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Long-Range Process Planning under Uncertainty via Parametric Programming

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Abstract

Scenario analysis within a multi-stage stochastic programming formulation offers an attractive framework for modelling uncertainties in long-range planning models. However, whether the expected outcome is implicitly / explicitly evaluated, such formulations lead to computationally intensive optimization problems. Focussing here on the scenario planning / multi-period approach for mixed integer linear programming (MILP) problems under uncertainty, this paper presents a novel decomposition strategy for its solution. The proposed algorithm circumvents the direct solution of the large-scale deterministic equivalent MILP problem by exploiting its block-angular structure. Through the use of parametric programming, separable subproblems are formulated and solved in parallel at a relatively low computational cost. Computational studies show that the algorithm is ideally suited for problems where a large number of scenarios inhibits the direct solution of the deterministic equivalent problem.

Keywords: Strategic Planning, Long-Range Capacity Optimization, Parametric Programming, Two-Stage Stochastic Programming, Scenario Analysis.

1. Introduction

Typically, optimization problems under uncertainty pose considerable challenges in both conceptual formulation and numerical solution. Within the area of long-range planning and strategic enterprise design, a number of contributions have been made towards solution algorithms for these types of optimization problems. Especially plant location and capacity planning models under uncertainty have received considerable attention, where in most applications stochastic programming with recourse has evolved as the preferred framework (Kall and Wallace, 1994; Sahinidis, 2004). In its most basic form, the two-stage stochastic programming problem with recourse groups decisions into two sets. Certain decisions must be made at present in the face of uncertainty (*first-stage*), while others can be taken as corrective recourse actions at a later stage based on the information that becomes available after uncertainties are revealed (*second-stage*). Often the second-stage decisions are seen as the *operational* measures that need to be taken to prevent any infeasibilities that may occur due to the realization of a specific uncertainty, with the goal being to choose the first stage *design* / *structural* variables in

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such a way that the sum of the first stage costs and the expected value of the second-stage costs is minimized.

In the scenario planning / multi-period approach, the uncertainties are captured as a set of discrete scenarios, each describing a different realization of the stochastic quantities (Ierapetritou et al., 1996, Clay and Grossmann, 1997; Ahmed and Sahinidis, 1998; Tsiakis et al., 2001). Also, each scenario has a relative probability of occurring (often derived from probability distribution functions if available), allowing the expectancy over all foreseen scenarios to be evaluated. The objective is then to find a robust network design and production plan that assures feasible operation over all scenarios. Its major advantage is that the discretization of the uncertainty into a number of scenarios allows the *stochastic* problem to be reformulated as a *deterministic equivalent* problem which can be solved directly using standard optimization techniques. However, while this offers an attractive modelling framework, its applicability is limited, since a large number of scenarios inevitably results in a large-scale deterministic problem that can be difficult to solve directly.

Despite the computational challenges, many applications in strategic planning are ideally suited for such an approach, since many of the unforeseen future market conditions can be naturally modelled as discrete scenarios. The increasing power of modern computing technologies has also facilitated the use of scenarios for strategic planning under uncertainty (Vladimirou and Zenios, 1997).

In this paper, a new algorithm is proposed for solving scenario analysis (multi-period) problems within two-stage stochastic programming formulations. The algorithm exploits the special block-angular structure of the recourse problem, thereby circumventing the direct solution of the large-scale deterministic equivalent problem. By using parametric programming, separable subproblems are formulated and solved in parallel at a relatively low computational cost. This allows analytical profiles to be obtained for each scenario, representing the second stage recourse actions as functions of the common first stage decisions.

2. The Scenario Planning Problem

Derivation of the scenario planning problem as a special case of the general two-stage stochastic programming problem requires firstly the approximation of the uncertain vector as a discrete and finite probability distribution according to a set of scenarios, $k \in \mathcal{K} := \{1,2,\ldots,NK\}$. This allows a one-to-one corresponds between any scenario and the uncertainty realization, $\omega^k \in \Omega := \{\omega^1,\omega^2,\ldots,\omega^{NK}\}$. A probability, p^k, is also assigned to the likelihood of scenario k occurring such that $p^k > 0$, for all $\omega^k \in \Omega$, and that $\Sigma_k\, p^k = 1$. For each scenario, a different recourse decision, y^k, must be determined. The expected cost of taking this recourse is then the weighted average of these decisions over all scenarios. Under this simplification, the general two-stage stochastic programming problem is reformulated into a large-scale *deterministic equivalent* problem (DEP). Typically, first-stage "*here-and-now*" variables can be either continuous, x_1 (for example, total available capacities), or binary, , x_2 (for example, whether capacity should be expanded or not), while second-stage "*wait-and-see*" variables, y^k (for example, production rates) are restricted to the continuous domain. With the use of scenarios, the stochastic two-stage recourse problem is translated into an embedded mixed integer linear programming (MILP) problem that can be solved (in principle) directly using standard techniques for deterministic optimization. In most cases, though, the large number of scenarios inhibits its direct solution of the DEP:

