

One-Stage Optimization Problem with Chance Constraints

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The one-stage optimization problem with chance constraints is considered. This problem is aroused by chemical processes design under uncertainties. We develop methods of solving the one-stage optimization problem with chance constraints based on transformation of a problem with chance constraints into a problem with deterministic constraints.

1. Introduction

We consider a problem of a chemical process (CP) design in the case of the presence of uncertainty in the process models. During chemical process design some design specifications (constraints) must be satisfied. Some of these are as follows:

- i) The specifications connected with safety of the CP.
- ii) Ecological specifications are the second type of specifications. The CP must be environmentally benign. One way to achieve this is to impose constraints on the maximum effluent flowrates of hazardous chemicals.
- iii) Performance targets in the CP (such as conversion in a catalytic reactor) are design specifications.

CP performance is estimated by some measure which includes the capital and operating costs. It can be a cost, revenue, product yield. Our goal is to minimize the cost of CP, which consists of the capital and operating costs (that include energy expenditures). The satisfaction of the design specifications is complicated by the presence of an uncertainty in the process models. Therefore, in process design we are forced to use inexact process models. Thus during CP design we must solve the following problem: it is necessary to find such values of the design and control variables under which some measure of the CP performance takes the minimal or maximal value and the design specifications are met with some probability. The mathematical formulation of this problem is of the form

$$\min_{d,z} E_{\theta} \{f(d,z,\theta)\} \quad (1)$$

$$\Pr\{g_j(d,z,\theta) \leq 0\} \leq \alpha_j, \quad j = 1, \dots, m, \quad (2)$$

where d is a vector of the design variables, z is a vector of the control variables, θ is p -vector of uncertain parameters, $f(d, z, \theta)$ is a goal function

$$\Pr\{g_j(d, z, \theta) \leq 0\} = \int_{\Omega_j} \rho(\theta) d\theta$$

$$\Omega_j = \{\theta : g_j(d, z, \theta) \leq 0, \theta \in T\}. \quad (3)$$

$\Pr\{g_j(x, \theta) \leq 0\}$ is the probability measure of the region Ω_j and α_j is a probability level. Problem (1) is the problem of finding a trade-off between the problems of minimization of CP cost and minimization of environment pollution. Indeed, if we increase the values α_j (the probability of satisfaction of the constraints) we diminish possible effluent flowrates of hazardous chemicals. However, one can prove that an increase of the values α_j worsens the optimal value of the objective function (particularly, energy expenditures) i.e. increases the price of CP and vice versa. Problem (1) is the one-stage optimization problem (OSOP) with chance constraints.

The main issue in solving the one-stage optimization problems is the calculation of multiple integrals that give expected value of the objective function and probability of constraints satisfaction. The use of the standard Gaussian quadrature for the calculation of multiple integrals is very intensive computationally even for small dimensionality of vector θ of the uncertain parameters. In connection with this the problem of simplification of a multidimensional integrals calculation is very important. One can note three groups of methods in which this problem is considered. The methods which improve the Gauss quadrature belong to the first group (Bernardo et al, 1999, Pintaric and Kravanja, 2004, Wey and Realf, 2004). The methods in which the sampling techniques (Monte-Carlo, Latin Hypercube or Hammersley Sequence Sampling - HSS) (Bernardo and Saraiva, 1998, Diwekar and Kalagnanam, 1997) are used belong to the second group. Diwekar and Kalagnanam (1997) have shown that the HSS technique is more efficient than other sampling techniques. Unfortunately, even the HSS technique requires several hundred approximation points to obtain a reasonable accuracy.

Methods permitting to transform chance constraints into deterministic ones belong to the third group. Li et al. (2008) developed method permitting to transform chance constraints into deterministic ones. It is based on the use of a monotone relationship between a constrained output and one of the uncertain parameters. Unfortunately, it is very difficult to prove that this property holds in process models of real processes. Besides, some process models do not have this property. We will develop a new method based on the approximate transformation of the chance constraints into deterministic ones. This permits to diminish significantly computational time of solving OSOP with chance constraints.

2. Approximate method of solving the TSOP with chance constraints

Transform problem (1). Consider some region T_{α_j} , which has the following property

$$\Pr\{\theta \in T_{\alpha_j}\} \geq \alpha_j \quad (4)$$

Condition (4) means that the probability measure of the region T_{α_j} is equal to α_j . It should be noted that, generally speaking, condition (4) determines not single region but some infinite set of regions. Designate this set by T_{α_j} . Consider the following constraint

$$\max_{\theta \in T_{\alpha_j}} g_j(d, z, \theta) \leq 0, \quad (5)$$

where T_{α_j} is one of the regions from the set T_{α_j} . If constraint (5) is met then the constraint $g_j(d, z, \theta) \leq 0$ is met at each point of the region T_{α_j} . Since a probability measure of the region T_{α_j} is at least α_j then the probability of satisfaction of the constraint $g_j(d, z, \theta) \leq 0$ is at least α_j . Consequently, constraint (2) can be substituted with the constraints (4), (5). Hence, problem (1) can be rewritten in the following form

$$f^* = \min_{d, z, T_{\alpha_j}} E[f(d, z, \theta)] \quad (6)$$

$$\max_{\theta \in T_{\alpha_j}} g_j(d, z, \theta) \leq 0, \quad j = 1, \dots, m$$

$$\Pr\{\theta \in T_{\alpha_j}\} \geq \alpha_j, \quad (7)$$

Unfortunately it is very difficult to look for the optimal form and location of the region T_{α_j} . Therefore, we will restrict the class of possible regions T_{α_j} and look for the optimal region in the form of a multidimensional rectangle. In connection with this we will consider two cases in which form of regions T_{α_j} will be given.

