

Stochastic MINLP Optimisation using Simplicial Approximation

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Abstract

Mathematical programming has long been recognized as a promising direction to the efficient solution of design, synthesis and operation problems that can gain industry the competitive advantage required to survive in today's difficult economic environment. Most of the engineering design problems can be modeled as MINLP problems with stochastic parameters. In this paper a novel decomposition algorithm is presented to solve convex stochastic MINLP problems. The proposed approach is an extension of the *simplicial-approximation* approach proposed by Goyal and Ierapetritou, (Goyal and Ierapetritou, 2004a, 2004b), for solving deterministic MINLP problems and is based on the idea of closely approximating the feasible region defined by the set of constraints by an approximation of its convex hull. A case study is also presented illustrating the applicability and efficiency of the proposed approach.

Keywords: Simplicial Approximation, Stochastic MINLP; Sample average approximation.

1. Introduction

A large number of the chemical engineering problems require decisions to be made under uncertainty which is often further complicated by the presence of integer decision to model logical or discrete decisions resulting in stochastic mixed integer nonlinear problems. A traditional process design under uncertainty problem can be modeled as a stochastic MINLP (Acevedo and Pistikopoulos, 1998).

$$v^* = \min_{x,y,z} E_{\theta}[f(x,y,z,\theta)] \quad (I)$$

$$s.t. \quad g_j(x,y,z,\theta) \leq 0 \quad \forall j \in J, x \in X, z \in Z, \theta \in \Theta, y \in \{0,1\}^m$$

where y is a vector of binary 0–1 variables denoting the choice of the units, x a vector of design variables such as unit sizes, z a vector of control/state variables, which can vary to accommodate changes of uncertain parameters θ . The objective is commonly chosen to minimize the expected value of total cost or maximize the expected value of profit. The constraint set g_j includes mass balances, unit design/operating models, design/operating specifications, and logical constraints. The exact evaluation of the

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expected value is not possible and is often approximated through sample averaging. Several papers in literature have addressed the various issues of solving such problems including: (i) integration methods, and (ii) sampling methods. A comparison of the different methods is available in Acevedo and Pistikopoulos, (1996).

Sampling-based algorithms can be further categorized as approaches that follow either internal or external sampling. The internal sampling methods perform sampling within the algorithm with new i.i.d. samples generated and accumulated over iterations (Norkin et al., 1998). External sampling approaches, (sample average approximation (SAA)), approximate problem (I) by the sample average problem (Kleywegt et al., (2001):

$$\hat{v}_N = \min_{x,y,z_i} \frac{1}{N} \sum_{i=1}^N [f(x,y,z_i,\theta_i)] \quad (\text{II})$$

$$s.t. \quad g_j(x,y,z_i,\theta_i) \leq 0, i \in I_k; j \in J, x \in X, z \in Z, y \in \{0,1\}^m$$

where the subscript i corresponds to each of the generated sample point. Hence, once the sample points are generated, the stochastic problem becomes a deterministic one, which can be solved by existing deterministic algorithms. The optimality gap of the solution, estimated by the difference between an upper bound (the objective value at any candidate solution) and a lower bound (average of replicated solutions), has been used to determine convergence. The validity of this lower bound has been proven by Mak et al, (1999). Kleywegt et al., (2001), used a smaller sample size N to make decisions (with M replications) and a larger sample size N' to re-compute the objective value with the decisions fixed at the values obtained from solving the smaller problems. Recently Wei and Realff, (2004) used this idea and proposed a Sample Average Approximation (SAA) approach for the solution of convex MINLP problems. They combined the above results with the OA algorithm proposed by Duran and Grossmann, (1986) to obtain optimal solutions for convex stochastic MINLP problems.

The approach described in this paper utilizes the idea of simplicial-based approach proposed by Goyal and Ierapetritou, (2004a, 2004b) and the basic idea of SAA approach, for the solution of convex stochastic MINLP problems. In particular, at each iteration of the simplicial-based algorithm, the SAA procedure is applied to all NLP sub-problems and the MILP problem.