$$\begin{aligned}
\min_{x_1,x_2,y^k} \quad & c_1^T x_1 + c_2^T x_2 + \sum_{k=1}^{NK} p^k q(\omega^k)^T y^k \\
\text{st}: \quad & A_1 x_1 + A_2 x_2 \le b \\
& T_1(\omega^k)x_1 + T_2(\omega^k)x_2 + W(\omega^k)y^k \le h(\omega^k), \qquad \forall k \in \mathcal{K} \\
& 0 \le x_1 \le u^{x_1} \\
& 0 \le y^k \le v^y, \qquad \forall k \in \mathcal{K} \\
& x_1 \in \Re^n,\ x_2 \in \{0,1\}^m,\ y \in \Re^l
\end{aligned} \tag{1}$$

with its block-angular structure being highlighted in a compact matrix representation:

$$\begin{pmatrix} A & & & & \\ T(\omega^1) & W(\omega^1) & & & \\ T(\omega^2) & & W(\omega^2) & & \\ \vdots & & & \ddots & \\ T(\omega^k) & & & & W(\omega^{NK}) \end{pmatrix} \begin{pmatrix} x \\ y^1 \\ y^2 \\ \vdots \\ y^{NK} \end{pmatrix} \le \begin{pmatrix} b \\ h(\omega^1) \\ h(\omega^2) \\ \vdots \\ h(\omega^{NK}) \end{pmatrix} \tag{2}$$

While the problem size of the DEP increases linearly with the number of scenarios and can, therefore, pose a significant computational challenge to solve directly, its special structure can readily be exploited through decomposition methods. Under a given set of first stage decisions, the problem decomposes into a set of *NK* scenario-specific separable subproblems. More specifically, for the special case where binary decisions do not occur in the second stage, these subproblems are linear programming (LP) problems of relatively low computational effort which can be solved in parallel (Vladimirou and Zenios, 1997).

3. Algorithmic Steps

Step 1: Parametric Programming Scenario Decomposition

Based upon this insight, the DEP can be decomposed into a set of scenario specific multi-parametric linear programming problems (SSmpLP) by decoupling the first stage variables through substitution with parameters, $x_1 \Rightarrow \theta_1$, $x_2 \Rightarrow \theta_2$:

$$\begin{aligned}
\forall k \in \mathcal{K}: \ \Phi^k(\theta_1,\theta_2) = \min_{y^k} \quad & q^T y^k \\
\text{st}: \quad & W(\omega^k)y^k \le h(\omega^k) - T_1(\omega^k)\theta_1 - T_2(\omega^k)\theta_2 \\
& \theta_1 \in [0, u^{x_1}],\ \theta_2 \in [0,1] \\
& 0 \le y^k \le v^y \\
& y \in \Re^l
\end{aligned} \tag{3}$$

Since the *NK* scenario specific problems are completely independent in the absence of the first stage variables, their solutions can be obtained irrespective of each other at a relatively low computational burden through recent developments in multi-parametric programming (Dua et al., 2002). More importantly, because the subproblems are separable and no non-anticipativity (linking) constraints are required, parallel computing can be employed to further reduce the solution time.

The solution of each `SSmpLP` is a unique set of piecewise linear convex parametric profiles, $\phi^k_i(\theta_1,\theta_2)$, and a set of corresponding *critical regions*, $i \in \mathcal{I}^k := \{1,2,\ldots,N_{reg}{}^k\}$. Each region is defined by a set of constraints, $CR^k{}_i$, over which each profile is valid. The variables describing these profiles in each region are expressed as a function of the parameters, *i.e.* $y^k_i(\theta_1,\theta_2)$. Recalling that the parameters are merely a substitution of the original first stage variables, it can be noted that the solution of each `SSmpLP` provides a set of profiles of the second stage variables in terms of the first stage variables, *i.e.* $y^k_i(x_1,x_2)$.

Step 2: Aggregation

Next, the individual solutions of the decomposed subproblems are aggregated together into a reduced formulation of the original deterministic equivalent problem. This is achieved by aggregating the scenario-specific parametric profiles of (3) and re-introducing the weighted probabilities of each scenario. First, θ_1 & θ_2 are substituted with x_1 & x_2 respectively in the parametric profiles, *i.e.* $y^k_i(\theta_1,\theta_2) \Rightarrow y^k_i(x_1,x_2)$. These profiles are then re-introduced into the original recourse problem (`DEP`). Finally, the objective function is modified to include the minimization of the piecewise linear parametric profiles through the introduction of a scenario-specific numerical variable, ε^k. This leads to the reduced form of the original deterministic MILP (`rDEP`):

$$\begin{aligned}
\chi = \min_{x_1,x_2,\epsilon^k} \quad & c_1^T x_1 + c_2^T x_2 + \sum_{k=1}^{NK} p^k \epsilon^k \\
\text{st}: \quad & A_1 x_1 + A_2 x_2 \le b \\
& \epsilon^k \ge q^T y_i^k(x_1,x_2), \qquad \forall i \in \mathcal{I}^k, \ \ \forall k \in \mathcal{K} \\
& 0 \le x \le u^x \\
& x_1 \in \Re^l, \ \ x_2 \in \{0,1\} \qquad\qquad (4)
\end{aligned}$$

An exact solution to the original problem can, therefore, be obtained through a reformulation that has a reduced number of decision variables. Only the first stage decision variables together with one additional variable per scenario constitute the decision space of `rDEP`.