Case 1: The uncertain parameters θ_i , $i = 1, \dots, p$, are independent, random variables having the normal distribution $N_1[E[\theta_i], \sigma_i]$ where $E[\theta_i]$ is the expected value of the parameters θ_i . In this case we will suppose that the regions T_{α_j} have a form of a multidimensional rectangle

$$T_{\alpha_j} = \{\theta_i : \theta_i^{L,j} \leq \theta_i \leq \theta_i^{U,j}, i = 1, \dots, p\}, \quad (8)$$

where $\theta_i^{L,j}, \theta_i^{U,j}$ are upper and lower bounds of sides of the multidimensional rectangles T_{α_j} . In this case the uncertainty region has the form (8), where the values θ_i^L, θ_i^U , $i = 1, \dots, p$, have the following form: $\theta_i^L = E[\theta_i] - k_i \sigma_i$, $\theta_i^U = E[\theta_i] + k_i \sigma_i$ and k_i are some large enough coefficients. In this case the search of the optimal forms and locations of the regions T_{α_j} is reduced to the search of the optimal upper and lower bounds $\theta_i^{L,j}, \theta_i^{U,j}$ of the sides of the multidimensional rectangles T_{α_j} . Since all the parameters θ_i are independent and have the normal distribution then the probability

measure of the multidimensional rectangle T_{α_j} is equal to multiplication of the probability measures of the intervals $I_i^j = \{\theta_i^{L,j} \leq \theta_i \leq \theta_i^{U,j}\}$. Thus, we have

$$\Pr\{\theta \in T_{\alpha_j}\} = \prod_{i=1}^p [\Phi(\tilde{\theta}_i^{U,j}) - \Phi(\tilde{\theta}_i^{L,j})] \quad , \quad (9)$$

where $\Phi(\eta)$ is the standard normal distribution function and $\tilde{\theta}_i^{L,j}, \tilde{\theta}_i^{U,j}$ have the following form

$$\tilde{\theta}_i^{L,j} = (\theta_i^{L,j} - E[\theta_i])\sigma_i^{-1}, \quad \tilde{\theta}_i^{U,j} = (\theta_i^{U,j} - E[\theta_i])\sigma_i^{-1}.$$

Replace $\Pr\{\theta \in T_{\alpha_j}\}$ in condition (7) by its expression from (9). Then problem (6) takes the form

$$\bar{f} = \min_{d,z,\theta_i^{L,j},\theta_i^{U,j}} E[f(d,z,\theta)], \quad (10)$$

$$\max_{\theta \in T_{\alpha_j}} g_j(d,z,\theta) \leq 0, \quad j=1,\dots,m, \quad (11)$$

$$[\Phi(\tilde{\theta}_1^{U,j}) - \Phi(\tilde{\theta}_1^{L,j})] \dots [\Phi(\tilde{\theta}_p^{U,j}) - \Phi(\tilde{\theta}_p^{L,j})] \geq \alpha_j, \quad j=1,\dots,m,$$

where the regions T_{α_j} are defined by the formulae (8). Problem (10) is the semi-infinite programming problems. For its solving one can use the outer approximation algorithm (Hettich and Kortanek, 1993).

For approximate calculation of the expected value of the function $f(d,z,\theta)$ we will use the iteration procedure based on partition of the region T . Let at the k -th iteration the region T consist of Q_k subregions $T_q^{(k)}, q=1,\dots,Q_k$. For an approximate calculation of the expected value of the function $f(d,z,\theta)$ we will use piecewise linear approximation of the function $f(d,z,\theta)$. For this at each subregion $T_q^{(k)}$ we will replace the function $f(d,z,\theta)$ by its linear approximation

$$\bar{f}(d,z,\theta,\theta^q) = f(d,z,\theta^q) + \sum_{i=1}^p (\partial f(d,z,\theta^q)/\partial \theta_i)(\theta_i - \theta_i^q). \quad (12)$$

where $\theta^q \in T_q^{(k)}$. Then one can show that some approximation $E_{ap}[f(d,z,\theta);T]$ of the expected value of the function $f(d,z,\theta)$ can be represented in the following form

$$E_{ap}[f(d,z,\theta);T] = \sum_{q=1}^{Q_k} (a_q f(d,z,\theta^q) + \sum_{i=1}^p (\partial f(d,z,\theta^q)/\partial \theta_i)(E[\theta_i;T_q^{(k)}] - a_q \theta_i^q)) \quad (13)$$