2. Proposed Approach

The proposed approach is based on the idea of closely approximating the feasible region by a set of linear constraints representing its convex hull. In summary, the convex hull approximation approach solves a series of line searches and linear programs to approximate the feasible region by a set of hyper-planes, representing its convex hull approximation. The objective function is then linearized at the simplicial boundary points. Using the linear representation of the feasible space and the linear approximation of the objective function, the global optimal solution is obtained by solving a single MILP followed by a NLP of the original problem with fixed binary variables. Detailed explanations of the steps of the algorithm are as follows:

Step 1: Relax the set of binary variables as $0 \leq y \leq 1$ and solve the resulting stochastic NLP to get a point inside the feasible region defined by the set of constraints.

To solve the stochastic optimization problems, the *Optimality Gap method (OGM)*, proposed by Wei and Realff, (2004) is utilized to obtain an optimal solution. In brief, the optimal solution of a stochastic NLP is obtained by iteratively solving the following series of sub-problems:

A smaller stochastic NLP (S-NLP) is solved M times, each at sample size N ;

A larger stochastic NLP (L-NLP) is solved at sample size N' with fixed continuous decision variables $\tilde{x}, \tilde{y}$.

$$\begin{aligned} \min_{x,y,z_i} \frac{1}{N} \sum_{k=1}^{N_k} [f(x,y,z_i,\theta_i)] \\ \text{s.t. } g_j(x,y,z_i,\theta_i) \leq 0 \quad \forall i \in I_k; \forall j \in J, x \in X, z \in Z, 0 \leq y \leq 1 \end{aligned} \quad (\text{S-NLP})$$

$$\begin{aligned} \min_{z_i} \frac{1}{N'_k} \sum_{k=1}^{N'_k} [f(\tilde{x},\tilde{y},z_i,\theta_i)] \\ \text{s.t. } g_j(\tilde{x},\tilde{y},z_i,\theta_i) \leq 0 \quad \forall i \in I'_k; \forall j \in J, z \in Z \end{aligned} \quad (\text{L-NLP})$$

(S-NLP) corresponds to a relaxation of problem (II) since the binary variables are relaxed ($0 \leq y \leq 1$). In the problem definitions above, different sample size N and N' are allowed at each iteration to enhance convergence. I_k and I'_k are the sets of the samples at the k^{th} iteration with sample size N_k and N'_k , respectively. In (L-NLP) the decision variables, $\tilde{x}, \tilde{y}$ are fixed at the solution of the (S-NLP). The convergence of the *OGM* is

explained as follows. If v^* is the optimal solution to a stochastic optimisation problem (I) and $\hat{v}_N$ denotes the optimal solution of the approximation problem (II) with sample size N , Mak et al., (1999) have shown that, $E[\hat{v}_N] \leq v^*$. Hence, a statistical lower estimate for true optimal value v^* is the expected value of the replicated SAA solutions,

which can be estimated by: $\bar{v}_{N,M} = \frac{1}{M} \sum_{m=1}^M \hat{v}_N^{(m)}$ where $\bar{v}_{N,M}$ denotes the average of

the M replicated solutions $\hat{v}_N^{(m)}$ ($m=1,...,M$), each with sample size N . The variance of the replicated solutions is denoted by the following

expression: $\frac{(\hat{S}_{N,M})^2}{M} = \frac{1}{M(M-1)} \sum_{m=1}^M (\hat{v}_N^{(m)} - \bar{v}_{N,M})^2$. So, the $(1-\alpha)$ confidence

interval of the lower estimate is $\bar{v}_{N,M} \pm t_{(M-1),(\alpha/2)} \frac{\hat{S}_{N,M}}{\sqrt{M}}$ where t is the Student's

t -test with $M-1$ degrees of freedom and $1-\alpha$ confidence level. Similarly, variance of the solutions for the upper estimate is denoted by:

$\frac{(\hat{S}_{N'})^2}{N'} = \frac{1}{N'(N'-1)} \sum_{i=1}^{N'} (\hat{f}_i - \hat{v}_{N'})^2$ where $\hat{v}_{N'}$ is the approximation solution of the

