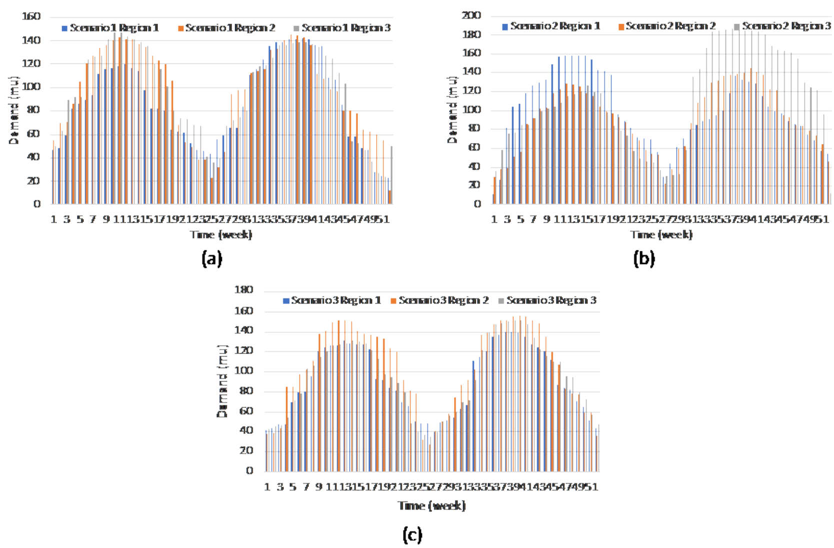

Figure 1. Bimodal demand curve for each market region under different scenarios.

Table 1. List of model parameters used in the illustrative case study.

Model parameters	**Values**
Initial capacity in each of the 5 AI production plants (mu)	100, 115, 100, 120, 110
Safety stock in each AI production plant (mu)	5, 5, 10, 10 ,5
Initial inventory level in each AI production plant (mu)	5, 5, 15, 0, 15
Transportation capacity from AI production plant to warehouse (mu)	400 for mode 1 350 for mode 2
Transportation capacity from warehouse to market region (mu)	100 for mode 3 200 for mode 4
Storage capacity in each of the 4 warehouses (mu)	550, 650, 500, 450
Initial inventory level in each warehouse (mu)	25, 20, 30, 10
Probability of the three possible scenarios	0.25, 0.45, 0.30
Fixed cost in each of the 5 AI production plants ($\times 10^3$ $)	75, 100, 150, 100, 75
Variable cost in each of the 5 AI production plants ($)	10, 15, 10, 5, 20
Expansion cost in each of the 5 AI production plants ($\times 10^3$ $)	10, 50, 25, 35, 15
Fixed transportation cost from AI production plant to warehouse ($)	25 for mode 1 30 for mode 2
Fixed transportation cost from warehouse to market region ($)	15 for mode 3 30 for mode 4
Variable transportation cost from AI production plant to warehouse ($/mu)	2 for mode 1 2.5 for mode 2
Variable transportation cost from warehouse to market region ($/mu)	1.5 for mode 3 2.5 for mode 4
Maximum total demand loss in each time period (mu)	15
Variable cost on demand loss ($/mu) for each of the 3 market regions	50, 55, 70

3. Discussion

The original MINLP model, which contains 9255 continuous variables and 1874 binary variables, has 14499 linear constraints and 2 nonlinear constraints of Equation (2) (one equality constraint and one inequality constraint). After the first iteration of adding perspective cuts, the reformulated MILP contains 14551 linear constraints (14499 linear constraints and 52 perspective cuts, each corresponding to one time period), 1874 binary variables, and 9254 continuous variables. We specify a solving time of 150 seconds, at which the original MINLP model has an objective function value of $\$1.509 \times 10^6$ and a gap of 2.39%, whereas the reformulated model shows an objective function value of $\$1.498 \times 10^6$ and a closer gap of 1.64%. We emphasize that the reformulated model always yields a feasible solution in the original formulation, suggesting that it provides a better optimal solution. This is due to the fact that the reformulated model is able to identify a solution with less overall demand loss $\sum_{s\in S}\sum_{t\in T}\chi_t^s$ compared to the solution obtained from the original MINLP. This suggests that the reformulated model produces a more efficient supply chain compared to the original model.

In a separate numerical study, we analyze the impact of problem size on the computational benefits of introducing perspective cuts. When we consider only 13 time periods (monthly) in the model, no significant computational speed improvement is observed in the reformulated model compared to the original MINLP. However, when considering 26 time periods (biweekly) in the model, the reformulated model solves to 1% gap in 29 seconds, whereas the original MINLP solves to the same objective function value as well as the same 1% gap in 41 seconds. This observation is consistent with that made by Bestuzheva et al. (2021), in the sense that the computational benefits of perspective cuts depend on the size of the problem. Perspective cuts should be accompanied by other reformulation strategies and bound-tightening constraints to maximize their benefits.

4. Conclusion

In this work, we optimize the supply chain of an agrochemical active ingredient by formulating and solving a scenario-based stochastic MINLP problem. The nonlinearity of the model comes from the CVaR constraint used to quantify risks associated with unforeseen demand loss. For the first time, we propose to reformulate the CVaR constraints using perspective reformulation techniques. The reformulated model, which is a MILP, always gives a feasible solution to the original MINLP model. Using a simple case study, we demonstrate the effectiveness of perspective cuts in fostering convergence and reducing computation time. In particular, we show that the reformulated model typically produces optimal solutions with less overall demand loss compared to the solution obtained from the original MINLP. Thus, adopting perspective reformulation could help identify a more efficient supply chain network and production/distribution plans with lower costs and carbon emissions. On the other hand, we point out that, depending on the problem size, adding perspective cuts for nonconvex MINLPs may not lead to significant computational time improvements. In this case, perspective cuts should be accompanied by other reformulation strategies and bound-tightening constraints to synergistically facilitate the solution of nonconvex MINLPs.

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