where

$$a_q = \int_{T_q^{(k)}} \rho(\theta) d\theta = [\Phi(\tilde{\theta}_1^{U,q}) - \Phi(\tilde{\theta}_1^{L,q})][\Phi(\tilde{\theta}_2^{U,q}) - \Phi(\tilde{\theta}_2^{L,q})] \dots [\Phi(\tilde{\theta}_p^{U,q}) - \Phi(\tilde{\theta}_p^{L,q})],$$

$$E[\theta_i; T_q^{(k)}] = \int_{T_q^{(k)}} \theta_i \rho(\theta) d\theta = I_1^{i-1} \left(\int_{\theta_i^{L,r}}^{\theta_i^{U,r}} \theta_i \rho(\theta_i) d\theta_i \right) I_{i+1}^p.$$

where

$$I_1^{i-1} = [\Phi(\tilde{\theta}_1^{U,r}) - \Phi(\tilde{\theta}_1^{L,r})] \cdots [\Phi(\tilde{\theta}_{i-1}^{U,r}) - \Phi(\tilde{\theta}_{i-1}^{L,r})],$$

$$I_{i+1}^p = [\Phi(\tilde{\theta}_{i+1}^{U,r}) - \Phi(\tilde{\theta}_{i+1}^{L,r})] \cdots [\Phi(\tilde{\theta}_p^{U,r}) - \Phi(\tilde{\theta}_p^{L,r})].$$

On the basis of above considerations we developed the iteration procedure of solving the OSOP with chance constraints. At each iteration we solve optimization problem (10) in which the value $E[f(d, z, \theta)]$ is replaced by the $E_{ap}[f(d, z, \theta)]$ (see (13)). For solving problem (10) we can use the outer approximations method (Hettich and Kortanek, 1993). Thus, it is seen that the considered method does not require the calculation of multiple integrals.

Case 2: The uncertain parameters θ_i , $i=1, \dots, p$, are dependent random variables having multivariate normal distribution $N_p[E[\theta_i], \Lambda]$, where Λ is a covariance matrix. It is known that the random variable y where

$$y = (\theta - \mu)^T \Lambda^{-1} (\theta - \mu)$$

(where μ is p -vector with components $\mu_i = E[\theta_i]$, $i=1, \dots, p$) has distribution χ^2 with p degrees of freedom. Take the regions T_{α_j} in the following forms

$$T_{\alpha_j} = \{\theta : (\theta - \mu)^T \Lambda^{-1} (\theta - \mu) \leq C(\alpha_j)\}, \quad j=1, \dots, m, \quad (14)$$

where $\chi^2(C(\alpha)) = \alpha$. In this case, the probability measure of the region T_{α_j} is equal to α_j . Consequently, only one region T_{α_j} satisfies constraint (7). Therefore, problem (6) is reduced to the following problem

$$f^* = \min_{d, z} E[f(d, z, \theta)], \quad (15)$$

$$\max_{\theta \in T_{\alpha_j}} g_j(d, z, \theta) \leq 0, \quad j=1, \dots, m.$$

Problem (15) is the semi-infinite programming problems. For its solving one can use the outer approximation algorithm (Hettich and Kortanek, 1993).

3. Computational experiment

As an illustration we consider a problem of a design of a chemical process (CP) consisting from a continuous stirred tank reactor and a heat exchanger. There is the detailed description of this CP in (Halemane and Grossmann, 1983). This CP has two design variables — a reactor volume V and a heat exchanger area A , two control variables — the reaction temperature T_1 and the temperature T_{w2} of a cold water on the

output of the heat exchanger and five uncertain parameters. The objective function f takes into account the capital and operating (energetic) expenditures. We solved the nominal optimization problem (NOP) and the OSOP for $\alpha_j = 0.5$, $j = 1, \dots, m$. The values of V , A and f obtained by solving NOP and OSOP are equal to 5.42, 5.21, 9003 and 7.40, 5.48, 9971. It is seen that in order to guarantee of satisfying the constraints with the given probability 0.5 we must increase the reactor volume and the heat exchanger area from 5.42, 5.21 up to 7.40, 5.48, respectively. This increases a cost of CP by 11%. It is interesting that if we use the straightforward way of solving problem (1) then the total CPU-time required only for the computation of multiple integrals used to determine the values of objective function (1) and constraints (2) is equal to approximately 40 minutes (using the Monte–Carlo method from the software package “Mathematica”). At the same time, the total CPU-time required to solve problem (10) with help of our approach is equal to 3.9 s.

4. Conclusion

We have developed the new approach to solving the chance constrained one-stage optimization problem for the case of normally distributed uncertain parameters. This approach is based on approximate transformation of chance constraints into deterministic ones and a piece-wise linear approximation of the original objective function. Partition of the uncertainty region into subregions is used to improve these approximate transformations.

The developed approach permits to solve one-stage optimization problems with chance constraints in the case when the uncertain parameters are normally distributed random variables without computationally intensive calculation of multivariate integrals.

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