L-NLP with fixed decision variables. Then, a $(1-\alpha)$ confidence interval for the upper

estimate is: $\hat{v}_{N'} \pm t_{(N'-1),(\alpha/2)} \frac{\hat{S}_{N'}}{\sqrt{N'}}$. Combining the confidence intervals of the

lower and upper estimates, the confidence interval of the optimality gap is obtained as:

$$\left(0, \hat{v}_{N'} - \bar{v}_{N,M} + t_{(M-1),(\alpha/2)} \frac{\hat{S}_{N,M}}{\sqrt{M}} + t_{(N'-1),(\alpha/2)} \frac{\hat{S}_{N'}}{\sqrt{N'}} \right)$$

The iterative process is thus carried out by increasing the sample size N , M and N' , until the gap and the variance of the gap are sufficiently small. In the proposed approach, tolerance is defined as, γv_{mean} , where γ is a small number between 0 and 1, and v_{mean} is the optimal value of the deterministic problem at the mean values of uncertain parameters.

Step 2: Using the solution obtained at step 1, perform the convex-hull approximation approach over the bounded feasible region to determine the equations of the outer-hull that approximate the feasible region. Details of the approximation approach are available in Goyal and Ierapetritou, 2004a.

Step 3: Linearize the objective function around the simplicial-boundary points obtained at step 2.

Step 4: Using the linear representation of the feasible region and the linearized objective function, a stochastic MILP (SAA-MILP; linear representation of the MINLP) is solved to determine the optimal set of binary variables for the MINLP.

$$\begin{aligned} \min_{x,y,z_i} \quad & \mu \\ \mu \geq \quad & \frac{1}{N} \sum_{k=1}^{N_k} \left(f(x_k^*, y_k^*, z_{i,k}^*, \theta_i) + \nabla f(x_k^*, y_k^*, z_{i,k}^*, \theta_i) \begin{bmatrix} x - x_k^* \\ y - y_k^* \\ z_i - z_{i,k}^* \end{bmatrix} \right), \quad k = 1, \dots, K \end{aligned} \quad (\text{SAA-MILP})$$

$$\text{s.t.} \quad \left(g_j(x_k^*, y_k^*, z_{i,k}^*, \theta_i) + \nabla g_j(x_k^*, y_k^*, z_{i,k}^*, \theta_i) \begin{bmatrix} x - x_k^* \\ y - y_k^* \\ z_i - z_{i,k}^* \end{bmatrix} \right) \leq 0, \quad k = 1, \dots, K; \forall i \in I_k; \forall j \in J$$

where the first set of constraints is the linearization of the objective function at the simplicial-boundary points and the second set of constraints denote the convex hull approximation cuts. The stochastic MILP is solved using the (OGM). The optimal solution of the stochastic MILP is obtained by iteratively solving a series of S-MILP/L-MILP until convergence is achieved.

Step 5: Fix the set of binary variables at the values obtained at step 4 and solve the final convex stochastic NLP to determine the set of continuous variables. The set of binary and continuous variables, obtained at steps 4 and 5 correspond to the optimal solution set.

Thus, the overall proposed approach integrates the OGM, into the deterministic simplicial-based approximation approach to allow the solution of the required stochastic NLP/MILP problems. It is important to note that the overall proposed approach requires the solution of two stochastic NLP problems, line searches and just one stochastic MILP problem for overall convergence as compared to the SAA-algorithm proposed by Wei

and Realff, (2004) which require the solution of a stochastic NLP/MILP at each iteration.

3. Case Study

In this section, the process synthesis/planning problem examined by Acevedo and Pistikopoulos, (1998), is considered to illustrate the efficiency of the proposed approach. The problem is modelled using GAMS with CONOPT and CPLEX as the NLP and MILP solver, respectively, and solved on a Dell 733MHz PC with Linux operating system.