Step 3: Recourse Action Look-Up (Post-Processing)

With the original set of second stage variables being omitted, it is necessary to perform a post-processing step to arrive at the optimal values of the recourse actions. Within each scenario set of $\varepsilon^k \ge q^T y^k_i(x_1,x_2), \ \forall\, i \in \mathcal{I}^k$ constraints, at least one constraint will be active. Since each constraint within a specific scenario realization corresponds to a particular critical region of its `SSmpLP` solution, the active constraint indicates in which particular critical region the solution of the first stage variables lies. Using the expressions of the critical regions as *look-up tables*, the scenario specific recourse actions are merely calculated through substitution of the optimal first stage decisions into the parametric profiles.

4. Parallelization & Software Implementation

Implementation of the algorithm is performed using MATLAB (The Mathworks Inc., 2000) running on the Linux Operating System. Each scenario specific multi-parametric programming problem is solved using the ParOS Ltd POP software written for MATLAB (Ross, 2003). Parallelization of the scenario specific problems is managed using the Sun Grid Engine software (Sun Microsystems Inc., 2002), submitted onto a cluster of 60 Pentium 4 machines with 1.8, 2.4 and 3.0 GHz processors. The final aggregation problem is solved using Cplex 7.5 (ILOG, 2002).

5. Application: Long-Range Capacity Planning under Uncertainty

The classical long-term capacity expansion and production planning problem with fixed-charge expansion costs tries to determine from a given extended network of continuous production processes and chemicals the optimum selection of processes and how their capacities should be expanded over a future horizon. Over this planning horizon, the demands, availabilities and prices of the chemicals are forecasted as stochastic quantities, while the process capital investment and operating costs and expansion bounds are deterministically known. Because of the presence of uncertainty in the forecasted market conditions, the expected demands, availabilities and prices of the chemicals are predicted according to a set of scenarios. In the absence of knowing the uncertainty, the strategic process selection and capacity planning decisions have to be made in the *first stage*, irrespective of the which scenario occurs. However, the production rates of the processes and the amounts of chemicals purchased and sold can be manipulated in the *second stage* to best satisfy the market conditions revealed under each scenario. The objective is to find the appropriate capacity plan to implement at the present time that maximizes the expected profit while still ensuring feasible plant operations over all the uncertain future realizations. The decision whether an expansion should take place or not is modelled through the use of a binary variable. The model is, therefore, formulated as a MILP problem.

The production network that will be used to illustrate the application of the algorithm to the stochastic capacity expansion problem is shown in Figure 1 and consists of 3 processes, 3 chemicals and 4 time periods - taken from Iyer and Grossmann (1998). Considering that the prices and demands/availabilities of each chemical can be forecasted as 2 possible outcomes, 64 unique scenario permutations representing the different realizations can be constructed. Table 1 contains a break-down of the solution via the decomposition algorithm. Other detailed examples and computational statistics can be found in Hugo (2005).

6. Conclusions

In this paper a new decomposition algorithm has been presented for the solution of two-stage stochastic programming problems that use scenario analysis to model uncertain expectations. The specific class of problems addressed by the algorithm is commonly found in long-range strategic process planning under uncertainty. The motivation behind developing the algorithm has been the realization that when using a large number of scenarios the problem becomes computationally intensive. It has, therefore, been proposed that the decomposition of the large-scale deterministic equivalent MILP problem into smaller multi-parametric LP's and their subsequent aggregation, pose a smaller computational challenge than solving the problem directly in its entirety.

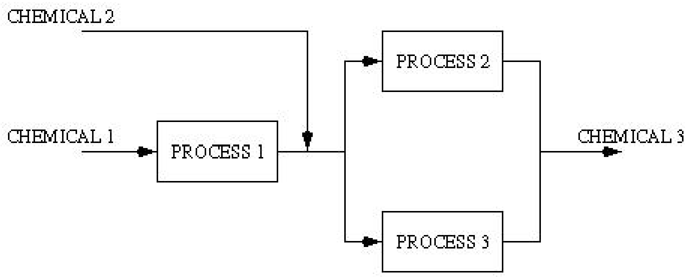

Figure 1. Capacity Planning Example

Table 1. Computational Statistics of the Capacity Planning Example

Step 1: Problem `SSmpLP` x 64		Step 2: Problem `rDEP`	
# of Continuous Variables:	27	# of Continuous Variables:	82
# of Bounded Parameters:	9	# of Binary Variables:	9
# of Inequality Constraints:	54	# of Inequality Constraints:	21997
# of Equality Constraints:	9	# of Equality Constraints:	9
Longest Individual CPU Seconds:	1336	CPU Seconds:	7.94
Average # of Critical Regions:	343		

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