Table 1. Case Study Parameters

Process k	1	2	3	4	5	6	7	8	9	10	11
PC _k	13	15	17	14	10	15	16	11	13	15	17
K _k	1.0	1.2	1.7	1.5	1.8	1.4	1.5	1.3	1.1	1.2	1.8
MI _k	18	20	15	20	20	21	15	15	25	15	20
OC _k	400	400	400	400	400	400	400	400	400	400	400
DC _k	2500	2500	2500	2500	2500	2500	2500	2500	2500	2500	2500
FC _k	4000	2500	3500	3000	4500	2500	3000	2200	2800	2700	2500
Q_k^{max}	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0	3.0
α_j	600		650	500		400		700			
D_i, RM_j^{max}	Normal Distribution ~ N(30,1.5), 25.5≤ D _i ≤34.5, N(35,1.5), 29.5≤ RM _j ^{max} ≤ 40.5										
β_i	200		320	230		250		300			

The problem involves the production of five products from five raw materials with 11 processes (Figure 1). The uncertain parameters are the maximum availabilities of raw materials, RM_j^{max} and demands for products, D_i , (i.e. 10 uncertainty parameters). The problem parameters are given in Table 1. The continuous decision variables are the capacities for the processes, Q_k . The mathematical model for the problem is as follows:

$$Objective : \max_{\theta} E \left[\sum_{i=1}^5 \beta_i P_i - \sum_{j=1}^5 \alpha_j RM_j - \sum_{k=1}^{11} OC_k IS_k \right] - \sum_{k=1}^{11} [DC_k Q_k + FC_k y_k]$$

$$1. Yield Relations: OK_k \leq PC_k \ln(1 + \frac{IS_k}{K_k}), \quad k = 1, \dots, 11$$

$$2. Desired Production: P_i \leq D_i, \quad i = 1, \dots, 5$$

$$3. Raw Material Availability: RM_j \leq RM_j^{max}, \quad j = 1, \dots, 5$$

$$4. Logical Constraints: IS_k \leq MI_k Q_k, \quad k = 1, \dots, 11$$

$$QS_k \leq y_k Q_k^{max}, \quad k = 1, \dots, 11$$

5. Material Balances Around Each Unit

where D_i is the uncertain demand of product i ; DC_k , FC_k and OC_k are the design, fixed and operating cost respectively for process k ; IS_k and OS_k are the input and output flow rates; α_j is the raw material cost; β_i is the price of product i ; MI_k and K_k are yield

parameters whereas y_k is a binary variables denoting the existence of process k . All the 10 uncertain parameters are assumed to follow normal distribution with: $D_i \sim N(30,1.5)$ and $RM_j^{\max} \sim N(35,1.5)$. The Hammersley Sequence Sampling (HSS) technique developed by Kalagnanam and Diwekar, (1997), has been utilized to generate the required samples. The problem was solved using the proposed stochastic simplicial approximation approach with $M=20$, $N=200$, $N'=1000$ and $\varepsilon=0.001$ for the convex-hull approximation step. Two simplicial iterations were required for convergence of the convex-hull approximation step and the overall approach requires 1840.6 CPU sec to converge to the optimal solution of $y_k = (0001011111)$ and a cost of \$30,840. The stochastic MILP converged with an optimality gap of 0.11% whereas the final stochastic NLP, obtained after fixing the binary variables, converged with a gap of 0.23%, both of which were within the tolerance level. To compare the optimal solution, the original MINLP was also solved with a large number of samples, $N=2000$ using GAMS/SBB and converged to the same optimal solution after 4 hours, illustrating the efficiency of the proposed approach.

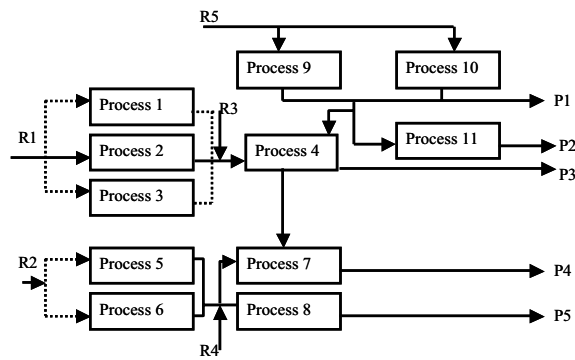


Figure 1. Process flow sheet for the case study

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Acknowledgements

The authors gratefully acknowledge financial support from the National Science Foundation under the NSF CAREER award CTS-998340 and CTS-0224745.